



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 09:21 AM EST

PDB ID : 7S3D  
EMDB ID : EMD-24821  
Title : Structure of photosystem I with bound ferredoxin from *Synechococcus* sp. PCC 7335 acclimated to far-red light  
Authors : Gisriel, C.J.; Flesher, D.A.; Shen, G.; Wang, J.; Ho, M.; Brudvig, G.W.; Bryant, D.A.  
Deposited on : 2021-09-05  
Resolution : 2.91 Å(reported)

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

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

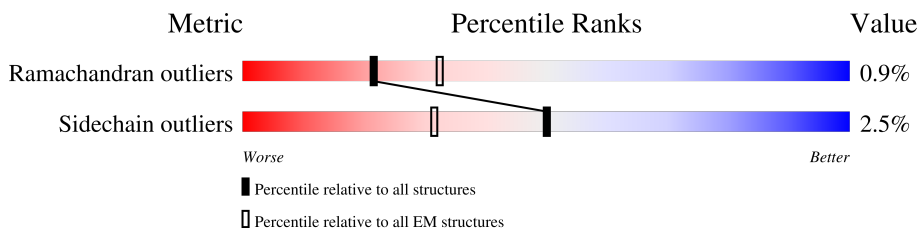
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.91 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 782    | <div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93%</p> |
| 1   | G     | 782    | <div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93%</p> |
| 1   | a     | 782    | <div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93%</p> |
| 2   | B     | 743    | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">99%</p>                                                                                         |
| 2   | H     | 743    | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">99%</p>                                                                                         |
| 2   | b     | 743    | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">99%</p>                                                                                         |
| 3   | C     | 81     | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">98%</p>                                                                                         |
| 3   | N     | 81     | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">98%</p>                                                                                         |
| 3   | c     | 81     | <div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">98%</p>                                                                                         |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 4   | D     | 155    | 12% 85% 6% • 8%   |
| 4   | O     | 155    | 12% 85% 6% • 8%   |
| 4   | d     | 155    | 12% 85% 6% • 8%   |
| 5   | E     | 71     | 23% 90% 10%       |
| 5   | P     | 71     | 21% 90% 10%       |
| 5   | e     | 71     | 24% 90% 10%       |
| 6   | F     | 168    | 74% 71% •• 26%    |
| 6   | Q     | 168    | 74% 71% •• 26%    |
| 6   | f     | 168    | 74% 71% •• 26%    |
| 7   | I     | 70     | 59% • 40%         |
| 7   | R     | 70     | 59% • 40%         |
| 7   | i     | 70     | 59% • 40%         |
| 8   | J     | 46     | 89% 83% 7% 11%    |
| 8   | S     | 46     | 89% 83% 7% 11%    |
| 8   | j     | 46     | 89% 83% 7% 11%    |
| 9   | K     | 84     | 31% 75% 12% • 11% |
| 9   | T     | 84     | 30% 75% 12% • 11% |
| 9   | k     | 84     | 30% 75% 12% • 11% |
| 10  | L     | 174    | 97% ••            |
| 10  | U     | 174    | 97% ••            |
| 10  | l     | 174    | 97% ••            |
| 11  | M     | 31     | 100%              |
| 11  | V     | 31     | 100%              |
| 11  | m     | 31     | 100%              |
| 12  | W     | 99     | 98% 83% 15% •     |

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| Mol | Chain | Length | Quality of chain       |
|-----|-------|--------|------------------------|
| 12  | X     | 99     | <p>98%<br/>83% 15%</p> |
| 12  | x     | 99     | <p>98%<br/>83% 15%</p> |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13  | CL0  | A     | 1011 | X         | -        | -       | -                |
| 13  | CL0  | G     | 1011 | X         | -        | -       | -                |
| 13  | CL0  | a     | 1011 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1012 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1013 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1101 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1102 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1103 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1104 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1105 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1106 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1107 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1108 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1109 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1110 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1111 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1112 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1113 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1114 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1115 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1116 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1117 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1118 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1119 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1120 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1122 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1123 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1124 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1125 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1126 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1127 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1128 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1129 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | A     | 1130 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1131 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1132 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1133 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1134 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1135 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1136 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1137 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1138 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1139 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1140 | X         | -        | -       | -                |
| 14  | CLA  | A     | 1141 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1021 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1022 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1023 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1201 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1202 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1203 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1204 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1205 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1206 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1208 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1209 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1210 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1211 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1212 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1213 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1214 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1215 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1216 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1217 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1218 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1220 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1221 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1222 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1223 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1224 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1225 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1226 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1227 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1228 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1229 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | B     | 1231 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1232 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1233 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1234 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1235 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1236 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1239 | X         | -        | -       | -                |
| 14  | CLA  | B     | 1240 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1012 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1013 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1101 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1102 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1103 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1104 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1105 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1106 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1107 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1108 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1109 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1110 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1111 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1112 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1113 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1114 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1115 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1116 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1117 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1118 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1119 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1120 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1122 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1123 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1124 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1125 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1126 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1127 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1128 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1129 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1130 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1131 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1132 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1133 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | G     | 1134 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1135 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1136 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1137 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1138 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1139 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1140 | X         | -        | -       | -                |
| 14  | CLA  | G     | 1141 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1021 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1022 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1023 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1201 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1202 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1203 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1204 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1205 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1206 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1208 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1209 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1210 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1211 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1212 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1213 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1214 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1215 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1216 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1217 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1218 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1220 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1221 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1222 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1223 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1224 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1225 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1226 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1227 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1228 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1229 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1231 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1232 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1233 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1234 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | H     | 1235 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1236 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1239 | X         | -        | -       | -                |
| 14  | CLA  | H     | 1240 | X         | -        | -       | -                |
| 14  | CLA  | K     | 1401 | X         | -        | -       | -                |
| 14  | CLA  | L     | 1501 | X         | -        | -       | -                |
| 14  | CLA  | L     | 1502 | X         | -        | -       | -                |
| 14  | CLA  | L     | 1503 | X         | -        | -       | -                |
| 14  | CLA  | M     | 1501 | X         | -        | -       | -                |
| 14  | CLA  | T     | 1401 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1501 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1502 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1503 | X         | -        | -       | -                |
| 14  | CLA  | V     | 1501 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1012 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1013 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1101 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1102 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1103 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1104 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1105 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1106 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1107 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1108 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1109 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1110 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1111 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1112 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1113 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1114 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1115 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1116 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1117 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1118 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1119 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1120 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1122 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1123 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1124 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1125 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1126 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1127 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | a     | 1128 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1129 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1130 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1131 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1132 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1133 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1134 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1135 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1136 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1137 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1138 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1139 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1140 | X         | -        | -       | -                |
| 14  | CLA  | a     | 1141 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1021 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1022 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1023 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1201 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1202 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1203 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1204 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1205 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1206 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1208 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1209 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1210 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1211 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1212 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1213 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1214 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1215 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1216 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1217 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1218 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1220 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1221 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1222 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1223 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1224 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1225 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1226 | X         | -        | -       | -                |
| 14  | CLA  | b     | 1227 | X         | -        | -       | -                |

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| <b>Mol</b> | <b>Type</b> | <b>Chain</b> | <b>Res</b> | <b>Chirality</b> | <b>Geometry</b> | <b>Clashes</b> | <b>Electron density</b> |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 14         | CLA         | b            | 1228       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1229       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1231       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1232       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1233       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1234       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1235       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1236       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1239       | X                | -               | -              | -                       |
| 14         | CLA         | b            | 1240       | X                | -               | -              | -                       |
| 14         | CLA         | k            | 1401       | X                | -               | -              | -                       |
| 14         | CLA         | l            | 1501       | X                | -               | -              | -                       |
| 14         | CLA         | l            | 1502       | X                | -               | -              | -                       |
| 14         | CLA         | l            | 1503       | X                | -               | -              | -                       |
| 14         | CLA         | m            | 1501       | X                | -               | -              | -                       |

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 75150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |      |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|----|---------|-------|
|     |       |          | Total | C    | N    | O   | S  |         |       |
| 1   | A     | 749      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5849  | 3818 | 1005 | 991 | 35 |         |       |
| 1   | G     | 749      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5849  | 3818 | 1005 | 991 | 35 |         |       |
| 1   | a     | 749      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5849  | 3818 | 1005 | 991 | 35 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
|     |       |          | Total | C    | N   | O    | S  |         |       |
| 2   | B     | 742      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5900  | 3883 | 988 | 1008 | 21 |         |       |
| 2   | H     | 742      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5900  | 3883 | 988 | 1008 | 21 |         |       |
| 2   | b     | 742      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5900  | 3883 | 988 | 1008 | 21 |         |       |

- Molecule 3 is a protein called PsaC.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | S  |         |       |
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 365 | 105 | 117 | 11 |         |       |
| 3   | N     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 365 | 105 | 117 | 11 |         |       |
| 3   | c     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 365 | 105 | 117 | 11 |         |       |

- Molecule 4 is a protein called Photosystem I 16 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 4   | D     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 695 | 189 | 213 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | O     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 695 | 189 | 213 | 5 |         |       |
| 4   | d     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 695 | 189 | 213 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | E     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 506   | 322 | 89 | 95 |   |         |       |
| 5   | P     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 506   | 322 | 89 | 95 |   |         |       |
| 5   | e     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 506   | 322 | 89 | 95 |   |         |       |

- Molecule 6 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 826   | 542 | 134 | 148 | 2 |         |       |
| 6   | Q     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 826   | 542 | 134 | 148 | 2 |         |       |
| 6   | f     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 826   | 542 | 134 | 148 | 2 |         |       |

- Molecule 7 is a protein called PsaI2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 237 | 49 | 55 | 2 |         |       |
| 7   | R     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 237 | 49 | 55 | 2 |         |       |
| 7   | i     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 237 | 49 | 55 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 296   | 197 | 46 | 52 | 1 |         |       |
| 8   | S     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 296   | 197 | 46 | 52 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | j     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 296   | 197 | 46 | 52 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | K     | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 516   | 343 | 85 | 86 | 2 |         |       |
| 9   | T     | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 516   | 343 | 85 | 86 | 2 |         |       |
| 9   | k     | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 516   | 343 | 85 | 86 | 2 |         |       |

- Molecule 10 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1291  | 830 | 220 | 238 | 3 |         |       |
| 10  | U     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1291  | 830 | 220 | 238 | 3 |         |       |
| 10  | l     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1291  | 830 | 220 | 238 | 3 |         |       |

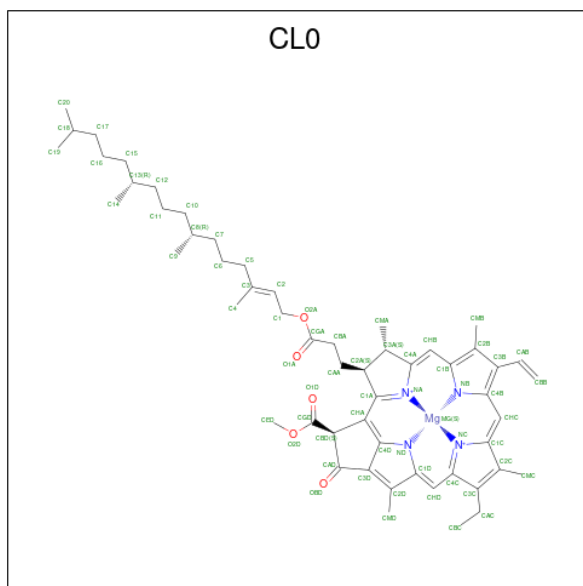
- Molecule 11 is a protein called PsaM.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 232   | 156 | 35 | 40 | 1 |         |       |
| 11  | V     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 232   | 156 | 35 | 40 | 1 |         |       |
| 11  | m     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 232   | 156 | 35 | 40 | 1 |         |       |

- Molecule 12 is a protein called 2Fe-2S ferredoxin-type domain-containing protein.

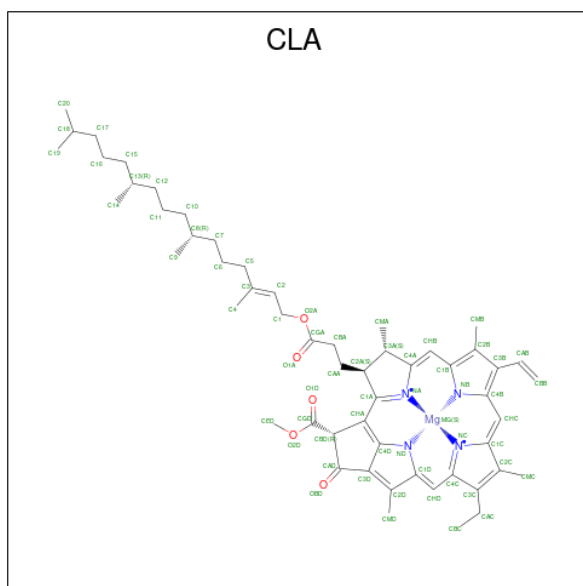
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | X     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 405 | 107 | 132 | 5 |         |       |
| 12  | W     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 405 | 107 | 132 | 5 |         |       |
| 12  | x     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 405 | 107 | 132 | 5 |         |       |

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---|
| 13  | A     | 1        | Total | C  | Mg | N | O       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |   |
| 13  | G     | 1        | Total | C  | Mg | N | O       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |   |
| 13  | a     | 1        | Total | C  | Mg | N | O       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |   |

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | A     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | A     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | B     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | B     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | K     | 1        | Total<br>45   | C<br>35   | Mg<br>1  | N<br>4   | O<br>5   | 0       |
| 14  | L     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 14  | L     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 14  | L     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 14  | M     | 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 |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | G     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | G     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | H     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | H     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | T     | 1        | Total<br>45   | C<br>35   | Mg<br>1  | N<br>4   | O<br>5   | 0       |
| 14  | U     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 14  | U     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 14  | U     | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 14  | V     | 1        | 50    | 40   | 1  | 4   | 5   | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |
| 14  | a     | 1        | 2330  | 1910 | 42 | 168 | 210 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 14  | a     | 1        | Total<br>2330 | C<br>1910 | Mg<br>42 | N<br>168 | O<br>210 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |
| 14  | b     | 1        | Total<br>2255 | C<br>1875 | Mg<br>38 | N<br>152 | O<br>190 | 0       |

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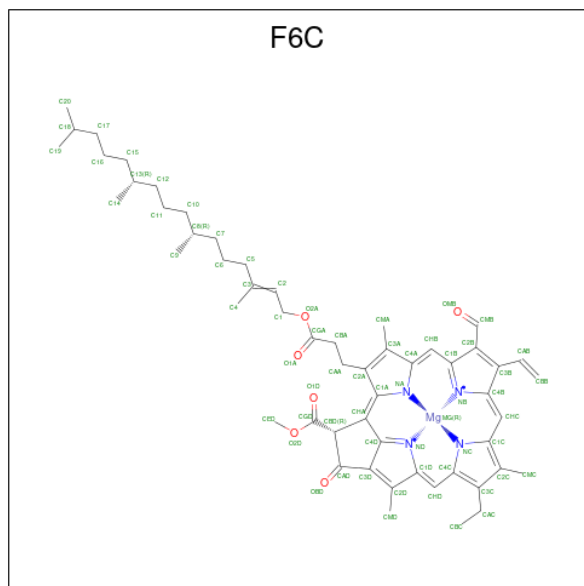
| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | b     | 1        | 2255  | 1875 | 38 | 152 | 190 | 0       |
| 14  | k     | 1        | 45    | 35   | 1  | 4   | 5   | 0       |
| 14  | l     | 1        | 190   | 160  | 3  | 12  | 15  | 0       |
| 14  | l     | 1        | 190   | 160  | 3  | 12  | 15  | 0       |

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| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 14  | l     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 190   | 160 | 3  | 12 | 15 |         |
| 14  | m     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 50    | 40  | 1  | 4  | 5  |         |

- Molecule 15 is Chlorophyll F (three-letter code: F6C) (formula:  $C_{55}H_{68}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



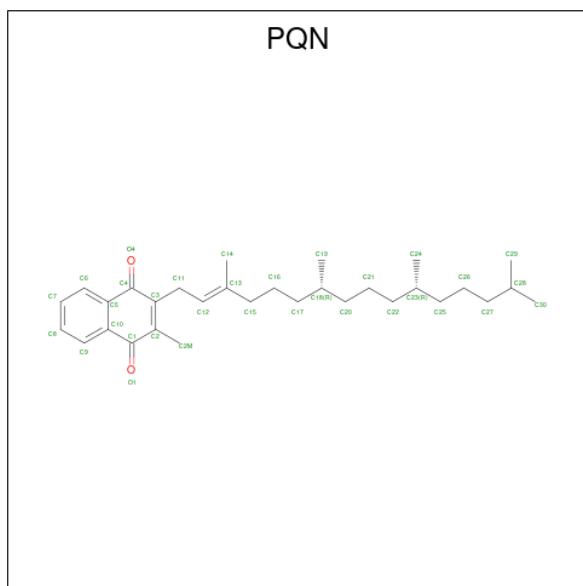
| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 15  | A     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 46    | 35  | 1  | 4  | 6  |         |
| 15  | B     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | B     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | B     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | B     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | B     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | G     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 46    | 35  | 1  | 4  | 6  |         |
| 15  | H     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |
| 15  | H     | 1        | Total | C   | Mg | N  | O  | 0       |
|     |       |          | 300   | 245 | 5  | 20 | 30 |         |

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| Mol | Chain | Residues | Atoms        |          |         |         |         | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|
|     |       |          | Total        | C        | Mg      | N       | O       |         |
| 15  | H     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | H     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | H     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | a     | 1        | Total<br>46  | C<br>35  | Mg<br>1 | N<br>4  | O<br>6  | 0       |
| 15  | b     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | b     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | b     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | b     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |
| 15  | b     | 1        | Total<br>300 | C<br>245 | Mg<br>5 | N<br>20 | O<br>30 | 0       |

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



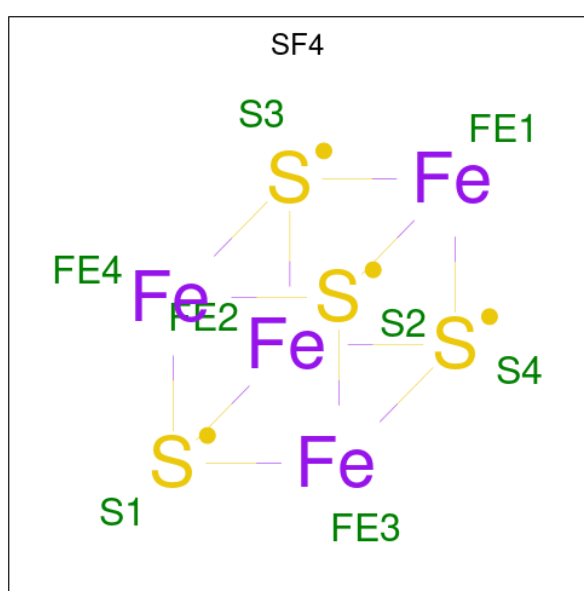
| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
|     |       |          | Total       | C       | O      |         |
| 16  | A     | 1        | Total<br>33 | C<br>31 | O<br>2 | 0       |
| 16  | B     | 1        | Total<br>33 | C<br>31 | O<br>2 | 0       |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | C  | O |         |
| 16  | G     | 1        | 33    | 31 | 2 | 0       |
| 16  | H     | 1        | 33    | 31 | 2 | 0       |
| 16  | a     | 1        | 33    | 31 | 2 | 0       |
| 16  | b     | 1        | 33    | 31 | 2 | 0       |

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



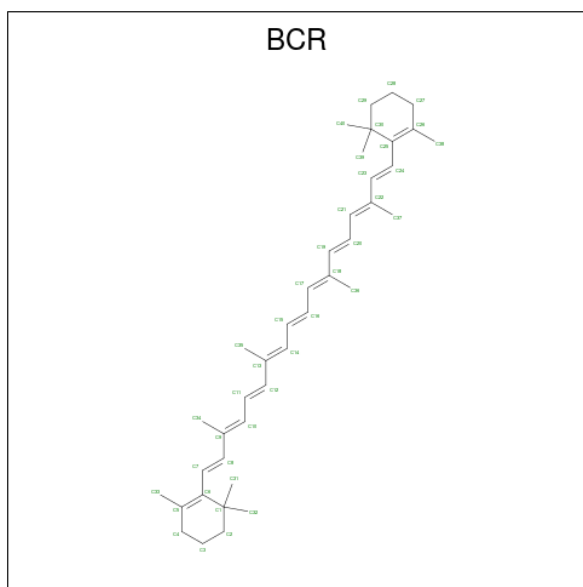
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | Fe | S |         |
| 17  | A     | 1        | 8     | 4  | 4 | 0       |
| 17  | C     | 1        | 16    | 8  | 8 | 0       |
| 17  | C     | 1        | 16    | 8  | 8 | 0       |
| 17  | G     | 1        | 8     | 4  | 4 | 0       |
| 17  | N     | 1        | 16    | 8  | 8 | 0       |
| 17  | N     | 1        | 16    | 8  | 8 | 0       |
| 17  | a     | 1        | 8     | 4  | 4 | 0       |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 17  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 16    | 8  | 8 |         |
| 17  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 16    | 8  | 8 |         |

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | A     | 1        | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 18  | B     | 1        | Total | C   | 0       |
|     |       |          | 280   | 280 |         |
| 18  | B     | 1        | Total | C   | 0       |
|     |       |          | 280   | 280 |         |
| 18  | B     | 1        | Total | C   | 0       |
|     |       |          | 280   | 280 |         |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 18  | B     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | B     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | B     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | B     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | I     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | I     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | K     | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | L     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | L     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | M     | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | G     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | H     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | R     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | R     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | T     | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | U     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | U     | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | V     | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | a     | 1        | Total<br>240 | C<br>240 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |
| 18  | b     | 1        | Total<br>280 | C<br>280 | 0       |

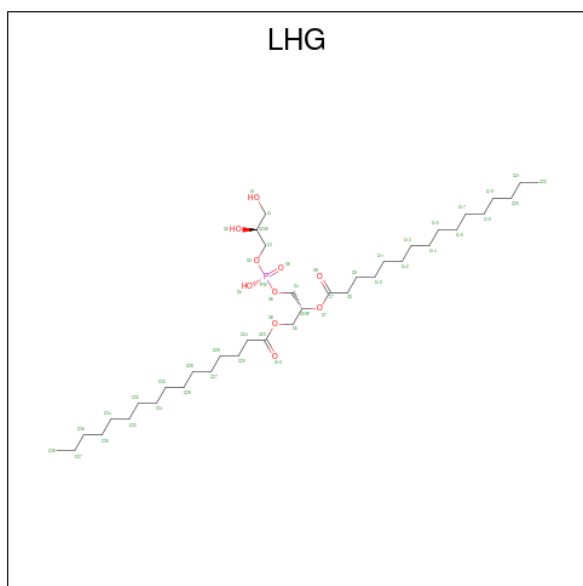
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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 18  | i     | 1        | Total | C  | 0       |
|     |       |          | 80    | 80 |         |
| 18  | i     | 1        | Total | C  | 0       |
|     |       |          | 80    | 80 |         |
| 18  | k     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 18  | l     | 1        | Total | C  | 0       |
|     |       |          | 80    | 80 |         |
| 18  | l     | 1        | Total | C  | 0       |
|     |       |          | 80    | 80 |         |
| 18  | m     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



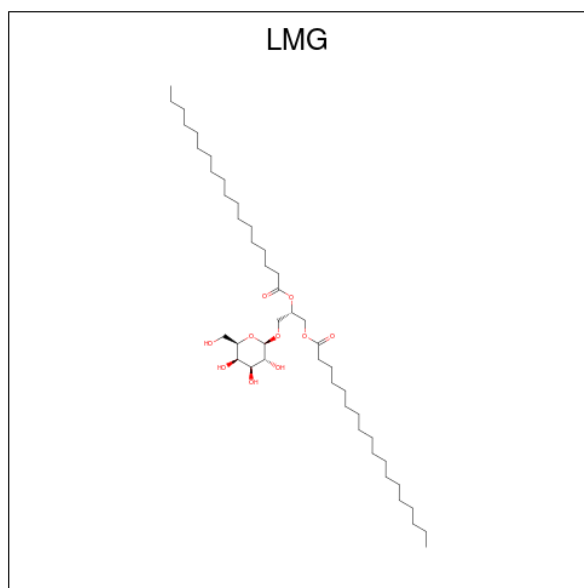
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 86    | 66 | 18 | 2 |         |
| 19  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 86    | 66 | 18 | 2 |         |
| 19  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 74    | 58 | 15 | 1 |         |
| 19  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 74    | 58 | 15 | 1 |         |
| 19  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 86    | 66 | 18 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
|     |       |          | Total       | C       | O       | P      |         |
| 19  | G     | 1        | Total<br>86 | C<br>66 | O<br>18 | P<br>2 | 0       |
| 19  | U     | 1        | Total<br>74 | C<br>58 | O<br>15 | P<br>1 | 0       |
| 19  | U     | 1        | Total<br>74 | C<br>58 | O<br>15 | P<br>1 | 0       |
| 19  | a     | 1        | Total<br>86 | C<br>66 | O<br>18 | P<br>2 | 0       |
| 19  | a     | 1        | Total<br>86 | C<br>66 | O<br>18 | P<br>2 | 0       |
| 19  | l     | 1        | Total<br>74 | C<br>58 | O<br>15 | P<br>1 | 0       |
| 19  | l     | 1        | Total<br>74 | C<br>58 | O<br>15 | P<br>1 | 0       |

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



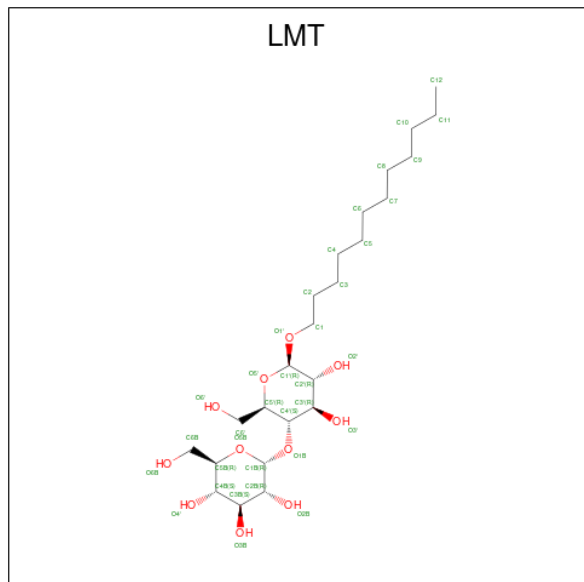
| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
|     |       |          | Total       | C       | O       |         |
| 20  | A     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 20  | B     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 20  | I     | 1        | Total<br>37 | C<br>27 | O<br>10 | 0       |
| 20  | G     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
|     |       |          | Total | C  | O  |         |
| 20  | H     | 1        | 46    | 36 | 10 | 0       |
| 20  | R     | 1        | 37    | 27 | 10 | 0       |
| 20  | a     | 1        | 46    | 36 | 10 | 0       |
| 20  | b     | 1        | 46    | 36 | 10 | 0       |
| 20  | i     | 1        | 37    | 27 | 10 | 0       |

- Molecule 21 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
|     |       |          | Total | C  | O  |         |
| 21  | A     | 1        | 115   | 76 | 39 | 0       |
| 21  | A     | 1        | 115   | 76 | 39 | 0       |
| 21  | A     | 1        | 115   | 76 | 39 | 0       |
| 21  | A     | 1        | 115   | 76 | 39 | 0       |
| 21  | B     | 1        | 136   | 92 | 44 | 0       |
| 21  | B     | 1        | 136   | 92 | 44 | 0       |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
|     |       |          | Total | C  | O  |         |
| 21  | B     | 1        | 136   | 92 | 44 | 0       |
| 21  | B     | 1        | 136   | 92 | 44 | 0       |
| 21  | I     | 1        | 35    | 24 | 11 | 0       |
| 21  | L     | 1        | 84    | 61 | 23 | 0       |
| 21  | L     | 1        | 84    | 61 | 23 | 0       |
| 21  | L     | 1        | 84    | 61 | 23 | 0       |
| 21  | M     | 1        | 35    | 24 | 11 | 0       |
| 21  | G     | 1        | 115   | 76 | 39 | 0       |
| 21  | G     | 1        | 115   | 76 | 39 | 0       |
| 21  | G     | 1        | 115   | 76 | 39 | 0       |
| 21  | G     | 1        | 115   | 76 | 39 | 0       |
| 21  | H     | 1        | 136   | 92 | 44 | 0       |
| 21  | H     | 1        | 136   | 92 | 44 | 0       |
| 21  | H     | 1        | 136   | 92 | 44 | 0       |
| 21  | H     | 1        | 136   | 92 | 44 | 0       |
| 21  | R     | 1        | 35    | 24 | 11 | 0       |
| 21  | U     | 1        | 84    | 61 | 23 | 0       |
| 21  | U     | 1        | 84    | 61 | 23 | 0       |
| 21  | U     | 1        | 84    | 61 | 23 | 0       |
| 21  | V     | 1        | 35    | 24 | 11 | 0       |
| 21  | a     | 1        | 115   | 76 | 39 | 0       |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 21  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 115   | 76 | 39 |         |
| 21  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 115   | 76 | 39 |         |
| 21  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 115   | 76 | 39 |         |
| 21  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 136   | 92 | 44 |         |
| 21  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 136   | 92 | 44 |         |
| 21  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 136   | 92 | 44 |         |
| 21  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 136   | 92 | 44 |         |
| 21  | i     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 21  | l     | 1        | Total | C  | O  | 0       |
|     |       |          | 84    | 61 | 23 |         |
| 21  | l     | 1        | Total | C  | O  | 0       |
|     |       |          | 84    | 61 | 23 |         |
| 21  | l     | 1        | Total | C  | O  | 0       |
|     |       |          | 84    | 61 | 23 |         |
| 21  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 22  | A     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 22  | G     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 22  | a     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

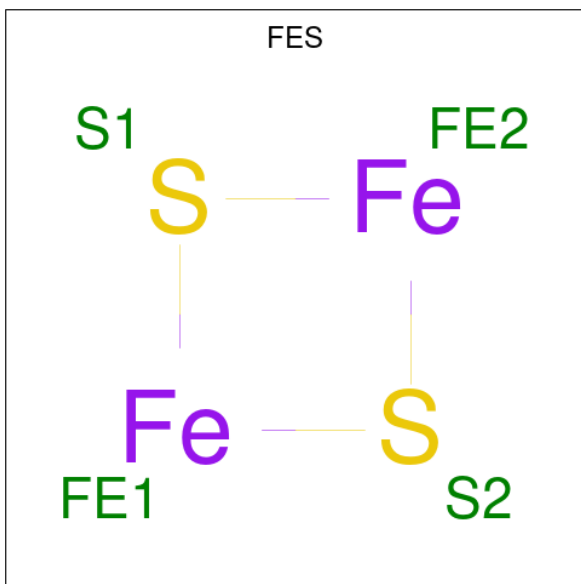
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | L     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 23  | U     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | 1     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | X     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 24  | W     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 24  | x     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 25  | A     | 35       | Total | O  | 0       |
|     |       |          | 35    | 35 |         |
| 25  | B     | 35       | Total | O  | 0       |
|     |       |          | 35    | 35 |         |
| 25  | C     | 9        | Total | O  | 0       |
|     |       |          | 9     | 9  |         |
| 25  | D     | 13       | Total | O  | 0       |
|     |       |          | 13    | 13 |         |
| 25  | I     | 4        | Total | O  | 0       |
|     |       |          | 4     | 4  |         |

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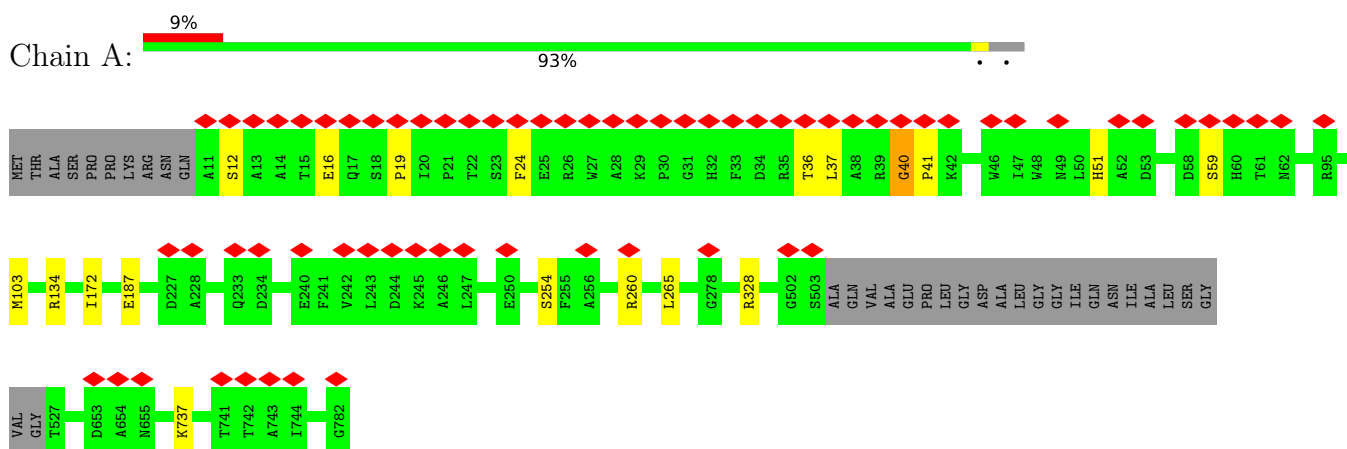
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 25  | L     | 15       | Total<br>15 | O<br>15 | 0       |
| 25  | G     | 35       | Total<br>35 | O<br>35 | 0       |
| 25  | H     | 35       | Total<br>35 | O<br>35 | 0       |
| 25  | N     | 9        | Total<br>9  | O<br>9  | 0       |
| 25  | O     | 13       | Total<br>13 | O<br>13 | 0       |
| 25  | R     | 4        | Total<br>4  | O<br>4  | 0       |
| 25  | U     | 15       | Total<br>15 | O<br>15 | 0       |
| 25  | a     | 35       | Total<br>35 | O<br>35 | 0       |
| 25  | b     | 35       | Total<br>35 | O<br>35 | 0       |
| 25  | c     | 9        | Total<br>9  | O<br>9  | 0       |
| 25  | d     | 13       | Total<br>13 | O<br>13 | 0       |
| 25  | i     | 4        | Total<br>4  | O<br>4  | 0       |
| 25  | l     | 15       | Total<br>15 | O<br>15 | 0       |

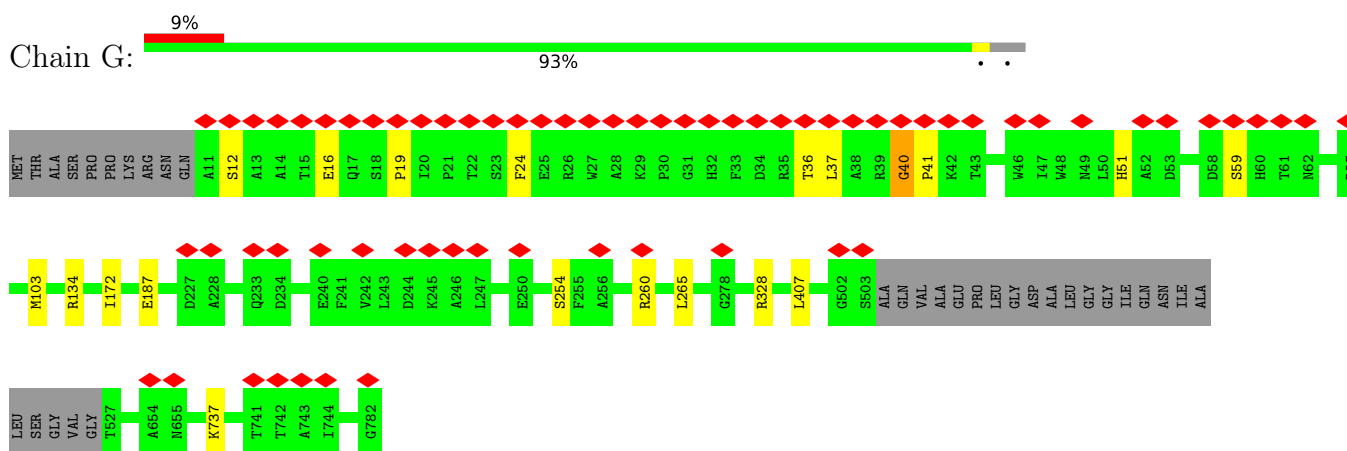
### 3 Residue-property plots [i](#)

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

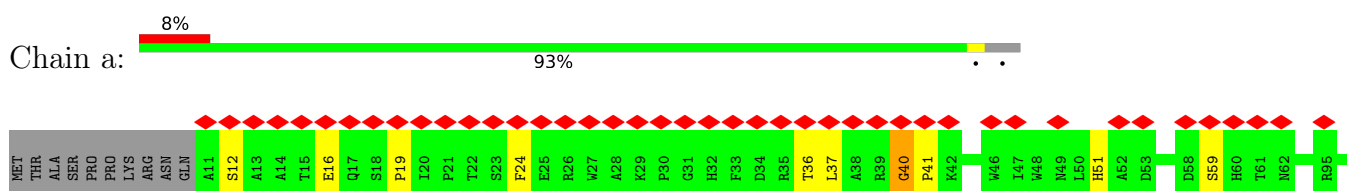
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



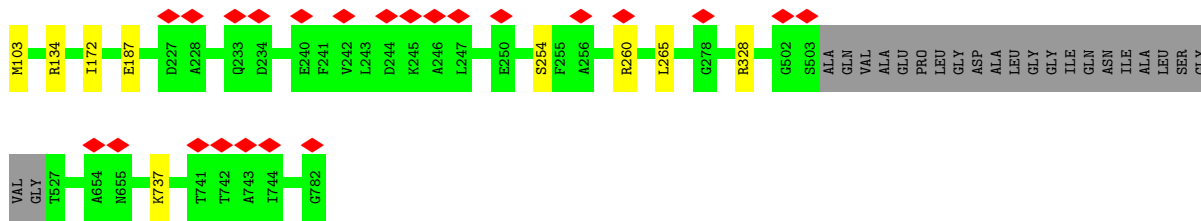
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



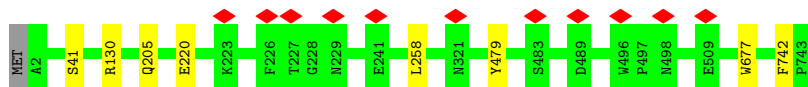
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



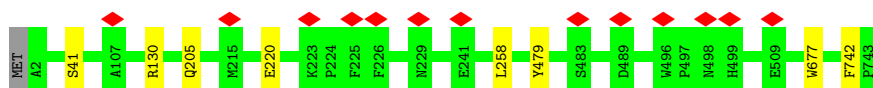




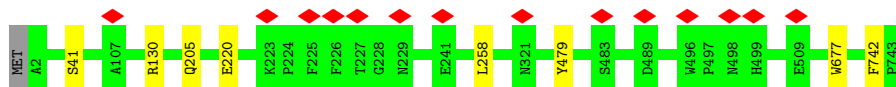
● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



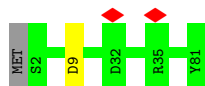
● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



● Molecule 3: PsaC

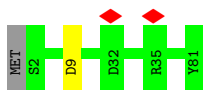


● Molecule 3: PsaC

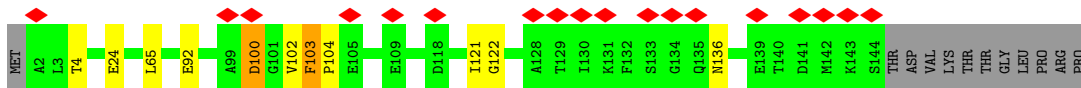
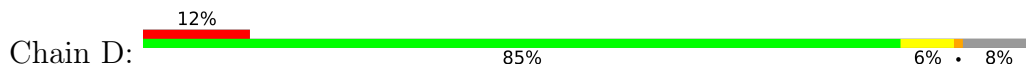


● Molecule 3: PsaC

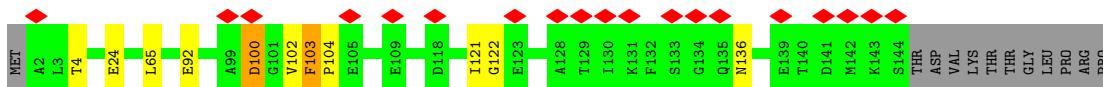
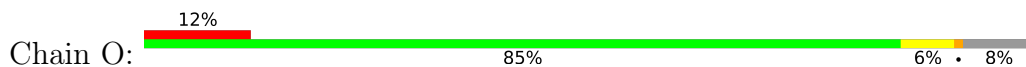




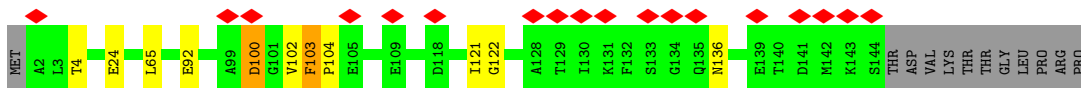
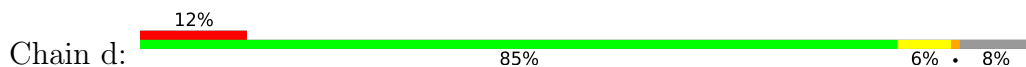
- Molecule 4: Photosystem I 16 kDa polypeptide



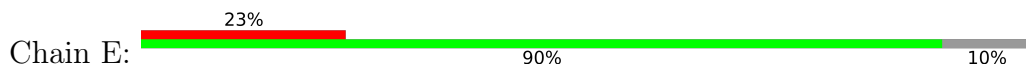
- Molecule 4: Photosystem I 16 kDa polypeptide



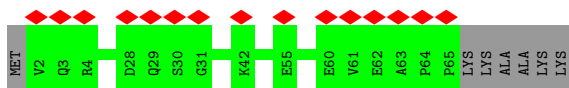
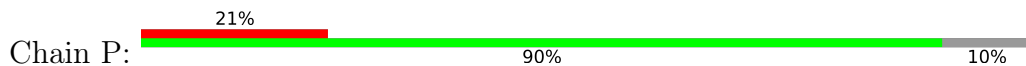
- Molecule 4: Photosystem I 16 kDa polypeptide



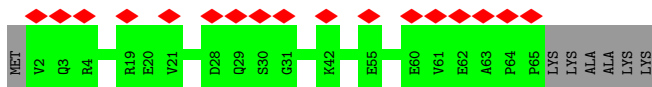
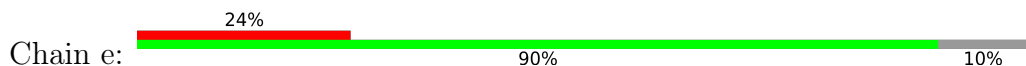
- Molecule 5: Photosystem I reaction center subunit IV



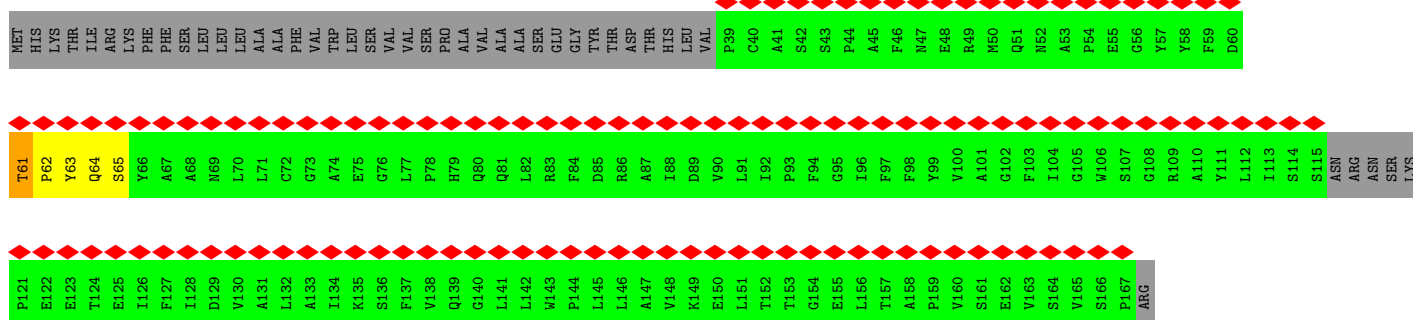
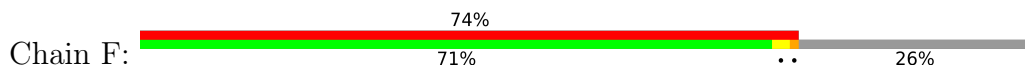
- Molecule 5: Photosystem I reaction center subunit IV



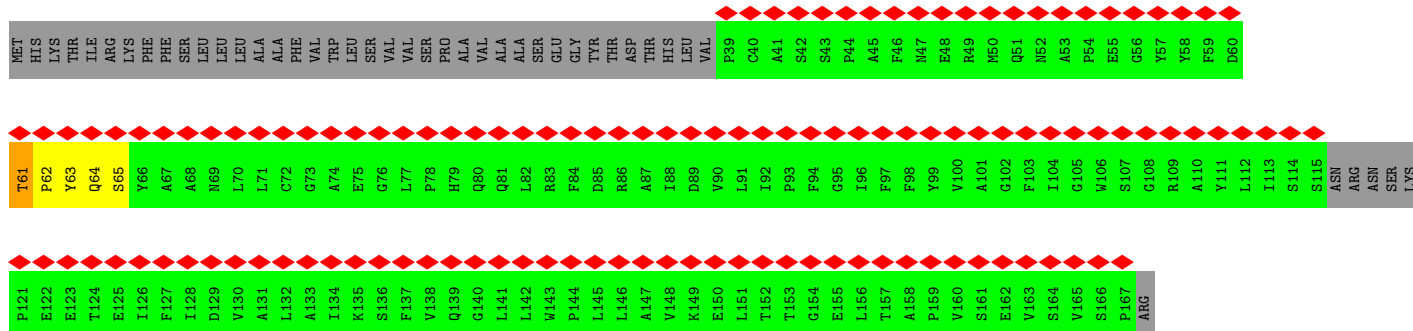
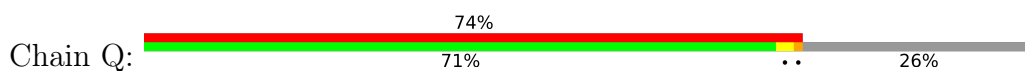
- Molecule 5: Photosystem I reaction center subunit IV



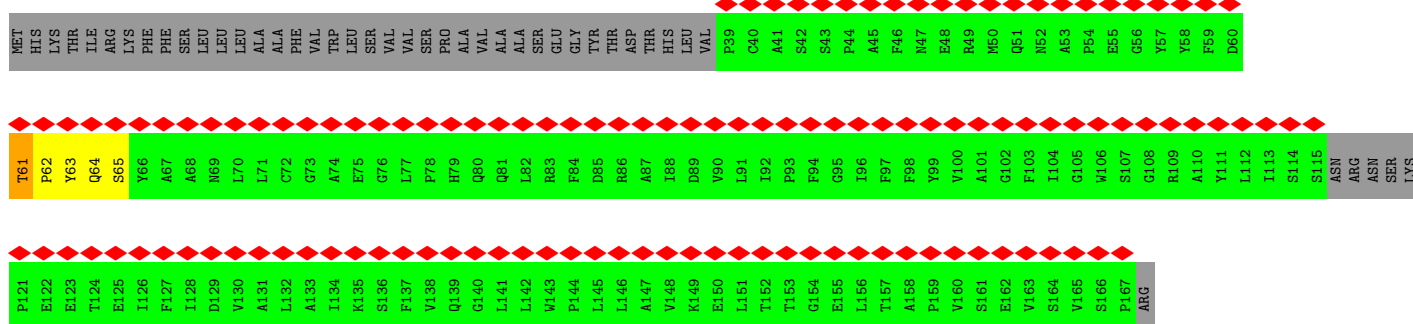
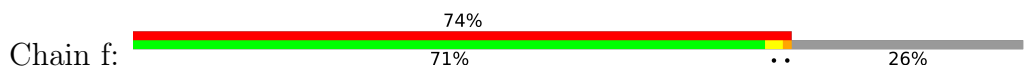
- Molecule 6: PSI-F



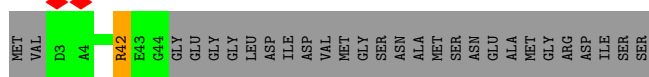
• Molecule 6: PSI-F



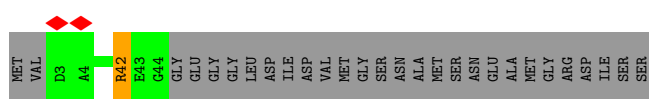
• Molecule 6: PSI-F



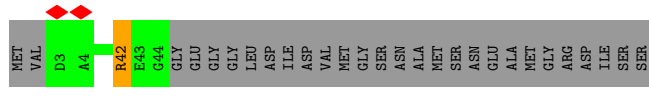
• Molecule 7: PsaI2



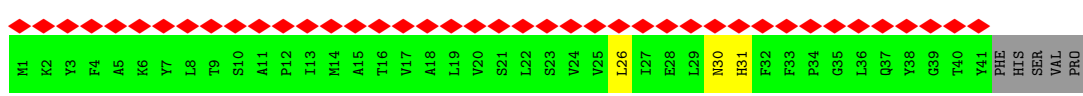
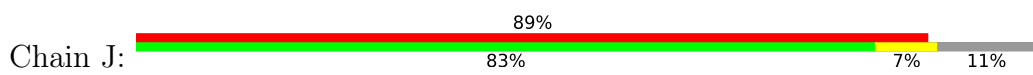
• Molecule 7: PsaI2



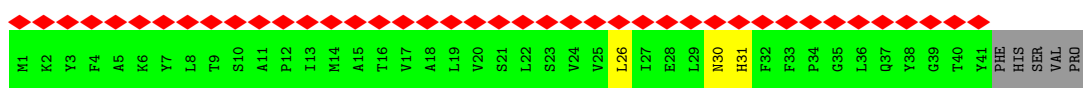
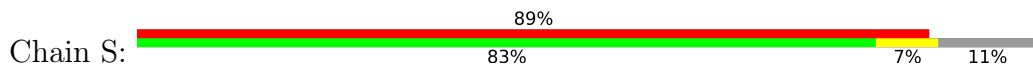
• Molecule 7: PsaI2



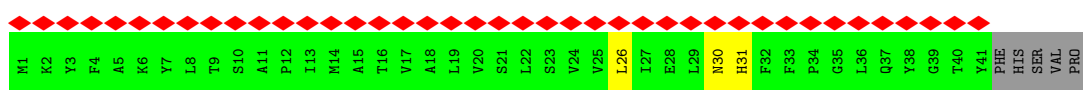
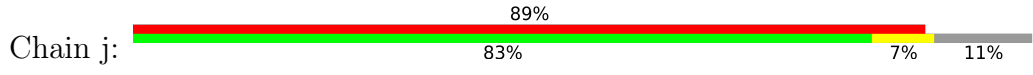
• Molecule 8: Photosystem I reaction center subunit IX



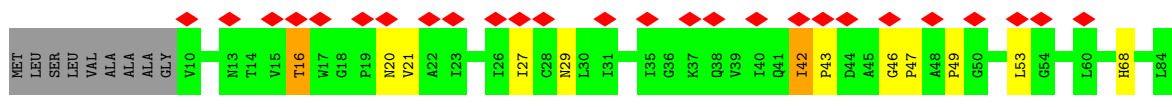
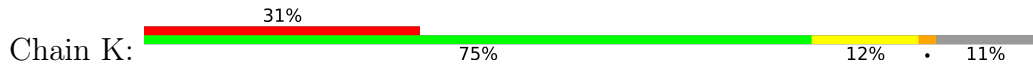
• Molecule 8: Photosystem I reaction center subunit IX



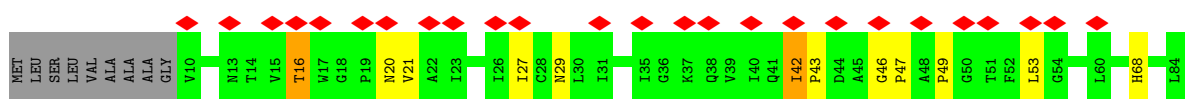
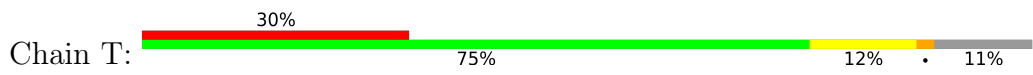
• Molecule 8: Photosystem I reaction center subunit IX



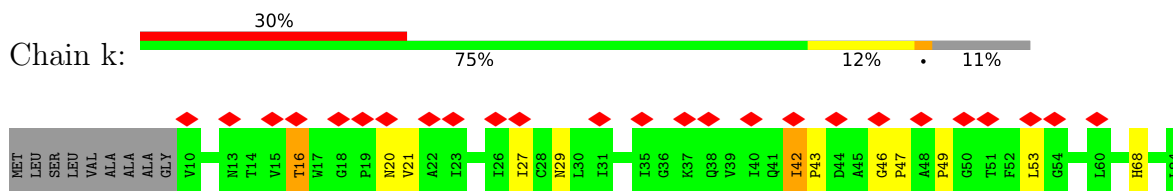
• Molecule 9: Photosystem I reaction center subunit PsaK



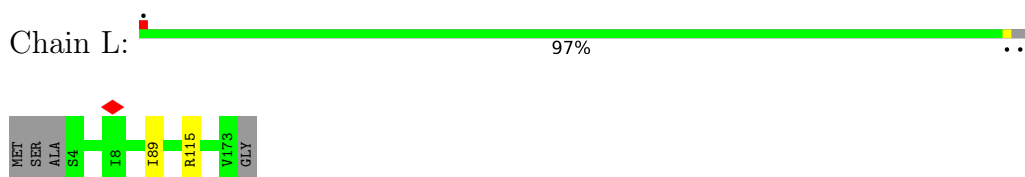
• Molecule 9: Photosystem I reaction center subunit PsaK



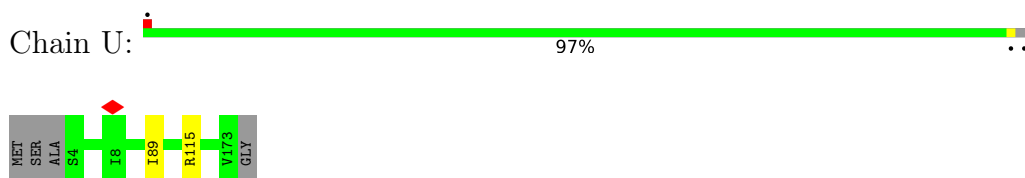
- Molecule 9: Photosystem I reaction center subunit PsaK



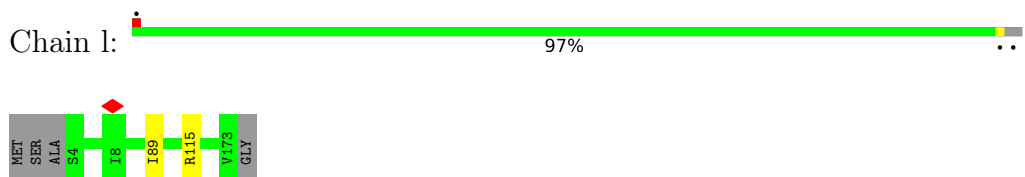
- Molecule 10: PSI subunit V



- Molecule 10: PSI subunit V



- Molecule 10: PSI subunit V



- Molecule 11: PsaM



There are no outlier residues recorded for this chain.

- Molecule 11: PsaM



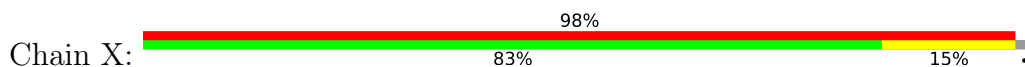
There are no outlier residues recorded for this chain.

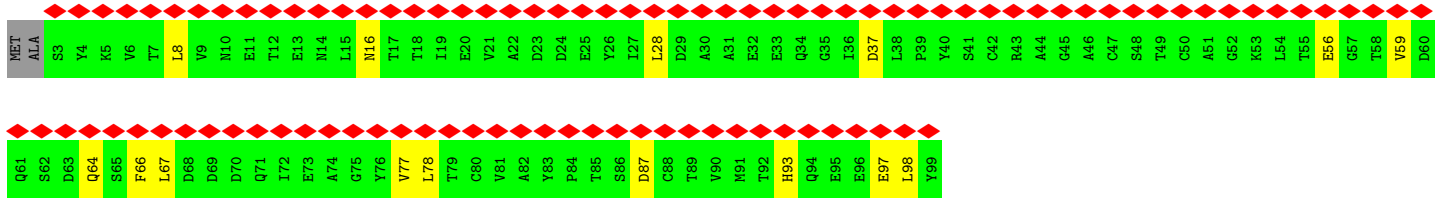
- Molecule 11: PsaM



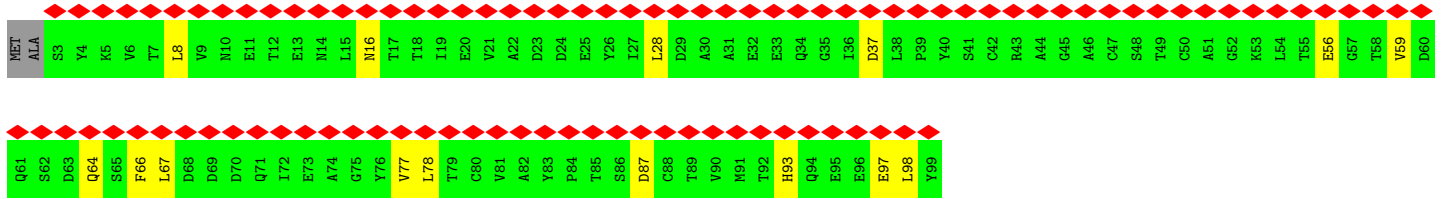
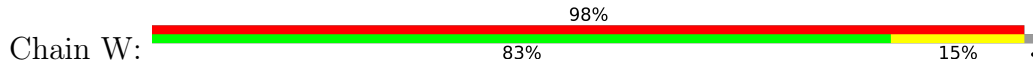
There are no outlier residues recorded for this chain.

- Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein

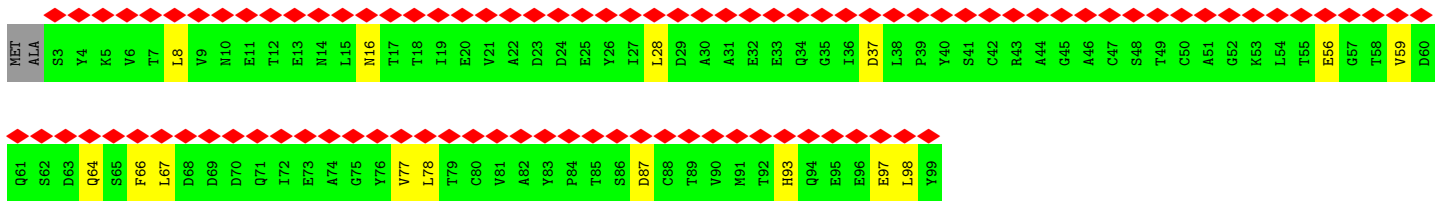
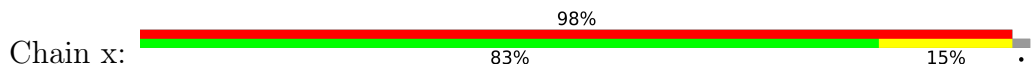




• Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein



• Molecule 12: 2Fe-2S ferredoxin-type domain-containing protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 286672                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40.8                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.315                                   | Depositor |
| Minimum map value                    | -0.201                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.010                                   | Depositor |
| Recommended contour level            | 0.0302                                  | Depositor |
| Map size (Å)                         | 316.8, 316.8, 316.8                     | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.825, 0.825, 0.825                     | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F6C, LHG, BCR, LMG, CLA, PQN, CA, FES, LMT, CL, CL0, SF4

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     | 0.48         | 0/6045  | 0.62        | 4/8233 (0.0%) |
| 1   | G     | 0.49         | 0/6045  | 0.62        | 5/8233 (0.1%) |
| 1   | a     | 0.48         | 0/6045  | 0.62        | 4/8233 (0.0%) |
| 2   | B     | 0.47         | 0/6124  | 0.59        | 1/8377 (0.0%) |
| 2   | H     | 0.47         | 0/6124  | 0.59        | 1/8377 (0.0%) |
| 2   | b     | 0.47         | 0/6124  | 0.59        | 1/8377 (0.0%) |
| 3   | C     | 0.50         | 0/608   | 0.65        | 1/823 (0.1%)  |
| 3   | N     | 0.50         | 0/608   | 0.65        | 1/823 (0.1%)  |
| 3   | c     | 0.50         | 0/608   | 0.65        | 1/823 (0.1%)  |
| 4   | D     | 0.44         | 0/1125  | 0.63        | 1/1515 (0.1%) |
| 4   | O     | 0.44         | 0/1125  | 0.63        | 1/1515 (0.1%) |
| 4   | d     | 0.44         | 0/1125  | 0.63        | 1/1515 (0.1%) |
| 5   | E     | 0.38         | 0/517   | 0.48        | 0/702         |
| 5   | P     | 0.38         | 0/517   | 0.48        | 0/702         |
| 5   | e     | 0.38         | 0/517   | 0.48        | 0/702         |
| 6   | F     | 0.31         | 0/847   | 0.90        | 1/1168 (0.1%) |
| 6   | Q     | 0.31         | 0/847   | 0.90        | 1/1168 (0.1%) |
| 6   | f     | 0.31         | 0/847   | 0.90        | 1/1168 (0.1%) |
| 7   | I     | 0.52         | 0/357   | 0.83        | 1/491 (0.2%)  |
| 7   | R     | 0.52         | 0/357   | 0.83        | 1/491 (0.2%)  |
| 7   | i     | 0.52         | 0/357   | 0.83        | 1/491 (0.2%)  |
| 8   | J     | 0.31         | 0/302   | 0.71        | 1/414 (0.2%)  |
| 8   | S     | 0.31         | 0/302   | 0.72        | 1/414 (0.2%)  |
| 8   | j     | 0.31         | 0/302   | 0.71        | 1/414 (0.2%)  |
| 9   | K     | 0.47         | 0/526   | 1.37        | 3/724 (0.4%)  |
| 9   | T     | 0.47         | 0/526   | 1.37        | 3/724 (0.4%)  |
| 9   | k     | 0.47         | 0/526   | 1.37        | 3/724 (0.4%)  |
| 10  | L     | 0.50         | 0/1322  | 0.59        | 1/1797 (0.1%) |
| 10  | U     | 0.50         | 0/1322  | 0.59        | 1/1797 (0.1%) |
| 10  | l     | 0.50         | 0/1322  | 0.59        | 1/1797 (0.1%) |
| 11  | M     | 0.34         | 0/235   | 0.62        | 0/319         |
| 11  | V     | 0.34         | 0/235   | 0.62        | 0/319         |



| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 11  | m     | 0.34         | 0/235   | 0.62        | 0/319           |
| 12  | W     | 0.66         | 0/657   | 0.58        | 0/900           |
| 12  | X     | 0.66         | 0/657   | 0.58        | 0/900           |
| 12  | x     | 0.67         | 0/657   | 0.58        | 0/900           |
| All | All   | 0.48         | 0/55995 | 0.66        | 43/76389 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |
| 2   | H     | 0                   | 2                   |
| 2   | b     | 0                   | 2                   |
| 4   | D     | 0                   | 2                   |
| 4   | O     | 0                   | 2                   |
| 4   | d     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

There are no bond length outliers.

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 9   | K     | 42  | ILE  | C-N-CD    | -24.85 | 65.92       | 120.60   |
| 9   | k     | 42  | ILE  | C-N-CD    | -24.85 | 65.92       | 120.60   |
| 9   | T     | 42  | ILE  | C-N-CD    | -24.84 | 65.96       | 120.60   |
| 6   | Q     | 61  | THR  | C-N-CD    | -24.79 | 66.07       | 120.60   |
| 6   | f     | 61  | THR  | C-N-CD    | -24.78 | 66.09       | 120.60   |
| 6   | F     | 61  | THR  | C-N-CD    | -24.77 | 66.11       | 120.60   |
| 9   | k     | 46  | GLY  | C-N-CD    | -19.48 | 77.73       | 120.60   |
| 9   | K     | 46  | GLY  | C-N-CD    | -19.48 | 77.75       | 120.60   |
| 9   | T     | 46  | GLY  | C-N-CD    | -19.47 | 77.76       | 120.60   |
| 1   | a     | 40  | GLY  | C-N-CD    | -14.97 | 87.67       | 120.60   |
| 1   | A     | 40  | GLY  | C-N-CD    | -14.95 | 87.71       | 120.60   |
| 1   | G     | 40  | GLY  | C-N-CD    | -14.94 | 87.72       | 120.60   |
| 1   | G     | 328 | ARG  | NE-CZ-NH1 | 8.13   | 124.37      | 120.30   |
| 7   | i     | 42  | ARG  | NE-CZ-NH1 | 8.13   | 124.37      | 120.30   |
| 7   | I     | 42  | ARG  | NE-CZ-NH1 | 8.13   | 124.36      | 120.30   |
| 7   | R     | 42  | ARG  | NE-CZ-NH1 | 8.11   | 124.36      | 120.30   |
| 1   | A     | 328 | ARG  | NE-CZ-NH1 | 8.07   | 124.33      | 120.30   |
| 1   | a     | 328 | ARG  | NE-CZ-NH1 | 8.06   | 124.33      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 103 | PHE  | C-N-CD     | -6.44 | 106.44      | 120.60   |
| 4   | d     | 103 | PHE  | C-N-CD     | -6.43 | 106.45      | 120.60   |
| 4   | O     | 103 | PHE  | C-N-CD     | -6.43 | 106.45      | 120.60   |
| 8   | S     | 26  | LEU  | CA-CB-CG   | 5.74  | 128.50      | 115.30   |
| 8   | j     | 26  | LEU  | CA-CB-CG   | 5.73  | 128.48      | 115.30   |
| 8   | J     | 26  | LEU  | CA-CB-CG   | 5.73  | 128.47      | 115.30   |
| 9   | k     | 53  | LEU  | CA-CB-CG   | 5.60  | 128.18      | 115.30   |
| 9   | K     | 53  | LEU  | CA-CB-CG   | 5.59  | 128.16      | 115.30   |
| 9   | T     | 53  | LEU  | CA-CB-CG   | 5.57  | 128.12      | 115.30   |
| 1   | A     | 265 | LEU  | CA-CB-CG   | 5.52  | 128.00      | 115.30   |
| 1   | G     | 265 | LEU  | CA-CB-CG   | 5.52  | 127.99      | 115.30   |
| 1   | a     | 265 | LEU  | CA-CB-CG   | 5.51  | 127.98      | 115.30   |
| 10  | U     | 89  | ILE  | CG1-CB-CG2 | -5.32 | 99.71       | 111.40   |
| 10  | L     | 89  | ILE  | CG1-CB-CG2 | -5.31 | 99.71       | 111.40   |
| 10  | l     | 89  | ILE  | CG1-CB-CG2 | -5.31 | 99.71       | 111.40   |
| 1   | G     | 328 | ARG  | NE-CZ-NH2  | -5.28 | 117.66      | 120.30   |
| 1   | A     | 328 | ARG  | NE-CZ-NH2  | -5.26 | 117.67      | 120.30   |
| 3   | N     | 9   | ASP  | CB-CG-OD2  | 5.26  | 123.04      | 118.30   |
| 1   | a     | 328 | ARG  | NE-CZ-NH2  | -5.25 | 117.68      | 120.30   |
| 3   | c     | 9   | ASP  | CB-CG-OD2  | 5.24  | 123.02      | 118.30   |
| 3   | C     | 9   | ASP  | CB-CG-OD2  | 5.22  | 123.00      | 118.30   |
| 2   | b     | 258 | LEU  | CA-CB-CG   | 5.15  | 127.14      | 115.30   |
| 2   | B     | 258 | LEU  | CA-CB-CG   | 5.15  | 127.14      | 115.30   |
| 2   | H     | 258 | LEU  | CA-CB-CG   | 5.12  | 127.09      | 115.30   |
| 1   | G     | 407 | LEU  | CA-CB-CG   | 5.00  | 126.80      | 115.30   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 677 | TRP  | Peptide   |
| 2   | B     | 742 | PHE  | Mainchain |
| 4   | D     | 100 | ASP  | Peptide   |
| 4   | D     | 136 | ASN  | Peptide   |
| 2   | H     | 677 | TRP  | Peptide   |
| 2   | H     | 742 | PHE  | Mainchain |
| 4   | O     | 100 | ASP  | Peptide   |
| 4   | O     | 136 | ASN  | Peptide   |
| 2   | b     | 677 | TRP  | Peptide   |
| 2   | b     | 742 | PHE  | Mainchain |
| 4   | d     | 100 | ASP  | Peptide   |
| 4   | d     | 136 | ASN  | Peptide   |

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 745/782 (95%)  | 708 (95%) | 31 (4%)  | 6 (1%)   | 19          | 49  |
| 1   | G     | 745/782 (95%)  | 708 (95%) | 31 (4%)  | 6 (1%)   | 19          | 49  |
| 1   | a     | 745/782 (95%)  | 708 (95%) | 31 (4%)  | 6 (1%)   | 19          | 49  |
| 2   | B     | 740/743 (100%) | 703 (95%) | 37 (5%)  | 0        | 100         | 100 |
| 2   | H     | 740/743 (100%) | 702 (95%) | 38 (5%)  | 0        | 100         | 100 |
| 2   | b     | 740/743 (100%) | 702 (95%) | 38 (5%)  | 0        | 100         | 100 |
| 3   | C     | 78/81 (96%)    | 74 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 3   | N     | 78/81 (96%)    | 74 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 3   | c     | 78/81 (96%)    | 74 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 4   | D     | 141/155 (91%)  | 119 (84%) | 17 (12%) | 5 (4%)   | 3           | 13  |
| 4   | O     | 141/155 (91%)  | 119 (84%) | 17 (12%) | 5 (4%)   | 3           | 13  |
| 4   | d     | 141/155 (91%)  | 119 (84%) | 17 (12%) | 5 (4%)   | 3           | 13  |
| 5   | E     | 62/71 (87%)    | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 5   | P     | 62/71 (87%)    | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 5   | e     | 62/71 (87%)    | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 6   | F     | 120/168 (71%)  | 106 (88%) | 10 (8%)  | 4 (3%)   | 4           | 14  |
| 6   | Q     | 120/168 (71%)  | 106 (88%) | 10 (8%)  | 4 (3%)   | 4           | 14  |
| 6   | f     | 120/168 (71%)  | 106 (88%) | 10 (8%)  | 4 (3%)   | 4           | 14  |
| 7   | I     | 40/70 (57%)    | 36 (90%)  | 4 (10%)  | 0        | 100         | 100 |
| 7   | R     | 40/70 (57%)    | 36 (90%)  | 4 (10%)  | 0        | 100         | 100 |
| 7   | i     | 40/70 (57%)    | 36 (90%)  | 4 (10%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8   | J     | 39/46 (85%)     | 34 (87%)   | 5 (13%)  | 0        | 100         | 100 |
| 8   | S     | 39/46 (85%)     | 34 (87%)   | 5 (13%)  | 0        | 100         | 100 |
| 8   | j     | 39/46 (85%)     | 34 (87%)   | 5 (13%)  | 0        | 100         | 100 |
| 9   | K     | 73/84 (87%)     | 57 (78%)   | 12 (16%) | 4 (6%)   | 2           | 5   |
| 9   | T     | 73/84 (87%)     | 57 (78%)   | 12 (16%) | 4 (6%)   | 2           | 5   |
| 9   | k     | 73/84 (87%)     | 57 (78%)   | 12 (16%) | 4 (6%)   | 2           | 5   |
| 10  | L     | 168/174 (97%)   | 165 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 10  | U     | 168/174 (97%)   | 165 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 10  | l     | 168/174 (97%)   | 165 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 11  | M     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 11  | V     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 11  | m     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 12  | W     | 95/99 (96%)     | 80 (84%)   | 13 (14%) | 2 (2%)   | 7           | 24  |
| 12  | X     | 95/99 (96%)     | 80 (84%)   | 13 (14%) | 2 (2%)   | 7           | 24  |
| 12  | x     | 95/99 (96%)     | 80 (84%)   | 13 (14%) | 2 (2%)   | 7           | 24  |
| All | All   | 6990/7512 (93%) | 6505 (93%) | 422 (6%) | 63 (1%)  | 21          | 46  |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | PRO  |
| 6   | F     | 62  | PRO  |
| 9   | K     | 43  | PRO  |
| 9   | K     | 47  | PRO  |
| 1   | G     | 41  | PRO  |
| 6   | Q     | 62  | PRO  |
| 9   | T     | 43  | PRO  |
| 9   | T     | 47  | PRO  |
| 1   | a     | 41  | PRO  |
| 6   | f     | 62  | PRO  |
| 9   | k     | 43  | PRO  |
| 9   | k     | 47  | PRO  |
| 1   | A     | 16  | GLU  |
| 1   | A     | 19  | PRO  |
| 4   | D     | 102 | VAL  |
| 4   | D     | 104 | PRO  |
| 1   | G     | 16  | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | G            | 19         | PRO         |
| 4          | O            | 102        | VAL         |
| 4          | O            | 104        | PRO         |
| 1          | a            | 16         | GLU         |
| 1          | a            | 19         | PRO         |
| 4          | d            | 102        | VAL         |
| 4          | d            | 104        | PRO         |
| 1          | A            | 40         | GLY         |
| 4          | D            | 100        | ASP         |
| 6          | F            | 65         | SER         |
| 1          | G            | 40         | GLY         |
| 4          | O            | 100        | ASP         |
| 6          | Q            | 65         | SER         |
| 1          | a            | 40         | GLY         |
| 4          | d            | 100        | ASP         |
| 6          | f            | 65         | SER         |
| 6          | F            | 64         | GLN         |
| 12         | X            | 66         | PHE         |
| 6          | Q            | 64         | GLN         |
| 12         | W            | 66         | PHE         |
| 6          | f            | 64         | GLN         |
| 12         | x            | 66         | PHE         |
| 1          | A            | 12         | SER         |
| 6          | F            | 61         | THR         |
| 9          | K            | 16         | THR         |
| 12         | X            | 87         | ASP         |
| 1          | G            | 12         | SER         |
| 6          | Q            | 61         | THR         |
| 9          | T            | 16         | THR         |
| 12         | W            | 87         | ASP         |
| 1          | a            | 12         | SER         |
| 6          | f            | 61         | THR         |
| 9          | k            | 16         | THR         |
| 12         | x            | 87         | ASP         |
| 9          | K            | 49         | PRO         |
| 9          | T            | 49         | PRO         |
| 9          | k            | 49         | PRO         |
| 1          | A            | 260        | ARG         |
| 4          | D            | 121        | ILE         |
| 1          | G            | 260        | ARG         |
| 4          | O            | 121        | ILE         |
| 1          | a            | 260        | ARG         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | d     | 121 | ILE  |
| 4   | D     | 122 | GLY  |
| 4   | O     | 122 | GLY  |
| 4   | d     | 122 | GLY  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | A     | 593/626 (95%)  | 582 (98%) | 11 (2%)  | 57          | 83  |
| 1   | G     | 593/626 (95%)  | 582 (98%) | 11 (2%)  | 57          | 83  |
| 1   | a     | 593/626 (95%)  | 582 (98%) | 11 (2%)  | 57          | 83  |
| 2   | B     | 598/599 (100%) | 593 (99%) | 5 (1%)   | 81          | 93  |
| 2   | H     | 598/599 (100%) | 593 (99%) | 5 (1%)   | 81          | 93  |
| 2   | b     | 598/599 (100%) | 593 (99%) | 5 (1%)   | 81          | 93  |
| 3   | C     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 3   | N     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 3   | c     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 4   | D     | 115/127 (91%)  | 110 (96%) | 5 (4%)   | 29          | 61  |
| 4   | O     | 115/127 (91%)  | 110 (96%) | 5 (4%)   | 29          | 61  |
| 4   | d     | 115/127 (91%)  | 110 (96%) | 5 (4%)   | 29          | 61  |
| 5   | E     | 56/61 (92%)    | 56 (100%) | 0        | 100         | 100 |
| 5   | P     | 56/61 (92%)    | 56 (100%) | 0        | 100         | 100 |
| 5   | e     | 56/61 (92%)    | 56 (100%) | 0        | 100         | 100 |
| 6   | F     | 63/140 (45%)   | 62 (98%)  | 1 (2%)   | 62          | 85  |
| 6   | Q     | 63/140 (45%)   | 62 (98%)  | 1 (2%)   | 62          | 85  |
| 6   | f     | 63/140 (45%)   | 62 (98%)  | 1 (2%)   | 62          | 85  |
| 7   | I     | 33/54 (61%)    | 32 (97%)  | 1 (3%)   | 41          | 73  |
| 7   | R     | 33/54 (61%)    | 32 (97%)  | 1 (3%)   | 41          | 73  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 7   | i     | 33/54 (61%)     | 32 (97%)   | 1 (3%)   | 41          | 73  |
| 8   | J     | 29/40 (72%)     | 27 (93%)   | 2 (7%)   | 15          | 40  |
| 8   | S     | 29/40 (72%)     | 27 (93%)   | 2 (7%)   | 15          | 40  |
| 8   | j     | 29/40 (72%)     | 27 (93%)   | 2 (7%)   | 15          | 40  |
| 9   | K     | 53/59 (90%)     | 46 (87%)   | 7 (13%)  | 4           | 11  |
| 9   | T     | 53/59 (90%)     | 46 (87%)   | 7 (13%)  | 4           | 11  |
| 9   | k     | 53/59 (90%)     | 46 (87%)   | 7 (13%)  | 4           | 11  |
| 10  | L     | 135/137 (98%)   | 134 (99%)  | 1 (1%)   | 84          | 95  |
| 10  | U     | 135/137 (98%)   | 134 (99%)  | 1 (1%)   | 84          | 95  |
| 10  | l     | 135/137 (98%)   | 134 (99%)  | 1 (1%)   | 84          | 95  |
| 11  | M     | 23/24 (96%)     | 23 (100%)  | 0        | 100         | 100 |
| 11  | V     | 23/24 (96%)     | 23 (100%)  | 0        | 100         | 100 |
| 11  | m     | 23/24 (96%)     | 23 (100%)  | 0        | 100         | 100 |
| 12  | W     | 52/85 (61%)     | 39 (75%)   | 13 (25%) | 0           | 1   |
| 12  | X     | 52/85 (61%)     | 39 (75%)   | 13 (25%) | 0           | 1   |
| 12  | x     | 52/85 (61%)     | 39 (75%)   | 13 (25%) | 0           | 1   |
| All | All   | 5451/6060 (90%) | 5313 (98%) | 138 (2%) | 50          | 77  |

All (138) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | PHE  |
| 1   | A     | 36  | THR  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 51  | HIS  |
| 1   | A     | 59  | SER  |
| 1   | A     | 103 | MET  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 172 | ILE  |
| 1   | A     | 187 | GLU  |
| 1   | A     | 254 | SER  |
| 1   | A     | 737 | LYS  |
| 2   | B     | 41  | SER  |
| 2   | B     | 130 | ARG  |
| 2   | B     | 205 | GLN  |
| 2   | B     | 220 | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | B            | 479        | TYR         |
| 4          | D            | 4          | THR         |
| 4          | D            | 24         | GLU         |
| 4          | D            | 65         | LEU         |
| 4          | D            | 92         | GLU         |
| 4          | D            | 103        | PHE         |
| 6          | F            | 63         | TYR         |
| 7          | I            | 42         | ARG         |
| 8          | J            | 30         | ASN         |
| 8          | J            | 31         | HIS         |
| 9          | K            | 16         | THR         |
| 9          | K            | 20         | ASN         |
| 9          | K            | 21         | VAL         |
| 9          | K            | 27         | ILE         |
| 9          | K            | 29         | ASN         |
| 9          | K            | 42         | ILE         |
| 9          | K            | 68         | HIS         |
| 10         | L            | 115        | ARG         |
| 12         | X            | 8          | LEU         |
| 12         | X            | 16         | ASN         |
| 12         | X            | 28         | LEU         |
| 12         | X            | 37         | ASP         |
| 12         | X            | 56         | GLU         |
| 12         | X            | 59         | VAL         |
| 12         | X            | 64         | GLN         |
| 12         | X            | 67         | LEU         |
| 12         | X            | 77         | VAL         |
| 12         | X            | 78         | LEU         |
| 12         | X            | 93         | HIS         |
| 12         | X            | 97         | GLU         |
| 12         | X            | 98         | LEU         |
| 1          | G            | 24         | PHE         |
| 1          | G            | 36         | THR         |
| 1          | G            | 37         | LEU         |
| 1          | G            | 51         | HIS         |
| 1          | G            | 59         | SER         |
| 1          | G            | 103        | MET         |
| 1          | G            | 134        | ARG         |
| 1          | G            | 172        | ILE         |
| 1          | G            | 187        | GLU         |
| 1          | G            | 254        | SER         |
| 1          | G            | 737        | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | H            | 41         | SER         |
| 2          | H            | 130        | ARG         |
| 2          | H            | 205        | GLN         |
| 2          | H            | 220        | GLU         |
| 2          | H            | 479        | TYR         |
| 4          | O            | 4          | THR         |
| 4          | O            | 24         | GLU         |
| 4          | O            | 65         | LEU         |
| 4          | O            | 92         | GLU         |
| 4          | O            | 103        | PHE         |
| 6          | Q            | 63         | TYR         |
| 7          | R            | 42         | ARG         |
| 8          | S            | 30         | ASN         |
| 8          | S            | 31         | HIS         |
| 9          | T            | 16         | THR         |
| 9          | T            | 20         | ASN         |
| 9          | T            | 21         | VAL         |
| 9          | T            | 27         | ILE         |
| 9          | T            | 29         | ASN         |
| 9          | T            | 42         | ILE         |
| 9          | T            | 68         | HIS         |
| 10         | U            | 115        | ARG         |
| 12         | W            | 8          | LEU         |
| 12         | W            | 16         | ASN         |
| 12         | W            | 28         | LEU         |
| 12         | W            | 37         | ASP         |
| 12         | W            | 56         | GLU         |
| 12         | W            | 59         | VAL         |
| 12         | W            | 64         | GLN         |
| 12         | W            | 67         | LEU         |
| 12         | W            | 77         | VAL         |
| 12         | W            | 78         | LEU         |
| 12         | W            | 93         | HIS         |
| 12         | W            | 97         | GLU         |
| 12         | W            | 98         | LEU         |
| 1          | a            | 24         | PHE         |
| 1          | a            | 36         | THR         |
| 1          | a            | 37         | LEU         |
| 1          | a            | 51         | HIS         |
| 1          | a            | 59         | SER         |
| 1          | a            | 103        | MET         |
| 1          | a            | 134        | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | a            | 172        | ILE         |
| 1          | a            | 187        | GLU         |
| 1          | a            | 254        | SER         |
| 1          | a            | 737        | LYS         |
| 2          | b            | 41         | SER         |
| 2          | b            | 130        | ARG         |
| 2          | b            | 205        | GLN         |
| 2          | b            | 220        | GLU         |
| 2          | b            | 479        | TYR         |
| 4          | d            | 4          | THR         |
| 4          | d            | 24         | GLU         |
| 4          | d            | 65         | LEU         |
| 4          | d            | 92         | GLU         |
| 4          | d            | 103        | PHE         |
| 6          | f            | 63         | TYR         |
| 7          | i            | 42         | ARG         |
| 8          | j            | 30         | ASN         |
| 8          | j            | 31         | HIS         |
| 9          | k            | 16         | THR         |
| 9          | k            | 20         | ASN         |
| 9          | k            | 21         | VAL         |
| 9          | k            | 27         | ILE         |
| 9          | k            | 29         | ASN         |
| 9          | k            | 42         | ILE         |
| 9          | k            | 68         | HIS         |
| 10         | l            | 115        | ARG         |
| 12         | x            | 8          | LEU         |
| 12         | x            | 16         | ASN         |
| 12         | x            | 28         | LEU         |
| 12         | x            | 37         | ASP         |
| 12         | x            | 56         | GLU         |
| 12         | x            | 59         | VAL         |
| 12         | x            | 64         | GLN         |
| 12         | x            | 67         | LEU         |
| 12         | x            | 77         | VAL         |
| 12         | x            | 78         | LEU         |
| 12         | x            | 93         | HIS         |
| 12         | x            | 97         | GLU         |
| 12         | x            | 98         | LEU         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | GLN  |
| 1   | A     | 92  | HIS  |
| 1   | A     | 108 | HIS  |
| 1   | A     | 137 | GLN  |
| 1   | A     | 180 | HIS  |
| 1   | A     | 190 | GLN  |
| 1   | A     | 329 | HIS  |
| 1   | A     | 400 | HIS  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 452 | GLN  |
| 1   | A     | 645 | GLN  |
| 1   | A     | 725 | GLN  |
| 1   | A     | 745 | GLN  |
| 2   | B     | 196 | HIS  |
| 2   | B     | 206 | HIS  |
| 2   | B     | 262 | HIS  |
| 2   | B     | 276 | HIS  |
| 2   | B     | 340 | GLN  |
| 2   | B     | 471 | GLN  |
| 2   | B     | 530 | HIS  |
| 2   | B     | 682 | GLN  |
| 2   | B     | 694 | ASN  |
| 3   | C     | 16  | GLN  |
| 4   | D     | 54  | ASN  |
| 4   | D     | 124 | ASN  |
| 9   | K     | 68  | HIS  |
| 10  | L     | 14  | GLN  |
| 10  | L     | 137 | GLN  |
| 10  | L     | 172 | ASN  |
| 12  | X     | 94  | GLN  |
| 1   | G     | 65  | GLN  |
| 1   | G     | 92  | HIS  |
| 1   | G     | 108 | HIS  |
| 1   | G     | 137 | GLN  |
| 1   | G     | 180 | HIS  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 257 | GLN  |
| 1   | G     | 329 | HIS  |
| 1   | G     | 400 | HIS  |
| 1   | G     | 428 | ASN  |
| 1   | G     | 452 | GLN  |
| 1   | G     | 645 | GLN  |
| 1   | G     | 725 | GLN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | G            | 745        | GLN         |
| 2          | H            | 196        | HIS         |
| 2          | H            | 206        | HIS         |
| 2          | H            | 262        | HIS         |
| 2          | H            | 276        | HIS         |
| 2          | H            | 340        | GLN         |
| 2          | H            | 471        | GLN         |
| 2          | H            | 530        | HIS         |
| 2          | H            | 682        | GLN         |
| 2          | H            | 694        | ASN         |
| 3          | N            | 16         | GLN         |
| 4          | O            | 54         | ASN         |
| 4          | O            | 124        | ASN         |
| 9          | T            | 68         | HIS         |
| 10         | U            | 14         | GLN         |
| 10         | U            | 137        | GLN         |
| 10         | U            | 172        | ASN         |
| 12         | W            | 93         | HIS         |
| 12         | W            | 94         | GLN         |
| 1          | a            | 60         | HIS         |
| 1          | a            | 65         | GLN         |
| 1          | a            | 92         | HIS         |
| 1          | a            | 108        | HIS         |
| 1          | a            | 137        | GLN         |
| 1          | a            | 180        | HIS         |
| 1          | a            | 190        | GLN         |
| 1          | a            | 329        | HIS         |
| 1          | a            | 400        | HIS         |
| 1          | a            | 428        | ASN         |
| 1          | a            | 452        | GLN         |
| 1          | a            | 645        | GLN         |
| 1          | a            | 725        | GLN         |
| 1          | a            | 745        | GLN         |
| 2          | b            | 196        | HIS         |
| 2          | b            | 206        | HIS         |
| 2          | b            | 262        | HIS         |
| 2          | b            | 276        | HIS         |
| 2          | b            | 340        | GLN         |
| 2          | b            | 471        | GLN         |
| 2          | b            | 530        | HIS         |
| 2          | b            | 682        | GLN         |
| 2          | b            | 694        | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | c     | 16  | GLN  |
| 4   | d     | 54  | ASN  |
| 4   | d     | 124 | ASN  |
| 9   | k     | 68  | HIS  |
| 10  | l     | 14  | GLN  |
| 10  | l     | 137 | GLN  |
| 10  | l     | 172 | ASN  |
| 12  | x     | 93  | HIS  |
| 12  | x     | 94  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 417 ligands modelled in this entry, 6 are monoatomic - leaving 411 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 | $\# Z  > 2$ |
| 14  | CLA  | H     | 1223 | -    | 65,73,73     | 2.23 | 18 (27%)    | 76,113,113  | 2.62 | 26 (34%)    |
| 14  | CLA  | a     | 1101 | -    | 45,53,73     | 2.58 | 19 (42%)    | 52,89,113   | 2.95 | 22 (42%)    |
| 15  | F6C  | H     | 1238 | 25   | 69,74,74     | 2.73 | 24 (34%)    | 70,114,114  | 3.11 | 29 (41%)    |
| 21  | LMT  | b     | 6003 | -    | 36,36,36     | 1.18 | 4 (11%)     | 47,47,47    | 1.60 | 7 (14%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 1123 | -    | 60,68,73     | 2.33 | 18 (30%) | 70,107,113  | 2.77 | 24 (34%) |
| 14  | CLA  | A     | 1103 | -    | 65,73,73     | 2.21 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 13  | CL0  | A     | 1011 | -    | 65,73,73     | 2.26 | 20 (30%) | 76,113,113  | 2.54 | 25 (32%) |
| 14  | CLA  | G     | 1133 | 1    | 60,68,73     | 2.32 | 18 (30%) | 70,107,113  | 2.77 | 20 (28%) |
| 18  | BCR  | H     | 4006 | -    | 41,41,41     | 2.82 | 6 (14%)  | 56,56,56    | 6.58 | 18 (32%) |
| 14  | CLA  | H     | 1220 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.58 | 22 (28%) |
| 18  | BCR  | b     | 4004 | -    | 41,41,41     | 2.82 | 6 (14%)  | 56,56,56    | 6.51 | 22 (39%) |
| 14  | CLA  | a     | 1138 | -    | 55,63,73     | 2.38 | 20 (36%) | 64,101,113  | 2.89 | 26 (40%) |
| 20  | LMG  | i     | 5006 | -    | 37,37,55     | 1.13 | 3 (8%)   | 45,45,63    | 1.21 | 5 (11%)  |
| 14  | CLA  | G     | 1107 | -    | 45,53,73     | 2.56 | 17 (37%) | 52,89,113   | 2.93 | 21 (40%) |
| 14  | CLA  | B     | 1227 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 2.99 | 19 (36%) |
| 14  | CLA  | a     | 1122 | -    | 55,63,73     | 2.35 | 19 (34%) | 64,101,113  | 2.71 | 24 (37%) |
| 14  | CLA  | A     | 1112 | -    | 55,63,73     | 2.44 | 20 (36%) | 64,101,113  | 2.79 | 22 (34%) |
| 20  | LMG  | B     | 5002 | -    | 46,46,55     | 1.29 | 6 (13%)  | 54,54,63    | 1.24 | 6 (11%)  |
| 21  | LMT  | U     | 6101 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.32 | 4 (8%)   |
| 21  | LMT  | l     | 6101 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.32 | 4 (8%)   |
| 14  | CLA  | G     | 1120 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 3.11 | 19 (36%) |
| 18  | BCR  | V     | 4021 | -    | 41,41,41     | 2.91 | 6 (14%)  | 56,56,56    | 6.64 | 19 (33%) |
| 14  | CLA  | b     | 1233 | -    | 45,53,73     | 2.57 | 19 (42%) | 52,89,113   | 2.91 | 20 (38%) |
| 14  | CLA  | A     | 1013 | -    | 60,68,73     | 2.30 | 19 (31%) | 70,107,113  | 2.80 | 22 (31%) |
| 15  | F6C  | H     | 1230 | -    | 49,54,74     | 3.18 | 25 (51%) | 46,90,114   | 3.80 | 25 (54%) |
| 21  | LMT  | A     | 6001 | -    | 32,32,36     | 1.30 | 6 (18%)  | 43,43,47    | 1.10 | 5 (11%)  |
| 15  | F6C  | H     | 1219 | -    | 59,64,74     | 2.96 | 26 (44%) | 58,102,114  | 3.52 | 28 (48%) |
| 21  | LMT  | U     | 6001 | -    | 13,13,36     | 0.44 | 0        | 12,12,47    | 0.90 | 0        |
| 14  | CLA  | H     | 1218 | -    | 45,53,73     | 2.57 | 18 (40%) | 52,89,113   | 3.08 | 21 (40%) |
| 14  | CLA  | H     | 1221 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.55 | 23 (30%) |
| 14  | CLA  | A     | 1136 | -    | 65,73,73     | 2.19 | 19 (29%) | 76,113,113  | 2.62 | 22 (28%) |
| 14  | CLA  | H     | 1239 | -    | 65,73,73     | 2.23 | 20 (30%) | 76,113,113  | 2.62 | 28 (36%) |
| 14  | CLA  | a     | 1106 | 1    | 60,68,73     | 2.31 | 19 (31%) | 70,107,113  | 2.76 | 25 (35%) |
| 14  | CLA  | G     | 1140 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.69 | 20 (31%) |
| 14  | CLA  | b     | 1209 | -    | 45,53,73     | 2.56 | 18 (40%) | 52,89,113   | 2.80 | 20 (38%) |
| 14  | CLA  | H     | 1233 | -    | 45,53,73     | 2.56 | 19 (42%) | 52,89,113   | 2.90 | 20 (38%) |
| 14  | CLA  | A     | 1109 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.67 | 23 (30%) |
| 19  | LHG  | A     | 5002 | -    | 43,43,48     | 1.00 | 2 (4%)   | 47,48,54    | 1.14 | 2 (4%)   |
| 14  | CLA  | B     | 1229 | -    | 60,68,73     | 2.33 | 19 (31%) | 70,107,113  | 2.69 | 23 (32%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | L     | 1503 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.56 | 23 (30%) |
| 14  | CLA  | B     | 1222 | 25   | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.66 | 24 (31%) |
| 18  | BCR  | I     | 4018 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.59 | 16 (28%) |
| 21  | LMT  | B     | 6004 | -    | 32,32,36     | 1.22 | 5 (15%)  | 43,43,47    | 1.16 | 4 (9%)   |
| 21  | LMT  | G     | 6003 | -    | 33,33,36     | 1.22 | 5 (15%)  | 44,44,47    | 0.95 | 1 (2%)   |
| 14  | CLA  | a     | 1110 | -    | 45,53,73     | 2.60 | 18 (40%) | 52,89,113   | 2.89 | 19 (36%) |
| 14  | CLA  | G     | 1117 | -    | 65,73,73     | 2.14 | 19 (29%) | 76,113,113  | 2.62 | 29 (38%) |
| 14  | CLA  | U     | 1501 | 10   | 65,73,73     | 2.18 | 18 (27%) | 76,113,113  | 2.61 | 23 (30%) |
| 15  | F6C  | b     | 1207 | -    | 69,74,74     | 2.75 | 24 (34%) | 70,114,114  | 3.17 | 28 (40%) |
| 14  | CLA  | B     | 1224 | -    | 65,73,73     | 2.22 | 17 (26%) | 76,113,113  | 2.64 | 24 (31%) |
| 14  | CLA  | b     | 1231 | -    | 65,73,73     | 2.18 | 19 (29%) | 76,113,113  | 2.57 | 21 (27%) |
| 14  | CLA  | b     | 1221 | -    | 65,73,73     | 2.24 | 19 (29%) | 76,113,113  | 2.55 | 23 (30%) |
| 14  | CLA  | B     | 1206 | -    | 65,73,73     | 2.23 | 18 (27%) | 76,113,113  | 2.60 | 24 (31%) |
| 17  | SF4  | C     | 3003 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | BCR  | B     | 4004 | -    | 41,41,41     | 2.82 | 6 (14%)  | 56,56,56    | 6.52 | 22 (39%) |
| 19  | LHG  | L     | 5101 | -    | 24,24,48     | 1.27 | 2 (8%)   | 26,26,54    | 1.48 | 4 (15%)  |
| 14  | CLA  | b     | 1223 | -    | 65,73,73     | 2.23 | 18 (27%) | 76,113,113  | 2.62 | 26 (34%) |
| 15  | F6C  | H     | 1207 | -    | 69,74,74     | 2.75 | 24 (34%) | 70,114,114  | 3.17 | 27 (38%) |
| 14  | CLA  | a     | 1141 | -    | 45,53,73     | 2.54 | 20 (44%) | 52,89,113   | 2.98 | 21 (40%) |
| 14  | CLA  | a     | 1131 | -    | 60,68,73     | 2.30 | 19 (31%) | 70,107,113  | 2.72 | 22 (31%) |
| 14  | CLA  | H     | 1227 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 3.00 | 19 (36%) |
| 14  | CLA  | B     | 1023 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.85 | 30 (39%) |
| 16  | PQN  | B     | 2002 | -    | 34,34,34     | 1.55 | 2 (5%)   | 42,45,45    | 1.12 | 2 (4%)   |
| 14  | CLA  | B     | 1233 | -    | 45,53,73     | 2.57 | 19 (42%) | 52,89,113   | 2.90 | 20 (38%) |
| 14  | CLA  | G     | 1111 | -    | 60,68,73     | 2.29 | 18 (30%) | 70,107,113  | 4.77 | 28 (40%) |
| 14  | CLA  | a     | 1119 | -    | 65,73,73     | 2.22 | 18 (27%) | 76,113,113  | 2.48 | 21 (27%) |
| 18  | BCR  | A     | 4005 | -    | 41,41,41     | 3.02 | 6 (14%)  | 56,56,56    | 6.52 | 23 (41%) |
| 21  | LMT  | b     | 6002 | -    | 36,36,36     | 1.21 | 6 (16%)  | 47,47,47    | 1.03 | 1 (2%)   |
| 14  | CLA  | B     | 1235 | -    | 60,68,73     | 2.29 | 19 (31%) | 70,107,113  | 2.77 | 26 (37%) |
| 14  | CLA  | B     | 1240 | 2    | 65,73,73     | 2.27 | 20 (30%) | 76,113,113  | 2.59 | 22 (28%) |
| 21  | LMT  | G     | 6001 | -    | 32,32,36     | 1.30 | 6 (18%)  | 43,43,47    | 1.10 | 5 (11%)  |
| 18  | BCR  | G     | 4001 | -    | 41,41,41     | 2.88 | 6 (14%)  | 56,56,56    | 6.56 | 17 (30%) |
| 19  | LHG  | a     | 5001 | -    | 41,41,48     | 1.05 | 2 (4%)   | 44,47,54    | 0.98 | 2 (4%)   |
| 18  | BCR  | G     | 4006 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.57 | 23 (41%) |
| 21  | LMT  | B     | 6001 | -    | 36,36,36     | 1.19 | 5 (13%)  | 47,47,47    | 0.96 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 1111 | -    | 60,68,73     | 2.30 | 18 (30%) | 70,107,113  | 4.77 | 27 (38%) |
| 17  | SF4  | c     | 3002 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 21  | LMT  | R     | 6001 | -    | 36,36,36     | 1.17 | 5 (13%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 15  | F6C  | A     | 1121 | -    | 49,54,74     | 3.13 | 24 (48%) | 46,90,114   | 3.77 | 27 (58%) |
| 15  | F6C  | b     | 1237 | 25   | 69,74,74     | 2.68 | 23 (33%) | 70,114,114  | 3.17 | 30 (42%) |
| 21  | LMT  | A     | 6002 | -    | 29,29,36     | 1.46 | 6 (20%)  | 40,40,47    | 1.24 | 4 (10%)  |
| 14  | CLA  | l     | 1501 | 10   | 65,73,73     | 2.18 | 18 (27%) | 76,113,113  | 2.60 | 23 (30%) |
| 14  | CLA  | B     | 1231 | -    | 65,73,73     | 2.19 | 19 (29%) | 76,113,113  | 2.57 | 21 (27%) |
| 21  | LMT  | H     | 6003 | -    | 36,36,36     | 1.18 | 3 (8%)   | 47,47,47    | 1.60 | 7 (14%)  |
| 18  | BCR  | b     | 4014 | -    | 41,41,41     | 2.81 | 6 (14%)  | 56,56,56    | 6.63 | 20 (35%) |
| 14  | CLA  | A     | 1102 | -    | 50,58,73     | 2.59 | 21 (42%) | 58,95,113   | 2.95 | 24 (41%) |
| 14  | CLA  | a     | 1130 | -    | 55,63,73     | 2.46 | 19 (34%) | 64,101,113  | 2.66 | 21 (32%) |
| 14  | CLA  | b     | 1206 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.61 | 24 (31%) |
| 21  | LMT  | H     | 6004 | -    | 32,32,36     | 1.21 | 4 (12%)  | 43,43,47    | 1.16 | 4 (9%)   |
| 14  | CLA  | H     | 1224 | -    | 65,73,73     | 2.23 | 17 (26%) | 76,113,113  | 2.65 | 24 (31%) |
| 14  | CLA  | b     | 1205 | -    | 65,73,73     | 2.17 | 17 (26%) | 76,113,113  | 2.67 | 24 (31%) |
| 16  | PQN  | A     | 2001 | -    | 34,34,34     | 1.50 | 2 (5%)   | 42,45,45    | 1.19 | 4 (9%)   |
| 20  | LMG  | a     | 5003 | -    | 46,46,55     | 1.29 | 5 (10%)  | 54,54,63    | 1.25 | 4 (7%)   |
| 14  | CLA  | V     | 1501 | -    | 50,58,73     | 2.53 | 18 (36%) | 58,95,113   | 2.91 | 24 (41%) |
| 14  | CLA  | G     | 1109 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.66 | 23 (30%) |
| 14  | CLA  | H     | 1231 | -    | 65,73,73     | 2.19 | 19 (29%) | 76,113,113  | 2.57 | 21 (27%) |
| 14  | CLA  | A     | 1120 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 3.11 | 19 (36%) |
| 14  | CLA  | G     | 1119 | -    | 65,73,73     | 2.23 | 18 (27%) | 76,113,113  | 2.48 | 21 (27%) |
| 14  | CLA  | a     | 1135 | -    | 50,58,73     | 2.56 | 20 (40%) | 58,95,113   | 2.94 | 24 (41%) |
| 14  | CLA  | H     | 1236 | -    | 55,63,73     | 2.33 | 19 (34%) | 64,101,113  | 2.98 | 23 (35%) |
| 15  | F6C  | B     | 1237 | 25   | 69,74,74     | 2.68 | 23 (33%) | 70,114,114  | 3.17 | 30 (42%) |
| 14  | CLA  | a     | 1013 | -    | 60,68,73     | 2.31 | 19 (31%) | 70,107,113  | 2.79 | 22 (31%) |
| 18  | BCR  | A     | 4003 | -    | 41,41,41     | 2.96 | 6 (14%)  | 56,56,56    | 6.84 | 25 (44%) |
| 21  | LMT  | m     | 6000 | -    | 36,36,36     | 1.19 | 6 (16%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 14  | CLA  | a     | 1107 | -    | 45,53,73     | 2.56 | 17 (37%) | 52,89,113   | 2.92 | 21 (40%) |
| 19  | LHG  | G     | 5001 | -    | 41,41,48     | 1.05 | 2 (4%)   | 44,47,54    | 0.98 | 2 (4%)   |
| 14  | CLA  | A     | 1108 | -    | 45,53,73     | 2.62 | 19 (42%) | 52,89,113   | 2.91 | 22 (42%) |
| 18  | BCR  | b     | 4006 | -    | 41,41,41     | 2.82 | 6 (14%)  | 56,56,56    | 6.58 | 18 (32%) |
| 14  | CLA  | b     | 1217 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 2.96 | 20 (38%) |
| 21  | LMT  | G     | 6004 | -    | 24,24,36     | 1.05 | 3 (12%)  | 29,29,47    | 1.07 | 2 (6%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | B     | 1204 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.60 | 23 (30%) |
| 14  | CLA  | A     | 1141 | -    | 45,53,73     | 2.55 | 20 (44%) | 52,89,113   | 2.98 | 21 (40%) |
| 14  | CLA  | A     | 1137 | -    | 50,58,73     | 2.52 | 18 (36%) | 58,95,113   | 3.01 | 22 (37%) |
| 20  | LMG  | H     | 5002 | -    | 46,46,55     | 1.29 | 6 (13%)  | 54,54,63    | 1.24 | 6 (11%)  |
| 21  | LMT  | U     | 6002 | -    | 36,36,36     | 1.29 | 5 (13%)  | 47,47,47    | 1.21 | 7 (14%)  |
| 14  | CLA  | b     | 1215 | -    | 60,68,73     | 2.28 | 19 (31%) | 70,107,113  | 2.62 | 20 (28%) |
| 17  | SF4  | a     | 3001 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | BCR  | l     | 4019 | -    | 41,41,41     | 3.08 | 7 (17%)  | 56,56,56    | 6.50 | 28 (50%) |
| 14  | CLA  | A     | 1129 | -    | 50,58,73     | 2.51 | 19 (38%) | 58,95,113   | 3.08 | 25 (43%) |
| 18  | BCR  | G     | 4005 | -    | 41,41,41     | 3.02 | 7 (17%)  | 56,56,56    | 6.51 | 23 (41%) |
| 15  | F6C  | B     | 1238 | 25   | 69,74,74     | 2.73 | 24 (34%) | 70,114,114  | 3.12 | 29 (41%) |
| 18  | BCR  | R     | 4018 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.59 | 16 (28%) |
| 14  | CLA  | H     | 1201 | -    | 65,73,73     | 2.20 | 20 (30%) | 76,113,113  | 2.71 | 25 (32%) |
| 21  | LMT  | l     | 6002 | -    | 36,36,36     | 1.29 | 5 (13%)  | 47,47,47    | 1.22 | 7 (14%)  |
| 15  | F6C  | H     | 1237 | 25   | 69,74,74     | 2.68 | 23 (33%) | 70,114,114  | 3.18 | 30 (42%) |
| 14  | CLA  | a     | 1116 | -    | 55,63,73     | 2.42 | 19 (34%) | 64,101,113  | 2.75 | 23 (35%) |
| 14  | CLA  | G     | 1129 | -    | 50,58,73     | 2.51 | 19 (38%) | 58,95,113   | 3.08 | 25 (43%) |
| 14  | CLA  | a     | 1105 | -    | 45,53,73     | 2.61 | 19 (42%) | 52,89,113   | 2.94 | 20 (38%) |
| 14  | CLA  | b     | 1021 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.47 | 27 (35%) |
| 20  | LMG  | G     | 5003 | -    | 46,46,55     | 1.29 | 5 (10%)  | 54,54,63    | 1.25 | 4 (7%)   |
| 14  | CLA  | A     | 1133 | 1    | 60,68,73     | 2.31 | 18 (30%) | 70,107,113  | 2.76 | 20 (28%) |
| 14  | CLA  | G     | 1126 | -    | 60,68,73     | 2.34 | 17 (28%) | 70,107,113  | 2.59 | 20 (28%) |
| 14  | CLA  | B     | 1215 | -    | 60,68,73     | 2.27 | 19 (31%) | 70,107,113  | 2.62 | 20 (28%) |
| 14  | CLA  | a     | 1114 | -    | 45,53,73     | 2.58 | 19 (42%) | 52,89,113   | 2.88 | 19 (36%) |
| 14  | CLA  | b     | 1023 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.86 | 30 (39%) |
| 14  | CLA  | G     | 1124 | 25   | 55,63,73     | 2.40 | 18 (32%) | 64,101,113  | 2.83 | 21 (32%) |
| 14  | CLA  | B     | 1214 | -    | 60,68,73     | 2.34 | 21 (35%) | 70,107,113  | 2.67 | 28 (40%) |
| 14  | CLA  | a     | 1128 | -    | 60,68,73     | 2.34 | 19 (31%) | 70,107,113  | 2.69 | 23 (32%) |
| 14  | CLA  | a     | 1126 | -    | 60,68,73     | 2.33 | 17 (28%) | 70,107,113  | 2.59 | 20 (28%) |
| 14  | CLA  | a     | 1118 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.79 | 22 (34%) |
| 14  | CLA  | b     | 1232 | -    | 45,53,73     | 2.58 | 20 (44%) | 52,89,113   | 2.89 | 20 (38%) |
| 21  | LMT  | H     | 6001 | -    | 36,36,36     | 1.19 | 5 (13%)  | 47,47,47    | 0.96 | 1 (2%)   |
| 14  | CLA  | B     | 1203 | -    | 65,73,73     | 2.17 | 19 (29%) | 76,113,113  | 2.69 | 22 (28%) |
| 21  | LMT  | L     | 6001 | -    | 13,13,36     | 0.44 | 0        | 12,12,47    | 0.90 | 0        |
| 14  | CLA  | H     | 1206 | -    | 65,73,73     | 2.24 | 19 (29%) | 76,113,113  | 2.60 | 24 (31%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 1103 | -    | 65,73,73     | 2.21 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 14  | CLA  | G     | 1122 | -    | 55,63,73     | 2.35 | 19 (34%) | 64,101,113  | 2.71 | 25 (39%) |
| 18  | BCR  | B     | 4014 | -    | 41,41,41     | 2.81 | 6 (14%)  | 56,56,56    | 6.63 | 20 (35%) |
| 19  | LHG  | L     | 5102 | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 14  | CLA  | B     | 1217 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 2.95 | 20 (38%) |
| 14  | CLA  | b     | 1234 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.54 | 24 (31%) |
| 14  | CLA  | B     | 1226 | -    | 65,73,73     | 2.27 | 18 (27%) | 76,113,113  | 2.62 | 24 (31%) |
| 18  | BCR  | U     | 4019 | -    | 41,41,41     | 3.09 | 7 (17%)  | 56,56,56    | 6.49 | 28 (50%) |
| 14  | CLA  | H     | 1023 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.85 | 30 (39%) |
| 14  | CLA  | A     | 1140 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.69 | 21 (32%) |
| 16  | PQN  | H     | 2002 | -    | 34,34,34     | 1.56 | 2 (5%)   | 42,45,45    | 1.12 | 2 (4%)   |
| 14  | CLA  | G     | 1102 | -    | 50,58,73     | 2.59 | 21 (42%) | 58,95,113   | 2.96 | 24 (41%) |
| 21  | LMT  | A     | 6004 | -    | 24,24,36     | 1.06 | 3 (12%)  | 29,29,47    | 1.07 | 2 (6%)   |
| 14  | CLA  | G     | 1116 | -    | 55,63,73     | 2.41 | 19 (34%) | 64,101,113  | 2.74 | 22 (34%) |
| 13  | CL0  | a     | 1011 | -    | 65,73,73     | 2.26 | 20 (30%) | 76,113,113  | 2.54 | 25 (32%) |
| 18  | BCR  | G     | 4003 | -    | 41,41,41     | 2.95 | 6 (14%)  | 56,56,56    | 6.84 | 25 (44%) |
| 16  | PQN  | a     | 2001 | -    | 34,34,34     | 1.50 | 2 (5%)   | 42,45,45    | 1.19 | 4 (9%)   |
| 14  | CLA  | G     | 1103 | -    | 65,73,73     | 2.21 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 14  | CLA  | L     | 1501 | 10   | 65,73,73     | 2.18 | 18 (27%) | 76,113,113  | 2.61 | 23 (30%) |
| 14  | CLA  | A     | 1123 | -    | 60,68,73     | 2.32 | 18 (30%) | 70,107,113  | 2.77 | 24 (34%) |
| 14  | CLA  | H     | 1240 | 2    | 65,73,73     | 2.27 | 20 (30%) | 76,113,113  | 2.59 | 22 (28%) |
| 14  | CLA  | A     | 1111 | -    | 60,68,73     | 2.29 | 18 (30%) | 70,107,113  | 4.77 | 28 (40%) |
| 15  | F6C  | B     | 1219 | -    | 59,64,74     | 2.96 | 26 (44%) | 58,102,114  | 3.52 | 27 (46%) |
| 14  | CLA  | a     | 1125 | -    | 65,73,73     | 2.16 | 18 (27%) | 76,113,113  | 2.69 | 23 (30%) |
| 18  | BCR  | B     | 4009 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.51 | 23 (41%) |
| 18  | BCR  | A     | 4001 | -    | 41,41,41     | 2.88 | 6 (14%)  | 56,56,56    | 6.56 | 17 (30%) |
| 18  | BCR  | T     | 4001 | -    | 41,41,41     | 2.90 | 6 (14%)  | 56,56,56    | 6.45 | 22 (39%) |
| 14  | CLA  | G     | 1138 | -    | 55,63,73     | 2.38 | 20 (36%) | 64,101,113  | 2.89 | 26 (40%) |
| 14  | CLA  | k     | 1401 | -    | 45,53,73     | 2.59 | 19 (42%) | 52,89,113   | 3.03 | 22 (42%) |
| 14  | CLA  | A     | 1138 | -    | 55,63,73     | 2.38 | 20 (36%) | 64,101,113  | 2.89 | 26 (40%) |
| 14  | CLA  | b     | 1236 | -    | 55,63,73     | 2.32 | 18 (32%) | 64,101,113  | 2.98 | 23 (35%) |
| 14  | CLA  | b     | 1216 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.42 | 21 (27%) |
| 14  | CLA  | a     | 1102 | -    | 50,58,73     | 2.59 | 21 (42%) | 58,95,113   | 2.96 | 24 (41%) |
| 14  | CLA  | b     | 1201 | -    | 65,73,73     | 2.20 | 20 (30%) | 76,113,113  | 2.71 | 25 (32%) |
| 14  | CLA  | a     | 1109 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.67 | 23 (30%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | BCR  | b     | 4017 | -    | 41,41,41     | 3.05 | 8 (19%)  | 56,56,56    | 6.72 | 20 (35%) |
| 14  | CLA  | H     | 1226 | -    | 65,73,73     | 2.27 | 18 (27%) | 76,113,113  | 2.63 | 24 (31%) |
| 18  | BCR  | m     | 4021 | -    | 41,41,41     | 2.91 | 6 (14%)  | 56,56,56    | 6.64 | 19 (33%) |
| 17  | SF4  | C     | 3002 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | a     | 1139 | -    | 45,53,73     | 2.57 | 20 (44%) | 52,89,113   | 2.84 | 20 (38%) |
| 24  | FES  | X     | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 1228 | -    | 55,63,73     | 2.45 | 20 (36%) | 64,101,113  | 2.66 | 26 (40%) |
| 14  | CLA  | A     | 1101 | -    | 45,53,73     | 2.57 | 19 (42%) | 52,89,113   | 2.94 | 22 (42%) |
| 14  | CLA  | b     | 1022 | -    | 55,63,73     | 2.38 | 17 (30%) | 64,101,113  | 2.73 | 24 (37%) |
| 14  | CLA  | H     | 1210 | -    | 65,73,73     | 2.21 | 18 (27%) | 76,113,113  | 2.82 | 25 (32%) |
| 14  | CLA  | G     | 1104 | -    | 65,73,73     | 2.15 | 19 (29%) | 76,113,113  | 2.80 | 24 (31%) |
| 14  | CLA  | a     | 1120 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 3.10 | 19 (36%) |
| 18  | BCR  | b     | 4005 | -    | 41,41,41     | 2.84 | 6 (14%)  | 56,56,56    | 6.53 | 20 (35%) |
| 14  | CLA  | G     | 1139 | -    | 45,53,73     | 2.56 | 20 (44%) | 52,89,113   | 2.84 | 20 (38%) |
| 14  | CLA  | U     | 1502 | -    | 60,68,73     | 2.28 | 18 (30%) | 70,107,113  | 2.69 | 21 (30%) |
| 14  | CLA  | a     | 1012 | 25   | 65,73,73     | 2.20 | 17 (26%) | 76,113,113  | 2.52 | 25 (32%) |
| 14  | CLA  | a     | 1132 | -    | 65,73,73     | 2.19 | 18 (27%) | 76,113,113  | 2.65 | 23 (30%) |
| 18  | BCR  | I     | 4020 | -    | 41,41,41     | 3.17 | 9 (21%)  | 56,56,56    | 6.78 | 21 (37%) |
| 21  | LMT  | l     | 6001 | -    | 13,13,36     | 0.44 | 0        | 12,12,47    | 0.91 | 0        |
| 13  | CL0  | G     | 1011 | -    | 65,73,73     | 2.26 | 20 (30%) | 76,113,113  | 2.54 | 25 (32%) |
| 14  | CLA  | G     | 1134 | 1    | 45,53,73     | 2.55 | 20 (44%) | 52,89,113   | 2.92 | 20 (38%) |
| 14  | CLA  | B     | 1234 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.54 | 24 (31%) |
| 18  | BCR  | G     | 4004 | -    | 41,41,41     | 3.04 | 6 (14%)  | 56,56,56    | 6.67 | 25 (44%) |
| 14  | CLA  | b     | 1224 | -    | 65,73,73     | 2.22 | 17 (26%) | 76,113,113  | 2.64 | 23 (30%) |
| 14  | CLA  | A     | 1106 | 1    | 60,68,73     | 2.31 | 18 (30%) | 70,107,113  | 2.76 | 25 (35%) |
| 14  | CLA  | a     | 1108 | -    | 45,53,73     | 2.61 | 19 (42%) | 52,89,113   | 2.90 | 22 (42%) |
| 21  | LMT  | L     | 6002 | -    | 36,36,36     | 1.29 | 5 (13%)  | 47,47,47    | 1.21 | 7 (14%)  |
| 14  | CLA  | G     | 1112 | -    | 55,63,73     | 2.44 | 20 (36%) | 64,101,113  | 2.79 | 22 (34%) |
| 14  | CLA  | b     | 1210 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.82 | 25 (32%) |
| 15  | F6C  | B     | 1207 | -    | 69,74,74     | 2.75 | 24 (34%) | 70,114,114  | 3.16 | 28 (40%) |
| 18  | BCR  | L     | 4022 | -    | 41,41,41     | 3.00 | 6 (14%)  | 56,56,56    | 6.39 | 22 (39%) |
| 14  | CLA  | A     | 1134 | 1    | 45,53,73     | 2.54 | 20 (44%) | 52,89,113   | 2.92 | 20 (38%) |
| 14  | CLA  | b     | 1239 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.63 | 27 (35%) |
| 21  | LMT  | V     | 6000 | -    | 36,36,36     | 1.19 | 6 (16%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 14  | CLA  | G     | 1135 | -    | 50,58,73     | 2.56 | 20 (40%) | 58,95,113   | 2.95 | 25 (43%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | b     | 1227 | -    | 45,53,73     | 2.52 | 18 (40%) | 52,89,113   | 2.99 | 19 (36%) |
| 18  | BCR  | M     | 4021 | -    | 41,41,41     | 2.91 | 6 (14%)  | 56,56,56    | 6.65 | 19 (33%) |
| 14  | CLA  | B     | 1216 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.42 | 21 (27%) |
| 14  | CLA  | B     | 1236 | -    | 55,63,73     | 2.33 | 18 (32%) | 64,101,113  | 2.98 | 23 (35%) |
| 18  | BCR  | B     | 4010 | -    | 41,41,41     | 3.03 | 7 (17%)  | 56,56,56    | 6.85 | 21 (37%) |
| 14  | CLA  | B     | 1210 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.82 | 25 (32%) |
| 14  | CLA  | b     | 1220 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.57 | 22 (28%) |
| 14  | CLA  | H     | 1214 | -    | 60,68,73     | 2.34 | 21 (35%) | 70,107,113  | 2.66 | 28 (40%) |
| 14  | CLA  | a     | 1117 | -    | 65,73,73     | 2.15 | 19 (29%) | 76,113,113  | 2.62 | 28 (36%) |
| 14  | CLA  | H     | 1021 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.47 | 27 (35%) |
| 18  | BCR  | B     | 4017 | -    | 41,41,41     | 3.05 | 8 (19%)  | 56,56,56    | 6.71 | 20 (35%) |
| 18  | BCR  | a     | 4002 | -    | 41,41,41     | 2.85 | 6 (14%)  | 56,56,56    | 6.52 | 25 (44%) |
| 14  | CLA  | B     | 1221 | -    | 65,73,73     | 2.24 | 19 (29%) | 76,113,113  | 2.55 | 23 (30%) |
| 14  | CLA  | a     | 1127 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.54 | 21 (27%) |
| 21  | LMT  | a     | 6002 | -    | 29,29,36     | 1.46 | 6 (20%)  | 40,40,47    | 1.23 | 4 (10%)  |
| 21  | LMT  | I     | 6001 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 18  | BCR  | L     | 4019 | -    | 41,41,41     | 3.09 | 7 (17%)  | 56,56,56    | 6.50 | 28 (50%) |
| 14  | CLA  | b     | 1225 | -    | 65,73,73     | 2.26 | 19 (29%) | 76,113,113  | 2.48 | 19 (25%) |
| 14  | CLA  | G     | 1123 | -    | 60,68,73     | 2.33 | 18 (30%) | 70,107,113  | 2.77 | 24 (34%) |
| 14  | CLA  | G     | 1101 | -    | 45,53,73     | 2.57 | 19 (42%) | 52,89,113   | 2.94 | 22 (42%) |
| 14  | CLA  | l     | 1502 | -    | 60,68,73     | 2.27 | 18 (30%) | 70,107,113  | 2.69 | 21 (30%) |
| 15  | F6C  | G     | 1121 | -    | 49,54,74     | 3.13 | 24 (48%) | 46,90,114   | 3.77 | 27 (58%) |
| 18  | BCR  | G     | 4002 | -    | 41,41,41     | 2.85 | 6 (14%)  | 56,56,56    | 6.52 | 25 (44%) |
| 14  | CLA  | G     | 1106 | 1    | 60,68,73     | 2.31 | 18 (30%) | 70,107,113  | 2.77 | 25 (35%) |
| 18  | BCR  | B     | 4005 | -    | 41,41,41     | 2.83 | 6 (14%)  | 56,56,56    | 6.53 | 20 (35%) |
| 18  | BCR  | a     | 4001 | -    | 41,41,41     | 2.88 | 6 (14%)  | 56,56,56    | 6.56 | 17 (30%) |
| 14  | CLA  | b     | 1229 | -    | 60,68,73     | 2.33 | 19 (31%) | 70,107,113  | 2.69 | 23 (32%) |
| 21  | LMT  | B     | 6003 | -    | 36,36,36     | 1.18 | 4 (11%)  | 47,47,47    | 1.60 | 7 (14%)  |
| 21  | LMT  | G     | 6002 | -    | 29,29,36     | 1.46 | 6 (20%)  | 40,40,47    | 1.23 | 4 (10%)  |
| 14  | CLA  | T     | 1401 | -    | 45,53,73     | 2.59 | 20 (44%) | 52,89,113   | 3.03 | 22 (42%) |
| 14  | CLA  | A     | 1124 | 25   | 55,63,73     | 2.40 | 18 (32%) | 64,101,113  | 2.83 | 21 (32%) |
| 14  | CLA  | B     | 1223 | -    | 65,73,73     | 2.23 | 18 (27%) | 76,113,113  | 2.62 | 26 (34%) |
| 14  | CLA  | b     | 1203 | -    | 65,73,73     | 2.17 | 19 (29%) | 76,113,113  | 2.69 | 22 (28%) |
| 21  | LMT  | b     | 6004 | -    | 32,32,36     | 1.22 | 5 (15%)  | 43,43,47    | 1.17 | 4 (9%)   |
| 14  | CLA  | A     | 1117 | -    | 65,73,73     | 2.15 | 19 (29%) | 76,113,113  | 2.62 | 28 (36%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | G     | 1110 | -    | 45,53,73     | 2.61 | 18 (40%) | 52,89,113   | 2.89 | 19 (36%) |
| 14  | CLA  | H     | 1212 | -    | 45,53,73     | 2.54 | 18 (40%) | 52,89,113   | 2.96 | 22 (42%) |
| 18  | BCR  | i     | 4018 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.59 | 16 (28%) |
| 14  | CLA  | A     | 1122 | -    | 55,63,73     | 2.35 | 19 (34%) | 64,101,113  | 2.71 | 24 (37%) |
| 14  | CLA  | H     | 1203 | -    | 65,73,73     | 2.17 | 19 (29%) | 76,113,113  | 2.69 | 22 (28%) |
| 14  | CLA  | H     | 1209 | -    | 45,53,73     | 2.55 | 18 (40%) | 52,89,113   | 2.80 | 20 (38%) |
| 18  | BCR  | A     | 4002 | -    | 41,41,41     | 2.85 | 6 (14%)  | 56,56,56    | 6.53 | 25 (44%) |
| 21  | LMT  | B     | 6002 | -    | 36,36,36     | 1.20 | 6 (16%)  | 47,47,47    | 1.02 | 1 (2%)   |
| 17  | SF4  | N     | 3002 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | BCR  | H     | 4014 | -    | 41,41,41     | 2.81 | 6 (14%)  | 56,56,56    | 6.63 | 20 (35%) |
| 18  | BCR  | A     | 4006 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.57 | 24 (42%) |
| 14  | CLA  | b     | 1226 | -    | 65,73,73     | 2.27 | 18 (27%) | 76,113,113  | 2.62 | 24 (31%) |
| 14  | CLA  | H     | 1022 | -    | 55,63,73     | 2.38 | 18 (32%) | 64,101,113  | 2.73 | 24 (37%) |
| 18  | BCR  | i     | 4020 | -    | 41,41,41     | 3.17 | 9 (21%)  | 56,56,56    | 6.78 | 21 (37%) |
| 21  | LMT  | a     | 6001 | -    | 32,32,36     | 1.31 | 6 (18%)  | 43,43,47    | 1.10 | 5 (11%)  |
| 14  | CLA  | a     | 1136 | -    | 65,73,73     | 2.19 | 19 (29%) | 76,113,113  | 2.61 | 22 (28%) |
| 14  | CLA  | B     | 1228 | -    | 55,63,73     | 2.45 | 20 (36%) | 64,101,113  | 2.66 | 26 (40%) |
| 14  | CLA  | b     | 1208 | -    | 60,68,73     | 2.34 | 19 (31%) | 70,107,113  | 2.75 | 26 (37%) |
| 14  | CLA  | H     | 1216 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.41 | 21 (27%) |
| 19  | LHG  | A     | 5001 | -    | 41,41,48     | 1.05 | 2 (4%)   | 44,47,54    | 0.98 | 2 (4%)   |
| 14  | CLA  | G     | 1127 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.53 | 21 (27%) |
| 14  | CLA  | H     | 1225 | -    | 65,73,73     | 2.26 | 19 (29%) | 76,113,113  | 2.48 | 19 (25%) |
| 18  | BCR  | K     | 4001 | -    | 41,41,41     | 2.90 | 6 (14%)  | 56,56,56    | 6.45 | 22 (39%) |
| 14  | CLA  | m     | 1501 | -    | 50,58,73     | 2.52 | 18 (36%) | 58,95,113   | 2.91 | 24 (41%) |
| 18  | BCR  | b     | 4010 | -    | 41,41,41     | 3.03 | 7 (17%)  | 56,56,56    | 6.86 | 21 (37%) |
| 14  | CLA  | H     | 1229 | -    | 60,68,73     | 2.33 | 19 (31%) | 70,107,113  | 2.70 | 23 (32%) |
| 18  | BCR  | A     | 4004 | -    | 41,41,41     | 3.04 | 6 (14%)  | 56,56,56    | 6.67 | 25 (44%) |
| 19  | LHG  | a     | 5002 | -    | 43,43,48     | 1.00 | 2 (4%)   | 47,48,54    | 1.13 | 2 (4%)   |
| 14  | CLA  | A     | 1104 | -    | 65,73,73     | 2.15 | 19 (29%) | 76,113,113  | 2.79 | 24 (31%) |
| 14  | CLA  | H     | 1228 | -    | 55,63,73     | 2.44 | 20 (36%) | 64,101,113  | 2.66 | 26 (40%) |
| 14  | CLA  | b     | 1222 | 25   | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.67 | 25 (32%) |
| 14  | CLA  | B     | 1212 | -    | 45,53,73     | 2.55 | 19 (42%) | 52,89,113   | 2.97 | 22 (42%) |
| 14  | CLA  | A     | 1113 | -    | 45,53,73     | 2.55 | 18 (40%) | 52,89,113   | 2.87 | 21 (40%) |
| 21  | LMT  | b     | 6001 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 0.96 | 2 (4%)   |
| 24  | FES  | W     | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | H     | 1215 | -    | 60,68,73     | 2.27 | 19 (31%) | 70,107,113  | 2.62 | 20 (28%) |
| 21  | LMT  | H     | 6002 | -    | 36,36,36     | 1.20 | 6 (16%)  | 47,47,47    | 1.02 | 1 (2%)   |
| 14  | CLA  | B     | 1022 | -    | 55,63,73     | 2.38 | 18 (32%) | 64,101,113  | 2.74 | 24 (37%) |
| 14  | CLA  | G     | 1132 | -    | 65,73,73     | 2.19 | 18 (27%) | 76,113,113  | 2.64 | 23 (30%) |
| 15  | F6C  | b     | 1230 | -    | 49,54,74     | 3.18 | 25 (51%) | 46,90,114   | 3.79 | 25 (54%) |
| 14  | CLA  | B     | 1225 | -    | 65,73,73     | 2.27 | 19 (29%) | 76,113,113  | 2.48 | 19 (25%) |
| 20  | LMG  | A     | 5003 | -    | 46,46,55     | 1.29 | 5 (10%)  | 54,54,63    | 1.25 | 4 (7%)   |
| 14  | CLA  | B     | 1205 | -    | 65,73,73     | 2.17 | 17 (26%) | 76,113,113  | 2.67 | 24 (31%) |
| 14  | CLA  | B     | 1201 | -    | 65,73,73     | 2.20 | 20 (30%) | 76,113,113  | 2.71 | 25 (32%) |
| 14  | CLA  | G     | 1130 | -    | 55,63,73     | 2.46 | 19 (34%) | 64,101,113  | 2.65 | 21 (32%) |
| 14  | CLA  | b     | 1240 | 2    | 65,73,73     | 2.27 | 20 (30%) | 76,113,113  | 2.59 | 22 (28%) |
| 21  | LMT  | L     | 6101 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.32 | 4 (8%)   |
| 14  | CLA  | L     | 1502 | -    | 60,68,73     | 2.27 | 18 (30%) | 70,107,113  | 2.69 | 21 (30%) |
| 14  | CLA  | A     | 1115 | -    | 65,73,73     | 2.26 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 14  | CLA  | a     | 1112 | -    | 55,63,73     | 2.44 | 20 (36%) | 64,101,113  | 2.80 | 22 (34%) |
| 14  | CLA  | H     | 1208 | -    | 60,68,73     | 2.33 | 19 (31%) | 70,107,113  | 2.76 | 26 (37%) |
| 18  | BCR  | l     | 4022 | -    | 41,41,41     | 3.01 | 6 (14%)  | 56,56,56    | 6.40 | 22 (39%) |
| 18  | BCR  | a     | 4005 | -    | 41,41,41     | 3.03 | 7 (17%)  | 56,56,56    | 6.52 | 23 (41%) |
| 14  | CLA  | G     | 1013 | -    | 60,68,73     | 2.30 | 19 (31%) | 70,107,113  | 2.80 | 22 (31%) |
| 14  | CLA  | A     | 1110 | -    | 45,53,73     | 2.60 | 18 (40%) | 52,89,113   | 2.89 | 19 (36%) |
| 14  | CLA  | A     | 1107 | -    | 45,53,73     | 2.57 | 17 (37%) | 52,89,113   | 2.92 | 21 (40%) |
| 20  | LMG  | R     | 5006 | -    | 37,37,55     | 1.13 | 3 (8%)   | 45,45,63    | 1.21 | 5 (11%)  |
| 14  | CLA  | H     | 1217 | -    | 45,53,73     | 2.53 | 18 (40%) | 52,89,113   | 2.95 | 20 (38%) |
| 21  | LMT  | a     | 6003 | -    | 33,33,36     | 1.22 | 5 (15%)  | 44,44,47    | 0.95 | 1 (2%)   |
| 14  | CLA  | H     | 1235 | -    | 60,68,73     | 2.29 | 19 (31%) | 70,107,113  | 2.76 | 26 (37%) |
| 24  | FES  | x     | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 15  | F6C  | a     | 1121 | -    | 49,54,74     | 3.13 | 24 (48%) | 46,90,114   | 3.77 | 27 (58%) |
| 18  | BCR  | B     | 4006 | -    | 41,41,41     | 2.82 | 6 (14%)  | 56,56,56    | 6.58 | 18 (32%) |
| 14  | CLA  | G     | 1115 | -    | 65,73,73     | 2.26 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 14  | CLA  | b     | 1212 | -    | 45,53,73     | 2.54 | 19 (42%) | 52,89,113   | 2.97 | 22 (42%) |
| 14  | CLA  | A     | 1012 | 25   | 65,73,73     | 2.19 | 17 (26%) | 76,113,113  | 2.52 | 25 (32%) |
| 14  | CLA  | M     | 1501 | -    | 50,58,73     | 2.53 | 18 (36%) | 58,95,113   | 2.91 | 24 (41%) |
| 17  | SF4  | N     | 3003 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | H     | 1234 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.54 | 24 (31%) |
| 17  | SF4  | c     | 3003 | 3    | 0,12,12      | -    | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 1118 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.79 | 22 (34%) |
| 21  | LMT  | i     | 6001 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 14  | CLA  | A     | 1119 | -    | 65,73,73     | 2.23 | 18 (27%) | 76,113,113  | 2.49 | 21 (27%) |
| 14  | CLA  | a     | 1124 | 25   | 55,63,73     | 2.40 | 19 (34%) | 64,101,113  | 2.82 | 21 (32%) |
| 14  | CLA  | G     | 1113 | -    | 45,53,73     | 2.55 | 18 (40%) | 52,89,113   | 2.88 | 21 (40%) |
| 17  | SF4  | A     | 3001 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 1218 | -    | 45,53,73     | 2.57 | 18 (40%) | 52,89,113   | 3.09 | 21 (40%) |
| 14  | CLA  | a     | 1115 | -    | 65,73,73     | 2.26 | 18 (27%) | 76,113,113  | 2.64 | 26 (34%) |
| 18  | BCR  | H     | 4009 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.51 | 23 (41%) |
| 14  | CLA  | U     | 1503 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.56 | 23 (30%) |
| 14  | CLA  | b     | 1204 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.59 | 23 (30%) |
| 14  | CLA  | B     | 1208 | -    | 60,68,73     | 2.34 | 19 (31%) | 70,107,113  | 2.76 | 26 (37%) |
| 14  | CLA  | b     | 1213 | -    | 45,53,73     | 2.58 | 19 (42%) | 52,89,113   | 2.93 | 20 (38%) |
| 14  | CLA  | H     | 1232 | -    | 45,53,73     | 2.58 | 20 (44%) | 52,89,113   | 2.89 | 20 (38%) |
| 18  | BCR  | H     | 4010 | -    | 41,41,41     | 3.03 | 7 (17%)  | 56,56,56    | 6.86 | 21 (37%) |
| 15  | F6C  | B     | 1230 | -    | 49,54,74     | 3.18 | 25 (51%) | 46,90,114   | 3.79 | 25 (54%) |
| 18  | BCR  | H     | 4017 | -    | 41,41,41     | 3.05 | 8 (19%)  | 56,56,56    | 6.71 | 20 (35%) |
| 14  | CLA  | H     | 1204 | -    | 65,73,73     | 2.21 | 19 (29%) | 76,113,113  | 2.59 | 23 (30%) |
| 14  | CLA  | A     | 1135 | -    | 50,58,73     | 2.56 | 20 (40%) | 58,95,113   | 2.95 | 25 (43%) |
| 18  | BCR  | a     | 4006 | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 6.58 | 24 (42%) |
| 14  | CLA  | B     | 1213 | -    | 45,53,73     | 2.58 | 19 (42%) | 52,89,113   | 2.93 | 20 (38%) |
| 14  | CLA  | H     | 1222 | 25   | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.67 | 24 (31%) |
| 21  | LMT  | M     | 6000 | -    | 36,36,36     | 1.19 | 6 (16%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 14  | CLA  | A     | 1116 | -    | 55,63,73     | 2.42 | 19 (34%) | 64,101,113  | 2.75 | 22 (34%) |
| 15  | F6C  | b     | 1238 | 25   | 69,74,74     | 2.74 | 24 (34%) | 70,114,114  | 3.12 | 29 (41%) |
| 14  | CLA  | a     | 1129 | -    | 50,58,73     | 2.52 | 19 (38%) | 58,95,113   | 3.08 | 25 (43%) |
| 14  | CLA  | B     | 1021 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.47 | 27 (35%) |
| 14  | CLA  | B     | 1239 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.63 | 27 (35%) |
| 14  | CLA  | A     | 1114 | -    | 45,53,73     | 2.58 | 19 (42%) | 52,89,113   | 2.88 | 19 (36%) |
| 16  | PQN  | G     | 2001 | -    | 34,34,34     | 1.50 | 2 (5%)   | 42,45,45    | 1.19 | 4 (9%)   |
| 14  | CLA  | l     | 1503 | -    | 65,73,73     | 2.23 | 19 (29%) | 76,113,113  | 2.56 | 23 (30%) |
| 14  | CLA  | G     | 1136 | -    | 65,73,73     | 2.19 | 19 (29%) | 76,113,113  | 2.62 | 22 (28%) |
| 21  | LMT  | A     | 6003 | -    | 33,33,36     | 1.22 | 5 (15%)  | 44,44,47    | 0.95 | 1 (2%)   |
| 14  | CLA  | B     | 1209 | -    | 45,53,73     | 2.56 | 18 (40%) | 52,89,113   | 2.80 | 20 (38%) |
| 18  | BCR  | H     | 4004 | -    | 41,41,41     | 2.83 | 6 (14%)  | 56,56,56    | 6.52 | 22 (39%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | LHG  | l     | 5102 | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 19  | LHG  | U     | 5102 | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 14  | CLA  | A     | 1125 | -    | 65,73,73     | 2.16 | 18 (27%) | 76,113,113  | 2.69 | 23 (30%) |
| 18  | BCR  | R     | 4020 | -    | 41,41,41     | 3.17 | 9 (21%)  | 56,56,56    | 6.77 | 21 (37%) |
| 18  | BCR  | a     | 4003 | -    | 41,41,41     | 2.95 | 6 (14%)  | 56,56,56    | 6.84 | 25 (44%) |
| 14  | CLA  | a     | 1104 | -    | 65,73,73     | 2.15 | 19 (29%) | 76,113,113  | 2.79 | 24 (31%) |
| 14  | CLA  | G     | 1114 | -    | 45,53,73     | 2.57 | 19 (42%) | 52,89,113   | 2.89 | 19 (36%) |
| 14  | CLA  | b     | 1211 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.52 | 25 (32%) |
| 14  | CLA  | B     | 1232 | -    | 45,53,73     | 2.58 | 20 (44%) | 52,89,113   | 2.89 | 20 (38%) |
| 20  | LMG  | b     | 5002 | -    | 46,46,55     | 1.29 | 6 (13%)  | 54,54,63    | 1.24 | 6 (11%)  |
| 18  | BCR  | H     | 4005 | -    | 41,41,41     | 2.83 | 6 (14%)  | 56,56,56    | 6.53 | 20 (35%) |
| 14  | CLA  | G     | 1108 | -    | 45,53,73     | 2.62 | 19 (42%) | 52,89,113   | 2.91 | 21 (40%) |
| 14  | CLA  | b     | 1214 | -    | 60,68,73     | 2.34 | 21 (35%) | 70,107,113  | 2.66 | 28 (40%) |
| 17  | SF4  | G     | 3001 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | A     | 1131 | -    | 60,68,73     | 2.30 | 19 (31%) | 70,107,113  | 2.72 | 21 (30%) |
| 14  | CLA  | H     | 1211 | -    | 65,73,73     | 2.23 | 20 (30%) | 76,113,113  | 2.52 | 25 (32%) |
| 14  | CLA  | b     | 1235 | -    | 60,68,73     | 2.29 | 19 (31%) | 70,107,113  | 2.76 | 26 (37%) |
| 14  | CLA  | G     | 1118 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.80 | 22 (34%) |
| 16  | PQN  | b     | 2002 | -    | 34,34,34     | 1.55 | 2 (5%)   | 42,45,45    | 1.12 | 2 (4%)   |
| 14  | CLA  | a     | 1137 | -    | 50,58,73     | 2.52 | 18 (36%) | 58,95,113   | 3.01 | 22 (37%) |
| 14  | CLA  | H     | 1202 | -    | 65,73,73     | 2.22 | 18 (27%) | 76,113,113  | 2.61 | 24 (31%) |
| 20  | LMG  | I     | 5006 | -    | 37,37,55     | 1.13 | 3 (8%)   | 45,45,63    | 1.21 | 5 (11%)  |
| 14  | CLA  | b     | 1202 | -    | 65,73,73     | 2.22 | 18 (27%) | 76,113,113  | 2.61 | 24 (31%) |
| 14  | CLA  | G     | 1137 | -    | 50,58,73     | 2.52 | 18 (36%) | 58,95,113   | 3.01 | 22 (37%) |
| 14  | CLA  | A     | 1139 | -    | 45,53,73     | 2.56 | 20 (44%) | 52,89,113   | 2.84 | 20 (38%) |
| 19  | LHG  | U     | 5101 | -    | 24,24,48     | 1.27 | 2 (8%)   | 26,26,54    | 1.48 | 4 (15%)  |
| 14  | CLA  | G     | 1141 | -    | 45,53,73     | 2.54 | 20 (44%) | 52,89,113   | 2.97 | 21 (40%) |
| 14  | CLA  | G     | 1105 | -    | 45,53,73     | 2.61 | 18 (40%) | 52,89,113   | 2.94 | 20 (38%) |
| 14  | CLA  | a     | 1134 | 1    | 45,53,73     | 2.55 | 20 (44%) | 52,89,113   | 2.93 | 20 (38%) |
| 19  | LHG  | G     | 5002 | -    | 43,43,48     | 1.00 | 2 (4%)   | 47,48,54    | 1.14 | 2 (4%)   |
| 14  | CLA  | G     | 1012 | 25   | 65,73,73     | 2.19 | 17 (26%) | 76,113,113  | 2.52 | 25 (32%) |
| 14  | CLA  | H     | 1205 | -    | 65,73,73     | 2.18 | 17 (26%) | 76,113,113  | 2.67 | 24 (31%) |
| 21  | LMT  | a     | 6004 | -    | 24,24,36     | 1.06 | 3 (12%)  | 29,29,47    | 1.07 | 2 (6%)   |
| 14  | CLA  | a     | 1133 | 1    | 60,68,73     | 2.31 | 19 (31%) | 70,107,113  | 2.75 | 20 (28%) |
| 14  | CLA  | G     | 1128 | -    | 60,68,73     | 2.35 | 19 (31%) | 70,107,113  | 2.70 | 23 (32%) |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | H     | 1213 | -    | 45,53,73     | 2.58 | 19 (42%) | 52,89,113   | 2.94 | 20 (38%) |
| 18  | BCR  | k     | 4001 | -    | 41,41,41     | 2.89 | 6 (14%)  | 56,56,56    | 6.45 | 22 (39%) |
| 15  | F6C  | b     | 1219 | -    | 59,64,74     | 2.96 | 26 (44%) | 58,102,114  | 3.52 | 27 (46%) |
| 18  | BCR  | b     | 4009 | -    | 41,41,41     | 2.93 | 6 (14%)  | 56,56,56    | 6.51 | 23 (41%) |
| 14  | CLA  | G     | 1125 | -    | 65,73,73     | 2.16 | 18 (27%) | 76,113,113  | 2.69 | 23 (30%) |
| 18  | BCR  | a     | 4004 | -    | 41,41,41     | 3.04 | 6 (14%)  | 56,56,56    | 6.66 | 25 (44%) |
| 14  | CLA  | B     | 1202 | -    | 65,73,73     | 2.22 | 18 (27%) | 76,113,113  | 2.62 | 24 (31%) |
| 14  | CLA  | B     | 1211 | -    | 65,73,73     | 2.24 | 20 (30%) | 76,113,113  | 2.53 | 25 (32%) |
| 14  | CLA  | a     | 1113 | -    | 45,53,73     | 2.54 | 18 (40%) | 52,89,113   | 2.87 | 20 (38%) |
| 14  | CLA  | B     | 1218 | -    | 45,53,73     | 2.57 | 18 (40%) | 52,89,113   | 3.08 | 21 (40%) |
| 14  | CLA  | B     | 1220 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.57 | 22 (28%) |
| 14  | CLA  | A     | 1130 | -    | 55,63,73     | 2.46 | 19 (34%) | 64,101,113  | 2.66 | 21 (32%) |
| 14  | CLA  | K     | 1401 | -    | 45,53,73     | 2.59 | 19 (42%) | 52,89,113   | 3.03 | 23 (44%) |
| 14  | CLA  | A     | 1105 | -    | 45,53,73     | 2.61 | 18 (40%) | 52,89,113   | 2.94 | 20 (38%) |
| 14  | CLA  | G     | 1131 | -    | 60,68,73     | 2.31 | 19 (31%) | 70,107,113  | 2.72 | 21 (30%) |
| 14  | CLA  | A     | 1127 | -    | 65,73,73     | 2.22 | 19 (29%) | 76,113,113  | 2.54 | 21 (27%) |
| 19  | LHG  | l     | 5101 | -    | 24,24,48     | 1.27 | 2 (8%)   | 26,26,54    | 1.48 | 4 (15%)  |
| 18  | BCR  | U     | 4022 | -    | 41,41,41     | 3.00 | 6 (14%)  | 56,56,56    | 6.39 | 22 (39%) |
| 14  | CLA  | A     | 1132 | -    | 65,73,73     | 2.18 | 18 (27%) | 76,113,113  | 2.64 | 23 (30%) |
| 14  | CLA  | A     | 1128 | -    | 60,68,73     | 2.35 | 19 (31%) | 70,107,113  | 2.69 | 23 (32%) |
| 14  | CLA  | A     | 1126 | -    | 60,68,73     | 2.33 | 17 (28%) | 70,107,113  | 2.58 | 20 (28%) |
| 14  | CLA  | a     | 1140 | -    | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.69 | 21 (32%) |

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

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | H     | 1223 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | a     | 1101 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 15  | F6C  | H     | 1238 | 25   | -         | 15/41/97/97   | -       |
| 21  | LMT  | b     | 6003 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 14  | CLA  | a     | 1123 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 14  | CLA  | A     | 1103 | -    | 1/1/15/20 | 23/37/115/115 | -       |
| 13  | CL0  | A     | 1011 | -    | 3/3/20/25 | 15/37/135/135 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | G     | 1133 | 1    | 1/1/14/20 | 21/31/109/115 | -       |
| 18  | BCR  | H     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 1220 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 18  | BCR  | b     | 4004 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 1138 | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 20  | LMG  | i     | 5006 | -    | -         | 13/32/52/70   | 0/1/1/1 |
| 14  | CLA  | G     | 1107 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | B     | 1227 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | a     | 1122 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 14  | CLA  | A     | 1112 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 20  | LMG  | B     | 5002 | -    | -         | 17/41/61/70   | 0/1/1/1 |
| 21  | LMT  | U     | 6101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 21  | LMT  | l     | 6101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 14  | CLA  | G     | 1120 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | BCR  | V     | 4021 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1233 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | A     | 1013 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 15  | F6C  | H     | 1230 | -    | -         | 9/17/73/97    | -       |
| 21  | LMT  | A     | 6001 | -    | -         | 9/17/57/61    | 0/2/2/2 |
| 15  | F6C  | H     | 1219 | -    | -         | 15/29/85/97   | -       |
| 21  | LMT  | U     | 6001 | -    | -         | 5/11/11/61    | -       |
| 14  | CLA  | H     | 1218 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | H     | 1221 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | A     | 1136 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | H     | 1239 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | a     | 1106 | 1    | 1/1/14/20 | 10/31/109/115 | -       |
| 14  | CLA  | G     | 1140 | -    | 1/1/13/20 | 14/25/103/115 | -       |
| 14  | CLA  | b     | 1209 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | H     | 1233 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | A     | 1109 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 19  | LHG  | A     | 5002 | -    | -         | 24/45/45/53   | -       |
| 14  | CLA  | B     | 1229 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | L     | 1503 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | B     | 1222 | 25   | 1/1/15/20 | 15/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 18  | BCR  | I     | 4018 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 21  | LMT  | B     | 6004 | -    | -         | 10/17/57/61   | 0/2/2/2 |
| 21  | LMT  | G     | 6003 | -    | -         | 7/18/58/61    | 0/2/2/2 |
| 14  | CLA  | a     | 1110 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | G     | 1117 | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | U     | 1501 | 10   | 1/1/15/20 | 8/37/115/115  | -       |
| 15  | F6C  | b     | 1207 | -    | -         | 19/41/97/97   | -       |
| 14  | CLA  | B     | 1224 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | b     | 1231 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | b     | 1221 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | B     | 1206 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 17  | SF4  | C     | 3003 | 3    | -         | -             | 0/6/5/5 |
| 18  | BCR  | B     | 4004 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 19  | LHG  | L     | 5101 | -    | -         | 15/26/26/53   | -       |
| 14  | CLA  | b     | 1223 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 15  | F6C  | H     | 1207 | -    | -         | 19/41/97/97   | -       |
| 14  | CLA  | a     | 1141 | -    | 1/1/11/20 | 10/13/91/115  | -       |
| 14  | CLA  | a     | 1131 | -    | 1/1/14/20 | 12/31/109/115 | -       |
| 14  | CLA  | H     | 1227 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | B     | 1023 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 16  | PQN  | B     | 2002 | -    | -         | 9/23/43/43    | 0/2/2/2 |
| 14  | CLA  | B     | 1233 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | G     | 1111 | -    | 1/1/14/20 | 16/31/109/115 | -       |
| 14  | CLA  | a     | 1119 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 18  | BCR  | A     | 4005 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 21  | LMT  | b     | 6002 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 14  | CLA  | B     | 1235 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 14  | CLA  | B     | 1240 | 2    | 1/1/15/20 | 18/37/115/115 | -       |
| 21  | LMT  | G     | 6001 | -    | -         | 9/17/57/61    | 0/2/2/2 |
| 18  | BCR  | G     | 4001 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 19  | LHG  | a     | 5001 | -    | -         | 23/46/46/53   | -       |
| 18  | BCR  | G     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 21  | LMT  | B     | 6001 | -    | -         | 7/21/61/61    | 0/2/2/2 |
| 14  | CLA  | a     | 1111 | -    | 1/1/14/20 | 16/31/109/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | SF4  | c     | 3002 | 3    | -         | -             | 0/6/5/5 |
| 21  | LMT  | R     | 6001 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 15  | F6C  | A     | 1121 | -    | -         | 10/17/73/97   | -       |
| 15  | F6C  | b     | 1237 | 25   | -         | 24/41/97/97   | -       |
| 21  | LMT  | A     | 6002 | -    | -         | 9/14/54/61    | 0/2/2/2 |
| 14  | CLA  | l     | 1501 | 10   | 1/1/15/20 | 8/37/115/115  | -       |
| 14  | CLA  | B     | 1231 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 21  | LMT  | H     | 6003 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 18  | BCR  | b     | 4014 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 1102 | -    | 1/1/12/20 | 10/19/97/115  | -       |
| 14  | CLA  | a     | 1130 | -    | 1/1/13/20 | 9/25/103/115  | -       |
| 14  | CLA  | b     | 1206 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 21  | LMT  | H     | 6004 | -    | -         | 10/17/57/61   | 0/2/2/2 |
| 14  | CLA  | H     | 1224 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | b     | 1205 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 16  | PQN  | A     | 2001 | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 20  | LMG  | a     | 5003 | -    | -         | 15/41/61/70   | 0/1/1/1 |
| 14  | CLA  | V     | 1501 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 14  | CLA  | G     | 1109 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | H     | 1231 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | A     | 1120 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | G     | 1119 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 1135 | -    | 1/1/12/20 | 8/19/97/115   | -       |
| 14  | CLA  | H     | 1236 | -    | 1/1/13/20 | 15/25/103/115 | -       |
| 15  | F6C  | B     | 1237 | 25   | -         | 24/41/97/97   | -       |
| 14  | CLA  | a     | 1013 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 18  | BCR  | A     | 4003 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 21  | LMT  | m     | 6000 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 14  | CLA  | a     | 1107 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 19  | LHG  | G     | 5001 | -    | -         | 23/46/46/53   | -       |
| 14  | CLA  | A     | 1108 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | BCR  | b     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1217 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 21  | LMT  | G     | 6004 | -    | -         | 6/15/35/61    | 0/1/1/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | B     | 1204 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | A     | 1141 | -    | 1/1/11/20 | 10/13/91/115  | -       |
| 14  | CLA  | A     | 1137 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 20  | LMG  | H     | 5002 | -    | -         | 17/41/61/70   | 0/1/1/1 |
| 21  | LMT  | U     | 6002 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 14  | CLA  | b     | 1215 | -    | 1/1/14/20 | 16/31/109/115 | -       |
| 17  | SF4  | a     | 3001 | 2,1  | -         | -             | 0/6/5/5 |
| 18  | BCR  | l     | 4019 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 1129 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 18  | BCR  | G     | 4005 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 15  | F6C  | B     | 1238 | 25   | -         | 15/41/97/97   | -       |
| 18  | BCR  | R     | 4018 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 1201 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 21  | LMT  | l     | 6002 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 15  | F6C  | H     | 1237 | 25   | -         | 24/41/97/97   | -       |
| 14  | CLA  | a     | 1116 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 14  | CLA  | G     | 1129 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 14  | CLA  | a     | 1105 | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 14  | CLA  | b     | 1021 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 20  | LMG  | G     | 5003 | -    | -         | 15/41/61/70   | 0/1/1/1 |
| 14  | CLA  | A     | 1133 | 1    | 1/1/14/20 | 21/31/109/115 | -       |
| 14  | CLA  | G     | 1126 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | B     | 1215 | -    | 1/1/14/20 | 16/31/109/115 | -       |
| 14  | CLA  | a     | 1114 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | b     | 1023 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | G     | 1124 | 25   | 1/1/13/20 | 5/25/103/115  | -       |
| 14  | CLA  | B     | 1214 | -    | 1/1/14/20 | 11/31/109/115 | -       |
| 14  | CLA  | a     | 1128 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | a     | 1126 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | a     | 1118 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 14  | CLA  | b     | 1232 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 21  | LMT  | H     | 6001 | -    | -         | 7/21/61/61    | 0/2/2/2 |
| 14  | CLA  | B     | 1203 | -    | 1/1/15/20 | 22/37/115/115 | -       |
| 21  | LMT  | L     | 6001 | -    | -         | 5/11/11/61    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | H     | 1206 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | a     | 1103 | -    | 1/1/15/20 | 23/37/115/115 | -       |
| 14  | CLA  | G     | 1122 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 18  | BCR  | B     | 4014 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 19  | LHG  | L     | 5102 | -    | -         | 26/53/53/53   | -       |
| 14  | CLA  | B     | 1217 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | b     | 1234 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | B     | 1226 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 18  | BCR  | U     | 4019 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 1023 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | A     | 1140 | -    | 1/1/13/20 | 14/25/103/115 | -       |
| 16  | PQN  | H     | 2002 | -    | -         | 9/23/43/43    | 0/2/2/2 |
| 14  | CLA  | G     | 1102 | -    | 1/1/12/20 | 10/19/97/115  | -       |
| 21  | LMT  | A     | 6004 | -    | -         | 6/15/35/61    | 0/1/1/2 |
| 14  | CLA  | G     | 1116 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 13  | CL0  | a     | 1011 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 18  | BCR  | G     | 4003 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 16  | PQN  | a     | 2001 | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 14  | CLA  | G     | 1103 | -    | 1/1/15/20 | 23/37/115/115 | -       |
| 14  | CLA  | L     | 1501 | 10   | 1/1/15/20 | 8/37/115/115  | -       |
| 14  | CLA  | A     | 1123 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 14  | CLA  | H     | 1240 | 2    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | A     | 1111 | -    | 1/1/14/20 | 16/31/109/115 | -       |
| 15  | F6C  | B     | 1219 | -    | -         | 15/29/85/97   | -       |
| 14  | CLA  | a     | 1125 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 18  | BCR  | B     | 4009 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 18  | BCR  | A     | 4001 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 18  | BCR  | T     | 4001 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 1138 | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 14  | CLA  | k     | 1401 | -    | 1/1/11/20 | 9/13/91/115   | -       |
| 14  | CLA  | A     | 1138 | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 14  | CLA  | b     | 1236 | -    | 1/1/13/20 | 15/25/103/115 | -       |
| 14  | CLA  | b     | 1216 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | a     | 1102 | -    | 1/1/12/20 | 10/19/97/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 1201 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | a     | 1109 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 18  | BCR  | b     | 4017 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 1226 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 18  | BCR  | m     | 4021 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 17  | SF4  | C     | 3002 | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | a     | 1139 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 24  | FES  | X     | 101  | 12   | -         | -             | 0/1/1/1 |
| 14  | CLA  | b     | 1228 | -    | 1/1/13/20 | 15/25/103/115 | -       |
| 14  | CLA  | A     | 1101 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | b     | 1022 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 14  | CLA  | H     | 1210 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | G     | 1104 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | a     | 1120 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | BCR  | b     | 4005 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 1139 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | U     | 1502 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 14  | CLA  | a     | 1012 | 25   | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | a     | 1132 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 18  | BCR  | I     | 4020 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 21  | LMT  | l     | 6001 | -    | -         | 5/11/11/61    | -       |
| 13  | CL0  | G     | 1011 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | G     | 1134 | 1    | 1/1/11/20 | 9/13/91/115   | -       |
| 14  | CLA  | B     | 1234 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 18  | BCR  | G     | 4004 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1224 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | A     | 1106 | 1    | 1/1/14/20 | 10/31/109/115 | -       |
| 14  | CLA  | a     | 1108 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 21  | LMT  | L     | 6002 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 14  | CLA  | G     | 1112 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 14  | CLA  | b     | 1210 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 15  | F6C  | B     | 1207 | -    | -         | 19/41/97/97   | -       |
| 18  | BCR  | L     | 4022 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 1134 | 1    | 1/1/11/20 | 9/13/91/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 1239 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 21  | LMT  | V     | 6000 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 14  | CLA  | G     | 1135 | -    | 1/1/12/20 | 8/19/97/115   | -       |
| 14  | CLA  | b     | 1227 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 18  | BCR  | M     | 4021 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 14  | CLA  | B     | 1216 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | B     | 1236 | -    | 1/1/13/20 | 15/25/103/115 | -       |
| 18  | BCR  | B     | 4010 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 1210 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | b     | 1220 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | H     | 1214 | -    | 1/1/14/20 | 11/31/109/115 | -       |
| 14  | CLA  | a     | 1117 | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | H     | 1021 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 18  | BCR  | B     | 4017 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 18  | BCR  | a     | 4002 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | B     | 1221 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | a     | 1127 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 21  | LMT  | a     | 6002 | -    | -         | 9/14/54/61    | 0/2/2/2 |
| 21  | LMT  | I     | 6001 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 18  | BCR  | L     | 4019 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1225 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | G     | 1123 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 14  | CLA  | G     | 1101 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | l     | 1502 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 15  | F6C  | G     | 1121 | -    | -         | 10/17/73/97   | -       |
| 18  | BCR  | G     | 4002 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 1106 | 1    | 1/1/14/20 | 10/31/109/115 | -       |
| 18  | BCR  | B     | 4005 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 18  | BCR  | a     | 4001 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1229 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 21  | LMT  | B     | 6003 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 21  | LMT  | G     | 6002 | -    | -         | 9/14/54/61    | 0/2/2/2 |
| 14  | CLA  | T     | 1401 | -    | 1/1/11/20 | 9/13/91/115   | -       |
| 14  | CLA  | A     | 1124 | 25   | 1/1/13/20 | 5/25/103/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | B     | 1223 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | b     | 1203 | -    | 1/1/15/20 | 22/37/115/115 | -       |
| 21  | LMT  | b     | 6004 | -    | -         | 10/17/57/61   | 0/2/2/2 |
| 14  | CLA  | A     | 1117 | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | G     | 1110 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | H     | 1212 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 18  | BCR  | i     | 4018 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 1122 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 14  | CLA  | H     | 1203 | -    | 1/1/15/20 | 22/37/115/115 | -       |
| 14  | CLA  | H     | 1209 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | BCR  | A     | 4002 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 21  | LMT  | B     | 6002 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 18  | BCR  | H     | 4014 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 17  | SF4  | N     | 3002 | 3    | -         | -             | 0/6/5/5 |
| 18  | BCR  | A     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 1226 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | H     | 1022 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 18  | BCR  | i     | 4020 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 21  | LMT  | a     | 6001 | -    | -         | 9/17/57/61    | 0/2/2/2 |
| 14  | CLA  | a     | 1136 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | B     | 1228 | -    | 1/1/13/20 | 15/25/103/115 | -       |
| 14  | CLA  | b     | 1208 | -    | 1/1/14/20 | 9/31/109/115  | -       |
| 14  | CLA  | H     | 1216 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 19  | LHG  | A     | 5001 | -    | -         | 23/46/46/53   | -       |
| 14  | CLA  | G     | 1127 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | H     | 1225 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 18  | BCR  | K     | 4001 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | m     | 1501 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 18  | BCR  | b     | 4010 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 1229 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 18  | BCR  | A     | 4004 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 19  | LHG  | a     | 5002 | -    | -         | 24/45/45/53   | -       |
| 14  | CLA  | A     | 1104 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | H     | 1228 | -    | 1/1/13/20 | 15/25/103/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 1222 | 25   | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | B     | 1212 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | A     | 1113 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 21  | LMT  | b     | 6001 | -    | -         | 7/21/61/61    | 0/2/2/2 |
| 24  | FES  | W     | 101  | 12   | -         | -             | 0/1/1/1 |
| 14  | CLA  | H     | 1215 | -    | 1/1/14/20 | 16/31/109/115 | -       |
| 21  | LMT  | H     | 6002 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 14  | CLA  | B     | 1022 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 14  | CLA  | G     | 1132 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 15  | F6C  | b     | 1230 | -    | -         | 9/17/73/97    | -       |
| 14  | CLA  | B     | 1225 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 20  | LMG  | A     | 5003 | -    | -         | 15/41/61/70   | 0/1/1/1 |
| 14  | CLA  | B     | 1205 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | B     | 1201 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | G     | 1130 | -    | 1/1/13/20 | 9/25/103/115  | -       |
| 14  | CLA  | b     | 1240 | 2    | 1/1/15/20 | 18/37/115/115 | -       |
| 21  | LMT  | L     | 6101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 14  | CLA  | L     | 1502 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 14  | CLA  | A     | 1115 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | a     | 1112 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 14  | CLA  | H     | 1208 | -    | 1/1/14/20 | 9/31/109/115  | -       |
| 18  | BCR  | l     | 4022 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 18  | BCR  | a     | 4005 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 1013 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 14  | CLA  | A     | 1110 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | A     | 1107 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 20  | LMG  | R     | 5006 | -    | -         | 13/32/52/70   | 0/1/1/1 |
| 14  | CLA  | H     | 1217 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 21  | LMT  | a     | 6003 | -    | -         | 7/18/58/61    | 0/2/2/2 |
| 14  | CLA  | H     | 1235 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 24  | FES  | x     | 101  | 12   | -         | -             | 0/1/1/1 |
| 15  | F6C  | a     | 1121 | -    | -         | 10/17/73/97   | -       |
| 18  | BCR  | B     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 1115 | -    | 1/1/15/20 | 19/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 1212 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | A     | 1012 | 25   | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | M     | 1501 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 17  | SF4  | N     | 3003 | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | H     | 1234 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 17  | SF4  | c     | 3003 | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | A     | 1118 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 21  | LMT  | i     | 6001 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 14  | CLA  | A     | 1119 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 1124 | 25   | 1/1/13/20 | 5/25/103/115  | -       |
| 14  | CLA  | G     | 1113 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 17  | SF4  | A     | 3001 | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 1218 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | a     | 1115 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 18  | BCR  | H     | 4009 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | U     | 1503 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | b     | 1204 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | B     | 1208 | -    | 1/1/14/20 | 9/31/109/115  | -       |
| 14  | CLA  | b     | 1213 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | H     | 1232 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | BCR  | H     | 4010 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 15  | F6C  | B     | 1230 | -    | -         | 9/17/73/97    | -       |
| 18  | BCR  | H     | 4017 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 1204 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | A     | 1135 | -    | 1/1/12/20 | 8/19/97/115   | -       |
| 18  | BCR  | a     | 4006 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | B     | 1213 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | H     | 1222 | 25   | 1/1/15/20 | 15/37/115/115 | -       |
| 21  | LMT  | M     | 6000 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 14  | CLA  | A     | 1116 | -    | 1/1/13/20 | 12/25/103/115 | -       |
| 15  | F6C  | b     | 1238 | 25   | -         | 15/41/97/97   | -       |
| 14  | CLA  | a     | 1129 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 14  | CLA  | B     | 1021 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | B     | 1239 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | A     | 1114 | -    | 1/1/11/20 | 4/13/91/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 16  | PQN  | G     | 2001 | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 14  | CLA  | l     | 1503 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | G     | 1136 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 21  | LMT  | A     | 6003 | -    | -         | 7/18/58/61    | 0/2/2/2 |
| 14  | CLA  | B     | 1209 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | BCR  | H     | 4004 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 19  | LHG  | l     | 5102 | -    | -         | 26/53/53/53   | -       |
| 19  | LHG  | U     | 5102 | -    | -         | 26/53/53/53   | -       |
| 14  | CLA  | A     | 1125 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 18  | BCR  | R     | 4020 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 18  | BCR  | a     | 4003 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 1104 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | G     | 1114 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | b     | 1211 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | B     | 1232 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 20  | LMG  | b     | 5002 | -    | -         | 17/41/61/70   | 0/1/1/1 |
| 18  | BCR  | H     | 4005 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 1108 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | b     | 1214 | -    | 1/1/14/20 | 11/31/109/115 | -       |
| 17  | SF4  | G     | 3001 | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CLA  | A     | 1131 | -    | 1/1/14/20 | 12/31/109/115 | -       |
| 14  | CLA  | H     | 1211 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | b     | 1235 | -    | 1/1/14/20 | 14/31/109/115 | -       |
| 14  | CLA  | G     | 1118 | -    | 1/1/13/20 | 11/25/103/115 | -       |
| 16  | PQN  | b     | 2002 | -    | -         | 9/23/43/43    | 0/2/2/2 |
| 14  | CLA  | a     | 1137 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 14  | CLA  | H     | 1202 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 20  | LMG  | I     | 5006 | -    | -         | 13/32/52/70   | 0/1/1/1 |
| 14  | CLA  | b     | 1202 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | G     | 1137 | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 14  | CLA  | A     | 1139 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 19  | LHG  | U     | 5101 | -    | -         | 15/26/26/53   | -       |
| 14  | CLA  | G     | 1141 | -    | 1/1/11/20 | 10/13/91/115  | -       |
| 14  | CLA  | G     | 1105 | -    | 1/1/11/20 | 3/13/91/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | a     | 1134 | 1    | 1/1/11/20 | 9/13/91/115   | -       |
| 19  | LHG  | G     | 5002 | -    | -         | 24/45/45/53   | -       |
| 14  | CLA  | G     | 1012 | 25   | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | H     | 1205 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 21  | LMT  | a     | 6004 | -    | -         | 6/15/35/61    | 0/1/1/2 |
| 14  | CLA  | a     | 1133 | 1    | 1/1/14/20 | 21/31/109/115 | -       |
| 14  | CLA  | G     | 1128 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | H     | 1213 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | BCR  | k     | 4001 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 15  | F6C  | b     | 1219 | -    | -         | 15/29/85/97   | -       |
| 18  | BCR  | b     | 4009 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 1125 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 18  | BCR  | a     | 4004 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | B     | 1202 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | B     | 1211 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | a     | 1113 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | B     | 1218 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 14  | CLA  | B     | 1220 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | A     | 1130 | -    | 1/1/13/20 | 9/25/103/115  | -       |
| 14  | CLA  | K     | 1401 | -    | 1/1/11/20 | 9/13/91/115   | -       |
| 14  | CLA  | A     | 1105 | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 14  | CLA  | G     | 1131 | -    | 1/1/14/20 | 12/31/109/115 | -       |
| 14  | CLA  | A     | 1127 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 19  | LHG  | l     | 5101 | -    | -         | 15/26/26/53   | -       |
| 18  | BCR  | U     | 4022 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 1132 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | A     | 1128 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | A     | 1126 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 14  | CLA  | a     | 1140 | -    | 1/1/13/20 | 14/25/103/115 | -       |

All (5905) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 15  | b     | 1207 | F6C  | MG-NA | 9.22 | 2.24        | 2.05     |
| 15  | H     | 1207 | F6C  | MG-NA | 9.19 | 2.24        | 2.05     |
| 15  | B     | 1207 | F6C  | MG-NA | 9.18 | 2.24        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | H     | 1219 | F6C  | MG-NA   | 9.11  | 2.23        | 2.05     |
| 15  | B     | 1219 | F6C  | MG-NA   | 9.08  | 2.23        | 2.05     |
| 15  | b     | 1219 | F6C  | MG-NA   | 9.06  | 2.23        | 2.05     |
| 15  | B     | 1230 | F6C  | MG-NA   | 9.03  | 2.23        | 2.05     |
| 15  | H     | 1230 | F6C  | MG-NA   | 9.02  | 2.23        | 2.05     |
| 15  | b     | 1230 | F6C  | MG-NA   | 9.01  | 2.23        | 2.05     |
| 15  | A     | 1121 | F6C  | MG-NA   | 8.97  | 2.23        | 2.05     |
| 15  | a     | 1121 | F6C  | MG-NA   | 8.96  | 2.23        | 2.05     |
| 15  | G     | 1121 | F6C  | MG-NA   | 8.96  | 2.23        | 2.05     |
| 15  | H     | 1238 | F6C  | MG-NA   | 8.92  | 2.23        | 2.05     |
| 15  | b     | 1238 | F6C  | MG-NA   | 8.92  | 2.23        | 2.05     |
| 15  | B     | 1238 | F6C  | MG-NA   | 8.91  | 2.23        | 2.05     |
| 18  | R     | 4020 | BCR  | C8-C9   | -8.91 | 1.26        | 1.45     |
| 18  | I     | 4020 | BCR  | C8-C9   | -8.90 | 1.26        | 1.45     |
| 18  | U     | 4019 | BCR  | C8-C9   | -8.90 | 1.26        | 1.45     |
| 18  | i     | 4020 | BCR  | C8-C9   | -8.88 | 1.26        | 1.45     |
| 18  | L     | 4019 | BCR  | C8-C9   | -8.88 | 1.26        | 1.45     |
| 18  | l     | 4019 | BCR  | C8-C9   | -8.86 | 1.26        | 1.45     |
| 18  | a     | 4004 | BCR  | C8-C9   | -8.82 | 1.27        | 1.45     |
| 18  | A     | 4004 | BCR  | C8-C9   | -8.81 | 1.27        | 1.45     |
| 18  | G     | 4004 | BCR  | C8-C9   | -8.78 | 1.27        | 1.45     |
| 18  | i     | 4020 | BCR  | C10-C9  | -8.78 | 1.24        | 1.35     |
| 18  | I     | 4020 | BCR  | C10-C9  | -8.75 | 1.24        | 1.35     |
| 18  | R     | 4020 | BCR  | C10-C9  | -8.73 | 1.24        | 1.35     |
| 15  | a     | 1121 | F6C  | C1A-CHA | 8.72  | 1.51        | 1.35     |
| 18  | G     | 4004 | BCR  | C10-C9  | -8.69 | 1.24        | 1.35     |
| 15  | A     | 1121 | F6C  | C1A-CHA | 8.68  | 1.51        | 1.35     |
| 18  | A     | 4004 | BCR  | C10-C9  | -8.68 | 1.24        | 1.35     |
| 18  | B     | 4017 | BCR  | C8-C9   | -8.67 | 1.27        | 1.45     |
| 18  | a     | 4004 | BCR  | C10-C9  | -8.67 | 1.24        | 1.35     |
| 18  | b     | 4017 | BCR  | C8-C9   | -8.67 | 1.27        | 1.45     |
| 18  | H     | 4017 | BCR  | C8-C9   | -8.66 | 1.27        | 1.45     |
| 15  | G     | 1121 | F6C  | C1A-CHA | 8.65  | 1.51        | 1.35     |
| 18  | B     | 4010 | BCR  | C10-C9  | -8.65 | 1.24        | 1.35     |
| 18  | m     | 4021 | BCR  | C8-C9   | -8.65 | 1.27        | 1.45     |
| 18  | l     | 4022 | BCR  | C8-C9   | -8.65 | 1.27        | 1.45     |
| 18  | M     | 4021 | BCR  | C8-C9   | -8.64 | 1.27        | 1.45     |
| 18  | V     | 4021 | BCR  | C8-C9   | -8.64 | 1.27        | 1.45     |
| 18  | b     | 4010 | BCR  | C10-C9  | -8.64 | 1.24        | 1.35     |
| 18  | H     | 4010 | BCR  | C10-C9  | -8.61 | 1.24        | 1.35     |
| 18  | L     | 4022 | BCR  | C8-C9   | -8.61 | 1.27        | 1.45     |
| 18  | U     | 4022 | BCR  | C8-C9   | -8.59 | 1.27        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | R     | 4020 | BCR  | C11-C10 | -8.57 | 1.16        | 1.43     |
| 18  | H     | 4009 | BCR  | C8-C9   | -8.57 | 1.27        | 1.45     |
| 18  | I     | 4020 | BCR  | C11-C10 | -8.56 | 1.16        | 1.43     |
| 18  | i     | 4020 | BCR  | C11-C10 | -8.56 | 1.16        | 1.43     |
| 18  | H     | 4010 | BCR  | C11-C10 | -8.56 | 1.16        | 1.43     |
| 18  | l     | 4019 | BCR  | C11-C10 | -8.56 | 1.16        | 1.43     |
| 18  | a     | 4006 | BCR  | C8-C9   | -8.55 | 1.27        | 1.45     |
| 18  | B     | 4009 | BCR  | C8-C9   | -8.55 | 1.27        | 1.45     |
| 18  | A     | 4006 | BCR  | C8-C9   | -8.55 | 1.27        | 1.45     |
| 18  | G     | 4006 | BCR  | C8-C9   | -8.54 | 1.27        | 1.45     |
| 18  | B     | 4010 | BCR  | C11-C10 | -8.54 | 1.17        | 1.43     |
| 18  | U     | 4019 | BCR  | C11-C10 | -8.54 | 1.17        | 1.43     |
| 18  | G     | 4004 | BCR  | C11-C10 | -8.54 | 1.17        | 1.43     |
| 18  | A     | 4004 | BCR  | C11-C10 | -8.53 | 1.17        | 1.43     |
| 18  | G     | 4005 | BCR  | C8-C9   | -8.53 | 1.27        | 1.45     |
| 18  | b     | 4010 | BCR  | C11-C10 | -8.53 | 1.17        | 1.43     |
| 18  | a     | 4004 | BCR  | C11-C10 | -8.53 | 1.17        | 1.43     |
| 18  | b     | 4009 | BCR  | C8-C9   | -8.53 | 1.27        | 1.45     |
| 18  | L     | 4019 | BCR  | C11-C10 | -8.52 | 1.17        | 1.43     |
| 18  | a     | 4005 | BCR  | C8-C9   | -8.52 | 1.27        | 1.45     |
| 15  | b     | 1237 | F6C  | MG-NA   | 8.52  | 2.22        | 2.05     |
| 18  | A     | 4005 | BCR  | C8-C9   | -8.51 | 1.27        | 1.45     |
| 15  | B     | 1237 | F6C  | MG-NA   | 8.51  | 2.22        | 2.05     |
| 15  | H     | 1237 | F6C  | MG-NA   | 8.50  | 2.22        | 2.05     |
| 18  | A     | 4003 | BCR  | C8-C9   | -8.50 | 1.27        | 1.45     |
| 18  | a     | 4003 | BCR  | C8-C9   | -8.49 | 1.27        | 1.45     |
| 15  | b     | 1237 | F6C  | C1A-CHA | 8.49  | 1.51        | 1.35     |
| 15  | H     | 1237 | F6C  | C1A-CHA | 8.48  | 1.51        | 1.35     |
| 18  | G     | 4003 | BCR  | C8-C9   | -8.48 | 1.27        | 1.45     |
| 15  | b     | 1238 | F6C  | C1A-CHA | 8.47  | 1.51        | 1.35     |
| 18  | a     | 4005 | BCR  | C10-C9  | -8.46 | 1.24        | 1.35     |
| 15  | B     | 1237 | F6C  | C1A-CHA | 8.46  | 1.51        | 1.35     |
| 18  | L     | 4019 | BCR  | C10-C9  | -8.46 | 1.24        | 1.35     |
| 18  | A     | 4005 | BCR  | C10-C9  | -8.46 | 1.24        | 1.35     |
| 18  | A     | 4001 | BCR  | C8-C9   | -8.46 | 1.27        | 1.45     |
| 18  | b     | 4006 | BCR  | C8-C9   | -8.45 | 1.27        | 1.45     |
| 18  | U     | 4019 | BCR  | C10-C9  | -8.45 | 1.24        | 1.35     |
| 18  | G     | 4001 | BCR  | C8-C9   | -8.45 | 1.27        | 1.45     |
| 15  | B     | 1238 | F6C  | C1A-CHA | 8.45  | 1.51        | 1.35     |
| 18  | a     | 4003 | BCR  | C11-C10 | -8.45 | 1.17        | 1.43     |
| 18  | R     | 4018 | BCR  | C8-C9   | -8.45 | 1.27        | 1.45     |
| 18  | H     | 4006 | BCR  | C8-C9   | -8.44 | 1.27        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | l     | 4019 | BCR  | C10-C9  | -8.44 | 1.24        | 1.35     |
| 18  | a     | 4001 | BCR  | C8-C9   | -8.44 | 1.27        | 1.45     |
| 15  | H     | 1238 | F6C  | C1A-CHA | 8.44  | 1.51        | 1.35     |
| 18  | i     | 4018 | BCR  | C8-C9   | -8.44 | 1.27        | 1.45     |
| 18  | a     | 4005 | BCR  | C11-C10 | -8.44 | 1.17        | 1.43     |
| 18  | I     | 4018 | BCR  | C8-C9   | -8.44 | 1.27        | 1.45     |
| 18  | B     | 4006 | BCR  | C8-C9   | -8.43 | 1.27        | 1.45     |
| 18  | A     | 4003 | BCR  | C11-C10 | -8.43 | 1.17        | 1.43     |
| 18  | H     | 4004 | BCR  | C8-C9   | -8.43 | 1.27        | 1.45     |
| 18  | G     | 4003 | BCR  | C11-C10 | -8.43 | 1.17        | 1.43     |
| 18  | A     | 4005 | BCR  | C11-C10 | -8.43 | 1.17        | 1.43     |
| 15  | B     | 1207 | F6C  | C1A-CHA | 8.43  | 1.51        | 1.35     |
| 18  | G     | 4005 | BCR  | C10-C9  | -8.42 | 1.24        | 1.35     |
| 15  | H     | 1207 | F6C  | C1A-CHA | 8.42  | 1.51        | 1.35     |
| 18  | G     | 4005 | BCR  | C11-C10 | -8.41 | 1.17        | 1.43     |
| 18  | B     | 4004 | BCR  | C8-C9   | -8.41 | 1.27        | 1.45     |
| 18  | B     | 4017 | BCR  | C10-C9  | -8.40 | 1.24        | 1.35     |
| 15  | b     | 1207 | F6C  | C1A-CHA | 8.40  | 1.51        | 1.35     |
| 18  | l     | 4022 | BCR  | C11-C10 | -8.39 | 1.17        | 1.43     |
| 18  | b     | 4004 | BCR  | C8-C9   | -8.39 | 1.27        | 1.45     |
| 18  | U     | 4022 | BCR  | C11-C10 | -8.37 | 1.17        | 1.43     |
| 18  | L     | 4022 | BCR  | C11-C10 | -8.37 | 1.17        | 1.43     |
| 18  | H     | 4017 | BCR  | C11-C10 | -8.36 | 1.17        | 1.43     |
| 18  | b     | 4017 | BCR  | C11-C10 | -8.36 | 1.17        | 1.43     |
| 18  | H     | 4017 | BCR  | C10-C9  | -8.36 | 1.24        | 1.35     |
| 18  | b     | 4017 | BCR  | C10-C9  | -8.35 | 1.24        | 1.35     |
| 18  | B     | 4017 | BCR  | C11-C10 | -8.34 | 1.17        | 1.43     |
| 18  | K     | 4001 | BCR  | C8-C9   | -8.33 | 1.28        | 1.45     |
| 18  | k     | 4001 | BCR  | C8-C9   | -8.32 | 1.28        | 1.45     |
| 18  | T     | 4001 | BCR  | C8-C9   | -8.32 | 1.28        | 1.45     |
| 18  | b     | 4010 | BCR  | C8-C9   | -8.26 | 1.28        | 1.45     |
| 18  | i     | 4018 | BCR  | C11-C10 | -8.26 | 1.17        | 1.43     |
| 18  | H     | 4010 | BCR  | C8-C9   | -8.25 | 1.28        | 1.45     |
| 18  | B     | 4010 | BCR  | C8-C9   | -8.25 | 1.28        | 1.45     |
| 18  | M     | 4021 | BCR  | C11-C10 | -8.25 | 1.17        | 1.43     |
| 18  | V     | 4021 | BCR  | C11-C10 | -8.24 | 1.17        | 1.43     |
| 18  | m     | 4021 | BCR  | C11-C10 | -8.24 | 1.17        | 1.43     |
| 18  | L     | 4022 | BCR  | C10-C9  | -8.24 | 1.24        | 1.35     |
| 18  | G     | 4006 | BCR  | C11-C10 | -8.24 | 1.17        | 1.43     |
| 18  | U     | 4022 | BCR  | C10-C9  | -8.23 | 1.24        | 1.35     |
| 18  | I     | 4018 | BCR  | C11-C10 | -8.23 | 1.18        | 1.43     |
| 18  | A     | 4006 | BCR  | C11-C10 | -8.22 | 1.18        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | a     | 4006 | BCR  | C11-C10 | -8.22 | 1.18        | 1.43     |
| 18  | R     | 4018 | BCR  | C11-C10 | -8.21 | 1.18        | 1.43     |
| 18  | l     | 4022 | BCR  | C10-C9  | -8.20 | 1.24        | 1.35     |
| 18  | G     | 4002 | BCR  | C8-C9   | -8.18 | 1.28        | 1.45     |
| 18  | A     | 4002 | BCR  | C8-C9   | -8.17 | 1.28        | 1.45     |
| 18  | a     | 4002 | BCR  | C8-C9   | -8.17 | 1.28        | 1.45     |
| 18  | T     | 4001 | BCR  | C11-C10 | -8.17 | 1.18        | 1.43     |
| 18  | G     | 4001 | BCR  | C11-C10 | -8.16 | 1.18        | 1.43     |
| 18  | K     | 4001 | BCR  | C11-C10 | -8.15 | 1.18        | 1.43     |
| 18  | k     | 4001 | BCR  | C11-C10 | -8.15 | 1.18        | 1.43     |
| 18  | A     | 4001 | BCR  | C11-C10 | -8.14 | 1.18        | 1.43     |
| 18  | H     | 4014 | BCR  | C8-C9   | -8.14 | 1.28        | 1.45     |
| 18  | b     | 4014 | BCR  | C8-C9   | -8.13 | 1.28        | 1.45     |
| 18  | a     | 4001 | BCR  | C11-C10 | -8.13 | 1.18        | 1.43     |
| 18  | b     | 4005 | BCR  | C11-C10 | -8.13 | 1.18        | 1.43     |
| 18  | B     | 4014 | BCR  | C8-C9   | -8.13 | 1.28        | 1.45     |
| 18  | b     | 4009 | BCR  | C11-C10 | -8.12 | 1.18        | 1.43     |
| 18  | H     | 4005 | BCR  | C11-C10 | -8.12 | 1.18        | 1.43     |
| 18  | a     | 4002 | BCR  | C11-C10 | -8.12 | 1.18        | 1.43     |
| 18  | B     | 4005 | BCR  | C11-C10 | -8.12 | 1.18        | 1.43     |
| 18  | A     | 4002 | BCR  | C11-C10 | -8.10 | 1.18        | 1.43     |
| 18  | B     | 4009 | BCR  | C11-C10 | -8.10 | 1.18        | 1.43     |
| 18  | G     | 4002 | BCR  | C11-C10 | -8.09 | 1.18        | 1.43     |
| 18  | H     | 4009 | BCR  | C11-C10 | -8.06 | 1.18        | 1.43     |
| 15  | B     | 1230 | F6C  | C1A-CHA | 8.06  | 1.50        | 1.35     |
| 18  | M     | 4021 | BCR  | C10-C9  | -8.06 | 1.25        | 1.35     |
| 18  | V     | 4021 | BCR  | C10-C9  | -8.05 | 1.25        | 1.35     |
| 15  | b     | 1230 | F6C  | C1A-CHA | 8.05  | 1.50        | 1.35     |
| 18  | U     | 4019 | BCR  | C20-C21 | -8.04 | 1.18        | 1.43     |
| 18  | A     | 4006 | BCR  | C10-C9  | -8.04 | 1.25        | 1.35     |
| 15  | H     | 1230 | F6C  | C1A-CHA | 8.03  | 1.50        | 1.35     |
| 18  | H     | 4014 | BCR  | C11-C10 | -8.03 | 1.18        | 1.43     |
| 18  | H     | 4006 | BCR  | C11-C10 | -8.03 | 1.18        | 1.43     |
| 18  | R     | 4018 | BCR  | C10-C9  | -8.02 | 1.25        | 1.35     |
| 18  | B     | 4006 | BCR  | C11-C10 | -8.02 | 1.18        | 1.43     |
| 18  | b     | 4005 | BCR  | C8-C9   | -8.02 | 1.28        | 1.45     |
| 18  | B     | 4014 | BCR  | C11-C10 | -8.02 | 1.18        | 1.43     |
| 18  | L     | 4019 | BCR  | C20-C21 | -8.02 | 1.18        | 1.43     |
| 18  | a     | 4006 | BCR  | C10-C9  | -8.02 | 1.25        | 1.35     |
| 18  | B     | 4005 | BCR  | C8-C9   | -8.01 | 1.28        | 1.45     |
| 18  | l     | 4019 | BCR  | C20-C21 | -8.01 | 1.18        | 1.43     |
| 18  | G     | 4006 | BCR  | C10-C9  | -8.01 | 1.25        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | b     | 4006 | BCR  | C11-C10 | -8.01 | 1.18        | 1.43     |
| 18  | b     | 4014 | BCR  | C11-C10 | -8.00 | 1.18        | 1.43     |
| 18  | m     | 4021 | BCR  | C10-C9  | -8.00 | 1.25        | 1.35     |
| 18  | B     | 4004 | BCR  | C11-C10 | -7.98 | 1.18        | 1.43     |
| 18  | I     | 4020 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 18  | R     | 4020 | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 18  | H     | 4005 | BCR  | C8-C9   | -7.98 | 1.28        | 1.45     |
| 18  | b     | 4004 | BCR  | C11-C10 | -7.97 | 1.18        | 1.43     |
| 18  | H     | 4004 | BCR  | C11-C10 | -7.97 | 1.18        | 1.43     |
| 18  | I     | 4020 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 18  | i     | 4020 | BCR  | C16-C17 | -7.97 | 1.18        | 1.43     |
| 18  | I     | 4018 | BCR  | C10-C9  | -7.96 | 1.25        | 1.35     |
| 18  | R     | 4020 | BCR  | C16-C17 | -7.96 | 1.18        | 1.43     |
| 18  | i     | 4018 | BCR  | C10-C9  | -7.96 | 1.25        | 1.35     |
| 18  | i     | 4020 | BCR  | C20-C21 | -7.96 | 1.18        | 1.43     |
| 18  | b     | 4010 | BCR  | C16-C17 | -7.95 | 1.18        | 1.43     |
| 18  | H     | 4010 | BCR  | C16-C17 | -7.95 | 1.18        | 1.43     |
| 18  | B     | 4010 | BCR  | C16-C17 | -7.94 | 1.18        | 1.43     |
| 18  | a     | 4001 | BCR  | C10-C9  | -7.92 | 1.25        | 1.35     |
| 18  | A     | 4001 | BCR  | C10-C9  | -7.90 | 1.25        | 1.35     |
| 18  | G     | 4001 | BCR  | C10-C9  | -7.87 | 1.25        | 1.35     |
| 18  | B     | 4017 | BCR  | C20-C21 | -7.87 | 1.19        | 1.43     |
| 18  | H     | 4017 | BCR  | C20-C21 | -7.86 | 1.19        | 1.43     |
| 18  | b     | 4017 | BCR  | C20-C21 | -7.86 | 1.19        | 1.43     |
| 18  | B     | 4017 | BCR  | C16-C17 | -7.86 | 1.19        | 1.43     |
| 18  | A     | 4003 | BCR  | C10-C9  | -7.86 | 1.25        | 1.35     |
| 18  | G     | 4003 | BCR  | C10-C9  | -7.85 | 1.25        | 1.35     |
| 18  | H     | 4017 | BCR  | C16-C17 | -7.85 | 1.19        | 1.43     |
| 18  | a     | 4003 | BCR  | C10-C9  | -7.85 | 1.25        | 1.35     |
| 18  | b     | 4017 | BCR  | C16-C17 | -7.84 | 1.19        | 1.43     |
| 18  | B     | 4009 | BCR  | C10-C9  | -7.83 | 1.25        | 1.35     |
| 18  | H     | 4009 | BCR  | C10-C9  | -7.82 | 1.25        | 1.35     |
| 18  | b     | 4009 | BCR  | C10-C9  | -7.80 | 1.25        | 1.35     |
| 18  | A     | 4003 | BCR  | C20-C21 | -7.78 | 1.19        | 1.43     |
| 18  | A     | 4002 | BCR  | C10-C9  | -7.78 | 1.25        | 1.35     |
| 15  | B     | 1219 | F6C  | C1A-CHA | 7.78  | 1.49        | 1.35     |
| 18  | G     | 4003 | BCR  | C20-C21 | -7.77 | 1.19        | 1.43     |
| 18  | a     | 4002 | BCR  | C10-C9  | -7.77 | 1.25        | 1.35     |
| 18  | G     | 4002 | BCR  | C10-C9  | -7.77 | 1.25        | 1.35     |
| 18  | G     | 4005 | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |
| 18  | A     | 4005 | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |
| 18  | a     | 4003 | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | l     | 4019 | BCR  | C16-C17 | -7.76 | 1.19        | 1.43     |
| 15  | b     | 1219 | F6C  | C1A-CHA | 7.76  | 1.49        | 1.35     |
| 18  | L     | 4019 | BCR  | C16-C17 | -7.76 | 1.19        | 1.43     |
| 18  | U     | 4019 | BCR  | C16-C17 | -7.75 | 1.19        | 1.43     |
| 18  | a     | 4005 | BCR  | C20-C21 | -7.75 | 1.19        | 1.43     |
| 18  | G     | 4006 | BCR  | C20-C21 | -7.75 | 1.19        | 1.43     |
| 18  | l     | 4022 | BCR  | C16-C17 | -7.75 | 1.19        | 1.43     |
| 18  | U     | 4022 | BCR  | C16-C17 | -7.74 | 1.19        | 1.43     |
| 18  | H     | 4009 | BCR  | C20-C21 | -7.74 | 1.19        | 1.43     |
| 18  | a     | 4006 | BCR  | C20-C21 | -7.74 | 1.19        | 1.43     |
| 18  | L     | 4022 | BCR  | C16-C17 | -7.74 | 1.19        | 1.43     |
| 15  | H     | 1219 | F6C  | C1A-CHA | 7.74  | 1.49        | 1.35     |
| 18  | a     | 4005 | BCR  | C16-C17 | -7.74 | 1.19        | 1.43     |
| 18  | A     | 4006 | BCR  | C20-C21 | -7.73 | 1.19        | 1.43     |
| 18  | b     | 4009 | BCR  | C20-C21 | -7.73 | 1.19        | 1.43     |
| 18  | B     | 4009 | BCR  | C20-C21 | -7.73 | 1.19        | 1.43     |
| 18  | H     | 4005 | BCR  | C10-C9  | -7.72 | 1.25        | 1.35     |
| 18  | A     | 4005 | BCR  | C16-C17 | -7.72 | 1.19        | 1.43     |
| 18  | G     | 4005 | BCR  | C16-C17 | -7.72 | 1.19        | 1.43     |
| 18  | b     | 4005 | BCR  | C10-C9  | -7.71 | 1.25        | 1.35     |
| 18  | B     | 4005 | BCR  | C10-C9  | -7.68 | 1.25        | 1.35     |
| 14  | G     | 1139 | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 18  | T     | 4001 | BCR  | C20-C21 | -7.67 | 1.19        | 1.43     |
| 14  | k     | 1401 | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 14  | T     | 1401 | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 18  | U     | 4022 | BCR  | C20-C21 | -7.66 | 1.19        | 1.43     |
| 14  | a     | 1139 | CLA  | MG-NA   | 7.66  | 2.24        | 2.06     |
| 14  | K     | 1401 | CLA  | MG-NA   | 7.66  | 2.24        | 2.06     |
| 18  | L     | 4022 | BCR  | C20-C21 | -7.66 | 1.19        | 1.43     |
| 18  | K     | 4001 | BCR  | C20-C21 | -7.65 | 1.19        | 1.43     |
| 18  | k     | 4001 | BCR  | C20-C21 | -7.65 | 1.19        | 1.43     |
| 14  | A     | 1139 | CLA  | MG-NA   | 7.65  | 2.24        | 2.06     |
| 18  | l     | 4022 | BCR  | C20-C21 | -7.64 | 1.19        | 1.43     |
| 18  | i     | 4018 | BCR  | C20-C21 | -7.64 | 1.19        | 1.43     |
| 18  | b     | 4006 | BCR  | C10-C9  | -7.63 | 1.25        | 1.35     |
| 18  | I     | 4018 | BCR  | C20-C21 | -7.62 | 1.19        | 1.43     |
| 18  | b     | 4010 | BCR  | C20-C21 | -7.61 | 1.19        | 1.43     |
| 18  | H     | 4010 | BCR  | C20-C21 | -7.61 | 1.19        | 1.43     |
| 18  | R     | 4018 | BCR  | C20-C21 | -7.61 | 1.19        | 1.43     |
| 18  | B     | 4010 | BCR  | C20-C21 | -7.60 | 1.19        | 1.43     |
| 14  | A     | 1109 | CLA  | MG-NA   | 7.60  | 2.24        | 2.06     |
| 18  | B     | 4006 | BCR  | C10-C9  | -7.60 | 1.25        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1109 | CLA  | MG-NA   | 7.60  | 2.24        | 2.06     |
| 18  | H     | 4009 | BCR  | C16-C17 | -7.60 | 1.19        | 1.43     |
| 18  | a     | 4003 | BCR  | C16-C17 | -7.59 | 1.19        | 1.43     |
| 14  | b     | 1233 | CLA  | MG-NA   | 7.59  | 2.24        | 2.06     |
| 14  | G     | 1141 | CLA  | MG-NA   | 7.59  | 2.24        | 2.06     |
| 18  | A     | 4003 | BCR  | C16-C17 | -7.59 | 1.19        | 1.43     |
| 14  | B     | 1233 | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | A     | 1134 | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | G     | 1109 | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | G     | 1134 | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | a     | 1141 | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 18  | a     | 4004 | BCR  | C16-C17 | -7.58 | 1.20        | 1.43     |
| 18  | T     | 4001 | BCR  | C16-C17 | -7.58 | 1.20        | 1.43     |
| 14  | a     | 1134 | CLA  | MG-NA   | 7.57  | 2.24        | 2.06     |
| 14  | H     | 1233 | CLA  | MG-NA   | 7.57  | 2.24        | 2.06     |
| 14  | A     | 1141 | CLA  | MG-NA   | 7.57  | 2.24        | 2.06     |
| 18  | K     | 4001 | BCR  | C16-C17 | -7.57 | 1.20        | 1.43     |
| 18  | B     | 4009 | BCR  | C16-C17 | -7.57 | 1.20        | 1.43     |
| 18  | G     | 4003 | BCR  | C16-C17 | -7.57 | 1.20        | 1.43     |
| 18  | A     | 4004 | BCR  | C16-C17 | -7.57 | 1.20        | 1.43     |
| 18  | H     | 4006 | BCR  | C10-C9  | -7.56 | 1.25        | 1.35     |
| 18  | b     | 4009 | BCR  | C16-C17 | -7.56 | 1.20        | 1.43     |
| 18  | G     | 4001 | BCR  | C20-C21 | -7.56 | 1.20        | 1.43     |
| 15  | B     | 1207 | F6C  | C2A-C3A | 7.55  | 1.52        | 1.36     |
| 15  | b     | 1207 | F6C  | C2A-C3A | 7.55  | 1.52        | 1.36     |
| 14  | b     | 1214 | CLA  | MG-NA   | 7.54  | 2.24        | 2.06     |
| 18  | k     | 4001 | BCR  | C16-C17 | -7.54 | 1.20        | 1.43     |
| 18  | K     | 4001 | BCR  | C10-C9  | -7.54 | 1.25        | 1.35     |
| 18  | G     | 4006 | BCR  | C16-C17 | -7.54 | 1.20        | 1.43     |
| 18  | G     | 4004 | BCR  | C16-C17 | -7.54 | 1.20        | 1.43     |
| 14  | V     | 1501 | CLA  | MG-NA   | 7.54  | 2.24        | 2.06     |
| 18  | T     | 4001 | BCR  | C10-C9  | -7.53 | 1.25        | 1.35     |
| 18  | a     | 4001 | BCR  | C20-C21 | -7.53 | 1.20        | 1.43     |
| 18  | A     | 4001 | BCR  | C20-C21 | -7.53 | 1.20        | 1.43     |
| 14  | a     | 1115 | CLA  | MG-NA   | 7.53  | 2.24        | 2.06     |
| 15  | H     | 1207 | F6C  | C2A-C3A | 7.52  | 1.52        | 1.36     |
| 14  | B     | 1214 | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |
| 18  | k     | 4001 | BCR  | C10-C9  | -7.52 | 1.25        | 1.35     |
| 15  | B     | 1219 | F6C  | C2A-C3A | 7.52  | 1.52        | 1.36     |
| 18  | b     | 4004 | BCR  | C20-C21 | -7.52 | 1.20        | 1.43     |
| 14  | H     | 1214 | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |
| 18  | a     | 4006 | BCR  | C16-C17 | -7.52 | 1.20        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | M     | 1501 | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |
| 14  | b     | 1223 | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |
| 18  | A     | 4006 | BCR  | C16-C17 | -7.51 | 1.20        | 1.43     |
| 18  | H     | 4004 | BCR  | C20-C21 | -7.51 | 1.20        | 1.43     |
| 14  | H     | 1223 | CLA  | MG-NA   | 7.51  | 2.24        | 2.06     |
| 18  | b     | 4014 | BCR  | C10-C9  | -7.51 | 1.25        | 1.35     |
| 18  | B     | 4004 | BCR  | C20-C21 | -7.51 | 1.20        | 1.43     |
| 15  | H     | 1219 | F6C  | C2A-C3A | 7.50  | 1.52        | 1.36     |
| 18  | a     | 4004 | BCR  | C20-C21 | -7.50 | 1.20        | 1.43     |
| 14  | B     | 1223 | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 18  | A     | 4004 | BCR  | C20-C21 | -7.50 | 1.20        | 1.43     |
| 14  | G     | 1115 | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 15  | b     | 1219 | F6C  | C2A-C3A | 7.49  | 1.52        | 1.36     |
| 18  | M     | 4021 | BCR  | C16-C17 | -7.49 | 1.20        | 1.43     |
| 14  | m     | 1501 | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 18  | G     | 4004 | BCR  | C20-C21 | -7.49 | 1.20        | 1.43     |
| 14  | A     | 1115 | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 14  | A     | 1114 | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 14  | B     | 1232 | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 14  | G     | 1114 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 14  | H     | 1022 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 18  | H     | 4014 | BCR  | C10-C9  | -7.48 | 1.25        | 1.35     |
| 14  | a     | 1101 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 14  | H     | 1232 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 14  | b     | 1022 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 18  | B     | 4014 | BCR  | C10-C9  | -7.48 | 1.25        | 1.35     |
| 14  | a     | 1114 | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 14  | B     | 1022 | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 18  | V     | 4021 | BCR  | C16-C17 | -7.47 | 1.20        | 1.43     |
| 14  | b     | 1217 | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 14  | b     | 1232 | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 18  | m     | 4021 | BCR  | C16-C17 | -7.47 | 1.20        | 1.43     |
| 14  | B     | 1217 | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 18  | b     | 4005 | BCR  | C20-C21 | -7.47 | 1.20        | 1.43     |
| 14  | a     | 1111 | CLA  | MG-NA   | 7.46  | 2.24        | 2.06     |
| 14  | H     | 1220 | CLA  | MG-NA   | 7.46  | 2.24        | 2.06     |
| 16  | H     | 2002 | PQN  | C3-C2   | 7.46  | 1.48        | 1.35     |
| 14  | A     | 1135 | CLA  | MG-NA   | 7.46  | 2.24        | 2.06     |
| 14  | B     | 1220 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | A     | 1101 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | H     | 1217 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | A     | 1140 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | a     | 4002 | BCR  | C20-C21 | -7.45 | 1.20        | 1.43     |
| 14  | G     | 1111 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | B     | 1209 | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 18  | A     | 4002 | BCR  | C20-C21 | -7.44 | 1.20        | 1.43     |
| 16  | B     | 2002 | PQN  | C3-C2   | 7.44  | 1.48        | 1.35     |
| 18  | H     | 4005 | BCR  | C20-C21 | -7.44 | 1.20        | 1.43     |
| 14  | G     | 1140 | CLA  | MG-NA   | 7.44  | 2.23        | 2.06     |
| 16  | b     | 2002 | PQN  | C3-C2   | 7.44  | 1.48        | 1.35     |
| 14  | G     | 1101 | CLA  | MG-NA   | 7.44  | 2.23        | 2.06     |
| 14  | G     | 1135 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 18  | B     | 4005 | BCR  | C20-C21 | -7.43 | 1.20        | 1.43     |
| 14  | a     | 1135 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | b     | 1209 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | B     | 1240 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 18  | G     | 4002 | BCR  | C20-C21 | -7.43 | 1.20        | 1.43     |
| 18  | G     | 4002 | BCR  | C16-C17 | -7.43 | 1.20        | 1.43     |
| 14  | a     | 1116 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | a     | 1140 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | H     | 1209 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 18  | A     | 4002 | BCR  | C16-C17 | -7.43 | 1.20        | 1.43     |
| 14  | A     | 1111 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | a     | 1113 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | H     | 1240 | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | b     | 1240 | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | G     | 1116 | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | b     | 1220 | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | A     | 1116 | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | A     | 1107 | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | b     | 1234 | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 18  | a     | 4002 | BCR  | C16-C17 | -7.41 | 1.20        | 1.43     |
| 14  | A     | 1113 | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | G     | 1107 | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | G     | 1123 | CLA  | MG-NA   | 7.40  | 2.23        | 2.06     |
| 14  | B     | 1234 | CLA  | MG-NA   | 7.40  | 2.23        | 2.06     |
| 14  | a     | 1123 | CLA  | MG-NA   | 7.39  | 2.23        | 2.06     |
| 18  | I     | 4018 | BCR  | C16-C17 | -7.39 | 1.20        | 1.43     |
| 14  | G     | 1113 | CLA  | MG-NA   | 7.39  | 2.23        | 2.06     |
| 14  | B     | 1221 | CLA  | MG-NA   | 7.39  | 2.23        | 2.06     |
| 14  | A     | 1123 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 14  | a     | 1107 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 18  | i     | 4018 | BCR  | C16-C17 | -7.38 | 1.20        | 1.43     |
| 14  | H     | 1221 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | H     | 4004 | BCR  | C16-C17 | -7.38 | 1.20        | 1.43     |
| 14  | H     | 1229 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 14  | a     | 1130 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 15  | H     | 1230 | F6C  | C2A-C3A | 7.37  | 1.52        | 1.36     |
| 14  | b     | 1221 | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 14  | B     | 1229 | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 18  | b     | 4004 | BCR  | C10-C9  | -7.36 | 1.26        | 1.35     |
| 18  | B     | 4004 | BCR  | C10-C9  | -7.36 | 1.26        | 1.35     |
| 18  | R     | 4018 | BCR  | C16-C17 | -7.36 | 1.20        | 1.43     |
| 15  | B     | 1230 | F6C  | C2A-C3A | 7.36  | 1.52        | 1.36     |
| 18  | B     | 4004 | BCR  | C16-C17 | -7.36 | 1.20        | 1.43     |
| 14  | b     | 1229 | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 14  | H     | 1234 | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 18  | b     | 4004 | BCR  | C16-C17 | -7.35 | 1.20        | 1.43     |
| 18  | H     | 4004 | BCR  | C10-C9  | -7.35 | 1.26        | 1.35     |
| 14  | U     | 1501 | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 14  | A     | 1130 | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 14  | l     | 1501 | CLA  | MG-NA   | 7.34  | 2.23        | 2.06     |
| 15  | b     | 1230 | F6C  | C2A-C3A | 7.34  | 1.52        | 1.36     |
| 18  | H     | 4014 | BCR  | C20-C21 | -7.34 | 1.20        | 1.43     |
| 18  | b     | 4014 | BCR  | C20-C21 | -7.34 | 1.20        | 1.43     |
| 14  | a     | 1102 | CLA  | MG-NA   | 7.34  | 2.23        | 2.06     |
| 14  | G     | 1130 | CLA  | MG-NA   | 7.34  | 2.23        | 2.06     |
| 18  | B     | 4006 | BCR  | C16-C17 | -7.34 | 1.20        | 1.43     |
| 18  | H     | 4006 | BCR  | C16-C17 | -7.34 | 1.20        | 1.43     |
| 14  | G     | 1102 | CLA  | MG-NA   | 7.34  | 2.23        | 2.06     |
| 14  | L     | 1501 | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 14  | B     | 1228 | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 18  | B     | 4014 | BCR  | C20-C21 | -7.33 | 1.20        | 1.43     |
| 14  | A     | 1102 | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 14  | H     | 1212 | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 18  | A     | 4001 | BCR  | C16-C17 | -7.33 | 1.20        | 1.43     |
| 14  | H     | 1228 | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 18  | b     | 4005 | BCR  | C16-C17 | -7.32 | 1.20        | 1.43     |
| 18  | b     | 4006 | BCR  | C16-C17 | -7.32 | 1.20        | 1.43     |
| 18  | B     | 4005 | BCR  | C16-C17 | -7.31 | 1.20        | 1.43     |
| 14  | a     | 1108 | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 18  | H     | 4005 | BCR  | C16-C17 | -7.31 | 1.20        | 1.43     |
| 14  | B     | 1212 | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 14  | a     | 1105 | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 18  | m     | 4021 | BCR  | C20-C21 | -7.31 | 1.20        | 1.43     |
| 14  | G     | 1108 | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | G     | 4001 | BCR  | C16-C17 | -7.31 | 1.20        | 1.43     |
| 18  | a     | 4001 | BCR  | C16-C17 | -7.30 | 1.20        | 1.43     |
| 14  | A     | 1105 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | G     | 1105 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | b     | 1228 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | b     | 1213 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | A     | 1136 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | A     | 1108 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | H     | 1213 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 15  | b     | 1207 | F6C  | C1A-NA  | -7.30 | 1.27        | 1.37     |
| 14  | G     | 1133 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | B     | 1213 | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 14  | A     | 1133 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | B     | 1236 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | b     | 1212 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | a     | 1136 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 18  | B     | 4006 | BCR  | C20-C21 | -7.29 | 1.20        | 1.43     |
| 15  | H     | 1207 | F6C  | C1A-NA  | -7.29 | 1.27        | 1.37     |
| 18  | b     | 4014 | BCR  | C16-C17 | -7.29 | 1.20        | 1.43     |
| 14  | G     | 1110 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 18  | H     | 4006 | BCR  | C20-C21 | -7.29 | 1.20        | 1.43     |
| 14  | G     | 1136 | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 18  | V     | 4021 | BCR  | C20-C21 | -7.28 | 1.20        | 1.43     |
| 14  | a     | 1133 | CLA  | MG-NA   | 7.28  | 2.23        | 2.06     |
| 18  | M     | 4021 | BCR  | C20-C21 | -7.28 | 1.20        | 1.43     |
| 14  | A     | 1110 | CLA  | MG-NA   | 7.28  | 2.23        | 2.06     |
| 18  | b     | 4006 | BCR  | C20-C21 | -7.28 | 1.20        | 1.43     |
| 18  | B     | 4014 | BCR  | C16-C17 | -7.28 | 1.20        | 1.43     |
| 14  | b     | 1236 | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 15  | B     | 1207 | F6C  | C1A-NA  | -7.27 | 1.27        | 1.37     |
| 18  | H     | 4014 | BCR  | C16-C17 | -7.27 | 1.20        | 1.43     |
| 14  | a     | 1110 | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 14  | a     | 1129 | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 14  | H     | 1236 | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 14  | G     | 1138 | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 14  | b     | 1211 | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 14  | B     | 1211 | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 14  | A     | 1138 | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | H     | 1210 | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | b     | 1210 | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | A     | 1129 | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | H     | 1211 | CLA  | MG-NA   | 7.24  | 2.23        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 16  | G     | 2001 | PQN  | C3-C2   | 7.24  | 1.48        | 1.35     |
| 14  | a     | 1138 | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 15  | B     | 1238 | F6C  | C2A-C3A | 7.23  | 1.52        | 1.36     |
| 14  | B     | 1210 | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 14  | G     | 1129 | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 15  | H     | 1238 | F6C  | C2A-C3A | 7.23  | 1.52        | 1.36     |
| 16  | a     | 2001 | PQN  | C3-C2   | 7.22  | 1.48        | 1.35     |
| 14  | G     | 1118 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 14  | B     | 1227 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 15  | b     | 1238 | F6C  | C2A-C3A | 7.22  | 1.52        | 1.36     |
| 14  | a     | 1012 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 14  | a     | 1118 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 14  | H     | 1227 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 15  | b     | 1219 | F6C  | C1A-NA  | -7.21 | 1.27        | 1.37     |
| 14  | b     | 1227 | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 14  | A     | 1118 | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 14  | l     | 1503 | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 16  | A     | 2001 | PQN  | C3-C2   | 7.20  | 1.48        | 1.35     |
| 14  | A     | 1012 | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 14  | G     | 1106 | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 14  | L     | 1503 | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 14  | a     | 1137 | CLA  | MG-NA   | 7.19  | 2.23        | 2.06     |
| 14  | G     | 1012 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 15  | B     | 1219 | F6C  | C1A-NA  | -7.18 | 1.27        | 1.37     |
| 14  | B     | 1208 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 14  | B     | 1216 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 14  | b     | 1208 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 14  | b     | 1216 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 14  | H     | 1208 | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 14  | U     | 1503 | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | H     | 1216 | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | A     | 1106 | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | b     | 1239 | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 15  | H     | 1219 | F6C  | C1A-NA  | -7.17 | 1.27        | 1.37     |
| 14  | a     | 1106 | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | G     | 1137 | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 14  | A     | 1137 | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 14  | G     | 1126 | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 14  | G     | 1112 | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 14  | a     | 1112 | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 14  | A     | 1119 | CLA  | MG-NA   | 7.15  | 2.23        | 2.06     |
| 14  | B     | 1239 | CLA  | MG-NA   | 7.15  | 2.23        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 1127 | CLA  | MG-NA   | 7.15 | 2.23        | 2.06     |
| 15  | G     | 1121 | F6C  | C2A-C3A | 7.15 | 1.51        | 1.36     |
| 14  | A     | 1112 | CLA  | MG-NA   | 7.15 | 2.23        | 2.06     |
| 14  | H     | 1224 | CLA  | MG-NA   | 7.15 | 2.23        | 2.06     |
| 14  | G     | 1127 | CLA  | MG-NA   | 7.15 | 2.23        | 2.06     |
| 15  | a     | 1121 | F6C  | C2A-C3A | 7.14 | 1.51        | 1.36     |
| 14  | B     | 1224 | CLA  | MG-NA   | 7.14 | 2.23        | 2.06     |
| 14  | a     | 1131 | CLA  | MG-NA   | 7.14 | 2.23        | 2.06     |
| 15  | A     | 1121 | F6C  | C2A-C3A | 7.14 | 1.51        | 1.36     |
| 14  | A     | 1131 | CLA  | MG-NA   | 7.14 | 2.23        | 2.06     |
| 14  | a     | 1126 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | G     | 1131 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | a     | 1119 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | a     | 1127 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | A     | 1126 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | G     | 1128 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | H     | 1239 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | G     | 1120 | CLA  | MG-NA   | 7.13 | 2.23        | 2.06     |
| 14  | a     | 1120 | CLA  | MG-NA   | 7.12 | 2.23        | 2.06     |
| 14  | G     | 1119 | CLA  | MG-NA   | 7.12 | 2.23        | 2.06     |
| 14  | A     | 1124 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | A     | 1128 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | a     | 1125 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | G     | 1125 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | A     | 1120 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | B     | 1235 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | a     | 1128 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | b     | 1224 | CLA  | MG-NA   | 7.11 | 2.23        | 2.06     |
| 14  | b     | 1201 | CLA  | MG-NA   | 7.10 | 2.23        | 2.06     |
| 14  | a     | 1124 | CLA  | MG-NA   | 7.10 | 2.23        | 2.06     |
| 14  | G     | 1122 | CLA  | MG-NA   | 7.10 | 2.23        | 2.06     |
| 14  | A     | 1122 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | G     | 1124 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | a     | 1122 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | B     | 1201 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | a     | 1132 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | b     | 1218 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | H     | 1235 | CLA  | MG-NA   | 7.09 | 2.23        | 2.06     |
| 14  | H     | 1201 | CLA  | MG-NA   | 7.08 | 2.23        | 2.06     |
| 13  | G     | 1011 | CL0  | MG-NA   | 7.08 | 2.23        | 2.06     |
| 14  | b     | 1235 | CLA  | MG-NA   | 7.08 | 2.23        | 2.06     |
| 14  | A     | 1125 | CLA  | MG-NA   | 7.08 | 2.23        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 14  | G     | 1132 | CLA  | MG-NA  | 7.08  | 2.23        | 2.06     |
| 13  | A     | 1011 | CL0  | MG-NA  | 7.08  | 2.23        | 2.06     |
| 14  | B     | 1215 | CLA  | MG-NA  | 7.07  | 2.23        | 2.06     |
| 14  | b     | 1215 | CLA  | MG-NA  | 7.07  | 2.23        | 2.06     |
| 14  | H     | 1218 | CLA  | MG-NA  | 7.07  | 2.23        | 2.06     |
| 13  | a     | 1011 | CL0  | MG-NA  | 7.07  | 2.23        | 2.06     |
| 15  | H     | 1237 | F6C  | C1A-NA | -7.07 | 1.28        | 1.37     |
| 14  | B     | 1218 | CLA  | MG-NA  | 7.07  | 2.23        | 2.06     |
| 14  | A     | 1132 | CLA  | MG-NA  | 7.06  | 2.23        | 2.06     |
| 15  | B     | 1230 | F6C  | C1A-NA | -7.06 | 1.28        | 1.37     |
| 15  | b     | 1237 | F6C  | C1A-NA | -7.06 | 1.28        | 1.37     |
| 14  | H     | 1215 | CLA  | MG-NA  | 7.06  | 2.23        | 2.06     |
| 14  | b     | 1204 | CLA  | MG-NA  | 7.05  | 2.23        | 2.06     |
| 14  | B     | 1231 | CLA  | MG-NA  | 7.05  | 2.23        | 2.06     |
| 14  | H     | 1206 | CLA  | MG-NA  | 7.05  | 2.23        | 2.06     |
| 15  | b     | 1230 | F6C  | C1A-NA | -7.05 | 1.28        | 1.37     |
| 14  | H     | 1231 | CLA  | MG-NA  | 7.04  | 2.23        | 2.06     |
| 14  | H     | 1205 | CLA  | MG-NA  | 7.03  | 2.23        | 2.06     |
| 15  | B     | 1237 | F6C  | C1A-NA | -7.03 | 1.28        | 1.37     |
| 14  | b     | 1206 | CLA  | MG-NA  | 7.03  | 2.23        | 2.06     |
| 14  | B     | 1204 | CLA  | MG-NA  | 7.03  | 2.23        | 2.06     |
| 15  | H     | 1230 | F6C  | C1A-NA | -7.02 | 1.28        | 1.37     |
| 14  | B     | 1206 | CLA  | MG-NA  | 7.02  | 2.22        | 2.06     |
| 14  | b     | 1231 | CLA  | MG-NA  | 7.02  | 2.22        | 2.06     |
| 15  | B     | 1238 | F6C  | C1A-NA | -7.02 | 1.28        | 1.37     |
| 14  | b     | 1205 | CLA  | MG-NA  | 7.01  | 2.22        | 2.06     |
| 15  | b     | 1238 | F6C  | C1A-NA | -7.01 | 1.28        | 1.37     |
| 14  | H     | 1222 | CLA  | MG-NA  | 7.01  | 2.22        | 2.06     |
| 14  | B     | 1205 | CLA  | MG-NA  | 7.01  | 2.22        | 2.06     |
| 14  | B     | 1222 | CLA  | MG-NA  | 7.00  | 2.22        | 2.06     |
| 14  | B     | 1225 | CLA  | MG-NA  | 7.00  | 2.22        | 2.06     |
| 14  | H     | 1204 | CLA  | MG-NA  | 7.00  | 2.22        | 2.06     |
| 14  | b     | 1222 | CLA  | MG-NA  | 7.00  | 2.22        | 2.06     |
| 14  | b     | 1203 | CLA  | MG-NA  | 6.98  | 2.22        | 2.06     |
| 14  | b     | 1225 | CLA  | MG-NA  | 6.98  | 2.22        | 2.06     |
| 14  | H     | 1225 | CLA  | MG-NA  | 6.98  | 2.22        | 2.06     |
| 14  | B     | 1203 | CLA  | MG-NA  | 6.97  | 2.22        | 2.06     |
| 14  | H     | 1226 | CLA  | MG-NA  | 6.96  | 2.22        | 2.06     |
| 14  | B     | 1226 | CLA  | MG-NA  | 6.95  | 2.22        | 2.06     |
| 14  | H     | 1203 | CLA  | MG-NA  | 6.95  | 2.22        | 2.06     |
| 14  | l     | 1502 | CLA  | MG-NA  | 6.95  | 2.22        | 2.06     |
| 14  | b     | 1226 | CLA  | MG-NA  | 6.94  | 2.22        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | H     | 1238 | F6C  | C1A-NA  | -6.94 | 1.28        | 1.37     |
| 14  | L     | 1502 | CLA  | MG-NA   | 6.93  | 2.22        | 2.06     |
| 14  | U     | 1502 | CLA  | MG-NA   | 6.93  | 2.22        | 2.06     |
| 14  | B     | 1021 | CLA  | MG-NA   | 6.93  | 2.22        | 2.06     |
| 14  | H     | 1021 | CLA  | MG-NA   | 6.92  | 2.22        | 2.06     |
| 14  | G     | 1117 | CLA  | MG-NA   | 6.91  | 2.22        | 2.06     |
| 14  | a     | 1117 | CLA  | MG-NA   | 6.91  | 2.22        | 2.06     |
| 14  | A     | 1117 | CLA  | MG-NA   | 6.90  | 2.22        | 2.06     |
| 14  | b     | 1021 | CLA  | MG-NA   | 6.89  | 2.22        | 2.06     |
| 14  | B     | 1202 | CLA  | MG-NA   | 6.86  | 2.22        | 2.06     |
| 14  | H     | 1202 | CLA  | MG-NA   | 6.86  | 2.22        | 2.06     |
| 14  | b     | 1202 | CLA  | MG-NA   | 6.85  | 2.22        | 2.06     |
| 14  | a     | 1104 | CLA  | MG-NA   | 6.77  | 2.22        | 2.06     |
| 14  | A     | 1104 | CLA  | MG-NA   | 6.75  | 2.22        | 2.06     |
| 14  | G     | 1104 | CLA  | MG-NA   | 6.74  | 2.22        | 2.06     |
| 14  | A     | 1013 | CLA  | MG-NA   | 6.72  | 2.22        | 2.06     |
| 14  | a     | 1013 | CLA  | MG-NA   | 6.72  | 2.22        | 2.06     |
| 14  | G     | 1013 | CLA  | MG-NA   | 6.72  | 2.22        | 2.06     |
| 14  | G     | 1103 | CLA  | MG-NA   | 6.65  | 2.22        | 2.06     |
| 14  | A     | 1103 | CLA  | MG-NA   | 6.61  | 2.22        | 2.06     |
| 14  | a     | 1103 | CLA  | MG-NA   | 6.61  | 2.22        | 2.06     |
| 15  | a     | 1121 | F6C  | C1A-NA  | -6.58 | 1.28        | 1.37     |
| 14  | B     | 1023 | CLA  | MG-NA   | 6.56  | 2.21        | 2.06     |
| 15  | G     | 1121 | F6C  | C1A-NA  | -6.56 | 1.28        | 1.37     |
| 15  | A     | 1121 | F6C  | C1A-NA  | -6.55 | 1.28        | 1.37     |
| 14  | b     | 1023 | CLA  | MG-NA   | 6.55  | 2.21        | 2.06     |
| 14  | H     | 1023 | CLA  | MG-NA   | 6.54  | 2.21        | 2.06     |
| 15  | H     | 1237 | F6C  | C2A-C3A | 6.25  | 1.50        | 1.36     |
| 15  | B     | 1237 | F6C  | C2A-C3A | 6.22  | 1.50        | 1.36     |
| 15  | b     | 1237 | F6C  | C2A-C3A | 6.21  | 1.49        | 1.36     |
| 14  | a     | 1115 | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 14  | H     | 1240 | CLA  | O2D-CGD | 5.29  | 1.46        | 1.33     |
| 14  | A     | 1115 | CLA  | C3B-C2B | 5.29  | 1.47        | 1.40     |
| 14  | H     | 1221 | CLA  | O2A-C1  | 5.29  | 1.61        | 1.46     |
| 14  | b     | 1240 | CLA  | O2D-CGD | 5.29  | 1.46        | 1.33     |
| 14  | B     | 1240 | CLA  | O2D-CGD | 5.28  | 1.46        | 1.33     |
| 14  | G     | 1115 | CLA  | C3B-C2B | 5.28  | 1.47        | 1.40     |
| 14  | b     | 1221 | CLA  | O2A-C1  | 5.27  | 1.61        | 1.46     |
| 14  | B     | 1221 | CLA  | O2A-C1  | 5.27  | 1.61        | 1.46     |
| 15  | b     | 1230 | F6C  | O2D-CGD | 5.26  | 1.46        | 1.33     |
| 15  | H     | 1230 | F6C  | O2D-CGD | 5.25  | 1.46        | 1.33     |
| 14  | a     | 1138 | CLA  | O2D-CGD | 5.24  | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1230 | F6C  | O2D-CGD | 5.24 | 1.46        | 1.33     |
| 14  | A     | 1102 | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 14  | k     | 1401 | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 14  | A     | 1138 | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 15  | b     | 1230 | F6C  | CHC-C4B | 5.22 | 1.48        | 1.35     |
| 14  | G     | 1138 | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 14  | a     | 1118 | CLA  | O2A-C1  | 5.22 | 1.60        | 1.46     |
| 14  | a     | 1102 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 14  | B     | 1211 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 14  | G     | 1102 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 15  | B     | 1230 | F6C  | CHC-C4B | 5.21 | 1.48        | 1.35     |
| 14  | b     | 1211 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 15  | H     | 1230 | F6C  | CHC-C4B | 5.21 | 1.48        | 1.35     |
| 14  | A     | 1123 | CLA  | O2A-C1  | 5.20 | 1.60        | 1.46     |
| 14  | G     | 1123 | CLA  | O2A-C1  | 5.20 | 1.60        | 1.46     |
| 14  | a     | 1123 | CLA  | O2A-C1  | 5.20 | 1.60        | 1.46     |
| 14  | b     | 1233 | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 14  | B     | 1233 | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | G     | 1118 | CLA  | O2A-C1  | 5.19 | 1.60        | 1.46     |
| 14  | b     | 1211 | CLA  | C3B-C2B | 5.19 | 1.47        | 1.40     |
| 14  | K     | 1401 | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | A     | 1118 | CLA  | O2A-C1  | 5.18 | 1.60        | 1.46     |
| 14  | H     | 1211 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 14  | H     | 1233 | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 14  | A     | 1102 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 14  | H     | 1234 | CLA  | O2A-C1  | 5.18 | 1.60        | 1.46     |
| 14  | A     | 1133 | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | G     | 1110 | CLA  | C3B-C2B | 5.17 | 1.47        | 1.40     |
| 14  | a     | 1110 | CLA  | C3B-C2B | 5.17 | 1.47        | 1.40     |
| 14  | b     | 1228 | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | A     | 1114 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | T     | 1401 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | G     | 1114 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | a     | 1133 | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | a     | 1013 | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | a     | 1102 | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 14  | B     | 1211 | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 14  | G     | 1106 | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 14  | G     | 1133 | CLA  | O2A-C1  | 5.16 | 1.60        | 1.46     |
| 14  | G     | 1140 | CLA  | O2A-C1  | 5.16 | 1.60        | 1.46     |
| 14  | B     | 1234 | CLA  | O2A-C1  | 5.16 | 1.60        | 1.46     |
| 14  | H     | 1218 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 1102 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 14  | H     | 1240 | CLA  | O2A-C1  | 5.15 | 1.60        | 1.46     |
| 14  | b     | 1225 | CLA  | O2A-C1  | 5.15 | 1.60        | 1.46     |
| 14  | B     | 1240 | CLA  | O2A-C1  | 5.15 | 1.60        | 1.46     |
| 14  | a     | 1114 | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 14  | H     | 1228 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | A     | 1105 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 14  | A     | 1140 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | B     | 1225 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | B     | 1228 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | H     | 1225 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | A     | 1013 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | a     | 1105 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 14  | G     | 1013 | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | H     | 1218 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 14  | A     | 1106 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 14  | G     | 1105 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 14  | H     | 1211 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 14  | a     | 1106 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | b     | 1240 | CLA  | O2A-C1  | 5.13 | 1.60        | 1.46     |
| 14  | B     | 1218 | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 14  | A     | 1110 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | G     | 1119 | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 14  | b     | 1234 | CLA  | O2A-C1  | 5.13 | 1.60        | 1.46     |
| 14  | b     | 1221 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | a     | 1140 | CLA  | O2A-C1  | 5.12 | 1.60        | 1.46     |
| 14  | H     | 1221 | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 14  | b     | 1218 | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 14  | H     | 1201 | CLA  | CHC-C1C | 5.11 | 1.48        | 1.35     |
| 15  | b     | 1219 | F6C  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | b     | 1211 | CLA  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 15  | H     | 1219 | F6C  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | B     | 1211 | CLA  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | A     | 1102 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | a     | 1119 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 14  | A     | 1119 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 14  | B     | 1221 | CLA  | C3B-C2B | 5.09 | 1.47        | 1.40     |
| 14  | A     | 1113 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 14  | G     | 1113 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 15  | B     | 1219 | F6C  | O2A-C1  | 5.09 | 1.60        | 1.46     |
| 14  | H     | 1213 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 14  | a     | 1113 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1229 | CLA  | O2A-C1  | 5.09  | 1.60        | 1.46     |
| 14  | G     | 1109 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 14  | H     | 1211 | CLA  | O2A-C1  | 5.09  | 1.60        | 1.46     |
| 14  | b     | 1022 | CLA  | CHC-C1C | 5.09  | 1.48        | 1.35     |
| 14  | G     | 1102 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 14  | a     | 1102 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 14  | H     | 1229 | CLA  | O2A-C1  | 5.08  | 1.60        | 1.46     |
| 14  | a     | 1131 | CLA  | O2A-C1  | 5.08  | 1.60        | 1.46     |
| 14  | B     | 1218 | CLA  | C3B-C2B | 5.08  | 1.47        | 1.40     |
| 14  | b     | 1229 | CLA  | O2A-C1  | 5.08  | 1.60        | 1.46     |
| 14  | b     | 1201 | CLA  | CHC-C1C | 5.08  | 1.48        | 1.35     |
| 14  | b     | 1214 | CLA  | O2A-C1  | 5.08  | 1.60        | 1.46     |
| 14  | b     | 1239 | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 14  | A     | 1109 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 14  | H     | 1232 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 14  | B     | 1022 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 14  | G     | 1131 | CLA  | O2A-C1  | 5.07  | 1.60        | 1.46     |
| 15  | b     | 1219 | F6C  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 14  | H     | 1216 | CLA  | O2A-C1  | 5.07  | 1.60        | 1.46     |
| 14  | B     | 1239 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 14  | H     | 1239 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 14  | G     | 1112 | CLA  | O2A-C1  | 5.07  | 1.60        | 1.46     |
| 14  | G     | 1112 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 14  | H     | 1214 | CLA  | O2A-C1  | 5.07  | 1.60        | 1.46     |
| 13  | a     | 1011 | CL0  | C1D-ND  | -5.07 | 1.31        | 1.37     |
| 14  | B     | 1201 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 14  | B     | 1213 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 14  | A     | 1131 | CLA  | O2A-C1  | 5.07  | 1.60        | 1.46     |
| 14  | G     | 1116 | CLA  | O2A-C1  | 5.06  | 1.60        | 1.46     |
| 14  | H     | 1022 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 14  | a     | 1112 | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 14  | A     | 1112 | CLA  | O2A-C1  | 5.06  | 1.60        | 1.46     |
| 14  | b     | 1218 | CLA  | C3B-C2B | 5.06  | 1.47        | 1.40     |
| 14  | b     | 1213 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 14  | B     | 1216 | CLA  | O2A-C1  | 5.06  | 1.60        | 1.46     |
| 14  | A     | 1108 | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 14  | b     | 1240 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 13  | A     | 1011 | CL0  | C1D-ND  | -5.06 | 1.31        | 1.37     |
| 14  | a     | 1139 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 14  | B     | 1214 | CLA  | O2A-C1  | 5.06  | 1.60        | 1.46     |
| 14  | a     | 1109 | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 14  | G     | 1109 | CLA  | O2A-C1  | 5.05  | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1216 | CLA  | O2A-C1  | 5.05  | 1.60        | 1.46     |
| 14  | A     | 1112 | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 13  | G     | 1011 | CL0  | C1D-ND  | -5.05 | 1.31        | 1.37     |
| 14  | a     | 1120 | CLA  | C3B-C2B | 5.05  | 1.47        | 1.40     |
| 14  | a     | 1013 | CLA  | C1D-ND  | -5.05 | 1.31        | 1.37     |
| 15  | B     | 1219 | F6C  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 14  | A     | 1109 | CLA  | O2A-C1  | 5.05  | 1.60        | 1.46     |
| 14  | a     | 1109 | CLA  | O2A-C1  | 5.05  | 1.60        | 1.46     |
| 14  | B     | 1232 | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 14  | A     | 1116 | CLA  | O2A-C1  | 5.05  | 1.60        | 1.46     |
| 14  | A     | 1139 | CLA  | CHC-C1C | 5.05  | 1.47        | 1.35     |
| 14  | B     | 1234 | CLA  | CHC-C1C | 5.05  | 1.47        | 1.35     |
| 14  | b     | 1234 | CLA  | CHC-C1C | 5.04  | 1.47        | 1.35     |
| 14  | B     | 1214 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 14  | a     | 1108 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 14  | H     | 1021 | CLA  | C1D-ND  | -5.04 | 1.31        | 1.37     |
| 14  | A     | 1013 | CLA  | CHC-C1C | 5.04  | 1.47        | 1.35     |
| 14  | G     | 1139 | CLA  | CHC-C1C | 5.04  | 1.47        | 1.35     |
| 14  | b     | 1214 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 14  | H     | 1234 | CLA  | CHC-C1C | 5.04  | 1.47        | 1.35     |
| 14  | H     | 1240 | CLA  | CHC-C1C | 5.04  | 1.47        | 1.35     |
| 14  | U     | 1503 | CLA  | O2A-C1  | 5.04  | 1.60        | 1.46     |
| 14  | a     | 1103 | CLA  | O2A-C1  | 5.04  | 1.60        | 1.46     |
| 14  | a     | 1119 | CLA  | O2A-C1  | 5.04  | 1.60        | 1.46     |
| 14  | G     | 1108 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 15  | H     | 1219 | F6C  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 14  | a     | 1112 | CLA  | O2A-C1  | 5.04  | 1.60        | 1.46     |
| 14  | G     | 1013 | CLA  | C1D-ND  | -5.04 | 1.31        | 1.37     |
| 14  | H     | 1208 | CLA  | O2A-C1  | 5.04  | 1.60        | 1.46     |
| 14  | b     | 1232 | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 14  | H     | 1236 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | G     | 1119 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | B     | 1021 | CLA  | C1D-ND  | -5.03 | 1.31        | 1.37     |
| 14  | B     | 1208 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | B     | 1236 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | b     | 1208 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | H     | 1214 | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 14  | B     | 1240 | CLA  | CHC-C1C | 5.03  | 1.47        | 1.35     |
| 14  | b     | 1021 | CLA  | C1D-ND  | -5.03 | 1.31        | 1.37     |
| 14  | H     | 1222 | CLA  | C3B-C2B | 5.03  | 1.47        | 1.40     |
| 14  | b     | 1213 | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 14  | G     | 1013 | CLA  | CHC-C1C | 5.03  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1236 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | A     | 1119 | CLA  | O2A-C1  | 5.03  | 1.60        | 1.46     |
| 14  | a     | 1123 | CLA  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 14  | a     | 1116 | CLA  | O2A-C1  | 5.02  | 1.60        | 1.46     |
| 14  | k     | 1401 | CLA  | CHC-C1C | 5.02  | 1.47        | 1.35     |
| 15  | b     | 1219 | F6C  | CHC-C4B | 5.02  | 1.47        | 1.35     |
| 14  | a     | 1141 | CLA  | CHC-C1C | 5.02  | 1.47        | 1.35     |
| 14  | A     | 1120 | CLA  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 14  | G     | 1123 | CLA  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 14  | G     | 1128 | CLA  | O2A-C1  | 5.02  | 1.60        | 1.46     |
| 14  | K     | 1401 | CLA  | CHC-C1C | 5.02  | 1.47        | 1.35     |
| 14  | G     | 1125 | CLA  | O2A-C1  | 5.02  | 1.60        | 1.46     |
| 14  | a     | 1130 | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 14  | A     | 1103 | CLA  | O2A-C1  | 5.02  | 1.60        | 1.46     |
| 14  | a     | 1133 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 15  | B     | 1219 | F6C  | CHC-C4B | 5.01  | 1.47        | 1.35     |
| 14  | G     | 1103 | CLA  | O2A-C1  | 5.01  | 1.60        | 1.46     |
| 14  | A     | 1133 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 14  | B     | 1222 | CLA  | C3B-C2B | 5.01  | 1.47        | 1.40     |
| 14  | b     | 1205 | CLA  | O2A-C1  | 5.01  | 1.60        | 1.46     |
| 14  | a     | 1013 | CLA  | CHC-C1C | 5.01  | 1.47        | 1.35     |
| 14  | T     | 1401 | CLA  | CHC-C1C | 5.01  | 1.47        | 1.35     |
| 14  | A     | 1013 | CLA  | C1D-ND  | -5.01 | 1.31        | 1.37     |
| 14  | G     | 1115 | CLA  | O2A-C1  | 5.01  | 1.60        | 1.46     |
| 14  | G     | 1120 | CLA  | C3B-C2B | 5.01  | 1.47        | 1.40     |
| 14  | B     | 1213 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 14  | G     | 1130 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 14  | B     | 1205 | CLA  | O2A-C1  | 5.01  | 1.60        | 1.46     |
| 14  | G     | 1101 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 14  | H     | 1231 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | A     | 1115 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | V     | 1501 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 14  | A     | 1141 | CLA  | CHC-C1C | 5.00  | 1.47        | 1.35     |
| 14  | A     | 1125 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | H     | 1213 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 14  | a     | 1119 | CLA  | CHC-C1C | 5.00  | 1.47        | 1.35     |
| 14  | G     | 1105 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 14  | G     | 1133 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 14  | H     | 1205 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | L     | 1503 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | l     | 1503 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |
| 14  | G     | 1136 | CLA  | O2A-C1  | 5.00  | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1105 | CLA  | CHC-C1C | 4.99  | 1.47        | 1.35     |
| 14  | b     | 1223 | CLA  | O2A-C1  | 4.99  | 1.60        | 1.46     |
| 14  | H     | 1235 | CLA  | CHC-C1C | 4.99  | 1.47        | 1.35     |
| 14  | A     | 1105 | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 15  | b     | 1237 | F6C  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 14  | H     | 1231 | CLA  | CHC-C1C | 4.99  | 1.47        | 1.35     |
| 15  | b     | 1238 | F6C  | C4A-NA  | -4.99 | 1.31        | 1.37     |
| 14  | a     | 1105 | CLA  | CHC-C1C | 4.99  | 1.47        | 1.35     |
| 15  | H     | 1219 | F6C  | CHC-C4B | 4.99  | 1.47        | 1.35     |
| 14  | A     | 1128 | CLA  | O2A-C1  | 4.99  | 1.60        | 1.46     |
| 14  | b     | 1239 | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 14  | A     | 1130 | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 14  | a     | 1101 | CLA  | CHC-C1C | 4.99  | 1.47        | 1.35     |
| 14  | B     | 1231 | CLA  | O2A-C1  | 4.99  | 1.60        | 1.46     |
| 14  | G     | 1105 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | A     | 1123 | CLA  | C3B-C2B | 4.98  | 1.47        | 1.40     |
| 14  | G     | 1107 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | G     | 1111 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | G     | 1126 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | a     | 1128 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | G     | 1101 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | G     | 1119 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | B     | 1223 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | A     | 1119 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 15  | b     | 1207 | F6C  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | M     | 1501 | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 14  | a     | 1136 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | G     | 1138 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | a     | 1105 | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 14  | b     | 1222 | CLA  | C3B-C2B | 4.98  | 1.47        | 1.40     |
| 14  | B     | 1235 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | G     | 1123 | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 15  | B     | 1237 | F6C  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 14  | A     | 1101 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | a     | 1115 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | G     | 1141 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | H     | 1229 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 14  | H     | 1223 | CLA  | O2A-C1  | 4.98  | 1.60        | 1.46     |
| 14  | B     | 1231 | CLA  | CHC-C1C | 4.98  | 1.47        | 1.35     |
| 15  | H     | 1238 | F6C  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 14  | A     | 1136 | CLA  | O2A-C1  | 4.97  | 1.60        | 1.46     |
| 14  | b     | 1226 | CLA  | O2A-C1  | 4.97  | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | b     | 1238 | F6C  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | A     | 1102 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 15  | H     | 1207 | F6C  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | a     | 1102 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | A     | 1123 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | a     | 1123 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 15  | B     | 1238 | F6C  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | A     | 1101 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | B     | 1229 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | b     | 1231 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | A     | 1126 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | H     | 1202 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | m     | 1501 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | A     | 1107 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | a     | 1107 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | a     | 1122 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 15  | B     | 1207 | F6C  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | b     | 1202 | CLA  | C3B-C2B | 4.97 | 1.47        | 1.40     |
| 14  | A     | 1106 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | a     | 1125 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | b     | 1231 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | a     | 1138 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | B     | 1202 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | H     | 1239 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | b     | 1235 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | b     | 1229 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | a     | 1101 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | B     | 1239 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | M     | 1501 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | B     | 1202 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 14  | H     | 1202 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 14  | B     | 1216 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | A     | 1138 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | b     | 1220 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | G     | 1110 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | m     | 1501 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | A     | 1139 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | H     | 1220 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | H     | 1216 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | B     | 1226 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | G     | 1130 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | G     | 1102 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1137 | CLA  | O2A-C1  | 4.96  | 1.60        | 1.46     |
| 14  | a     | 1135 | CLA  | C3B-C2B | 4.96  | 1.47        | 1.40     |
| 14  | G     | 1106 | CLA  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 15  | H     | 1237 | F6C  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 14  | A     | 1122 | CLA  | O2A-C1  | 4.96  | 1.60        | 1.46     |
| 14  | A     | 1116 | CLA  | CHC-C1C | 4.96  | 1.47        | 1.35     |
| 14  | B     | 1220 | CLA  | O2A-C1  | 4.96  | 1.60        | 1.46     |
| 14  | a     | 1111 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | A     | 1111 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | A     | 1130 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | V     | 1501 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | H     | 1226 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | A     | 1126 | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 14  | a     | 1126 | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 14  | H     | 1210 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | A     | 1137 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | a     | 1116 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | G     | 1122 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | a     | 1137 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | G     | 1116 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | b     | 1202 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | B     | 1204 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | a     | 1130 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | a     | 1126 | CLA  | O2A-C1  | 4.95  | 1.60        | 1.46     |
| 14  | G     | 1126 | CLA  | CHC-C1C | 4.95  | 1.47        | 1.35     |
| 14  | B     | 1225 | CLA  | C3B-C2B | 4.95  | 1.47        | 1.40     |
| 14  | a     | 1106 | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 14  | b     | 1216 | CLA  | CHC-C1C | 4.94  | 1.47        | 1.35     |
| 14  | A     | 1135 | CLA  | C3B-C2B | 4.94  | 1.47        | 1.40     |
| 14  | a     | 1126 | CLA  | CHC-C1C | 4.94  | 1.47        | 1.35     |
| 14  | G     | 1139 | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 14  | G     | 1112 | CLA  | CHC-C1C | 4.94  | 1.47        | 1.35     |
| 14  | B     | 1210 | CLA  | CHC-C1C | 4.94  | 1.47        | 1.35     |
| 14  | G     | 1126 | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 14  | B     | 1201 | CLA  | C3B-C2B | 4.94  | 1.47        | 1.40     |
| 14  | A     | 1120 | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 14  | b     | 1210 | CLA  | CHC-C1C | 4.94  | 1.47        | 1.35     |
| 14  | G     | 1129 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |
| 14  | b     | 1210 | CLA  | C3B-C2B | 4.93  | 1.47        | 1.40     |
| 15  | H     | 1238 | F6C  | C4A-NA  | -4.93 | 1.31        | 1.37     |
| 14  | A     | 1110 | CLA  | CHC-C1C | 4.93  | 1.47        | 1.35     |
| 14  | b     | 1202 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1110 | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 14  | b     | 1224 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |
| 14  | a     | 1139 | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 14  | H     | 1220 | CLA  | C3B-C2B | 4.93  | 1.47        | 1.40     |
| 14  | a     | 1127 | CLA  | C3B-C2B | 4.93  | 1.47        | 1.40     |
| 14  | H     | 1204 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |
| 14  | A     | 1118 | CLA  | CHC-C1C | 4.93  | 1.47        | 1.35     |
| 14  | a     | 1129 | CLA  | CHC-C1C | 4.93  | 1.47        | 1.35     |
| 14  | a     | 1110 | CLA  | CHC-C1C | 4.93  | 1.47        | 1.35     |
| 14  | A     | 1129 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |
| 14  | a     | 1132 | CLA  | O2A-C1  | 4.93  | 1.60        | 1.46     |
| 15  | G     | 1121 | F6C  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | U     | 1501 | CLA  | C3D-C4D | -4.92 | 1.33        | 1.44     |
| 14  | a     | 1129 | CLA  | O2A-C1  | 4.92  | 1.60        | 1.46     |
| 14  | a     | 1120 | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 15  | A     | 1121 | F6C  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | G     | 1112 | CLA  | C3B-C2B | 4.92  | 1.47        | 1.40     |
| 14  | b     | 1208 | CLA  | C3B-C2B | 4.92  | 1.47        | 1.40     |
| 14  | b     | 1204 | CLA  | O2A-C1  | 4.92  | 1.60        | 1.46     |
| 15  | a     | 1121 | F6C  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | H     | 1228 | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | A     | 1104 | CLA  | O2A-C1  | 4.92  | 1.60        | 1.46     |
| 14  | b     | 1226 | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 14  | A     | 1127 | CLA  | C3B-C2B | 4.92  | 1.47        | 1.40     |
| 14  | H     | 1201 | CLA  | C3B-C2B | 4.92  | 1.47        | 1.40     |
| 14  | A     | 1129 | CLA  | CHC-C1C | 4.92  | 1.47        | 1.35     |
| 14  | H     | 1202 | CLA  | O2A-C1  | 4.92  | 1.60        | 1.46     |
| 14  | G     | 1127 | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | G     | 1120 | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 14  | A     | 1126 | CLA  | CHC-C1C | 4.92  | 1.47        | 1.35     |
| 14  | b     | 1201 | CLA  | C3B-C2B | 4.91  | 1.47        | 1.40     |
| 14  | H     | 1224 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | A     | 1110 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 14  | G     | 1104 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | A     | 1127 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 14  | a     | 1127 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 14  | G     | 1116 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 14  | B     | 1208 | CLA  | C3B-C2B | 4.91  | 1.47        | 1.40     |
| 14  | G     | 1106 | CLA  | CHC-C1C | 4.91  | 1.47        | 1.35     |
| 14  | U     | 1502 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | G     | 1118 | CLA  | CHC-C1C | 4.91  | 1.47        | 1.35     |
| 14  | b     | 1228 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1104 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | B     | 1202 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | B     | 1220 | CLA  | C3B-C2B | 4.91  | 1.47        | 1.40     |
| 14  | G     | 1132 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | b     | 1206 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | B     | 1206 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | A     | 1106 | CLA  | CHC-C1C | 4.91  | 1.47        | 1.35     |
| 15  | B     | 1238 | F6C  | C4A-NA  | -4.91 | 1.31        | 1.37     |
| 14  | H     | 1206 | CLA  | O2A-C1  | 4.91  | 1.60        | 1.46     |
| 14  | a     | 1110 | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 14  | L     | 1501 | CLA  | C3D-C4D | -4.90 | 1.33        | 1.44     |
| 14  | A     | 1108 | CLA  | C3B-C2B | 4.90  | 1.47        | 1.40     |
| 14  | a     | 1111 | CLA  | O2A-C1  | 4.90  | 1.60        | 1.46     |
| 14  | B     | 1213 | CLA  | C3B-C2B | 4.90  | 1.47        | 1.40     |
| 14  | l     | 1501 | CLA  | C3D-C4D | -4.90 | 1.33        | 1.44     |
| 14  | b     | 1220 | CLA  | C3B-C2B | 4.90  | 1.47        | 1.40     |
| 14  | a     | 1116 | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 14  | A     | 1132 | CLA  | O2A-C1  | 4.90  | 1.60        | 1.46     |
| 14  | B     | 1224 | CLA  | O2A-C1  | 4.90  | 1.60        | 1.46     |
| 14  | B     | 1228 | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 14  | a     | 1118 | CLA  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 14  | G     | 1115 | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 14  | A     | 1112 | CLA  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 14  | l     | 1502 | CLA  | O2A-C1  | 4.90  | 1.59        | 1.46     |
| 14  | A     | 1112 | CLA  | C3B-C2B | 4.90  | 1.47        | 1.40     |
| 14  | G     | 1129 | CLA  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 14  | a     | 1106 | CLA  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 14  | a     | 1112 | CLA  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 14  | A     | 1116 | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 14  | b     | 1216 | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 14  | G     | 1135 | CLA  | C3B-C2B | 4.90  | 1.47        | 1.40     |
| 14  | B     | 1216 | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 14  | L     | 1502 | CLA  | O2A-C1  | 4.89  | 1.59        | 1.46     |
| 14  | H     | 1225 | CLA  | C3B-C2B | 4.89  | 1.47        | 1.40     |
| 14  | G     | 1115 | CLA  | CHC-C1C | 4.89  | 1.47        | 1.35     |
| 14  | H     | 1216 | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 14  | A     | 1115 | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 14  | A     | 1115 | CLA  | CHC-C1C | 4.89  | 1.47        | 1.35     |
| 14  | H     | 1213 | CLA  | C3B-C2B | 4.89  | 1.47        | 1.40     |
| 14  | A     | 1113 | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 14  | a     | 1115 | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 14  | B     | 1210 | CLA  | C3B-C2B | 4.89  | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1232 | CLA  | CHC-C1C | 4.89  | 1.47        | 1.35     |
| 14  | A     | 1123 | CLA  | CHC-C1C | 4.89  | 1.47        | 1.35     |
| 14  | B     | 1235 | CLA  | O2A-C1  | 4.89  | 1.59        | 1.46     |
| 14  | G     | 1123 | CLA  | CHC-C1C | 4.88  | 1.47        | 1.35     |
| 14  | A     | 1111 | CLA  | O2A-C1  | 4.88  | 1.59        | 1.46     |
| 14  | a     | 1112 | CLA  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 14  | b     | 1221 | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 15  | B     | 1237 | F6C  | C4A-NA  | -4.88 | 1.31        | 1.37     |
| 14  | B     | 1226 | CLA  | C3C-C2C | 4.88  | 1.47        | 1.36     |
| 14  | b     | 1223 | CLA  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 14  | A     | 1132 | CLA  | CHC-C1C | 4.88  | 1.47        | 1.35     |
| 15  | H     | 1238 | F6C  | CHC-C4B | 4.88  | 1.47        | 1.35     |
| 14  | b     | 1225 | CLA  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 14  | b     | 1235 | CLA  | O2A-C1  | 4.88  | 1.59        | 1.46     |
| 14  | H     | 1208 | CLA  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 14  | H     | 1235 | CLA  | O2A-C1  | 4.88  | 1.59        | 1.46     |
| 14  | G     | 1132 | CLA  | CHC-C1C | 4.88  | 1.47        | 1.35     |
| 14  | b     | 1218 | CLA  | CHC-C1C | 4.88  | 1.47        | 1.35     |
| 15  | B     | 1238 | F6C  | CHC-C4B | 4.88  | 1.47        | 1.35     |
| 15  | b     | 1238 | F6C  | O2A-C1  | 4.88  | 1.59        | 1.46     |
| 14  | a     | 1108 | CLA  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 14  | G     | 1108 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | a     | 1012 | CLA  | C3D-C4D | -4.87 | 1.33        | 1.44     |
| 14  | H     | 1221 | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 14  | G     | 1111 | CLA  | O2A-C1  | 4.87  | 1.59        | 1.46     |
| 14  | B     | 1232 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | G     | 1128 | CLA  | C3C-C2C | 4.87  | 1.47        | 1.36     |
| 14  | B     | 1223 | CLA  | C3B-C2B | 4.87  | 1.47        | 1.40     |
| 14  | a     | 1123 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | H     | 1208 | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 14  | G     | 1118 | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 14  | A     | 1108 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | a     | 1117 | CLA  | O2A-C1  | 4.87  | 1.59        | 1.46     |
| 14  | b     | 1215 | CLA  | O2A-C1  | 4.87  | 1.59        | 1.46     |
| 14  | a     | 1132 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | a     | 1108 | CLA  | CHC-C1C | 4.87  | 1.47        | 1.35     |
| 14  | A     | 1012 | CLA  | C3D-C4D | -4.86 | 1.33        | 1.44     |
| 14  | A     | 1117 | CLA  | O2A-C1  | 4.86  | 1.59        | 1.46     |
| 14  | G     | 1117 | CLA  | O2A-C1  | 4.86  | 1.59        | 1.46     |
| 14  | G     | 1108 | CLA  | C3B-C2B | 4.86  | 1.47        | 1.40     |
| 14  | B     | 1221 | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 14  | G     | 1113 | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1232 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | B     | 1223 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | a     | 1113 | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 14  | b     | 1213 | CLA  | C3B-C2B | 4.86  | 1.47        | 1.40     |
| 14  | H     | 1221 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | H     | 1226 | CLA  | C3C-C2C | 4.86  | 1.47        | 1.36     |
| 14  | a     | 1128 | CLA  | C3C-C2C | 4.86  | 1.47        | 1.36     |
| 14  | a     | 1115 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | a     | 1124 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | b     | 1208 | CLA  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 14  | H     | 1210 | CLA  | C3B-C2B | 4.86  | 1.47        | 1.40     |
| 14  | b     | 1209 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | G     | 1124 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | G     | 1127 | CLA  | C3B-C2B | 4.85  | 1.47        | 1.40     |
| 14  | b     | 1208 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | B     | 1225 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | b     | 1225 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | a     | 1134 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | B     | 1208 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | B     | 1221 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | H     | 1223 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | b     | 1223 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 15  | B     | 1238 | F6C  | O2A-C1  | 4.85  | 1.59        | 1.46     |
| 15  | b     | 1238 | F6C  | CHC-C4B | 4.85  | 1.47        | 1.35     |
| 14  | b     | 1203 | CLA  | O2A-C1  | 4.85  | 1.59        | 1.46     |
| 14  | A     | 1134 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | b     | 1236 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | A     | 1128 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 14  | H     | 1203 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | G     | 1134 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | B     | 1222 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | B     | 1209 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | A     | 1118 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | G     | 1012 | CLA  | C3D-C4D | -4.85 | 1.33        | 1.44     |
| 14  | G     | 1125 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | b     | 1217 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 15  | H     | 1237 | F6C  | C4A-NA  | -4.85 | 1.31        | 1.37     |
| 14  | B     | 1215 | CLA  | O2A-C1  | 4.85  | 1.59        | 1.46     |
| 14  | G     | 1107 | CLA  | C3B-C2B | 4.85  | 1.47        | 1.40     |
| 14  | H     | 1218 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | a     | 1140 | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 14  | B     | 1218 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1208 | CLA  | CHC-C1C | 4.85  | 1.47        | 1.35     |
| 14  | b     | 1203 | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 14  | a     | 1130 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 14  | H     | 1229 | CLA  | C3B-C2B | 4.84  | 1.47        | 1.40     |
| 14  | A     | 1124 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 14  | B     | 1203 | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 14  | b     | 1222 | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 14  | B     | 1217 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 14  | U     | 1501 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 15  | H     | 1238 | F6C  | O2A-C1  | 4.84  | 1.59        | 1.46     |
| 14  | H     | 1208 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 15  | b     | 1237 | F6C  | C4A-NA  | -4.84 | 1.31        | 1.37     |
| 14  | H     | 1225 | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 14  | b     | 1221 | CLA  | CHC-C1C | 4.84  | 1.47        | 1.35     |
| 14  | H     | 1236 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | a     | 1104 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | H     | 1204 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | A     | 1125 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | A     | 1140 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | a     | 1125 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | a     | 1118 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | b     | 1214 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | A     | 1107 | CLA  | C3B-C2B | 4.83  | 1.47        | 1.40     |
| 14  | H     | 1203 | CLA  | O2A-C1  | 4.83  | 1.59        | 1.46     |
| 14  | B     | 1214 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | H     | 1209 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | a     | 1125 | CLA  | C3B-C2B | 4.83  | 1.47        | 1.40     |
| 14  | B     | 1236 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | B     | 1204 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | H     | 1222 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 14  | H     | 1223 | CLA  | C3B-C2B | 4.83  | 1.47        | 1.40     |
| 14  | G     | 1130 | CLA  | CHC-C1C | 4.83  | 1.47        | 1.35     |
| 14  | H     | 1215 | CLA  | O2A-C1  | 4.82  | 1.59        | 1.46     |
| 14  | H     | 1217 | CLA  | CHC-C1C | 4.82  | 1.47        | 1.35     |
| 14  | H     | 1214 | CLA  | CHC-C1C | 4.82  | 1.47        | 1.35     |
| 14  | A     | 1125 | CLA  | C3B-C2B | 4.82  | 1.47        | 1.40     |
| 14  | b     | 1204 | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 14  | B     | 1215 | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 14  | A     | 1130 | CLA  | CHC-C1C | 4.82  | 1.47        | 1.35     |
| 14  | A     | 1104 | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 14  | B     | 1203 | CLA  | O2A-C1  | 4.82  | 1.59        | 1.46     |
| 14  | a     | 1107 | CLA  | C3B-C2B | 4.82  | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1234 | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 14  | G     | 1104 | CLA  | O2D-CGD | 4.81  | 1.44        | 1.33     |
| 14  | B     | 1229 | CLA  | C3B-C2B | 4.81  | 1.47        | 1.40     |
| 13  | A     | 1011 | CL0  | O2A-C1  | 4.81  | 1.59        | 1.46     |
| 14  | L     | 1501 | CLA  | CHC-C1C | 4.81  | 1.47        | 1.35     |
| 14  | b     | 1227 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 14  | H     | 1224 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 14  | B     | 1228 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 15  | B     | 1237 | F6C  | CHC-C4B | 4.80  | 1.47        | 1.35     |
| 14  | b     | 1215 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 14  | G     | 1135 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 14  | H     | 1215 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 13  | a     | 1011 | CL0  | O2A-C1  | 4.80  | 1.59        | 1.46     |
| 13  | G     | 1011 | CL0  | O2A-C1  | 4.80  | 1.59        | 1.46     |
| 14  | A     | 1135 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 15  | H     | 1237 | F6C  | O2A-C1  | 4.80  | 1.59        | 1.46     |
| 14  | L     | 1502 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 14  | B     | 1224 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 14  | l     | 1501 | CLA  | CHC-C1C | 4.79  | 1.47        | 1.35     |
| 15  | A     | 1121 | F6C  | CHD-C1D | 4.79  | 1.47        | 1.35     |
| 15  | a     | 1121 | F6C  | CHD-C1D | 4.79  | 1.47        | 1.35     |
| 14  | a     | 1124 | CLA  | O2A-C1  | 4.79  | 1.59        | 1.46     |
| 14  | b     | 1224 | CLA  | CHC-C1C | 4.79  | 1.47        | 1.35     |
| 14  | H     | 1228 | CLA  | CHC-C1C | 4.79  | 1.47        | 1.35     |
| 14  | A     | 1124 | CLA  | O2A-C1  | 4.79  | 1.59        | 1.46     |
| 15  | b     | 1219 | F6C  | CHD-C1D | 4.79  | 1.47        | 1.35     |
| 14  | B     | 1227 | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 14  | G     | 1106 | CLA  | O2A-C1  | 4.79  | 1.59        | 1.46     |
| 14  | G     | 1140 | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 14  | G     | 1125 | CLA  | C3B-C2B | 4.79  | 1.47        | 1.40     |
| 14  | G     | 1124 | CLA  | O2A-C1  | 4.79  | 1.59        | 1.46     |
| 14  | A     | 1136 | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 15  | B     | 1219 | F6C  | CHD-C1D | 4.79  | 1.47        | 1.35     |
| 14  | l     | 1502 | CLA  | CHC-C1C | 4.79  | 1.47        | 1.35     |
| 15  | B     | 1237 | F6C  | O2A-C1  | 4.79  | 1.59        | 1.46     |
| 14  | A     | 1103 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | B     | 1234 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | a     | 1103 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | H     | 1227 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 15  | b     | 1237 | F6C  | O2A-C1  | 4.78  | 1.59        | 1.46     |
| 15  | H     | 1219 | F6C  | CHD-C1D | 4.78  | 1.47        | 1.35     |
| 15  | b     | 1237 | F6C  | CHC-C4B | 4.78  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1107 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 15  | H     | 1237 | F6C  | CHC-C4B | 4.78  | 1.47        | 1.35     |
| 14  | G     | 1136 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | a     | 1125 | CLA  | C3D-C4D | -4.78 | 1.33        | 1.44     |
| 14  | B     | 1223 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | B     | 1217 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | A     | 1104 | CLA  | C3B-C2B | 4.78  | 1.47        | 1.40     |
| 14  | A     | 1120 | CLA  | CHC-C1C | 4.78  | 1.47        | 1.35     |
| 14  | U     | 1502 | CLA  | CHC-C1C | 4.78  | 1.47        | 1.35     |
| 14  | a     | 1135 | CLA  | C3D-C4D | -4.78 | 1.33        | 1.44     |
| 14  | a     | 1136 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | b     | 1229 | CLA  | C3B-C2B | 4.78  | 1.47        | 1.40     |
| 15  | G     | 1121 | F6C  | CHD-C1D | 4.78  | 1.47        | 1.35     |
| 14  | A     | 1106 | CLA  | O2A-C1  | 4.78  | 1.59        | 1.46     |
| 14  | b     | 1223 | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 14  | a     | 1135 | CLA  | O2A-C1  | 4.77  | 1.59        | 1.46     |
| 14  | G     | 1107 | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 14  | H     | 1233 | CLA  | CHC-C1C | 4.77  | 1.47        | 1.35     |
| 14  | b     | 1228 | CLA  | CHC-C1C | 4.77  | 1.47        | 1.35     |
| 14  | G     | 1120 | CLA  | CHC-C1C | 4.77  | 1.47        | 1.35     |
| 14  | G     | 1103 | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 14  | b     | 1234 | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 13  | a     | 1011 | CL0  | C3C-C2C | 4.77  | 1.46        | 1.36     |
| 14  | a     | 1120 | CLA  | CHC-C1C | 4.77  | 1.47        | 1.35     |
| 14  | a     | 1104 | CLA  | C3B-C2B | 4.76  | 1.47        | 1.40     |
| 13  | A     | 1011 | CL0  | C3C-C2C | 4.76  | 1.46        | 1.36     |
| 14  | V     | 1501 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | A     | 1122 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 14  | m     | 1501 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | b     | 1216 | CLA  | C3C-C2C | 4.76  | 1.46        | 1.36     |
| 14  | A     | 1125 | CLA  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 14  | B     | 1233 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | H     | 1217 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 14  | G     | 1122 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 14  | a     | 1107 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 14  | M     | 1501 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | b     | 1233 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | a     | 1106 | CLA  | O2A-C1  | 4.76  | 1.59        | 1.46     |
| 14  | H     | 1227 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 14  | A     | 1135 | CLA  | O2A-C1  | 4.76  | 1.59        | 1.46     |
| 14  | G     | 1125 | CLA  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 14  | G     | 1124 | CLA  | C3C-C2C | 4.76  | 1.46        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1217 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 14  | A     | 1127 | CLA  | O2A-C1  | 4.76  | 1.59        | 1.46     |
| 14  | H     | 1021 | CLA  | C3B-C2B | 4.75  | 1.47        | 1.40     |
| 14  | H     | 1223 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 14  | a     | 1122 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 14  | G     | 1135 | CLA  | O2A-C1  | 4.75  | 1.59        | 1.46     |
| 15  | H     | 1207 | F6C  | CHC-C4B | 4.75  | 1.47        | 1.35     |
| 14  | a     | 1013 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 14  | a     | 1127 | CLA  | O2A-C1  | 4.75  | 1.59        | 1.46     |
| 15  | B     | 1207 | F6C  | CHC-C4B | 4.74  | 1.47        | 1.35     |
| 14  | b     | 1205 | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 14  | A     | 1103 | CLA  | C3B-C2B | 4.74  | 1.47        | 1.40     |
| 13  | G     | 1011 | CL0  | C3C-C2C | 4.74  | 1.46        | 1.36     |
| 14  | B     | 1240 | CLA  | C3B-C2B | 4.74  | 1.47        | 1.40     |
| 14  | B     | 1216 | CLA  | C3C-C2C | 4.74  | 1.46        | 1.36     |
| 14  | G     | 1127 | CLA  | O2A-C1  | 4.74  | 1.59        | 1.46     |
| 14  | a     | 1103 | CLA  | C3B-C2B | 4.74  | 1.46        | 1.40     |
| 14  | B     | 1204 | CLA  | CHC-C1C | 4.74  | 1.47        | 1.35     |
| 14  | b     | 1214 | CLA  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 14  | H     | 1205 | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 15  | b     | 1207 | F6C  | CHC-C4B | 4.74  | 1.47        | 1.35     |
| 14  | B     | 1227 | CLA  | CHC-C1C | 4.74  | 1.47        | 1.35     |
| 14  | G     | 1104 | CLA  | C3B-C2B | 4.74  | 1.46        | 1.40     |
| 14  | b     | 1021 | CLA  | C3B-C2B | 4.74  | 1.46        | 1.40     |
| 14  | b     | 1203 | CLA  | CHC-C1C | 4.74  | 1.47        | 1.35     |
| 14  | U     | 1502 | CLA  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 14  | A     | 1124 | CLA  | C3C-C2C | 4.73  | 1.46        | 1.36     |
| 14  | B     | 1021 | CLA  | C3B-C2B | 4.73  | 1.46        | 1.40     |
| 14  | H     | 1204 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 14  | H     | 1222 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 14  | G     | 1103 | CLA  | C3B-C2B | 4.73  | 1.46        | 1.40     |
| 14  | B     | 1205 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 13  | A     | 1011 | CL0  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | H     | 1235 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | B     | 1240 | CLA  | CHD-C1D | 4.73  | 1.47        | 1.38     |
| 14  | H     | 1240 | CLA  | C3B-C2B | 4.73  | 1.46        | 1.40     |
| 14  | A     | 1013 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | A     | 1114 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 14  | B     | 1203 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 14  | H     | 1203 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 13  | a     | 1011 | CL0  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | B     | 1235 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1235 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | B     | 1202 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 14  | H     | 1225 | CLA  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 14  | A     | 1130 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 14  | B     | 1214 | CLA  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 14  | b     | 1227 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | H     | 1023 | CLA  | O2A-C1  | 4.72  | 1.59        | 1.46     |
| 14  | a     | 1103 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | b     | 1023 | CLA  | O2A-C1  | 4.72  | 1.59        | 1.46     |
| 14  | b     | 1240 | CLA  | C3B-C2B | 4.72  | 1.46        | 1.40     |
| 14  | b     | 1223 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 14  | a     | 1114 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | b     | 1205 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | G     | 1130 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 14  | a     | 1124 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 14  | B     | 1225 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | a     | 1127 | CLA  | CHC-C1C | 4.72  | 1.47        | 1.35     |
| 14  | a     | 1137 | CLA  | C3B-C2B | 4.72  | 1.46        | 1.40     |
| 14  | L     | 1502 | CLA  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 14  | H     | 1216 | CLA  | C3C-C2C | 4.71  | 1.46        | 1.36     |
| 14  | B     | 1023 | CLA  | O2A-C1  | 4.71  | 1.59        | 1.46     |
| 14  | G     | 1137 | CLA  | C3B-C2B | 4.71  | 1.46        | 1.40     |
| 14  | G     | 1137 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | B     | 1222 | CLA  | CHC-C1C | 4.71  | 1.47        | 1.35     |
| 14  | G     | 1012 | CLA  | CHC-C1C | 4.71  | 1.47        | 1.35     |
| 15  | b     | 1230 | F6C  | CHD-C1D | 4.71  | 1.47        | 1.35     |
| 14  | H     | 1214 | CLA  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 14  | A     | 1137 | CLA  | C3B-C2B | 4.71  | 1.46        | 1.40     |
| 14  | G     | 1013 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | B     | 1223 | CLA  | C3C-C2C | 4.71  | 1.46        | 1.36     |
| 14  | A     | 1141 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | B     | 1023 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | G     | 1103 | CLA  | CHC-C1C | 4.71  | 1.47        | 1.35     |
| 14  | G     | 1012 | CLA  | O2A-C1  | 4.71  | 1.59        | 1.46     |
| 14  | a     | 1141 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | H     | 1240 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 14  | B     | 1220 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | H     | 1220 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | H     | 1226 | CLA  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 14  | a     | 1137 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | A     | 1103 | CLA  | CHC-C1C | 4.71  | 1.47        | 1.35     |
| 15  | B     | 1230 | F6C  | CHD-C1D | 4.71  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | G     | 1011 | CL0  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 14  | A     | 1104 | CLA  | CHC-C1C | 4.71  | 1.47        | 1.35     |
| 14  | H     | 1023 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 14  | H     | 1224 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 14  | a     | 1117 | CLA  | C3B-C2B | 4.70  | 1.46        | 1.40     |
| 14  | A     | 1137 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 14  | b     | 1204 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | G     | 1138 | CLA  | CHD-C1D | 4.70  | 1.47        | 1.38     |
| 14  | G     | 1140 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | b     | 1202 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 14  | a     | 1138 | CLA  | CHD-C1D | 4.70  | 1.47        | 1.38     |
| 14  | A     | 1012 | CLA  | O2A-C1  | 4.70  | 1.59        | 1.46     |
| 14  | B     | 1224 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 14  | H     | 1202 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 14  | H     | 1204 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 14  | b     | 1225 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 15  | H     | 1230 | F6C  | CHD-C1D | 4.70  | 1.47        | 1.35     |
| 14  | k     | 1401 | CLA  | C3C-C2C | 4.70  | 1.46        | 1.36     |
| 14  | b     | 1220 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 14  | a     | 1114 | CLA  | C3C-C2C | 4.70  | 1.46        | 1.36     |
| 14  | G     | 1104 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | B     | 1226 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 14  | G     | 1114 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | a     | 1012 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | b     | 1222 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | A     | 1140 | CLA  | CHC-C1C | 4.70  | 1.47        | 1.35     |
| 14  | A     | 1114 | CLA  | C3C-C2C | 4.70  | 1.46        | 1.36     |
| 14  | B     | 1212 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 14  | H     | 1212 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 14  | T     | 1401 | CLA  | C3C-C2C | 4.69  | 1.46        | 1.36     |
| 14  | a     | 1130 | CLA  | C3C-C2C | 4.69  | 1.46        | 1.36     |
| 14  | H     | 1226 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 14  | B     | 1205 | CLA  | CHC-C1C | 4.69  | 1.47        | 1.35     |
| 14  | a     | 1012 | CLA  | O2A-C1  | 4.69  | 1.59        | 1.46     |
| 14  | a     | 1140 | CLA  | CHC-C1C | 4.69  | 1.47        | 1.35     |
| 14  | b     | 1224 | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 14  | K     | 1401 | CLA  | C3C-C2C | 4.69  | 1.46        | 1.36     |
| 14  | a     | 1124 | CLA  | C3B-C2B | 4.69  | 1.46        | 1.40     |
| 14  | G     | 1141 | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 14  | A     | 1012 | CLA  | CHC-C1C | 4.69  | 1.47        | 1.35     |
| 14  | b     | 1226 | CLA  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 14  | A     | 1103 | CLA  | C3D-C4D | -4.69 | 1.33        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | l     | 1502 | CLA  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 14  | H     | 1234 | CLA  | C3C-C2C | 4.69  | 1.46        | 1.36     |
| 14  | B     | 1226 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 14  | b     | 1224 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 14  | G     | 1103 | CLA  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 14  | b     | 1023 | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 14  | G     | 1111 | CLA  | C3B-C2B | 4.68  | 1.46        | 1.40     |
| 14  | A     | 1138 | CLA  | CHD-C1D | 4.68  | 1.47        | 1.38     |
| 14  | A     | 1127 | CLA  | CHC-C1C | 4.68  | 1.47        | 1.35     |
| 14  | B     | 1209 | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 14  | b     | 1240 | CLA  | CHD-C1D | 4.68  | 1.47        | 1.38     |
| 14  | b     | 1239 | CLA  | C1D-ND  | -4.68 | 1.32        | 1.37     |
| 14  | B     | 1021 | CLA  | O2A-C1  | 4.68  | 1.59        | 1.46     |
| 14  | H     | 1021 | CLA  | O2A-C1  | 4.68  | 1.59        | 1.46     |
| 14  | H     | 1223 | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 14  | H     | 1205 | CLA  | CHC-C1C | 4.68  | 1.47        | 1.35     |
| 14  | A     | 1117 | CLA  | C3B-C2B | 4.68  | 1.46        | 1.40     |
| 14  | G     | 1105 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 14  | b     | 1212 | CLA  | CHD-C1D | 4.67  | 1.47        | 1.38     |
| 13  | a     | 1011 | CL0  | CHC-C1C | 4.67  | 1.47        | 1.35     |
| 14  | b     | 1209 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | B     | 1224 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | b     | 1021 | CLA  | O2A-C1  | 4.67  | 1.59        | 1.46     |
| 14  | B     | 1234 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 14  | H     | 1209 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | B     | 1212 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | B     | 1204 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 14  | B     | 1220 | CLA  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 14  | A     | 1111 | CLA  | C3B-C2B | 4.67  | 1.46        | 1.40     |
| 14  | b     | 1212 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | A     | 1137 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 14  | a     | 1105 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 14  | a     | 1104 | CLA  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 13  | G     | 1011 | CL0  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 14  | A     | 1105 | CLA  | C3C-C2C | 4.67  | 1.46        | 1.36     |
| 14  | H     | 1228 | CLA  | C3B-C2B | 4.67  | 1.46        | 1.40     |
| 14  | G     | 1135 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 14  | G     | 1127 | CLA  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 14  | l     | 1503 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 14  | G     | 1109 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 14  | b     | 1228 | CLA  | C3B-C2B | 4.66  | 1.46        | 1.40     |
| 14  | b     | 1226 | CLA  | CHD-C1D | 4.66  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1109 | CLA  | C3C-C2C | 4.66  | 1.46        | 1.36     |
| 14  | L     | 1502 | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 14  | A     | 1124 | CLA  | C3B-C2B | 4.66  | 1.46        | 1.40     |
| 14  | G     | 1124 | CLA  | C3B-C2B | 4.66  | 1.46        | 1.40     |
| 14  | b     | 1220 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 14  | b     | 1204 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 14  | a     | 1137 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 14  | b     | 1023 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 15  | b     | 1230 | F6C  | C4A-NA  | -4.66 | 1.32        | 1.37     |
| 14  | L     | 1503 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 14  | A     | 1109 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 14  | H     | 1236 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 14  | H     | 1210 | CLA  | O2A-C1  | 4.65  | 1.59        | 1.46     |
| 13  | A     | 1011 | CL0  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | b     | 1202 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 14  | a     | 1135 | CLA  | O2D-CGD | 4.65  | 1.44        | 1.33     |
| 14  | G     | 1114 | CLA  | C3C-C2C | 4.65  | 1.46        | 1.36     |
| 14  | G     | 1128 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 14  | a     | 1109 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 15  | B     | 1230 | F6C  | C4A-NA  | -4.65 | 1.32        | 1.37     |
| 14  | A     | 1136 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | b     | 1234 | CLA  | C3C-C2C | 4.65  | 1.46        | 1.36     |
| 14  | a     | 1124 | CLA  | O2D-CGD | 4.65  | 1.44        | 1.33     |
| 14  | B     | 1239 | CLA  | C1D-ND  | -4.65 | 1.32        | 1.37     |
| 14  | H     | 1023 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | b     | 1235 | CLA  | C3B-C2B | 4.65  | 1.46        | 1.40     |
| 14  | G     | 1124 | CLA  | O2D-CGD | 4.65  | 1.44        | 1.33     |
| 14  | B     | 1023 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | G     | 1137 | CLA  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 14  | A     | 1124 | CLA  | O2D-CGD | 4.65  | 1.44        | 1.33     |
| 14  | H     | 1239 | CLA  | C1D-ND  | -4.65 | 1.32        | 1.37     |
| 14  | H     | 1220 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | U     | 1503 | CLA  | CHC-C1C | 4.65  | 1.46        | 1.35     |
| 14  | a     | 1111 | CLA  | C3B-C2B | 4.65  | 1.46        | 1.40     |
| 14  | G     | 1129 | CLA  | C3C-C2C | 4.65  | 1.46        | 1.36     |
| 14  | G     | 1136 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | b     | 1206 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | b     | 1210 | CLA  | O2A-C1  | 4.64  | 1.59        | 1.46     |
| 14  | H     | 1212 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | b     | 1236 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 14  | A     | 1135 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | A     | 1135 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1135 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | a     | 1135 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | A     | 1126 | CLA  | C3C-C2C | 4.64  | 1.46        | 1.36     |
| 14  | b     | 1203 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 14  | H     | 1212 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | H     | 1224 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | B     | 1228 | CLA  | C3B-C2B | 4.64  | 1.46        | 1.40     |
| 14  | U     | 1502 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | B     | 1226 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | a     | 1103 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 14  | B     | 1210 | CLA  | O2A-C1  | 4.64  | 1.59        | 1.46     |
| 14  | l     | 1502 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | U     | 1503 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 14  | B     | 1212 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | b     | 1226 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 14  | B     | 1202 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 14  | a     | 1136 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 14  | A     | 1109 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 14  | a     | 1126 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 14  | H     | 1235 | CLA  | C3B-C2B | 4.63  | 1.46        | 1.40     |
| 14  | H     | 1234 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 15  | H     | 1230 | F6C  | C4A-NA  | -4.63 | 1.32        | 1.37     |
| 14  | H     | 1202 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 14  | A     | 1129 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 14  | L     | 1503 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 14  | B     | 1233 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 14  | B     | 1236 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 14  | b     | 1212 | CLA  | CHC-C1C | 4.63  | 1.46        | 1.35     |
| 14  | b     | 1201 | CLA  | O2A-C1  | 4.63  | 1.59        | 1.46     |
| 14  | G     | 1131 | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 14  | b     | 1229 | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 14  | b     | 1224 | CLA  | C3B-C2B | 4.63  | 1.46        | 1.40     |
| 14  | b     | 1234 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 14  | b     | 1233 | CLA  | C3C-C2C | 4.63  | 1.46        | 1.36     |
| 14  | a     | 1130 | CLA  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 14  | H     | 1226 | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 14  | b     | 1233 | CLA  | CHD-C1D | 4.63  | 1.47        | 1.38     |
| 14  | a     | 1122 | CLA  | CHC-C1C | 4.62  | 1.46        | 1.35     |
| 14  | G     | 1109 | CLA  | C3C-C2C | 4.62  | 1.46        | 1.36     |
| 14  | G     | 1126 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | G     | 1110 | CLA  | C3C-C2C | 4.62  | 1.46        | 1.36     |
| 14  | B     | 1201 | CLA  | O2A-C1  | 4.62  | 1.59        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1114 | CLA  | CHD-C1D | 4.62  | 1.47        | 1.38     |
| 14  | H     | 1233 | CLA  | C3C-C2C | 4.62  | 1.46        | 1.36     |
| 14  | H     | 1215 | CLA  | CHC-C1C | 4.62  | 1.46        | 1.35     |
| 14  | G     | 1126 | CLA  | C3C-C2C | 4.62  | 1.46        | 1.36     |
| 14  | A     | 1128 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | G     | 1122 | CLA  | CHC-C1C | 4.62  | 1.46        | 1.35     |
| 14  | b     | 1205 | CLA  | C1D-ND  | -4.62 | 1.32        | 1.37     |
| 14  | a     | 1129 | CLA  | C3C-C2C | 4.62  | 1.46        | 1.36     |
| 14  | G     | 1127 | CLA  | C1D-ND  | -4.62 | 1.32        | 1.37     |
| 14  | b     | 1215 | CLA  | CHC-C1C | 4.62  | 1.46        | 1.35     |
| 14  | B     | 1225 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | H     | 1021 | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 14  | B     | 1234 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | l     | 1501 | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 14  | a     | 1126 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | A     | 1126 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | b     | 1228 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | b     | 1225 | CLA  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 14  | H     | 1228 | CLA  | C3C-C2C | 4.61  | 1.46        | 1.36     |
| 14  | B     | 1235 | CLA  | C3B-C2B | 4.61  | 1.46        | 1.40     |
| 14  | B     | 1203 | CLA  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 14  | H     | 1239 | CLA  | O2A-C1  | 4.61  | 1.59        | 1.46     |
| 14  | A     | 1131 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 14  | b     | 1217 | CLA  | C3B-C2B | 4.61  | 1.46        | 1.40     |
| 14  | H     | 1225 | CLA  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 14  | a     | 1131 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 14  | B     | 1229 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 14  | B     | 1233 | CLA  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 14  | H     | 1233 | CLA  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 14  | H     | 1206 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 14  | A     | 1130 | CLA  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 14  | B     | 1206 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 14  | B     | 1205 | CLA  | C1D-ND  | -4.61 | 1.32        | 1.37     |
| 14  | H     | 1226 | CLA  | CHC-C1C | 4.61  | 1.46        | 1.35     |
| 16  | A     | 2001 | PQN  | C10-C5  | 4.61  | 1.48        | 1.40     |
| 14  | b     | 1240 | CLA  | C3C-C2C | 4.61  | 1.46        | 1.36     |
| 14  | H     | 1201 | CLA  | O2A-C1  | 4.61  | 1.59        | 1.46     |
| 14  | A     | 1127 | CLA  | C1D-ND  | -4.60 | 1.32        | 1.37     |
| 14  | H     | 1224 | CLA  | C3B-C2B | 4.60  | 1.46        | 1.40     |
| 14  | A     | 1129 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | A     | 1130 | CLA  | C3B-C2B | 4.60  | 1.46        | 1.40     |
| 14  | b     | 1226 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1231 | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 14  | H     | 1203 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | a     | 1129 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | B     | 1228 | CLA  | C3C-C2C | 4.60  | 1.46        | 1.36     |
| 14  | l     | 1503 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | B     | 1239 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | A     | 1110 | CLA  | C3C-C2C | 4.60  | 1.46        | 1.36     |
| 14  | a     | 1110 | CLA  | C3C-C2C | 4.60  | 1.46        | 1.36     |
| 14  | B     | 1232 | CLA  | CHD-C1D | 4.60  | 1.47        | 1.38     |
| 14  | B     | 1228 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | b     | 1239 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | H     | 1225 | CLA  | C3C-C2C | 4.60  | 1.46        | 1.36     |
| 14  | A     | 1122 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | H     | 1231 | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 14  | A     | 1138 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | b     | 1227 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | b     | 1228 | CLA  | C3C-C2C | 4.60  | 1.46        | 1.36     |
| 14  | B     | 1215 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | H     | 1239 | CLA  | CHC-C1C | 4.60  | 1.46        | 1.35     |
| 14  | G     | 1130 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | b     | 1232 | CLA  | CHD-C1D | 4.60  | 1.47        | 1.38     |
| 14  | A     | 1114 | CLA  | CHD-C1D | 4.60  | 1.47        | 1.38     |
| 14  | V     | 1501 | CLA  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 14  | b     | 1228 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 14  | H     | 1205 | CLA  | C1D-ND  | -4.59 | 1.32        | 1.37     |
| 14  | H     | 1208 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | b     | 1231 | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 14  | B     | 1222 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | B     | 1227 | CLA  | C3D-C4D | -4.59 | 1.33        | 1.44     |
| 14  | B     | 1239 | CLA  | O2A-C1  | 4.59  | 1.59        | 1.46     |
| 14  | G     | 1117 | CLA  | C3B-C2B | 4.59  | 1.46        | 1.40     |
| 14  | B     | 1226 | CLA  | CHC-C1C | 4.59  | 1.46        | 1.35     |
| 14  | B     | 1224 | CLA  | C3B-C2B | 4.59  | 1.46        | 1.40     |
| 14  | H     | 1228 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 14  | H     | 1232 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 14  | B     | 1208 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | b     | 1203 | CLA  | C3B-C2B | 4.59  | 1.46        | 1.40     |
| 14  | a     | 1128 | CLA  | C3D-C4D | -4.59 | 1.33        | 1.44     |
| 14  | H     | 1240 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | b     | 1222 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | b     | 1239 | CLA  | O2A-C1  | 4.59  | 1.59        | 1.46     |
| 14  | H     | 1235 | CLA  | C3D-C4D | -4.59 | 1.33        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1228 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 14  | H     | 1227 | CLA  | C3D-C4D | -4.59 | 1.33        | 1.44     |
| 14  | B     | 1225 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 14  | G     | 1133 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | a     | 1141 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | B     | 1021 | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 14  | b     | 1225 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | L     | 1501 | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 14  | B     | 1203 | CLA  | C3B-C2B | 4.58  | 1.46        | 1.40     |
| 14  | G     | 1131 | CLA  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 14  | B     | 1240 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | a     | 1130 | CLA  | C3B-C2B | 4.58  | 1.46        | 1.40     |
| 14  | H     | 1214 | CLA  | CHD-C1D | 4.58  | 1.47        | 1.38     |
| 14  | H     | 1236 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 16  | G     | 2001 | PQN  | C10-C5  | 4.58  | 1.48        | 1.40     |
| 14  | H     | 1229 | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 14  | M     | 1501 | CLA  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 14  | G     | 1136 | CLA  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 14  | b     | 1222 | CLA  | O2A-C1  | 4.58  | 1.59        | 1.46     |
| 15  | a     | 1121 | F6C  | CHC-C4B | 4.58  | 1.46        | 1.35     |
| 14  | b     | 1209 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | G     | 1138 | CLA  | CHC-C1C | 4.58  | 1.46        | 1.35     |
| 14  | G     | 1112 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | a     | 1112 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | A     | 1108 | CLA  | C3C-C2C | 4.58  | 1.46        | 1.36     |
| 14  | a     | 1138 | CLA  | CHC-C1C | 4.57  | 1.46        | 1.35     |
| 14  | B     | 1214 | CLA  | CHD-C1D | 4.57  | 1.47        | 1.38     |
| 14  | A     | 1131 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 14  | G     | 1129 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 14  | G     | 1117 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 14  | H     | 1228 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 14  | B     | 1222 | CLA  | O2A-C1  | 4.57  | 1.59        | 1.46     |
| 14  | a     | 1131 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 15  | A     | 1121 | F6C  | CHC-C4B | 4.57  | 1.46        | 1.35     |
| 14  | U     | 1501 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 14  | b     | 1235 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 14  | a     | 1127 | CLA  | C1D-ND  | -4.57 | 1.32        | 1.37     |
| 14  | H     | 1211 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 16  | a     | 2001 | PQN  | C10-C5  | 4.57  | 1.48        | 1.40     |
| 14  | H     | 1222 | CLA  | O2A-C1  | 4.57  | 1.59        | 1.46     |
| 14  | B     | 1217 | CLA  | C3B-C2B | 4.57  | 1.46        | 1.40     |
| 14  | l     | 1503 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1136 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 14  | a     | 1117 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 14  | G     | 1137 | CLA  | CHC-C1C | 4.57  | 1.46        | 1.35     |
| 14  | B     | 1236 | CLA  | C3C-C2C | 4.57  | 1.46        | 1.36     |
| 14  | a     | 1108 | CLA  | C3C-C2C | 4.57  | 1.46        | 1.36     |
| 14  | A     | 1141 | CLA  | C3C-C2C | 4.57  | 1.46        | 1.36     |
| 15  | G     | 1121 | F6C  | CHC-C4B | 4.57  | 1.46        | 1.35     |
| 14  | G     | 1130 | CLA  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 14  | A     | 1112 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | H     | 1223 | CLA  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 14  | A     | 1117 | CLA  | O2D-CGD | 4.56  | 1.44        | 1.33     |
| 14  | B     | 1235 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | b     | 1023 | CLA  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 14  | A     | 1119 | CLA  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 14  | H     | 1203 | CLA  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 14  | B     | 1223 | CLA  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 14  | B     | 1211 | CLA  | O2D-CGD | 4.56  | 1.44        | 1.33     |
| 14  | B     | 1209 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | B     | 1235 | CLA  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 14  | H     | 1209 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | b     | 1021 | CLA  | O2D-CGD | 4.56  | 1.44        | 1.33     |
| 14  | a     | 1101 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | b     | 1235 | CLA  | C3C-C2C | 4.56  | 1.46        | 1.36     |
| 14  | H     | 1222 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | b     | 1236 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | L     | 1503 | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 14  | B     | 1023 | CLA  | C3D-C4D | -4.55 | 1.33        | 1.44     |
| 14  | G     | 1119 | CLA  | C3B-C2B | 4.55  | 1.46        | 1.40     |
| 14  | A     | 1101 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | G     | 1102 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | a     | 1114 | CLA  | CHD-C1D | 4.55  | 1.47        | 1.38     |
| 14  | A     | 1140 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | b     | 1208 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | H     | 1022 | CLA  | C1D-ND  | -4.55 | 1.32        | 1.37     |
| 14  | a     | 1136 | CLA  | C3D-C4D | -4.55 | 1.33        | 1.44     |
| 14  | U     | 1503 | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 14  | G     | 1108 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | b     | 1211 | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 14  | L     | 1503 | CLA  | C3C-C2C | 4.55  | 1.46        | 1.36     |
| 14  | B     | 1022 | CLA  | C1D-ND  | -4.55 | 1.32        | 1.37     |
| 14  | A     | 1102 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | a     | 1102 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1140 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | H     | 1235 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | G     | 1124 | CLA  | C3D-C4D | -4.54 | 1.33        | 1.44     |
| 14  | G     | 1140 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | a     | 1137 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | G     | 1113 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | a     | 1101 | CLA  | C3B-C2B | 4.54  | 1.46        | 1.40     |
| 14  | G     | 1141 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | b     | 1214 | CLA  | CHD-C1D | 4.54  | 1.47        | 1.38     |
| 14  | H     | 1224 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | G     | 1101 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | H     | 1229 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | G     | 1132 | CLA  | C3D-C4D | -4.54 | 1.33        | 1.44     |
| 14  | m     | 1501 | CLA  | C3D-C4D | -4.54 | 1.33        | 1.44     |
| 14  | A     | 1131 | CLA  | CHC-C1C | 4.54  | 1.46        | 1.35     |
| 14  | a     | 1105 | CLA  | C3D-C4D | -4.54 | 1.33        | 1.44     |
| 14  | G     | 1134 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 14  | b     | 1231 | CLA  | C3D-C4D | -4.53 | 1.33        | 1.44     |
| 14  | B     | 1022 | CLA  | O2A-C1  | 4.53  | 1.58        | 1.46     |
| 14  | H     | 1023 | CLA  | C3D-C4D | -4.53 | 1.33        | 1.44     |
| 14  | a     | 1132 | CLA  | C3D-C4D | -4.53 | 1.33        | 1.44     |
| 14  | B     | 1224 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | b     | 1022 | CLA  | O2A-C1  | 4.53  | 1.58        | 1.46     |
| 14  | A     | 1119 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | a     | 1131 | CLA  | CHC-C1C | 4.53  | 1.46        | 1.35     |
| 14  | B     | 1229 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | B     | 1231 | CLA  | C3D-C4D | -4.53 | 1.34        | 1.44     |
| 14  | A     | 1137 | CLA  | CHC-C1C | 4.53  | 1.46        | 1.35     |
| 14  | G     | 1131 | CLA  | CHC-C1C | 4.53  | 1.46        | 1.35     |
| 14  | b     | 1214 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | G     | 1129 | CLA  | O2D-CGD | 4.53  | 1.44        | 1.33     |
| 14  | A     | 1134 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | a     | 1140 | CLA  | C3D-C4D | -4.53 | 1.34        | 1.44     |
| 14  | A     | 1132 | CLA  | C3D-C4D | -4.53 | 1.34        | 1.44     |
| 14  | A     | 1133 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | G     | 1119 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | U     | 1503 | CLA  | C3C-C2C | 4.53  | 1.46        | 1.36     |
| 14  | G     | 1105 | CLA  | C3D-C4D | -4.53 | 1.34        | 1.44     |
| 14  | G     | 1140 | CLA  | C3D-C4D | -4.53 | 1.34        | 1.44     |
| 14  | B     | 1021 | CLA  | CHC-C1C | 4.53  | 1.46        | 1.35     |
| 14  | G     | 1013 | CLA  | C3B-C2B | 4.52  | 1.46        | 1.40     |
| 14  | a     | 1129 | CLA  | O2D-CGD | 4.52  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | a     | 1011 | CL0  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 13  | A     | 1011 | CL0  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | A     | 1140 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | a     | 1012 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | a     | 1134 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | A     | 1105 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | b     | 1223 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | G     | 1132 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | B     | 1225 | CLA  | C1D-ND  | -4.52 | 1.32        | 1.37     |
| 16  | H     | 2002 | PQN  | C10-C5  | 4.52  | 1.48        | 1.40     |
| 14  | A     | 1124 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | A     | 1132 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | l     | 1501 | CLA  | O2A-C1  | 4.52  | 1.58        | 1.46     |
| 14  | B     | 1214 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | H     | 1217 | CLA  | C3B-C2B | 4.52  | 1.46        | 1.40     |
| 14  | A     | 1137 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | a     | 1104 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | l     | 1502 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | H     | 1022 | CLA  | O2A-C1  | 4.52  | 1.58        | 1.46     |
| 14  | U     | 1502 | CLA  | C3C-C2C | 4.52  | 1.46        | 1.36     |
| 14  | B     | 1215 | CLA  | C3B-C2B | 4.52  | 1.46        | 1.40     |
| 14  | G     | 1128 | CLA  | CHC-C1C | 4.52  | 1.46        | 1.35     |
| 14  | b     | 1215 | CLA  | C3B-C2B | 4.52  | 1.46        | 1.40     |
| 14  | G     | 1118 | CLA  | C3D-C4D | -4.52 | 1.34        | 1.44     |
| 14  | A     | 1108 | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 14  | L     | 1501 | CLA  | O2A-C1  | 4.51  | 1.58        | 1.46     |
| 14  | A     | 1128 | CLA  | CHC-C1C | 4.51  | 1.46        | 1.35     |
| 13  | G     | 1011 | CL0  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | a     | 1119 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | a     | 1118 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | b     | 1021 | CLA  | CHC-C1C | 4.51  | 1.46        | 1.35     |
| 14  | a     | 1113 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | b     | 1224 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | B     | 1212 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | H     | 1021 | CLA  | CHC-C1C | 4.51  | 1.46        | 1.35     |
| 14  | a     | 1132 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | G     | 1115 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 16  | B     | 2002 | PQN  | C10-C5  | 4.51  | 1.48        | 1.40     |
| 14  | U     | 1501 | CLA  | O2A-C1  | 4.51  | 1.58        | 1.46     |
| 13  | G     | 1011 | CL0  | C3B-C2B | 4.51  | 1.46        | 1.40     |
| 14  | H     | 1231 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | A     | 1129 | CLA  | O2D-CGD | 4.51  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | l     | 1503 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | A     | 1101 | CLA  | C3B-C2B | 4.51  | 1.46        | 1.40     |
| 14  | b     | 1201 | CLA  | O2D-CGD | 4.51  | 1.44        | 1.33     |
| 14  | a     | 1137 | CLA  | CHC-C1C | 4.51  | 1.46        | 1.35     |
| 14  | a     | 1119 | CLA  | C3B-C2B | 4.51  | 1.46        | 1.40     |
| 14  | a     | 1108 | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 14  | A     | 1113 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 16  | b     | 2002 | PQN  | C10-C5  | 4.51  | 1.48        | 1.40     |
| 14  | G     | 1113 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | b     | 1229 | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 14  | G     | 1108 | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 14  | H     | 1229 | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 14  | a     | 1124 | CLA  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 14  | b     | 1216 | CLA  | CHD-C1D | 4.50  | 1.47        | 1.38     |
| 14  | G     | 1012 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | A     | 1113 | CLA  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 14  | G     | 1137 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | H     | 1214 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | A     | 1012 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | G     | 1106 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | H     | 1212 | CLA  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 14  | a     | 1123 | CLA  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 14  | A     | 1111 | CLA  | O2D-CGD | 4.50  | 1.44        | 1.33     |
| 14  | b     | 1022 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | A     | 1118 | CLA  | C3B-C2B | 4.50  | 1.46        | 1.40     |
| 14  | A     | 1123 | CLA  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 14  | L     | 1502 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | H     | 1202 | CLA  | C3C-C2C | 4.50  | 1.46        | 1.36     |
| 14  | a     | 1133 | CLA  | C3B-C2B | 4.50  | 1.46        | 1.40     |
| 14  | A     | 1104 | CLA  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 13  | A     | 1011 | CL0  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 14  | a     | 1128 | CLA  | CHC-C1C | 4.49  | 1.46        | 1.35     |
| 14  | a     | 1013 | CLA  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 14  | a     | 1103 | CLA  | CHD-C1D | 4.49  | 1.47        | 1.38     |
| 14  | B     | 1229 | CLA  | CHD-C1D | 4.49  | 1.47        | 1.38     |
| 14  | b     | 1212 | CLA  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 14  | a     | 1106 | CLA  | C3C-C2C | 4.49  | 1.46        | 1.36     |
| 14  | A     | 1118 | CLA  | C3D-C4D | -4.49 | 1.34        | 1.44     |
| 14  | B     | 1216 | CLA  | CHD-C1D | 4.49  | 1.47        | 1.38     |
| 14  | G     | 1103 | CLA  | CHD-C1D | 4.49  | 1.47        | 1.38     |
| 14  | H     | 1022 | CLA  | C3C-C2C | 4.49  | 1.46        | 1.36     |
| 14  | G     | 1119 | CLA  | C3D-C4D | -4.49 | 1.34        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1215 | CLA  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 14  | b     | 1232 | CLA  | C3B-C2B | 4.49  | 1.46        | 1.40     |
| 14  | b     | 1022 | CLA  | C1D-ND  | -4.49 | 1.32        | 1.37     |
| 14  | A     | 1103 | CLA  | CHD-C1D | 4.49  | 1.47        | 1.38     |
| 14  | H     | 1222 | CLA  | C3D-C4D | -4.49 | 1.34        | 1.44     |
| 14  | a     | 1111 | CLA  | O2D-CGD | 4.49  | 1.44        | 1.33     |
| 14  | H     | 1206 | CLA  | C3C-C2C | 4.49  | 1.46        | 1.36     |
| 14  | A     | 1013 | CLA  | C3B-C2B | 4.48  | 1.46        | 1.40     |
| 14  | a     | 1133 | CLA  | C3C-C2C | 4.48  | 1.46        | 1.36     |
| 14  | A     | 1106 | CLA  | C3C-C2C | 4.48  | 1.46        | 1.36     |
| 14  | B     | 1201 | CLA  | O2D-CGD | 4.48  | 1.44        | 1.33     |
| 14  | A     | 1115 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | G     | 1111 | CLA  | O2D-CGD | 4.48  | 1.44        | 1.33     |
| 14  | A     | 1113 | CLA  | CHD-C1D | 4.48  | 1.47        | 1.38     |
| 14  | B     | 1212 | CLA  | C3B-C2B | 4.48  | 1.46        | 1.40     |
| 14  | a     | 1113 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | B     | 1202 | CLA  | C3C-C2C | 4.48  | 1.46        | 1.36     |
| 14  | B     | 1206 | CLA  | C3C-C2C | 4.48  | 1.46        | 1.36     |
| 14  | b     | 1208 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | b     | 1232 | CLA  | C3C-C2C | 4.48  | 1.46        | 1.36     |
| 14  | H     | 1215 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | G     | 1123 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | H     | 1201 | CLA  | O2D-CGD | 4.48  | 1.44        | 1.33     |
| 14  | A     | 1119 | CLA  | C3D-C4D | -4.48 | 1.34        | 1.44     |
| 14  | H     | 1225 | CLA  | C1D-ND  | -4.47 | 1.32        | 1.37     |
| 14  | G     | 1104 | CLA  | C3D-C4D | -4.47 | 1.34        | 1.44     |
| 14  | H     | 1232 | CLA  | C3C-C2C | 4.47  | 1.46        | 1.36     |
| 14  | b     | 1232 | CLA  | C3D-C4D | -4.47 | 1.34        | 1.44     |
| 14  | b     | 1212 | CLA  | C3D-C4D | -4.47 | 1.34        | 1.44     |
| 14  | B     | 1022 | CLA  | C3C-C2C | 4.47  | 1.46        | 1.36     |
| 14  | A     | 1128 | CLA  | O2D-CGD | 4.47  | 1.44        | 1.33     |
| 13  | a     | 1011 | CL0  | C3B-C2B | 4.47  | 1.46        | 1.40     |
| 14  | b     | 1206 | CLA  | C3C-C2C | 4.47  | 1.46        | 1.36     |
| 14  | H     | 1206 | CLA  | CHC-C1C | 4.47  | 1.46        | 1.35     |
| 14  | G     | 1101 | CLA  | C3B-C2B | 4.47  | 1.46        | 1.40     |
| 14  | G     | 1128 | CLA  | O2D-CGD | 4.47  | 1.44        | 1.33     |
| 14  | b     | 1225 | CLA  | C1D-ND  | -4.47 | 1.32        | 1.37     |
| 14  | H     | 1232 | CLA  | C3B-C2B | 4.47  | 1.46        | 1.40     |
| 14  | G     | 1101 | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 14  | G     | 1113 | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 14  | b     | 1229 | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 14  | G     | 1133 | CLA  | C3B-C2B | 4.46  | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1133 | CLA  | CHC-C1C | 4.46  | 1.46        | 1.35     |
| 14  | G     | 1139 | CLA  | C3C-C2C | 4.46  | 1.46        | 1.36     |
| 14  | b     | 1023 | CLA  | C3B-C2B | 4.46  | 1.46        | 1.40     |
| 14  | H     | 1216 | CLA  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 14  | A     | 1109 | CLA  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 14  | B     | 1211 | CLA  | C3C-C2C | 4.46  | 1.46        | 1.36     |
| 14  | B     | 1232 | CLA  | C3B-C2B | 4.46  | 1.46        | 1.40     |
| 14  | a     | 1113 | CLA  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 14  | b     | 1201 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | a     | 1109 | CLA  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 14  | A     | 1107 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | B     | 1206 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | A     | 1133 | CLA  | C3B-C2B | 4.46  | 1.46        | 1.40     |
| 15  | B     | 1207 | F6C  | O2D-CGD | 4.46  | 1.44        | 1.33     |
| 14  | b     | 1202 | CLA  | C3C-C2C | 4.46  | 1.46        | 1.36     |
| 15  | B     | 1207 | F6C  | CHD-C1D | 4.46  | 1.46        | 1.35     |
| 14  | a     | 1115 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | b     | 1215 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | a     | 1118 | CLA  | C3B-C2B | 4.46  | 1.46        | 1.40     |
| 15  | b     | 1207 | F6C  | O2D-CGD | 4.46  | 1.44        | 1.33     |
| 14  | B     | 1206 | CLA  | CHC-C1C | 4.46  | 1.46        | 1.35     |
| 14  | B     | 1222 | CLA  | C3D-C4D | -4.46 | 1.34        | 1.44     |
| 14  | a     | 1107 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 14  | B     | 1210 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 14  | G     | 1109 | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |
| 14  | B     | 1232 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | A     | 1125 | CLA  | O2D-CGD | 4.45  | 1.44        | 1.33     |
| 14  | a     | 1107 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | a     | 1128 | CLA  | O2D-CGD | 4.45  | 1.44        | 1.33     |
| 14  | H     | 1206 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 15  | b     | 1207 | F6C  | CHD-C1D | 4.45  | 1.46        | 1.35     |
| 14  | A     | 1139 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | a     | 1119 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 14  | G     | 1118 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | b     | 1211 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | a     | 1101 | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |
| 15  | H     | 1238 | F6C  | CHD-C1D | 4.45  | 1.46        | 1.35     |
| 14  | H     | 1218 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | b     | 1210 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 15  | H     | 1207 | F6C  | O2D-CGD | 4.45  | 1.44        | 1.33     |
| 14  | G     | 1106 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |
| 14  | B     | 1208 | CLA  | C3D-C4D | -4.45 | 1.34        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1116 | CLA  | C3C-C2C | 4.45  | 1.46        | 1.36     |
| 14  | a     | 1105 | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 14  | B     | 1232 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | H     | 1210 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | K     | 1401 | CLA  | C3B-C2B | 4.44  | 1.46        | 1.40     |
| 14  | H     | 1208 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | A     | 1101 | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 14  | B     | 1208 | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 14  | H     | 1229 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | B     | 1215 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | a     | 1131 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | b     | 1206 | CLA  | CHC-C1C | 4.44  | 1.46        | 1.35     |
| 14  | B     | 1023 | CLA  | C3B-C2B | 4.44  | 1.46        | 1.40     |
| 14  | A     | 1131 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | H     | 1232 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 19  | a     | 5001 | LHG  | O8-C23  | 4.44  | 1.46        | 1.33     |
| 14  | b     | 1222 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | b     | 1206 | CLA  | C3D-C4D | -4.44 | 1.34        | 1.44     |
| 14  | a     | 1125 | CLA  | O2D-CGD | 4.44  | 1.44        | 1.33     |
| 14  | H     | 1211 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | A     | 1107 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 15  | H     | 1207 | F6C  | CHD-C1D | 4.44  | 1.46        | 1.35     |
| 14  | G     | 1136 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | G     | 1131 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | a     | 1139 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 14  | a     | 1110 | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 14  | G     | 1125 | CLA  | O2D-CGD | 4.44  | 1.44        | 1.33     |
| 14  | G     | 1117 | CLA  | CHC-C1C | 4.43  | 1.46        | 1.35     |
| 15  | B     | 1238 | F6C  | CHD-C1D | 4.43  | 1.46        | 1.35     |
| 14  | B     | 1218 | CLA  | C3C-C2C | 4.43  | 1.46        | 1.36     |
| 14  | B     | 1229 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | G     | 1118 | CLA  | C3B-C2B | 4.43  | 1.46        | 1.40     |
| 14  | A     | 1117 | CLA  | CHC-C1C | 4.43  | 1.46        | 1.35     |
| 14  | a     | 1117 | CLA  | CHC-C1C | 4.43  | 1.46        | 1.35     |
| 14  | A     | 1136 | CLA  | C3C-C2C | 4.43  | 1.46        | 1.36     |
| 14  | T     | 1401 | CLA  | C3B-C2B | 4.43  | 1.46        | 1.40     |
| 14  | G     | 1107 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | A     | 1133 | CLA  | CHC-C1C | 4.43  | 1.46        | 1.35     |
| 14  | a     | 1129 | CLA  | C3B-C2B | 4.43  | 1.46        | 1.40     |
| 14  | A     | 1106 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | G     | 1107 | CLA  | C3C-C2C | 4.43  | 1.46        | 1.36     |
| 14  | k     | 1401 | CLA  | C3B-C2B | 4.43  | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1201 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | H     | 1023 | CLA  | C3B-C2B | 4.43  | 1.46        | 1.40     |
| 14  | H     | 1021 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | B     | 1201 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | B     | 1213 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 14  | G     | 1108 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | A     | 1105 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 14  | b     | 1227 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | A     | 1135 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 15  | b     | 1238 | F6C  | CHD-C1D | 4.42  | 1.46        | 1.35     |
| 14  | b     | 1218 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | b     | 1218 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | H     | 1231 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | b     | 1231 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | b     | 1021 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | a     | 1102 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 14  | b     | 1229 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | a     | 1106 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | b     | 1240 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | H     | 1212 | CLA  | C3B-C2B | 4.42  | 1.46        | 1.40     |
| 14  | H     | 1213 | CLA  | C3D-C4D | -4.42 | 1.34        | 1.44     |
| 14  | A     | 1116 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | B     | 1227 | CLA  | C3C-C2C | 4.42  | 1.46        | 1.36     |
| 14  | G     | 1102 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 14  | a     | 1130 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 19  | A     | 5001 | LHG  | O8-C23  | 4.42  | 1.46        | 1.33     |
| 14  | A     | 1111 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | B     | 1218 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | b     | 1213 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | H     | 1240 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | G     | 1112 | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 14  | G     | 1133 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | A     | 1129 | CLA  | C3B-C2B | 4.41  | 1.46        | 1.40     |
| 14  | H     | 1208 | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 14  | a     | 1111 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | G     | 1133 | CLA  | CHC-C1C | 4.41  | 1.46        | 1.35     |
| 14  | G     | 1135 | CLA  | CHD-C1D | 4.41  | 1.46        | 1.38     |
| 14  | A     | 1108 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | G     | 1132 | CLA  | O2D-CGD | 4.41  | 1.44        | 1.33     |
| 14  | H     | 1227 | CLA  | C3C-C2C | 4.41  | 1.46        | 1.36     |
| 14  | G     | 1129 | CLA  | C3B-C2B | 4.41  | 1.46        | 1.40     |
| 14  | G     | 1135 | CLA  | C3C-C2C | 4.41  | 1.46        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1105 | CLA  | CHD-C1D | 4.41  | 1.46        | 1.38     |
| 19  | G     | 5001 | LHG  | O8-C23  | 4.41  | 1.46        | 1.33     |
| 14  | A     | 1122 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | a     | 1122 | CLA  | C3D-C4D | -4.41 | 1.34        | 1.44     |
| 14  | a     | 1136 | CLA  | C3C-C2C | 4.41  | 1.46        | 1.36     |
| 14  | A     | 1118 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | b     | 1208 | CLA  | CHD-C1D | 4.40  | 1.46        | 1.38     |
| 14  | a     | 1116 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | A     | 1112 | CLA  | CHD-C1D | 4.40  | 1.46        | 1.38     |
| 14  | G     | 1111 | CLA  | C3D-C4D | -4.40 | 1.34        | 1.44     |
| 14  | a     | 1118 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | B     | 1021 | CLA  | C3D-C4D | -4.40 | 1.34        | 1.44     |
| 14  | A     | 1102 | CLA  | CHD-C1D | 4.40  | 1.46        | 1.38     |
| 14  | A     | 1110 | CLA  | CHD-C1D | 4.40  | 1.46        | 1.38     |
| 14  | B     | 1231 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | L     | 1501 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | H     | 1206 | CLA  | C1D-ND  | -4.40 | 1.32        | 1.37     |
| 14  | b     | 1217 | CLA  | C3C-C2C | 4.40  | 1.46        | 1.36     |
| 14  | a     | 1114 | CLA  | C3D-C4D | -4.40 | 1.34        | 1.44     |
| 14  | a     | 1132 | CLA  | O2D-CGD | 4.40  | 1.43        | 1.33     |
| 14  | A     | 1132 | CLA  | O2D-CGD | 4.39  | 1.43        | 1.33     |
| 14  | G     | 1139 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 14  | B     | 1231 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 14  | b     | 1023 | CLA  | C1C-NC  | -4.39 | 1.31        | 1.37     |
| 14  | a     | 1116 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | G     | 1122 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | A     | 1116 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | A     | 1139 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 14  | U     | 1501 | CLA  | C3C-C2C | 4.39  | 1.46        | 1.36     |
| 14  | A     | 1117 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | A     | 1133 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | a     | 1135 | CLA  | C3C-C2C | 4.39  | 1.46        | 1.36     |
| 14  | G     | 1110 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 14  | G     | 1114 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | A     | 1114 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 14  | a     | 1117 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | b     | 1211 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | B     | 1212 | CLA  | C3C-C2C | 4.38  | 1.46        | 1.36     |
| 14  | B     | 1217 | CLA  | C3C-C2C | 4.38  | 1.46        | 1.36     |
| 14  | H     | 1218 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | H     | 1210 | CLA  | O2D-CGD | 4.38  | 1.43        | 1.33     |
| 14  | a     | 1138 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1240 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | A     | 1135 | CLA  | C3C-C2C | 4.38  | 1.46        | 1.36     |
| 14  | H     | 1209 | CLA  | CHD-C1D | 4.38  | 1.46        | 1.38     |
| 14  | b     | 1209 | CLA  | CHD-C1D | 4.38  | 1.46        | 1.38     |
| 14  | a     | 1108 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | B     | 1211 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | G     | 1126 | CLA  | CHD-C1D | 4.38  | 1.46        | 1.38     |
| 14  | a     | 1139 | CLA  | CHD-C1D | 4.38  | 1.46        | 1.38     |
| 14  | G     | 1112 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | a     | 1112 | CLA  | CHD-C1D | 4.38  | 1.46        | 1.38     |
| 14  | b     | 1212 | CLA  | C3C-C2C | 4.38  | 1.46        | 1.36     |
| 14  | a     | 1109 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | B     | 1209 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | B     | 1216 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | A     | 1110 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | H     | 1022 | CLA  | C3D-C4D | -4.38 | 1.34        | 1.44     |
| 14  | l     | 1501 | CLA  | C3C-C2C | 4.37  | 1.46        | 1.36     |
| 14  | H     | 1220 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | B     | 1206 | CLA  | C1D-ND  | -4.37 | 1.32        | 1.37     |
| 14  | a     | 1135 | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 14  | B     | 1209 | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 14  | a     | 1126 | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 14  | b     | 1220 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | H     | 1231 | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 14  | H     | 1212 | CLA  | C3C-C2C | 4.37  | 1.46        | 1.36     |
| 14  | B     | 1022 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | A     | 1138 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | H     | 1211 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 15  | G     | 1121 | F6C  | C4A-NA  | -4.37 | 1.32        | 1.37     |
| 14  | M     | 1501 | CLA  | C3C-C2C | 4.37  | 1.46        | 1.36     |
| 14  | A     | 1130 | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 14  | A     | 1112 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 15  | H     | 1219 | F6C  | C4A-NA  | -4.37 | 1.32        | 1.37     |
| 14  | B     | 1023 | CLA  | C1C-NC  | -4.37 | 1.31        | 1.37     |
| 14  | G     | 1110 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | G     | 1116 | CLA  | C3D-C4D | -4.37 | 1.34        | 1.44     |
| 14  | B     | 1210 | CLA  | O2D-CGD | 4.36  | 1.43        | 1.33     |
| 14  | b     | 1220 | CLA  | C3C-C2C | 4.36  | 1.46        | 1.36     |
| 14  | H     | 1209 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | a     | 1112 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | G     | 1120 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | b     | 1216 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1220 | CLA  | C3C-C2C | 4.36  | 1.46        | 1.36     |
| 14  | b     | 1231 | CLA  | CHD-C1D | 4.36  | 1.46        | 1.38     |
| 14  | a     | 1102 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | a     | 1110 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | a     | 1133 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | H     | 1217 | CLA  | C3C-C2C | 4.36  | 1.46        | 1.36     |
| 14  | B     | 1220 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | G     | 1130 | CLA  | CHD-C1D | 4.36  | 1.46        | 1.38     |
| 14  | b     | 1209 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | H     | 1221 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | a     | 1134 | CLA  | C3D-C4D | -4.36 | 1.34        | 1.44     |
| 14  | m     | 1501 | CLA  | C3C-C2C | 4.36  | 1.46        | 1.36     |
| 14  | b     | 1022 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | G     | 1127 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | G     | 1138 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | G     | 1117 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | b     | 1221 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | B     | 1221 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |
| 14  | a     | 1131 | CLA  | CHD-C1D | 4.35  | 1.46        | 1.38     |
| 14  | H     | 1220 | CLA  | C3C-C2C | 4.35  | 1.46        | 1.36     |
| 14  | A     | 1117 | CLA  | CHD-C1D | 4.35  | 1.46        | 1.38     |
| 14  | G     | 1134 | CLA  | O2D-CGD | 4.35  | 1.43        | 1.33     |
| 14  | A     | 1126 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | a     | 1117 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | H     | 1204 | CLA  | C3B-C2B | 4.34  | 1.46        | 1.40     |
| 14  | B     | 1201 | CLA  | C3C-C2C | 4.34  | 1.46        | 1.36     |
| 15  | A     | 1121 | F6C  | C4A-NA  | -4.34 | 1.32        | 1.37     |
| 14  | H     | 1205 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | B     | 1204 | CLA  | C3B-C2B | 4.34  | 1.46        | 1.40     |
| 14  | H     | 1216 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | G     | 1136 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | G     | 1117 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | G     | 1131 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | b     | 1206 | CLA  | C1D-ND  | -4.34 | 1.32        | 1.37     |
| 14  | A     | 1109 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | A     | 1134 | CLA  | O2D-CGD | 4.34  | 1.43        | 1.33     |
| 14  | V     | 1501 | CLA  | C3C-C2C | 4.34  | 1.45        | 1.36     |
| 14  | A     | 1102 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | A     | 1127 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | A     | 1120 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | G     | 1109 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | H     | 1023 | CLA  | C1C-NC  | -4.34 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1134 | CLA  | C3D-C4D | -4.34 | 1.34        | 1.44     |
| 14  | A     | 1131 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 14  | a     | 1120 | CLA  | C3D-C4D | -4.33 | 1.34        | 1.44     |
| 15  | a     | 1121 | F6C  | C4A-NA  | -4.33 | 1.32        | 1.37     |
| 14  | A     | 1101 | CLA  | C3D-C4D | -4.33 | 1.34        | 1.44     |
| 14  | b     | 1210 | CLA  | O2D-CGD | 4.33  | 1.43        | 1.33     |
| 14  | a     | 1101 | CLA  | C3D-C4D | -4.33 | 1.34        | 1.44     |
| 14  | H     | 1201 | CLA  | C3C-C2C | 4.33  | 1.45        | 1.36     |
| 14  | b     | 1220 | CLA  | CHD-C1D | 4.33  | 1.46        | 1.38     |
| 14  | a     | 1128 | CLA  | C1D-ND  | -4.33 | 1.32        | 1.37     |
| 20  | H     | 5002 | LMG  | O8-C28  | 4.33  | 1.46        | 1.33     |
| 14  | a     | 1127 | CLA  | C3D-C4D | -4.33 | 1.34        | 1.44     |
| 14  | H     | 1220 | CLA  | CHD-C1D | 4.33  | 1.46        | 1.38     |
| 14  | G     | 1128 | CLA  | CHD-C1D | 4.33  | 1.46        | 1.38     |
| 14  | b     | 1215 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 14  | b     | 1201 | CLA  | C3C-C2C | 4.32  | 1.45        | 1.36     |
| 15  | B     | 1219 | F6C  | C4A-NA  | -4.32 | 1.32        | 1.37     |
| 14  | G     | 1134 | CLA  | C3D-C4D | -4.32 | 1.34        | 1.44     |
| 14  | B     | 1210 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 14  | B     | 1205 | CLA  | C3D-C4D | -4.32 | 1.34        | 1.44     |
| 14  | B     | 1220 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 14  | H     | 1210 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 20  | B     | 5002 | LMG  | O8-C28  | 4.32  | 1.46        | 1.33     |
| 14  | G     | 1126 | CLA  | C3B-C2B | 4.32  | 1.46        | 1.40     |
| 14  | H     | 1221 | CLA  | C3C-C2C | 4.32  | 1.45        | 1.36     |
| 14  | a     | 1128 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 14  | a     | 1134 | CLA  | O2D-CGD | 4.32  | 1.43        | 1.33     |
| 14  | G     | 1101 | CLA  | C3D-C4D | -4.32 | 1.34        | 1.44     |
| 14  | a     | 1116 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | b     | 1205 | CLA  | C3D-C4D | -4.31 | 1.34        | 1.44     |
| 14  | B     | 1215 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 20  | b     | 5002 | LMG  | O8-C28  | 4.31  | 1.45        | 1.33     |
| 14  | A     | 1136 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | H     | 1022 | CLA  | C3B-C2B | 4.31  | 1.46        | 1.40     |
| 14  | m     | 1501 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | B     | 1221 | CLA  | C3C-C2C | 4.31  | 1.45        | 1.36     |
| 14  | A     | 1116 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | a     | 1136 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | M     | 1501 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 14  | a     | 1113 | CLA  | C3B-C2B | 4.30  | 1.46        | 1.40     |
| 14  | V     | 1501 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 14  | G     | 1102 | CLA  | C3D-C4D | -4.30 | 1.34        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1203 | CLA  | C3C-C2C | 4.30  | 1.45        | 1.36     |
| 14  | G     | 1128 | CLA  | C1D-ND  | -4.30 | 1.32        | 1.37     |
| 14  | A     | 1141 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 14  | A     | 1113 | CLA  | C3B-C2B | 4.30  | 1.46        | 1.40     |
| 14  | K     | 1401 | CLA  | C3D-C4D | -4.30 | 1.34        | 1.44     |
| 14  | b     | 1221 | CLA  | C3C-C2C | 4.30  | 1.45        | 1.36     |
| 14  | G     | 1125 | CLA  | C3C-C2C | 4.30  | 1.45        | 1.36     |
| 14  | b     | 1204 | CLA  | C3B-C2B | 4.30  | 1.46        | 1.40     |
| 20  | I     | 5006 | LMG  | O8-C28  | 4.29  | 1.45        | 1.33     |
| 14  | G     | 1113 | CLA  | C3B-C2B | 4.29  | 1.46        | 1.40     |
| 14  | A     | 1119 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | H     | 1224 | CLA  | C1D-ND  | -4.29 | 1.32        | 1.37     |
| 20  | R     | 5006 | LMG  | O8-C28  | 4.29  | 1.45        | 1.33     |
| 14  | H     | 1203 | CLA  | C3C-C2C | 4.29  | 1.45        | 1.36     |
| 14  | a     | 1119 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | H     | 1217 | CLA  | C3D-C4D | -4.29 | 1.34        | 1.44     |
| 14  | b     | 1233 | CLA  | C3D-C4D | -4.29 | 1.34        | 1.44     |
| 14  | a     | 1115 | CLA  | C3C-C2C | 4.29  | 1.45        | 1.36     |
| 14  | G     | 1119 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | b     | 1210 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | A     | 1125 | CLA  | C3C-C2C | 4.29  | 1.45        | 1.36     |
| 14  | A     | 1128 | CLA  | C1D-ND  | -4.29 | 1.32        | 1.37     |
| 14  | B     | 1203 | CLA  | C3C-C2C | 4.29  | 1.45        | 1.36     |
| 14  | A     | 1128 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | k     | 1401 | CLA  | C3D-C4D | -4.29 | 1.34        | 1.44     |
| 14  | H     | 1217 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 14  | G     | 1141 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 15  | b     | 1238 | F6C  | C3D-C4D | -4.28 | 1.33        | 1.43     |
| 14  | A     | 1141 | CLA  | C3B-C2B | 4.28  | 1.46        | 1.40     |
| 14  | G     | 1012 | CLA  | O2D-CGD | 4.28  | 1.43        | 1.33     |
| 20  | i     | 5006 | LMG  | O8-C28  | 4.28  | 1.45        | 1.33     |
| 14  | a     | 1012 | CLA  | O2D-CGD | 4.28  | 1.43        | 1.33     |
| 14  | B     | 1233 | CLA  | C3D-C4D | -4.28 | 1.34        | 1.44     |
| 14  | L     | 1503 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 14  | G     | 1116 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 14  | T     | 1401 | CLA  | C3D-C4D | -4.28 | 1.34        | 1.44     |
| 14  | B     | 1204 | CLA  | C1D-ND  | -4.28 | 1.32        | 1.37     |
| 14  | A     | 1012 | CLA  | O2D-CGD | 4.28  | 1.43        | 1.33     |
| 14  | a     | 1133 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 14  | a     | 1141 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 14  | b     | 1217 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 15  | B     | 1238 | F6C  | C3D-C4D | -4.28 | 1.33        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1239 | CLA  | C3D-C4D | -4.28 | 1.34        | 1.44     |
| 14  | l     | 1503 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 14  | H     | 1239 | CLA  | C3D-C4D | -4.27 | 1.34        | 1.44     |
| 14  | b     | 1217 | CLA  | C3D-C4D | -4.27 | 1.34        | 1.44     |
| 14  | b     | 1239 | CLA  | C3D-C4D | -4.27 | 1.34        | 1.44     |
| 14  | H     | 1233 | CLA  | C3D-C4D | -4.27 | 1.34        | 1.44     |
| 14  | A     | 1115 | CLA  | C3C-C2C | 4.27  | 1.45        | 1.36     |
| 14  | U     | 1503 | CLA  | C3B-C2B | 4.27  | 1.46        | 1.40     |
| 14  | a     | 1134 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 14  | b     | 1224 | CLA  | C1D-ND  | -4.27 | 1.32        | 1.37     |
| 14  | B     | 1217 | CLA  | C3D-C4D | -4.27 | 1.34        | 1.44     |
| 14  | a     | 1125 | CLA  | C3C-C2C | 4.27  | 1.45        | 1.36     |
| 14  | a     | 1127 | CLA  | C3C-C2C | 4.27  | 1.45        | 1.36     |
| 14  | H     | 1215 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | B     | 1217 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | b     | 1239 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | b     | 1213 | CLA  | C3C-C2C | 4.26  | 1.45        | 1.36     |
| 14  | A     | 1126 | CLA  | C3B-C2B | 4.26  | 1.46        | 1.40     |
| 14  | a     | 1132 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | G     | 1106 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | B     | 1224 | CLA  | C1D-ND  | -4.26 | 1.32        | 1.37     |
| 14  | U     | 1503 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 14  | G     | 1115 | CLA  | C3C-C2C | 4.26  | 1.45        | 1.36     |
| 15  | b     | 1219 | F6C  | C4A-NA  | -4.26 | 1.32        | 1.37     |
| 14  | A     | 1139 | CLA  | C3B-C2B | 4.26  | 1.46        | 1.40     |
| 15  | H     | 1238 | F6C  | C3D-C4D | -4.26 | 1.33        | 1.43     |
| 14  | a     | 1139 | CLA  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 14  | G     | 1132 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 14  | a     | 1126 | CLA  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 14  | G     | 1013 | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 14  | B     | 1022 | CLA  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 14  | B     | 1213 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 14  | A     | 1103 | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 14  | G     | 1133 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 14  | A     | 1134 | CLA  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 14  | a     | 1134 | CLA  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 14  | a     | 1012 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 20  | G     | 5003 | LMG  | O7-C10  | 4.25  | 1.46        | 1.34     |
| 14  | A     | 1127 | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 20  | A     | 5003 | LMG  | O7-C10  | 4.25  | 1.46        | 1.34     |
| 14  | b     | 1204 | CLA  | C1D-ND  | -4.25 | 1.32        | 1.37     |
| 14  | H     | 1213 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1213 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 14  | A     | 1134 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 14  | A     | 1013 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | b     | 1022 | CLA  | C3B-C2B | 4.24  | 1.46        | 1.40     |
| 14  | b     | 1201 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 14  | a     | 1013 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | G     | 1134 | CLA  | C3B-C2B | 4.24  | 1.46        | 1.40     |
| 14  | A     | 1012 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 14  | A     | 1133 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 14  | G     | 1140 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 14  | B     | 1204 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | a     | 1103 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 20  | a     | 5003 | LMG  | O7-C10  | 4.24  | 1.46        | 1.34     |
| 14  | A     | 1013 | CLA  | C3D-C4D | -4.24 | 1.34        | 1.44     |
| 14  | a     | 1139 | CLA  | C3D-C4D | -4.24 | 1.34        | 1.44     |
| 14  | G     | 1120 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | A     | 1106 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 14  | H     | 1213 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | B     | 1239 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | a     | 1141 | CLA  | C3B-C2B | 4.23  | 1.46        | 1.40     |
| 14  | G     | 1013 | CLA  | C3D-C4D | -4.23 | 1.34        | 1.44     |
| 20  | A     | 5003 | LMG  | O8-C28  | 4.23  | 1.45        | 1.33     |
| 14  | H     | 1204 | CLA  | C1D-ND  | -4.23 | 1.32        | 1.37     |
| 20  | a     | 5003 | LMG  | O8-C28  | 4.23  | 1.45        | 1.33     |
| 14  | L     | 1503 | CLA  | C3B-C2B | 4.23  | 1.46        | 1.40     |
| 14  | B     | 1201 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | G     | 1134 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 19  | a     | 5001 | LHG  | O7-C7   | 4.23  | 1.46        | 1.34     |
| 14  | H     | 1201 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | a     | 1109 | CLA  | C3B-C2B | 4.23  | 1.46        | 1.40     |
| 14  | b     | 1023 | CLA  | C1D-ND  | -4.23 | 1.32        | 1.37     |
| 14  | A     | 1120 | CLA  | C3C-C2C | 4.23  | 1.45        | 1.36     |
| 14  | a     | 1106 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | A     | 1140 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | A     | 1132 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | a     | 1140 | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 14  | B     | 1213 | CLA  | C3C-C2C | 4.23  | 1.45        | 1.36     |
| 14  | G     | 1115 | CLA  | CHD-C1D | 4.22  | 1.46        | 1.38     |
| 14  | G     | 1139 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | A     | 1116 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | G     | 1141 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | G     | 1127 | CLA  | C3C-C2C | 4.22  | 1.45        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | L     | 1501 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | U     | 1501 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | a     | 1013 | CLA  | C3D-C4D | -4.22 | 1.34        | 1.44     |
| 14  | G     | 1109 | CLA  | C3B-C2B | 4.22  | 1.46        | 1.40     |
| 14  | a     | 1115 | CLA  | CHD-C1D | 4.22  | 1.46        | 1.38     |
| 14  | A     | 1139 | CLA  | C3D-C4D | -4.22 | 1.34        | 1.44     |
| 14  | a     | 1116 | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | G     | 1103 | CLA  | C3C-C2C | 4.21  | 1.45        | 1.36     |
| 14  | G     | 1012 | CLA  | CHD-C1D | 4.21  | 1.46        | 1.38     |
| 14  | a     | 1122 | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | A     | 1115 | CLA  | CHD-C1D | 4.21  | 1.46        | 1.38     |
| 20  | G     | 5003 | LMG  | O8-C28  | 4.21  | 1.45        | 1.33     |
| 14  | H     | 1239 | CLA  | CHD-C1D | 4.21  | 1.46        | 1.38     |
| 14  | H     | 1204 | CLA  | C3C-C2C | 4.21  | 1.45        | 1.36     |
| 14  | a     | 1123 | CLA  | C3C-C2C | 4.21  | 1.45        | 1.36     |
| 14  | B     | 1022 | CLA  | O2D-CGD | 4.21  | 1.43        | 1.33     |
| 14  | a     | 1138 | CLA  | C3C-C2C | 4.21  | 1.45        | 1.36     |
| 19  | A     | 5001 | LHG  | O7-C7   | 4.21  | 1.46        | 1.34     |
| 14  | H     | 1235 | CLA  | CHD-C1D | 4.21  | 1.46        | 1.38     |
| 14  | B     | 1023 | CLA  | C1D-ND  | -4.21 | 1.32        | 1.37     |
| 14  | a     | 1140 | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | B     | 1227 | CLA  | CHD-C1D | 4.20  | 1.46        | 1.38     |
| 14  | A     | 1123 | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |
| 14  | a     | 1120 | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |
| 14  | G     | 1116 | CLA  | C3B-C2B | 4.20  | 1.46        | 1.40     |
| 14  | G     | 1139 | CLA  | C3D-C4D | -4.20 | 1.34        | 1.44     |
| 14  | l     | 1503 | CLA  | C3B-C2B | 4.20  | 1.46        | 1.40     |
| 14  | B     | 1235 | CLA  | CHD-C1D | 4.20  | 1.46        | 1.38     |
| 14  | b     | 1204 | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |
| 14  | A     | 1109 | CLA  | C3B-C2B | 4.20  | 1.46        | 1.40     |
| 14  | H     | 1023 | CLA  | C1D-ND  | -4.20 | 1.32        | 1.37     |
| 14  | l     | 1501 | CLA  | C3B-C2B | 4.20  | 1.46        | 1.40     |
| 14  | G     | 1138 | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |
| 14  | H     | 1227 | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 14  | G     | 1123 | CLA  | C3C-C2C | 4.19  | 1.45        | 1.36     |
| 19  | G     | 5001 | LHG  | O7-C7   | 4.19  | 1.46        | 1.34     |
| 14  | B     | 1205 | CLA  | C3C-C2C | 4.19  | 1.45        | 1.36     |
| 14  | A     | 1138 | CLA  | C3C-C2C | 4.19  | 1.45        | 1.36     |
| 14  | H     | 1022 | CLA  | O2D-CGD | 4.19  | 1.43        | 1.33     |
| 14  | a     | 1117 | CLA  | C3C-C2C | 4.19  | 1.45        | 1.36     |
| 14  | H     | 1205 | CLA  | C3C-C2C | 4.18  | 1.45        | 1.36     |
| 14  | b     | 1022 | CLA  | O2D-CGD | 4.18  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1234 | CLA  | C3B-C2B | 4.17  | 1.46        | 1.40     |
| 14  | A     | 1122 | CLA  | CHD-C1D | 4.17  | 1.46        | 1.38     |
| 14  | b     | 1234 | CLA  | C3B-C2B | 4.17  | 1.46        | 1.40     |
| 14  | A     | 1141 | CLA  | C3D-C4D | -4.17 | 1.34        | 1.44     |
| 14  | a     | 1130 | CLA  | C1D-ND  | -4.17 | 1.32        | 1.37     |
| 14  | A     | 1122 | CLA  | C3B-C2B | 4.17  | 1.46        | 1.40     |
| 14  | G     | 1122 | CLA  | CHD-C1D | 4.17  | 1.46        | 1.38     |
| 14  | A     | 1117 | CLA  | C3C-C2C | 4.17  | 1.45        | 1.36     |
| 14  | G     | 1117 | CLA  | C3C-C2C | 4.17  | 1.45        | 1.36     |
| 14  | H     | 1215 | CLA  | C3C-C2C | 4.16  | 1.45        | 1.36     |
| 14  | a     | 1141 | CLA  | C3D-C4D | -4.16 | 1.34        | 1.44     |
| 14  | A     | 1138 | CLA  | CHD-C4C | 4.16  | 1.48        | 1.39     |
| 14  | A     | 1140 | CLA  | C3B-C2B | 4.16  | 1.46        | 1.40     |
| 14  | B     | 1225 | CLA  | CHD-C1D | 4.16  | 1.46        | 1.38     |
| 14  | G     | 1138 | CLA  | CHD-C4C | 4.16  | 1.48        | 1.39     |
| 14  | b     | 1227 | CLA  | CHD-C1D | 4.16  | 1.46        | 1.38     |
| 14  | b     | 1235 | CLA  | CHD-C1D | 4.16  | 1.46        | 1.38     |
| 14  | G     | 1104 | CLA  | C3C-C2C | 4.16  | 1.45        | 1.36     |
| 14  | G     | 1140 | CLA  | C3B-C2B | 4.16  | 1.46        | 1.40     |
| 15  | H     | 1237 | F6C  | CHD-C1D | 4.16  | 1.45        | 1.35     |
| 14  | H     | 1234 | CLA  | C3B-C2B | 4.16  | 1.46        | 1.40     |
| 14  | G     | 1141 | CLA  | C3D-C4D | -4.16 | 1.34        | 1.44     |
| 19  | l     | 5101 | LHG  | O8-C23  | 4.15  | 1.45        | 1.33     |
| 14  | H     | 1021 | CLA  | C3C-C2C | 4.15  | 1.45        | 1.36     |
| 14  | b     | 1226 | CLA  | C1D-ND  | -4.15 | 1.32        | 1.37     |
| 14  | a     | 1138 | CLA  | CHD-C4C | 4.15  | 1.48        | 1.39     |
| 14  | b     | 1205 | CLA  | C3C-C2C | 4.15  | 1.45        | 1.36     |
| 14  | b     | 1021 | CLA  | C3C-C2C | 4.15  | 1.45        | 1.36     |
| 14  | a     | 1122 | CLA  | CHD-C1D | 4.14  | 1.46        | 1.38     |
| 14  | H     | 1023 | CLA  | C3C-C2C | 4.14  | 1.45        | 1.36     |
| 15  | B     | 1237 | F6C  | CHD-C1D | 4.14  | 1.45        | 1.35     |
| 14  | a     | 1104 | CLA  | C3C-C2C | 4.14  | 1.45        | 1.36     |
| 14  | b     | 1225 | CLA  | CHD-C1D | 4.14  | 1.46        | 1.38     |
| 14  | H     | 1240 | CLA  | CHD-C4C | 4.14  | 1.48        | 1.39     |
| 14  | B     | 1023 | CLA  | C3C-C2C | 4.14  | 1.45        | 1.36     |
| 14  | B     | 1215 | CLA  | C3C-C2C | 4.13  | 1.45        | 1.36     |
| 14  | G     | 1137 | CLA  | C1D-ND  | -4.13 | 1.32        | 1.37     |
| 14  | B     | 1021 | CLA  | C3C-C2C | 4.13  | 1.45        | 1.36     |
| 19  | L     | 5101 | LHG  | O8-C23  | 4.13  | 1.45        | 1.33     |
| 14  | A     | 1130 | CLA  | C1D-ND  | -4.13 | 1.32        | 1.37     |
| 14  | H     | 1225 | CLA  | CHD-C1D | 4.13  | 1.46        | 1.38     |
| 14  | A     | 1104 | CLA  | C3C-C2C | 4.13  | 1.45        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1103 | CLA  | CHD-C4C | 4.13  | 1.48        | 1.39     |
| 14  | b     | 1240 | CLA  | CHD-C4C | 4.12  | 1.48        | 1.39     |
| 14  | a     | 1111 | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 14  | G     | 1130 | CLA  | C1D-ND  | -4.12 | 1.32        | 1.37     |
| 14  | b     | 1215 | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 14  | b     | 1222 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 14  | b     | 1023 | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 15  | b     | 1237 | F6C  | CHD-C1D | 4.12  | 1.45        | 1.35     |
| 14  | U     | 1502 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 14  | B     | 1240 | CLA  | CHD-C4C | 4.12  | 1.48        | 1.39     |
| 19  | U     | 5101 | LHG  | O8-C23  | 4.11  | 1.45        | 1.33     |
| 14  | G     | 1111 | CLA  | C3C-C2C | 4.11  | 1.45        | 1.36     |
| 14  | A     | 1111 | CLA  | C3C-C2C | 4.11  | 1.45        | 1.36     |
| 14  | a     | 1107 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 14  | B     | 1236 | CLA  | C3B-C2B | 4.11  | 1.46        | 1.40     |
| 14  | A     | 1137 | CLA  | C1D-ND  | -4.11 | 1.32        | 1.37     |
| 14  | L     | 1502 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 14  | G     | 1122 | CLA  | C3B-C2B | 4.11  | 1.46        | 1.40     |
| 14  | G     | 1103 | CLA  | CHD-C4C | 4.11  | 1.48        | 1.39     |
| 14  | b     | 1202 | CLA  | C1D-ND  | -4.10 | 1.32        | 1.37     |
| 14  | b     | 1227 | CLA  | C3B-C2B | 4.10  | 1.46        | 1.40     |
| 14  | b     | 1209 | CLA  | C3B-C2B | 4.10  | 1.46        | 1.40     |
| 14  | a     | 1137 | CLA  | C1D-ND  | -4.10 | 1.32        | 1.37     |
| 14  | A     | 1103 | CLA  | CHD-C4C | 4.10  | 1.48        | 1.39     |
| 19  | A     | 5002 | LHG  | O8-C23  | 4.10  | 1.45        | 1.33     |
| 14  | B     | 1222 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 14  | a     | 1129 | CLA  | C1D-ND  | -4.09 | 1.32        | 1.37     |
| 19  | a     | 5002 | LHG  | O8-C23  | 4.09  | 1.45        | 1.33     |
| 14  | G     | 1115 | CLA  | C1D-ND  | -4.09 | 1.32        | 1.37     |
| 14  | H     | 1236 | CLA  | O2D-CGD | 4.09  | 1.43        | 1.33     |
| 14  | l     | 1501 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 14  | H     | 1222 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 14  | B     | 1227 | CLA  | C3B-C2B | 4.09  | 1.46        | 1.40     |
| 14  | l     | 1502 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 14  | b     | 1236 | CLA  | C3B-C2B | 4.08  | 1.46        | 1.40     |
| 14  | H     | 1236 | CLA  | C3B-C2B | 4.08  | 1.46        | 1.40     |
| 14  | H     | 1236 | CLA  | C1D-ND  | -4.08 | 1.32        | 1.37     |
| 14  | b     | 1236 | CLA  | O2D-CGD | 4.08  | 1.43        | 1.33     |
| 14  | A     | 1129 | CLA  | C1D-ND  | -4.08 | 1.32        | 1.37     |
| 19  | G     | 5002 | LHG  | O8-C23  | 4.08  | 1.45        | 1.33     |
| 19  | a     | 5002 | LHG  | O7-C7   | 4.08  | 1.45        | 1.34     |
| 14  | L     | 1501 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1236 | CLA  | C1D-ND  | -4.08 | 1.32        | 1.37     |
| 14  | b     | 1221 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 14  | U     | 1501 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 14  | a     | 1131 | CLA  | C3B-C2B | 4.07  | 1.46        | 1.40     |
| 14  | B     | 1209 | CLA  | C3B-C2B | 4.07  | 1.46        | 1.40     |
| 14  | k     | 1401 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 19  | l     | 5102 | LHG  | O8-C23  | 4.07  | 1.45        | 1.33     |
| 14  | B     | 1236 | CLA  | O2D-CGD | 4.07  | 1.43        | 1.33     |
| 14  | B     | 1202 | CLA  | C1D-ND  | -4.07 | 1.32        | 1.37     |
| 19  | L     | 5102 | LHG  | O8-C23  | 4.07  | 1.45        | 1.33     |
| 14  | A     | 1107 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 14  | b     | 1206 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 14  | b     | 1211 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 14  | B     | 1210 | CLA  | C3C-C2C | 4.07  | 1.45        | 1.36     |
| 15  | b     | 1207 | F6C  | C3D-C4D | -4.07 | 1.33        | 1.43     |
| 14  | A     | 1111 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 14  | A     | 1115 | CLA  | C1D-ND  | -4.06 | 1.32        | 1.37     |
| 14  | B     | 1226 | CLA  | C1D-ND  | -4.06 | 1.32        | 1.37     |
| 15  | H     | 1207 | F6C  | C3D-C4D | -4.06 | 1.33        | 1.43     |
| 19  | A     | 5002 | LHG  | O7-C7   | 4.06  | 1.45        | 1.34     |
| 14  | B     | 1211 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 14  | H     | 1227 | CLA  | C3B-C2B | 4.06  | 1.46        | 1.40     |
| 14  | a     | 1012 | CLA  | C1D-ND  | -4.06 | 1.32        | 1.37     |
| 14  | G     | 1107 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 15  | B     | 1207 | F6C  | C3D-C4D | -4.06 | 1.33        | 1.43     |
| 14  | H     | 1209 | CLA  | C3B-C2B | 4.06  | 1.46        | 1.40     |
| 14  | K     | 1401 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | b     | 1204 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | b     | 1210 | CLA  | C3C-C2C | 4.05  | 1.45        | 1.36     |
| 19  | G     | 5002 | LHG  | O7-C7   | 4.05  | 1.45        | 1.34     |
| 19  | U     | 5102 | LHG  | O8-C23  | 4.05  | 1.45        | 1.33     |
| 14  | H     | 1210 | CLA  | C3C-C2C | 4.05  | 1.45        | 1.36     |
| 14  | G     | 1111 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | T     | 1401 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | b     | 1236 | CLA  | C1D-ND  | -4.05 | 1.32        | 1.37     |
| 14  | a     | 1129 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | H     | 1226 | CLA  | C1D-ND  | -4.05 | 1.32        | 1.37     |
| 14  | a     | 1111 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 14  | a     | 1114 | CLA  | C3B-C2B | 4.05  | 1.46        | 1.40     |
| 14  | B     | 1206 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 14  | H     | 1202 | CLA  | C1D-ND  | -4.04 | 1.32        | 1.37     |
| 14  | G     | 1129 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1114 | CLA  | C3B-C2B | 4.04  | 1.46        | 1.40     |
| 14  | G     | 1125 | CLA  | C1C-NC  | -4.04 | 1.31        | 1.37     |
| 14  | H     | 1218 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 15  | H     | 1237 | F6C  | C1D-ND  | -4.04 | 1.31        | 1.37     |
| 14  | G     | 1123 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | A     | 1128 | CLA  | C3B-C2B | 4.03  | 1.46        | 1.40     |
| 14  | H     | 1223 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | G     | 1131 | CLA  | C3B-C2B | 4.03  | 1.46        | 1.40     |
| 14  | a     | 1115 | CLA  | C1D-ND  | -4.03 | 1.32        | 1.37     |
| 14  | A     | 1129 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | B     | 1221 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | a     | 1125 | CLA  | C1C-NC  | -4.03 | 1.31        | 1.37     |
| 14  | B     | 1204 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | b     | 1223 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 14  | A     | 1125 | CLA  | C1C-NC  | -4.03 | 1.31        | 1.37     |
| 14  | B     | 1223 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 14  | a     | 1128 | CLA  | C3B-C2B | 4.02  | 1.46        | 1.40     |
| 14  | H     | 1206 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 14  | b     | 1218 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 14  | H     | 1221 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 14  | G     | 1131 | CLA  | C1D-ND  | -4.02 | 1.32        | 1.37     |
| 14  | H     | 1211 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 18  | R     | 4020 | BCR  | C11-C12 | -4.02 | 1.24        | 1.34     |
| 14  | A     | 1114 | CLA  | C3B-C2B | 4.02  | 1.45        | 1.40     |
| 14  | B     | 1218 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 14  | b     | 1228 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 15  | b     | 1207 | F6C  | C4A-NA  | -4.01 | 1.32        | 1.37     |
| 14  | A     | 1123 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 14  | H     | 1204 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 14  | a     | 1131 | CLA  | C1D-ND  | -4.01 | 1.32        | 1.37     |
| 18  | I     | 4020 | BCR  | C11-C12 | -4.01 | 1.24        | 1.34     |
| 14  | G     | 1129 | CLA  | C1D-ND  | -4.01 | 1.32        | 1.37     |
| 14  | H     | 1206 | CLA  | C3B-C2B | 4.01  | 1.45        | 1.40     |
| 14  | A     | 1131 | CLA  | C3B-C2B | 4.00  | 1.45        | 1.40     |
| 14  | G     | 1138 | CLA  | C3B-C2B | 4.00  | 1.45        | 1.40     |
| 14  | G     | 1128 | CLA  | C3B-C2B | 4.00  | 1.45        | 1.40     |
| 14  | a     | 1118 | CLA  | C1D-ND  | -4.00 | 1.32        | 1.37     |
| 18  | i     | 4020 | BCR  | C11-C12 | -3.99 | 1.24        | 1.34     |
| 14  | a     | 1132 | CLA  | C3B-C2B | 3.99  | 1.45        | 1.40     |
| 14  | A     | 1012 | CLA  | C1D-ND  | -3.99 | 1.32        | 1.37     |
| 14  | B     | 1228 | CLA  | CHD-C4C | 3.99  | 1.48        | 1.39     |
| 14  | G     | 1118 | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1138 | CLA  | C3B-C2B | 3.99  | 1.45        | 1.40     |
| 15  | B     | 1207 | F6C  | C4A-NA  | -3.99 | 1.32        | 1.37     |
| 14  | A     | 1132 | CLA  | C3B-C2B | 3.99  | 1.45        | 1.40     |
| 14  | a     | 1138 | CLA  | C3B-C2B | 3.99  | 1.45        | 1.40     |
| 15  | b     | 1237 | F6C  | C1D-ND  | -3.99 | 1.31        | 1.37     |
| 14  | G     | 1012 | CLA  | C1D-ND  | -3.99 | 1.32        | 1.37     |
| 15  | B     | 1237 | F6C  | C1D-ND  | -3.99 | 1.31        | 1.37     |
| 14  | a     | 1109 | CLA  | CHD-C4C | 3.99  | 1.48        | 1.39     |
| 14  | A     | 1137 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 15  | b     | 1237 | F6C  | C3D-C4D | -3.98 | 1.34        | 1.43     |
| 15  | B     | 1237 | F6C  | C3D-C4D | -3.98 | 1.34        | 1.43     |
| 14  | A     | 1118 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | H     | 1228 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 14  | U     | 1502 | CLA  | C3B-C2B | 3.98  | 1.45        | 1.40     |
| 14  | G     | 1124 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 15  | H     | 1207 | F6C  | C4A-NA  | -3.98 | 1.32        | 1.37     |
| 14  | B     | 1202 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | A     | 1131 | CLA  | C1D-ND  | -3.98 | 1.32        | 1.37     |
| 14  | A     | 1124 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | a     | 1118 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | G     | 1132 | CLA  | C3B-C2B | 3.98  | 1.45        | 1.40     |
| 14  | a     | 1123 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | H     | 1232 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 14  | H     | 1202 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 14  | L     | 1502 | CLA  | C3B-C2B | 3.98  | 1.45        | 1.40     |
| 14  | B     | 1216 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 14  | a     | 1124 | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 14  | B     | 1231 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 14  | b     | 1232 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 14  | A     | 1109 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 14  | b     | 1206 | CLA  | C3B-C2B | 3.97  | 1.45        | 1.40     |
| 14  | b     | 1202 | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 14  | H     | 1218 | CLA  | C1D-ND  | -3.96 | 1.32        | 1.37     |
| 20  | I     | 5006 | LMG  | O7-C10  | 3.96  | 1.45        | 1.34     |
| 14  | G     | 1137 | CLA  | CHD-C1D | 3.96  | 1.46        | 1.38     |
| 14  | H     | 1239 | CLA  | C3B-C2B | 3.96  | 1.45        | 1.40     |
| 14  | H     | 1231 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 14  | a     | 1114 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 14  | H     | 1216 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 14  | G     | 1127 | CLA  | CHD-C1D | 3.96  | 1.46        | 1.38     |
| 14  | l     | 1502 | CLA  | C3B-C2B | 3.96  | 1.45        | 1.40     |
| 14  | B     | 1206 | CLA  | C3B-C2B | 3.96  | 1.45        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1137 | CLA  | CHD-C1D | 3.96  | 1.46        | 1.38     |
| 14  | b     | 1216 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 14  | M     | 1501 | CLA  | C3B-C2B | 3.96  | 1.45        | 1.40     |
| 15  | H     | 1237 | F6C  | C3D-C4D | -3.96 | 1.34        | 1.43     |
| 20  | i     | 5006 | LMG  | O7-C10  | 3.96  | 1.45        | 1.34     |
| 14  | V     | 1501 | CLA  | C3B-C2B | 3.96  | 1.45        | 1.40     |
| 14  | A     | 1118 | CLA  | C1D-ND  | -3.95 | 1.32        | 1.37     |
| 14  | A     | 1124 | CLA  | C1D-ND  | -3.95 | 1.32        | 1.37     |
| 20  | R     | 5006 | LMG  | O7-C10  | 3.95  | 1.45        | 1.34     |
| 14  | B     | 1232 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 14  | a     | 1117 | CLA  | C1D-ND  | -3.95 | 1.32        | 1.37     |
| 18  | L     | 4019 | BCR  | C11-C12 | -3.95 | 1.24        | 1.34     |
| 14  | G     | 1109 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 14  | b     | 1231 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 14  | G     | 1114 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 14  | H     | 1204 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 18  | G     | 4004 | BCR  | C11-C12 | -3.95 | 1.24        | 1.34     |
| 14  | B     | 1234 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 14  | b     | 1226 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 14  | G     | 1124 | CLA  | C1D-ND  | -3.94 | 1.32        | 1.37     |
| 14  | b     | 1212 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 14  | B     | 1226 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 14  | B     | 1204 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 14  | G     | 1120 | CLA  | C1D-ND  | -3.94 | 1.32        | 1.37     |
| 14  | A     | 1114 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 14  | A     | 1127 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 18  | a     | 4004 | BCR  | C11-C12 | -3.94 | 1.24        | 1.34     |
| 14  | H     | 1234 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 14  | a     | 1124 | CLA  | C1D-ND  | -3.93 | 1.32        | 1.37     |
| 18  | U     | 4019 | BCR  | C11-C12 | -3.93 | 1.24        | 1.34     |
| 14  | b     | 1204 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 14  | G     | 1117 | CLA  | C1D-ND  | -3.93 | 1.32        | 1.37     |
| 14  | B     | 1212 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 14  | a     | 1107 | CLA  | C1D-ND  | -3.93 | 1.32        | 1.37     |
| 14  | A     | 1117 | CLA  | C1D-ND  | -3.93 | 1.33        | 1.37     |
| 14  | G     | 1118 | CLA  | C1D-ND  | -3.93 | 1.33        | 1.37     |
| 14  | H     | 1212 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 14  | B     | 1239 | CLA  | C3B-C2B | 3.93  | 1.45        | 1.40     |
| 14  | b     | 1234 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 18  | A     | 4004 | BCR  | C11-C12 | -3.93 | 1.24        | 1.34     |
| 14  | H     | 1226 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 14  | b     | 1214 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1218 | CLA  | C1D-ND  | -3.92 | 1.33        | 1.37     |
| 18  | l     | 4019 | BCR  | C11-C12 | -3.92 | 1.24        | 1.34     |
| 14  | B     | 1214 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 14  | b     | 1229 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 19  | l     | 5102 | LHG  | O7-C7   | 3.92  | 1.45        | 1.34     |
| 14  | U     | 1502 | CLA  | C1D-ND  | -3.92 | 1.33        | 1.37     |
| 14  | B     | 1229 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 14  | m     | 1501 | CLA  | C3B-C2B | 3.91  | 1.45        | 1.40     |
| 15  | H     | 1219 | F6C  | C3D-C4D | -3.91 | 1.34        | 1.43     |
| 19  | U     | 5102 | LHG  | O7-C7   | 3.91  | 1.45        | 1.34     |
| 14  | A     | 1120 | CLA  | C1D-ND  | -3.91 | 1.33        | 1.37     |
| 14  | b     | 1218 | CLA  | C1D-ND  | -3.91 | 1.33        | 1.37     |
| 14  | A     | 1102 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 19  | L     | 5102 | LHG  | O7-C7   | 3.91  | 1.45        | 1.34     |
| 14  | H     | 1229 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 14  | a     | 1102 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 19  | l     | 5101 | LHG  | O7-C7   | 3.90  | 1.45        | 1.34     |
| 14  | a     | 1127 | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 14  | G     | 1136 | CLA  | C3B-C2B | 3.89  | 1.45        | 1.40     |
| 14  | b     | 1213 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 14  | A     | 1136 | CLA  | C3B-C2B | 3.89  | 1.45        | 1.40     |
| 19  | L     | 5101 | LHG  | O7-C7   | 3.89  | 1.45        | 1.34     |
| 15  | B     | 1219 | F6C  | C3D-C4D | -3.89 | 1.34        | 1.43     |
| 14  | B     | 1231 | CLA  | C3B-C2B | 3.89  | 1.45        | 1.40     |
| 14  | G     | 1102 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 14  | l     | 1503 | CLA  | C1D-ND  | -3.89 | 1.33        | 1.37     |
| 14  | U     | 1503 | CLA  | C1D-ND  | -3.89 | 1.33        | 1.37     |
| 14  | H     | 1214 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 14  | b     | 1224 | CLA  | CHD-C1D | 3.88  | 1.45        | 1.38     |
| 14  | G     | 1141 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 14  | b     | 1233 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 14  | a     | 1136 | CLA  | C3B-C2B | 3.88  | 1.45        | 1.40     |
| 15  | b     | 1219 | F6C  | C3D-C4D | -3.88 | 1.34        | 1.43     |
| 14  | H     | 1231 | CLA  | C3B-C2B | 3.88  | 1.45        | 1.40     |
| 19  | U     | 5101 | LHG  | O7-C7   | 3.88  | 1.45        | 1.34     |
| 14  | H     | 1233 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 14  | A     | 1139 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 14  | H     | 1213 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 14  | A     | 1107 | CLA  | C1D-ND  | -3.87 | 1.33        | 1.37     |
| 14  | H     | 1205 | CLA  | CHD-C1D | 3.87  | 1.45        | 1.38     |
| 14  | G     | 1139 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 14  | H     | 1224 | CLA  | CHD-C1D | 3.87  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | L     | 1503 | CLA  | C1D-ND  | -3.87 | 1.33        | 1.37     |
| 14  | G     | 1104 | CLA  | C1D-ND  | -3.87 | 1.33        | 1.37     |
| 14  | G     | 1107 | CLA  | C1D-ND  | -3.87 | 1.33        | 1.37     |
| 14  | G     | 1126 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 14  | a     | 1135 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 15  | a     | 1121 | F6C  | C3D-C4D | -3.86 | 1.34        | 1.43     |
| 14  | B     | 1221 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | l     | 1502 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | b     | 1239 | CLA  | C3B-C2B | 3.86  | 1.45        | 1.40     |
| 14  | G     | 1126 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | B     | 1224 | CLA  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 14  | A     | 1135 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 14  | L     | 1502 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | b     | 1221 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | a     | 1141 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 14  | B     | 1233 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 14  | G     | 1130 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 14  | A     | 1141 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 14  | H     | 1221 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | a     | 1120 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | a     | 1126 | CLA  | C1D-ND  | -3.86 | 1.33        | 1.37     |
| 14  | a     | 1112 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | a     | 1139 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | a     | 1130 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | B     | 1213 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | B     | 1205 | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |
| 14  | k     | 1401 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | b     | 1233 | CLA  | C3B-C2B | 3.85  | 1.45        | 1.40     |
| 14  | B     | 1233 | CLA  | C3B-C2B | 3.85  | 1.45        | 1.40     |
| 14  | A     | 1130 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | A     | 1126 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | A     | 1108 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 14  | a     | 1126 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 14  | G     | 1135 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 14  | K     | 1401 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 14  | a     | 1108 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 14  | b     | 1208 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 14  | b     | 1239 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 15  | A     | 1121 | F6C  | C3D-C4D | -3.84 | 1.34        | 1.43     |
| 14  | B     | 1239 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 14  | H     | 1233 | CLA  | C3B-C2B | 3.83  | 1.45        | 1.40     |
| 14  | H     | 1218 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1231 | CLA  | C3B-C2B | 3.83  | 1.45        | 1.40     |
| 14  | G     | 1108 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 14  | T     | 1401 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | H     | 1208 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | a     | 1120 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | A     | 1105 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | A     | 1120 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | B     | 1218 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | G     | 1120 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 14  | B     | 1227 | CLA  | C1D-ND  | -3.82 | 1.33        | 1.37     |
| 14  | A     | 1112 | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 18  | b     | 4010 | BCR  | C11-C12 | -3.82 | 1.24        | 1.34     |
| 15  | H     | 1230 | F6C  | C3D-C4D | -3.82 | 1.34        | 1.43     |
| 18  | B     | 4010 | BCR  | C11-C12 | -3.82 | 1.24        | 1.34     |
| 14  | b     | 1215 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 14  | A     | 1110 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 15  | G     | 1121 | F6C  | C3D-C4D | -3.81 | 1.34        | 1.43     |
| 14  | G     | 1110 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 15  | b     | 1230 | F6C  | C3D-C4D | -3.81 | 1.34        | 1.43     |
| 14  | b     | 1218 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 14  | B     | 1215 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 15  | B     | 1230 | F6C  | C3D-C4D | -3.81 | 1.34        | 1.43     |
| 14  | B     | 1208 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 14  | b     | 1205 | CLA  | CHD-C1D | 3.81  | 1.45        | 1.38     |
| 14  | A     | 1126 | CLA  | C1D-ND  | -3.81 | 1.33        | 1.37     |
| 14  | H     | 1215 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 14  | H     | 1239 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 14  | H     | 1226 | CLA  | C3B-C2B | 3.80  | 1.45        | 1.40     |
| 14  | H     | 1227 | CLA  | C1D-ND  | -3.80 | 1.33        | 1.37     |
| 14  | a     | 1104 | CLA  | C1D-ND  | -3.80 | 1.33        | 1.37     |
| 14  | G     | 1105 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 14  | B     | 1226 | CLA  | C3B-C2B | 3.80  | 1.45        | 1.40     |
| 14  | a     | 1105 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 14  | G     | 1112 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 14  | G     | 1131 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 20  | H     | 5002 | LMG  | O7-C10  | 3.79  | 1.45        | 1.34     |
| 18  | H     | 4010 | BCR  | C11-C12 | -3.79 | 1.24        | 1.34     |
| 14  | a     | 1110 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 14  | a     | 1133 | CLA  | C1D-ND  | -3.79 | 1.33        | 1.37     |
| 14  | a     | 1131 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 14  | b     | 1227 | CLA  | C1D-ND  | -3.78 | 1.33        | 1.37     |
| 18  | G     | 4005 | BCR  | C11-C12 | -3.78 | 1.24        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1131 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 14  | a     | 1140 | CLA  | C1D-ND  | -3.78 | 1.33        | 1.37     |
| 14  | G     | 1115 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 20  | B     | 5002 | LMG  | O7-C10  | 3.77  | 1.44        | 1.34     |
| 14  | A     | 1115 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | A     | 1104 | CLA  | C1D-ND  | -3.77 | 1.33        | 1.37     |
| 14  | a     | 1101 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | G     | 1133 | CLA  | C1D-ND  | -3.77 | 1.33        | 1.37     |
| 14  | b     | 1203 | CLA  | C1D-ND  | -3.77 | 1.33        | 1.37     |
| 14  | G     | 1122 | CLA  | C1D-ND  | -3.77 | 1.33        | 1.37     |
| 14  | b     | 1226 | CLA  | C3B-C2B | 3.77  | 1.45        | 1.40     |
| 14  | G     | 1101 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | A     | 1119 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | a     | 1115 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | a     | 1119 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | G     | 1119 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 14  | A     | 1136 | CLA  | C1D-ND  | -3.76 | 1.33        | 1.37     |
| 14  | A     | 1140 | CLA  | C1D-ND  | -3.76 | 1.33        | 1.37     |
| 20  | b     | 5002 | LMG  | O7-C10  | 3.76  | 1.44        | 1.34     |
| 14  | G     | 1136 | CLA  | C1D-ND  | -3.76 | 1.33        | 1.37     |
| 14  | A     | 1101 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 14  | a     | 1136 | CLA  | C1D-ND  | -3.76 | 1.33        | 1.37     |
| 14  | A     | 1133 | CLA  | C1D-ND  | -3.76 | 1.33        | 1.37     |
| 18  | B     | 4017 | BCR  | C11-C12 | -3.75 | 1.24        | 1.34     |
| 14  | b     | 1215 | CLA  | C1D-ND  | -3.75 | 1.33        | 1.37     |
| 15  | H     | 1219 | F6C  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 18  | A     | 4005 | BCR  | C11-C12 | -3.75 | 1.24        | 1.34     |
| 14  | G     | 1140 | CLA  | C1D-ND  | -3.75 | 1.33        | 1.37     |
| 14  | b     | 1209 | CLA  | C1D-ND  | -3.75 | 1.33        | 1.37     |
| 14  | H     | 1203 | CLA  | C1D-ND  | -3.75 | 1.33        | 1.37     |
| 14  | B     | 1203 | CLA  | C1D-ND  | -3.75 | 1.33        | 1.37     |
| 14  | H     | 1202 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 14  | A     | 1122 | CLA  | C1D-ND  | -3.74 | 1.33        | 1.37     |
| 14  | a     | 1118 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 15  | B     | 1219 | F6C  | CHB-C1B | 3.74  | 1.47        | 1.39     |
| 18  | a     | 4005 | BCR  | C11-C12 | -3.74 | 1.24        | 1.34     |
| 14  | A     | 1116 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 14  | a     | 1101 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 14  | a     | 1116 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 14  | A     | 1103 | CLA  | C1D-ND  | -3.74 | 1.33        | 1.37     |
| 14  | B     | 1203 | CLA  | CHD-C1D | 3.73  | 1.45        | 1.38     |
| 14  | A     | 1118 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1132 | CLA  | C1D-ND  | -3.73 | 1.33        | 1.37     |
| 14  | B     | 1202 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 14  | G     | 1103 | CLA  | C1D-ND  | -3.73 | 1.33        | 1.37     |
| 14  | U     | 1501 | CLA  | C1D-ND  | -3.73 | 1.33        | 1.37     |
| 14  | H     | 1021 | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 14  | a     | 1103 | CLA  | C1D-ND  | -3.73 | 1.33        | 1.37     |
| 14  | G     | 1116 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 18  | H     | 4017 | BCR  | C11-C12 | -3.73 | 1.25        | 1.34     |
| 14  | H     | 1209 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 14  | b     | 1203 | CLA  | CHD-C1D | 3.73  | 1.45        | 1.38     |
| 14  | H     | 1215 | CLA  | C1D-ND  | -3.73 | 1.33        | 1.37     |
| 18  | G     | 4003 | BCR  | C11-C12 | -3.72 | 1.25        | 1.34     |
| 14  | G     | 1101 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 14  | G     | 1118 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 14  | A     | 1101 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 14  | A     | 1104 | CLA  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 14  | B     | 1235 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 14  | H     | 1203 | CLA  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 14  | G     | 1104 | CLA  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 14  | H     | 1235 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 14  | b     | 1235 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 18  | b     | 4017 | BCR  | C11-C12 | -3.72 | 1.25        | 1.34     |
| 14  | a     | 1122 | CLA  | C1D-ND  | -3.72 | 1.33        | 1.37     |
| 14  | A     | 1122 | CLA  | C3C-C2C | 3.72  | 1.44        | 1.36     |
| 14  | H     | 1222 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 14  | a     | 1104 | CLA  | CHD-C1D | 3.71  | 1.45        | 1.38     |
| 18  | A     | 4003 | BCR  | C11-C12 | -3.71 | 1.25        | 1.34     |
| 14  | b     | 1209 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 14  | l     | 1503 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 14  | B     | 1215 | CLA  | C1D-ND  | -3.71 | 1.33        | 1.37     |
| 14  | b     | 1202 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 14  | H     | 1233 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 14  | B     | 1209 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 14  | b     | 1222 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 14  | a     | 1139 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 15  | b     | 1219 | F6C  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 14  | G     | 1122 | CLA  | C3C-C2C | 3.70  | 1.44        | 1.36     |
| 14  | B     | 1209 | CLA  | C1D-ND  | -3.70 | 1.33        | 1.37     |
| 14  | B     | 1222 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 18  | a     | 4003 | BCR  | C11-C12 | -3.70 | 1.25        | 1.34     |
| 14  | A     | 1102 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 14  | H     | 1211 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1136 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 14  | a     | 1122 | CLA  | C3C-C2C | 3.69  | 1.44        | 1.36     |
| 14  | H     | 1209 | CLA  | C1D-ND  | -3.69 | 1.33        | 1.37     |
| 14  | A     | 1132 | CLA  | C1D-ND  | -3.69 | 1.33        | 1.37     |
| 14  | B     | 1211 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 14  | a     | 1136 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 14  | B     | 1021 | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 14  | b     | 1021 | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 14  | B     | 1233 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 14  | H     | 1210 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 14  | G     | 1136 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 13  | a     | 1011 | CL0  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 14  | L     | 1503 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 14  | U     | 1502 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 14  | G     | 1102 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 14  | b     | 1210 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 14  | A     | 1012 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | B     | 1220 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | a     | 1132 | CLA  | C1D-ND  | -3.68 | 1.33        | 1.37     |
| 14  | A     | 1120 | CLA  | CHD-C1D | 3.68  | 1.45        | 1.38     |
| 14  | l     | 1502 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | G     | 1012 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 13  | A     | 1011 | CL0  | CHD-C1D | 3.68  | 1.45        | 1.38     |
| 14  | M     | 1501 | CLA  | C1D-ND  | -3.68 | 1.33        | 1.37     |
| 14  | a     | 1110 | CLA  | C1D-ND  | -3.68 | 1.33        | 1.37     |
| 14  | V     | 1501 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | a     | 1120 | CLA  | CHD-C1D | 3.68  | 1.45        | 1.38     |
| 14  | a     | 1102 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 14  | B     | 1210 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 15  | H     | 1219 | F6C  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 14  | G     | 1140 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | a     | 1012 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 14  | b     | 1233 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 14  | B     | 1205 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 14  | b     | 1220 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 14  | b     | 1205 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 14  | U     | 1503 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 14  | m     | 1501 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 14  | M     | 1501 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 15  | B     | 1219 | F6C  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 14  | H     | 1201 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 14  | a     | 1116 | CLA  | C1D-ND  | -3.67 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1022 | CLA  | CHD-C1D | 3.67  | 1.45        | 1.38     |
| 13  | G     | 1011 | CL0  | CHD-C1D | 3.67  | 1.45        | 1.38     |
| 14  | L     | 1501 | CLA  | C1D-ND  | -3.67 | 1.33        | 1.37     |
| 14  | G     | 1124 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 14  | G     | 1120 | CLA  | CHD-C1D | 3.66  | 1.45        | 1.38     |
| 14  | b     | 1211 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 14  | A     | 1116 | CLA  | C1D-ND  | -3.66 | 1.33        | 1.37     |
| 14  | A     | 1113 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 14  | L     | 1502 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 14  | a     | 1106 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 14  | l     | 1501 | CLA  | C1D-ND  | -3.66 | 1.33        | 1.37     |
| 15  | b     | 1219 | F6C  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 14  | H     | 1022 | CLA  | CHD-C1D | 3.66  | 1.45        | 1.38     |
| 14  | A     | 1140 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 14  | H     | 1220 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 14  | H     | 1205 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 14  | A     | 1139 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 14  | H     | 1208 | CLA  | C1D-ND  | -3.66 | 1.33        | 1.37     |
| 14  | G     | 1113 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 14  | H     | 1223 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | G     | 1139 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 14  | B     | 1210 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | G     | 1135 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | A     | 1113 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 14  | H     | 1210 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | a     | 1140 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 14  | G     | 1110 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | A     | 1110 | CLA  | C1D-ND  | -3.65 | 1.33        | 1.37     |
| 14  | G     | 1113 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 14  | b     | 1208 | CLA  | C1D-ND  | -3.64 | 1.33        | 1.37     |
| 14  | b     | 1210 | CLA  | C1D-ND  | -3.64 | 1.33        | 1.37     |
| 14  | B     | 1208 | CLA  | C1D-ND  | -3.64 | 1.33        | 1.37     |
| 14  | b     | 1022 | CLA  | CHD-C1D | 3.64  | 1.45        | 1.38     |
| 18  | L     | 4022 | BCR  | C11-C12 | -3.64 | 1.25        | 1.34     |
| 14  | a     | 1113 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 14  | H     | 1235 | CLA  | C1D-ND  | -3.64 | 1.33        | 1.37     |
| 14  | G     | 1134 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 14  | A     | 1124 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 14  | B     | 1201 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 14  | A     | 1106 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 14  | H     | 1217 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 14  | V     | 1501 | CLA  | C1D-ND  | -3.63 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1023 | CLA  | CHD-C1D | 3.63  | 1.45        | 1.38     |
| 14  | a     | 1124 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 15  | G     | 1121 | F6C  | CHB-C1B | 3.63  | 1.47        | 1.39     |
| 18  | U     | 4022 | BCR  | C11-C12 | -3.63 | 1.25        | 1.34     |
| 14  | a     | 1113 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 14  | M     | 1501 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 14  | B     | 1217 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 14  | m     | 1501 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 14  | H     | 1229 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 14  | b     | 1217 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 15  | A     | 1121 | F6C  | CHB-C1B | 3.62  | 1.47        | 1.39     |
| 14  | B     | 1214 | CLA  | C1D-ND  | -3.62 | 1.33        | 1.37     |
| 14  | b     | 1201 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 14  | b     | 1229 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 14  | H     | 1227 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 14  | H     | 1201 | CLA  | C1D-ND  | -3.62 | 1.33        | 1.37     |
| 14  | G     | 1116 | CLA  | C1D-ND  | -3.62 | 1.33        | 1.37     |
| 14  | b     | 1223 | CLA  | C1D-ND  | -3.62 | 1.33        | 1.37     |
| 18  | l     | 4022 | BCR  | C11-C12 | -3.62 | 1.25        | 1.34     |
| 14  | A     | 1129 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 14  | B     | 1235 | CLA  | C1D-ND  | -3.62 | 1.33        | 1.37     |
| 14  | b     | 1021 | CLA  | CHD-C1D | 3.62  | 1.45        | 1.38     |
| 14  | U     | 1501 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 14  | a     | 1129 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 14  | G     | 1106 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 15  | a     | 1121 | F6C  | CHB-C1B | 3.61  | 1.47        | 1.39     |
| 14  | G     | 1109 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 18  | a     | 4006 | BCR  | C11-C12 | -3.61 | 1.25        | 1.34     |
| 14  | H     | 1214 | CLA  | C3B-C2B | 3.61  | 1.45        | 1.40     |
| 14  | B     | 1229 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 14  | a     | 1117 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 14  | G     | 1123 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 14  | H     | 1214 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 14  | A     | 1134 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 14  | H     | 1231 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 14  | A     | 1123 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 14  | b     | 1214 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 14  | L     | 1501 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 14  | A     | 1135 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 18  | A     | 4006 | BCR  | C11-C12 | -3.61 | 1.25        | 1.34     |
| 14  | A     | 1117 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 14  | B     | 1021 | CLA  | CHD-C1D | 3.61  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1021 | CLA  | CHD-C1D | 3.60  | 1.45        | 1.38     |
| 14  | a     | 1123 | CLA  | C1D-ND  | -3.60 | 1.33        | 1.37     |
| 14  | b     | 1214 | CLA  | C3B-C2B | 3.60  | 1.45        | 1.40     |
| 14  | V     | 1501 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 14  | a     | 1134 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 14  | H     | 1234 | CLA  | C1D-ND  | -3.60 | 1.33        | 1.37     |
| 14  | G     | 1132 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 14  | B     | 1214 | CLA  | C3B-C2B | 3.60  | 1.45        | 1.40     |
| 14  | G     | 1137 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 14  | H     | 1206 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 14  | G     | 1122 | CLA  | C1C-NC  | -3.60 | 1.32        | 1.37     |
| 18  | G     | 4006 | BCR  | C11-C12 | -3.60 | 1.25        | 1.34     |
| 14  | B     | 1227 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 14  | B     | 1223 | CLA  | C1D-ND  | -3.60 | 1.33        | 1.37     |
| 14  | A     | 1109 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 14  | B     | 1231 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 14  | B     | 1023 | CLA  | CHD-C1D | 3.59  | 1.45        | 1.38     |
| 14  | G     | 1104 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 14  | b     | 1208 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 14  | A     | 1137 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 14  | m     | 1501 | CLA  | C1D-ND  | -3.59 | 1.33        | 1.37     |
| 14  | A     | 1132 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 14  | G     | 1129 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 14  | a     | 1137 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 14  | a     | 1112 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 14  | G     | 1111 | CLA  | C1D-ND  | -3.59 | 1.33        | 1.37     |
| 14  | B     | 1240 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 14  | G     | 1112 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 14  | a     | 1111 | CLA  | C1D-ND  | -3.58 | 1.33        | 1.37     |
| 14  | G     | 1117 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 14  | A     | 1111 | CLA  | C1D-ND  | -3.58 | 1.33        | 1.37     |
| 14  | a     | 1104 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 14  | b     | 1227 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 14  | H     | 1240 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 14  | a     | 1109 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 14  | A     | 1122 | CLA  | C1C-NC  | -3.57 | 1.32        | 1.37     |
| 14  | l     | 1501 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 14  | A     | 1112 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 14  | a     | 1132 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 14  | H     | 1023 | CLA  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 14  | A     | 1104 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 14  | b     | 1206 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1213 | CLA  | C1D-ND  | -3.57 | 1.33        | 1.37     |
| 14  | b     | 1231 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 14  | b     | 1240 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 14  | B     | 1201 | CLA  | C1D-ND  | -3.56 | 1.33        | 1.37     |
| 14  | a     | 1122 | CLA  | C1C-NC  | -3.56 | 1.32        | 1.37     |
| 18  | m     | 4021 | BCR  | C11-C12 | -3.56 | 1.25        | 1.34     |
| 14  | B     | 1234 | CLA  | C1D-ND  | -3.56 | 1.33        | 1.37     |
| 14  | b     | 1213 | CLA  | C1D-ND  | -3.56 | 1.33        | 1.37     |
| 14  | a     | 1135 | CLA  | C1D-ND  | -3.56 | 1.33        | 1.37     |
| 14  | B     | 1206 | CLA  | CHD-C4C | 3.56  | 1.47        | 1.39     |
| 14  | a     | 1114 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 18  | R     | 4018 | BCR  | C11-C12 | -3.56 | 1.25        | 1.34     |
| 14  | b     | 1211 | CLA  | C1D-ND  | -3.56 | 1.33        | 1.37     |
| 14  | a     | 1107 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 18  | V     | 4021 | BCR  | C11-C12 | -3.55 | 1.25        | 1.34     |
| 18  | I     | 4018 | BCR  | C11-C12 | -3.55 | 1.25        | 1.34     |
| 14  | A     | 1107 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 14  | G     | 1013 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 14  | k     | 1401 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 14  | B     | 1222 | CLA  | C1D-ND  | -3.55 | 1.33        | 1.37     |
| 14  | b     | 1235 | CLA  | C1D-ND  | -3.55 | 1.33        | 1.37     |
| 14  | B     | 1208 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 18  | M     | 4021 | BCR  | C11-C12 | -3.54 | 1.25        | 1.34     |
| 14  | B     | 1223 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 14  | B     | 1213 | CLA  | C1D-ND  | -3.54 | 1.33        | 1.37     |
| 14  | G     | 1108 | CLA  | C1D-ND  | -3.54 | 1.33        | 1.37     |
| 14  | G     | 1107 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | H     | 1223 | CLA  | CHD-C4C | 3.53  | 1.47        | 1.39     |
| 14  | H     | 1224 | CLA  | CHD-C4C | 3.53  | 1.47        | 1.39     |
| 14  | b     | 1232 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | A     | 1013 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | l     | 1502 | CLA  | C1C-NC  | -3.53 | 1.32        | 1.37     |
| 14  | G     | 1114 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | b     | 1213 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | a     | 1118 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 14  | b     | 1234 | CLA  | C1D-ND  | -3.52 | 1.33        | 1.37     |
| 14  | a     | 1134 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | a     | 1119 | CLA  | C1D-ND  | -3.52 | 1.33        | 1.37     |
| 14  | A     | 1114 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | B     | 1224 | CLA  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 14  | H     | 1208 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | H     | 1213 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1222 | CLA  | C1D-ND  | -3.52 | 1.33        | 1.37     |
| 14  | K     | 1401 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | A     | 1140 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | H     | 1232 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | b     | 1224 | CLA  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 14  | G     | 1140 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | A     | 1134 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | B     | 1232 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 18  | i     | 4018 | BCR  | C11-C12 | -3.52 | 1.25        | 1.34     |
| 14  | G     | 1134 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | a     | 1140 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 14  | B     | 1213 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | B     | 1211 | CLA  | C1D-ND  | -3.51 | 1.33        | 1.37     |
| 14  | G     | 1120 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | G     | 1141 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | H     | 1206 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | G     | 1107 | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 14  | B     | 1234 | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 14  | b     | 1223 | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 14  | A     | 1108 | CLA  | C1D-ND  | -3.51 | 1.33        | 1.37     |
| 14  | A     | 1118 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | a     | 1111 | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 14  | L     | 1502 | CLA  | C1C-NC  | -3.51 | 1.32        | 1.37     |
| 14  | a     | 1141 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 14  | G     | 1105 | CLA  | C1D-ND  | -3.51 | 1.33        | 1.37     |
| 14  | H     | 1222 | CLA  | C1D-ND  | -3.50 | 1.33        | 1.37     |
| 14  | A     | 1120 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 14  | a     | 1128 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 14  | G     | 1119 | CLA  | C1D-ND  | -3.50 | 1.33        | 1.37     |
| 14  | a     | 1122 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 15  | H     | 1230 | F6C  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 14  | G     | 1122 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 14  | A     | 1133 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 14  | H     | 1211 | CLA  | C1D-ND  | -3.49 | 1.33        | 1.37     |
| 14  | A     | 1107 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 14  | A     | 1128 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 15  | b     | 1207 | F6C  | C1C-NC  | -3.49 | 1.32        | 1.35     |
| 14  | b     | 1201 | CLA  | C1D-ND  | -3.49 | 1.33        | 1.37     |
| 14  | H     | 1234 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 14  | A     | 1119 | CLA  | C1D-ND  | -3.49 | 1.33        | 1.37     |
| 14  | a     | 1108 | CLA  | C1D-ND  | -3.49 | 1.33        | 1.37     |
| 14  | a     | 1013 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1234 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 14  | A     | 1141 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 14  | A     | 1111 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 14  | G     | 1108 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 14  | U     | 1502 | CLA  | C1C-NC  | -3.49 | 1.32        | 1.37     |
| 14  | a     | 1120 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 14  | G     | 1133 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 14  | G     | 1128 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 14  | G     | 1111 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 14  | A     | 1122 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 14  | H     | 1210 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 14  | a     | 1107 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 15  | b     | 1230 | F6C  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 15  | B     | 1230 | F6C  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 14  | B     | 1206 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 14  | H     | 1216 | CLA  | C3B-C2B | 3.47  | 1.45        | 1.40     |
| 14  | T     | 1401 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | a     | 1108 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | b     | 1210 | CLA  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 14  | B     | 1203 | CLA  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 14  | b     | 1226 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | b     | 1205 | CLA  | C1C-NC  | -3.47 | 1.32        | 1.37     |
| 14  | H     | 1226 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | U     | 1503 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | H     | 1236 | CLA  | CHD-C1D | 3.47  | 1.45        | 1.38     |
| 14  | G     | 1118 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | B     | 1210 | CLA  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 14  | A     | 1108 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | H     | 1220 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 14  | a     | 1133 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 14  | B     | 1226 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 14  | A     | 1105 | CLA  | C1D-ND  | -3.46 | 1.33        | 1.37     |
| 14  | L     | 1503 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 14  | b     | 1209 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 14  | b     | 1203 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 14  | b     | 1206 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 14  | a     | 1123 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 14  | B     | 1205 | CLA  | C1C-NC  | -3.46 | 1.32        | 1.37     |
| 14  | H     | 1203 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 13  | G     | 1011 | CL0  | MG-ND   | -3.46 | 1.98        | 2.05     |
| 14  | H     | 1231 | CLA  | C1D-ND  | -3.46 | 1.33        | 1.37     |
| 14  | b     | 1220 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1216 | CLA  | C3B-C2B | 3.45  | 1.45        | 1.40     |
| 14  | B     | 1216 | CLA  | C3B-C2B | 3.45  | 1.45        | 1.40     |
| 14  | G     | 1128 | CLA  | MG-ND   | -3.45 | 1.98        | 2.05     |
| 13  | a     | 1011 | CL0  | MG-ND   | -3.45 | 1.98        | 2.05     |
| 14  | B     | 1209 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 14  | H     | 1205 | CLA  | C1C-NC  | -3.45 | 1.32        | 1.37     |
| 14  | B     | 1205 | CLA  | C3B-C2B | 3.45  | 1.45        | 1.40     |
| 14  | G     | 1110 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 15  | A     | 1121 | F6C  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 14  | b     | 1202 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 18  | H     | 4009 | BCR  | C11-C12 | -3.45 | 1.25        | 1.34     |
| 13  | A     | 1011 | CL0  | MG-ND   | -3.44 | 1.99        | 2.05     |
| 14  | A     | 1138 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 14  | B     | 1202 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 14  | b     | 1212 | CLA  | C1C-NC  | -3.44 | 1.32        | 1.37     |
| 18  | a     | 4001 | BCR  | C11-C12 | -3.44 | 1.25        | 1.34     |
| 15  | G     | 1121 | F6C  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 14  | B     | 1212 | CLA  | C1C-NC  | -3.44 | 1.32        | 1.37     |
| 14  | b     | 1225 | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 18  | B     | 4005 | BCR  | C11-C12 | -3.44 | 1.25        | 1.34     |
| 14  | b     | 1236 | CLA  | CHD-C1D | 3.44  | 1.45        | 1.38     |
| 14  | B     | 1220 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 14  | H     | 1215 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 18  | A     | 4001 | BCR  | C11-C12 | -3.44 | 1.25        | 1.34     |
| 14  | H     | 1202 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 18  | b     | 4005 | BCR  | C11-C12 | -3.44 | 1.25        | 1.34     |
| 14  | B     | 1231 | CLA  | C1D-ND  | -3.44 | 1.33        | 1.37     |
| 14  | B     | 1221 | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 14  | H     | 1221 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 14  | H     | 1205 | CLA  | C3B-C2B | 3.43  | 1.45        | 1.40     |
| 14  | B     | 1236 | CLA  | CHD-C1D | 3.43  | 1.45        | 1.38     |
| 14  | b     | 1218 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 18  | T     | 4001 | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 14  | G     | 1106 | CLA  | C1D-ND  | -3.43 | 1.33        | 1.37     |
| 14  | H     | 1209 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 14  | a     | 1111 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 14  | A     | 1106 | CLA  | C1D-ND  | -3.43 | 1.33        | 1.37     |
| 14  | a     | 1106 | CLA  | C1D-ND  | -3.43 | 1.33        | 1.37     |
| 18  | G     | 4001 | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 14  | A     | 1128 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 15  | a     | 1121 | F6C  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 14  | H     | 1221 | CLA  | CHD-C4C | 3.43  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1128 | CLA  | MG-ND   | -3.43 | 1.99        | 2.05     |
| 14  | a     | 1132 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 14  | A     | 1123 | CLA  | CHD-C4C | 3.43  | 1.47        | 1.39     |
| 15  | b     | 1237 | F6C  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 18  | k     | 4001 | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 18  | H     | 4005 | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 14  | A     | 1128 | CLA  | MG-ND   | -3.43 | 1.99        | 2.05     |
| 14  | A     | 1111 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 14  | H     | 1220 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | A     | 1110 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 14  | B     | 1221 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 18  | K     | 4001 | BCR  | C11-C12 | -3.42 | 1.25        | 1.34     |
| 14  | G     | 1125 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | U     | 1503 | CLA  | C1C-NC  | -3.42 | 1.32        | 1.37     |
| 14  | B     | 1215 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 14  | A     | 1128 | CLA  | C1C-NC  | -3.42 | 1.32        | 1.37     |
| 14  | H     | 1212 | CLA  | C1C-NC  | -3.42 | 1.32        | 1.37     |
| 14  | G     | 1128 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 15  | B     | 1237 | F6C  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 14  | G     | 1138 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 14  | b     | 1231 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | b     | 1221 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 14  | G     | 1123 | CLA  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 14  | A     | 1132 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 14  | b     | 1221 | CLA  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 14  | a     | 1105 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | A     | 1126 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 14  | G     | 1128 | CLA  | C1C-NC  | -3.41 | 1.32        | 1.37     |
| 14  | a     | 1138 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 14  | B     | 1218 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 14  | A     | 1125 | CLA  | C1D-ND  | -3.41 | 1.33        | 1.37     |
| 14  | b     | 1215 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 15  | H     | 1237 | F6C  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 14  | H     | 1218 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 14  | G     | 1132 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 14  | b     | 1220 | CLA  | C1D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | G     | 1013 | CLA  | CHD-C4C | 3.40  | 1.47        | 1.39     |
| 14  | a     | 1013 | CLA  | CHD-C4C | 3.40  | 1.47        | 1.39     |
| 14  | H     | 1226 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 14  | b     | 1205 | CLA  | C3B-C2B | 3.40  | 1.45        | 1.40     |
| 14  | B     | 1239 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 14  | a     | 1110 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | b     | 4006 | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 18  | G     | 4002 | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 14  | G     | 1111 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 14  | B     | 1220 | CLA  | C1D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | a     | 1133 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 14  | A     | 1125 | CLA  | CHD-C1D | 3.40  | 1.45        | 1.38     |
| 18  | B     | 4006 | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 18  | H     | 4006 | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 14  | A     | 1127 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 14  | a     | 1126 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 14  | H     | 1239 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 18  | B     | 4009 | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 14  | B     | 1225 | CLA  | CHD-C4C | 3.40  | 1.47        | 1.39     |
| 14  | a     | 1122 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 14  | l     | 1503 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 14  | a     | 1125 | CLA  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 14  | B     | 1226 | CLA  | C1C-NC  | -3.39 | 1.32        | 1.37     |
| 14  | G     | 1126 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 14  | a     | 1128 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 14  | B     | 1023 | CLA  | C4B-NB  | -3.39 | 1.32        | 1.35     |
| 15  | B     | 1207 | F6C  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 14  | H     | 1224 | CLA  | MG-ND   | -3.39 | 1.99        | 2.05     |
| 14  | A     | 1013 | CLA  | CHD-C4C | 3.39  | 1.47        | 1.39     |
| 15  | B     | 1207 | F6C  | C1C-NC  | -3.39 | 1.32        | 1.35     |
| 14  | a     | 1012 | CLA  | MG-ND   | -3.39 | 1.99        | 2.05     |
| 14  | G     | 1133 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 14  | b     | 1226 | CLA  | C1C-NC  | -3.39 | 1.32        | 1.37     |
| 14  | b     | 1224 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 14  | G     | 1125 | CLA  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 14  | A     | 1105 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 14  | B     | 1201 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 13  | a     | 1011 | CL0  | CHD-C4C | 3.38  | 1.47        | 1.39     |
| 14  | A     | 1013 | CLA  | CHD-C1D | 3.38  | 1.45        | 1.38     |
| 18  | A     | 4002 | BCR  | C11-C12 | -3.38 | 1.25        | 1.34     |
| 14  | B     | 1224 | CLA  | MG-ND   | -3.38 | 1.99        | 2.05     |
| 14  | H     | 1201 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 14  | b     | 1224 | CLA  | MG-ND   | -3.38 | 1.99        | 2.05     |
| 18  | a     | 4002 | BCR  | C11-C12 | -3.38 | 1.25        | 1.34     |
| 14  | L     | 1503 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 14  | G     | 1105 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 14  | a     | 1127 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 15  | b     | 1207 | F6C  | CHB-C1B | 3.38  | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1128 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 14  | H     | 1226 | CLA  | MG-ND   | -3.38 | 1.99        | 2.05     |
| 14  | G     | 1127 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 14  | b     | 1239 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 14  | A     | 1012 | CLA  | MG-ND   | -3.37 | 1.99        | 2.05     |
| 14  | b     | 1226 | CLA  | MG-ND   | -3.37 | 1.99        | 2.05     |
| 14  | G     | 1013 | CLA  | CHD-C1D | 3.37  | 1.44        | 1.38     |
| 14  | H     | 1023 | CLA  | C4B-NB  | -3.37 | 1.32        | 1.35     |
| 14  | b     | 1021 | CLA  | C1C-NC  | -3.37 | 1.32        | 1.37     |
| 14  | A     | 1122 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 14  | B     | 1021 | CLA  | C1C-NC  | -3.37 | 1.32        | 1.37     |
| 15  | H     | 1207 | F6C  | CHB-C1B | 3.37  | 1.46        | 1.39     |
| 15  | H     | 1238 | F6C  | C1D-ND  | -3.37 | 1.32        | 1.37     |
| 14  | H     | 1225 | CLA  | CHD-C4C | 3.37  | 1.46        | 1.39     |
| 14  | a     | 1127 | CLA  | CHD-C4C | 3.36  | 1.46        | 1.39     |
| 14  | G     | 1131 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 14  | B     | 1023 | CLA  | CHD-C4C | 3.36  | 1.46        | 1.39     |
| 14  | A     | 1133 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 14  | b     | 1201 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 18  | b     | 4009 | BCR  | C11-C12 | -3.36 | 1.25        | 1.34     |
| 14  | a     | 1131 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 14  | a     | 1013 | CLA  | CHD-C1D | 3.36  | 1.44        | 1.38     |
| 14  | a     | 1125 | CLA  | C1D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | G     | 1012 | CLA  | MG-ND   | -3.36 | 1.99        | 2.05     |
| 14  | b     | 1222 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 14  | H     | 1206 | CLA  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 14  | B     | 1226 | CLA  | MG-ND   | -3.35 | 1.99        | 2.05     |
| 14  | A     | 1131 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 14  | B     | 1224 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 14  | H     | 1224 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 13  | G     | 1011 | CL0  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 13  | A     | 1011 | CL0  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 14  | H     | 1023 | CLA  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 14  | b     | 1023 | CLA  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 15  | B     | 1238 | F6C  | C1D-ND  | -3.34 | 1.32        | 1.37     |
| 14  | G     | 1106 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 14  | A     | 1106 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 14  | b     | 1023 | CLA  | C4B-NB  | -3.34 | 1.32        | 1.35     |
| 14  | K     | 1401 | CLA  | C1D-ND  | -3.34 | 1.33        | 1.37     |
| 15  | H     | 1207 | F6C  | C1C-NC  | -3.34 | 1.32        | 1.35     |
| 14  | l     | 1503 | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 14  | a     | 1105 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1222 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 15  | b     | 1238 | F6C  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 14  | B     | 1239 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | G     | 1116 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | b     | 1022 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | G     | 1127 | CLA  | CHD-C4C | 3.33  | 1.46        | 1.39     |
| 14  | A     | 1127 | CLA  | CHD-C4C | 3.33  | 1.46        | 1.39     |
| 14  | H     | 1225 | CLA  | MG-ND   | -3.33 | 1.99        | 2.05     |
| 15  | b     | 1238 | F6C  | C1D-ND  | -3.33 | 1.32        | 1.37     |
| 14  | b     | 1226 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 14  | B     | 1222 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | b     | 1239 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | H     | 1021 | CLA  | C1C-NC  | -3.33 | 1.32        | 1.37     |
| 14  | H     | 1239 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | k     | 1401 | CLA  | C1D-ND  | -3.33 | 1.33        | 1.37     |
| 14  | G     | 1122 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 14  | b     | 1228 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 14  | T     | 1401 | CLA  | C1D-ND  | -3.32 | 1.33        | 1.37     |
| 14  | H     | 1216 | CLA  | C1D-ND  | -3.32 | 1.33        | 1.37     |
| 14  | b     | 1023 | CLA  | MG-ND   | -3.32 | 1.99        | 2.05     |
| 15  | B     | 1238 | F6C  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 15  | b     | 1237 | F6C  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 14  | a     | 1106 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | b     | 1206 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 14  | B     | 1023 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 14  | B     | 1206 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 14  | B     | 1228 | CLA  | C1D-ND  | -3.31 | 1.33        | 1.37     |
| 14  | B     | 1022 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | H     | 1217 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | a     | 1116 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | a     | 1127 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 14  | b     | 1022 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 15  | B     | 1237 | F6C  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | B     | 1226 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 14  | H     | 1022 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 14  | b     | 1225 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 15  | H     | 1238 | F6C  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 14  | B     | 1228 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 15  | H     | 1237 | F6C  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | B     | 1206 | CLA  | MG-ND   | -3.30 | 1.99        | 2.05     |
| 14  | G     | 1124 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | H     | 1228 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1023 | CLA  | MG-ND   | -3.30 | 1.99        | 2.05     |
| 14  | B     | 1236 | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 14  | A     | 1116 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | H     | 1228 | CLA  | C1D-ND  | -3.30 | 1.33        | 1.37     |
| 14  | b     | 1236 | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 14  | A     | 1012 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | b     | 1023 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | H     | 1236 | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 15  | b     | 1230 | F6C  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 14  | G     | 1012 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 14  | A     | 1127 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | B     | 1225 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | H     | 1206 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | H     | 1226 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 14  | B     | 1205 | CLA  | CHD-C4C | 3.29  | 1.46        | 1.39     |
| 15  | B     | 1230 | F6C  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 18  | b     | 4014 | BCR  | C11-C12 | -3.29 | 1.26        | 1.34     |
| 20  | H     | 5002 | LMG  | C37-C36 | -3.29 | 1.33        | 1.51     |
| 14  | H     | 1205 | CLA  | CHD-C4C | 3.29  | 1.46        | 1.39     |
| 20  | B     | 5002 | LMG  | C37-C36 | -3.29 | 1.33        | 1.51     |
| 14  | B     | 1022 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | B     | 1221 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | b     | 1228 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 15  | H     | 1230 | F6C  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 14  | G     | 1115 | CLA  | MG-ND   | -3.29 | 1.99        | 2.05     |
| 14  | B     | 1225 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 14  | B     | 1216 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 20  | a     | 5003 | LMG  | C40-C39 | -3.29 | 1.33        | 1.51     |
| 20  | b     | 5002 | LMG  | C37-C36 | -3.29 | 1.33        | 1.51     |
| 14  | G     | 1102 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | H     | 1023 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 14  | b     | 1225 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | a     | 1103 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | G     | 1012 | CLA  | C3B-C2B | 3.28  | 1.44        | 1.40     |
| 14  | H     | 1022 | CLA  | MG-ND   | -3.28 | 1.99        | 2.05     |
| 20  | B     | 5002 | LMG  | C22-C21 | -3.28 | 1.33        | 1.51     |
| 14  | A     | 1104 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | A     | 1123 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | B     | 1239 | CLA  | MG-ND   | -3.28 | 1.99        | 2.05     |
| 14  | H     | 1239 | CLA  | MG-ND   | -3.28 | 1.99        | 2.05     |
| 14  | G     | 1103 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | a     | 1104 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1012 | CLA  | C3B-C2B | 3.28  | 1.44        | 1.40     |
| 14  | b     | 1205 | CLA  | CHD-C4C | 3.28  | 1.46        | 1.39     |
| 14  | B     | 1023 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 14  | b     | 1239 | CLA  | MG-ND   | -3.28 | 1.99        | 2.05     |
| 20  | b     | 5002 | LMG  | C22-C21 | -3.28 | 1.33        | 1.51     |
| 20  | A     | 5003 | LMG  | C40-C39 | -3.28 | 1.33        | 1.51     |
| 14  | B     | 1232 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | a     | 1102 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | G     | 1123 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 14  | b     | 1206 | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 20  | G     | 5003 | LMG  | C40-C39 | -3.27 | 1.33        | 1.51     |
| 14  | b     | 1216 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | G     | 1127 | CLA  | MG-ND   | -3.27 | 1.99        | 2.05     |
| 14  | G     | 1104 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 14  | A     | 1103 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 14  | a     | 1115 | CLA  | MG-ND   | -3.27 | 1.99        | 2.05     |
| 14  | A     | 1124 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 14  | H     | 1229 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | b     | 1221 | CLA  | MG-ND   | -3.27 | 1.99        | 2.05     |
| 14  | a     | 1123 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 14  | A     | 1115 | CLA  | MG-ND   | -3.27 | 1.99        | 2.05     |
| 14  | A     | 1012 | CLA  | C3B-C2B | 3.27  | 1.44        | 1.40     |
| 20  | H     | 5002 | LMG  | C22-C21 | -3.27 | 1.33        | 1.51     |
| 14  | b     | 1217 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 15  | b     | 1238 | F6C  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 14  | H     | 1225 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 14  | B     | 1229 | CLA  | C1D-ND  | -3.26 | 1.33        | 1.37     |
| 18  | B     | 4014 | BCR  | C11-C12 | -3.26 | 1.26        | 1.34     |
| 14  | B     | 1217 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 14  | G     | 1012 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 14  | A     | 1115 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 14  | A     | 1012 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 14  | G     | 1126 | CLA  | MG-ND   | -3.26 | 1.99        | 2.05     |
| 14  | H     | 1221 | CLA  | MG-ND   | -3.26 | 1.99        | 2.05     |
| 20  | G     | 5003 | LMG  | C43-C42 | -3.26 | 1.33        | 1.51     |
| 14  | B     | 1214 | CLA  | MG-ND   | -3.26 | 1.99        | 2.05     |
| 20  | a     | 5003 | LMG  | C43-C42 | -3.26 | 1.33        | 1.51     |
| 14  | G     | 1115 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 14  | H     | 1232 | CLA  | C1D-ND  | -3.25 | 1.33        | 1.37     |
| 18  | H     | 4014 | BCR  | C11-C12 | -3.25 | 1.26        | 1.34     |
| 14  | b     | 1232 | CLA  | C1D-ND  | -3.25 | 1.33        | 1.37     |
| 14  | b     | 1214 | CLA  | MG-ND   | -3.25 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | T     | 1401 | CLA  | MG-NC   | 3.25  | 2.14        | 2.06     |
| 14  | a     | 1012 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 14  | b     | 1021 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 20  | A     | 5003 | LMG  | C43-C42 | -3.25 | 1.33        | 1.51     |
| 14  | a     | 1137 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 14  | a     | 1115 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 14  | a     | 1135 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 20  | G     | 5003 | LMG  | C37-C36 | -3.25 | 1.33        | 1.51     |
| 14  | B     | 1021 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 20  | A     | 5003 | LMG  | C37-C36 | -3.24 | 1.33        | 1.51     |
| 14  | A     | 1126 | CLA  | MG-ND   | -3.24 | 1.99        | 2.05     |
| 14  | A     | 1135 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 20  | a     | 5003 | LMG  | C37-C36 | -3.24 | 1.33        | 1.51     |
| 20  | H     | 5002 | LMG  | C19-C18 | -3.24 | 1.33        | 1.51     |
| 14  | b     | 1223 | CLA  | MG-ND   | -3.24 | 1.99        | 2.05     |
| 14  | a     | 1124 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 14  | K     | 1401 | CLA  | MG-NC   | 3.24  | 2.14        | 2.06     |
| 14  | b     | 1217 | CLA  | C1D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | a     | 1130 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 15  | B     | 1238 | F6C  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 20  | B     | 5002 | LMG  | C19-C18 | -3.24 | 1.33        | 1.51     |
| 14  | a     | 1012 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 14  | H     | 1214 | CLA  | MG-ND   | -3.24 | 1.99        | 2.05     |
| 14  | H     | 1224 | CLA  | C1C-NC  | -3.24 | 1.33        | 1.37     |
| 14  | b     | 1204 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 14  | a     | 1138 | CLA  | C1D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | B     | 1204 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 14  | H     | 1204 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 14  | G     | 1137 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 14  | G     | 1134 | CLA  | C1D-ND  | -3.23 | 1.33        | 1.37     |
| 14  | a     | 1112 | CLA  | C1D-ND  | -3.23 | 1.33        | 1.37     |
| 20  | b     | 5002 | LMG  | C19-C18 | -3.23 | 1.33        | 1.51     |
| 14  | G     | 1135 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 14  | H     | 1217 | CLA  | C1D-ND  | -3.23 | 1.33        | 1.37     |
| 14  | G     | 1130 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 14  | B     | 1217 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | a     | 1134 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | b     | 1211 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 14  | b     | 1229 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | A     | 1130 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 14  | A     | 1137 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 14  | H     | 1223 | CLA  | MG-ND   | -3.21 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1013 | CLA  | C1C-NC  | -3.21 | 1.33        | 1.37     |
| 14  | k     | 1401 | CLA  | MG-NC   | 3.21  | 2.13        | 2.06     |
| 14  | G     | 1138 | CLA  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | B     | 1224 | CLA  | C1C-NC  | -3.21 | 1.33        | 1.37     |
| 14  | a     | 1126 | CLA  | MG-ND   | -3.21 | 1.99        | 2.05     |
| 14  | H     | 1227 | CLA  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 14  | A     | 1134 | CLA  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 15  | B     | 1237 | F6C  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 14  | G     | 1140 | CLA  | MG-ND   | -3.20 | 1.99        | 2.05     |
| 14  | A     | 1102 | CLA  | C1D-ND  | -3.20 | 1.33        | 1.37     |
| 14  | A     | 1138 | CLA  | C1D-ND  | -3.20 | 1.33        | 1.37     |
| 14  | H     | 1021 | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 14  | B     | 1223 | CLA  | MG-ND   | -3.20 | 1.99        | 2.05     |
| 15  | b     | 1219 | F6C  | C3B-C2B | 3.20  | 1.46        | 1.39     |
| 14  | b     | 1216 | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 14  | B     | 1211 | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 14  | a     | 1140 | CLA  | MG-ND   | -3.20 | 1.99        | 2.05     |
| 14  | A     | 1140 | CLA  | MG-ND   | -3.20 | 1.99        | 2.05     |
| 15  | b     | 1237 | F6C  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 14  | G     | 1013 | CLA  | C1C-NC  | -3.19 | 1.33        | 1.37     |
| 14  | a     | 1117 | CLA  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 15  | H     | 1237 | F6C  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 15  | B     | 1219 | F6C  | C3B-C2B | 3.19  | 1.46        | 1.39     |
| 14  | H     | 1206 | CLA  | C1B-NB  | -3.19 | 1.32        | 1.35     |
| 14  | B     | 1226 | CLA  | C1B-NB  | -3.19 | 1.32        | 1.35     |
| 14  | b     | 1224 | CLA  | C1C-NC  | -3.19 | 1.33        | 1.37     |
| 15  | H     | 1238 | F6C  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 14  | G     | 1124 | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 18  | H     | 4004 | BCR  | C11-C12 | -3.18 | 1.26        | 1.34     |
| 14  | B     | 1022 | CLA  | CHD-C4C | 3.18  | 1.46        | 1.39     |
| 14  | H     | 1227 | CLA  | MG-ND   | -3.18 | 1.99        | 2.05     |
| 14  | a     | 1013 | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 14  | a     | 1122 | CLA  | MG-ND   | -3.18 | 1.99        | 2.05     |
| 14  | a     | 1117 | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 14  | a     | 1136 | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 14  | B     | 1227 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 14  | B     | 1222 | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 14  | H     | 1216 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 14  | H     | 1022 | CLA  | CHD-C4C | 3.18  | 1.46        | 1.39     |
| 14  | H     | 1217 | CLA  | MG-NC   | 3.17  | 2.13        | 2.06     |
| 14  | H     | 1222 | CLA  | C1C-NC  | -3.17 | 1.33        | 1.37     |
| 14  | G     | 1118 | CLA  | MG-ND   | -3.17 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1022 | CLA  | CHD-C4C | 3.17  | 1.46        | 1.39     |
| 14  | A     | 1124 | CLA  | C1C-NC  | -3.17 | 1.33        | 1.37     |
| 14  | A     | 1122 | CLA  | MG-ND   | -3.17 | 1.99        | 2.05     |
| 14  | L     | 1502 | CLA  | MG-ND   | -3.17 | 1.99        | 2.05     |
| 14  | B     | 1214 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 14  | H     | 1022 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 18  | B     | 4004 | BCR  | C11-C12 | -3.17 | 1.26        | 1.34     |
| 15  | H     | 1219 | F6C  | C3B-C2B | 3.17  | 1.46        | 1.39     |
| 14  | A     | 1119 | CLA  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 15  | H     | 1237 | F6C  | C3B-C2B | 3.16  | 1.46        | 1.39     |
| 14  | A     | 1137 | CLA  | MG-ND   | -3.16 | 1.99        | 2.05     |
| 14  | b     | 1222 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 18  | b     | 4004 | BCR  | C11-C12 | -3.16 | 1.26        | 1.34     |
| 14  | H     | 1234 | CLA  | MG-NC   | 3.16  | 2.13        | 2.06     |
| 14  | G     | 1117 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 14  | B     | 1210 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 14  | G     | 1136 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 14  | A     | 1117 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 14  | B     | 1216 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 15  | B     | 1237 | F6C  | C3B-C2B | 3.16  | 1.46        | 1.39     |
| 14  | A     | 1112 | CLA  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | a     | 1124 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 14  | G     | 1112 | CLA  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | A     | 1136 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 14  | b     | 1210 | CLA  | C1C-NC  | -3.16 | 1.33        | 1.37     |
| 14  | B     | 1022 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 14  | a     | 1119 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 14  | b     | 1227 | CLA  | MG-ND   | -3.15 | 1.99        | 2.05     |
| 14  | b     | 1214 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 14  | A     | 1118 | CLA  | MG-ND   | -3.15 | 1.99        | 2.05     |
| 14  | b     | 1217 | CLA  | MG-NC   | 3.15  | 2.13        | 2.06     |
| 14  | B     | 1217 | CLA  | MG-NC   | 3.15  | 2.13        | 2.06     |
| 14  | a     | 1137 | CLA  | MG-ND   | -3.15 | 1.99        | 2.05     |
| 14  | H     | 1211 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 14  | H     | 1214 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 14  | B     | 1227 | CLA  | MG-ND   | -3.15 | 1.99        | 2.05     |
| 14  | l     | 1502 | CLA  | MG-ND   | -3.15 | 1.99        | 2.05     |
| 14  | U     | 1502 | CLA  | MG-ND   | -3.14 | 1.99        | 2.05     |
| 14  | a     | 1133 | CLA  | C1C-NC  | -3.14 | 1.33        | 1.37     |
| 14  | G     | 1122 | CLA  | MG-ND   | -3.14 | 1.99        | 2.05     |
| 14  | H     | 1226 | CLA  | C1B-NB  | -3.14 | 1.32        | 1.35     |
| 14  | b     | 1206 | CLA  | C1B-NB  | -3.14 | 1.32        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | b     | 1237 | F6C  | C3B-C2B | 3.14  | 1.46        | 1.39     |
| 14  | A     | 1133 | CLA  | C1C-NC  | -3.14 | 1.33        | 1.37     |
| 14  | G     | 1133 | CLA  | C1C-NC  | -3.14 | 1.33        | 1.37     |
| 14  | b     | 1227 | CLA  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 14  | b     | 1022 | CLA  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 14  | A     | 1117 | CLA  | C1C-NC  | -3.14 | 1.33        | 1.37     |
| 14  | H     | 1206 | CLA  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 14  | B     | 1234 | CLA  | MG-NC   | 3.13  | 2.13        | 2.06     |
| 15  | H     | 1207 | F6C  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 14  | b     | 1234 | CLA  | MG-NC   | 3.13  | 2.13        | 2.06     |
| 14  | G     | 1119 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 14  | B     | 1234 | CLA  | OBD-CAD | 3.13  | 1.27        | 1.22     |
| 15  | B     | 1207 | F6C  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 14  | G     | 1103 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 14  | H     | 1225 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 14  | G     | 1128 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 14  | A     | 1128 | CLA  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 14  | G     | 1114 | CLA  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 13  | A     | 1011 | CL0  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 14  | G     | 1137 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | H     | 1210 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | G     | 1137 | CLA  | MG-ND   | -3.12 | 1.99        | 2.05     |
| 14  | H     | 1203 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | H     | 1234 | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 14  | H     | 1215 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | H     | 1222 | CLA  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 14  | B     | 1225 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | B     | 1206 | CLA  | C1B-NB  | -3.12 | 1.32        | 1.35     |
| 14  | A     | 1137 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | G     | 1128 | CLA  | C1B-NB  | -3.12 | 1.32        | 1.35     |
| 14  | a     | 1137 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | A     | 1103 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | b     | 1234 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 14  | G     | 1117 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 14  | A     | 1114 | CLA  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 14  | H     | 1204 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 14  | a     | 1118 | CLA  | MG-ND   | -3.11 | 1.99        | 2.05     |
| 13  | G     | 1011 | CL0  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 14  | L     | 1502 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 14  | a     | 1141 | CLA  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 13  | a     | 1011 | CL0  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 14  | l     | 1502 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | a     | 1011 | CL0  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 14  | b     | 1212 | CLA  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 14  | a     | 1128 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 14  | U     | 1502 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 14  | b     | 1223 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 14  | A     | 1123 | CLA  | MG-NC   | 3.11  | 2.13        | 2.06     |
| 14  | G     | 1102 | CLA  | MG-NC   | 3.10  | 2.13        | 2.06     |
| 13  | G     | 1011 | CL0  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 14  | b     | 1222 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | G     | 1133 | CLA  | MG-ND   | -3.10 | 1.99        | 2.05     |
| 14  | a     | 1130 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | G     | 1141 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 14  | a     | 1114 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 14  | B     | 1215 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 14  | b     | 1204 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 15  | b     | 1207 | F6C  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 14  | B     | 1222 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | U     | 1502 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | B     | 1223 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 14  | b     | 1226 | CLA  | C1B-NB  | -3.10 | 1.32        | 1.35     |
| 14  | a     | 1131 | CLA  | MG-ND   | -3.10 | 1.99        | 2.05     |
| 14  | A     | 1130 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | a     | 1123 | CLA  | MG-NC   | 3.10  | 2.13        | 2.06     |
| 14  | G     | 1130 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | b     | 1206 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 14  | B     | 1206 | CLA  | C3D-C2D | 3.09  | 1.47        | 1.39     |
| 14  | H     | 1220 | CLA  | C3D-C2D | 3.09  | 1.47        | 1.39     |
| 14  | a     | 1126 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | H     | 1216 | CLA  | C3D-C2D | 3.09  | 1.47        | 1.39     |
| 14  | A     | 1135 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 1102 | CLA  | MG-NC   | 3.09  | 2.13        | 2.06     |
| 14  | B     | 1204 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | B     | 1228 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 1133 | CLA  | MG-ND   | -3.09 | 1.99        | 2.05     |
| 14  | A     | 1141 | CLA  | MG-NC   | 3.09  | 2.13        | 2.06     |
| 14  | G     | 1131 | CLA  | MG-ND   | -3.09 | 1.99        | 2.05     |
| 14  | b     | 1228 | CLA  | MG-ND   | -3.09 | 1.99        | 2.05     |
| 14  | G     | 1123 | CLA  | MG-NC   | 3.09  | 2.13        | 2.06     |
| 14  | A     | 1141 | CLA  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 14  | L     | 1502 | CLA  | OBD-CAD | 3.09  | 1.27        | 1.22     |
| 14  | b     | 1215 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | a     | 1013 | CLA  | MG-ND   | -3.09 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1013 | CLA  | MG-ND   | -3.09 | 1.99        | 2.05     |
| 14  | a     | 1112 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | H     | 1228 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 1131 | CLA  | MG-ND   | -3.08 | 1.99        | 2.05     |
| 14  | b     | 1225 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | l     | 1502 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 14  | G     | 1013 | CLA  | MG-ND   | -3.08 | 1.99        | 2.05     |
| 14  | a     | 1102 | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | m     | 1501 | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | B     | 1203 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | G     | 1126 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | H     | 1220 | CLA  | MG-ND   | -3.08 | 1.99        | 2.05     |
| 14  | a     | 1103 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | H     | 1215 | CLA  | MG-ND   | -3.08 | 1.99        | 2.05     |
| 14  | A     | 1126 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | B     | 1216 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 14  | H     | 1223 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 1212 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 14  | b     | 1228 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 1209 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | G     | 1129 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 1215 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | H     | 1236 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | A     | 1130 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | b     | 1216 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 14  | a     | 1141 | CLA  | MG-NC   | 3.07  | 2.13        | 2.06     |
| 14  | H     | 1240 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 14  | B     | 1220 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 14  | G     | 1141 | CLA  | MG-NC   | 3.07  | 2.13        | 2.06     |
| 13  | A     | 1011 | CL0  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | H     | 1209 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | b     | 1202 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | G     | 1130 | CLA  | MG-ND   | -3.07 | 1.99        | 2.05     |
| 14  | A     | 1115 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 14  | b     | 1220 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 14  | V     | 1501 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | B     | 1236 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 14  | A     | 1101 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | G     | 1135 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 14  | b     | 1240 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 14  | a     | 1123 | CLA  | MG-ND   | -3.06 | 1.99        | 2.05     |
| 14  | b     | 1209 | CLA  | MG-ND   | -3.06 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1212 | CLA  | C1D-ND  | -3.06 | 1.34        | 1.37     |
| 14  | b     | 1203 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 15  | H     | 1207 | F6C  | C3B-C2B | 3.06  | 1.46        | 1.39     |
| 14  | G     | 1115 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 14  | G     | 1101 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | B     | 1240 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 14  | M     | 1501 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | b     | 1236 | CLA  | MG-ND   | -3.06 | 1.99        | 2.05     |
| 14  | a     | 1135 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 14  | l     | 1503 | CLA  | MG-ND   | -3.06 | 1.99        | 2.05     |
| 14  | G     | 1123 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 14  | H     | 1202 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 14  | l     | 1501 | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 14  | a     | 1115 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 14  | b     | 1202 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 14  | b     | 1236 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | b     | 1220 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 14  | m     | 1501 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 14  | b     | 1021 | CLA  | CHD-C4C | 3.05  | 1.46        | 1.39     |
| 14  | B     | 1203 | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 14  | B     | 1021 | CLA  | CHD-C4C | 3.05  | 1.46        | 1.39     |
| 14  | A     | 1013 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 14  | b     | 1022 | CLA  | MG-NC   | 3.05  | 2.13        | 2.06     |
| 14  | H     | 1203 | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 14  | a     | 1132 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | B     | 1022 | CLA  | MG-NC   | 3.05  | 2.13        | 2.06     |
| 14  | A     | 1129 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | a     | 1129 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | B     | 1202 | CLA  | MG-ND   | -3.05 | 1.99        | 2.05     |
| 15  | b     | 1207 | F6C  | C3B-C2B | 3.05  | 1.46        | 1.39     |
| 14  | H     | 1236 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | b     | 1216 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | a     | 1133 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | A     | 1108 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 14  | B     | 1202 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 14  | B     | 1220 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | B     | 1236 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | H     | 1202 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 14  | b     | 1215 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | a     | 1108 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 14  | G     | 1112 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 14  | A     | 1128 | CLA  | C1B-NB  | -3.04 | 1.32        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | L     | 1503 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | H     | 1021 | CLA  | CHD-C4C | 3.04  | 1.46        | 1.39     |
| 14  | H     | 1221 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 14  | U     | 1501 | CLA  | OBD-CAD | 3.04  | 1.27        | 1.22     |
| 14  | H     | 1205 | CLA  | OBD-CAD | 3.04  | 1.27        | 1.22     |
| 14  | L     | 1501 | CLA  | OBD-CAD | 3.04  | 1.27        | 1.22     |
| 14  | A     | 1139 | CLA  | MG-NC   | 3.04  | 2.13        | 2.06     |
| 14  | b     | 1228 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 15  | B     | 1207 | F6C  | C3B-C2B | 3.04  | 1.46        | 1.39     |
| 14  | a     | 1139 | CLA  | MG-NC   | 3.04  | 2.13        | 2.06     |
| 14  | H     | 1215 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 14  | a     | 1101 | CLA  | MG-NC   | 3.04  | 2.13        | 2.06     |
| 14  | B     | 1228 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | b     | 1221 | CLA  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 14  | U     | 1503 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 14  | A     | 1138 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 14  | B     | 1221 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 14  | G     | 1138 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 15  | H     | 1207 | F6C  | OBD-CAD | 3.03  | 1.27        | 1.22     |
| 14  | G     | 1139 | CLA  | MG-NC   | 3.03  | 2.13        | 2.06     |
| 14  | M     | 1501 | CLA  | MG-ND   | -3.03 | 1.99        | 2.05     |
| 14  | H     | 1216 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 14  | H     | 1022 | CLA  | MG-NC   | 3.03  | 2.13        | 2.06     |
| 14  | a     | 1138 | CLA  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 14  | A     | 1132 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 14  | a     | 1128 | CLA  | C1B-NB  | -3.02 | 1.32        | 1.35     |
| 14  | G     | 1013 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 14  | A     | 1123 | CLA  | MG-ND   | -3.02 | 1.99        | 2.05     |
| 14  | a     | 1013 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 14  | b     | 1232 | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 15  | H     | 1238 | F6C  | C3B-C2B | 3.02  | 1.46        | 1.39     |
| 14  | B     | 1216 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 14  | V     | 1501 | CLA  | MG-ND   | -3.02 | 1.99        | 2.05     |
| 15  | b     | 1238 | F6C  | C3B-C2B | 3.02  | 1.46        | 1.39     |
| 14  | A     | 1112 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 15  | B     | 1238 | F6C  | C3B-C2B | 3.02  | 1.46        | 1.39     |
| 14  | H     | 1214 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 14  | B     | 1232 | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 14  | b     | 1215 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 14  | a     | 1116 | CLA  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 14  | H     | 1228 | CLA  | MG-ND   | -3.02 | 1.99        | 2.05     |
| 14  | a     | 1130 | CLA  | MG-ND   | -3.02 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1228 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 14  | H     | 1232 | CLA  | MG-NC   | 3.01  | 2.13        | 2.06     |
| 14  | B     | 1205 | CLA  | OBD-CAD | 3.01  | 1.27        | 1.22     |
| 14  | a     | 1129 | CLA  | MG-ND   | -3.01 | 1.99        | 2.05     |
| 14  | G     | 1108 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 14  | a     | 1125 | CLA  | MG-ND   | -3.01 | 1.99        | 2.05     |
| 15  | H     | 1230 | F6C  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 14  | G     | 1136 | CLA  | MG-ND   | -3.01 | 1.99        | 2.05     |
| 14  | G     | 1129 | CLA  | MG-ND   | -3.01 | 1.99        | 2.05     |
| 14  | B     | 1215 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 15  | H     | 1207 | F6C  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 14  | G     | 1120 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | b     | 1214 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 15  | B     | 1230 | F6C  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 14  | H     | 1233 | CLA  | C1D-ND  | -3.00 | 1.34        | 1.37     |
| 14  | B     | 1214 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 14  | b     | 1205 | CLA  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 14  | A     | 1119 | CLA  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 14  | l     | 1501 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | A     | 1106 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | G     | 1109 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 14  | U     | 1501 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | b     | 1234 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | A     | 1113 | CLA  | MG-NC   | 3.00  | 2.13        | 2.06     |
| 14  | l     | 1501 | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | G     | 1131 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 14  | A     | 1116 | CLA  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 14  | G     | 1103 | CLA  | MG-ND   | -2.99 | 1.99        | 2.05     |
| 14  | a     | 1120 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 14  | B     | 1234 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 14  | L     | 1501 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 14  | G     | 1113 | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | A     | 1140 | CLA  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 14  | A     | 1109 | CLA  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 14  | G     | 1116 | CLA  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 14  | A     | 1118 | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | a     | 1135 | CLA  | MG-ND   | -2.99 | 1.99        | 2.05     |
| 14  | A     | 1120 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 14  | A     | 1136 | CLA  | MG-ND   | -2.99 | 1.99        | 2.05     |
| 14  | G     | 1119 | CLA  | MG-ND   | -2.99 | 1.99        | 2.05     |
| 14  | A     | 1129 | CLA  | MG-ND   | -2.99 | 1.99        | 2.05     |
| 14  | b     | 1203 | CLA  | OBD-CAD | 2.99  | 1.27        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1118 | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | L     | 1501 | CLA  | MG-NC   | 2.98  | 2.13        | 2.06     |
| 14  | a     | 1118 | CLA  | MG-NC   | 2.98  | 2.13        | 2.06     |
| 15  | b     | 1230 | F6C  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 14  | a     | 1140 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 14  | G     | 1132 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 21  | a     | 6001 | LMT  | O3'-C3' | -2.98 | 1.36        | 1.43     |
| 14  | a     | 1109 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 15  | B     | 1230 | F6C  | C3C-C2C | 2.98  | 1.46        | 1.37     |
| 14  | A     | 1125 | CLA  | MG-ND   | -2.98 | 1.99        | 2.05     |
| 14  | A     | 1101 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 14  | A     | 1109 | CLA  | MG-ND   | -2.98 | 1.99        | 2.05     |
| 15  | B     | 1207 | F6C  | OBD-CAD | 2.98  | 1.27        | 1.22     |
| 15  | b     | 1207 | F6C  | OBD-CAD | 2.98  | 1.27        | 1.22     |
| 14  | a     | 1109 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 14  | H     | 1234 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 14  | a     | 1102 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 14  | A     | 1103 | CLA  | MG-ND   | -2.98 | 1.99        | 2.05     |
| 14  | A     | 1113 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 14  | B     | 1212 | CLA  | MG-ND   | -2.98 | 1.99        | 2.05     |
| 15  | H     | 1230 | F6C  | C3C-C2C | 2.98  | 1.46        | 1.37     |
| 14  | A     | 1102 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 14  | G     | 1131 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 15  | b     | 1230 | F6C  | C3C-C2C | 2.97  | 1.46        | 1.37     |
| 14  | a     | 1105 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | H     | 1204 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 14  | B     | 1204 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 14  | H     | 1228 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 14  | G     | 1102 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 21  | A     | 6001 | LMT  | O3'-C3' | -2.97 | 1.36        | 1.43     |
| 14  | G     | 1106 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 14  | B     | 1233 | CLA  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 14  | G     | 1101 | CLA  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 14  | a     | 1109 | CLA  | MG-ND   | -2.97 | 1.99        | 2.05     |
| 14  | H     | 1201 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 21  | G     | 6001 | LMT  | O3'-C3' | -2.97 | 1.36        | 1.43     |
| 14  | G     | 1140 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 15  | B     | 1207 | F6C  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 14  | b     | 1221 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | B     | 1214 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | G     | 1105 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | B     | 1201 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1119 | CLA  | OBD-CAD | 2.96  | 1.27        | 1.22     |
| 14  | a     | 1136 | CLA  | OBD-CAD | 2.96  | 1.27        | 1.22     |
| 14  | b     | 1211 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | a     | 1113 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | H     | 1208 | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 14  | B     | 1223 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | A     | 1109 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 15  | H     | 1219 | F6C  | C3C-C2C | 2.96  | 1.46        | 1.37     |
| 14  | H     | 1204 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | a     | 1136 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | b     | 1204 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 14  | H     | 1221 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | A     | 1107 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 15  | b     | 1207 | F6C  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 15  | B     | 1219 | F6C  | C3C-C2C | 2.96  | 1.46        | 1.37     |
| 14  | G     | 1116 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | a     | 1103 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | a     | 1106 | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 14  | H     | 1235 | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 14  | G     | 1125 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | U     | 1501 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | b     | 1233 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | a     | 1131 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 14  | b     | 1240 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 14  | A     | 1105 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | H     | 1212 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | b     | 1208 | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 14  | G     | 1107 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | G     | 1109 | CLA  | MG-ND   | -2.96 | 1.99        | 2.05     |
| 14  | G     | 1113 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 14  | A     | 1126 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 14  | a     | 1126 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 15  | H     | 1219 | F6C  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 14  | b     | 1201 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | B     | 1208 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 14  | H     | 1210 | CLA  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 14  | a     | 1101 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | b     | 1233 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | A     | 1139 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | B     | 1240 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | A     | 1119 | CLA  | MG-ND   | -2.95 | 1.99        | 2.05     |
| 14  | G     | 1139 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1116 | CLA  | MG-ND   | -2.95 | 1.99        | 2.05     |
| 14  | b     | 1212 | CLA  | MG-ND   | -2.95 | 1.99        | 2.05     |
| 14  | B     | 1221 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | B     | 1233 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | H     | 1214 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | a     | 1139 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | A     | 1131 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 14  | b     | 1210 | CLA  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 14  | b     | 1214 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | b     | 1220 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | H     | 1240 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | A     | 1135 | CLA  | MG-ND   | -2.95 | 1.99        | 2.05     |
| 14  | B     | 1211 | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | a     | 1113 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 14  | G     | 1126 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | a     | 1116 | CLA  | MG-ND   | -2.94 | 1.99        | 2.05     |
| 14  | G     | 1109 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 14  | A     | 1131 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | b     | 1234 | CLA  | MG-ND   | -2.94 | 2.00        | 2.05     |
| 14  | a     | 1119 | CLA  | OBD-CAD | 2.94  | 1.27        | 1.22     |
| 14  | A     | 1127 | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 14  | A     | 1140 | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 14  | B     | 1210 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 21  | a     | 6002 | LMT  | O3'-C3' | -2.94 | 1.36        | 1.43     |
| 14  | b     | 1204 | CLA  | MG-ND   | -2.94 | 2.00        | 2.05     |
| 14  | a     | 1134 | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 14  | G     | 1114 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | H     | 1211 | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | H     | 1229 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | a     | 1130 | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 14  | H     | 1223 | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | a     | 1135 | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | B     | 1235 | CLA  | OBD-CAD | 2.94  | 1.27        | 1.22     |
| 14  | G     | 1135 | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | a     | 1125 | CLA  | CHD-C4C | 2.94  | 1.45        | 1.39     |
| 14  | b     | 1203 | CLA  | MG-ND   | -2.94 | 2.00        | 2.05     |
| 14  | H     | 1021 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | l     | 1503 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 14  | a     | 1119 | CLA  | MG-ND   | -2.93 | 2.00        | 2.05     |
| 14  | A     | 1130 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | A     | 1114 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | B     | 1212 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | b     | 1219 | F6C  | C3C-C2C | 2.93  | 1.46        | 1.37     |
| 14  | B     | 1235 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | H     | 1235 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |
| 21  | G     | 6002 | LMT  | O4'-C4B | -2.93 | 1.36        | 1.43     |
| 21  | G     | 6002 | LMT  | O3'-C3' | -2.93 | 1.36        | 1.43     |
| 14  | A     | 1125 | CLA  | CHD-C4C | 2.93  | 1.45        | 1.39     |
| 14  | B     | 1021 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | G     | 1135 | CLA  | MG-ND   | -2.93 | 2.00        | 2.05     |
| 14  | b     | 1212 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 15  | B     | 1219 | F6C  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | H     | 1229 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | G     | 1127 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | G     | 1109 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 21  | A     | 6002 | LMT  | O4'-C4B | -2.93 | 1.36        | 1.43     |
| 14  | A     | 1116 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | B     | 1234 | CLA  | MG-ND   | -2.93 | 2.00        | 2.05     |
| 14  | a     | 1114 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | A     | 1135 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | G     | 1140 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | H     | 1233 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | b     | 1021 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | b     | 1212 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |
| 14  | a     | 1127 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | A     | 1136 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |
| 14  | a     | 1112 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | b     | 1223 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | b     | 1227 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 14  | H     | 1233 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | U     | 1503 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 15  | b     | 1219 | F6C  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 14  | a     | 1111 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 14  | B     | 1229 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 14  | a     | 1141 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | a     | 1131 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 15  | B     | 1207 | F6C  | C1D-ND  | -2.92 | 1.33        | 1.37     |
| 14  | H     | 1023 | CLA  | C1B-NB  | -2.92 | 1.32        | 1.35     |
| 21  | A     | 6002 | LMT  | O3'-C3' | -2.92 | 1.36        | 1.43     |
| 21  | l     | 6002 | LMT  | O2B-C2B | -2.92 | 1.36        | 1.43     |
| 14  | A     | 1112 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | L     | 1503 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | a     | 1140 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 14  | G     | 1125 | CLA  | CHD-C4C | 2.92  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1229 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 14  | B     | 1217 | CLA  | MG-ND   | -2.92 | 2.00        | 2.05     |
| 14  | A     | 1113 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | B     | 1204 | CLA  | MG-ND   | -2.92 | 2.00        | 2.05     |
| 14  | b     | 1229 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | a     | 1107 | CLA  | MG-ND   | -2.92 | 2.00        | 2.05     |
| 14  | H     | 1212 | CLA  | OBD-CAD | 2.92  | 1.27        | 1.22     |
| 13  | A     | 1011 | CL0  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | b     | 1235 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 15  | a     | 1121 | F6C  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | H     | 1227 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 14  | A     | 1141 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 14  | G     | 1130 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 13  | G     | 1011 | CL0  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 21  | L     | 6002 | LMT  | O2B-C2B | -2.92 | 1.36        | 1.43     |
| 14  | b     | 1235 | CLA  | OBD-CAD | 2.92  | 1.27        | 1.22     |
| 14  | H     | 1220 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 21  | a     | 6002 | LMT  | O4'-C4B | -2.92 | 1.36        | 1.43     |
| 14  | A     | 1140 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | G     | 1114 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 13  | a     | 1011 | CL0  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | G     | 1108 | CLA  | C1C-NC  | -2.91 | 1.33        | 1.37     |
| 14  | H     | 1234 | CLA  | MG-ND   | -2.91 | 2.00        | 2.05     |
| 15  | b     | 1207 | F6C  | C1D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | G     | 1141 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | B     | 1220 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | a     | 1140 | CLA  | C1C-NC  | -2.91 | 1.33        | 1.37     |
| 14  | B     | 1212 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 14  | H     | 1217 | CLA  | MG-ND   | -2.91 | 2.00        | 2.05     |
| 14  | A     | 1108 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | B     | 1212 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | G     | 1113 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | H     | 1208 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | A     | 1139 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 14  | a     | 1116 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | B     | 1203 | CLA  | MG-ND   | -2.91 | 2.00        | 2.05     |
| 14  | A     | 1114 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | H     | 1212 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 14  | A     | 1109 | CLA  | C1D-ND  | -2.90 | 1.34        | 1.37     |
| 14  | B     | 1208 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | G     | 1108 | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 14  | A     | 1134 | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1139 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 15  | b     | 1238 | F6C  | MG-ND   | -2.90 | 1.99        | 2.06     |
| 14  | B     | 1229 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 15  | B     | 1238 | F6C  | MG-ND   | -2.90 | 1.99        | 2.06     |
| 14  | H     | 1209 | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 14  | G     | 1116 | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 15  | H     | 1207 | F6C  | C1D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | B     | 1233 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | b     | 1233 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | b     | 1212 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 14  | G     | 1136 | CLA  | OBD-CAD | 2.90  | 1.27        | 1.22     |
| 14  | G     | 1112 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | A     | 1108 | CLA  | MG-ND   | -2.90 | 2.00        | 2.05     |
| 15  | H     | 1230 | F6C  | C3B-C2B | 2.90  | 1.46        | 1.39     |
| 14  | H     | 1212 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | A     | 1133 | CLA  | C3D-C2D | 2.90  | 1.47        | 1.39     |
| 14  | A     | 1109 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | G     | 1134 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | G     | 1104 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | H     | 1240 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 15  | A     | 1121 | F6C  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | G     | 1139 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | G     | 1132 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | a     | 1113 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | a     | 1133 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | G     | 1111 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | a     | 1109 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | a     | 1132 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 21  | U     | 6002 | LMT  | O2B-C2B | -2.89 | 1.36        | 1.43     |
| 14  | b     | 1208 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | b     | 1217 | CLA  | MG-ND   | -2.89 | 2.00        | 2.05     |
| 14  | A     | 1119 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | A     | 1132 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | H     | 1213 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | a     | 1108 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 14  | G     | 1133 | CLA  | C3D-C2D | 2.89  | 1.47        | 1.39     |
| 14  | A     | 1134 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 14  | H     | 1203 | CLA  | MG-ND   | -2.89 | 2.00        | 2.05     |
| 14  | b     | 1229 | CLA  | MG-ND   | -2.89 | 2.00        | 2.05     |
| 14  | A     | 1111 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 21  | U     | 6002 | LMT  | O3'-C3' | -2.89 | 1.36        | 1.43     |
| 14  | a     | 1114 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1209 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | b     | 1209 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | a     | 1132 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 14  | G     | 1110 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 15  | B     | 1237 | F6C  | MG-ND   | -2.88 | 1.99        | 2.06     |
| 14  | A     | 1132 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 14  | G     | 1134 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | G     | 1131 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | b     | 1209 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | H     | 1218 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | a     | 1134 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 15  | b     | 1230 | F6C  | C3B-C2B | 2.88  | 1.46        | 1.39     |
| 14  | b     | 1240 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 14  | A     | 1111 | CLA  | C1C-NC  | -2.88 | 1.33        | 1.37     |
| 14  | G     | 1140 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 21  | m     | 6000 | LMT  | O3'-C3' | -2.88 | 1.36        | 1.43     |
| 14  | A     | 1136 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | G     | 1120 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | G     | 1124 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 14  | a     | 1109 | CLA  | C1D-ND  | -2.88 | 1.34        | 1.37     |
| 14  | b     | 1217 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | a     | 1110 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 14  | B     | 1240 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 14  | B     | 1209 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 14  | H     | 1220 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 21  | M     | 6000 | LMT  | O3'-C3' | -2.87 | 1.36        | 1.43     |
| 14  | a     | 1110 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 14  | a     | 1111 | CLA  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 14  | a     | 1122 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 14  | A     | 1108 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | A     | 1131 | CLA  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 14  | B     | 1213 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 15  | G     | 1121 | F6C  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 14  | A     | 1110 | CLA  | MG-ND   | -2.87 | 2.00        | 2.05     |
| 14  | G     | 1108 | CLA  | MG-ND   | -2.87 | 2.00        | 2.05     |
| 15  | B     | 1230 | F6C  | C3B-C2B | 2.87  | 1.46        | 1.39     |
| 14  | B     | 1211 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 21  | V     | 6000 | LMT  | O3'-C3' | -2.87 | 1.36        | 1.43     |
| 14  | a     | 1136 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 15  | H     | 1237 | F6C  | MG-ND   | -2.87 | 1.99        | 2.06     |
| 14  | b     | 1213 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 14  | G     | 1132 | CLA  | MG-ND   | -2.87 | 2.00        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1108 | CLA  | MG-ND   | -2.87 | 2.00        | 2.05     |
| 14  | B     | 1209 | CLA  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 14  | B     | 1240 | CLA  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 21  | L     | 6002 | LMT  | O3'-C3' | -2.87 | 1.36        | 1.43     |
| 14  | A     | 1104 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | A     | 1122 | CLA  | C3D-C2D | 2.87  | 1.46        | 1.39     |
| 14  | b     | 1218 | CLA  | C3D-C2D | 2.87  | 1.46        | 1.39     |
| 14  | b     | 1211 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | G     | 1119 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 15  | H     | 1238 | F6C  | MG-ND   | -2.86 | 1.99        | 2.06     |
| 14  | B     | 1227 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | G     | 1109 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | b     | 1235 | CLA  | MG-ND   | -2.86 | 2.00        | 2.05     |
| 14  | G     | 1136 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | B     | 1220 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | a     | 1119 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | H     | 1223 | CLA  | OBD-CAD | 2.86  | 1.27        | 1.22     |
| 14  | a     | 1119 | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 15  | b     | 1237 | F6C  | C1C-NC  | -2.86 | 1.32        | 1.35     |
| 14  | b     | 1220 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 15  | b     | 1237 | F6C  | MG-ND   | -2.86 | 1.99        | 2.06     |
| 14  | G     | 1111 | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 14  | B     | 1223 | CLA  | OBD-CAD | 2.86  | 1.27        | 1.22     |
| 14  | A     | 1110 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | B     | 1023 | CLA  | C1B-NB  | -2.86 | 1.32        | 1.35     |
| 14  | A     | 1141 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 14  | H     | 1201 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | b     | 1211 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | b     | 1216 | CLA  | MG-ND   | -2.86 | 2.00        | 2.05     |
| 14  | A     | 1127 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | B     | 1023 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | b     | 1201 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | H     | 1023 | CLA  | C4C-C3C | 2.86  | 1.50        | 1.45     |
| 15  | a     | 1121 | F6C  | C3B-C2B | 2.86  | 1.46        | 1.39     |
| 14  | B     | 1217 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | U     | 1503 | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 14  | H     | 1213 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | B     | 1211 | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | B     | 1023 | CLA  | C4C-C3C | 2.86  | 1.50        | 1.45     |
| 14  | H     | 1211 | CLA  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 14  | a     | 1104 | CLA  | C1C-NC  | -2.85 | 1.33        | 1.37     |
| 14  | A     | 1120 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1229 | CLA  | MG-ND   | -2.85 | 2.00        | 2.05     |
| 14  | b     | 1023 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 21  | l     | 6002 | LMT  | O3'-C3' | -2.85 | 1.36        | 1.43     |
| 14  | H     | 1232 | CLA  | MG-ND   | -2.85 | 2.00        | 2.05     |
| 14  | a     | 1106 | CLA  | MG-ND   | -2.85 | 2.00        | 2.05     |
| 14  | b     | 1240 | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | a     | 1118 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 14  | B     | 1225 | CLA  | C1B-NB  | -2.85 | 1.32        | 1.35     |
| 14  | B     | 1218 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 14  | B     | 1232 | CLA  | MG-ND   | -2.85 | 2.00        | 2.05     |
| 14  | G     | 1115 | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | H     | 1240 | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | G     | 1141 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 14  | B     | 1201 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 15  | a     | 1121 | F6C  | C3C-C2C | 2.85  | 1.46        | 1.37     |
| 14  | H     | 1229 | CLA  | MG-ND   | -2.85 | 2.00        | 2.05     |
| 14  | b     | 1023 | CLA  | C1B-NB  | -2.85 | 1.32        | 1.35     |
| 14  | a     | 1127 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 14  | b     | 1023 | CLA  | C4C-C3C | 2.85  | 1.49        | 1.45     |
| 14  | a     | 1115 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 14  | A     | 1119 | CLA  | MG-NC   | 2.84  | 2.13        | 2.06     |
| 14  | G     | 1119 | CLA  | MG-NC   | 2.84  | 2.13        | 2.06     |
| 14  | H     | 1023 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 14  | a     | 1110 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 15  | A     | 1121 | F6C  | C3C-C2C | 2.84  | 1.46        | 1.37     |
| 14  | a     | 1120 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 14  | G     | 1110 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 14  | G     | 1110 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 14  | a     | 1141 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 14  | a     | 1108 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 14  | b     | 1235 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 14  | a     | 1114 | CLA  | MG-ND   | -2.84 | 2.00        | 2.05     |
| 14  | G     | 1122 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 14  | b     | 1225 | CLA  | C1B-NB  | -2.84 | 1.32        | 1.35     |
| 14  | G     | 1123 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 15  | H     | 1219 | F6C  | C1D-C2D | 2.84  | 1.50        | 1.44     |
| 14  | G     | 1106 | CLA  | MG-ND   | -2.84 | 2.00        | 2.05     |
| 14  | b     | 1223 | CLA  | OBD-CAD | 2.84  | 1.27        | 1.22     |
| 14  | H     | 1217 | CLA  | C3D-C2D | 2.84  | 1.46        | 1.39     |
| 15  | B     | 1237 | F6C  | C4B-NB  | -2.84 | 1.33        | 1.37     |
| 14  | A     | 1124 | CLA  | MG-ND   | -2.84 | 2.00        | 2.05     |
| 14  | H     | 1223 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1216 | CLA  | MG-ND   | -2.84 | 2.00        | 2.05     |
| 15  | H     | 1238 | F6C  | C4B-NB  | -2.83 | 1.33        | 1.37     |
| 14  | B     | 1213 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 15  | a     | 1121 | F6C  | C1D-ND  | -2.83 | 1.33        | 1.37     |
| 14  | A     | 1012 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | B     | 1235 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | G     | 1127 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 15  | A     | 1121 | F6C  | C1D-ND  | -2.83 | 1.33        | 1.37     |
| 14  | G     | 1106 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 14  | a     | 1131 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | H     | 1235 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 14  | H     | 1216 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | A     | 1106 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | b     | 1232 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 15  | G     | 1121 | F6C  | C1D-ND  | -2.83 | 1.33        | 1.37     |
| 14  | B     | 1223 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 14  | B     | 1208 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | b     | 1213 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | a     | 1112 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | H     | 1213 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | a     | 1120 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 14  | b     | 1205 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 14  | G     | 1012 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | a     | 1115 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | a     | 1127 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | A     | 1115 | CLA  | C1C-NC  | -2.83 | 1.33        | 1.37     |
| 15  | G     | 1121 | F6C  | C3C-C2C | 2.83  | 1.46        | 1.37     |
| 14  | b     | 1232 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 14  | L     | 1503 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 15  | B     | 1219 | F6C  | C1D-C2D | 2.83  | 1.50        | 1.44     |
| 14  | A     | 1118 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 14  | b     | 1233 | CLA  | C1C-NC  | -2.83 | 1.33        | 1.37     |
| 14  | B     | 1235 | CLA  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 14  | G     | 1101 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 14  | G     | 1115 | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 14  | A     | 1115 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | a     | 1124 | CLA  | MG-ND   | -2.82 | 2.00        | 2.05     |
| 14  | H     | 1232 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 14  | H     | 1213 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 15  | A     | 1121 | F6C  | C3B-C2B | 2.82  | 1.45        | 1.39     |
| 14  | G     | 1118 | CLA  | C3D-C2D | 2.82  | 1.46        | 1.39     |
| 14  | G     | 1129 | CLA  | OBD-CAD | 2.82  | 1.27        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1223 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 14  | a     | 1111 | CLA  | C3D-C2D | 2.82  | 1.46        | 1.39     |
| 14  | A     | 1123 | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 14  | G     | 1109 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 15  | b     | 1219 | F6C  | C1D-C2D | 2.82  | 1.50        | 1.44     |
| 14  | B     | 1232 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 14  | A     | 1112 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | G     | 1138 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 14  | B     | 1205 | CLA  | C3D-C2D | 2.82  | 1.46        | 1.39     |
| 14  | A     | 1127 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | G     | 1111 | CLA  | C3D-C2D | 2.81  | 1.46        | 1.39     |
| 14  | a     | 1129 | CLA  | OBD-CAD | 2.81  | 1.27        | 1.22     |
| 14  | A     | 1129 | CLA  | OBD-CAD | 2.81  | 1.27        | 1.22     |
| 14  | a     | 1140 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 14  | G     | 1127 | CLA  | MG-NC   | 2.81  | 2.13        | 2.06     |
| 14  | H     | 1211 | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | A     | 1101 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 14  | b     | 1221 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 14  | B     | 1213 | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 15  | b     | 1237 | F6C  | C4B-NB  | -2.81 | 1.33        | 1.37     |
| 14  | b     | 1218 | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | H     | 1208 | CLA  | MG-ND   | -2.81 | 2.00        | 2.05     |
| 14  | H     | 1211 | CLA  | MG-ND   | -2.81 | 2.00        | 2.05     |
| 14  | a     | 1139 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 14  | A     | 1107 | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | a     | 1124 | CLA  | C3D-C2D | 2.81  | 1.46        | 1.39     |
| 14  | G     | 1112 | CLA  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 14  | A     | 1120 | CLA  | MG-ND   | -2.81 | 2.00        | 2.05     |
| 14  | G     | 1114 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 14  | B     | 1233 | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | B     | 1213 | CLA  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 14  | G     | 1134 | CLA  | MG-ND   | -2.81 | 2.00        | 2.05     |
| 14  | a     | 1109 | CLA  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 14  | A     | 1111 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | a     | 1101 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 14  | G     | 1107 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | G     | 1114 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | a     | 1012 | CLA  | MG-NC   | 2.80  | 2.12        | 2.06     |
| 14  | b     | 1201 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | b     | 1210 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 15  | H     | 1207 | F6C  | MG-ND   | -2.80 | 1.99        | 2.06     |
| 14  | H     | 1225 | CLA  | C1B-NB  | -2.80 | 1.32        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1205 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | b     | 1232 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 15  | G     | 1121 | F6C  | C3B-C2B | 2.80  | 1.45        | 1.39     |
| 14  | A     | 1107 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | l     | 1503 | CLA  | MG-NC   | 2.80  | 2.12        | 2.06     |
| 14  | G     | 1139 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 14  | A     | 1106 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | A     | 1111 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | A     | 1114 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | a     | 1111 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | H     | 1235 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | G     | 1111 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | a     | 1112 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | A     | 1123 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | B     | 1221 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 14  | A     | 1139 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 14  | B     | 1211 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 14  | B     | 1218 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 15  | H     | 1237 | F6C  | C4B-NB  | -2.80 | 1.33        | 1.37     |
| 14  | A     | 1124 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 14  | B     | 1210 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 15  | b     | 1238 | F6C  | C4B-NB  | -2.79 | 1.33        | 1.37     |
| 21  | a     | 6001 | LMT  | O2'-C2' | -2.79 | 1.36        | 1.43     |
| 14  | a     | 1107 | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 14  | G     | 1124 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | A     | 1124 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | b     | 1227 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | K     | 1401 | CLA  | C3D-C2D | 2.79  | 1.46        | 1.39     |
| 14  | A     | 1138 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 14  | a     | 1138 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 14  | A     | 1109 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | A     | 1114 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 14  | A     | 1110 | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 14  | a     | 1107 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | H     | 1218 | CLA  | MG-ND   | -2.79 | 2.00        | 2.05     |
| 14  | a     | 1101 | CLA  | MG-ND   | -2.79 | 2.00        | 2.05     |
| 14  | a     | 1114 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 14  | a     | 1123 | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 14  | G     | 1116 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 14  | A     | 1140 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 15  | H     | 1207 | F6C  | C3C-C2C | 2.79  | 1.45        | 1.37     |
| 14  | G     | 1101 | CLA  | MG-ND   | -2.79 | 2.00        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1139 | CLA  | MG-ND   | -2.79 | 2.00        | 2.05     |
| 15  | B     | 1207 | F6C  | MG-ND   | -2.78 | 1.99        | 2.06     |
| 14  | B     | 1210 | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | G     | 1120 | CLA  | MG-ND   | -2.78 | 2.00        | 2.05     |
| 14  | G     | 1123 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 14  | G     | 1124 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 15  | B     | 1238 | F6C  | C4B-NB  | -2.78 | 1.33        | 1.37     |
| 21  | G     | 6001 | LMT  | O2'-C2' | -2.78 | 1.36        | 1.43     |
| 14  | b     | 1217 | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 14  | a     | 1107 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 21  | A     | 6001 | LMT  | O2'-C2' | -2.78 | 1.36        | 1.43     |
| 14  | k     | 1401 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 14  | a     | 1123 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 14  | H     | 1227 | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | B     | 1217 | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 14  | B     | 1227 | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | G     | 1105 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 14  | A     | 1112 | CLA  | MG-ND   | -2.78 | 2.00        | 2.05     |
| 14  | b     | 1213 | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | H     | 1210 | CLA  | MG-ND   | -2.78 | 2.00        | 2.05     |
| 14  | a     | 1013 | CLA  | C1B-NB  | -2.78 | 1.32        | 1.35     |
| 14  | T     | 1401 | CLA  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 14  | b     | 1208 | CLA  | MG-ND   | -2.78 | 2.00        | 2.05     |
| 15  | b     | 1207 | F6C  | MG-ND   | -2.78 | 1.99        | 2.06     |
| 14  | H     | 1223 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | a     | 1124 | CLA  | MG-NC   | 2.77  | 2.12        | 2.06     |
| 15  | b     | 1207 | F6C  | C3C-C2C | 2.77  | 1.45        | 1.37     |
| 14  | G     | 1140 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | b     | 1224 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | b     | 1239 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | G     | 1107 | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 14  | A     | 1105 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | B     | 1201 | CLA  | MG-ND   | -2.77 | 2.00        | 2.05     |
| 14  | B     | 1232 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | a     | 1106 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | H     | 1221 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | H     | 1224 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | H     | 1234 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | B     | 1218 | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 14  | G     | 1112 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | H     | 1217 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | H     | 1201 | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1223 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | G     | 1117 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | A     | 1116 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | A     | 1101 | CLA  | MG-ND   | -2.77 | 2.00        | 2.05     |
| 14  | a     | 1116 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 14  | a     | 1105 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | A     | 1134 | CLA  | MG-ND   | -2.77 | 2.00        | 2.05     |
| 14  | B     | 1239 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 15  | B     | 1207 | F6C  | C3C-C2C | 2.77  | 1.45        | 1.37     |
| 14  | A     | 1117 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 15  | b     | 1207 | F6C  | C1A-C2A | 2.77  | 1.51        | 1.45     |
| 14  | b     | 1218 | CLA  | MG-ND   | -2.77 | 2.00        | 2.05     |
| 14  | B     | 1224 | CLA  | C3D-C2D | 2.77  | 1.46        | 1.39     |
| 14  | a     | 1122 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | H     | 1232 | CLA  | C3D-C2D | 2.76  | 1.46        | 1.39     |
| 14  | a     | 1134 | CLA  | MG-ND   | -2.76 | 2.00        | 2.05     |
| 14  | H     | 1239 | CLA  | C3D-C2D | 2.76  | 1.46        | 1.39     |
| 14  | A     | 1112 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | b     | 1213 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | A     | 1107 | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | A     | 1131 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | b     | 1209 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | A     | 1103 | CLA  | C3D-C2D | 2.76  | 1.46        | 1.39     |
| 14  | G     | 1134 | CLA  | C3D-C2D | 2.76  | 1.46        | 1.39     |
| 14  | G     | 1111 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | A     | 1128 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | G     | 1131 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | H     | 1233 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | G     | 1110 | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | a     | 1103 | CLA  | C3D-C2D | 2.76  | 1.46        | 1.39     |
| 14  | A     | 1111 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | A     | 1122 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | H     | 1209 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | a     | 1139 | CLA  | MG-ND   | -2.76 | 2.00        | 2.05     |
| 13  | A     | 1011 | CL0  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | G     | 1107 | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | k     | 1401 | CLA  | MG-ND   | -2.76 | 2.00        | 2.05     |
| 14  | b     | 1210 | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | G     | 1128 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 14  | b     | 1211 | CLA  | MG-ND   | -2.76 | 2.00        | 2.05     |
| 14  | H     | 1235 | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | a     | 1110 | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | R     | 6001 | LMT  | O3'-C3' | -2.75 | 1.36        | 1.43     |
| 14  | B     | 1234 | CLA  | C3D-C2D | 2.75  | 1.46        | 1.39     |
| 14  | B     | 1209 | CLA  | C1C-NC  | -2.75 | 1.33        | 1.37     |
| 13  | a     | 1011 | CL0  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | G     | 1105 | CLA  | C1C-NC  | -2.75 | 1.33        | 1.37     |
| 13  | G     | 1011 | CL0  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | K     | 1401 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 15  | B     | 1237 | F6C  | C1C-NC  | -2.75 | 1.32        | 1.35     |
| 14  | G     | 1105 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 14  | A     | 1105 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 14  | A     | 1110 | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | a     | 1111 | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 14  | G     | 1122 | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 14  | a     | 1102 | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 14  | a     | 1128 | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 21  | i     | 6001 | LMT  | O3'-C3' | -2.75 | 1.36        | 1.43     |
| 14  | b     | 1235 | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | A     | 1134 | CLA  | C3D-C2D | 2.75  | 1.46        | 1.39     |
| 14  | G     | 1137 | CLA  | C3D-C2D | 2.75  | 1.46        | 1.39     |
| 15  | B     | 1238 | F6C  | C3C-C2C | 2.75  | 1.45        | 1.37     |
| 14  | G     | 1112 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 14  | T     | 1401 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 14  | H     | 1210 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | G     | 1102 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | H     | 1218 | CLA  | C1C-NC  | -2.74 | 1.33        | 1.37     |
| 15  | H     | 1207 | F6C  | C1A-C2A | 2.74  | 1.51        | 1.45     |
| 14  | B     | 1235 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | A     | 1139 | CLA  | MG-ND   | -2.74 | 2.00        | 2.05     |
| 14  | G     | 1103 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | a     | 1112 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 21  | I     | 6001 | LMT  | O3'-C3' | -2.74 | 1.36        | 1.43     |
| 14  | a     | 1131 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | a     | 1134 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | a     | 1117 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | B     | 1220 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | a     | 1137 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | H     | 1225 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | b     | 1223 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | A     | 1102 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | a     | 1105 | CLA  | MG-ND   | -2.74 | 2.00        | 2.05     |
| 14  | H     | 1220 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | G     | 1101 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1201 | CLA  | C1C-NC  | -2.74 | 1.33        | 1.37     |
| 14  | b     | 1225 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | B     | 1226 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 14  | a     | 1105 | CLA  | C1C-NC  | -2.74 | 1.33        | 1.37     |
| 14  | H     | 1239 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | A     | 1101 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 14  | B     | 1225 | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 15  | H     | 1238 | F6C  | C3C-C2C | 2.73  | 1.45        | 1.37     |
| 14  | A     | 1013 | CLA  | C1B-NB  | -2.73 | 1.32        | 1.35     |
| 14  | G     | 1137 | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | H     | 1224 | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | B     | 1022 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 14  | A     | 1132 | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 15  | b     | 1238 | F6C  | C3C-C2C | 2.73  | 1.45        | 1.37     |
| 14  | A     | 1137 | CLA  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 14  | b     | 1220 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 14  | H     | 1022 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 14  | a     | 1136 | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 15  | H     | 1230 | F6C  | C1D-C2D | 2.73  | 1.49        | 1.44     |
| 14  | m     | 1501 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 14  | b     | 1234 | CLA  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 14  | a     | 1101 | CLA  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 14  | b     | 1233 | CLA  | MG-ND   | -2.72 | 2.00        | 2.05     |
| 14  | A     | 1105 | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 15  | B     | 1207 | F6C  | C1A-C2A | 2.72  | 1.51        | 1.45     |
| 15  | H     | 1237 | F6C  | C1C-NC  | -2.72 | 1.32        | 1.35     |
| 14  | M     | 1501 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | G     | 1136 | CLA  | MG-NC   | 2.72  | 2.12        | 2.06     |
| 14  | H     | 1201 | CLA  | MG-ND   | -2.72 | 2.00        | 2.05     |
| 14  | H     | 1233 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | b     | 1022 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | B     | 1201 | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 14  | a     | 1104 | CLA  | MG-ND   | -2.72 | 2.00        | 2.05     |
| 14  | U     | 1501 | CLA  | C3D-C2D | 2.72  | 1.46        | 1.39     |
| 14  | H     | 1226 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | B     | 1233 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | H     | 1222 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 21  | G     | 6003 | LMT  | O3'-C3' | -2.72 | 1.36        | 1.43     |
| 14  | G     | 1133 | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 14  | b     | 1224 | CLA  | MG-NC   | 2.72  | 2.12        | 2.06     |
| 21  | B     | 6001 | LMT  | O3'-C3' | -2.72 | 1.36        | 1.43     |
| 14  | L     | 1501 | CLA  | C3D-C2D | 2.72  | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | l     | 1501 | CLA  | C3D-C2D | 2.72  | 1.46        | 1.39     |
| 14  | b     | 1231 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | G     | 1141 | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 14  | A     | 1137 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | a     | 1138 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | A     | 1104 | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 14  | G     | 1104 | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 14  | B     | 1215 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | b     | 1226 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 21  | H     | 6001 | LMT  | O3'-C3' | -2.71 | 1.36        | 1.43     |
| 14  | B     | 1206 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | H     | 1222 | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 14  | A     | 1127 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | G     | 1138 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | b     | 1233 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | A     | 1136 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | A     | 1012 | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | H     | 1215 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | V     | 1501 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | a     | 1136 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | b     | 1222 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | H     | 1208 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | H     | 1208 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | B     | 1231 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | A     | 1138 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | B     | 1224 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | A     | 1106 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | B     | 1208 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | A     | 1141 | CLA  | MG-ND   | -2.70 | 2.00        | 2.05     |
| 14  | a     | 1134 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | H     | 1203 | CLA  | C3D-C2D | 2.70  | 1.46        | 1.39     |
| 14  | H     | 1206 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | b     | 1215 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 21  | G     | 6002 | LMT  | O3B-C3B | -2.70 | 1.36        | 1.43     |
| 14  | B     | 1222 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | B     | 1239 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | B     | 1208 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | a     | 1110 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | G     | 1127 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | a     | 1133 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | b     | 1206 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | a     | 1127 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1133 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | G     | 1123 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | G     | 1132 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | b     | 1208 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 21  | A     | 6003 | LMT  | O3'-C3' | -2.70 | 1.36        | 1.43     |
| 14  | a     | 1106 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | b     | 1231 | CLA  | C3D-C2D | 2.70  | 1.46        | 1.39     |
| 14  | G     | 1105 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | b     | 1222 | CLA  | MG-ND   | -2.70 | 2.00        | 2.05     |
| 14  | G     | 1110 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 21  | A     | 6002 | LMT  | O3B-C3B | -2.70 | 1.36        | 1.43     |
| 14  | A     | 1136 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | G     | 1106 | CLA  | C4D-CHA | 2.70  | 1.48        | 1.38     |
| 14  | H     | 1231 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | A     | 1134 | CLA  | C4D-CHA | 2.69  | 1.48        | 1.38     |
| 14  | B     | 1214 | CLA  | C4D-CHA | 2.69  | 1.48        | 1.38     |
| 14  | a     | 1132 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | a     | 1118 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 14  | B     | 1233 | CLA  | MG-ND   | -2.69 | 2.00        | 2.05     |
| 14  | b     | 1214 | CLA  | C4D-CHA | 2.69  | 1.48        | 1.38     |
| 14  | A     | 1118 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 15  | H     | 1237 | F6C  | C3C-C2C | 2.69  | 1.45        | 1.37     |
| 14  | A     | 1114 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 21  | a     | 6002 | LMT  | O3B-C3B | -2.69 | 1.36        | 1.43     |
| 14  | b     | 1208 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | B     | 1225 | CLA  | C3D-C2D | 2.69  | 1.46        | 1.39     |
| 14  | b     | 1239 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | G     | 1136 | CLA  | C4D-CHA | 2.69  | 1.48        | 1.38     |
| 14  | a     | 1133 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | G     | 1012 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 15  | B     | 1237 | F6C  | C3C-C2C | 2.69  | 1.45        | 1.37     |
| 15  | b     | 1237 | F6C  | C3C-C2C | 2.69  | 1.45        | 1.37     |
| 14  | a     | 1105 | CLA  | C4D-CHA | 2.69  | 1.48        | 1.38     |
| 21  | b     | 6001 | LMT  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 14  | G     | 1133 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | B     | 1222 | CLA  | MG-ND   | -2.69 | 2.00        | 2.05     |
| 14  | H     | 1233 | CLA  | MG-ND   | -2.69 | 2.00        | 2.05     |
| 14  | B     | 1203 | CLA  | C3D-C2D | 2.69  | 1.46        | 1.39     |
| 14  | a     | 1106 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 14  | A     | 1106 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 14  | G     | 1134 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 14  | A     | 1126 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1118 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 14  | A     | 1123 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | A     | 1110 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | A     | 1125 | CLA  | OBD-CAD | 2.68  | 1.27        | 1.22     |
| 14  | a     | 1126 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | A     | 1133 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | G     | 1130 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | B     | 1240 | CLA  | MG-ND   | -2.68 | 2.00        | 2.05     |
| 21  | H     | 6002 | LMT  | O3'-C3' | -2.68 | 1.36        | 1.43     |
| 14  | b     | 1225 | CLA  | C3D-C2D | 2.68  | 1.46        | 1.39     |
| 21  | B     | 6002 | LMT  | O3'-C3' | -2.68 | 1.36        | 1.43     |
| 21  | A     | 6001 | LMT  | O3B-C3B | -2.68 | 1.36        | 1.43     |
| 14  | B     | 1213 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | a     | 1141 | CLA  | MG-ND   | -2.68 | 2.00        | 2.05     |
| 14  | A     | 1105 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | H     | 1214 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | G     | 1114 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 14  | G     | 1126 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | a     | 1123 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | H     | 1202 | CLA  | C3D-C2D | 2.68  | 1.46        | 1.39     |
| 14  | b     | 1213 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 14  | H     | 1231 | CLA  | C3D-C2D | 2.68  | 1.46        | 1.39     |
| 21  | a     | 6003 | LMT  | O3'-C3' | -2.68 | 1.36        | 1.43     |
| 14  | a     | 1132 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 15  | B     | 1230 | F6C  | C1C-CHC | 2.68  | 1.48        | 1.41     |
| 14  | b     | 1222 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 21  | b     | 6002 | LMT  | O3'-C3' | -2.67 | 1.36        | 1.43     |
| 14  | H     | 1228 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 14  | B     | 1222 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 14  | H     | 1225 | CLA  | C3D-C2D | 2.67  | 1.46        | 1.39     |
| 14  | H     | 1240 | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 14  | b     | 1228 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 14  | B     | 1202 | CLA  | C3D-C2D | 2.67  | 1.46        | 1.39     |
| 14  | B     | 1231 | CLA  | C3D-C2D | 2.67  | 1.46        | 1.39     |
| 15  | B     | 1230 | F6C  | C1D-C2D | 2.67  | 1.49        | 1.44     |
| 14  | H     | 1222 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 14  | a     | 1137 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 14  | b     | 1203 | CLA  | C3D-C2D | 2.67  | 1.46        | 1.39     |
| 21  | a     | 6001 | LMT  | O3B-C3B | -2.67 | 1.36        | 1.43     |
| 21  | G     | 6001 | LMT  | O3B-C3B | -2.67 | 1.36        | 1.43     |
| 14  | a     | 1012 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | B     | 1228 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1210 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 15  | H     | 1230 | F6C  | C1C-CHC | 2.66  | 1.48        | 1.41     |
| 14  | b     | 1239 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 14  | A     | 1102 | CLA  | MG-ND   | -2.66 | 2.00        | 2.05     |
| 14  | b     | 1240 | CLA  | MG-ND   | -2.66 | 2.00        | 2.05     |
| 15  | B     | 1238 | F6C  | C3D-C2D | 2.66  | 1.46        | 1.39     |
| 14  | a     | 1114 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 15  | b     | 1230 | F6C  | C1C-CHC | 2.66  | 1.48        | 1.41     |
| 15  | H     | 1238 | F6C  | C3D-C2D | 2.66  | 1.46        | 1.39     |
| 14  | G     | 1125 | CLA  | OBD-CAD | 2.66  | 1.27        | 1.22     |
| 14  | a     | 1130 | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 15  | b     | 1230 | F6C  | C1D-C2D | 2.66  | 1.49        | 1.44     |
| 14  | B     | 1205 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 14  | B     | 1221 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 14  | G     | 1102 | CLA  | MG-ND   | -2.66 | 2.00        | 2.05     |
| 14  | b     | 1210 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 14  | B     | 1210 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 14  | H     | 1213 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 14  | G     | 1013 | CLA  | C1B-NB  | -2.66 | 1.32        | 1.35     |
| 21  | a     | 6001 | LMT  | O2B-C2B | -2.66 | 1.36        | 1.43     |
| 21  | a     | 6004 | LMT  | O3'-C3' | -2.66 | 1.36        | 1.43     |
| 14  | G     | 1106 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | H     | 1236 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | a     | 1125 | CLA  | OBD-CAD | 2.65  | 1.27        | 1.22     |
| 14  | B     | 1239 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | K     | 1401 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | G     | 1120 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | T     | 1401 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | G     | 1102 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 21  | A     | 6004 | LMT  | O3'-C3' | -2.65 | 1.36        | 1.43     |
| 14  | B     | 1216 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | b     | 1221 | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 14  | A     | 1132 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 21  | L     | 6101 | LMT  | O3'-C3' | -2.65 | 1.36        | 1.43     |
| 14  | A     | 1126 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | G     | 1132 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 15  | b     | 1230 | F6C  | CHB-C4A | -2.65 | 1.33        | 1.38     |
| 14  | A     | 1130 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | H     | 1204 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | A     | 1120 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | b     | 1205 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | a     | 1102 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1120 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | a     | 1115 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | b     | 1209 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | H     | 1216 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | k     | 1401 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 14  | B     | 1228 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | b     | 1228 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | G     | 1124 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 21  | b     | 6004 | LMT  | O2'-C2' | -2.65 | 1.36        | 1.43     |
| 14  | A     | 1102 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | b     | 1236 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | G     | 1119 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | B     | 1209 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | a     | 1104 | CLA  | C3D-C2D | 2.64  | 1.46        | 1.39     |
| 14  | K     | 1401 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 14  | a     | 1120 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 21  | G     | 6001 | LMT  | O2B-C2B | -2.64 | 1.36        | 1.43     |
| 14  | G     | 1126 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | H     | 1239 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | A     | 1104 | CLA  | C3D-C2D | 2.64  | 1.46        | 1.39     |
| 21  | l     | 6101 | LMT  | O3'-C3' | -2.64 | 1.36        | 1.43     |
| 14  | B     | 1203 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | a     | 1117 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | a     | 1102 | CLA  | MG-ND   | -2.64 | 2.00        | 2.05     |
| 14  | a     | 1125 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 21  | G     | 6004 | LMT  | O3'-C3' | -2.64 | 1.36        | 1.43     |
| 14  | b     | 1202 | CLA  | C3D-C2D | 2.64  | 1.46        | 1.39     |
| 15  | b     | 1238 | F6C  | C3D-C2D | 2.64  | 1.46        | 1.39     |
| 14  | b     | 1216 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | H     | 1205 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | B     | 1231 | CLA  | MG-ND   | -2.64 | 2.00        | 2.05     |
| 14  | A     | 1124 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | A     | 1107 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | H     | 1215 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | a     | 1124 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | G     | 1125 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | A     | 1117 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 15  | B     | 1207 | F6C  | CMB-C2B | 2.64  | 1.50        | 1.45     |
| 15  | b     | 1207 | F6C  | CMB-C2B | 2.64  | 1.50        | 1.45     |
| 14  | a     | 1107 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 14  | G     | 1120 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | G     | 1134 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | a     | 6002 | LMT  | O2B-C2B | -2.64 | 1.36        | 1.43     |
| 14  | a     | 1119 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 21  | U     | 6101 | LMT  | O3'-C3' | -2.63 | 1.36        | 1.43     |
| 14  | A     | 1113 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 14  | a     | 1126 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | B     | 1236 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | b     | 1201 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | H     | 1211 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 15  | B     | 1230 | F6C  | CHB-C4A | -2.63 | 1.33        | 1.38     |
| 14  | B     | 1227 | CLA  | C3D-C2D | 2.63  | 1.46        | 1.39     |
| 14  | A     | 1129 | CLA  | C3D-C2D | 2.63  | 1.46        | 1.39     |
| 14  | b     | 1231 | CLA  | MG-ND   | -2.63 | 2.00        | 2.05     |
| 21  | G     | 6002 | LMT  | O2B-C2B | -2.63 | 1.36        | 1.43     |
| 14  | H     | 1221 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 14  | A     | 1113 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | G     | 1129 | CLA  | C3D-C2D | 2.63  | 1.46        | 1.39     |
| 14  | b     | 1203 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | a     | 1139 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 14  | G     | 1117 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | H     | 1209 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | B     | 1217 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 14  | a     | 1134 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 14  | V     | 1501 | CLA  | C3D-C2D | 2.63  | 1.46        | 1.39     |
| 14  | A     | 1119 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | G     | 1113 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | A     | 1134 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 14  | G     | 1108 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | L     | 1502 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | b     | 1225 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | B     | 1211 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 21  | A     | 6002 | LMT  | O2B-C2B | -2.63 | 1.36        | 1.43     |
| 14  | A     | 1108 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 14  | G     | 1117 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | B     | 1227 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | a     | 1129 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | H     | 1229 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | H     | 1217 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | b     | 1217 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | H     | 1228 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | H     | 1227 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | U     | 1502 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 15  | H     | 1230 | F6C  | C4C-CHD | 2.62  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1137 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | G     | 1107 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | H     | 1201 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 21  | A     | 6001 | LMT  | O2B-C2B | -2.62 | 1.36        | 1.43     |
| 14  | H     | 1203 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | B     | 1236 | CLA  | OBD-CAD | 2.62  | 1.27        | 1.22     |
| 14  | G     | 1104 | CLA  | C3D-C2D | 2.62  | 1.46        | 1.39     |
| 14  | B     | 1215 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | B     | 1229 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | G     | 1129 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | B     | 1240 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | A     | 1129 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | B     | 1201 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | G     | 1129 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | b     | 1204 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | A     | 1125 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | A     | 1115 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | B     | 1204 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 21  | b     | 6003 | LMT  | O3'-C3' | -2.62 | 1.36        | 1.43     |
| 14  | b     | 1227 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | a     | 1113 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 14  | b     | 1227 | CLA  | C3D-C2D | 2.62  | 1.46        | 1.39     |
| 14  | a     | 1117 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | a     | 1120 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | l     | 1502 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | b     | 1211 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 15  | H     | 1230 | F6C  | CHB-C4A | -2.61 | 1.33        | 1.38     |
| 14  | M     | 1501 | CLA  | C3D-C2D | 2.61  | 1.46        | 1.39     |
| 14  | b     | 1236 | CLA  | OBD-CAD | 2.61  | 1.27        | 1.22     |
| 21  | a     | 6002 | LMT  | O2'-C2' | -2.61 | 1.36        | 1.43     |
| 15  | H     | 1207 | F6C  | CMB-C2B | 2.61  | 1.50        | 1.45     |
| 15  | A     | 1121 | F6C  | C1A-C2A | 2.61  | 1.51        | 1.45     |
| 14  | A     | 1117 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 21  | B     | 6003 | LMT  | O3'-C3' | -2.61 | 1.36        | 1.43     |
| 21  | H     | 6003 | LMT  | O3'-C3' | -2.61 | 1.36        | 1.43     |
| 14  | H     | 1203 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | G     | 1115 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | A     | 1129 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | a     | 1113 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 14  | b     | 1240 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 14  | H     | 1231 | CLA  | MG-ND   | -2.61 | 2.00        | 2.05     |
| 14  | b     | 1215 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | B     | 6004 | LMT  | O2'-C2' | -2.61 | 1.36        | 1.43     |
| 14  | B     | 1203 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | B     | 1216 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | a     | 1108 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | B     | 1218 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | A     | 1137 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 15  | G     | 1121 | F6C  | C1A-C2A | 2.61  | 1.51        | 1.45     |
| 14  | B     | 1225 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | b     | 1211 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 14  | A     | 1130 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 21  | G     | 6002 | LMT  | O2'-C2' | -2.60 | 1.36        | 1.43     |
| 14  | k     | 1401 | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 14  | a     | 1129 | CLA  | C3D-C2D | 2.60  | 1.46        | 1.39     |
| 14  | b     | 1231 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | T     | 1401 | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 14  | b     | 1234 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | b     | 1216 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | G     | 1130 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1225 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | A     | 1122 | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |
| 14  | A     | 1139 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 14  | B     | 1231 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | B     | 1211 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1240 | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 14  | a     | 1122 | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |
| 14  | a     | 1130 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | b     | 1021 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 15  | b     | 1219 | F6C  | CMB-C2B | 2.60  | 1.50        | 1.45     |
| 14  | H     | 1227 | CLA  | C3D-C2D | 2.60  | 1.46        | 1.39     |
| 14  | b     | 1218 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1218 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1211 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1021 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | b     | 1229 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 14  | H     | 1234 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 21  | H     | 6004 | LMT  | O2'-C2' | -2.59 | 1.36        | 1.43     |
| 14  | B     | 1021 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 14  | L     | 1503 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 14  | B     | 1212 | CLA  | MG-NC   | 2.59  | 2.12        | 2.06     |
| 14  | a     | 1012 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 14  | b     | 1212 | CLA  | MG-NC   | 2.59  | 2.12        | 2.06     |
| 14  | H     | 1216 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1234 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 14  | H     | 1231 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 14  | m     | 1501 | CLA  | C3D-C2D | 2.59  | 1.46        | 1.39     |
| 15  | a     | 1121 | F6C  | C1A-C2A | 2.59  | 1.51        | 1.45     |
| 14  | G     | 1137 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 21  | A     | 6002 | LMT  | O2'-C2' | -2.59 | 1.36        | 1.43     |
| 14  | G     | 1135 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 15  | H     | 1219 | F6C  | CMB-C2B | 2.59  | 1.50        | 1.45     |
| 15  | b     | 1230 | F6C  | CMB-C2B | 2.59  | 1.50        | 1.45     |
| 14  | B     | 1236 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | H     | 1236 | CLA  | OBD-CAD | 2.59  | 1.26        | 1.22     |
| 14  | G     | 1139 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | b     | 1236 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | G     | 1122 | CLA  | MG-NC   | 2.58  | 2.12        | 2.06     |
| 18  | R     | 4020 | BCR  | C21-C22 | -2.58 | 1.32        | 1.35     |
| 14  | A     | 1012 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 14  | a     | 1135 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 14  | a     | 1129 | CLA  | MG-NC   | 2.58  | 2.12        | 2.06     |
| 15  | B     | 1230 | F6C  | CMB-C2B | 2.58  | 1.50        | 1.45     |
| 15  | B     | 1230 | F6C  | C4C-CHD | 2.58  | 1.48        | 1.41     |
| 15  | B     | 1219 | F6C  | CMB-C2B | 2.58  | 1.50        | 1.45     |
| 15  | H     | 1230 | F6C  | CMB-C2B | 2.58  | 1.50        | 1.45     |
| 14  | l     | 1503 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 14  | A     | 1125 | CLA  | C3D-C2D | 2.58  | 1.46        | 1.39     |
| 14  | b     | 1022 | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 14  | U     | 1503 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 14  | M     | 1501 | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 15  | b     | 1230 | F6C  | C4C-CHD | 2.58  | 1.48        | 1.41     |
| 14  | A     | 1135 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 18  | i     | 4020 | BCR  | C17-C18 | -2.58 | 1.32        | 1.35     |
| 18  | i     | 4020 | BCR  | C21-C22 | -2.57 | 1.32        | 1.35     |
| 14  | H     | 1212 | CLA  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 14  | H     | 1229 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | G     | 1113 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | b     | 1205 | CLA  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 14  | B     | 1022 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | G     | 1012 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 14  | A     | 1013 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 14  | b     | 1203 | CLA  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 14  | G     | 1013 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 14  | B     | 1205 | CLA  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 21  | G     | 6003 | LMT  | O2'-C2' | -2.57 | 1.36        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | I     | 4020 | BCR  | C17-C18 | -2.57 | 1.32        | 1.35     |
| 14  | G     | 1125 | CLA  | C3D-C2D | 2.57  | 1.46        | 1.39     |
| 14  | A     | 1116 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | a     | 1125 | CLA  | C3D-C2D | 2.57  | 1.46        | 1.39     |
| 15  | B     | 1219 | F6C  | C1C-CHC | 2.57  | 1.48        | 1.41     |
| 14  | a     | 1118 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 15  | H     | 1219 | F6C  | C1C-CHC | 2.57  | 1.48        | 1.41     |
| 21  | B     | 6001 | LMT  | O2'-C2' | -2.56 | 1.36        | 1.43     |
| 21  | H     | 6001 | LMT  | O2'-C2' | -2.56 | 1.36        | 1.43     |
| 14  | B     | 1206 | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | m     | 1501 | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 18  | I     | 4020 | BCR  | C21-C22 | -2.56 | 1.32        | 1.35     |
| 15  | H     | 1230 | F6C  | C1D-ND  | -2.56 | 1.34        | 1.37     |
| 14  | B     | 1022 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | H     | 1206 | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | B     | 1218 | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | H     | 1224 | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 14  | a     | 1013 | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 14  | H     | 1022 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | H     | 1236 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | b     | 1218 | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | A     | 1101 | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 14  | b     | 1224 | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 15  | b     | 1219 | F6C  | C4C-CHD | 2.56  | 1.48        | 1.41     |
| 14  | V     | 1501 | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 14  | a     | 1116 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 21  | U     | 6002 | LMT  | O2'-C2' | -2.55 | 1.37        | 1.43     |
| 14  | M     | 1501 | CLA  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 21  | b     | 6001 | LMT  | O2'-C2' | -2.55 | 1.37        | 1.43     |
| 14  | b     | 1233 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 14  | B     | 1224 | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 18  | L     | 4019 | BCR  | C21-C22 | -2.55 | 1.32        | 1.35     |
| 14  | a     | 1101 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | G     | 1116 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 15  | b     | 1219 | F6C  | C1C-CHC | 2.55  | 1.48        | 1.41     |
| 14  | a     | 1138 | CLA  | MG-ND   | -2.55 | 2.00        | 2.05     |
| 15  | B     | 1219 | F6C  | C4C-CHD | 2.55  | 1.48        | 1.41     |
| 14  | G     | 1118 | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 14  | G     | 1103 | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 14  | H     | 1205 | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | V     | 1501 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | b     | 1022 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1116 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 21  | b     | 6002 | LMT  | O2'-C2' | -2.54 | 1.37        | 1.43     |
| 21  | l     | 6002 | LMT  | O2'-C2' | -2.54 | 1.37        | 1.43     |
| 14  | B     | 1229 | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 14  | b     | 1229 | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 14  | H     | 1218 | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 14  | A     | 1101 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | m     | 1501 | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 21  | V     | 6000 | LMT  | O3B-C3B | -2.54 | 1.37        | 1.43     |
| 15  | H     | 1219 | F6C  | C4C-CHD | 2.54  | 1.48        | 1.41     |
| 21  | M     | 6000 | LMT  | O3B-C3B | -2.54 | 1.37        | 1.43     |
| 14  | B     | 1233 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | A     | 1118 | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 15  | B     | 1230 | F6C  | C1D-ND  | -2.54 | 1.34        | 1.37     |
| 21  | a     | 6003 | LMT  | O2'-C2' | -2.54 | 1.37        | 1.43     |
| 14  | H     | 1023 | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 14  | A     | 1128 | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 21  | L     | 6002 | LMT  | O2'-C2' | -2.54 | 1.37        | 1.43     |
| 14  | U     | 1502 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 21  | B     | 6002 | LMT  | O2'-C2' | -2.53 | 1.37        | 1.43     |
| 14  | H     | 1235 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 14  | H     | 1022 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 14  | G     | 1113 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | l     | 1501 | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 15  | B     | 1238 | F6C  | CHB-C4A | -2.53 | 1.33        | 1.38     |
| 14  | b     | 1236 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 14  | H     | 1202 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 14  | U     | 1501 | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 14  | G     | 1101 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 15  | a     | 1121 | F6C  | C1D-C2D | 2.53  | 1.49        | 1.44     |
| 14  | b     | 1202 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 14  | b     | 1235 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 15  | G     | 1121 | F6C  | C1D-C2D | 2.53  | 1.49        | 1.44     |
| 14  | A     | 1116 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | G     | 1101 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | L     | 1501 | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 14  | B     | 1202 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 21  | A     | 6003 | LMT  | O2'-C2' | -2.53 | 1.37        | 1.43     |
| 14  | b     | 1202 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | L     | 1502 | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 14  | A     | 1138 | CLA  | MG-ND   | -2.52 | 2.00        | 2.05     |
| 14  | l     | 1502 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1138 | CLA  | MG-ND   | -2.52 | 2.00        | 2.05     |
| 14  | a     | 1101 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | A     | 1103 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 14  | a     | 1116 | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 14  | B     | 1235 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 14  | G     | 1128 | CLA  | MG-NC   | 2.52  | 2.12        | 2.06     |
| 15  | A     | 1121 | F6C  | C1D-C2D | 2.52  | 1.49        | 1.44     |
| 14  | B     | 1236 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 21  | m     | 6000 | LMT  | O3B-C3B | -2.52 | 1.37        | 1.43     |
| 14  | A     | 1117 | CLA  | MG-ND   | -2.52 | 2.00        | 2.05     |
| 21  | H     | 6002 | LMT  | O2'-C2' | -2.52 | 1.37        | 1.43     |
| 15  | b     | 1230 | F6C  | C1D-ND  | -2.52 | 1.34        | 1.37     |
| 18  | R     | 4020 | BCR  | C17-C18 | -2.52 | 1.32        | 1.35     |
| 14  | a     | 1103 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 14  | B     | 1202 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | B     | 1234 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | b     | 1206 | CLA  | MG-NC   | 2.52  | 2.12        | 2.06     |
| 14  | A     | 1113 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | B     | 1214 | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 15  | H     | 1238 | F6C  | CHB-C4A | -2.52 | 1.33        | 1.38     |
| 14  | H     | 1236 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 14  | G     | 1139 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 14  | L     | 1501 | CLA  | C4D-CHA | 2.51  | 1.47        | 1.38     |
| 14  | H     | 1233 | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 15  | b     | 1238 | F6C  | CHB-C4A | -2.51 | 1.33        | 1.38     |
| 14  | b     | 1214 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 14  | B     | 1023 | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | a     | 1128 | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | l     | 1501 | CLA  | C4D-CHA | 2.51  | 1.47        | 1.38     |
| 14  | G     | 1141 | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 15  | a     | 1121 | F6C  | MG-ND   | -2.51 | 2.00        | 2.06     |
| 14  | b     | 1231 | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 14  | H     | 1240 | CLA  | C1D-C2D | 2.50  | 1.50        | 1.45     |
| 14  | G     | 1104 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 14  | H     | 1234 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 18  | l     | 4019 | BCR  | C21-C22 | -2.50 | 1.32        | 1.35     |
| 15  | G     | 1121 | F6C  | MG-ND   | -2.50 | 2.00        | 2.06     |
| 14  | b     | 1021 | CLA  | MG-NC   | 2.50  | 2.12        | 2.06     |
| 14  | a     | 1117 | CLA  | MG-ND   | -2.50 | 2.00        | 2.05     |
| 14  | H     | 1201 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 14  | U     | 1501 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 13  | A     | 1011 | CL0  | C4D-CHA | 2.50  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1104 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 14  | b     | 1234 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 14  | b     | 1023 | CLA  | MG-NC   | 2.50  | 2.12        | 2.06     |
| 14  | A     | 1104 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 14  | a     | 1113 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 13  | G     | 1011 | CL0  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 14  | b     | 1201 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 13  | a     | 1011 | CL0  | C4D-CHA | 2.49  | 1.47        | 1.38     |
| 14  | B     | 1201 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 18  | U     | 4019 | BCR  | C21-C22 | -2.49 | 1.32        | 1.35     |
| 14  | b     | 1213 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | B     | 1213 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | H     | 1202 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | k     | 1401 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 13  | a     | 1011 | CL0  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 15  | A     | 1121 | F6C  | MG-ND   | -2.49 | 2.00        | 2.06     |
| 14  | a     | 1115 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | T     | 1401 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 14  | H     | 1214 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 14  | K     | 1401 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 15  | G     | 1121 | F6C  | C4C-CHD | 2.48  | 1.47        | 1.41     |
| 14  | H     | 1231 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | a     | 1139 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 14  | G     | 1117 | CLA  | MG-ND   | -2.48 | 2.00        | 2.05     |
| 14  | b     | 1240 | CLA  | C1D-C2D | 2.48  | 1.50        | 1.45     |
| 14  | B     | 1021 | CLA  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 14  | a     | 1110 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 21  | V     | 6000 | LMT  | O2'-C2' | -2.48 | 1.37        | 1.43     |
| 14  | G     | 1107 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | A     | 1141 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | H     | 1213 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | B     | 1231 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | b     | 1023 | CLA  | C4D-CHA | 2.48  | 1.47        | 1.38     |
| 14  | l     | 1501 | CLA  | MG-ND   | -2.48 | 2.00        | 2.05     |
| 14  | k     | 1401 | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 13  | A     | 1011 | CL0  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | A     | 1139 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 14  | A     | 1107 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 14  | T     | 1401 | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | a     | 1141 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 14  | A     | 1110 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 14  | A     | 1141 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | G     | 1011 | CL0  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | L     | 1501 | CLA  | MG-ND   | -2.47 | 2.00        | 2.05     |
| 14  | H     | 1223 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 14  | a     | 1107 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 15  | A     | 1121 | F6C  | C4C-CHD | 2.47  | 1.47        | 1.41     |
| 15  | b     | 1230 | F6C  | C1A-C2A | 2.47  | 1.50        | 1.45     |
| 14  | B     | 1240 | CLA  | C1D-C2D | 2.46  | 1.50        | 1.45     |
| 14  | U     | 1501 | CLA  | MG-ND   | -2.46 | 2.00        | 2.05     |
| 14  | T     | 1401 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 14  | A     | 1115 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 14  | B     | 1023 | CLA  | C4D-CHA | 2.46  | 1.47        | 1.38     |
| 21  | M     | 6000 | LMT  | O2'-C2' | -2.46 | 1.37        | 1.43     |
| 14  | G     | 1110 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 21  | m     | 6000 | LMT  | O2'-C2' | -2.46 | 1.37        | 1.43     |
| 14  | B     | 1232 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 15  | H     | 1230 | F6C  | C1A-C2A | 2.45  | 1.50        | 1.45     |
| 14  | H     | 1229 | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 15  | a     | 1121 | F6C  | C4C-CHD | 2.45  | 1.47        | 1.41     |
| 14  | K     | 1401 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 14  | K     | 1401 | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 21  | i     | 6001 | LMT  | O2'-C2' | -2.45 | 1.37        | 1.43     |
| 14  | H     | 1021 | CLA  | MG-NC   | 2.45  | 2.12        | 2.06     |
| 14  | A     | 1135 | CLA  | C3D-C2D | 2.45  | 1.45        | 1.39     |
| 14  | H     | 1021 | CLA  | C1B-NB  | -2.45 | 1.33        | 1.35     |
| 14  | G     | 1113 | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 14  | G     | 1101 | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 14  | B     | 1223 | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 14  | B     | 1021 | CLA  | C3A-C2A | -2.45 | 1.47        | 1.54     |
| 14  | G     | 1135 | CLA  | C3D-C2D | 2.45  | 1.45        | 1.39     |
| 14  | G     | 1119 | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 14  | B     | 1021 | CLA  | C1B-NB  | -2.44 | 1.33        | 1.35     |
| 14  | G     | 1115 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | a     | 1141 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 14  | H     | 1232 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 14  | b     | 1223 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | b     | 1021 | CLA  | C1B-NB  | -2.44 | 1.33        | 1.35     |
| 14  | b     | 1204 | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 14  | b     | 1231 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 14  | k     | 1401 | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 14  | A     | 1111 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | a     | 1101 | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 15  | B     | 1230 | F6C  | C1A-C2A | 2.44  | 1.50        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1119 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | a     | 1135 | CLA  | C3D-C2D | 2.44  | 1.45        | 1.39     |
| 14  | b     | 1229 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | G     | 1141 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 14  | H     | 1023 | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 14  | B     | 1204 | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 14  | B     | 1229 | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 14  | b     | 1021 | CLA  | C3A-C2A | -2.43 | 1.47        | 1.54     |
| 14  | a     | 1111 | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 21  | R     | 6001 | LMT  | O2'-C2' | -2.43 | 1.37        | 1.43     |
| 21  | I     | 6001 | LMT  | O2'-C2' | -2.43 | 1.37        | 1.43     |
| 14  | b     | 1232 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | A     | 1101 | CLA  | C1B-CHB | 2.43  | 1.47        | 1.41     |
| 14  | H     | 1231 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | H     | 1021 | CLA  | C3A-C2A | -2.43 | 1.47        | 1.54     |
| 21  | l     | 6002 | LMT  | O3B-C3B | -2.43 | 1.37        | 1.43     |
| 14  | H     | 1204 | CLA  | C4D-CHA | 2.43  | 1.47        | 1.38     |
| 14  | G     | 1111 | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 14  | B     | 1231 | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 14  | H     | 1209 | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 14  | a     | 1113 | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 14  | a     | 1119 | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 21  | b     | 6002 | LMT  | O2B-C2B | -2.42 | 1.37        | 1.43     |
| 14  | a     | 1138 | CLA  | C1D-C2D | 2.42  | 1.50        | 1.45     |
| 21  | l     | 6002 | LMT  | O4'-C4B | -2.42 | 1.37        | 1.43     |
| 14  | G     | 1108 | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 14  | G     | 1133 | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 14  | a     | 1114 | CLA  | C1D-C2D | 2.41  | 1.50        | 1.45     |
| 14  | A     | 1113 | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 14  | H     | 1217 | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 21  | L     | 6002 | LMT  | O4'-C4B | -2.41 | 1.37        | 1.43     |
| 14  | G     | 1118 | CLA  | C4B-CHC | 2.41  | 1.47        | 1.41     |
| 14  | b     | 1202 | CLA  | MG-NC   | 2.41  | 2.12        | 2.06     |
| 14  | B     | 1202 | CLA  | MG-NC   | 2.41  | 2.12        | 2.06     |
| 14  | H     | 1202 | CLA  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 14  | G     | 1102 | CLA  | C1D-C2D | 2.40  | 1.50        | 1.45     |
| 14  | B     | 1217 | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | a     | 1013 | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 14  | H     | 1221 | CLA  | C1B-NB  | -2.40 | 1.33        | 1.35     |
| 14  | A     | 1133 | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 21  | B     | 6004 | LMT  | O3'-C3' | -2.40 | 1.37        | 1.43     |
| 14  | A     | 1114 | CLA  | C1D-C2D | 2.40  | 1.50        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1236 | CLA  | C3D-C2D | 2.40  | 1.45        | 1.39     |
| 14  | A     | 1108 | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 15  | B     | 1230 | F6C  | MG-ND   | -2.40 | 2.00        | 2.06     |
| 14  | b     | 1218 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 21  | L     | 6002 | LMT  | O3B-C3B | -2.39 | 1.37        | 1.43     |
| 14  | H     | 1218 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 21  | i     | 6001 | LMT  | O3B-C3B | -2.39 | 1.37        | 1.43     |
| 14  | b     | 1210 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | B     | 1209 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 21  | U     | 6002 | LMT  | O3B-C3B | -2.39 | 1.37        | 1.43     |
| 21  | U     | 6002 | LMT  | O4'-C4B | -2.39 | 1.37        | 1.43     |
| 14  | A     | 1113 | CLA  | MG-ND   | -2.39 | 2.01        | 2.05     |
| 14  | G     | 1113 | CLA  | MG-ND   | -2.39 | 2.01        | 2.05     |
| 14  | A     | 1118 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | G     | 1013 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 21  | G     | 6003 | LMT  | O3B-C3B | -2.39 | 1.37        | 1.43     |
| 14  | B     | 1218 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | H     | 1235 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 21  | B     | 6002 | LMT  | O2B-C2B | -2.39 | 1.37        | 1.43     |
| 14  | B     | 1210 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | H     | 1210 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | a     | 1108 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | a     | 1129 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | a     | 1123 | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |
| 21  | m     | 6000 | LMT  | O2B-C2B | -2.38 | 1.37        | 1.43     |
| 14  | a     | 1118 | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | A     | 1013 | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | H     | 1236 | CLA  | C3D-C2D | 2.38  | 1.45        | 1.39     |
| 21  | a     | 6003 | LMT  | O2B-C2B | -2.38 | 1.37        | 1.43     |
| 15  | b     | 1230 | F6C  | MG-ND   | -2.38 | 2.00        | 2.06     |
| 14  | G     | 1114 | CLA  | C1D-C2D | 2.38  | 1.50        | 1.45     |
| 15  | H     | 1230 | F6C  | MG-ND   | -2.38 | 2.00        | 2.06     |
| 14  | b     | 1209 | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 21  | H     | 6004 | LMT  | O3'-C3' | -2.38 | 1.37        | 1.43     |
| 14  | b     | 1236 | CLA  | C3D-C2D | 2.38  | 1.45        | 1.39     |
| 14  | B     | 1235 | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | A     | 1102 | CLA  | C1D-C2D | 2.38  | 1.50        | 1.45     |
| 15  | b     | 1238 | F6C  | CMB-C2B | 2.38  | 1.50        | 1.45     |
| 14  | a     | 1113 | CLA  | MG-ND   | -2.38 | 2.01        | 2.05     |
| 21  | I     | 6001 | LMT  | O3B-C3B | -2.38 | 1.37        | 1.43     |
| 14  | a     | 1114 | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | A     | 1123 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | G     | 1011 | CL0  | C1B-NB  | -2.37 | 1.33        | 1.35     |
| 14  | A     | 1125 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1123 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 21  | b     | 6004 | LMT  | O3'-C3' | -2.37 | 1.37        | 1.43     |
| 14  | A     | 1138 | CLA  | C1D-C2D | 2.37  | 1.50        | 1.45     |
| 14  | A     | 1129 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | a     | 1105 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 13  | A     | 1011 | CL0  | C1B-NB  | -2.37 | 1.33        | 1.35     |
| 14  | a     | 1107 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 14  | a     | 1133 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 14  | b     | 1235 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1129 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1125 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1127 | CLA  | C1B-NB  | -2.37 | 1.33        | 1.35     |
| 21  | A     | 6003 | LMT  | O2B-C2B | -2.37 | 1.37        | 1.43     |
| 14  | A     | 1105 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 21  | V     | 6000 | LMT  | O2B-C2B | -2.37 | 1.37        | 1.43     |
| 14  | b     | 1234 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 14  | A     | 1107 | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1105 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | G     | 1108 | CLA  | C1D-C2D | 2.37  | 1.50        | 1.45     |
| 14  | H     | 1216 | CLA  | C1D-C2D | 2.37  | 1.50        | 1.45     |
| 14  | a     | 1125 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | G     | 1114 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | G     | 1107 | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | b     | 1217 | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | B     | 1221 | CLA  | C1B-NB  | -2.36 | 1.33        | 1.35     |
| 14  | b     | 1226 | CLA  | MG-NC   | 2.36  | 2.11        | 2.06     |
| 21  | M     | 6000 | LMT  | O2B-C2B | -2.36 | 1.37        | 1.43     |
| 13  | a     | 1011 | CL0  | C1B-NB  | -2.36 | 1.33        | 1.35     |
| 14  | a     | 1140 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | A     | 1140 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | B     | 1217 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | G     | 1109 | CLA  | C1D-C2D | 2.36  | 1.50        | 1.45     |
| 21  | H     | 6002 | LMT  | O2B-C2B | -2.36 | 1.37        | 1.43     |
| 14  | A     | 1141 | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 15  | H     | 1238 | F6C  | CMB-C2B | 2.36  | 1.50        | 1.45     |
| 14  | A     | 1125 | CLA  | MG-NC   | 2.36  | 2.11        | 2.06     |
| 14  | B     | 1226 | CLA  | MG-NC   | 2.36  | 2.11        | 2.06     |
| 14  | G     | 1141 | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | A     | 1109 | CLA  | C1D-C2D | 2.36  | 1.50        | 1.45     |
| 21  | A     | 6003 | LMT  | O3B-C3B | -2.36 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | B     | 1238 | F6C  | CMB-C2B | 2.36  | 1.50        | 1.45     |
| 14  | H     | 1217 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | B     | 1240 | CLA  | C4B-CHC | 2.35  | 1.47        | 1.41     |
| 15  | H     | 1207 | F6C  | CHB-C4A | -2.35 | 1.33        | 1.38     |
| 21  | H     | 6002 | LMT  | O3B-C3B | -2.35 | 1.37        | 1.43     |
| 14  | a     | 1141 | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 14  | a     | 1102 | CLA  | C1D-C2D | 2.35  | 1.50        | 1.45     |
| 14  | b     | 1231 | CLA  | C1D-C2D | 2.35  | 1.50        | 1.45     |
| 15  | B     | 1219 | F6C  | C4B-NB  | -2.35 | 1.34        | 1.37     |
| 15  | b     | 1219 | F6C  | C4B-NB  | -2.35 | 1.34        | 1.37     |
| 14  | B     | 1234 | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 21  | R     | 6001 | LMT  | O3B-C3B | -2.35 | 1.37        | 1.43     |
| 21  | l     | 6101 | LMT  | O2'-C2' | -2.35 | 1.37        | 1.43     |
| 21  | H     | 6001 | LMT  | O2B-C2B | -2.35 | 1.37        | 1.43     |
| 14  | a     | 1109 | CLA  | C1D-C2D | 2.35  | 1.50        | 1.45     |
| 14  | G     | 1130 | CLA  | C1B-NB  | -2.35 | 1.33        | 1.35     |
| 14  | b     | 1221 | CLA  | C1B-NB  | -2.34 | 1.33        | 1.35     |
| 14  | A     | 1114 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 15  | B     | 1207 | F6C  | CHB-C4A | -2.34 | 1.33        | 1.38     |
| 14  | H     | 1221 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | b     | 1217 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 15  | H     | 1219 | F6C  | C4B-NB  | -2.34 | 1.34        | 1.37     |
| 14  | H     | 1226 | CLA  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 14  | a     | 1125 | CLA  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 14  | G     | 1125 | CLA  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 14  | U     | 1502 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | b     | 1240 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | A     | 1108 | CLA  | C1D-C2D | 2.34  | 1.49        | 1.45     |
| 14  | H     | 1234 | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 15  | a     | 1121 | F6C  | C2B-C1B | 2.34  | 1.49        | 1.44     |
| 21  | a     | 6003 | LMT  | O3B-C3B | -2.34 | 1.37        | 1.43     |
| 15  | b     | 1238 | F6C  | C1C-CHC | 2.34  | 1.47        | 1.41     |
| 14  | B     | 1233 | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | H     | 1233 | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 15  | b     | 1207 | F6C  | CHB-C4A | -2.34 | 1.33        | 1.38     |
| 15  | G     | 1121 | F6C  | C2B-C1B | 2.34  | 1.49        | 1.44     |
| 14  | a     | 1118 | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | G     | 1140 | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 14  | H     | 1240 | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 14  | G     | 1138 | CLA  | C1D-C2D | 2.33  | 1.49        | 1.45     |
| 14  | B     | 1221 | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 14  | G     | 1118 | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1231 | CLA  | C1D-C2D | 2.33  | 1.49        | 1.45     |
| 21  | b     | 6002 | LMT  | O3B-C3B | -2.33 | 1.37        | 1.43     |
| 21  | B     | 6002 | LMT  | O3B-C3B | -2.33 | 1.37        | 1.43     |
| 14  | A     | 1127 | CLA  | C1B-NB  | -2.33 | 1.33        | 1.35     |
| 21  | G     | 6003 | LMT  | O2B-C2B | -2.33 | 1.37        | 1.43     |
| 14  | B     | 1216 | CLA  | C1D-C2D | 2.33  | 1.49        | 1.45     |
| 14  | H     | 1239 | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 14  | H     | 1231 | CLA  | C1D-C2D | 2.33  | 1.49        | 1.45     |
| 21  | B     | 6001 | LMT  | O2B-C2B | -2.33 | 1.37        | 1.43     |
| 14  | A     | 1102 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 21  | L     | 6101 | LMT  | O2'-C2' | -2.33 | 1.37        | 1.43     |
| 14  | a     | 1108 | CLA  | C1D-C2D | 2.33  | 1.49        | 1.45     |
| 14  | A     | 1013 | CLA  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 14  | G     | 1013 | CLA  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 14  | a     | 1132 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | A     | 1132 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | b     | 1233 | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 14  | b     | 1216 | CLA  | C1D-C2D | 2.32  | 1.49        | 1.45     |
| 21  | H     | 6003 | LMT  | O3B-C3B | -2.32 | 1.37        | 1.43     |
| 14  | G     | 1106 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | l     | 1501 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | L     | 1502 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 21  | b     | 6001 | LMT  | O2B-C2B | -2.32 | 1.37        | 1.43     |
| 14  | L     | 1501 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | U     | 1501 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 14  | A     | 1118 | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 15  | A     | 1121 | F6C  | C2B-C1B | 2.32  | 1.49        | 1.44     |
| 14  | A     | 1138 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 14  | A     | 1135 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 14  | B     | 1220 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | b     | 1216 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | b     | 1220 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | a     | 1140 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | a     | 1125 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 15  | b     | 1219 | F6C  | C2B-C1B | 2.31  | 1.49        | 1.44     |
| 14  | a     | 1102 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | a     | 1102 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 14  | A     | 1108 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | G     | 1132 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | G     | 1140 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 21  | b     | 6004 | LMT  | O2B-C2B | -2.31 | 1.37        | 1.43     |
| 14  | a     | 1116 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 1125 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | b     | 1221 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | l     | 1502 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | B     | 1208 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | B     | 1239 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | A     | 1106 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | a     | 1136 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | G     | 1104 | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | G     | 1124 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | a     | 1106 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | A     | 1130 | CLA  | C1B-NB  | -2.30 | 1.33        | 1.35     |
| 15  | H     | 1219 | F6C  | C1D-ND  | -2.30 | 1.34        | 1.37     |
| 14  | A     | 1140 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | b     | 1239 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | B     | 1232 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | G     | 1135 | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 14  | l     | 1503 | CLA  | C1B-NB  | -2.30 | 1.33        | 1.35     |
| 14  | a     | 1104 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | H     | 1216 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | m     | 1501 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | H     | 1232 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | G     | 1102 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | G     | 1106 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | b     | 1208 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | G     | 1105 | CLA  | C1D-C2D | 2.30  | 1.49        | 1.45     |
| 14  | G     | 1138 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | V     | 1501 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | B     | 1228 | CLA  | C1D-C2D | 2.30  | 1.49        | 1.45     |
| 14  | A     | 1136 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | A     | 1124 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 15  | B     | 1238 | F6C  | C1C-CHC | 2.30  | 1.47        | 1.41     |
| 14  | G     | 1102 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | b     | 1232 | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 14  | A     | 1103 | CLA  | MG-NC   | 2.30  | 2.11        | 2.06     |
| 21  | B     | 6004 | LMT  | O3B-C3B | -2.30 | 1.37        | 1.43     |
| 14  | a     | 1103 | CLA  | MG-NC   | 2.30  | 2.11        | 2.06     |
| 15  | b     | 1219 | F6C  | C4A-C3A | 2.29  | 1.49        | 1.45     |
| 14  | A     | 1116 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | G     | 1136 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | a     | 1135 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 14  | H     | 1218 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | G     | 1109 | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1104 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | B     | 1216 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | a     | 1124 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | G     | 1108 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | a     | 1013 | CLA  | MG-NC   | 2.29  | 2.11        | 2.06     |
| 15  | H     | 1238 | F6C  | C1C-CHC | 2.29  | 1.47        | 1.41     |
| 14  | G     | 1103 | CLA  | MG-NC   | 2.29  | 2.11        | 2.06     |
| 14  | A     | 1102 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | H     | 1208 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | b     | 1229 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | A     | 1125 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | H     | 1224 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | b     | 1224 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | A     | 1106 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | B     | 1224 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | H     | 1220 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | a     | 1138 | CLA  | C1C-NC  | -2.29 | 1.34        | 1.37     |
| 21  | H     | 6001 | LMT  | O3B-C3B | -2.29 | 1.37        | 1.43     |
| 21  | H     | 6004 | LMT  | O3B-C3B | -2.29 | 1.37        | 1.43     |
| 21  | b     | 6004 | LMT  | O3B-C3B | -2.29 | 1.37        | 1.43     |
| 21  | B     | 6003 | LMT  | O3B-C3B | -2.28 | 1.37        | 1.43     |
| 14  | a     | 1127 | CLA  | C1B-NB  | -2.28 | 1.33        | 1.35     |
| 14  | G     | 1120 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 21  | U     | 6101 | LMT  | O2'-C2' | -2.28 | 1.37        | 1.43     |
| 13  | G     | 1011 | CL0  | C3A-C2A | -2.28 | 1.48        | 1.54     |
| 14  | A     | 1123 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 14  | a     | 1108 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 21  | b     | 6003 | LMT  | O3B-C3B | -2.28 | 1.37        | 1.43     |
| 14  | G     | 1123 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 14  | M     | 1501 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 14  | A     | 1105 | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 14  | B     | 1229 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 14  | a     | 1106 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 14  | b     | 1218 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 15  | B     | 1219 | F6C  | C4A-C3A | 2.28  | 1.49        | 1.45     |
| 21  | B     | 6004 | LMT  | O2B-C2B | -2.28 | 1.37        | 1.43     |
| 14  | G     | 1116 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 15  | H     | 1219 | F6C  | C4A-C3A | 2.28  | 1.49        | 1.45     |
| 14  | a     | 1115 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 18  | i     | 4020 | BCR  | C14-C13 | -2.28 | 1.32        | 1.35     |
| 14  | H     | 1229 | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 14  | a     | 1126 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | B     | 6001 | LMT  | O3B-C3B | -2.28 | 1.37        | 1.43     |
| 14  | b     | 1227 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 14  | G     | 1115 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 14  | A     | 1109 | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 15  | b     | 1219 | F6C  | C1D-ND  | -2.28 | 1.34        | 1.37     |
| 14  | B     | 1233 | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 14  | b     | 1228 | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 14  | a     | 1112 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | A     | 1112 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | B     | 1218 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 15  | B     | 1219 | F6C  | C2B-C1B | 2.27  | 1.49        | 1.44     |
| 14  | A     | 1126 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | B     | 1227 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | G     | 1105 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 15  | B     | 1219 | F6C  | C1D-ND  | -2.27 | 1.34        | 1.37     |
| 14  | A     | 1115 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 14  | G     | 1126 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | a     | 1123 | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | H     | 1228 | CLA  | C1D-C2D | 2.27  | 1.49        | 1.45     |
| 21  | A     | 6004 | LMT  | O2'-C2' | -2.27 | 1.37        | 1.43     |
| 14  | H     | 1236 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 14  | a     | 1120 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 14  | a     | 1109 | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 14  | B     | 1236 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 14  | A     | 1120 | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 21  | b     | 6001 | LMT  | O3B-C3B | -2.27 | 1.37        | 1.43     |
| 15  | b     | 1238 | F6C  | C4C-CHD | 2.26  | 1.47        | 1.41     |
| 14  | a     | 1105 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | a     | 1129 | CLA  | C1B-NB  | -2.26 | 1.33        | 1.35     |
| 14  | H     | 1227 | CLA  | C4B-CHC | 2.26  | 1.47        | 1.41     |
| 14  | H     | 1233 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 14  | H     | 1212 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | a     | 1137 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | H     | 1229 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | b     | 1236 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | B     | 1229 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | A     | 1105 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 13  | A     | 1011 | CL0  | C3A-C2A | -2.26 | 1.48        | 1.54     |
| 18  | H     | 4017 | BCR  | C21-C22 | -2.26 | 1.32        | 1.35     |
| 14  | b     | 1229 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | H     | 1233 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 21  | i     | 6001 | LMT  | O2B-C2B | -2.26 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1110 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | L     | 1503 | CLA  | C1B-NB  | -2.26 | 1.33        | 1.35     |
| 14  | G     | 1112 | CLA  | C4B-CHC | 2.26  | 1.47        | 1.41     |
| 14  | a     | 1130 | CLA  | C1B-NB  | -2.26 | 1.33        | 1.35     |
| 13  | a     | 1011 | CL0  | C3A-C2A | -2.26 | 1.48        | 1.54     |
| 21  | I     | 6001 | LMT  | O2B-C2B | -2.26 | 1.37        | 1.43     |
| 14  | B     | 1222 | CLA  | C4B-CHC | 2.26  | 1.47        | 1.41     |
| 14  | G     | 1135 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | a     | 1105 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | B     | 1212 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | b     | 1212 | CLA  | C1D-C2D | 2.26  | 1.49        | 1.45     |
| 14  | a     | 1110 | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 21  | H     | 6004 | LMT  | O2B-C2B | -2.25 | 1.37        | 1.43     |
| 14  | G     | 1104 | CLA  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 15  | H     | 1219 | F6C  | C2B-C1B | 2.25  | 1.49        | 1.44     |
| 14  | b     | 1214 | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 15  | b     | 1238 | F6C  | C1C-NC  | -2.25 | 1.33        | 1.35     |
| 14  | b     | 1228 | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 18  | b     | 4017 | BCR  | C21-C22 | -2.25 | 1.32        | 1.35     |
| 21  | a     | 6004 | LMT  | O2'-C2' | -2.25 | 1.37        | 1.43     |
| 14  | G     | 1139 | CLA  | C1D-C2D | 2.25  | 1.49        | 1.45     |
| 14  | b     | 1222 | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 14  | G     | 1110 | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | G     | 1134 | CLA  | C1D-C2D | 2.25  | 1.49        | 1.45     |
| 14  | a     | 1120 | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 14  | B     | 1233 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 21  | R     | 6001 | LMT  | O2B-C2B | -2.25 | 1.37        | 1.43     |
| 14  | H     | 1231 | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | G     | 1109 | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | a     | 1113 | CLA  | C1D-C2D | 2.25  | 1.49        | 1.45     |
| 14  | A     | 1137 | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | G     | 1137 | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | A     | 1113 | CLA  | C1D-C2D | 2.24  | 1.49        | 1.45     |
| 15  | H     | 1238 | F6C  | C4C-CHD | 2.24  | 1.47        | 1.41     |
| 14  | G     | 1113 | CLA  | C1D-C2D | 2.24  | 1.49        | 1.45     |
| 15  | b     | 1230 | F6C  | C3B-C4B | 2.24  | 1.49        | 1.44     |
| 15  | B     | 1238 | F6C  | C4C-CHD | 2.24  | 1.47        | 1.41     |
| 14  | B     | 1228 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | A     | 1109 | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | G     | 1120 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | B     | 1226 | CLA  | CMB-C2B | -2.24 | 1.47        | 1.51     |
| 14  | B     | 1214 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1104 | CLA  | MG-NC   | 2.24  | 2.11        | 2.06     |
| 14  | H     | 1222 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | A     | 1139 | CLA  | C1D-C2D | 2.24  | 1.49        | 1.45     |
| 14  | H     | 1209 | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | b     | 1233 | CLA  | C1D-C2D | 2.24  | 1.49        | 1.45     |
| 15  | B     | 1238 | F6C  | C1A-C2A | 2.24  | 1.50        | 1.45     |
| 14  | A     | 1135 | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | H     | 1220 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | b     | 1209 | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | a     | 1109 | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | a     | 1104 | CLA  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 14  | B     | 1209 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | A     | 1127 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | B     | 1231 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | G     | 1114 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 15  | b     | 1237 | F6C  | CMB-C2B | 2.23  | 1.49        | 1.45     |
| 21  | G     | 6004 | LMT  | O2'-C2' | -2.23 | 1.37        | 1.43     |
| 14  | b     | 1235 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | a     | 1135 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | b     | 1228 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 15  | H     | 1230 | F6C  | C3B-C4B | 2.23  | 1.49        | 1.44     |
| 15  | b     | 1238 | F6C  | C1A-C2A | 2.23  | 1.50        | 1.45     |
| 21  | a     | 6001 | LMT  | O1'-C1' | -2.23 | 1.36        | 1.40     |
| 14  | G     | 1129 | CLA  | C1B-NB  | -2.23 | 1.33        | 1.35     |
| 14  | A     | 1114 | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 18  | I     | 4020 | BCR  | C14-C13 | -2.23 | 1.32        | 1.35     |
| 14  | H     | 1228 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 14  | b     | 1216 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 21  | A     | 6001 | LMT  | O1'-C1' | -2.23 | 1.36        | 1.40     |
| 14  | B     | 1228 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 15  | G     | 1121 | F6C  | C1C-NC  | -2.22 | 1.33        | 1.35     |
| 14  | a     | 1139 | CLA  | C1D-C2D | 2.22  | 1.49        | 1.45     |
| 15  | B     | 1230 | F6C  | C3B-C4B | 2.22  | 1.49        | 1.44     |
| 14  | a     | 1127 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 14  | a     | 1134 | CLA  | C1D-C2D | 2.22  | 1.49        | 1.45     |
| 14  | A     | 1120 | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 14  | b     | 1232 | CLA  | C1D-C2D | 2.22  | 1.49        | 1.45     |
| 14  | l     | 1503 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 15  | a     | 1121 | F6C  | C1C-NC  | -2.22 | 1.33        | 1.35     |
| 14  | G     | 1127 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 14  | A     | 1129 | CLA  | C1B-NB  | -2.22 | 1.33        | 1.35     |
| 14  | a     | 1114 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 1232 | CLA  | C1D-C2D | 2.22  | 1.49        | 1.45     |
| 14  | B     | 1220 | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 14  | H     | 1214 | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 15  | B     | 1237 | F6C  | CMB-C2B | 2.22  | 1.49        | 1.45     |
| 14  | U     | 1503 | CLA  | C1B-NB  | -2.22 | 1.33        | 1.35     |
| 14  | G     | 1128 | CLA  | CMB-C2B | -2.22 | 1.47        | 1.51     |
| 14  | L     | 1503 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 14  | H     | 1228 | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 14  | G     | 1111 | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 14  | B     | 1211 | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 18  | B     | 4017 | BCR  | C21-C22 | -2.21 | 1.32        | 1.35     |
| 15  | H     | 1238 | F6C  | C1A-C2A | 2.21  | 1.50        | 1.45     |
| 14  | A     | 1102 | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | G     | 1102 | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | b     | 1211 | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 14  | H     | 1232 | CLA  | C1D-C2D | 2.21  | 1.49        | 1.45     |
| 15  | H     | 1237 | F6C  | CMB-C2B | 2.21  | 1.49        | 1.45     |
| 14  | b     | 1220 | CLA  | C4B-CHC | 2.21  | 1.47        | 1.41     |
| 14  | b     | 1233 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 14  | H     | 1214 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 14  | H     | 1226 | CLA  | CMB-C2B | -2.21 | 1.47        | 1.51     |
| 14  | a     | 1102 | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | b     | 1231 | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 14  | G     | 1109 | CLA  | C4B-CHC | 2.21  | 1.47        | 1.41     |
| 14  | a     | 1112 | CLA  | C1D-C2D | 2.21  | 1.49        | 1.45     |
| 14  | B     | 1216 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 14  | A     | 1134 | CLA  | C1D-C2D | 2.21  | 1.49        | 1.45     |
| 14  | B     | 1222 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 21  | I     | 6001 | LMT  | O4'-C4B | -2.20 | 1.37        | 1.43     |
| 14  | A     | 1128 | CLA  | CMB-C2B | -2.20 | 1.47        | 1.51     |
| 14  | H     | 1211 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | a     | 1128 | CLA  | CMB-C2B | -2.20 | 1.47        | 1.51     |
| 14  | G     | 1103 | CLA  | C4B-CHC | 2.20  | 1.47        | 1.41     |
| 14  | U     | 1503 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | G     | 1130 | CLA  | C4B-CHC | 2.20  | 1.47        | 1.41     |
| 14  | H     | 1222 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | H     | 1208 | CLA  | C1D-C2D | 2.20  | 1.49        | 1.45     |
| 18  | R     | 4020 | BCR  | C14-C13 | -2.20 | 1.32        | 1.35     |
| 15  | b     | 1219 | F6C  | MG-ND   | -2.20 | 2.01        | 2.06     |
| 14  | H     | 1235 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | B     | 1235 | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | A     | 1111 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1203 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 14  | b     | 1214 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 14  | b     | 1222 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 21  | U     | 6101 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 21  | i     | 6001 | LMT  | O4'-C4B | -2.19 | 1.37        | 1.43     |
| 21  | L     | 6101 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 14  | B     | 1227 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 21  | b     | 6002 | LMT  | O4'-C4B | -2.19 | 1.37        | 1.43     |
| 21  | l     | 6101 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 14  | G     | 1139 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 14  | A     | 1109 | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 21  | G     | 6001 | LMT  | O1'-C1' | -2.19 | 1.36        | 1.40     |
| 14  | b     | 1226 | CLA  | CMB-C2B | -2.19 | 1.47        | 1.51     |
| 14  | A     | 1101 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 14  | a     | 1111 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 14  | a     | 1103 | CLA  | C1D-C2D | 2.19  | 1.49        | 1.45     |
| 14  | a     | 1109 | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 14  | G     | 1104 | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 21  | H     | 6002 | LMT  | O4'-C4B | -2.19 | 1.37        | 1.43     |
| 15  | b     | 1207 | F6C  | C4C-CHD | 2.19  | 1.47        | 1.41     |
| 21  | l     | 6101 | LMT  | O2B-C2B | -2.19 | 1.37        | 1.43     |
| 14  | A     | 1103 | CLA  | C1D-C2D | 2.19  | 1.49        | 1.45     |
| 21  | b     | 6002 | LMT  | O1'-C1' | -2.19 | 1.36        | 1.40     |
| 14  | H     | 1227 | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 14  | G     | 1104 | CLA  | C1B-NB  | -2.19 | 1.33        | 1.35     |
| 15  | H     | 1238 | F6C  | C1C-NC  | -2.19 | 1.33        | 1.35     |
| 14  | b     | 1208 | CLA  | C1D-C2D | 2.19  | 1.49        | 1.45     |
| 14  | A     | 1103 | CLA  | C4B-CHC | 2.18  | 1.47        | 1.41     |
| 14  | A     | 1139 | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 14  | a     | 1139 | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 14  | A     | 1130 | CLA  | C4B-CHC | 2.18  | 1.47        | 1.41     |
| 15  | B     | 1219 | F6C  | MG-ND   | -2.18 | 2.01        | 2.06     |
| 15  | G     | 1121 | F6C  | C4B-NB  | -2.18 | 1.34        | 1.37     |
| 14  | A     | 1112 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 14  | a     | 1134 | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 21  | B     | 6002 | LMT  | O1'-C1' | -2.18 | 1.36        | 1.40     |
| 14  | B     | 1208 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 14  | G     | 1103 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 15  | G     | 1121 | F6C  | C4D-CHA | 2.18  | 1.48        | 1.42     |
| 15  | B     | 1238 | F6C  | C1C-NC  | -2.18 | 1.33        | 1.35     |
| 14  | a     | 1101 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 14  | b     | 1227 | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1141 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 14  | a     | 1104 | CLA  | C4B-CHC | 2.18  | 1.47        | 1.41     |
| 14  | b     | 1208 | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 21  | R     | 6001 | LMT  | O4'-C4B | -2.18 | 1.37        | 1.43     |
| 21  | B     | 6002 | LMT  | O4'-C4B | -2.17 | 1.37        | 1.43     |
| 21  | L     | 6101 | LMT  | O2B-C2B | -2.17 | 1.37        | 1.43     |
| 14  | a     | 1141 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 14  | a     | 1131 | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 14  | B     | 1214 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 18  | B     | 4010 | BCR  | C17-C18 | -2.17 | 1.32        | 1.35     |
| 15  | B     | 1207 | F6C  | C4C-CHD | 2.17  | 1.47        | 1.41     |
| 14  | G     | 1112 | CLA  | C1D-C2D | 2.17  | 1.49        | 1.45     |
| 14  | a     | 1130 | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 15  | H     | 1207 | F6C  | C4C-CHD | 2.17  | 1.47        | 1.41     |
| 14  | G     | 1136 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 15  | H     | 1219 | F6C  | MG-ND   | -2.17 | 2.01        | 2.06     |
| 21  | m     | 6000 | LMT  | O4'-C4B | -2.17 | 1.37        | 1.43     |
| 14  | a     | 1103 | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 21  | H     | 6002 | LMT  | O1'-C1' | -2.17 | 1.36        | 1.40     |
| 14  | b     | 1021 | CLA  | C1B-CHB | 2.17  | 1.47        | 1.41     |
| 21  | M     | 6000 | LMT  | O4'-C4B | -2.17 | 1.37        | 1.43     |
| 14  | G     | 1141 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 14  | A     | 1131 | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 15  | H     | 1237 | F6C  | C1A-C2A | 2.17  | 1.50        | 1.45     |
| 21  | U     | 6101 | LMT  | O2B-C2B | -2.17 | 1.37        | 1.43     |
| 14  | H     | 1208 | CLA  | C1B-CHB | 2.17  | 1.47        | 1.41     |
| 14  | B     | 1208 | CLA  | C1B-CHB | 2.17  | 1.47        | 1.41     |
| 14  | H     | 1216 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 14  | H     | 1213 | CLA  | C1D-C2D | 2.17  | 1.49        | 1.45     |
| 18  | H     | 4010 | BCR  | C17-C18 | -2.16 | 1.32        | 1.35     |
| 14  | B     | 1203 | CLA  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 21  | G     | 6002 | LMT  | O1'-C1' | -2.16 | 1.36        | 1.40     |
| 14  | B     | 1021 | CLA  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 21  | A     | 6002 | LMT  | O1'-C1' | -2.16 | 1.36        | 1.40     |
| 14  | A     | 1104 | CLA  | C4B-CHC | 2.16  | 1.47        | 1.41     |
| 14  | H     | 1232 | CLA  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 15  | A     | 1121 | F6C  | C4D-CHA | 2.16  | 1.48        | 1.42     |
| 14  | b     | 1203 | CLA  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 14  | a     | 1117 | CLA  | C4B-CHC | 2.16  | 1.47        | 1.41     |
| 15  | B     | 1237 | F6C  | C1A-C2A | 2.16  | 1.50        | 1.45     |
| 14  | H     | 1214 | CLA  | C1D-C2D | 2.16  | 1.49        | 1.45     |
| 15  | A     | 1121 | F6C  | C1C-NC  | -2.16 | 1.33        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms                | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|----------------------|-------|-------------|----------|
| 14  | G     | 1138 | CLA  | C1A-CHA              | 2.16  | 1.52        | 1.43     |
| 14  | b     | 1232 | CLA  | C1B-CHB              | 2.16  | 1.47        | 1.41     |
| 14  | a     | 1104 | CLA  | C1B-NB               | -2.16 | 1.33        | 1.35     |
| 14  | A     | 1138 | CLA  | C1A-CHA              | 2.16  | 1.52        | 1.43     |
| 14  | a     | 1138 | CLA  | C1A-CHA              | 2.16  | 1.52        | 1.43     |
| 14  | A     | 1012 | CLA  | C4B-CHC              | 2.16  | 1.47        | 1.41     |
| 14  | B     | 1213 | CLA  | C1D-C2D              | 2.16  | 1.49        | 1.45     |
| 14  | B     | 1232 | CLA  | C1B-CHB              | 2.16  | 1.47        | 1.41     |
| 14  | G     | 1131 | CLA  | C4B-CHC              | 2.16  | 1.47        | 1.41     |
| 14  | b     | 1225 | CLA  | C1B-CHB              | 2.16  | 1.47        | 1.41     |
| 14  | H     | 1021 | CLA  | C1B-CHB              | 2.16  | 1.47        | 1.41     |
| 14  | K     | 1401 | CLA  | C1D-C2D              | 2.15  | 1.49        | 1.45     |
| 14  | A     | 1136 | CLA  | C1A-CHA              | 2.15  | 1.52        | 1.43     |
| 14  | G     | 1117 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 14  | b     | 1217 | CLA  | C1A-CHA              | 2.15  | 1.52        | 1.43     |
| 14  | G     | 1012 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 15  | a     | 1121 | F6C  | C4B-NB               | -2.15 | 1.34        | 1.37     |
| 14  | U     | 1503 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 14  | l     | 1503 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 14  | A     | 1134 | CLA  | C1B-CHB              | 2.15  | 1.47        | 1.41     |
| 14  | G     | 1131 | CLA  | C1B-CHB              | 2.15  | 1.47        | 1.41     |
| 15  | b     | 1237 | F6C  | C1A-C2A              | 2.15  | 1.50        | 1.45     |
| 14  | b     | 1214 | CLA  | C1D-C2D              | 2.15  | 1.49        | 1.45     |
| 14  | B     | 1239 | CLA  | C1B-CHB              | 2.15  | 1.47        | 1.41     |
| 14  | b     | 1204 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 14  | b     | 1239 | CLA  | C1B-CHB              | 2.15  | 1.47        | 1.41     |
| 14  | a     | 1012 | CLA  | C4B-CHC              | 2.15  | 1.47        | 1.41     |
| 14  | A     | 1117 | CLA  | C4B-CHC              | 2.14  | 1.47        | 1.41     |
| 14  | b     | 1240 | CLA  | C4C-C3C              | 2.14  | 1.48        | 1.45     |
| 15  | A     | 1121 | F6C  | C4B-NB               | -2.14 | 1.34        | 1.37     |
| 14  | b     | 1213 | CLA  | C1D-C2D              | 2.14  | 1.49        | 1.45     |
| 14  | L     | 1503 | CLA  | C4B-CHC              | 2.14  | 1.47        | 1.41     |
| 14  | B     | 1214 | CLA  | C1B-NB               | -2.14 | 1.33        | 1.35     |
| 14  | B     | 1225 | CLA  | C1B-CHB              | 2.14  | 1.46        | 1.41     |
| 14  | B     | 1214 | CLA  | C1D-C2D              | 2.14  | 1.49        | 1.45     |
| 14  | A     | 1101 | CLA  | C1D-C2D              | 2.14  | 1.49        | 1.45     |
| 14  | B     | 1217 | CLA  | C1A-CHA              | 2.14  | 1.52        | 1.43     |
| 14  | b     | 1203 | CLA  | C4B-CHC              | 2.14  | 1.46        | 1.41     |
| 14  | T     | 1401 | CLA  | C1D-C2D              | 2.14  | 1.49        | 1.45     |
| 15  | a     | 1121 | F6C  | C4D-CHA              | 2.14  | 1.48        | 1.42     |
| 21  | V     | 6000 | LMT  | O4 <sup>2</sup> -C4B | -2.14 | 1.37        | 1.43     |
| 13  | G     | 1011 | CL0  | C4B-CHC              | 2.14  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | B     | 1230 | F6C  | C4B-NB  | -2.14 | 1.34        | 1.37     |
| 21  | a     | 6002 | LMT  | O1'-C1' | -2.14 | 1.36        | 1.40     |
| 14  | b     | 1227 | CLA  | C1D-C2D | 2.14  | 1.49        | 1.45     |
| 14  | a     | 1136 | CLA  | C1A-CHA | 2.14  | 1.52        | 1.43     |
| 14  | a     | 1114 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 13  | A     | 1011 | CL0  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 14  | A     | 1131 | CLA  | C1B-CHB | 2.14  | 1.46        | 1.41     |
| 14  | B     | 1203 | CLA  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 13  | a     | 1011 | CL0  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 14  | G     | 1101 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 14  | G     | 1141 | CLA  | C1A-CHA | 2.13  | 1.52        | 1.43     |
| 14  | A     | 1141 | CLA  | C1A-CHA | 2.13  | 1.52        | 1.43     |
| 14  | H     | 1203 | CLA  | C1B-NB  | -2.13 | 1.33        | 1.35     |
| 14  | b     | 1214 | CLA  | C1B-NB  | -2.13 | 1.33        | 1.35     |
| 14  | B     | 1218 | CLA  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 14  | A     | 1114 | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 14  | b     | 1210 | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | B     | 1204 | CLA  | C4B-CHC | 2.13  | 1.46        | 1.41     |
| 14  | G     | 1141 | CLA  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 21  | b     | 6001 | LMT  | O4'-C4B | -2.13 | 1.38        | 1.43     |
| 14  | H     | 1217 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 18  | b     | 4010 | BCR  | C17-C18 | -2.13 | 1.33        | 1.35     |
| 21  | V     | 6000 | LMT  | O1'-C1' | -2.13 | 1.36        | 1.40     |
| 14  | a     | 1141 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 14  | H     | 1227 | CLA  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 14  | a     | 1137 | CLA  | C4B-CHC | 2.13  | 1.46        | 1.41     |
| 14  | A     | 1141 | CLA  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 14  | B     | 1227 | CLA  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 14  | G     | 1134 | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | H     | 1225 | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | B     | 1204 | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | b     | 1215 | CLA  | C4B-CHC | 2.13  | 1.46        | 1.41     |
| 14  | H     | 1239 | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 21  | B     | 6001 | LMT  | O4'-C4B | -2.13 | 1.38        | 1.43     |
| 14  | B     | 1211 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 15  | b     | 1237 | F6C  | CHB-C4A | -2.12 | 1.34        | 1.38     |
| 15  | H     | 1230 | F6C  | C4B-NB  | -2.12 | 1.34        | 1.37     |
| 14  | B     | 1210 | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 15  | b     | 1230 | F6C  | C4B-NB  | -2.12 | 1.34        | 1.37     |
| 14  | k     | 1401 | CLA  | C1D-C2D | 2.12  | 1.49        | 1.45     |
| 14  | H     | 1201 | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | H     | 1203 | CLA  | C4B-CHC | 2.12  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1215 | CLA  | C4B-CHC | 2.12  | 1.46        | 1.41     |
| 15  | B     | 1207 | F6C  | C4D-CHA | 2.12  | 1.48        | 1.42     |
| 14  | G     | 1101 | CLA  | C1D-C2D | 2.12  | 1.49        | 1.45     |
| 14  | H     | 1210 | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | B     | 1240 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 14  | H     | 1204 | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | b     | 1204 | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 21  | A     | 6003 | LMT  | O4'-C4B | -2.12 | 1.38        | 1.43     |
| 14  | B     | 1215 | CLA  | C4B-CHC | 2.12  | 1.46        | 1.41     |
| 21  | M     | 6000 | LMT  | O1'-C1' | -2.12 | 1.36        | 1.40     |
| 14  | a     | 1131 | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |
| 14  | A     | 1137 | CLA  | C4B-CHC | 2.11  | 1.46        | 1.41     |
| 14  | b     | 1211 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 14  | b     | 1218 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 14  | b     | 1214 | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |
| 14  | H     | 1218 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 14  | b     | 1211 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 14  | G     | 1013 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 14  | A     | 1104 | CLA  | C1B-NB  | -2.11 | 1.33        | 1.35     |
| 14  | a     | 1141 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 21  | m     | 6000 | LMT  | O1'-C1' | -2.11 | 1.36        | 1.40     |
| 21  | l     | 6101 | LMT  | O1'-C1' | -2.11 | 1.36        | 1.40     |
| 14  | a     | 1101 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 15  | B     | 1237 | F6C  | CHB-C4A | -2.11 | 1.34        | 1.38     |
| 21  | G     | 6003 | LMT  | O4'-C4B | -2.11 | 1.38        | 1.43     |
| 21  | H     | 6001 | LMT  | O4'-C4B | -2.11 | 1.38        | 1.43     |
| 14  | H     | 1214 | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |
| 14  | H     | 1204 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 14  | H     | 1211 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 14  | G     | 1137 | CLA  | C4B-CHC | 2.11  | 1.46        | 1.41     |
| 21  | a     | 6003 | LMT  | O4'-C4B | -2.11 | 1.38        | 1.43     |
| 14  | A     | 1122 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 15  | A     | 1121 | F6C  | CMB-C2B | 2.10  | 1.49        | 1.45     |
| 14  | H     | 1204 | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 14  | a     | 1013 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 14  | G     | 1122 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | G     | 1128 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 15  | H     | 1219 | F6C  | C4D-CHA | 2.10  | 1.48        | 1.42     |
| 14  | G     | 1112 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | H     | 1211 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 14  | A     | 1135 | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 15  | H     | 1230 | F6C  | C4D-CHA | 2.10  | 1.48        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 1220 | CLA  | C1D-C2D | 2.10  | 1.49        | 1.45     |
| 15  | b     | 1207 | F6C  | C4D-CHA | 2.10  | 1.47        | 1.42     |
| 14  | b     | 1204 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 14  | A     | 1013 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 14  | H     | 1228 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | H     | 1214 | CLA  | C1B-NB  | -2.10 | 1.33        | 1.35     |
| 15  | H     | 1219 | F6C  | C1A-C2A | 2.10  | 1.50        | 1.45     |
| 14  | B     | 1204 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 20  | B     | 5002 | LMG  | O1-C1   | 2.09  | 1.43        | 1.40     |
| 14  | A     | 1132 | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 14  | B     | 1228 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | A     | 1112 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 15  | H     | 1207 | F6C  | C4D-CHA | 2.09  | 1.47        | 1.42     |
| 15  | b     | 1219 | F6C  | C4D-CHA | 2.09  | 1.47        | 1.42     |
| 14  | b     | 1235 | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 20  | b     | 5002 | LMG  | O1-C1   | 2.09  | 1.43        | 1.40     |
| 14  | H     | 1223 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | G     | 1132 | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 14  | a     | 1134 | CLA  | C1B-NB  | -2.09 | 1.33        | 1.35     |
| 14  | B     | 1235 | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 15  | G     | 1121 | F6C  | CMB-C2B | 2.09  | 1.49        | 1.45     |
| 14  | B     | 1201 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | a     | 1108 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 14  | A     | 1128 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | B     | 1214 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | H     | 1235 | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 14  | b     | 1232 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 15  | B     | 1230 | F6C  | C4D-CHA | 2.09  | 1.47        | 1.42     |
| 14  | a     | 1135 | CLA  | C1B-NB  | -2.09 | 1.33        | 1.35     |
| 14  | l     | 1502 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | B     | 1211 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 14  | b     | 1203 | CLA  | C1B-NB  | -2.09 | 1.33        | 1.35     |
| 14  | A     | 1108 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 14  | b     | 1223 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | G     | 1114 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 14  | G     | 1110 | CLA  | C1D-C2D | 2.08  | 1.49        | 1.45     |
| 14  | B     | 1223 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | b     | 1201 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | a     | 1135 | CLA  | C4B-CHC | 2.08  | 1.46        | 1.41     |
| 14  | B     | 1232 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 14  | A     | 1127 | CLA  | C4B-CHC | 2.08  | 1.46        | 1.41     |
| 14  | U     | 1502 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1240 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 21  | G     | 6001 | LMT  | O4'-C4B | -2.08 | 1.38        | 1.43     |
| 14  | a     | 1129 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 21  | U     | 6101 | LMT  | O1'-C1' | -2.08 | 1.36        | 1.40     |
| 14  | H     | 1023 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | A     | 1136 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | G     | 1135 | CLA  | C4B-CHC | 2.08  | 1.46        | 1.41     |
| 14  | B     | 1232 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 15  | B     | 1219 | F6C  | C4D-CHA | 2.08  | 1.47        | 1.42     |
| 14  | G     | 1129 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | H     | 1221 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 15  | b     | 1219 | F6C  | C1A-C2A | 2.08  | 1.50        | 1.45     |
| 14  | G     | 1139 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 14  | a     | 1136 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | B     | 1220 | CLA  | C1D-C2D | 2.08  | 1.49        | 1.45     |
| 14  | B     | 1240 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | A     | 1116 | CLA  | C1D-C2D | 2.07  | 1.49        | 1.45     |
| 14  | H     | 1232 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 14  | A     | 1119 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | B     | 1023 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | a     | 1122 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | H     | 1220 | CLA  | C1D-C2D | 2.07  | 1.49        | 1.45     |
| 14  | b     | 1240 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | b     | 1212 | CLA  | C4B-CHC | 2.07  | 1.46        | 1.41     |
| 15  | B     | 1219 | F6C  | C1A-C2A | 2.07  | 1.50        | 1.45     |
| 14  | H     | 1232 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 14  | b     | 1201 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 14  | a     | 1112 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 15  | H     | 1237 | F6C  | CHB-C4A | -2.07 | 1.34        | 1.38     |
| 21  | b     | 6003 | LMT  | C3'-C2' | 2.07  | 1.57        | 1.52     |
| 14  | G     | 1136 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | a     | 1128 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 21  | L     | 6101 | LMT  | O1'-C1' | -2.07 | 1.36        | 1.40     |
| 14  | L     | 1502 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | B     | 1203 | CLA  | C1B-NB  | -2.07 | 1.33        | 1.35     |
| 14  | G     | 1127 | CLA  | C4B-CHC | 2.07  | 1.46        | 1.41     |
| 14  | H     | 1240 | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | B     | 1221 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 14  | b     | 1221 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 14  | G     | 1119 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | G     | 1122 | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | G     | 1116 | CLA  | C1D-C2D | 2.06  | 1.49        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1139 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 14  | H     | 1201 | CLA  | C1D-C2D | 2.06  | 1.49        | 1.45     |
| 14  | a     | 1119 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 21  | a     | 6001 | LMT  | O4'-C4B | -2.06 | 1.38        | 1.43     |
| 14  | a     | 1112 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | A     | 1134 | CLA  | C1B-NB  | -2.06 | 1.33        | 1.35     |
| 14  | G     | 1134 | CLA  | C1B-NB  | -2.06 | 1.33        | 1.35     |
| 14  | H     | 1201 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 14  | H     | 1225 | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | B     | 1209 | CLA  | C1D-C2D | 2.06  | 1.49        | 1.45     |
| 14  | A     | 1122 | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | b     | 1023 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | b     | 1225 | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | a     | 1120 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 14  | B     | 1201 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 15  | a     | 1121 | F6C  | CMB-C2B | 2.06  | 1.49        | 1.45     |
| 14  | b     | 1228 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | B     | 1225 | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | A     | 1129 | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | H     | 1239 | CLA  | C1D-C2D | 2.06  | 1.49        | 1.45     |
| 18  | B     | 4017 | BCR  | C14-C13 | -2.06 | 1.33        | 1.35     |
| 15  | b     | 1237 | F6C  | C1C-CHC | 2.06  | 1.46        | 1.41     |
| 20  | H     | 5002 | LMG  | O1-C1   | 2.06  | 1.43        | 1.40     |
| 14  | a     | 1132 | CLA  | C1D-C2D | 2.05  | 1.49        | 1.45     |
| 14  | a     | 1116 | CLA  | C1D-C2D | 2.05  | 1.49        | 1.45     |
| 14  | G     | 1108 | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 14  | b     | 1232 | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 14  | H     | 1212 | CLA  | C4B-CHC | 2.05  | 1.46        | 1.41     |
| 14  | A     | 1112 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 15  | b     | 1230 | F6C  | C4D-CHA | 2.05  | 1.47        | 1.42     |
| 14  | a     | 1139 | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 14  | b     | 1234 | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 21  | a     | 6004 | LMT  | O1'-C1' | -2.05 | 1.36        | 1.40     |
| 14  | G     | 1112 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 14  | H     | 1202 | CLA  | C1B-CHB | 2.05  | 1.46        | 1.41     |
| 14  | H     | 1206 | CLA  | C1B-CHB | 2.05  | 1.46        | 1.41     |
| 21  | A     | 6001 | LMT  | O4'-C4B | -2.05 | 1.38        | 1.43     |
| 18  | b     | 4017 | BCR  | C14-C13 | -2.05 | 1.33        | 1.35     |
| 14  | G     | 1117 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 14  | B     | 1205 | CLA  | C4B-CHC | 2.05  | 1.46        | 1.41     |
| 14  | B     | 1212 | CLA  | C4B-CHC | 2.05  | 1.46        | 1.41     |
| 14  | H     | 1205 | CLA  | C4B-CHC | 2.05  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 1117 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 14  | A     | 1135 | CLA  | C1B-NB  | -2.05 | 1.33        | 1.35     |
| 14  | a     | 1117 | CLA  | C1D-C2D | 2.05  | 1.49        | 1.45     |
| 21  | A     | 6004 | LMT  | O1'-C1' | -2.05 | 1.36        | 1.40     |
| 14  | a     | 1117 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 14  | B     | 1213 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | b     | 1209 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 14  | b     | 1239 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 21  | B     | 6003 | LMT  | C3'-C2' | 2.04  | 1.57        | 1.52     |
| 20  | i     | 5006 | LMG  | C37-C36 | -2.04 | 1.33        | 1.49     |
| 14  | B     | 1234 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 14  | B     | 1206 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | a     | 1122 | CLA  | C4B-CHC | 2.04  | 1.46        | 1.41     |
| 14  | A     | 1110 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 20  | I     | 5006 | LMG  | C37-C36 | -2.04 | 1.33        | 1.49     |
| 15  | H     | 1237 | F6C  | C1C-CHC | 2.04  | 1.46        | 1.41     |
| 15  | B     | 1237 | F6C  | C1C-CHC | 2.04  | 1.46        | 1.41     |
| 20  | R     | 5006 | LMG  | C37-C36 | -2.04 | 1.33        | 1.49     |
| 14  | G     | 1102 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 14  | B     | 1239 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 14  | H     | 1213 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | A     | 1138 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | a     | 1127 | CLA  | C4B-CHC | 2.04  | 1.46        | 1.41     |
| 14  | A     | 1120 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 14  | a     | 1139 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 14  | a     | 1122 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | b     | 1213 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | B     | 1201 | CLA  | C1D-C2D | 2.03  | 1.49        | 1.45     |
| 14  | a     | 1138 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | A     | 1133 | CLA  | C4B-CHC | 2.03  | 1.46        | 1.41     |
| 14  | H     | 1234 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | a     | 1110 | CLA  | C1D-C2D | 2.03  | 1.49        | 1.45     |
| 14  | G     | 1133 | CLA  | C4B-CHC | 2.03  | 1.46        | 1.41     |
| 14  | b     | 1210 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | A     | 1138 | CLA  | C4B-CHC | 2.03  | 1.46        | 1.41     |
| 14  | B     | 1202 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | b     | 1212 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | G     | 1131 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | A     | 1134 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | b     | 1215 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 18  | a     | 4005 | BCR  | C14-C13 | -2.03 | 1.33        | 1.35     |
| 14  | A     | 1102 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 1130 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | G     | 1138 | CLA  | C4B-CHC | 2.03  | 1.46        | 1.41     |
| 14  | a     | 1124 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | a     | 1138 | CLA  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 14  | A     | 1117 | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 14  | b     | 1205 | CLA  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 14  | b     | 1206 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | G     | 1138 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | a     | 1133 | CLA  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 14  | A     | 1122 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | B     | 1022 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 14  | H     | 1236 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 18  | H     | 4017 | BCR  | C14-C13 | -2.02 | 1.33        | 1.35     |
| 21  | H     | 6003 | LMT  | C3'-C2' | 2.02  | 1.57        | 1.52     |
| 14  | b     | 1202 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | G     | 1120 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | B     | 1210 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | H     | 1215 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | H     | 1215 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | G     | 1122 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | b     | 1213 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | a     | 1134 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | b     | 1212 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | a     | 1124 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | a     | 1106 | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 14  | A     | 1139 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | a     | 1102 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | a     | 1105 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | H     | 1213 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | G     | 1117 | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 14  | B     | 1215 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | A     | 1131 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 14  | G     | 1130 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | H     | 1212 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | H     | 1222 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | G     | 1134 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | a     | 1131 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 21  | G     | 6004 | LMT  | O1'-C1' | -2.01 | 1.36        | 1.40     |
| 21  | B     | 6004 | LMT  | O4'-C4B | -2.01 | 1.38        | 1.43     |
| 14  | A     | 1124 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | A     | 1130 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | G     | 1135 | CLA  | C1D-C2D | 2.01  | 1.49        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1022 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 14  | B     | 1215 | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 14  | b     | 1215 | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 14  | B     | 1213 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | H     | 1206 | CLA  | C4B-CHC | 2.01  | 1.46        | 1.41     |
| 14  | b     | 1222 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | B     | 1212 | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 14  | G     | 1124 | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 21  | b     | 6004 | LMT  | O4'-C4B | -2.01 | 1.38        | 1.43     |
| 14  | H     | 1239 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | H     | 1221 | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 14  | G     | 1139 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 14  | b     | 1206 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 18  | G     | 4005 | BCR  | C14-C13 | -2.00 | 1.33        | 1.35     |
| 14  | a     | 1133 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 14  | H     | 1209 | CLA  | C1D-C2D | 2.00  | 1.49        | 1.45     |
| 14  | b     | 1201 | CLA  | C1D-C2D | 2.00  | 1.49        | 1.45     |
| 21  | B     | 6003 | LMT  | O2'-C2' | -2.00 | 1.38        | 1.43     |
| 21  | b     | 6003 | LMT  | O2'-C2' | -2.00 | 1.38        | 1.43     |
| 14  | B     | 1212 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 14  | B     | 1222 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 14  | T     | 1401 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |

All (7844) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | i     | 4020 | BCR  | C20-C21-C22 | 27.22 | 166.15      | 127.31   |
| 18  | I     | 4020 | BCR  | C20-C21-C22 | 27.20 | 166.13      | 127.31   |
| 18  | R     | 4020 | BCR  | C20-C21-C22 | 27.18 | 166.10      | 127.31   |
| 18  | b     | 4010 | BCR  | C16-C17-C18 | 27.11 | 166.00      | 127.31   |
| 18  | H     | 4010 | BCR  | C16-C17-C18 | 27.09 | 165.97      | 127.31   |
| 18  | B     | 4010 | BCR  | C16-C17-C18 | 27.09 | 165.97      | 127.31   |
| 18  | A     | 4003 | BCR  | C20-C21-C22 | 25.97 | 164.37      | 127.31   |
| 18  | a     | 4003 | BCR  | C20-C21-C22 | 25.97 | 164.37      | 127.31   |
| 18  | G     | 4003 | BCR  | C20-C21-C22 | 25.95 | 164.34      | 127.31   |
| 18  | b     | 4017 | BCR  | C20-C21-C22 | 25.84 | 164.19      | 127.31   |
| 18  | H     | 4017 | BCR  | C20-C21-C22 | 25.83 | 164.17      | 127.31   |
| 18  | B     | 4017 | BCR  | C20-C21-C22 | 25.80 | 164.13      | 127.31   |
| 18  | G     | 4004 | BCR  | C16-C17-C18 | 23.98 | 161.54      | 127.31   |
| 18  | A     | 4004 | BCR  | C16-C17-C18 | 23.96 | 161.51      | 127.31   |
| 18  | a     | 4004 | BCR  | C16-C17-C18 | 23.96 | 161.50      | 127.31   |
| 18  | i     | 4018 | BCR  | C16-C17-C18 | 23.13 | 160.32      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | I     | 4018 | BCR  | C16-C17-C18 | 23.12 | 160.30      | 127.31   |
| 18  | R     | 4018 | BCR  | C16-C17-C18 | 23.10 | 160.27      | 127.31   |
| 18  | B     | 4006 | BCR  | C20-C21-C22 | 22.68 | 159.68      | 127.31   |
| 18  | H     | 4006 | BCR  | C20-C21-C22 | 22.68 | 159.67      | 127.31   |
| 18  | b     | 4006 | BCR  | C20-C21-C22 | 22.67 | 159.67      | 127.31   |
| 18  | K     | 4001 | BCR  | C20-C21-C22 | 22.62 | 159.59      | 127.31   |
| 18  | T     | 4001 | BCR  | C20-C21-C22 | 22.60 | 159.56      | 127.31   |
| 18  | k     | 4001 | BCR  | C20-C21-C22 | 22.57 | 159.52      | 127.31   |
| 18  | M     | 4021 | BCR  | C20-C21-C22 | 22.44 | 159.33      | 127.31   |
| 18  | m     | 4021 | BCR  | C20-C21-C22 | 22.43 | 159.32      | 127.31   |
| 18  | V     | 4021 | BCR  | C20-C21-C22 | 22.41 | 159.29      | 127.31   |
| 18  | b     | 4014 | BCR  | C20-C21-C22 | 22.13 | 158.89      | 127.31   |
| 18  | B     | 4014 | BCR  | C20-C21-C22 | 22.12 | 158.88      | 127.31   |
| 18  | H     | 4014 | BCR  | C20-C21-C22 | 22.12 | 158.88      | 127.31   |
| 18  | a     | 4004 | BCR  | C20-C21-C22 | 22.11 | 158.86      | 127.31   |
| 18  | A     | 4004 | BCR  | C20-C21-C22 | 22.06 | 158.79      | 127.31   |
| 18  | G     | 4004 | BCR  | C20-C21-C22 | 22.05 | 158.77      | 127.31   |
| 18  | a     | 4001 | BCR  | C16-C17-C18 | 21.92 | 158.60      | 127.31   |
| 18  | A     | 4001 | BCR  | C16-C17-C18 | 21.90 | 158.57      | 127.31   |
| 18  | G     | 4001 | BCR  | C16-C17-C18 | 21.88 | 158.54      | 127.31   |
| 18  | a     | 4006 | BCR  | C16-C17-C18 | 21.80 | 158.42      | 127.31   |
| 18  | A     | 4006 | BCR  | C16-C17-C18 | 21.78 | 158.39      | 127.31   |
| 18  | G     | 4006 | BCR  | C16-C17-C18 | 21.77 | 158.37      | 127.31   |
| 18  | G     | 4001 | BCR  | C20-C21-C22 | 21.74 | 158.34      | 127.31   |
| 18  | a     | 4001 | BCR  | C20-C21-C22 | 21.74 | 158.34      | 127.31   |
| 18  | A     | 4001 | BCR  | C20-C21-C22 | 21.73 | 158.32      | 127.31   |
| 18  | B     | 4014 | BCR  | C15-C16-C17 | 21.69 | 167.91      | 123.47   |
| 18  | H     | 4014 | BCR  | C15-C16-C17 | 21.69 | 167.90      | 123.47   |
| 18  | b     | 4014 | BCR  | C15-C16-C17 | 21.66 | 167.85      | 123.47   |
| 18  | H     | 4010 | BCR  | C20-C21-C22 | 21.48 | 157.96      | 127.31   |
| 18  | G     | 4002 | BCR  | C16-C17-C18 | 21.47 | 157.95      | 127.31   |
| 18  | a     | 4002 | BCR  | C16-C17-C18 | 21.46 | 157.94      | 127.31   |
| 18  | b     | 4010 | BCR  | C20-C21-C22 | 21.45 | 157.93      | 127.31   |
| 18  | A     | 4002 | BCR  | C16-C17-C18 | 21.44 | 157.91      | 127.31   |
| 18  | B     | 4010 | BCR  | C20-C21-C22 | 21.44 | 157.91      | 127.31   |
| 18  | M     | 4021 | BCR  | C15-C16-C17 | 21.35 | 167.21      | 123.47   |
| 18  | m     | 4021 | BCR  | C15-C16-C17 | 21.35 | 167.21      | 123.47   |
| 18  | V     | 4021 | BCR  | C15-C16-C17 | 21.35 | 167.21      | 123.47   |
| 18  | B     | 4004 | BCR  | C20-C21-C22 | 21.34 | 157.76      | 127.31   |
| 18  | H     | 4004 | BCR  | C20-C21-C22 | 21.32 | 157.73      | 127.31   |
| 18  | b     | 4004 | BCR  | C20-C21-C22 | 21.31 | 157.72      | 127.31   |
| 18  | b     | 4006 | BCR  | C16-C17-C18 | 21.20 | 157.56      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | B     | 4006 | BCR  | C16-C17-C18 | 21.18 | 157.54      | 127.31   |
| 18  | H     | 4006 | BCR  | C16-C17-C18 | 21.18 | 157.53      | 127.31   |
| 18  | H     | 4009 | BCR  | C16-C17-C18 | 21.06 | 157.37      | 127.31   |
| 18  | B     | 4009 | BCR  | C16-C17-C18 | 21.04 | 157.34      | 127.31   |
| 18  | b     | 4009 | BCR  | C16-C17-C18 | 21.02 | 157.31      | 127.31   |
| 18  | B     | 4005 | BCR  | C20-C21-C22 | 20.86 | 157.08      | 127.31   |
| 18  | b     | 4005 | BCR  | C20-C21-C22 | 20.85 | 157.07      | 127.31   |
| 18  | H     | 4005 | BCR  | C20-C21-C22 | 20.84 | 157.05      | 127.31   |
| 18  | H     | 4009 | BCR  | C20-C21-C22 | 20.41 | 156.43      | 127.31   |
| 18  | H     | 4005 | BCR  | C15-C16-C17 | 20.39 | 165.25      | 123.47   |
| 18  | b     | 4005 | BCR  | C15-C16-C17 | 20.39 | 165.24      | 123.47   |
| 18  | K     | 4001 | BCR  | C15-C16-C17 | 20.39 | 165.23      | 123.47   |
| 18  | T     | 4001 | BCR  | C15-C16-C17 | 20.39 | 165.23      | 123.47   |
| 18  | B     | 4009 | BCR  | C20-C21-C22 | 20.38 | 156.40      | 127.31   |
| 18  | B     | 4005 | BCR  | C15-C16-C17 | 20.38 | 165.23      | 123.47   |
| 18  | G     | 4005 | BCR  | C15-C16-C17 | 20.38 | 165.22      | 123.47   |
| 18  | a     | 4005 | BCR  | C15-C16-C17 | 20.38 | 165.21      | 123.47   |
| 18  | I     | 4018 | BCR  | C20-C21-C22 | 20.37 | 156.39      | 127.31   |
| 18  | b     | 4014 | BCR  | C16-C17-C18 | 20.37 | 156.39      | 127.31   |
| 18  | i     | 4018 | BCR  | C20-C21-C22 | 20.37 | 156.38      | 127.31   |
| 18  | k     | 4001 | BCR  | C15-C16-C17 | 20.37 | 165.20      | 123.47   |
| 18  | b     | 4009 | BCR  | C20-C21-C22 | 20.37 | 156.38      | 127.31   |
| 18  | B     | 4014 | BCR  | C16-C17-C18 | 20.37 | 156.38      | 127.31   |
| 18  | A     | 4005 | BCR  | C15-C16-C17 | 20.35 | 165.16      | 123.47   |
| 18  | H     | 4014 | BCR  | C16-C17-C18 | 20.35 | 156.35      | 127.31   |
| 18  | R     | 4018 | BCR  | C20-C21-C22 | 20.34 | 156.33      | 127.31   |
| 18  | a     | 4003 | BCR  | C16-C17-C18 | 20.31 | 156.30      | 127.31   |
| 18  | A     | 4003 | BCR  | C16-C17-C18 | 20.30 | 156.28      | 127.31   |
| 18  | A     | 4003 | BCR  | C15-C16-C17 | 20.29 | 165.04      | 123.47   |
| 18  | G     | 4003 | BCR  | C16-C17-C18 | 20.29 | 156.27      | 127.31   |
| 18  | a     | 4003 | BCR  | C15-C16-C17 | 20.29 | 165.03      | 123.47   |
| 18  | G     | 4003 | BCR  | C15-C16-C17 | 20.29 | 165.03      | 123.47   |
| 18  | b     | 4017 | BCR  | C16-C17-C18 | 20.26 | 156.22      | 127.31   |
| 18  | B     | 4017 | BCR  | C16-C17-C18 | 20.22 | 156.17      | 127.31   |
| 18  | I     | 4020 | BCR  | C15-C16-C17 | 20.22 | 164.89      | 123.47   |
| 18  | R     | 4020 | BCR  | C15-C16-C17 | 20.21 | 164.88      | 123.47   |
| 18  | i     | 4020 | BCR  | C15-C16-C17 | 20.21 | 164.87      | 123.47   |
| 18  | b     | 4004 | BCR  | C15-C16-C17 | 20.21 | 164.86      | 123.47   |
| 18  | H     | 4004 | BCR  | C15-C16-C17 | 20.20 | 164.86      | 123.47   |
| 18  | B     | 4004 | BCR  | C15-C16-C17 | 20.20 | 164.85      | 123.47   |
| 18  | H     | 4017 | BCR  | C16-C17-C18 | 20.18 | 156.11      | 127.31   |
| 18  | L     | 4019 | BCR  | C20-C21-C22 | 20.16 | 156.08      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | L     | 4022 | BCR  | C15-C16-C17 | 20.15  | 164.75      | 123.47   |
| 14  | a     | 1111 | CLA  | C4-C3-C5    | -20.15 | 81.38       | 115.27   |
| 18  | l     | 4022 | BCR  | C15-C16-C17 | 20.14  | 164.74      | 123.47   |
| 18  | U     | 4022 | BCR  | C15-C16-C17 | 20.14  | 164.72      | 123.47   |
| 18  | l     | 4019 | BCR  | C20-C21-C22 | 20.14  | 156.05      | 127.31   |
| 18  | U     | 4019 | BCR  | C20-C21-C22 | 20.13  | 156.04      | 127.31   |
| 14  | A     | 1111 | CLA  | C4-C3-C5    | -20.13 | 81.40       | 115.27   |
| 14  | G     | 1111 | CLA  | C4-C3-C5    | -20.12 | 81.43       | 115.27   |
| 18  | I     | 4020 | BCR  | C16-C17-C18 | 20.09  | 155.99      | 127.31   |
| 18  | i     | 4020 | BCR  | C16-C17-C18 | 20.08  | 155.97      | 127.31   |
| 18  | K     | 4001 | BCR  | C16-C17-C18 | 20.08  | 155.96      | 127.31   |
| 18  | R     | 4020 | BCR  | C16-C17-C18 | 20.06  | 155.94      | 127.31   |
| 18  | T     | 4001 | BCR  | C16-C17-C18 | 20.06  | 155.94      | 127.31   |
| 18  | k     | 4001 | BCR  | C16-C17-C18 | 20.04  | 155.92      | 127.31   |
| 18  | A     | 4002 | BCR  | C20-C21-C22 | 19.98  | 155.82      | 127.31   |
| 18  | G     | 4002 | BCR  | C20-C21-C22 | 19.95  | 155.78      | 127.31   |
| 18  | a     | 4002 | BCR  | C20-C21-C22 | 19.93  | 155.76      | 127.31   |
| 18  | l     | 4022 | BCR  | C20-C21-C22 | 19.92  | 155.75      | 127.31   |
| 18  | L     | 4022 | BCR  | C20-C21-C22 | 19.91  | 155.72      | 127.31   |
| 18  | U     | 4022 | BCR  | C20-C21-C22 | 19.89  | 155.70      | 127.31   |
| 18  | L     | 4019 | BCR  | C16-C17-C18 | 19.85  | 155.64      | 127.31   |
| 18  | l     | 4019 | BCR  | C16-C17-C18 | 19.84  | 155.62      | 127.31   |
| 18  | U     | 4019 | BCR  | C16-C17-C18 | 19.83  | 155.61      | 127.31   |
| 18  | L     | 4019 | BCR  | C15-C16-C17 | 19.79  | 164.00      | 123.47   |
| 18  | l     | 4019 | BCR  | C15-C16-C17 | 19.77  | 163.97      | 123.47   |
| 18  | U     | 4019 | BCR  | C15-C16-C17 | 19.76  | 163.95      | 123.47   |
| 18  | A     | 4005 | BCR  | C20-C21-C22 | 19.75  | 155.50      | 127.31   |
| 18  | a     | 4005 | BCR  | C20-C21-C22 | 19.74  | 155.49      | 127.31   |
| 18  | G     | 4005 | BCR  | C20-C21-C22 | 19.72  | 155.46      | 127.31   |
| 18  | b     | 4005 | BCR  | C16-C17-C18 | 19.71  | 155.44      | 127.31   |
| 18  | b     | 4017 | BCR  | C15-C16-C17 | 19.70  | 163.84      | 123.47   |
| 18  | B     | 4017 | BCR  | C15-C16-C17 | 19.69  | 163.81      | 123.47   |
| 18  | B     | 4005 | BCR  | C16-C17-C18 | 19.68  | 155.40      | 127.31   |
| 18  | H     | 4017 | BCR  | C15-C16-C17 | 19.66  | 163.75      | 123.47   |
| 18  | H     | 4005 | BCR  | C16-C17-C18 | 19.66  | 155.37      | 127.31   |
| 18  | a     | 4005 | BCR  | C16-C17-C18 | 19.61  | 155.30      | 127.31   |
| 18  | G     | 4005 | BCR  | C16-C17-C18 | 19.59  | 155.28      | 127.31   |
| 18  | A     | 4005 | BCR  | C16-C17-C18 | 19.58  | 155.26      | 127.31   |
| 18  | B     | 4006 | BCR  | C15-C16-C17 | 19.54  | 163.49      | 123.47   |
| 18  | b     | 4006 | BCR  | C15-C16-C17 | 19.54  | 163.49      | 123.47   |
| 18  | H     | 4006 | BCR  | C15-C16-C17 | 19.54  | 163.49      | 123.47   |
| 18  | H     | 4009 | BCR  | C15-C16-C17 | 19.47  | 163.36      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | B     | 4009 | BCR  | C15-C16-C17 | 19.44  | 163.31      | 123.47   |
| 18  | b     | 4009 | BCR  | C15-C16-C17 | 19.43  | 163.27      | 123.47   |
| 18  | a     | 4006 | BCR  | C20-C21-C22 | 19.42  | 155.03      | 127.31   |
| 18  | A     | 4006 | BCR  | C20-C21-C22 | 19.40  | 154.99      | 127.31   |
| 18  | G     | 4006 | BCR  | C20-C21-C22 | 19.39  | 154.98      | 127.31   |
| 14  | G     | 1111 | CLA  | C5-C3-C2    | 19.22  | 160.01      | 121.12   |
| 14  | A     | 1111 | CLA  | C5-C3-C2    | 19.21  | 159.99      | 121.12   |
| 14  | a     | 1111 | CLA  | C5-C3-C2    | 19.19  | 159.95      | 121.12   |
| 18  | l     | 4022 | BCR  | C16-C17-C18 | 19.14  | 154.62      | 127.31   |
| 18  | L     | 4022 | BCR  | C16-C17-C18 | 19.12  | 154.59      | 127.31   |
| 18  | U     | 4022 | BCR  | C16-C17-C18 | 19.09  | 154.56      | 127.31   |
| 18  | a     | 4006 | BCR  | C15-C16-C17 | 18.92  | 162.24      | 123.47   |
| 18  | A     | 4006 | BCR  | C15-C16-C17 | 18.91  | 162.20      | 123.47   |
| 18  | G     | 4006 | BCR  | C15-C16-C17 | 18.90  | 162.19      | 123.47   |
| 18  | R     | 4018 | BCR  | C15-C16-C17 | 18.42  | 161.22      | 123.47   |
| 18  | i     | 4018 | BCR  | C15-C16-C17 | 18.40  | 161.16      | 123.47   |
| 18  | I     | 4018 | BCR  | C15-C16-C17 | 18.39  | 161.15      | 123.47   |
| 18  | b     | 4004 | BCR  | C16-C17-C18 | 18.34  | 153.48      | 127.31   |
| 18  | H     | 4004 | BCR  | C16-C17-C18 | 18.33  | 153.47      | 127.31   |
| 18  | B     | 4004 | BCR  | C16-C17-C18 | 18.33  | 153.47      | 127.31   |
| 18  | H     | 4010 | BCR  | C10-C11-C12 | 17.84  | 178.90      | 123.22   |
| 18  | B     | 4010 | BCR  | C10-C11-C12 | 17.83  | 178.87      | 123.22   |
| 18  | G     | 4001 | BCR  | C15-C16-C17 | 17.83  | 159.99      | 123.47   |
| 18  | b     | 4010 | BCR  | C10-C11-C12 | 17.83  | 178.84      | 123.22   |
| 18  | A     | 4001 | BCR  | C15-C16-C17 | 17.82  | 159.98      | 123.47   |
| 18  | a     | 4001 | BCR  | C15-C16-C17 | 17.81  | 159.95      | 123.47   |
| 18  | a     | 4003 | BCR  | C10-C11-C12 | 17.80  | 178.76      | 123.22   |
| 18  | A     | 4003 | BCR  | C10-C11-C12 | 17.79  | 178.74      | 123.22   |
| 18  | G     | 4003 | BCR  | C10-C11-C12 | 17.79  | 178.74      | 123.22   |
| 14  | a     | 1111 | CLA  | C4-C3-C2    | -17.56 | 78.62       | 123.68   |
| 14  | G     | 1111 | CLA  | C4-C3-C2    | -17.56 | 78.63       | 123.68   |
| 14  | A     | 1111 | CLA  | C4-C3-C2    | -17.56 | 78.64       | 123.68   |
| 18  | b     | 4009 | BCR  | C10-C11-C12 | 17.52  | 177.89      | 123.22   |
| 18  | B     | 4009 | BCR  | C10-C11-C12 | 17.51  | 177.85      | 123.22   |
| 18  | H     | 4009 | BCR  | C10-C11-C12 | 17.49  | 177.81      | 123.22   |
| 18  | a     | 4001 | BCR  | C10-C11-C12 | 17.41  | 177.54      | 123.22   |
| 18  | b     | 4017 | BCR  | C10-C11-C12 | 17.40  | 177.51      | 123.22   |
| 18  | A     | 4001 | BCR  | C10-C11-C12 | 17.40  | 177.51      | 123.22   |
| 18  | H     | 4004 | BCR  | C10-C11-C12 | 17.40  | 177.50      | 123.22   |
| 18  | B     | 4017 | BCR  | C10-C11-C12 | 17.40  | 177.50      | 123.22   |
| 18  | H     | 4017 | BCR  | C10-C11-C12 | 17.39  | 177.50      | 123.22   |
| 18  | B     | 4004 | BCR  | C10-C11-C12 | 17.39  | 177.47      | 123.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4001 | BCR  | C10-C11-C12 | 17.38 | 177.46      | 123.22   |
| 18  | b     | 4004 | BCR  | C10-C11-C12 | 17.38 | 177.44      | 123.22   |
| 18  | R     | 4018 | BCR  | C10-C11-C12 | 17.23 | 177.00      | 123.22   |
| 18  | i     | 4018 | BCR  | C10-C11-C12 | 17.22 | 176.95      | 123.22   |
| 18  | I     | 4018 | BCR  | C10-C11-C12 | 17.21 | 176.94      | 123.22   |
| 18  | l     | 4022 | BCR  | C10-C11-C12 | 17.20 | 176.90      | 123.22   |
| 18  | L     | 4022 | BCR  | C10-C11-C12 | 17.20 | 176.90      | 123.22   |
| 18  | U     | 4022 | BCR  | C10-C11-C12 | 17.20 | 176.89      | 123.22   |
| 18  | V     | 4021 | BCR  | C10-C11-C12 | 17.20 | 176.89      | 123.22   |
| 18  | M     | 4021 | BCR  | C10-C11-C12 | 17.19 | 176.87      | 123.22   |
| 18  | m     | 4021 | BCR  | C10-C11-C12 | 17.19 | 176.85      | 123.22   |
| 18  | a     | 4002 | BCR  | C10-C11-C12 | 17.16 | 176.75      | 123.22   |
| 18  | A     | 4002 | BCR  | C10-C11-C12 | 17.15 | 176.74      | 123.22   |
| 18  | G     | 4002 | BCR  | C10-C11-C12 | 17.15 | 176.73      | 123.22   |
| 18  | G     | 4004 | BCR  | C10-C11-C12 | 17.11 | 176.62      | 123.22   |
| 18  | A     | 4004 | BCR  | C10-C11-C12 | 17.10 | 176.58      | 123.22   |
| 18  | a     | 4004 | BCR  | C10-C11-C12 | 17.08 | 176.52      | 123.22   |
| 18  | b     | 4006 | BCR  | C10-C11-C12 | 17.03 | 176.35      | 123.22   |
| 18  | B     | 4006 | BCR  | C10-C11-C12 | 17.02 | 176.34      | 123.22   |
| 18  | H     | 4006 | BCR  | C10-C11-C12 | 17.02 | 176.34      | 123.22   |
| 18  | T     | 4001 | BCR  | C10-C11-C12 | 17.00 | 176.27      | 123.22   |
| 18  | K     | 4001 | BCR  | C10-C11-C12 | 16.99 | 176.25      | 123.22   |
| 18  | k     | 4001 | BCR  | C10-C11-C12 | 16.99 | 176.24      | 123.22   |
| 18  | m     | 4021 | BCR  | C16-C17-C18 | 16.97 | 151.53      | 127.31   |
| 18  | M     | 4021 | BCR  | C16-C17-C18 | 16.97 | 151.53      | 127.31   |
| 18  | V     | 4021 | BCR  | C16-C17-C18 | 16.94 | 151.48      | 127.31   |
| 18  | i     | 4020 | BCR  | C10-C11-C12 | 16.90 | 175.96      | 123.22   |
| 18  | I     | 4020 | BCR  | C10-C11-C12 | 16.90 | 175.95      | 123.22   |
| 18  | R     | 4020 | BCR  | C10-C11-C12 | 16.90 | 175.95      | 123.22   |
| 18  | A     | 4002 | BCR  | C15-C16-C17 | 16.86 | 158.00      | 123.47   |
| 18  | a     | 4002 | BCR  | C15-C16-C17 | 16.84 | 157.98      | 123.47   |
| 18  | G     | 4002 | BCR  | C15-C16-C17 | 16.81 | 157.92      | 123.47   |
| 18  | B     | 4005 | BCR  | C10-C11-C12 | 16.80 | 175.64      | 123.22   |
| 18  | H     | 4005 | BCR  | C10-C11-C12 | 16.79 | 175.63      | 123.22   |
| 18  | b     | 4005 | BCR  | C10-C11-C12 | 16.79 | 175.62      | 123.22   |
| 18  | M     | 4021 | BCR  | C16-C15-C14 | 16.78 | 157.85      | 123.47   |
| 18  | m     | 4021 | BCR  | C16-C15-C14 | 16.78 | 157.84      | 123.47   |
| 18  | V     | 4021 | BCR  | C16-C15-C14 | 16.76 | 157.81      | 123.47   |
| 18  | a     | 4005 | BCR  | C10-C11-C12 | 16.71 | 175.37      | 123.22   |
| 18  | A     | 4005 | BCR  | C10-C11-C12 | 16.70 | 175.32      | 123.22   |
| 18  | G     | 4005 | BCR  | C10-C11-C12 | 16.69 | 175.31      | 123.22   |
| 18  | l     | 4019 | BCR  | C10-C11-C12 | 16.50 | 174.71      | 123.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | H     | 4014 | BCR  | C10-C11-C12 | 16.49 | 174.67      | 123.22   |
| 18  | L     | 4019 | BCR  | C10-C11-C12 | 16.49 | 174.67      | 123.22   |
| 18  | U     | 4019 | BCR  | C10-C11-C12 | 16.48 | 174.64      | 123.22   |
| 18  | B     | 4014 | BCR  | C10-C11-C12 | 16.48 | 174.63      | 123.22   |
| 18  | b     | 4014 | BCR  | C10-C11-C12 | 16.47 | 174.62      | 123.22   |
| 18  | A     | 4004 | BCR  | C15-C16-C17 | 16.37 | 157.01      | 123.47   |
| 18  | G     | 4004 | BCR  | C15-C16-C17 | 16.37 | 157.00      | 123.47   |
| 18  | a     | 4004 | BCR  | C15-C16-C17 | 16.36 | 156.99      | 123.47   |
| 18  | a     | 4002 | BCR  | C16-C15-C14 | 16.05 | 156.36      | 123.47   |
| 18  | A     | 4002 | BCR  | C16-C15-C14 | 16.05 | 156.35      | 123.47   |
| 18  | G     | 4002 | BCR  | C16-C15-C14 | 16.02 | 156.30      | 123.47   |
| 18  | G     | 4006 | BCR  | C10-C11-C12 | 15.94 | 172.95      | 123.22   |
| 18  | A     | 4006 | BCR  | C10-C11-C12 | 15.93 | 172.94      | 123.22   |
| 18  | a     | 4006 | BCR  | C10-C11-C12 | 15.93 | 172.93      | 123.22   |
| 18  | b     | 4010 | BCR  | C15-C16-C17 | 15.46 | 155.15      | 123.47   |
| 18  | H     | 4010 | BCR  | C15-C16-C17 | 15.44 | 155.10      | 123.47   |
| 18  | B     | 4010 | BCR  | C15-C16-C17 | 15.43 | 155.07      | 123.47   |
| 18  | i     | 4018 | BCR  | C16-C15-C14 | 14.99 | 154.19      | 123.47   |
| 18  | I     | 4018 | BCR  | C16-C15-C14 | 14.99 | 154.18      | 123.47   |
| 18  | R     | 4018 | BCR  | C16-C15-C14 | 14.98 | 154.16      | 123.47   |
| 18  | a     | 4001 | BCR  | C16-C15-C14 | 14.95 | 154.09      | 123.47   |
| 18  | a     | 4006 | BCR  | C11-C10-C9  | 14.95 | 148.64      | 127.31   |
| 18  | A     | 4001 | BCR  | C16-C15-C14 | 14.93 | 154.06      | 123.47   |
| 18  | A     | 4006 | BCR  | C11-C10-C9  | 14.93 | 148.62      | 127.31   |
| 18  | G     | 4001 | BCR  | C16-C15-C14 | 14.93 | 154.06      | 123.47   |
| 18  | G     | 4006 | BCR  | C11-C10-C9  | 14.92 | 148.61      | 127.31   |
| 18  | l     | 4019 | BCR  | C11-C10-C9  | 14.70 | 148.29      | 127.31   |
| 18  | U     | 4019 | BCR  | C11-C10-C9  | 14.70 | 148.28      | 127.31   |
| 18  | L     | 4019 | BCR  | C11-C10-C9  | 14.66 | 148.24      | 127.31   |
| 18  | H     | 4004 | BCR  | C11-C10-C9  | 14.50 | 148.00      | 127.31   |
| 18  | H     | 4005 | BCR  | C11-C10-C9  | 14.49 | 147.99      | 127.31   |
| 18  | B     | 4005 | BCR  | C11-C10-C9  | 14.49 | 147.99      | 127.31   |
| 18  | b     | 4005 | BCR  | C11-C10-C9  | 14.48 | 147.97      | 127.31   |
| 18  | B     | 4004 | BCR  | C11-C10-C9  | 14.47 | 147.96      | 127.31   |
| 18  | b     | 4004 | BCR  | C11-C10-C9  | 14.45 | 147.94      | 127.31   |
| 18  | H     | 4014 | BCR  | C11-C10-C9  | 13.99 | 147.28      | 127.31   |
| 18  | b     | 4014 | BCR  | C11-C10-C9  | 13.97 | 147.25      | 127.31   |
| 18  | B     | 4014 | BCR  | C11-C10-C9  | 13.97 | 147.24      | 127.31   |
| 18  | L     | 4019 | BCR  | C21-C20-C19 | 13.96 | 166.77      | 123.22   |
| 18  | l     | 4019 | BCR  | C21-C20-C19 | 13.94 | 166.73      | 123.22   |
| 18  | U     | 4019 | BCR  | C21-C20-C19 | 13.94 | 166.73      | 123.22   |
| 18  | L     | 4022 | BCR  | C21-C20-C19 | 13.71 | 166.00      | 123.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | B     | 4004 | BCR  | C21-C20-C19 | 13.71 | 165.99      | 123.22   |
| 18  | l     | 4022 | BCR  | C21-C20-C19 | 13.71 | 165.99      | 123.22   |
| 18  | U     | 4022 | BCR  | C21-C20-C19 | 13.70 | 165.98      | 123.22   |
| 18  | H     | 4004 | BCR  | C21-C20-C19 | 13.70 | 165.96      | 123.22   |
| 18  | b     | 4004 | BCR  | C21-C20-C19 | 13.70 | 165.96      | 123.22   |
| 18  | a     | 4005 | BCR  | C11-C10-C9  | 13.67 | 146.82      | 127.31   |
| 18  | A     | 4005 | BCR  | C11-C10-C9  | 13.65 | 146.78      | 127.31   |
| 18  | G     | 4005 | BCR  | C11-C10-C9  | 13.63 | 146.77      | 127.31   |
| 18  | B     | 4010 | BCR  | C16-C15-C14 | 13.62 | 151.37      | 123.47   |
| 18  | H     | 4010 | BCR  | C16-C15-C14 | 13.61 | 151.35      | 123.47   |
| 18  | b     | 4010 | BCR  | C16-C15-C14 | 13.60 | 151.33      | 123.47   |
| 18  | R     | 4018 | BCR  | C11-C10-C9  | 13.54 | 146.63      | 127.31   |
| 18  | i     | 4018 | BCR  | C11-C10-C9  | 13.52 | 146.61      | 127.31   |
| 18  | R     | 4020 | BCR  | C11-C10-C9  | 13.51 | 146.59      | 127.31   |
| 18  | I     | 4020 | BCR  | C11-C10-C9  | 13.51 | 146.58      | 127.31   |
| 18  | I     | 4018 | BCR  | C11-C10-C9  | 13.50 | 146.58      | 127.31   |
| 18  | i     | 4020 | BCR  | C11-C10-C9  | 13.48 | 146.55      | 127.31   |
| 18  | a     | 4003 | BCR  | C11-C10-C9  | 13.45 | 146.50      | 127.31   |
| 18  | H     | 4010 | BCR  | C21-C20-C19 | 13.44 | 165.17      | 123.22   |
| 18  | A     | 4003 | BCR  | C11-C10-C9  | 13.43 | 146.48      | 127.31   |
| 18  | G     | 4001 | BCR  | C21-C20-C19 | 13.43 | 165.13      | 123.22   |
| 18  | B     | 4010 | BCR  | C21-C20-C19 | 13.43 | 165.13      | 123.22   |
| 18  | a     | 4006 | BCR  | C16-C15-C14 | 13.43 | 150.98      | 123.47   |
| 18  | b     | 4010 | BCR  | C21-C20-C19 | 13.43 | 165.11      | 123.22   |
| 18  | A     | 4001 | BCR  | C21-C20-C19 | 13.42 | 165.10      | 123.22   |
| 18  | G     | 4003 | BCR  | C11-C10-C9  | 13.42 | 146.46      | 127.31   |
| 18  | M     | 4021 | BCR  | C11-C10-C9  | 13.41 | 146.45      | 127.31   |
| 18  | A     | 4006 | BCR  | C16-C15-C14 | 13.41 | 150.95      | 123.47   |
| 18  | G     | 4006 | BCR  | C16-C15-C14 | 13.40 | 150.93      | 123.47   |
| 18  | a     | 4001 | BCR  | C21-C20-C19 | 13.40 | 165.04      | 123.22   |
| 18  | V     | 4021 | BCR  | C11-C10-C9  | 13.40 | 146.44      | 127.31   |
| 18  | m     | 4021 | BCR  | C11-C10-C9  | 13.39 | 146.42      | 127.31   |
| 18  | a     | 4005 | BCR  | C21-C20-C19 | 13.37 | 164.94      | 123.22   |
| 18  | A     | 4005 | BCR  | C21-C20-C19 | 13.37 | 164.93      | 123.22   |
| 18  | G     | 4005 | BCR  | C21-C20-C19 | 13.35 | 164.87      | 123.22   |
| 18  | H     | 4010 | BCR  | C11-C10-C9  | 13.27 | 146.25      | 127.31   |
| 18  | B     | 4010 | BCR  | C11-C10-C9  | 13.26 | 146.24      | 127.31   |
| 18  | b     | 4010 | BCR  | C11-C10-C9  | 13.23 | 146.19      | 127.31   |
| 18  | b     | 4004 | BCR  | C16-C15-C14 | 13.14 | 150.38      | 123.47   |
| 18  | G     | 4004 | BCR  | C16-C15-C14 | 13.13 | 150.38      | 123.47   |
| 18  | B     | 4004 | BCR  | C16-C15-C14 | 13.13 | 150.37      | 123.47   |
| 18  | H     | 4004 | BCR  | C16-C15-C14 | 13.13 | 150.37      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 4004 | BCR  | C16-C15-C14 | 13.12 | 150.35      | 123.47   |
| 18  | a     | 4004 | BCR  | C16-C15-C14 | 13.12 | 150.35      | 123.47   |
| 18  | b     | 4009 | BCR  | C21-C20-C19 | 13.07 | 164.00      | 123.22   |
| 18  | H     | 4009 | BCR  | C16-C15-C14 | 13.07 | 150.24      | 123.47   |
| 18  | B     | 4009 | BCR  | C21-C20-C19 | 13.06 | 163.96      | 123.22   |
| 18  | H     | 4009 | BCR  | C21-C20-C19 | 13.05 | 163.93      | 123.22   |
| 18  | B     | 4009 | BCR  | C16-C15-C14 | 13.04 | 150.18      | 123.47   |
| 18  | b     | 4009 | BCR  | C16-C15-C14 | 13.02 | 150.15      | 123.47   |
| 18  | H     | 4017 | BCR  | C11-C10-C9  | 12.92 | 145.74      | 127.31   |
| 18  | B     | 4017 | BCR  | C11-C10-C9  | 12.91 | 145.73      | 127.31   |
| 18  | b     | 4017 | BCR  | C11-C10-C9  | 12.88 | 145.69      | 127.31   |
| 18  | G     | 4004 | BCR  | C11-C10-C9  | 12.86 | 145.67      | 127.31   |
| 18  | A     | 4004 | BCR  | C11-C10-C9  | 12.85 | 145.64      | 127.31   |
| 18  | a     | 4004 | BCR  | C11-C10-C9  | 12.81 | 145.59      | 127.31   |
| 18  | B     | 4006 | BCR  | C11-C10-C9  | 12.80 | 145.58      | 127.31   |
| 18  | H     | 4006 | BCR  | C11-C10-C9  | 12.80 | 145.58      | 127.31   |
| 18  | b     | 4006 | BCR  | C11-C10-C9  | 12.80 | 145.58      | 127.31   |
| 18  | B     | 4006 | BCR  | C16-C15-C14 | 12.78 | 149.66      | 123.47   |
| 18  | b     | 4006 | BCR  | C16-C15-C14 | 12.78 | 149.65      | 123.47   |
| 18  | H     | 4006 | BCR  | C16-C15-C14 | 12.76 | 149.61      | 123.47   |
| 18  | a     | 4003 | BCR  | C21-C20-C19 | 12.70 | 162.84      | 123.22   |
| 18  | G     | 4003 | BCR  | C21-C20-C19 | 12.69 | 162.82      | 123.22   |
| 18  | A     | 4003 | BCR  | C21-C20-C19 | 12.69 | 162.82      | 123.22   |
| 18  | K     | 4001 | BCR  | C21-C20-C19 | 12.65 | 162.69      | 123.22   |
| 18  | T     | 4001 | BCR  | C21-C20-C19 | 12.64 | 162.68      | 123.22   |
| 18  | A     | 4002 | BCR  | C21-C20-C19 | 12.64 | 162.68      | 123.22   |
| 18  | k     | 4001 | BCR  | C21-C20-C19 | 12.64 | 162.67      | 123.22   |
| 18  | G     | 4002 | BCR  | C21-C20-C19 | 12.63 | 162.63      | 123.22   |
| 18  | a     | 4002 | BCR  | C21-C20-C19 | 12.63 | 162.62      | 123.22   |
| 18  | b     | 4005 | BCR  | C21-C20-C19 | 12.61 | 162.56      | 123.22   |
| 18  | B     | 4005 | BCR  | C21-C20-C19 | 12.61 | 162.55      | 123.22   |
| 18  | H     | 4005 | BCR  | C21-C20-C19 | 12.60 | 162.53      | 123.22   |
| 18  | l     | 4022 | BCR  | C11-C10-C9  | 12.57 | 145.25      | 127.31   |
| 18  | L     | 4022 | BCR  | C11-C10-C9  | 12.56 | 145.24      | 127.31   |
| 18  | U     | 4022 | BCR  | C11-C10-C9  | 12.55 | 145.22      | 127.31   |
| 18  | a     | 4001 | BCR  | C11-C10-C9  | 12.55 | 145.22      | 127.31   |
| 18  | A     | 4001 | BCR  | C11-C10-C9  | 12.53 | 145.19      | 127.31   |
| 18  | G     | 4001 | BCR  | C11-C10-C9  | 12.50 | 145.16      | 127.31   |
| 18  | H     | 4005 | BCR  | C16-C15-C14 | 12.47 | 149.01      | 123.47   |
| 18  | B     | 4005 | BCR  | C16-C15-C14 | 12.46 | 149.00      | 123.47   |
| 18  | b     | 4005 | BCR  | C16-C15-C14 | 12.46 | 148.99      | 123.47   |
| 18  | a     | 4006 | BCR  | C21-C20-C19 | 12.45 | 162.07      | 123.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 4006 | BCR  | C21-C20-C19 | 12.43 | 162.02      | 123.22   |
| 18  | G     | 4006 | BCR  | C21-C20-C19 | 12.43 | 162.00      | 123.22   |
| 18  | b     | 4014 | BCR  | C21-C20-C19 | 12.43 | 162.00      | 123.22   |
| 18  | a     | 4005 | BCR  | C16-C15-C14 | 12.42 | 148.92      | 123.47   |
| 18  | G     | 4005 | BCR  | C16-C15-C14 | 12.42 | 148.92      | 123.47   |
| 18  | B     | 4014 | BCR  | C21-C20-C19 | 12.42 | 161.97      | 123.22   |
| 18  | H     | 4017 | BCR  | C21-C20-C19 | 12.42 | 161.97      | 123.22   |
| 18  | H     | 4014 | BCR  | C21-C20-C19 | 12.42 | 161.97      | 123.22   |
| 18  | B     | 4017 | BCR  | C21-C20-C19 | 12.42 | 161.96      | 123.22   |
| 18  | b     | 4017 | BCR  | C21-C20-C19 | 12.41 | 161.96      | 123.22   |
| 18  | A     | 4005 | BCR  | C16-C15-C14 | 12.39 | 148.86      | 123.47   |
| 18  | a     | 4002 | BCR  | C11-C10-C9  | 12.39 | 144.99      | 127.31   |
| 18  | i     | 4020 | BCR  | C16-C15-C14 | 12.37 | 148.82      | 123.47   |
| 18  | I     | 4020 | BCR  | C16-C15-C14 | 12.36 | 148.80      | 123.47   |
| 18  | A     | 4002 | BCR  | C11-C10-C9  | 12.35 | 144.94      | 127.31   |
| 18  | R     | 4020 | BCR  | C16-C15-C14 | 12.35 | 148.77      | 123.47   |
| 18  | B     | 4017 | BCR  | C16-C15-C14 | 12.34 | 148.75      | 123.47   |
| 18  | b     | 4017 | BCR  | C16-C15-C14 | 12.33 | 148.74      | 123.47   |
| 18  | H     | 4017 | BCR  | C16-C15-C14 | 12.33 | 148.73      | 123.47   |
| 18  | G     | 4002 | BCR  | C11-C10-C9  | 12.32 | 144.89      | 127.31   |
| 18  | L     | 4019 | BCR  | C16-C15-C14 | 12.30 | 148.68      | 123.47   |
| 18  | K     | 4001 | BCR  | C16-C15-C14 | 12.29 | 148.66      | 123.47   |
| 18  | U     | 4019 | BCR  | C16-C15-C14 | 12.29 | 148.65      | 123.47   |
| 18  | T     | 4001 | BCR  | C16-C15-C14 | 12.29 | 148.64      | 123.47   |
| 18  | l     | 4019 | BCR  | C16-C15-C14 | 12.29 | 148.64      | 123.47   |
| 18  | k     | 4001 | BCR  | C16-C15-C14 | 12.28 | 148.63      | 123.47   |
| 18  | l     | 4022 | BCR  | C16-C15-C14 | 12.26 | 148.59      | 123.47   |
| 18  | L     | 4022 | BCR  | C16-C15-C14 | 12.26 | 148.58      | 123.47   |
| 18  | U     | 4022 | BCR  | C16-C15-C14 | 12.25 | 148.56      | 123.47   |
| 18  | H     | 4006 | BCR  | C21-C20-C19 | 12.22 | 161.34      | 123.22   |
| 18  | B     | 4006 | BCR  | C21-C20-C19 | 12.22 | 161.34      | 123.22   |
| 18  | b     | 4006 | BCR  | C21-C20-C19 | 12.20 | 161.28      | 123.22   |
| 18  | G     | 4006 | BCR  | C11-C12-C13 | 11.93 | 159.93      | 126.42   |
| 18  | A     | 4006 | BCR  | C11-C12-C13 | 11.91 | 159.87      | 126.42   |
| 18  | a     | 4006 | BCR  | C11-C12-C13 | 11.90 | 159.84      | 126.42   |
| 18  | A     | 4004 | BCR  | C21-C20-C19 | 11.86 | 160.24      | 123.22   |
| 18  | a     | 4004 | BCR  | C21-C20-C19 | 11.85 | 160.21      | 123.22   |
| 18  | G     | 4004 | BCR  | C21-C20-C19 | 11.85 | 160.20      | 123.22   |
| 18  | b     | 4009 | BCR  | C11-C10-C9  | 11.85 | 144.22      | 127.31   |
| 18  | B     | 4009 | BCR  | C11-C10-C9  | 11.84 | 144.20      | 127.31   |
| 18  | H     | 4009 | BCR  | C11-C10-C9  | 11.81 | 144.17      | 127.31   |
| 18  | H     | 4014 | BCR  | C16-C15-C14 | 11.74 | 147.51      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | B     | 4014 | BCR  | C16-C15-C14 | 11.72  | 147.48      | 123.47   |
| 18  | b     | 4014 | BCR  | C16-C15-C14 | 11.70  | 147.45      | 123.47   |
| 18  | b     | 4010 | BCR  | C11-C12-C13 | 11.65  | 159.13      | 126.42   |
| 18  | B     | 4010 | BCR  | C11-C12-C13 | 11.65  | 159.13      | 126.42   |
| 18  | H     | 4010 | BCR  | C11-C12-C13 | 11.64  | 159.12      | 126.42   |
| 18  | A     | 4003 | BCR  | C16-C15-C14 | 11.64  | 147.32      | 123.47   |
| 18  | a     | 4003 | BCR  | C16-C15-C14 | 11.63  | 147.30      | 123.47   |
| 18  | G     | 4003 | BCR  | C16-C15-C14 | 11.63  | 147.30      | 123.47   |
| 18  | b     | 4014 | BCR  | C11-C12-C13 | 11.63  | 159.09      | 126.42   |
| 18  | l     | 4019 | BCR  | C11-C12-C13 | 11.63  | 159.08      | 126.42   |
| 18  | L     | 4019 | BCR  | C11-C12-C13 | 11.62  | 159.06      | 126.42   |
| 18  | B     | 4014 | BCR  | C11-C12-C13 | 11.61  | 159.04      | 126.42   |
| 18  | H     | 4014 | BCR  | C11-C12-C13 | 11.61  | 159.03      | 126.42   |
| 18  | U     | 4019 | BCR  | C11-C12-C13 | 11.61  | 159.03      | 126.42   |
| 18  | i     | 4018 | BCR  | C21-C20-C19 | 11.61  | 159.44      | 123.22   |
| 18  | I     | 4018 | BCR  | C21-C20-C19 | 11.60  | 159.43      | 123.22   |
| 18  | R     | 4018 | BCR  | C21-C20-C19 | 11.60  | 159.40      | 123.22   |
| 18  | m     | 4021 | BCR  | C21-C20-C19 | 11.59  | 159.38      | 123.22   |
| 18  | M     | 4021 | BCR  | C21-C20-C19 | 11.59  | 159.38      | 123.22   |
| 18  | a     | 4005 | BCR  | C11-C12-C13 | 11.58  | 158.94      | 126.42   |
| 18  | V     | 4021 | BCR  | C21-C20-C19 | 11.57  | 159.33      | 123.22   |
| 18  | A     | 4005 | BCR  | C11-C12-C13 | 11.56  | 158.90      | 126.42   |
| 18  | G     | 4005 | BCR  | C11-C12-C13 | 11.56  | 158.89      | 126.42   |
| 15  | b     | 1230 | F6C  | CAA-C2A-C3A | -11.35 | 106.74      | 127.88   |
| 15  | B     | 1230 | F6C  | CAA-C2A-C3A | -11.35 | 106.75      | 127.88   |
| 15  | H     | 1230 | F6C  | CAA-C2A-C3A | -11.33 | 106.78      | 127.88   |
| 18  | K     | 4001 | BCR  | C11-C12-C13 | 11.16  | 157.78      | 126.42   |
| 18  | T     | 4001 | BCR  | C11-C12-C13 | 11.16  | 157.77      | 126.42   |
| 18  | k     | 4001 | BCR  | C11-C12-C13 | 11.16  | 157.77      | 126.42   |
| 18  | l     | 4022 | BCR  | C11-C12-C13 | 11.05  | 157.46      | 126.42   |
| 18  | L     | 4022 | BCR  | C11-C12-C13 | 11.04  | 157.43      | 126.42   |
| 18  | U     | 4022 | BCR  | C11-C12-C13 | 11.04  | 157.42      | 126.42   |
| 15  | b     | 1237 | F6C  | CAA-C2A-C3A | -10.91 | 107.56      | 127.88   |
| 15  | H     | 1237 | F6C  | CAA-C2A-C3A | -10.91 | 107.57      | 127.88   |
| 15  | B     | 1237 | F6C  | CAA-C2A-C3A | -10.89 | 107.59      | 127.88   |
| 18  | G     | 4004 | BCR  | C11-C12-C13 | 10.82  | 156.82      | 126.42   |
| 18  | A     | 4004 | BCR  | C11-C12-C13 | 10.81  | 156.79      | 126.42   |
| 18  | b     | 4009 | BCR  | C11-C12-C13 | 10.80  | 156.76      | 126.42   |
| 18  | B     | 4009 | BCR  | C11-C12-C13 | 10.80  | 156.75      | 126.42   |
| 18  | a     | 4004 | BCR  | C11-C12-C13 | 10.80  | 156.74      | 126.42   |
| 18  | H     | 4009 | BCR  | C11-C12-C13 | 10.80  | 156.74      | 126.42   |
| 18  | b     | 4005 | BCR  | C11-C12-C13 | 10.79  | 156.74      | 126.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | H     | 4005 | BCR  | C11-C12-C13 | 10.79  | 156.73      | 126.42   |
| 18  | B     | 4005 | BCR  | C11-C12-C13 | 10.79  | 156.73      | 126.42   |
| 15  | H     | 1238 | F6C  | CAA-C2A-C3A | -10.74 | 107.88      | 127.88   |
| 15  | B     | 1238 | F6C  | CAA-C2A-C3A | -10.73 | 107.90      | 127.88   |
| 15  | b     | 1238 | F6C  | CAA-C2A-C3A | -10.72 | 107.91      | 127.88   |
| 18  | R     | 4020 | BCR  | C11-C12-C13 | 10.69  | 156.46      | 126.42   |
| 18  | I     | 4020 | BCR  | C11-C12-C13 | 10.69  | 156.46      | 126.42   |
| 18  | i     | 4020 | BCR  | C11-C12-C13 | 10.69  | 156.45      | 126.42   |
| 18  | H     | 4006 | BCR  | C11-C12-C13 | 10.66  | 156.37      | 126.42   |
| 18  | B     | 4006 | BCR  | C11-C12-C13 | 10.66  | 156.37      | 126.42   |
| 18  | b     | 4006 | BCR  | C11-C12-C13 | 10.65  | 156.34      | 126.42   |
| 18  | a     | 4003 | BCR  | C11-C12-C13 | 10.64  | 156.30      | 126.42   |
| 18  | A     | 4003 | BCR  | C11-C12-C13 | 10.64  | 156.30      | 126.42   |
| 18  | G     | 4003 | BCR  | C11-C12-C13 | 10.64  | 156.30      | 126.42   |
| 18  | a     | 4001 | BCR  | C11-C12-C13 | 10.38  | 155.57      | 126.42   |
| 18  | A     | 4001 | BCR  | C11-C12-C13 | 10.37  | 155.54      | 126.42   |
| 18  | G     | 4001 | BCR  | C11-C12-C13 | 10.36  | 155.52      | 126.42   |
| 18  | H     | 4017 | BCR  | C11-C12-C13 | 10.24  | 155.17      | 126.42   |
| 18  | b     | 4017 | BCR  | C11-C12-C13 | 10.24  | 155.17      | 126.42   |
| 18  | B     | 4017 | BCR  | C11-C12-C13 | 10.23  | 155.15      | 126.42   |
| 18  | V     | 4021 | BCR  | C11-C12-C13 | 10.22  | 155.13      | 126.42   |
| 18  | M     | 4021 | BCR  | C11-C12-C13 | 10.21  | 155.09      | 126.42   |
| 18  | m     | 4021 | BCR  | C11-C12-C13 | 10.20  | 155.06      | 126.42   |
| 18  | H     | 4004 | BCR  | C11-C12-C13 | 10.17  | 154.98      | 126.42   |
| 18  | B     | 4004 | BCR  | C11-C12-C13 | 10.17  | 154.98      | 126.42   |
| 18  | b     | 4004 | BCR  | C11-C12-C13 | 10.16  | 154.95      | 126.42   |
| 18  | R     | 4020 | BCR  | C21-C20-C19 | 10.10  | 154.75      | 123.22   |
| 18  | I     | 4020 | BCR  | C21-C20-C19 | 10.09  | 154.71      | 123.22   |
| 18  | i     | 4020 | BCR  | C21-C20-C19 | 10.08  | 154.69      | 123.22   |
| 18  | R     | 4018 | BCR  | C11-C12-C13 | 10.08  | 154.74      | 126.42   |
| 18  | I     | 4018 | BCR  | C11-C12-C13 | 10.07  | 154.70      | 126.42   |
| 18  | i     | 4018 | BCR  | C11-C12-C13 | 10.07  | 154.69      | 126.42   |
| 15  | B     | 1219 | F6C  | CAA-C2A-C3A | -9.54  | 110.10      | 127.88   |
| 15  | b     | 1219 | F6C  | CAA-C2A-C3A | -9.54  | 110.12      | 127.88   |
| 15  | H     | 1219 | F6C  | CAA-C2A-C3A | -9.53  | 110.13      | 127.88   |
| 18  | a     | 4002 | BCR  | C11-C12-C13 | 9.39   | 152.78      | 126.42   |
| 18  | G     | 4002 | BCR  | C11-C12-C13 | 9.38   | 152.76      | 126.42   |
| 18  | A     | 4002 | BCR  | C11-C12-C13 | 9.37   | 152.75      | 126.42   |
| 15  | b     | 1219 | F6C  | C1D-ND-C4D  | -9.26  | 102.54      | 106.71   |
| 15  | B     | 1219 | F6C  | C1D-ND-C4D  | -9.19  | 102.57      | 106.71   |
| 15  | H     | 1219 | F6C  | C1D-ND-C4D  | -9.18  | 102.58      | 106.71   |
| 14  | A     | 1013 | CLA  | C2D-C1D-ND  | 9.11   | 116.82      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | a     | 1121 | F6C  | C1C-C2C-C3C | -9.11 | 100.66      | 107.00   |
| 15  | H     | 1219 | F6C  | CMD-C2D-C1D | 9.09  | 138.89      | 125.04   |
| 14  | G     | 1013 | CLA  | C2D-C1D-ND  | 9.09  | 116.80      | 110.10   |
| 15  | B     | 1219 | F6C  | CMD-C2D-C1D | 9.07  | 138.85      | 125.04   |
| 18  | T     | 4001 | BCR  | C11-C10-C9  | 9.07  | 140.25      | 127.31   |
| 14  | a     | 1013 | CLA  | C2D-C1D-ND  | 9.06  | 116.78      | 110.10   |
| 15  | b     | 1219 | F6C  | CMD-C2D-C1D | 9.05  | 138.83      | 125.04   |
| 18  | K     | 4001 | BCR  | C11-C10-C9  | 9.05  | 140.23      | 127.31   |
| 18  | k     | 4001 | BCR  | C11-C10-C9  | 9.04  | 140.22      | 127.31   |
| 15  | G     | 1121 | F6C  | C1C-C2C-C3C | -9.03 | 100.71      | 107.00   |
| 15  | A     | 1121 | F6C  | C1C-C2C-C3C | -9.02 | 100.72      | 107.00   |
| 15  | a     | 1121 | F6C  | CAA-C2A-C3A | -9.00 | 111.11      | 127.88   |
| 15  | A     | 1121 | F6C  | CAA-C2A-C3A | -9.00 | 111.12      | 127.88   |
| 15  | G     | 1121 | F6C  | CAA-C2A-C3A | -8.99 | 111.13      | 127.88   |
| 14  | G     | 1135 | CLA  | CMD-C2D-C1D | 8.95  | 140.49      | 124.71   |
| 14  | A     | 1135 | CLA  | CMD-C2D-C1D | 8.95  | 140.48      | 124.71   |
| 15  | b     | 1207 | F6C  | C1C-C2C-C3C | -8.93 | 100.78      | 107.00   |
| 14  | a     | 1135 | CLA  | CMD-C2D-C1D | 8.92  | 140.44      | 124.71   |
| 15  | H     | 1207 | F6C  | C1C-C2C-C3C | -8.90 | 100.80      | 107.00   |
| 15  | B     | 1207 | F6C  | C1C-C2C-C3C | -8.88 | 100.82      | 107.00   |
| 18  | G     | 4003 | BCR  | C20-C19-C18 | 8.83  | 151.23      | 126.42   |
| 18  | a     | 4003 | BCR  | C20-C19-C18 | 8.83  | 151.23      | 126.42   |
| 18  | A     | 4003 | BCR  | C20-C19-C18 | 8.83  | 151.23      | 126.42   |
| 15  | a     | 1121 | F6C  | CMD-C2D-C1D | 8.78  | 138.41      | 125.04   |
| 15  | A     | 1121 | F6C  | CMD-C2D-C1D | 8.76  | 138.38      | 125.04   |
| 15  | H     | 1230 | F6C  | CMD-C2D-C1D | 8.74  | 138.35      | 125.04   |
| 15  | G     | 1121 | F6C  | CMD-C2D-C1D | 8.74  | 138.35      | 125.04   |
| 15  | b     | 1230 | F6C  | CMD-C2D-C1D | 8.73  | 138.34      | 125.04   |
| 15  | B     | 1230 | F6C  | CMD-C2D-C1D | 8.73  | 138.33      | 125.04   |
| 18  | b     | 4006 | BCR  | C20-C19-C18 | 8.61  | 150.61      | 126.42   |
| 18  | B     | 4006 | BCR  | C20-C19-C18 | 8.59  | 150.55      | 126.42   |
| 14  | a     | 1125 | CLA  | C2D-C1D-ND  | 8.59  | 116.43      | 110.10   |
| 18  | H     | 4006 | BCR  | C20-C19-C18 | 8.58  | 150.52      | 126.42   |
| 14  | G     | 1125 | CLA  | C2D-C1D-ND  | 8.57  | 116.42      | 110.10   |
| 14  | A     | 1125 | CLA  | C2D-C1D-ND  | 8.57  | 116.42      | 110.10   |
| 14  | H     | 1231 | CLA  | CMD-C2D-C1D | 8.55  | 139.78      | 124.71   |
| 14  | B     | 1231 | CLA  | CMD-C2D-C1D | 8.55  | 139.77      | 124.71   |
| 14  | b     | 1231 | CLA  | CMD-C2D-C1D | 8.54  | 139.77      | 124.71   |
| 14  | A     | 1109 | CLA  | CMD-C2D-C1D | 8.52  | 139.72      | 124.71   |
| 14  | G     | 1109 | CLA  | CMD-C2D-C1D | 8.52  | 139.72      | 124.71   |
| 18  | i     | 4018 | BCR  | C20-C19-C18 | 8.51  | 150.32      | 126.42   |
| 14  | a     | 1109 | CLA  | CMD-C2D-C1D | 8.49  | 139.68      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | I     | 4018 | BCR  | C20-C19-C18 | 8.49  | 150.27      | 126.42   |
| 18  | R     | 4018 | BCR  | C20-C19-C18 | 8.49  | 150.26      | 126.42   |
| 15  | b     | 1207 | F6C  | CAA-C2A-C3A | -8.47 | 112.10      | 127.88   |
| 15  | B     | 1207 | F6C  | CAA-C2A-C3A | -8.47 | 112.11      | 127.88   |
| 15  | H     | 1207 | F6C  | CAA-C2A-C3A | -8.46 | 112.13      | 127.88   |
| 14  | G     | 1105 | CLA  | CMD-C2D-C1D | 8.45  | 139.61      | 124.71   |
| 14  | A     | 1105 | CLA  | CMD-C2D-C1D | 8.45  | 139.61      | 124.71   |
| 14  | a     | 1105 | CLA  | CMD-C2D-C1D | 8.45  | 139.61      | 124.71   |
| 15  | B     | 1238 | F6C  | CMD-C2D-C1D | 8.41  | 137.85      | 125.04   |
| 15  | H     | 1238 | F6C  | CMD-C2D-C1D | 8.40  | 137.83      | 125.04   |
| 15  | b     | 1238 | F6C  | CMD-C2D-C1D | 8.40  | 137.83      | 125.04   |
| 14  | B     | 1227 | CLA  | CMD-C2D-C1D | 8.39  | 139.49      | 124.71   |
| 14  | H     | 1227 | CLA  | CMD-C2D-C1D | 8.38  | 139.49      | 124.71   |
| 14  | b     | 1227 | CLA  | CMD-C2D-C1D | 8.38  | 139.47      | 124.71   |
| 18  | a     | 4004 | BCR  | C20-C19-C18 | 8.34  | 149.85      | 126.42   |
| 18  | A     | 4004 | BCR  | C20-C19-C18 | 8.34  | 149.84      | 126.42   |
| 18  | G     | 4004 | BCR  | C20-C19-C18 | 8.33  | 149.83      | 126.42   |
| 14  | a     | 1103 | CLA  | CMD-C2D-C1D | 8.33  | 139.39      | 124.71   |
| 14  | H     | 1236 | CLA  | C2D-C1D-ND  | 8.31  | 116.23      | 110.10   |
| 14  | b     | 1236 | CLA  | C2D-C1D-ND  | 8.31  | 116.23      | 110.10   |
| 14  | B     | 1236 | CLA  | C2D-C1D-ND  | 8.31  | 116.22      | 110.10   |
| 14  | b     | 1232 | CLA  | CMD-C2D-C1D | 8.31  | 139.35      | 124.71   |
| 14  | H     | 1232 | CLA  | CMD-C2D-C1D | 8.30  | 139.34      | 124.71   |
| 14  | A     | 1103 | CLA  | CMD-C2D-C1D | 8.29  | 139.33      | 124.71   |
| 14  | G     | 1103 | CLA  | CMD-C2D-C1D | 8.29  | 139.33      | 124.71   |
| 14  | B     | 1232 | CLA  | CMD-C2D-C1D | 8.29  | 139.32      | 124.71   |
| 14  | M     | 1501 | CLA  | CMD-C2D-C1D | 8.24  | 139.24      | 124.71   |
| 15  | H     | 1230 | F6C  | C1D-ND-C4D  | -8.23 | 103.00      | 106.71   |
| 14  | V     | 1501 | CLA  | CMD-C2D-C1D | 8.23  | 139.21      | 124.71   |
| 14  | m     | 1501 | CLA  | CMD-C2D-C1D | 8.23  | 139.21      | 124.71   |
| 14  | b     | 1023 | CLA  | C2D-C1D-ND  | 8.22  | 116.16      | 110.10   |
| 15  | b     | 1230 | F6C  | C1D-ND-C4D  | -8.21 | 103.02      | 106.71   |
| 14  | G     | 1134 | CLA  | CMD-C2D-C1D | 8.20  | 139.17      | 124.71   |
| 14  | B     | 1023 | CLA  | CAC-C3C-C4C | 8.20  | 135.45      | 124.81   |
| 14  | b     | 1023 | CLA  | CAC-C3C-C4C | 8.20  | 135.45      | 124.81   |
| 15  | B     | 1230 | F6C  | C1D-ND-C4D  | -8.19 | 103.02      | 106.71   |
| 14  | A     | 1134 | CLA  | CMD-C2D-C1D | 8.19  | 139.15      | 124.71   |
| 14  | H     | 1023 | CLA  | CAC-C3C-C4C | 8.19  | 135.44      | 124.81   |
| 14  | G     | 1104 | CLA  | CMD-C2D-C1D | 8.19  | 139.14      | 124.71   |
| 14  | G     | 1138 | CLA  | CMD-C2D-C1D | 8.19  | 139.14      | 124.71   |
| 14  | H     | 1022 | CLA  | C2D-C1D-ND  | 8.18  | 116.13      | 110.10   |
| 14  | A     | 1104 | CLA  | CMD-C2D-C1D | 8.18  | 139.12      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1104 | CLA  | CMD-C2D-C1D | 8.18  | 139.12      | 124.71   |
| 14  | a     | 1134 | CLA  | CMD-C2D-C1D | 8.18  | 139.12      | 124.71   |
| 14  | k     | 1401 | CLA  | CMD-C2D-C1D | 8.17  | 139.12      | 124.71   |
| 14  | T     | 1401 | CLA  | CMD-C2D-C1D | 8.17  | 139.12      | 124.71   |
| 14  | A     | 1138 | CLA  | CMD-C2D-C1D | 8.17  | 139.12      | 124.71   |
| 14  | a     | 1138 | CLA  | CMD-C2D-C1D | 8.17  | 139.11      | 124.71   |
| 14  | B     | 1022 | CLA  | C2D-C1D-ND  | 8.16  | 116.12      | 110.10   |
| 14  | K     | 1401 | CLA  | CMD-C2D-C1D | 8.16  | 139.10      | 124.71   |
| 14  | B     | 1023 | CLA  | C2D-C1D-ND  | 8.15  | 116.11      | 110.10   |
| 14  | G     | 1114 | CLA  | CMD-C2D-C1D | 8.13  | 139.04      | 124.71   |
| 14  | H     | 1233 | CLA  | CMD-C2D-C1D | 8.13  | 139.04      | 124.71   |
| 14  | H     | 1023 | CLA  | C2D-C1D-ND  | 8.13  | 116.09      | 110.10   |
| 14  | b     | 1228 | CLA  | CMD-C2D-C1D | 8.12  | 139.03      | 124.71   |
| 14  | b     | 1022 | CLA  | C2D-C1D-ND  | 8.11  | 116.08      | 110.10   |
| 14  | A     | 1114 | CLA  | CMD-C2D-C1D | 8.11  | 139.01      | 124.71   |
| 14  | b     | 1236 | CLA  | CMD-C2D-C1D | 8.11  | 139.01      | 124.71   |
| 14  | a     | 1114 | CLA  | CMD-C2D-C1D | 8.11  | 139.00      | 124.71   |
| 14  | B     | 1236 | CLA  | CMD-C2D-C1D | 8.11  | 139.00      | 124.71   |
| 15  | b     | 1219 | F6C  | C1C-C2C-C3C | -8.11 | 101.36      | 107.00   |
| 15  | H     | 1219 | F6C  | C1C-C2C-C3C | -8.10 | 101.36      | 107.00   |
| 14  | G     | 1120 | CLA  | C2D-C1D-ND  | 8.10  | 116.08      | 110.10   |
| 14  | H     | 1236 | CLA  | CMD-C2D-C1D | 8.10  | 139.00      | 124.71   |
| 15  | B     | 1219 | F6C  | C1C-C2C-C3C | -8.10 | 101.36      | 107.00   |
| 14  | B     | 1233 | CLA  | CMD-C2D-C1D | 8.10  | 138.99      | 124.71   |
| 14  | a     | 1102 | CLA  | CMD-C2D-C1D | 8.10  | 138.99      | 124.71   |
| 14  | A     | 1120 | CLA  | C2D-C1D-ND  | 8.09  | 116.07      | 110.10   |
| 14  | b     | 1240 | CLA  | CMD-C2D-C1D | 8.09  | 138.98      | 124.71   |
| 14  | a     | 1120 | CLA  | C2D-C1D-ND  | 8.09  | 116.07      | 110.10   |
| 14  | H     | 1240 | CLA  | CMD-C2D-C1D | 8.09  | 138.97      | 124.71   |
| 14  | b     | 1233 | CLA  | CMD-C2D-C1D | 8.09  | 138.97      | 124.71   |
| 14  | a     | 1101 | CLA  | CMD-C2D-C1D | 8.09  | 138.97      | 124.71   |
| 14  | B     | 1240 | CLA  | CMD-C2D-C1D | 8.08  | 138.96      | 124.71   |
| 14  | B     | 1201 | CLA  | CMD-C2D-C1D | 8.08  | 138.96      | 124.71   |
| 14  | B     | 1228 | CLA  | CMD-C2D-C1D | 8.08  | 138.96      | 124.71   |
| 14  | G     | 1101 | CLA  | CMD-C2D-C1D | 8.08  | 138.96      | 124.71   |
| 14  | H     | 1201 | CLA  | CMD-C2D-C1D | 8.08  | 138.95      | 124.71   |
| 14  | b     | 1213 | CLA  | CMD-C2D-C1D | 8.08  | 138.95      | 124.71   |
| 14  | A     | 1101 | CLA  | CMD-C2D-C1D | 8.08  | 138.94      | 124.71   |
| 14  | G     | 1102 | CLA  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 14  | b     | 1201 | CLA  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 14  | H     | 1213 | CLA  | CMD-C2D-C1D | 8.07  | 138.93      | 124.71   |
| 14  | A     | 1102 | CLA  | CMD-C2D-C1D | 8.07  | 138.93      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1139 | CLA  | CMD-C2D-C1D | 8.07  | 138.93      | 124.71   |
| 15  | H     | 1238 | F6C  | C1C-C2C-C3C | -8.07 | 101.39      | 107.00   |
| 14  | B     | 1213 | CLA  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 15  | b     | 1238 | F6C  | C1C-C2C-C3C | -8.06 | 101.39      | 107.00   |
| 14  | H     | 1228 | CLA  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 15  | B     | 1238 | F6C  | C1C-C2C-C3C | -8.06 | 101.39      | 107.00   |
| 14  | a     | 1139 | CLA  | CMD-C2D-C1D | 8.06  | 138.91      | 124.71   |
| 14  | H     | 1218 | CLA  | CMD-C2D-C1D | 8.05  | 138.91      | 124.71   |
| 15  | H     | 1207 | F6C  | CMD-C2D-C1D | 8.05  | 137.30      | 125.04   |
| 14  | G     | 1139 | CLA  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 14  | b     | 1212 | CLA  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 15  | B     | 1207 | F6C  | CMD-C2D-C1D | 8.03  | 137.27      | 125.04   |
| 14  | H     | 1229 | CLA  | CMD-C2D-C1D | 8.03  | 138.87      | 124.71   |
| 15  | B     | 1237 | F6C  | C1D-ND-C4D  | -8.03 | 103.09      | 106.71   |
| 14  | B     | 1212 | CLA  | CMD-C2D-C1D | 8.03  | 138.86      | 124.71   |
| 15  | b     | 1207 | F6C  | CMD-C2D-C1D | 8.02  | 137.26      | 125.04   |
| 14  | b     | 1229 | CLA  | CMD-C2D-C1D | 8.02  | 138.85      | 124.71   |
| 14  | G     | 1104 | CLA  | C2D-C1D-ND  | 8.02  | 116.02      | 110.10   |
| 14  | b     | 1218 | CLA  | CMD-C2D-C1D | 8.02  | 138.84      | 124.71   |
| 14  | B     | 1229 | CLA  | CMD-C2D-C1D | 8.02  | 138.84      | 124.71   |
| 15  | H     | 1237 | F6C  | C1D-ND-C4D  | -8.01 | 103.10      | 106.71   |
| 14  | B     | 1218 | CLA  | CMD-C2D-C1D | 8.01  | 138.83      | 124.71   |
| 14  | a     | 1104 | CLA  | C2D-C1D-ND  | 8.01  | 116.01      | 110.10   |
| 14  | H     | 1212 | CLA  | CMD-C2D-C1D | 8.00  | 138.82      | 124.71   |
| 14  | A     | 1129 | CLA  | CMD-C2D-C1D | 7.98  | 138.78      | 124.71   |
| 14  | G     | 1129 | CLA  | CMD-C2D-C1D | 7.98  | 138.78      | 124.71   |
| 14  | A     | 1104 | CLA  | C2D-C1D-ND  | 7.98  | 115.98      | 110.10   |
| 14  | a     | 1129 | CLA  | CMD-C2D-C1D | 7.97  | 138.76      | 124.71   |
| 14  | G     | 1106 | CLA  | CMD-C2D-C1D | 7.97  | 138.76      | 124.71   |
| 14  | a     | 1112 | CLA  | CMD-C2D-C1D | 7.96  | 138.75      | 124.71   |
| 14  | A     | 1112 | CLA  | CMD-C2D-C1D | 7.96  | 138.74      | 124.71   |
| 14  | G     | 1112 | CLA  | CMD-C2D-C1D | 7.95  | 138.73      | 124.71   |
| 14  | A     | 1111 | CLA  | CMD-C2D-C1D | 7.95  | 138.72      | 124.71   |
| 14  | G     | 1111 | CLA  | CMD-C2D-C1D | 7.95  | 138.72      | 124.71   |
| 14  | B     | 1205 | CLA  | C2D-C1D-ND  | 7.94  | 115.95      | 110.10   |
| 14  | H     | 1205 | CLA  | C2D-C1D-ND  | 7.94  | 115.95      | 110.10   |
| 14  | a     | 1111 | CLA  | CMD-C2D-C1D | 7.94  | 138.70      | 124.71   |
| 14  | B     | 1214 | CLA  | CMD-C2D-C1D | 7.93  | 138.69      | 124.71   |
| 14  | A     | 1106 | CLA  | CMD-C2D-C1D | 7.93  | 138.69      | 124.71   |
| 14  | H     | 1214 | CLA  | CMD-C2D-C1D | 7.92  | 138.68      | 124.71   |
| 14  | A     | 1129 | CLA  | O2D-CGD-CBD | 7.92  | 125.35      | 111.27   |
| 14  | G     | 1132 | CLA  | CMD-C2D-C1D | 7.92  | 138.67      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | b     | 1237 | F6C  | C1D-ND-C4D  | -7.92 | 103.15      | 106.71   |
| 14  | a     | 1129 | CLA  | O2D-CGD-CBD | 7.92  | 125.34      | 111.27   |
| 14  | a     | 1141 | CLA  | CMD-C2D-C1D | 7.92  | 138.67      | 124.71   |
| 14  | b     | 1214 | CLA  | CMD-C2D-C1D | 7.92  | 138.67      | 124.71   |
| 14  | a     | 1106 | CLA  | CMD-C2D-C1D | 7.91  | 138.66      | 124.71   |
| 14  | A     | 1132 | CLA  | CMD-C2D-C1D | 7.91  | 138.66      | 124.71   |
| 14  | b     | 1205 | CLA  | C2D-C1D-ND  | 7.91  | 115.93      | 110.10   |
| 14  | a     | 1132 | CLA  | CMD-C2D-C1D | 7.91  | 138.65      | 124.71   |
| 14  | G     | 1129 | CLA  | O2D-CGD-CBD | 7.91  | 125.32      | 111.27   |
| 14  | A     | 1141 | CLA  | CMD-C2D-C1D | 7.90  | 138.63      | 124.71   |
| 14  | G     | 1141 | CLA  | CMD-C2D-C1D | 7.90  | 138.63      | 124.71   |
| 14  | B     | 1208 | CLA  | CMD-C2D-C1D | 7.88  | 138.59      | 124.71   |
| 14  | B     | 1239 | CLA  | CMD-C2D-C1D | 7.87  | 138.59      | 124.71   |
| 14  | H     | 1208 | CLA  | CMD-C2D-C1D | 7.87  | 138.58      | 124.71   |
| 14  | b     | 1239 | CLA  | CMD-C2D-C1D | 7.86  | 138.57      | 124.71   |
| 14  | b     | 1208 | CLA  | CMD-C2D-C1D | 7.86  | 138.57      | 124.71   |
| 14  | H     | 1239 | CLA  | CMD-C2D-C1D | 7.85  | 138.55      | 124.71   |
| 14  | A     | 1137 | CLA  | CMD-C2D-C1D | 7.83  | 138.51      | 124.71   |
| 14  | a     | 1137 | CLA  | CMD-C2D-C1D | 7.83  | 138.51      | 124.71   |
| 14  | G     | 1137 | CLA  | CMD-C2D-C1D | 7.82  | 138.50      | 124.71   |
| 14  | B     | 1203 | CLA  | C2D-C1D-ND  | 7.82  | 115.87      | 110.10   |
| 14  | b     | 1235 | CLA  | CMD-C2D-C1D | 7.82  | 138.49      | 124.71   |
| 14  | B     | 1235 | CLA  | CMD-C2D-C1D | 7.82  | 138.49      | 124.71   |
| 14  | H     | 1235 | CLA  | CMD-C2D-C1D | 7.81  | 138.48      | 124.71   |
| 14  | b     | 1203 | CLA  | C2D-C1D-ND  | 7.81  | 115.86      | 110.10   |
| 14  | H     | 1203 | CLA  | C2D-C1D-ND  | 7.81  | 115.86      | 110.10   |
| 14  | A     | 1117 | CLA  | CMD-C2D-C1D | 7.80  | 138.47      | 124.71   |
| 18  | b     | 4017 | BCR  | C20-C19-C18 | 7.80  | 148.33      | 126.42   |
| 18  | B     | 4017 | BCR  | C20-C19-C18 | 7.80  | 148.33      | 126.42   |
| 14  | G     | 1117 | CLA  | CMD-C2D-C1D | 7.80  | 138.45      | 124.71   |
| 18  | H     | 4017 | BCR  | C20-C19-C18 | 7.79  | 148.31      | 126.42   |
| 14  | a     | 1117 | CLA  | CMD-C2D-C1D | 7.79  | 138.44      | 124.71   |
| 14  | G     | 1113 | CLA  | CMD-C2D-C1D | 7.78  | 138.42      | 124.71   |
| 14  | A     | 1113 | CLA  | CMD-C2D-C1D | 7.78  | 138.42      | 124.71   |
| 14  | k     | 1401 | CLA  | C2D-C1D-ND  | 7.77  | 115.83      | 110.10   |
| 15  | A     | 1121 | F6C  | C1D-ND-C4D  | -7.76 | 103.22      | 106.71   |
| 14  | K     | 1401 | CLA  | C2D-C1D-ND  | 7.76  | 115.82      | 110.10   |
| 14  | a     | 1113 | CLA  | CMD-C2D-C1D | 7.75  | 138.38      | 124.71   |
| 15  | a     | 1121 | F6C  | C1D-ND-C4D  | -7.75 | 103.22      | 106.71   |
| 14  | T     | 1401 | CLA  | C2D-C1D-ND  | 7.75  | 115.81      | 110.10   |
| 14  | A     | 1107 | CLA  | CMD-C2D-C1D | 7.74  | 138.36      | 124.71   |
| 15  | G     | 1121 | F6C  | C1D-ND-C4D  | -7.74 | 103.23      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | a     | 1107 | CLA  | CMD-C2D-C1D | 7.74 | 138.35      | 124.71   |
| 14  | G     | 1107 | CLA  | CMD-C2D-C1D | 7.73 | 138.33      | 124.71   |
| 14  | H     | 1210 | CLA  | O2A-C1-C2   | 7.73 | 128.94      | 108.64   |
| 14  | B     | 1210 | CLA  | O2A-C1-C2   | 7.72 | 128.93      | 108.64   |
| 14  | A     | 1116 | CLA  | CMD-C2D-C1D | 7.72 | 138.32      | 124.71   |
| 14  | a     | 1116 | CLA  | CMD-C2D-C1D | 7.72 | 138.32      | 124.71   |
| 14  | a     | 1126 | CLA  | CMD-C2D-C1D | 7.72 | 138.32      | 124.71   |
| 14  | G     | 1116 | CLA  | CMD-C2D-C1D | 7.72 | 138.31      | 124.71   |
| 14  | H     | 1202 | CLA  | CMD-C2D-C1D | 7.72 | 138.31      | 124.71   |
| 14  | B     | 1202 | CLA  | CMD-C2D-C1D | 7.71 | 138.31      | 124.71   |
| 14  | G     | 1136 | CLA  | CMD-C2D-C1D | 7.71 | 138.30      | 124.71   |
| 14  | G     | 1110 | CLA  | CMD-C2D-C1D | 7.70 | 138.29      | 124.71   |
| 14  | a     | 1136 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | H     | 1234 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | H     | 1216 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | b     | 1210 | CLA  | O2A-C1-C2   | 7.70 | 128.87      | 108.64   |
| 14  | A     | 1136 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | A     | 1110 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | a     | 1110 | CLA  | CMD-C2D-C1D | 7.70 | 138.28      | 124.71   |
| 14  | b     | 1202 | CLA  | CMD-C2D-C1D | 7.69 | 138.26      | 124.71   |
| 14  | H     | 1215 | CLA  | CMD-C2D-C1D | 7.68 | 138.26      | 124.71   |
| 14  | A     | 1126 | CLA  | CMD-C2D-C1D | 7.68 | 138.25      | 124.71   |
| 14  | B     | 1234 | CLA  | CMD-C2D-C1D | 7.68 | 138.25      | 124.71   |
| 14  | a     | 1108 | CLA  | CMD-C2D-C1D | 7.68 | 138.25      | 124.71   |
| 14  | B     | 1215 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | A     | 1108 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | b     | 1215 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | H     | 1218 | CLA  | C2D-C1D-ND  | 7.67 | 115.76      | 110.10   |
| 14  | A     | 1125 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | G     | 1125 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | G     | 1126 | CLA  | CMD-C2D-C1D | 7.67 | 138.23      | 124.71   |
| 14  | B     | 1216 | CLA  | CMD-C2D-C1D | 7.67 | 138.22      | 124.71   |
| 14  | b     | 1218 | CLA  | C2D-C1D-ND  | 7.66 | 115.75      | 110.10   |
| 14  | b     | 1216 | CLA  | CMD-C2D-C1D | 7.66 | 138.22      | 124.71   |
| 14  | B     | 1203 | CLA  | CMD-C2D-C1D | 7.66 | 138.21      | 124.71   |
| 14  | a     | 1125 | CLA  | CMD-C2D-C1D | 7.66 | 138.21      | 124.71   |
| 14  | b     | 1203 | CLA  | CMD-C2D-C1D | 7.66 | 138.21      | 124.71   |
| 14  | b     | 1234 | CLA  | CMD-C2D-C1D | 7.66 | 138.21      | 124.71   |
| 14  | H     | 1203 | CLA  | CMD-C2D-C1D | 7.65 | 138.20      | 124.71   |
| 14  | G     | 1108 | CLA  | CMD-C2D-C1D | 7.64 | 138.18      | 124.71   |
| 14  | B     | 1218 | CLA  | C2D-C1D-ND  | 7.63 | 115.73      | 110.10   |
| 14  | B     | 1204 | CLA  | CMD-C2D-C1D | 7.63 | 138.15      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1204 | CLA  | CMD-C2D-C1D | 7.62  | 138.15      | 124.71   |
| 14  | L     | 1501 | CLA  | CMD-C2D-C1D | 7.62  | 138.15      | 124.71   |
| 14  | G     | 1131 | CLA  | CMD-C2D-C1D | 7.62  | 138.15      | 124.71   |
| 14  | U     | 1501 | CLA  | CMD-C2D-C1D | 7.62  | 138.14      | 124.71   |
| 14  | a     | 1131 | CLA  | CMD-C2D-C1D | 7.62  | 138.14      | 124.71   |
| 14  | l     | 1501 | CLA  | CMD-C2D-C1D | 7.61  | 138.12      | 124.71   |
| 14  | H     | 1204 | CLA  | CMD-C2D-C1D | 7.61  | 138.12      | 124.71   |
| 14  | A     | 1131 | CLA  | CMD-C2D-C1D | 7.60  | 138.11      | 124.71   |
| 18  | G     | 4005 | BCR  | C24-C23-C22 | -7.60 | 114.75      | 126.23   |
| 18  | A     | 4005 | BCR  | C24-C23-C22 | -7.60 | 114.76      | 126.23   |
| 18  | a     | 4005 | BCR  | C24-C23-C22 | -7.58 | 114.78      | 126.23   |
| 14  | B     | 1211 | CLA  | CMD-C2D-C1D | 7.57  | 138.05      | 124.71   |
| 14  | H     | 1223 | CLA  | CMD-C2D-C1D | 7.57  | 138.05      | 124.71   |
| 14  | b     | 1224 | CLA  | CMD-C2D-C1D | 7.57  | 138.05      | 124.71   |
| 14  | b     | 1217 | CLA  | CMD-C2D-C1D | 7.57  | 138.05      | 124.71   |
| 15  | b     | 1237 | F6C  | C1C-C2C-C3C | -7.56 | 101.74      | 107.00   |
| 14  | B     | 1217 | CLA  | CMD-C2D-C1D | 7.55  | 138.03      | 124.71   |
| 14  | b     | 1211 | CLA  | CMD-C2D-C1D | 7.55  | 138.03      | 124.71   |
| 14  | H     | 1211 | CLA  | CMD-C2D-C1D | 7.55  | 138.03      | 124.71   |
| 14  | b     | 1223 | CLA  | CMD-C2D-C1D | 7.55  | 138.02      | 124.71   |
| 14  | B     | 1223 | CLA  | CMD-C2D-C1D | 7.55  | 138.02      | 124.71   |
| 14  | B     | 1224 | CLA  | CMD-C2D-C1D | 7.55  | 138.01      | 124.71   |
| 15  | H     | 1237 | F6C  | C1C-C2C-C3C | -7.55 | 101.75      | 107.00   |
| 14  | B     | 1210 | CLA  | O2D-CGD-CBD | 7.54  | 124.67      | 111.27   |
| 14  | b     | 1210 | CLA  | O2D-CGD-CBD | 7.54  | 124.66      | 111.27   |
| 14  | H     | 1217 | CLA  | CMD-C2D-C1D | 7.53  | 137.99      | 124.71   |
| 14  | H     | 1224 | CLA  | CMD-C2D-C1D | 7.53  | 137.99      | 124.71   |
| 14  | H     | 1210 | CLA  | O2D-CGD-CBD | 7.53  | 124.65      | 111.27   |
| 14  | H     | 1220 | CLA  | CMD-C2D-C1D | 7.51  | 137.96      | 124.71   |
| 15  | B     | 1237 | F6C  | C1C-C2C-C3C | -7.51 | 101.77      | 107.00   |
| 14  | G     | 1120 | CLA  | CMD-C2D-C1D | 7.51  | 137.95      | 124.71   |
| 14  | A     | 1120 | CLA  | CMD-C2D-C1D | 7.51  | 137.94      | 124.71   |
| 14  | a     | 1120 | CLA  | CMD-C2D-C1D | 7.50  | 137.93      | 124.71   |
| 18  | b     | 4005 | BCR  | C20-C19-C18 | 7.49  | 147.45      | 126.42   |
| 18  | B     | 4005 | BCR  | C20-C19-C18 | 7.49  | 147.45      | 126.42   |
| 14  | b     | 1220 | CLA  | CMD-C2D-C1D | 7.49  | 137.91      | 124.71   |
| 14  | B     | 1220 | CLA  | CMD-C2D-C1D | 7.48  | 137.90      | 124.71   |
| 18  | H     | 4005 | BCR  | C20-C19-C18 | 7.48  | 147.43      | 126.42   |
| 14  | G     | 1124 | CLA  | C2D-C1D-ND  | 7.47  | 115.61      | 110.10   |
| 14  | A     | 1124 | CLA  | C2D-C1D-ND  | 7.47  | 115.61      | 110.10   |
| 14  | B     | 1210 | CLA  | CMD-C2D-C1D | 7.46  | 137.87      | 124.71   |
| 14  | H     | 1210 | CLA  | CMD-C2D-C1D | 7.46  | 137.86      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | a     | 1124 | CLA  | C2D-C1D-ND  | 7.45 | 115.59      | 110.10   |
| 14  | b     | 1210 | CLA  | CMD-C2D-C1D | 7.45 | 137.84      | 124.71   |
| 14  | a     | 1124 | CLA  | CMD-C2D-C1D | 7.44 | 137.82      | 124.71   |
| 14  | G     | 1124 | CLA  | CMD-C2D-C1D | 7.43 | 137.81      | 124.71   |
| 14  | a     | 1111 | CLA  | C2D-C1D-ND  | 7.43 | 115.58      | 110.10   |
| 14  | A     | 1135 | CLA  | C2C-C1C-NC  | 7.43 | 116.93      | 109.97   |
| 14  | A     | 1124 | CLA  | CMD-C2D-C1D | 7.42 | 137.80      | 124.71   |
| 14  | b     | 1209 | CLA  | CMD-C2D-C1D | 7.42 | 137.79      | 124.71   |
| 14  | G     | 1135 | CLA  | C2C-C1C-NC  | 7.42 | 116.92      | 109.97   |
| 14  | A     | 1111 | CLA  | C2D-C1D-ND  | 7.41 | 115.57      | 110.10   |
| 14  | B     | 1209 | CLA  | CMD-C2D-C1D | 7.40 | 137.76      | 124.71   |
| 14  | H     | 1209 | CLA  | CMD-C2D-C1D | 7.40 | 137.76      | 124.71   |
| 14  | G     | 1111 | CLA  | C2D-C1D-ND  | 7.40 | 115.56      | 110.10   |
| 14  | a     | 1132 | CLA  | O2D-CGD-CBD | 7.39 | 124.40      | 111.27   |
| 14  | A     | 1132 | CLA  | O2D-CGD-CBD | 7.39 | 124.39      | 111.27   |
| 14  | a     | 1135 | CLA  | C2C-C1C-NC  | 7.38 | 116.89      | 109.97   |
| 14  | G     | 1132 | CLA  | O2D-CGD-CBD | 7.38 | 124.38      | 111.27   |
| 14  | B     | 1239 | CLA  | C2C-C1C-NC  | 7.37 | 116.88      | 109.97   |
| 14  | H     | 1239 | CLA  | C2C-C1C-NC  | 7.37 | 116.88      | 109.97   |
| 14  | A     | 1122 | CLA  | CMD-C2D-C1D | 7.37 | 137.69      | 124.71   |
| 14  | a     | 1122 | CLA  | CMD-C2D-C1D | 7.36 | 137.69      | 124.71   |
| 18  | a     | 4002 | BCR  | C20-C19-C18 | 7.35 | 147.08      | 126.42   |
| 18  | G     | 4002 | BCR  | C20-C19-C18 | 7.35 | 147.07      | 126.42   |
| 14  | b     | 1239 | CLA  | C2C-C1C-NC  | 7.35 | 116.86      | 109.97   |
| 18  | A     | 4002 | BCR  | C20-C19-C18 | 7.35 | 147.06      | 126.42   |
| 14  | G     | 1122 | CLA  | CMD-C2D-C1D | 7.34 | 137.66      | 124.71   |
| 14  | H     | 1206 | CLA  | C2D-C1D-ND  | 7.34 | 115.51      | 110.10   |
| 14  | b     | 1206 | CLA  | C2D-C1D-ND  | 7.34 | 115.51      | 110.10   |
| 14  | A     | 1133 | CLA  | C2C-C1C-NC  | 7.34 | 116.85      | 109.97   |
| 14  | B     | 1234 | CLA  | C2D-C1D-ND  | 7.34 | 115.51      | 110.10   |
| 14  | G     | 1133 | CLA  | C2C-C1C-NC  | 7.34 | 116.84      | 109.97   |
| 14  | a     | 1114 | CLA  | C2C-C1C-NC  | 7.34 | 116.84      | 109.97   |
| 14  | A     | 1114 | CLA  | C2C-C1C-NC  | 7.33 | 116.84      | 109.97   |
| 14  | G     | 1140 | CLA  | CMD-C2D-C1D | 7.33 | 137.62      | 124.71   |
| 14  | b     | 1221 | CLA  | C2D-C1D-ND  | 7.32 | 115.50      | 110.10   |
| 14  | H     | 1234 | CLA  | C2D-C1D-ND  | 7.32 | 115.50      | 110.10   |
| 14  | B     | 1206 | CLA  | C2D-C1D-ND  | 7.32 | 115.50      | 110.10   |
| 14  | a     | 1140 | CLA  | CMD-C2D-C1D | 7.32 | 137.61      | 124.71   |
| 14  | a     | 1133 | CLA  | C2C-C1C-NC  | 7.32 | 116.83      | 109.97   |
| 14  | A     | 1140 | CLA  | CMD-C2D-C1D | 7.32 | 137.61      | 124.71   |
| 18  | b     | 4014 | BCR  | C20-C19-C18 | 7.32 | 146.97      | 126.42   |
| 18  | B     | 4014 | BCR  | C20-C19-C18 | 7.31 | 146.94      | 126.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1013 | CLA  | C4A-NA-C1A  | 7.30  | 109.99      | 106.71   |
| 15  | H     | 1219 | F6C  | CAA-C2A-C1A | -7.30 | 108.00      | 128.11   |
| 14  | A     | 1013 | CLA  | C4A-NA-C1A  | 7.30  | 109.99      | 106.71   |
| 14  | A     | 1131 | CLA  | O2A-C1-C2   | 7.30  | 127.81      | 108.64   |
| 18  | H     | 4014 | BCR  | C20-C19-C18 | 7.30  | 146.91      | 126.42   |
| 14  | a     | 1131 | CLA  | O2A-C1-C2   | 7.29  | 127.80      | 108.64   |
| 15  | b     | 1219 | F6C  | CAA-C2A-C1A | -7.29 | 108.03      | 128.11   |
| 14  | G     | 1114 | CLA  | C2C-C1C-NC  | 7.29  | 116.80      | 109.97   |
| 15  | B     | 1219 | F6C  | CAA-C2A-C1A | -7.29 | 108.04      | 128.11   |
| 14  | B     | 1221 | CLA  | C2D-C1D-ND  | 7.29  | 115.47      | 110.10   |
| 14  | b     | 1204 | CLA  | C2D-C1D-ND  | 7.28  | 115.47      | 110.10   |
| 14  | G     | 1131 | CLA  | O2A-C1-C2   | 7.28  | 127.76      | 108.64   |
| 14  | B     | 1204 | CLA  | C2D-C1D-ND  | 7.28  | 115.47      | 110.10   |
| 14  | b     | 1234 | CLA  | C2D-C1D-ND  | 7.27  | 115.47      | 110.10   |
| 14  | a     | 1118 | CLA  | CMD-C2D-C1D | 7.27  | 137.53      | 124.71   |
| 14  | H     | 1221 | CLA  | C2D-C1D-ND  | 7.26  | 115.46      | 110.10   |
| 14  | A     | 1118 | CLA  | CMD-C2D-C1D | 7.25  | 137.50      | 124.71   |
| 14  | A     | 1123 | CLA  | CMD-C2D-C1D | 7.25  | 137.49      | 124.71   |
| 14  | H     | 1204 | CLA  | C2D-C1D-ND  | 7.25  | 115.44      | 110.10   |
| 14  | a     | 1123 | CLA  | CMD-C2D-C1D | 7.25  | 137.48      | 124.71   |
| 14  | H     | 1222 | CLA  | C2D-C1D-ND  | 7.24  | 115.44      | 110.10   |
| 14  | a     | 1137 | CLA  | C2C-C1C-NC  | 7.24  | 116.75      | 109.97   |
| 14  | G     | 1118 | CLA  | CMD-C2D-C1D | 7.24  | 137.47      | 124.71   |
| 14  | A     | 1141 | CLA  | C2D-C1D-ND  | 7.24  | 115.44      | 110.10   |
| 14  | G     | 1141 | CLA  | C2D-C1D-ND  | 7.23  | 115.43      | 110.10   |
| 14  | a     | 1141 | CLA  | C2D-C1D-ND  | 7.23  | 115.43      | 110.10   |
| 14  | G     | 1123 | CLA  | CMD-C2D-C1D | 7.23  | 137.46      | 124.71   |
| 14  | b     | 1233 | CLA  | C2C-C1C-NC  | 7.23  | 116.75      | 109.97   |
| 14  | H     | 1233 | CLA  | C2C-C1C-NC  | 7.23  | 116.74      | 109.97   |
| 13  | G     | 1011 | CL0  | C2D-C1D-ND  | 7.23  | 115.43      | 110.10   |
| 14  | H     | 1222 | CLA  | CMD-C2D-C1D | 7.22  | 137.44      | 124.71   |
| 14  | a     | 1013 | CLA  | C4A-NA-C1A  | 7.22  | 109.95      | 106.71   |
| 14  | A     | 1119 | CLA  | CMD-C2D-C1D | 7.22  | 137.43      | 124.71   |
| 14  | b     | 1222 | CLA  | CMD-C2D-C1D | 7.22  | 137.43      | 124.71   |
| 14  | G     | 1137 | CLA  | C2C-C1C-NC  | 7.21  | 116.73      | 109.97   |
| 13  | A     | 1011 | CL0  | C2D-C1D-ND  | 7.21  | 115.42      | 110.10   |
| 14  | G     | 1119 | CLA  | CMD-C2D-C1D | 7.21  | 137.43      | 124.71   |
| 14  | U     | 1501 | CLA  | C2C-C1C-NC  | 7.21  | 116.73      | 109.97   |
| 14  | a     | 1119 | CLA  | CMD-C2D-C1D | 7.21  | 137.42      | 124.71   |
| 14  | H     | 1206 | CLA  | C2C-C1C-NC  | 7.21  | 116.72      | 109.97   |
| 14  | B     | 1222 | CLA  | CMD-C2D-C1D | 7.20  | 137.41      | 124.71   |
| 14  | A     | 1127 | CLA  | C2D-C1D-ND  | 7.20  | 115.41      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1206 | CLA  | C2C-C1C-NC  | 7.20  | 116.72      | 109.97   |
| 14  | U     | 1502 | CLA  | C2D-C1D-ND  | 7.20  | 115.41      | 110.10   |
| 14  | b     | 1222 | CLA  | C2D-C1D-ND  | 7.20  | 115.41      | 110.10   |
| 14  | A     | 1137 | CLA  | C2C-C1C-NC  | 7.20  | 116.72      | 109.97   |
| 14  | M     | 1501 | CLA  | C2C-C1C-NC  | 7.20  | 116.72      | 109.97   |
| 14  | B     | 1233 | CLA  | C2C-C1C-NC  | 7.20  | 116.72      | 109.97   |
| 14  | L     | 1502 | CLA  | C2D-C1D-ND  | 7.19  | 115.41      | 110.10   |
| 14  | V     | 1501 | CLA  | C2C-C1C-NC  | 7.19  | 116.71      | 109.97   |
| 14  | B     | 1206 | CLA  | C2C-C1C-NC  | 7.19  | 116.71      | 109.97   |
| 13  | a     | 1011 | CL0  | C2D-C1D-ND  | 7.19  | 115.40      | 110.10   |
| 14  | H     | 1223 | CLA  | C2D-C1D-ND  | 7.18  | 115.40      | 110.10   |
| 14  | m     | 1501 | CLA  | C2C-C1C-NC  | 7.18  | 116.70      | 109.97   |
| 14  | B     | 1222 | CLA  | C2D-C1D-ND  | 7.18  | 115.39      | 110.10   |
| 15  | b     | 1207 | F6C  | C1D-ND-C4D  | -7.17 | 103.48      | 106.71   |
| 14  | G     | 1127 | CLA  | C2D-C1D-ND  | 7.17  | 115.39      | 110.10   |
| 14  | G     | 1133 | CLA  | C2D-C1D-ND  | 7.17  | 115.39      | 110.10   |
| 14  | b     | 1223 | CLA  | C2D-C1D-ND  | 7.17  | 115.39      | 110.10   |
| 14  | l     | 1502 | CLA  | C2D-C1D-ND  | 7.17  | 115.39      | 110.10   |
| 14  | a     | 1127 | CLA  | C2D-C1D-ND  | 7.17  | 115.39      | 110.10   |
| 15  | B     | 1207 | F6C  | C1D-ND-C4D  | -7.16 | 103.49      | 106.71   |
| 15  | H     | 1207 | F6C  | C1D-ND-C4D  | -7.16 | 103.49      | 106.71   |
| 14  | L     | 1501 | CLA  | C2C-C1C-NC  | 7.15  | 116.67      | 109.97   |
| 18  | a     | 4006 | BCR  | C20-C19-C18 | 7.15  | 146.51      | 126.42   |
| 18  | A     | 4006 | BCR  | C20-C19-C18 | 7.15  | 146.49      | 126.42   |
| 18  | G     | 4006 | BCR  | C20-C19-C18 | 7.14  | 146.48      | 126.42   |
| 14  | a     | 1133 | CLA  | C2D-C1D-ND  | 7.14  | 115.37      | 110.10   |
| 14  | A     | 1133 | CLA  | C2D-C1D-ND  | 7.14  | 115.37      | 110.10   |
| 14  | a     | 1133 | CLA  | CMD-C2D-C1D | 7.14  | 137.29      | 124.71   |
| 14  | A     | 1133 | CLA  | CMD-C2D-C1D | 7.12  | 137.26      | 124.71   |
| 14  | B     | 1210 | CLA  | C2D-C1D-ND  | 7.11  | 115.35      | 110.10   |
| 14  | H     | 1210 | CLA  | C2D-C1D-ND  | 7.11  | 115.35      | 110.10   |
| 14  | G     | 1133 | CLA  | CMD-C2D-C1D | 7.11  | 137.25      | 124.71   |
| 14  | l     | 1501 | CLA  | C2C-C1C-NC  | 7.11  | 116.63      | 109.97   |
| 14  | a     | 1130 | CLA  | CMD-C2D-C1D | 7.10  | 137.23      | 124.71   |
| 14  | B     | 1223 | CLA  | C2D-C1D-ND  | 7.10  | 115.34      | 110.10   |
| 14  | A     | 1130 | CLA  | CMD-C2D-C1D | 7.10  | 137.23      | 124.71   |
| 14  | b     | 1210 | CLA  | C2D-C1D-ND  | 7.08  | 115.33      | 110.10   |
| 14  | a     | 1129 | CLA  | C2D-C1D-ND  | 7.08  | 115.32      | 110.10   |
| 14  | G     | 1129 | CLA  | C2D-C1D-ND  | 7.08  | 115.32      | 110.10   |
| 14  | G     | 1130 | CLA  | CMD-C2D-C1D | 7.07  | 137.17      | 124.71   |
| 14  | b     | 1212 | CLA  | O2D-CGD-CBD | 7.06  | 123.82      | 111.27   |
| 14  | B     | 1212 | CLA  | O2D-CGD-CBD | 7.06  | 123.82      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | H     | 1212 | CLA  | O2D-CGD-CBD | 7.06 | 123.82      | 111.27   |
| 14  | b     | 1021 | CLA  | C2D-C1D-ND  | 7.06 | 115.31      | 110.10   |
| 14  | L     | 1503 | CLA  | CMD-C2D-C1D | 7.06 | 137.15      | 124.71   |
| 14  | b     | 1205 | CLA  | C4A-NA-C1A  | 7.06 | 109.88      | 106.71   |
| 14  | A     | 1129 | CLA  | C2D-C1D-ND  | 7.05 | 115.30      | 110.10   |
| 14  | B     | 1211 | CLA  | C2D-C1D-ND  | 7.05 | 115.30      | 110.10   |
| 14  | l     | 1503 | CLA  | CMD-C2D-C1D | 7.05 | 137.13      | 124.71   |
| 14  | U     | 1503 | CLA  | CMD-C2D-C1D | 7.05 | 137.13      | 124.71   |
| 14  | B     | 1021 | CLA  | C2D-C1D-ND  | 7.04 | 115.30      | 110.10   |
| 14  | b     | 1224 | CLA  | C2D-C1D-ND  | 7.04 | 115.29      | 110.10   |
| 14  | G     | 1133 | CLA  | C4A-NA-C1A  | 7.04 | 109.87      | 106.71   |
| 14  | U     | 1502 | CLA  | CMD-C2D-C1D | 7.03 | 137.11      | 124.71   |
| 14  | G     | 1106 | CLA  | C2D-C1D-ND  | 7.03 | 115.29      | 110.10   |
| 14  | A     | 1109 | CLA  | C2C-C1C-NC  | 7.03 | 116.56      | 109.97   |
| 14  | a     | 1132 | CLA  | C2D-C1D-ND  | 7.02 | 115.28      | 110.10   |
| 14  | a     | 1109 | CLA  | C2C-C1C-NC  | 7.02 | 116.55      | 109.97   |
| 14  | b     | 1211 | CLA  | C2D-C1D-ND  | 7.02 | 115.28      | 110.10   |
| 14  | H     | 1021 | CLA  | C2D-C1D-ND  | 7.02 | 115.28      | 110.10   |
| 14  | L     | 1502 | CLA  | CMD-C2D-C1D | 7.01 | 137.08      | 124.71   |
| 14  | G     | 1132 | CLA  | C2D-C1D-ND  | 7.01 | 115.27      | 110.10   |
| 14  | H     | 1022 | CLA  | O2D-CGD-CBD | 7.00 | 123.71      | 111.27   |
| 14  | b     | 1022 | CLA  | O2D-CGD-CBD | 7.00 | 123.71      | 111.27   |
| 14  | H     | 1211 | CLA  | C2D-C1D-ND  | 7.00 | 115.26      | 110.10   |
| 14  | B     | 1224 | CLA  | C2D-C1D-ND  | 7.00 | 115.26      | 110.10   |
| 14  | B     | 1022 | CLA  | O2D-CGD-CBD | 7.00 | 123.70      | 111.27   |
| 14  | A     | 1132 | CLA  | C2D-C1D-ND  | 6.99 | 115.26      | 110.10   |
| 14  | G     | 1109 | CLA  | C2C-C1C-NC  | 6.99 | 116.52      | 109.97   |
| 14  | a     | 1117 | CLA  | C2C-C1C-NC  | 6.99 | 116.52      | 109.97   |
| 14  | H     | 1224 | CLA  | C2D-C1D-ND  | 6.99 | 115.26      | 110.10   |
| 14  | l     | 1502 | CLA  | CMD-C2D-C1D | 6.99 | 137.03      | 124.71   |
| 14  | A     | 1106 | CLA  | C2D-C1D-ND  | 6.99 | 115.25      | 110.10   |
| 14  | H     | 1205 | CLA  | C4A-NA-C1A  | 6.98 | 109.84      | 106.71   |
| 14  | b     | 1220 | CLA  | C2C-C1C-NC  | 6.98 | 116.51      | 109.97   |
| 14  | G     | 1117 | CLA  | C2C-C1C-NC  | 6.98 | 116.51      | 109.97   |
| 14  | B     | 1220 | CLA  | C2C-C1C-NC  | 6.97 | 116.50      | 109.97   |
| 14  | A     | 1113 | CLA  | C2D-C1D-ND  | 6.97 | 115.24      | 110.10   |
| 14  | a     | 1116 | CLA  | C2D-C1D-ND  | 6.97 | 115.24      | 110.10   |
| 14  | b     | 1201 | CLA  | C2D-C1D-ND  | 6.96 | 115.23      | 110.10   |
| 14  | G     | 1118 | CLA  | C2D-C1D-ND  | 6.96 | 115.23      | 110.10   |
| 14  | A     | 1133 | CLA  | C4A-NA-C1A  | 6.96 | 109.83      | 106.71   |
| 14  | a     | 1131 | CLA  | C2C-C1C-NC  | 6.96 | 116.49      | 109.97   |
| 14  | A     | 1117 | CLA  | C2C-C1C-NC  | 6.96 | 116.49      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | B     | 1201 | CLA  | C2D-C1D-ND  | 6.95 | 115.22      | 110.10   |
| 14  | G     | 1113 | CLA  | C2D-C1D-ND  | 6.95 | 115.22      | 110.10   |
| 14  | H     | 1220 | CLA  | C2C-C1C-NC  | 6.95 | 116.48      | 109.97   |
| 14  | a     | 1106 | CLA  | C2D-C1D-ND  | 6.94 | 115.22      | 110.10   |
| 14  | A     | 1118 | CLA  | C2D-C1D-ND  | 6.94 | 115.22      | 110.10   |
| 14  | G     | 1131 | CLA  | C2C-C1C-NC  | 6.94 | 116.47      | 109.97   |
| 14  | A     | 1116 | CLA  | C2D-C1D-ND  | 6.93 | 115.21      | 110.10   |
| 14  | A     | 1138 | CLA  | C2C-C1C-NC  | 6.93 | 116.47      | 109.97   |
| 14  | b     | 1023 | CLA  | CMD-C2D-C1D | 6.93 | 136.92      | 124.71   |
| 14  | H     | 1201 | CLA  | C2D-C1D-ND  | 6.92 | 115.21      | 110.10   |
| 14  | a     | 1118 | CLA  | C2D-C1D-ND  | 6.92 | 115.21      | 110.10   |
| 14  | B     | 1235 | CLA  | C2D-C1D-ND  | 6.92 | 115.20      | 110.10   |
| 14  | b     | 1217 | CLA  | C2C-C1C-NC  | 6.91 | 116.45      | 109.97   |
| 14  | A     | 1131 | CLA  | C2C-C1C-NC  | 6.91 | 116.45      | 109.97   |
| 14  | B     | 1023 | CLA  | CMD-C2D-C1D | 6.91 | 136.89      | 124.71   |
| 14  | G     | 1128 | CLA  | C2C-C1C-NC  | 6.91 | 116.44      | 109.97   |
| 14  | A     | 1128 | CLA  | C2C-C1C-NC  | 6.91 | 116.44      | 109.97   |
| 14  | a     | 1138 | CLA  | C2C-C1C-NC  | 6.91 | 116.44      | 109.97   |
| 14  | B     | 1217 | CLA  | C2C-C1C-NC  | 6.91 | 116.44      | 109.97   |
| 14  | b     | 1235 | CLA  | C2D-C1D-ND  | 6.90 | 115.19      | 110.10   |
| 14  | a     | 1107 | CLA  | C2D-C1D-ND  | 6.90 | 115.19      | 110.10   |
| 14  | a     | 1113 | CLA  | C2D-C1D-ND  | 6.90 | 115.19      | 110.10   |
| 14  | H     | 1023 | CLA  | CMD-C2D-C1D | 6.90 | 136.87      | 124.71   |
| 14  | A     | 1107 | CLA  | C2D-C1D-ND  | 6.89 | 115.18      | 110.10   |
| 14  | G     | 1107 | CLA  | C2D-C1D-ND  | 6.89 | 115.18      | 110.10   |
| 14  | B     | 1205 | CLA  | C4A-NA-C1A  | 6.89 | 109.80      | 106.71   |
| 14  | b     | 1223 | CLA  | C2C-C1C-NC  | 6.88 | 116.42      | 109.97   |
| 14  | G     | 1116 | CLA  | C2D-C1D-ND  | 6.88 | 115.18      | 110.10   |
| 14  | G     | 1138 | CLA  | C2C-C1C-NC  | 6.88 | 116.42      | 109.97   |
| 14  | H     | 1217 | CLA  | C2C-C1C-NC  | 6.88 | 116.41      | 109.97   |
| 14  | A     | 1115 | CLA  | CMD-C2D-C1D | 6.87 | 136.83      | 124.71   |
| 14  | a     | 1128 | CLA  | C2C-C1C-NC  | 6.87 | 116.41      | 109.97   |
| 14  | G     | 1115 | CLA  | CMD-C2D-C1D | 6.87 | 136.82      | 124.71   |
| 14  | B     | 1223 | CLA  | C2C-C1C-NC  | 6.87 | 116.41      | 109.97   |
| 14  | a     | 1115 | CLA  | CMD-C2D-C1D | 6.87 | 136.81      | 124.71   |
| 14  | H     | 1226 | CLA  | C2C-C1C-NC  | 6.86 | 116.40      | 109.97   |
| 14  | b     | 1240 | CLA  | C2C-C1C-NC  | 6.86 | 116.40      | 109.97   |
| 14  | G     | 1134 | CLA  | C2D-C1D-ND  | 6.86 | 115.16      | 110.10   |
| 14  | H     | 1235 | CLA  | C2D-C1D-ND  | 6.86 | 115.16      | 110.10   |
| 14  | a     | 1101 | CLA  | C2C-C1C-NC  | 6.86 | 116.40      | 109.97   |
| 14  | L     | 1503 | CLA  | C2C-C1C-NC  | 6.86 | 116.40      | 109.97   |
| 14  | l     | 1503 | CLA  | C2C-C1C-NC  | 6.85 | 116.39      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | A     | 1134 | CLA  | C2D-C1D-ND  | 6.85 | 115.15      | 110.10   |
| 14  | B     | 1217 | CLA  | C2D-C1D-ND  | 6.85 | 115.15      | 110.10   |
| 14  | H     | 1240 | CLA  | C2C-C1C-NC  | 6.85 | 116.39      | 109.97   |
| 14  | H     | 1217 | CLA  | C2D-C1D-ND  | 6.84 | 115.15      | 110.10   |
| 14  | A     | 1101 | CLA  | C2C-C1C-NC  | 6.84 | 116.38      | 109.97   |
| 14  | G     | 1139 | CLA  | C2D-C1D-ND  | 6.83 | 115.14      | 110.10   |
| 14  | H     | 1223 | CLA  | C2C-C1C-NC  | 6.83 | 116.37      | 109.97   |
| 14  | b     | 1226 | CLA  | CMD-C2D-C1D | 6.83 | 136.75      | 124.71   |
| 14  | H     | 1227 | CLA  | C2D-C1D-ND  | 6.83 | 115.14      | 110.10   |
| 14  | a     | 1134 | CLA  | C2D-C1D-ND  | 6.83 | 115.14      | 110.10   |
| 14  | b     | 1217 | CLA  | C2D-C1D-ND  | 6.82 | 115.13      | 110.10   |
| 14  | B     | 1226 | CLA  | C2C-C1C-NC  | 6.82 | 116.36      | 109.97   |
| 14  | B     | 1240 | CLA  | C2C-C1C-NC  | 6.82 | 116.36      | 109.97   |
| 14  | B     | 1227 | CLA  | C2D-C1D-ND  | 6.81 | 115.13      | 110.10   |
| 14  | b     | 1226 | CLA  | C2C-C1C-NC  | 6.81 | 116.36      | 109.97   |
| 14  | L     | 1501 | CLA  | C2D-C1D-ND  | 6.81 | 115.12      | 110.10   |
| 14  | b     | 1213 | CLA  | C2D-C1D-ND  | 6.81 | 115.12      | 110.10   |
| 14  | B     | 1226 | CLA  | CMD-C2D-C1D | 6.81 | 136.72      | 124.71   |
| 14  | U     | 1503 | CLA  | C2C-C1C-NC  | 6.81 | 116.35      | 109.97   |
| 14  | b     | 1203 | CLA  | C2C-C1C-NC  | 6.81 | 116.35      | 109.97   |
| 14  | G     | 1101 | CLA  | C2C-C1C-NC  | 6.81 | 116.35      | 109.97   |
| 14  | b     | 1214 | CLA  | C2C-C1C-NC  | 6.81 | 116.35      | 109.97   |
| 14  | H     | 1226 | CLA  | CMD-C2D-C1D | 6.81 | 136.71      | 124.71   |
| 14  | B     | 1023 | CLA  | C4A-NA-C1A  | 6.80 | 109.77      | 106.71   |
| 14  | H     | 1213 | CLA  | C2D-C1D-ND  | 6.80 | 115.11      | 110.10   |
| 14  | U     | 1501 | CLA  | C2D-C1D-ND  | 6.80 | 115.11      | 110.10   |
| 14  | a     | 1102 | CLA  | C2D-C1D-ND  | 6.80 | 115.11      | 110.10   |
| 14  | a     | 1133 | CLA  | C4A-NA-C1A  | 6.80 | 109.76      | 106.71   |
| 14  | G     | 1117 | CLA  | O2D-CGD-CBD | 6.80 | 123.35      | 111.27   |
| 14  | A     | 1139 | CLA  | C2D-C1D-ND  | 6.80 | 115.11      | 110.10   |
| 14  | l     | 1501 | CLA  | C2D-C1D-ND  | 6.79 | 115.11      | 110.10   |
| 14  | a     | 1117 | CLA  | O2D-CGD-CBD | 6.79 | 123.33      | 111.27   |
| 14  | a     | 1139 | CLA  | C2D-C1D-ND  | 6.79 | 115.11      | 110.10   |
| 13  | A     | 1011 | CL0  | C2C-C1C-NC  | 6.79 | 116.33      | 109.97   |
| 14  | B     | 1214 | CLA  | C2C-C1C-NC  | 6.79 | 116.33      | 109.97   |
| 14  | H     | 1203 | CLA  | C2C-C1C-NC  | 6.79 | 116.33      | 109.97   |
| 13  | a     | 1011 | CL0  | C2C-C1C-NC  | 6.78 | 116.33      | 109.97   |
| 14  | B     | 1021 | CLA  | C4A-NA-C1A  | 6.78 | 109.75      | 106.71   |
| 14  | B     | 1213 | CLA  | C2D-C1D-ND  | 6.78 | 115.10      | 110.10   |
| 14  | H     | 1021 | CLA  | C4A-NA-C1A  | 6.78 | 109.75      | 106.71   |
| 14  | b     | 1227 | CLA  | C2D-C1D-ND  | 6.78 | 115.10      | 110.10   |
| 14  | B     | 1203 | CLA  | C2C-C1C-NC  | 6.78 | 116.32      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1239 | CLA  | C2D-C1D-ND  | 6.78  | 115.10      | 110.10   |
| 13  | G     | 1011 | CL0  | C2C-C1C-NC  | 6.78  | 116.32      | 109.97   |
| 14  | b     | 1215 | CLA  | C2D-C1D-ND  | 6.78  | 115.10      | 110.10   |
| 14  | G     | 1123 | CLA  | C2D-C1D-ND  | 6.77  | 115.09      | 110.10   |
| 14  | A     | 1012 | CLA  | CMD-C2D-C1D | 6.77  | 136.65      | 124.71   |
| 14  | B     | 1239 | CLA  | C2D-C1D-ND  | 6.77  | 115.09      | 110.10   |
| 14  | H     | 1227 | CLA  | C2C-C1C-NC  | 6.76  | 116.31      | 109.97   |
| 14  | A     | 1117 | CLA  | O2D-CGD-CBD | 6.76  | 123.29      | 111.27   |
| 14  | G     | 1102 | CLA  | C2D-C1D-ND  | 6.76  | 115.09      | 110.10   |
| 14  | a     | 1106 | CLA  | O2D-CGD-CBD | 6.76  | 123.28      | 111.27   |
| 14  | a     | 1012 | CLA  | CMD-C2D-C1D | 6.76  | 136.63      | 124.71   |
| 14  | H     | 1214 | CLA  | C2C-C1C-NC  | 6.76  | 116.30      | 109.97   |
| 14  | b     | 1023 | CLA  | C4A-NA-C1A  | 6.76  | 109.74      | 106.71   |
| 15  | b     | 1238 | F6C  | C1D-ND-C4D  | -6.76 | 103.67      | 106.71   |
| 14  | G     | 1123 | CLA  | C2C-C1C-NC  | 6.76  | 116.30      | 109.97   |
| 14  | G     | 1140 | CLA  | C2C-C1C-NC  | 6.76  | 116.30      | 109.97   |
| 14  | H     | 1023 | CLA  | C4A-NA-C1A  | 6.75  | 109.74      | 106.71   |
| 14  | G     | 1106 | CLA  | O2D-CGD-CBD | 6.75  | 123.26      | 111.27   |
| 14  | G     | 1012 | CLA  | CMD-C2D-C1D | 6.75  | 136.60      | 124.71   |
| 14  | A     | 1106 | CLA  | O2D-CGD-CBD | 6.75  | 123.26      | 111.27   |
| 14  | A     | 1137 | CLA  | C2D-C1D-ND  | 6.75  | 115.08      | 110.10   |
| 15  | B     | 1238 | F6C  | C1D-ND-C4D  | -6.74 | 103.67      | 106.71   |
| 14  | A     | 1140 | CLA  | C2C-C1C-NC  | 6.74  | 116.29      | 109.97   |
| 14  | a     | 1127 | CLA  | C2C-C1C-NC  | 6.74  | 116.29      | 109.97   |
| 14  | B     | 1215 | CLA  | C2D-C1D-ND  | 6.74  | 115.07      | 110.10   |
| 14  | G     | 1137 | CLA  | C2D-C1D-ND  | 6.73  | 115.07      | 110.10   |
| 14  | B     | 1227 | CLA  | C2C-C1C-NC  | 6.73  | 116.28      | 109.97   |
| 14  | A     | 1123 | CLA  | C2C-C1C-NC  | 6.73  | 116.28      | 109.97   |
| 14  | H     | 1215 | CLA  | C2D-C1D-ND  | 6.73  | 115.06      | 110.10   |
| 14  | A     | 1108 | CLA  | C2D-C1D-ND  | 6.73  | 115.06      | 110.10   |
| 14  | A     | 1127 | CLA  | C2C-C1C-NC  | 6.73  | 116.27      | 109.97   |
| 14  | A     | 1123 | CLA  | C2D-C1D-ND  | 6.73  | 115.06      | 110.10   |
| 14  | a     | 1123 | CLA  | C2D-C1D-ND  | 6.73  | 115.06      | 110.10   |
| 14  | G     | 1108 | CLA  | C2D-C1D-ND  | 6.73  | 115.06      | 110.10   |
| 14  | b     | 1021 | CLA  | C4A-NA-C1A  | 6.72  | 109.73      | 106.71   |
| 14  | H     | 1239 | CLA  | C2D-C1D-ND  | 6.72  | 115.06      | 110.10   |
| 14  | a     | 1137 | CLA  | C2D-C1D-ND  | 6.72  | 115.06      | 110.10   |
| 14  | A     | 1102 | CLA  | C2D-C1D-ND  | 6.72  | 115.06      | 110.10   |
| 14  | H     | 1240 | CLA  | O2A-C1-C2   | 6.72  | 126.29      | 108.64   |
| 14  | a     | 1123 | CLA  | C2C-C1C-NC  | 6.72  | 116.26      | 109.97   |
| 14  | B     | 1240 | CLA  | O2A-C1-C2   | 6.71  | 126.28      | 108.64   |
| 14  | b     | 1240 | CLA  | O2A-C1-C2   | 6.71  | 126.27      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1140 | CLA  | C2C-C1C-NC  | 6.71  | 116.25      | 109.97   |
| 14  | a     | 1108 | CLA  | C2D-C1D-ND  | 6.71  | 115.05      | 110.10   |
| 14  | b     | 1227 | CLA  | C2C-C1C-NC  | 6.71  | 116.25      | 109.97   |
| 18  | G     | 4001 | BCR  | C20-C19-C18 | 6.70  | 145.24      | 126.42   |
| 14  | G     | 1127 | CLA  | C2C-C1C-NC  | 6.70  | 116.25      | 109.97   |
| 14  | H     | 1220 | CLA  | C2D-C1D-ND  | 6.70  | 115.04      | 110.10   |
| 18  | A     | 4001 | BCR  | C20-C19-C18 | 6.69  | 145.21      | 126.42   |
| 14  | G     | 1136 | CLA  | C2D-C1D-ND  | 6.68  | 115.03      | 110.10   |
| 14  | A     | 1136 | CLA  | C2D-C1D-ND  | 6.67  | 115.02      | 110.10   |
| 18  | i     | 4020 | BCR  | C20-C19-C18 | 6.67  | 145.16      | 126.42   |
| 14  | A     | 1136 | CLA  | C2C-C1C-NC  | 6.67  | 116.22      | 109.97   |
| 14  | a     | 1134 | CLA  | C2C-C1C-NC  | 6.67  | 116.22      | 109.97   |
| 18  | I     | 4020 | BCR  | C20-C19-C18 | 6.67  | 145.14      | 126.42   |
| 18  | a     | 4001 | BCR  | C20-C19-C18 | 6.66  | 145.13      | 126.42   |
| 14  | G     | 1136 | CLA  | C2C-C1C-NC  | 6.65  | 116.21      | 109.97   |
| 15  | H     | 1238 | F6C  | C1D-ND-C4D  | -6.65 | 103.72      | 106.71   |
| 14  | a     | 1136 | CLA  | C2D-C1D-ND  | 6.65  | 115.00      | 110.10   |
| 14  | H     | 1225 | CLA  | C2C-C1C-NC  | 6.64  | 116.19      | 109.97   |
| 14  | a     | 1110 | CLA  | C2D-C1D-ND  | 6.64  | 115.00      | 110.10   |
| 14  | k     | 1401 | CLA  | C2C-C1C-NC  | 6.64  | 116.19      | 109.97   |
| 14  | a     | 1136 | CLA  | C2C-C1C-NC  | 6.64  | 116.19      | 109.97   |
| 18  | R     | 4020 | BCR  | C20-C19-C18 | 6.64  | 145.06      | 126.42   |
| 14  | B     | 1208 | CLA  | C2D-C1D-ND  | 6.63  | 114.99      | 110.10   |
| 14  | A     | 1122 | CLA  | C2D-C1D-ND  | 6.63  | 114.99      | 110.10   |
| 14  | B     | 1204 | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | G     | 1012 | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | B     | 1231 | CLA  | C2D-C1D-ND  | 6.62  | 114.99      | 110.10   |
| 14  | K     | 1401 | CLA  | C2C-C1C-NC  | 6.62  | 116.18      | 109.97   |
| 14  | G     | 1115 | CLA  | C2D-C1D-ND  | 6.62  | 114.98      | 110.10   |
| 14  | b     | 1232 | CLA  | C2C-C1C-NC  | 6.62  | 116.17      | 109.97   |
| 14  | A     | 1134 | CLA  | C2C-C1C-NC  | 6.62  | 116.17      | 109.97   |
| 14  | a     | 1104 | CLA  | C4A-NA-C1A  | 6.62  | 109.68      | 106.71   |
| 14  | G     | 1134 | CLA  | C2C-C1C-NC  | 6.61  | 116.17      | 109.97   |
| 14  | B     | 1225 | CLA  | C2C-C1C-NC  | 6.61  | 116.16      | 109.97   |
| 14  | a     | 1122 | CLA  | C2D-C1D-ND  | 6.61  | 114.97      | 110.10   |
| 14  | b     | 1220 | CLA  | C2D-C1D-ND  | 6.60  | 114.97      | 110.10   |
| 14  | B     | 1220 | CLA  | C2D-C1D-ND  | 6.60  | 114.97      | 110.10   |
| 14  | H     | 1215 | CLA  | C2C-C1C-NC  | 6.60  | 116.16      | 109.97   |
| 14  | H     | 1208 | CLA  | C2D-C1D-ND  | 6.60  | 114.97      | 110.10   |
| 14  | A     | 1012 | CLA  | C2C-C1C-NC  | 6.60  | 116.15      | 109.97   |
| 14  | H     | 1232 | CLA  | C2C-C1C-NC  | 6.60  | 116.15      | 109.97   |
| 14  | B     | 1221 | CLA  | C2C-C1C-NC  | 6.60  | 116.15      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | H     | 1221 | CLA  | C2C-C1C-NC  | 6.59 | 116.15      | 109.97   |
| 14  | A     | 1110 | CLA  | C2D-C1D-ND  | 6.59 | 114.96      | 110.10   |
| 14  | H     | 1231 | CLA  | C2D-C1D-ND  | 6.59 | 114.96      | 110.10   |
| 14  | a     | 1012 | CLA  | C2C-C1C-NC  | 6.59 | 116.14      | 109.97   |
| 14  | b     | 1225 | CLA  | C2C-C1C-NC  | 6.59 | 116.14      | 109.97   |
| 14  | G     | 1110 | CLA  | C2D-C1D-ND  | 6.59 | 114.96      | 110.10   |
| 14  | T     | 1401 | CLA  | C2C-C1C-NC  | 6.59 | 116.14      | 109.97   |
| 14  | G     | 1122 | CLA  | C2D-C1D-ND  | 6.59 | 114.96      | 110.10   |
| 14  | b     | 1231 | CLA  | C2D-C1D-ND  | 6.59 | 114.96      | 110.10   |
| 14  | B     | 1232 | CLA  | C2C-C1C-NC  | 6.59 | 116.14      | 109.97   |
| 14  | b     | 1215 | CLA  | C2C-C1C-NC  | 6.59 | 116.14      | 109.97   |
| 14  | A     | 1115 | CLA  | C2D-C1D-ND  | 6.58 | 114.95      | 110.10   |
| 14  | B     | 1236 | CLA  | C2C-C1C-NC  | 6.58 | 116.14      | 109.97   |
| 14  | H     | 1204 | CLA  | C2C-C1C-NC  | 6.58 | 116.14      | 109.97   |
| 14  | G     | 1119 | CLA  | C2D-C1D-ND  | 6.57 | 114.95      | 110.10   |
| 14  | G     | 1104 | CLA  | C4A-NA-C1A  | 6.57 | 109.66      | 106.71   |
| 14  | b     | 1204 | CLA  | C2C-C1C-NC  | 6.57 | 116.13      | 109.97   |
| 14  | B     | 1215 | CLA  | C2C-C1C-NC  | 6.57 | 116.12      | 109.97   |
| 14  | b     | 1221 | CLA  | C2C-C1C-NC  | 6.57 | 116.12      | 109.97   |
| 14  | b     | 1236 | CLA  | C2C-C1C-NC  | 6.57 | 116.12      | 109.97   |
| 14  | A     | 1119 | CLA  | C2D-C1D-ND  | 6.56 | 114.94      | 110.10   |
| 14  | B     | 1202 | CLA  | O2D-CGD-CBD | 6.56 | 122.92      | 111.27   |
| 14  | H     | 1236 | CLA  | C2C-C1C-NC  | 6.56 | 116.12      | 109.97   |
| 14  | a     | 1101 | CLA  | O2D-CGD-CBD | 6.56 | 122.92      | 111.27   |
| 14  | A     | 1101 | CLA  | O2D-CGD-CBD | 6.56 | 122.92      | 111.27   |
| 14  | H     | 1202 | CLA  | O2D-CGD-CBD | 6.55 | 122.91      | 111.27   |
| 14  | a     | 1115 | CLA  | C2D-C1D-ND  | 6.55 | 114.93      | 110.10   |
| 14  | G     | 1101 | CLA  | O2D-CGD-CBD | 6.55 | 122.91      | 111.27   |
| 18  | V     | 4021 | BCR  | C20-C19-C18 | 6.55 | 144.82      | 126.42   |
| 14  | b     | 1202 | CLA  | O2D-CGD-CBD | 6.54 | 122.90      | 111.27   |
| 14  | G     | 1112 | CLA  | C2C-C1C-NC  | 6.54 | 116.10      | 109.97   |
| 18  | M     | 4021 | BCR  | C20-C19-C18 | 6.54 | 144.79      | 126.42   |
| 14  | A     | 1104 | CLA  | C4A-NA-C1A  | 6.54 | 109.65      | 106.71   |
| 14  | B     | 1214 | CLA  | O2A-C1-C2   | 6.54 | 125.82      | 108.64   |
| 14  | b     | 1214 | CLA  | O2A-C1-C2   | 6.54 | 125.82      | 108.64   |
| 14  | H     | 1214 | CLA  | O2A-C1-C2   | 6.54 | 125.81      | 108.64   |
| 18  | m     | 4021 | BCR  | C20-C19-C18 | 6.53 | 144.76      | 126.42   |
| 14  | b     | 1208 | CLA  | C2D-C1D-ND  | 6.53 | 114.92      | 110.10   |
| 14  | a     | 1012 | CLA  | C2D-C1D-ND  | 6.53 | 114.91      | 110.10   |
| 14  | a     | 1141 | CLA  | C2C-C1C-NC  | 6.52 | 116.08      | 109.97   |
| 14  | b     | 1202 | CLA  | C2D-C1D-ND  | 6.52 | 114.91      | 110.10   |
| 14  | A     | 1128 | CLA  | CMD-C2D-C1D | 6.52 | 136.21      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1202 | CLA  | C2D-C1D-ND  | 6.52  | 114.91      | 110.10   |
| 14  | a     | 1112 | CLA  | C2C-C1C-NC  | 6.52  | 116.08      | 109.97   |
| 14  | b     | 1208 | CLA  | C2C-C1C-NC  | 6.52  | 116.08      | 109.97   |
| 14  | G     | 1128 | CLA  | CMD-C2D-C1D | 6.52  | 136.20      | 124.71   |
| 14  | a     | 1128 | CLA  | CMD-C2D-C1D | 6.52  | 136.20      | 124.71   |
| 14  | a     | 1119 | CLA  | C2D-C1D-ND  | 6.52  | 114.91      | 110.10   |
| 14  | a     | 1138 | CLA  | C2D-C1D-ND  | 6.51  | 114.91      | 110.10   |
| 14  | A     | 1012 | CLA  | C2D-C1D-ND  | 6.51  | 114.90      | 110.10   |
| 14  | G     | 1120 | CLA  | C2C-C1C-NC  | 6.51  | 116.07      | 109.97   |
| 14  | b     | 1222 | CLA  | C2C-C1C-NC  | 6.51  | 116.07      | 109.97   |
| 14  | A     | 1112 | CLA  | C2C-C1C-NC  | 6.51  | 116.07      | 109.97   |
| 14  | a     | 1105 | CLA  | C2D-C1D-ND  | 6.51  | 114.90      | 110.10   |
| 14  | A     | 1141 | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 14  | b     | 1212 | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 14  | G     | 1105 | CLA  | C2D-C1D-ND  | 6.50  | 114.89      | 110.10   |
| 15  | H     | 1230 | F6C  | C1C-C2C-C3C | -6.50 | 102.47      | 107.00   |
| 14  | G     | 1105 | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 14  | B     | 1209 | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 14  | H     | 1202 | CLA  | C2D-C1D-ND  | 6.50  | 114.89      | 110.10   |
| 14  | A     | 1120 | CLA  | C2C-C1C-NC  | 6.49  | 116.06      | 109.97   |
| 14  | A     | 1105 | CLA  | C2D-C1D-ND  | 6.49  | 114.89      | 110.10   |
| 14  | B     | 1222 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 14  | a     | 1120 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 14  | a     | 1139 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 14  | B     | 1202 | CLA  | C4A-NA-C1A  | 6.49  | 109.62      | 106.71   |
| 14  | A     | 1109 | CLA  | C2D-C1D-ND  | 6.49  | 114.89      | 110.10   |
| 14  | G     | 1138 | CLA  | C2D-C1D-ND  | 6.49  | 114.89      | 110.10   |
| 14  | H     | 1233 | CLA  | C2D-C1D-ND  | 6.49  | 114.89      | 110.10   |
| 14  | A     | 1105 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 14  | G     | 1012 | CLA  | C2D-C1D-ND  | 6.49  | 114.89      | 110.10   |
| 14  | A     | 1139 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 14  | G     | 1139 | CLA  | C2C-C1C-NC  | 6.49  | 116.05      | 109.97   |
| 15  | B     | 1230 | F6C  | C1C-C2C-C3C | -6.48 | 102.48      | 107.00   |
| 14  | G     | 1109 | CLA  | C2D-C1D-ND  | 6.48  | 114.88      | 110.10   |
| 14  | A     | 1138 | CLA  | C2D-C1D-ND  | 6.48  | 114.88      | 110.10   |
| 14  | H     | 1229 | CLA  | C2D-C1D-ND  | 6.48  | 114.88      | 110.10   |
| 14  | G     | 1106 | CLA  | C2C-C1C-NC  | 6.48  | 116.04      | 109.97   |
| 14  | b     | 1209 | CLA  | C2C-C1C-NC  | 6.48  | 116.04      | 109.97   |
| 14  | a     | 1109 | CLA  | C2D-C1D-ND  | 6.48  | 114.88      | 110.10   |
| 14  | b     | 1233 | CLA  | C2D-C1D-ND  | 6.47  | 114.87      | 110.10   |
| 14  | b     | 1216 | CLA  | C2C-C1C-NC  | 6.47  | 116.03      | 109.97   |
| 14  | G     | 1141 | CLA  | C2C-C1C-NC  | 6.47  | 116.03      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1115 | CLA  | O2D-CGD-CBD | 6.47  | 122.76      | 111.27   |
| 14  | B     | 1208 | CLA  | C2C-C1C-NC  | 6.47  | 116.03      | 109.97   |
| 14  | B     | 1212 | CLA  | C2C-C1C-NC  | 6.47  | 116.03      | 109.97   |
| 14  | a     | 1112 | CLA  | C2D-C1D-ND  | 6.47  | 114.87      | 110.10   |
| 14  | A     | 1118 | CLA  | C2C-C1C-NC  | 6.46  | 116.03      | 109.97   |
| 14  | H     | 1222 | CLA  | C2C-C1C-NC  | 6.46  | 116.03      | 109.97   |
| 14  | H     | 1212 | CLA  | C2C-C1C-NC  | 6.46  | 116.02      | 109.97   |
| 14  | G     | 1128 | CLA  | C2D-C1D-ND  | 6.46  | 114.86      | 110.10   |
| 14  | B     | 1233 | CLA  | C2D-C1D-ND  | 6.45  | 114.86      | 110.10   |
| 14  | G     | 1104 | CLA  | C2C-C1C-NC  | 6.45  | 116.02      | 109.97   |
| 14  | A     | 1115 | CLA  | O2D-CGD-CBD | 6.45  | 122.73      | 111.27   |
| 14  | l     | 1502 | CLA  | O2D-CGD-CBD | 6.45  | 122.73      | 111.27   |
| 14  | A     | 1106 | CLA  | C2C-C1C-NC  | 6.45  | 116.01      | 109.97   |
| 14  | a     | 1128 | CLA  | C2D-C1D-ND  | 6.45  | 114.85      | 110.10   |
| 14  | B     | 1216 | CLA  | C2C-C1C-NC  | 6.45  | 116.01      | 109.97   |
| 14  | H     | 1218 | CLA  | C2C-C1C-NC  | 6.45  | 116.01      | 109.97   |
| 15  | b     | 1230 | F6C  | C1C-C2C-C3C | -6.45 | 102.51      | 107.00   |
| 14  | G     | 1118 | CLA  | C2C-C1C-NC  | 6.44  | 116.01      | 109.97   |
| 14  | H     | 1209 | CLA  | C2C-C1C-NC  | 6.44  | 116.01      | 109.97   |
| 14  | A     | 1104 | CLA  | C2C-C1C-NC  | 6.44  | 116.01      | 109.97   |
| 14  | G     | 1115 | CLA  | O2D-CGD-CBD | 6.44  | 122.72      | 111.27   |
| 14  | a     | 1140 | CLA  | C2D-C1D-ND  | 6.44  | 114.85      | 110.10   |
| 14  | a     | 1123 | CLA  | O2D-CGD-CBD | 6.44  | 122.72      | 111.27   |
| 14  | b     | 1218 | CLA  | CHD-C1D-ND  | -6.44 | 118.53      | 124.45   |
| 14  | L     | 1502 | CLA  | O2D-CGD-CBD | 6.44  | 122.72      | 111.27   |
| 14  | G     | 1124 | CLA  | C2C-C1C-NC  | 6.44  | 116.01      | 109.97   |
| 14  | a     | 1105 | CLA  | C2C-C1C-NC  | 6.44  | 116.00      | 109.97   |
| 14  | a     | 1106 | CLA  | C2C-C1C-NC  | 6.44  | 116.00      | 109.97   |
| 14  | B     | 1229 | CLA  | C2D-C1D-ND  | 6.44  | 114.85      | 110.10   |
| 14  | a     | 1118 | CLA  | C2C-C1C-NC  | 6.43  | 116.00      | 109.97   |
| 14  | H     | 1216 | CLA  | C2C-C1C-NC  | 6.43  | 116.00      | 109.97   |
| 14  | A     | 1112 | CLA  | C2D-C1D-ND  | 6.43  | 114.84      | 110.10   |
| 14  | U     | 1502 | CLA  | O2D-CGD-CBD | 6.43  | 122.69      | 111.27   |
| 14  | b     | 1218 | CLA  | C2C-C1C-NC  | 6.43  | 116.00      | 109.97   |
| 18  | L     | 4019 | BCR  | C20-C19-C18 | 6.43  | 144.47      | 126.42   |
| 14  | G     | 1140 | CLA  | C2D-C1D-ND  | 6.43  | 114.84      | 110.10   |
| 14  | H     | 1208 | CLA  | C2C-C1C-NC  | 6.42  | 115.99      | 109.97   |
| 14  | a     | 1130 | CLA  | C2D-C1D-ND  | 6.42  | 114.84      | 110.10   |
| 14  | H     | 1201 | CLA  | O2D-CGD-CBD | 6.42  | 122.68      | 111.27   |
| 18  | U     | 4019 | BCR  | C20-C19-C18 | 6.42  | 144.46      | 126.42   |
| 14  | B     | 1201 | CLA  | O2D-CGD-CBD | 6.42  | 122.68      | 111.27   |
| 14  | b     | 1221 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1140 | CLA  | C2D-C1D-ND  | 6.42  | 114.83      | 110.10   |
| 14  | A     | 1130 | CLA  | C2D-C1D-ND  | 6.41  | 114.83      | 110.10   |
| 14  | A     | 1103 | CLA  | C2C-C1C-NC  | 6.41  | 115.98      | 109.97   |
| 14  | B     | 1218 | CLA  | C2C-C1C-NC  | 6.41  | 115.98      | 109.97   |
| 14  | A     | 1128 | CLA  | C2D-C1D-ND  | 6.41  | 114.83      | 110.10   |
| 14  | b     | 1202 | CLA  | C4A-NA-C1A  | 6.41  | 109.59      | 106.71   |
| 14  | G     | 1107 | CLA  | C2C-C1C-NC  | 6.41  | 115.98      | 109.97   |
| 14  | G     | 1112 | CLA  | C2D-C1D-ND  | 6.41  | 114.83      | 110.10   |
| 14  | a     | 1103 | CLA  | C2C-C1C-NC  | 6.41  | 115.97      | 109.97   |
| 14  | A     | 1123 | CLA  | O2D-CGD-CBD | 6.41  | 122.65      | 111.27   |
| 18  | l     | 4019 | BCR  | C20-C19-C18 | 6.41  | 144.41      | 126.42   |
| 14  | b     | 1229 | CLA  | C2D-C1D-ND  | 6.41  | 114.83      | 110.10   |
| 14  | B     | 1221 | CLA  | CMD-C2D-C1D | 6.41  | 136.00      | 124.71   |
| 14  | H     | 1202 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 14  | H     | 1221 | CLA  | CMD-C2D-C1D | 6.40  | 136.00      | 124.71   |
| 14  | G     | 1123 | CLA  | O2D-CGD-CBD | 6.40  | 122.64      | 111.27   |
| 14  | b     | 1201 | CLA  | O2D-CGD-CBD | 6.40  | 122.63      | 111.27   |
| 14  | b     | 1205 | CLA  | O2D-CGD-CBD | 6.39  | 122.63      | 111.27   |
| 14  | B     | 1218 | CLA  | CHD-C1D-ND  | -6.39 | 118.58      | 124.45   |
| 14  | H     | 1205 | CLA  | O2D-CGD-CBD | 6.39  | 122.63      | 111.27   |
| 14  | G     | 1103 | CLA  | C2C-C1C-NC  | 6.39  | 115.96      | 109.97   |
| 14  | a     | 1104 | CLA  | C2C-C1C-NC  | 6.39  | 115.96      | 109.97   |
| 14  | A     | 1124 | CLA  | C2C-C1C-NC  | 6.39  | 115.96      | 109.97   |
| 14  | H     | 1206 | CLA  | CMD-C2D-C1D | 6.39  | 135.97      | 124.71   |
| 14  | b     | 1206 | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.71   |
| 14  | a     | 1107 | CLA  | C2C-C1C-NC  | 6.38  | 115.95      | 109.97   |
| 14  | G     | 1138 | CLA  | CHD-C1D-ND  | -6.38 | 118.59      | 124.45   |
| 14  | H     | 1218 | CLA  | CHD-C1D-ND  | -6.38 | 118.59      | 124.45   |
| 14  | a     | 1126 | CLA  | C2C-C1C-NC  | 6.38  | 115.95      | 109.97   |
| 14  | B     | 1205 | CLA  | O2D-CGD-CBD | 6.38  | 122.61      | 111.27   |
| 14  | b     | 1225 | CLA  | O2A-C1-C2   | 6.38  | 125.40      | 108.64   |
| 14  | A     | 1138 | CLA  | CHD-C1D-ND  | -6.38 | 118.59      | 124.45   |
| 14  | B     | 1206 | CLA  | CMD-C2D-C1D | 6.38  | 135.95      | 124.71   |
| 14  | B     | 1225 | CLA  | O2A-C1-C2   | 6.37  | 125.39      | 108.64   |
| 14  | A     | 1107 | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 14  | a     | 1124 | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 18  | b     | 4009 | BCR  | C20-C19-C18 | 6.37  | 144.31      | 126.42   |
| 14  | B     | 1228 | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 14  | G     | 1104 | CLA  | C1C-C2C-C3C | -6.37 | 100.26      | 106.96   |
| 14  | G     | 1125 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 14  | a     | 1138 | CLA  | CHD-C1D-ND  | -6.37 | 118.60      | 124.45   |
| 14  | H     | 1225 | CLA  | O2A-C1-C2   | 6.37  | 125.36      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1229 | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 14  | H     | 1228 | CLA  | C2C-C1C-NC  | 6.36  | 115.93      | 109.97   |
| 18  | B     | 4009 | BCR  | C20-C19-C18 | 6.36  | 144.28      | 126.42   |
| 14  | A     | 1104 | CLA  | C1C-C2C-C3C | -6.36 | 100.27      | 106.96   |
| 14  | a     | 1104 | CLA  | C1C-C2C-C3C | -6.35 | 100.28      | 106.96   |
| 14  | a     | 1125 | CLA  | C3D-C2D-C1D | -6.35 | 97.17       | 105.83   |
| 14  | A     | 1125 | CLA  | C3D-C2D-C1D | -6.34 | 97.17       | 105.83   |
| 14  | b     | 1228 | CLA  | C2C-C1C-NC  | 6.34  | 115.91      | 109.97   |
| 14  | G     | 1141 | CLA  | O2D-CGD-CBD | 6.34  | 122.54      | 111.27   |
| 14  | A     | 1125 | CLA  | C4A-NA-C1A  | 6.34  | 109.56      | 106.71   |
| 14  | a     | 1141 | CLA  | O2D-CGD-CBD | 6.34  | 122.53      | 111.27   |
| 18  | H     | 4009 | BCR  | C20-C19-C18 | 6.34  | 144.22      | 126.42   |
| 14  | b     | 1227 | CLA  | O2D-CGD-CBD | 6.34  | 122.53      | 111.27   |
| 14  | G     | 1126 | CLA  | C2C-C1C-NC  | 6.34  | 115.91      | 109.97   |
| 14  | a     | 1101 | CLA  | C2D-C1D-ND  | 6.34  | 114.77      | 110.10   |
| 14  | A     | 1126 | CLA  | C2C-C1C-NC  | 6.33  | 115.91      | 109.97   |
| 14  | B     | 1234 | CLA  | C2C-C1C-NC  | 6.33  | 115.91      | 109.97   |
| 14  | A     | 1108 | CLA  | C2C-C1C-NC  | 6.33  | 115.91      | 109.97   |
| 14  | G     | 1125 | CLA  | C3D-C2D-C1D | -6.33 | 97.19       | 105.83   |
| 14  | G     | 1108 | CLA  | C2C-C1C-NC  | 6.33  | 115.90      | 109.97   |
| 14  | A     | 1141 | CLA  | O2D-CGD-CBD | 6.33  | 122.52      | 111.27   |
| 14  | G     | 1130 | CLA  | C2D-C1D-ND  | 6.33  | 114.77      | 110.10   |
| 14  | B     | 1229 | CLA  | C2C-C1C-NC  | 6.33  | 115.90      | 109.97   |
| 14  | B     | 1227 | CLA  | O2D-CGD-CBD | 6.33  | 122.51      | 111.27   |
| 14  | b     | 1216 | CLA  | C2D-C1D-ND  | 6.32  | 114.77      | 110.10   |
| 14  | a     | 1108 | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 14  | H     | 1226 | CLA  | O2A-C1-C2   | 6.32  | 125.25      | 108.64   |
| 14  | H     | 1234 | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 14  | b     | 1229 | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 14  | B     | 1226 | CLA  | O2A-C1-C2   | 6.32  | 125.24      | 108.64   |
| 14  | b     | 1226 | CLA  | O2A-C1-C2   | 6.30  | 125.20      | 108.64   |
| 14  | a     | 1125 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 15  | H     | 1237 | F6C  | C2D-C1D-ND  | 6.30  | 115.88      | 109.97   |
| 14  | a     | 1131 | CLA  | C2D-C1D-ND  | 6.30  | 114.75      | 110.10   |
| 14  | b     | 1234 | CLA  | C2C-C1C-NC  | 6.30  | 115.87      | 109.97   |
| 14  | H     | 1227 | CLA  | O2D-CGD-CBD | 6.29  | 122.45      | 111.27   |
| 14  | A     | 1130 | CLA  | C2C-C1C-NC  | 6.28  | 115.86      | 109.97   |
| 14  | H     | 1216 | CLA  | C2D-C1D-ND  | 6.28  | 114.73      | 110.10   |
| 14  | a     | 1130 | CLA  | C2C-C1C-NC  | 6.27  | 115.85      | 109.97   |
| 14  | a     | 1103 | CLA  | O2D-CGD-CBD | 6.27  | 122.42      | 111.27   |
| 14  | G     | 1110 | CLA  | C2C-C1C-NC  | 6.27  | 115.85      | 109.97   |
| 14  | A     | 1101 | CLA  | C2D-C1D-ND  | 6.27  | 114.73      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1216 | CLA  | C2D-C1D-ND  | 6.27  | 114.73      | 110.10   |
| 15  | B     | 1237 | F6C  | C2D-C1D-ND  | 6.27  | 115.85      | 109.97   |
| 15  | b     | 1207 | F6C  | O2D-CGD-CBD | 6.27  | 122.41      | 111.27   |
| 14  | A     | 1110 | CLA  | C2C-C1C-NC  | 6.26  | 115.84      | 109.97   |
| 15  | b     | 1238 | F6C  | CAA-C2A-C1A | -6.26 | 110.86      | 128.11   |
| 14  | G     | 1101 | CLA  | C2D-C1D-ND  | 6.26  | 114.72      | 110.10   |
| 14  | b     | 1209 | CLA  | C2D-C1D-ND  | 6.26  | 114.72      | 110.10   |
| 14  | G     | 1103 | CLA  | O2D-CGD-CBD | 6.26  | 122.39      | 111.27   |
| 14  | G     | 1131 | CLA  | C2D-C1D-ND  | 6.26  | 114.72      | 110.10   |
| 15  | B     | 1238 | F6C  | CAA-C2A-C1A | -6.26 | 110.88      | 128.11   |
| 14  | A     | 1103 | CLA  | O2D-CGD-CBD | 6.26  | 122.39      | 111.27   |
| 15  | B     | 1207 | F6C  | O2D-CGD-CBD | 6.25  | 122.38      | 111.27   |
| 14  | a     | 1110 | CLA  | C2C-C1C-NC  | 6.25  | 115.83      | 109.97   |
| 14  | B     | 1225 | CLA  | C2D-C1D-ND  | 6.25  | 114.71      | 110.10   |
| 14  | H     | 1209 | CLA  | C2D-C1D-ND  | 6.25  | 114.71      | 110.10   |
| 15  | H     | 1207 | F6C  | O2D-CGD-CBD | 6.25  | 122.37      | 111.27   |
| 14  | B     | 1240 | CLA  | C2D-C1D-ND  | 6.25  | 114.71      | 110.10   |
| 14  | G     | 1119 | CLA  | O2A-C1-C2   | 6.25  | 125.05      | 108.64   |
| 15  | H     | 1238 | F6C  | CAA-C2A-C1A | -6.25 | 110.91      | 128.11   |
| 14  | A     | 1138 | CLA  | C1C-C2C-C3C | -6.24 | 100.39      | 106.96   |
| 14  | H     | 1224 | CLA  | C2C-C1C-NC  | 6.24  | 115.82      | 109.97   |
| 14  | B     | 1209 | CLA  | C2D-C1D-ND  | 6.24  | 114.70      | 110.10   |
| 14  | H     | 1206 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 14  | G     | 1138 | CLA  | C1C-C2C-C3C | -6.23 | 100.40      | 106.96   |
| 14  | A     | 1131 | CLA  | C2D-C1D-ND  | 6.23  | 114.70      | 110.10   |
| 14  | H     | 1240 | CLA  | C2D-C1D-ND  | 6.23  | 114.70      | 110.10   |
| 14  | A     | 1119 | CLA  | O2A-C1-C2   | 6.23  | 125.00      | 108.64   |
| 14  | b     | 1240 | CLA  | C2D-C1D-ND  | 6.23  | 114.69      | 110.10   |
| 14  | a     | 1138 | CLA  | C1C-C2C-C3C | -6.23 | 100.41      | 106.96   |
| 14  | B     | 1224 | CLA  | C2C-C1C-NC  | 6.22  | 115.80      | 109.97   |
| 14  | G     | 1130 | CLA  | C2C-C1C-NC  | 6.22  | 115.80      | 109.97   |
| 15  | B     | 1207 | F6C  | C3A-C4A-NA  | 6.22  | 114.69      | 110.10   |
| 14  | b     | 1211 | CLA  | O2D-CGD-CBD | 6.22  | 122.33      | 111.27   |
| 14  | B     | 1225 | CLA  | CMD-C2D-C1D | 6.22  | 135.68      | 124.71   |
| 14  | b     | 1224 | CLA  | C2C-C1C-NC  | 6.22  | 115.80      | 109.97   |
| 14  | a     | 1119 | CLA  | O2A-C1-C2   | 6.22  | 124.97      | 108.64   |
| 14  | H     | 1229 | CLA  | O2D-CGD-CBD | 6.21  | 122.31      | 111.27   |
| 14  | H     | 1225 | CLA  | CMD-C2D-C1D | 6.21  | 135.66      | 124.71   |
| 14  | b     | 1225 | CLA  | C2D-C1D-ND  | 6.21  | 114.68      | 110.10   |
| 14  | b     | 1225 | CLA  | CMD-C2D-C1D | 6.20  | 135.65      | 124.71   |
| 14  | H     | 1235 | CLA  | C2C-C1C-NC  | 6.20  | 115.78      | 109.97   |
| 18  | k     | 4001 | BCR  | C20-C19-C18 | 6.20  | 143.83      | 126.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1211 | CLA  | O2D-CGD-CBD | 6.20  | 122.28      | 111.27   |
| 14  | B     | 1211 | CLA  | O2D-CGD-CBD | 6.20  | 122.28      | 111.27   |
| 15  | b     | 1237 | F6C  | C2D-C1D-ND  | 6.20  | 115.78      | 109.97   |
| 14  | B     | 1206 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | b     | 1205 | CLA  | C2C-C1C-NC  | 6.19  | 115.78      | 109.97   |
| 15  | H     | 1207 | F6C  | C3A-C4A-NA  | 6.19  | 114.67      | 110.10   |
| 18  | K     | 4001 | BCR  | C20-C19-C18 | 6.19  | 143.81      | 126.42   |
| 14  | b     | 1222 | CLA  | O2D-CGD-CBD | 6.19  | 122.26      | 111.27   |
| 14  | B     | 1229 | CLA  | O2D-CGD-CBD | 6.19  | 122.26      | 111.27   |
| 14  | H     | 1235 | CLA  | O2A-C1-C2   | 6.18  | 124.89      | 108.64   |
| 14  | G     | 1103 | CLA  | C4A-NA-C1A  | 6.18  | 109.49      | 106.71   |
| 18  | T     | 4001 | BCR  | C20-C19-C18 | 6.18  | 143.78      | 126.42   |
| 14  | b     | 1235 | CLA  | O2A-C1-C2   | 6.18  | 124.88      | 108.64   |
| 14  | B     | 1235 | CLA  | O2A-C1-C2   | 6.18  | 124.88      | 108.64   |
| 14  | b     | 1217 | CLA  | O2D-CGD-CBD | 6.18  | 122.25      | 111.27   |
| 18  | K     | 4001 | BCR  | C7-C8-C9    | -6.18 | 116.90      | 126.23   |
| 14  | b     | 1206 | CLA  | C4A-NA-C1A  | 6.18  | 109.48      | 106.71   |
| 14  | H     | 1217 | CLA  | O2D-CGD-CBD | 6.18  | 122.24      | 111.27   |
| 14  | B     | 1222 | CLA  | O2D-CGD-CBD | 6.18  | 122.24      | 111.27   |
| 18  | a     | 4005 | BCR  | C20-C19-C18 | 6.18  | 143.77      | 126.42   |
| 14  | b     | 1229 | CLA  | O2D-CGD-CBD | 6.18  | 122.24      | 111.27   |
| 14  | L     | 1503 | CLA  | C2D-C1D-ND  | 6.18  | 114.66      | 110.10   |
| 15  | B     | 1207 | F6C  | O2A-CGA-O1A | -6.17 | 108.01      | 123.59   |
| 14  | U     | 1503 | CLA  | C2D-C1D-ND  | 6.17  | 114.65      | 110.10   |
| 14  | H     | 1222 | CLA  | O2D-CGD-CBD | 6.17  | 122.24      | 111.27   |
| 14  | H     | 1225 | CLA  | C2D-C1D-ND  | 6.17  | 114.65      | 110.10   |
| 14  | a     | 1132 | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 18  | A     | 4005 | BCR  | C20-C19-C18 | 6.17  | 143.74      | 126.42   |
| 14  | l     | 1503 | CLA  | C2D-C1D-ND  | 6.17  | 114.65      | 110.10   |
| 14  | B     | 1205 | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 15  | b     | 1207 | F6C  | C3A-C4A-NA  | 6.17  | 114.65      | 110.10   |
| 18  | k     | 4001 | BCR  | C7-C8-C9    | -6.17 | 116.92      | 126.23   |
| 14  | a     | 1103 | CLA  | C4A-NA-C1A  | 6.17  | 109.48      | 106.71   |
| 14  | A     | 1119 | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 14  | H     | 1205 | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 14  | B     | 1217 | CLA  | O2D-CGD-CBD | 6.16  | 122.22      | 111.27   |
| 14  | A     | 1132 | CLA  | C2C-C1C-NC  | 6.16  | 115.75      | 109.97   |
| 14  | a     | 1118 | CLA  | O2D-CGD-CBD | 6.16  | 122.22      | 111.27   |
| 18  | T     | 4001 | BCR  | C7-C8-C9    | -6.16 | 116.92      | 126.23   |
| 14  | B     | 1235 | CLA  | C2C-C1C-NC  | 6.16  | 115.75      | 109.97   |
| 15  | H     | 1207 | F6C  | O2A-CGA-O1A | -6.16 | 108.05      | 123.59   |
| 15  | b     | 1207 | F6C  | O2A-CGA-O1A | -6.16 | 108.06      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1123 | CLA  | O2A-C1-C2   | 6.15  | 124.81      | 108.64   |
| 14  | G     | 1119 | CLA  | C2C-C1C-NC  | 6.15  | 115.74      | 109.97   |
| 14  | a     | 1119 | CLA  | C2C-C1C-NC  | 6.15  | 115.74      | 109.97   |
| 14  | G     | 1127 | CLA  | C4A-NA-C1A  | 6.15  | 109.47      | 106.71   |
| 14  | A     | 1123 | CLA  | O2A-C1-C2   | 6.15  | 124.80      | 108.64   |
| 18  | G     | 4005 | BCR  | C20-C19-C18 | 6.15  | 143.69      | 126.42   |
| 14  | a     | 1123 | CLA  | O2A-C1-C2   | 6.15  | 124.79      | 108.64   |
| 14  | G     | 1132 | CLA  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 14  | G     | 1128 | CLA  | O2D-CGD-CBD | 6.14  | 122.19      | 111.27   |
| 14  | a     | 1128 | CLA  | O2D-CGD-CBD | 6.14  | 122.18      | 111.27   |
| 14  | G     | 1133 | CLA  | C1C-C2C-C3C | -6.14 | 100.50      | 106.96   |
| 14  | A     | 1133 | CLA  | C1C-C2C-C3C | -6.14 | 100.50      | 106.96   |
| 14  | A     | 1128 | CLA  | O2D-CGD-CBD | 6.13  | 122.17      | 111.27   |
| 14  | A     | 1118 | CLA  | O2D-CGD-CBD | 6.13  | 122.17      | 111.27   |
| 14  | a     | 1113 | CLA  | C2C-C1C-NC  | 6.13  | 115.72      | 109.97   |
| 14  | b     | 1235 | CLA  | C2C-C1C-NC  | 6.13  | 115.72      | 109.97   |
| 18  | G     | 4002 | BCR  | C15-C14-C13 | -6.13 | 118.57      | 127.31   |
| 15  | H     | 1230 | F6C  | O2D-CGD-CBD | 6.12  | 122.15      | 111.27   |
| 14  | G     | 1113 | CLA  | C2C-C1C-NC  | 6.12  | 115.71      | 109.97   |
| 14  | G     | 1116 | CLA  | C2C-C1C-NC  | 6.12  | 115.71      | 109.97   |
| 14  | a     | 1133 | CLA  | C1C-C2C-C3C | -6.12 | 100.52      | 106.96   |
| 15  | B     | 1230 | F6C  | O2D-CGD-CBD | 6.12  | 122.14      | 111.27   |
| 14  | A     | 1120 | CLA  | C4A-NA-C1A  | 6.12  | 109.46      | 106.71   |
| 14  | G     | 1118 | CLA  | O2D-CGD-CBD | 6.12  | 122.14      | 111.27   |
| 14  | B     | 1232 | CLA  | C2D-C1D-ND  | 6.11  | 114.61      | 110.10   |
| 18  | A     | 4002 | BCR  | C15-C14-C13 | -6.11 | 118.58      | 127.31   |
| 14  | A     | 1124 | CLA  | C4A-NA-C1A  | 6.11  | 109.45      | 106.71   |
| 14  | U     | 1502 | CLA  | O2A-C1-C2   | 6.11  | 124.69      | 108.64   |
| 14  | b     | 1021 | CLA  | C2C-C1C-NC  | 6.10  | 115.69      | 109.97   |
| 14  | a     | 1129 | CLA  | C2C-C1C-NC  | 6.10  | 115.69      | 109.97   |
| 14  | H     | 1021 | CLA  | C2C-C1C-NC  | 6.10  | 115.68      | 109.97   |
| 14  | A     | 1113 | CLA  | C2C-C1C-NC  | 6.10  | 115.68      | 109.97   |
| 14  | A     | 1127 | CLA  | C4A-NA-C1A  | 6.09  | 109.45      | 106.71   |
| 14  | a     | 1116 | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 14  | L     | 1502 | CLA  | O2A-C1-C2   | 6.09  | 124.65      | 108.64   |
| 18  | a     | 4002 | BCR  | C15-C14-C13 | -6.09 | 118.62      | 127.31   |
| 14  | B     | 1021 | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 14  | l     | 1502 | CLA  | O2A-C1-C2   | 6.09  | 124.64      | 108.64   |
| 14  | G     | 1138 | CLA  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 14  | G     | 1137 | CLA  | O2D-CGD-CBD | 6.09  | 122.08      | 111.27   |
| 15  | b     | 1230 | F6C  | O2D-CGD-CBD | 6.09  | 122.08      | 111.27   |
| 14  | b     | 1232 | CLA  | C2D-C1D-ND  | 6.08  | 114.59      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | U     | 4022 | BCR  | C20-C19-C18 | 6.08  | 143.51      | 126.42   |
| 14  | a     | 1137 | CLA  | O2D-CGD-CBD | 6.08  | 122.08      | 111.27   |
| 18  | L     | 4022 | BCR  | C20-C19-C18 | 6.08  | 143.50      | 126.42   |
| 14  | A     | 1103 | CLA  | C4A-NA-C1A  | 6.08  | 109.44      | 106.71   |
| 14  | A     | 1137 | CLA  | O2D-CGD-CBD | 6.08  | 122.07      | 111.27   |
| 14  | H     | 1232 | CLA  | C2D-C1D-ND  | 6.08  | 114.58      | 110.10   |
| 14  | A     | 1116 | CLA  | C2C-C1C-NC  | 6.08  | 115.66      | 109.97   |
| 14  | G     | 1133 | CLA  | O2A-C1-C2   | 6.08  | 124.60      | 108.64   |
| 18  | l     | 4022 | BCR  | C20-C19-C18 | 6.07  | 143.48      | 126.42   |
| 14  | G     | 1124 | CLA  | C4A-NA-C1A  | 6.07  | 109.44      | 106.71   |
| 14  | G     | 1120 | CLA  | C4A-NA-C1A  | 6.07  | 109.44      | 106.71   |
| 14  | B     | 1204 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 14  | B     | 1201 | CLA  | C4A-NA-C1A  | 6.07  | 109.43      | 106.71   |
| 14  | B     | 1222 | CLA  | C4A-NA-C1A  | 6.07  | 109.43      | 106.71   |
| 14  | H     | 1204 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 14  | b     | 1204 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 14  | b     | 1023 | CLA  | C2C-C1C-NC  | 6.07  | 115.65      | 109.97   |
| 14  | b     | 1222 | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 14  | A     | 1129 | CLA  | C2C-C1C-NC  | 6.06  | 115.65      | 109.97   |
| 14  | A     | 1133 | CLA  | O2A-C1-C2   | 6.06  | 124.55      | 108.64   |
| 14  | a     | 1133 | CLA  | O2A-C1-C2   | 6.06  | 124.55      | 108.64   |
| 14  | H     | 1023 | CLA  | C2C-C1C-NC  | 6.05  | 115.64      | 109.97   |
| 14  | B     | 1023 | CLA  | C2C-C1C-NC  | 6.05  | 115.64      | 109.97   |
| 14  | G     | 1122 | CLA  | C2C-C1C-NC  | 6.04  | 115.64      | 109.97   |
| 14  | b     | 1228 | CLA  | C2D-C1D-ND  | 6.04  | 114.56      | 110.10   |
| 14  | A     | 1138 | CLA  | C4A-NA-C1A  | 6.04  | 109.42      | 106.71   |
| 14  | L     | 1501 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | G     | 1140 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | b     | 1220 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | a     | 1124 | CLA  | C4A-NA-C1A  | 6.04  | 109.42      | 106.71   |
| 14  | U     | 1501 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | b     | 1208 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | B     | 1220 | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 14  | a     | 1127 | CLA  | C4A-NA-C1A  | 6.04  | 109.42      | 106.71   |
| 14  | H     | 1231 | CLA  | O2D-CGD-CBD | 6.03  | 121.99      | 111.27   |
| 14  | a     | 1122 | CLA  | C2C-C1C-NC  | 6.03  | 115.62      | 109.97   |
| 14  | A     | 1140 | CLA  | O2D-CGD-CBD | 6.03  | 121.99      | 111.27   |
| 14  | H     | 1220 | CLA  | O2D-CGD-CBD | 6.03  | 121.99      | 111.27   |
| 14  | B     | 1212 | CLA  | C2D-C1D-ND  | 6.03  | 114.55      | 110.10   |
| 14  | b     | 1212 | CLA  | C2D-C1D-ND  | 6.03  | 114.55      | 110.10   |
| 14  | l     | 1501 | CLA  | O2D-CGD-CBD | 6.03  | 121.98      | 111.27   |
| 14  | b     | 1217 | CLA  | C4A-NA-C1A  | 6.03  | 109.42      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1231 | CLA  | O2D-CGD-CBD | 6.03  | 121.98      | 111.27   |
| 14  | H     | 1217 | CLA  | C4A-NA-C1A  | 6.03  | 109.42      | 106.71   |
| 14  | G     | 1129 | CLA  | C2C-C1C-NC  | 6.02  | 115.61      | 109.97   |
| 14  | a     | 1140 | CLA  | O2D-CGD-CBD | 6.02  | 121.97      | 111.27   |
| 14  | a     | 1138 | CLA  | C4A-NA-C1A  | 6.02  | 109.41      | 106.71   |
| 14  | B     | 1208 | CLA  | O2D-CGD-CBD | 6.02  | 121.97      | 111.27   |
| 14  | G     | 1114 | CLA  | C2D-C1D-ND  | 6.02  | 114.54      | 110.10   |
| 14  | B     | 1217 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | G     | 1122 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | b     | 1201 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | A     | 1122 | CLA  | C2C-C1C-NC  | 6.01  | 115.61      | 109.97   |
| 14  | a     | 1120 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | H     | 1201 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | H     | 1222 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | a     | 1114 | CLA  | C2D-C1D-ND  | 6.01  | 114.53      | 110.10   |
| 14  | B     | 1231 | CLA  | O2D-CGD-CBD | 6.01  | 121.94      | 111.27   |
| 14  | A     | 1127 | CLA  | CMD-C2D-C1D | 6.01  | 135.30      | 124.71   |
| 14  | B     | 1223 | CLA  | O2D-CGD-CBD | 6.01  | 121.94      | 111.27   |
| 14  | G     | 1137 | CLA  | C4A-NA-C1A  | 6.00  | 109.41      | 106.71   |
| 14  | H     | 1208 | CLA  | O2D-CGD-CBD | 6.00  | 121.93      | 111.27   |
| 14  | A     | 1122 | CLA  | C4A-NA-C1A  | 6.00  | 109.40      | 106.71   |
| 14  | H     | 1223 | CLA  | O2D-CGD-CBD | 6.00  | 121.92      | 111.27   |
| 14  | G     | 1127 | CLA  | CMD-C2D-C1D | 5.99  | 135.27      | 124.71   |
| 14  | H     | 1212 | CLA  | C2D-C1D-ND  | 5.99  | 114.52      | 110.10   |
| 14  | a     | 1127 | CLA  | CMD-C2D-C1D | 5.99  | 135.27      | 124.71   |
| 14  | a     | 1123 | CLA  | C4A-NA-C1A  | 5.99  | 109.40      | 106.71   |
| 14  | A     | 1114 | CLA  | C2D-C1D-ND  | 5.99  | 114.52      | 110.10   |
| 14  | b     | 1223 | CLA  | O2D-CGD-CBD | 5.99  | 121.91      | 111.27   |
| 14  | U     | 1503 | CLA  | O2D-CGD-CBD | 5.98  | 121.90      | 111.27   |
| 14  | b     | 1218 | CLA  | C1C-C2C-C3C | -5.98 | 100.67      | 106.96   |
| 14  | a     | 1114 | CLA  | C1C-C2C-C3C | -5.98 | 100.67      | 106.96   |
| 14  | a     | 1109 | CLA  | C4A-NA-C1A  | 5.98  | 109.39      | 106.71   |
| 14  | a     | 1122 | CLA  | C4A-NA-C1A  | 5.98  | 109.39      | 106.71   |
| 15  | B     | 1230 | F6C  | C3A-C4A-NA  | 5.97  | 114.50      | 110.10   |
| 14  | L     | 1503 | CLA  | O2D-CGD-CBD | 5.97  | 121.87      | 111.27   |
| 14  | H     | 1203 | CLA  | C1C-C2C-C3C | -5.96 | 100.69      | 106.96   |
| 14  | l     | 1503 | CLA  | O2D-CGD-CBD | 5.96  | 121.86      | 111.27   |
| 14  | M     | 1501 | CLA  | C2D-C1D-ND  | 5.96  | 114.50      | 110.10   |
| 14  | a     | 1120 | CLA  | CHD-C1D-ND  | -5.96 | 118.98      | 124.45   |
| 14  | B     | 1203 | CLA  | C1C-C2C-C3C | -5.96 | 100.69      | 106.96   |
| 15  | H     | 1230 | F6C  | C3A-C4A-NA  | 5.96  | 114.50      | 110.10   |
| 14  | A     | 1131 | CLA  | O2D-CGD-CBD | 5.96  | 121.85      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1236 | CLA  | O2D-CGD-CBD | 5.96  | 121.85      | 111.27   |
| 14  | H     | 1228 | CLA  | C2D-C1D-ND  | 5.96  | 114.49      | 110.10   |
| 14  | H     | 1218 | CLA  | C1C-C2C-C3C | -5.95 | 100.70      | 106.96   |
| 14  | G     | 1120 | CLA  | CHD-C1D-ND  | -5.95 | 118.98      | 124.45   |
| 14  | A     | 1114 | CLA  | C1C-C2C-C3C | -5.95 | 100.70      | 106.96   |
| 14  | b     | 1239 | CLA  | O2D-CGD-CBD | 5.95  | 121.84      | 111.27   |
| 14  | B     | 1204 | CLA  | O2D-CGD-CBD | 5.95  | 121.84      | 111.27   |
| 14  | A     | 1120 | CLA  | CHD-C1D-ND  | -5.95 | 118.99      | 124.45   |
| 14  | A     | 1137 | CLA  | C4A-NA-C1A  | 5.95  | 109.38      | 106.71   |
| 14  | H     | 1204 | CLA  | O2D-CGD-CBD | 5.95  | 121.83      | 111.27   |
| 14  | b     | 1203 | CLA  | C1C-C2C-C3C | -5.95 | 100.71      | 106.96   |
| 14  | H     | 1236 | CLA  | O2D-CGD-CBD | 5.94  | 121.83      | 111.27   |
| 14  | a     | 1131 | CLA  | O2D-CGD-CBD | 5.94  | 121.83      | 111.27   |
| 14  | G     | 1131 | CLA  | O2D-CGD-CBD | 5.94  | 121.83      | 111.27   |
| 14  | B     | 1218 | CLA  | C1C-C2C-C3C | -5.94 | 100.71      | 106.96   |
| 14  | G     | 1114 | CLA  | C1C-C2C-C3C | -5.94 | 100.71      | 106.96   |
| 14  | b     | 1204 | CLA  | O2D-CGD-CBD | 5.94  | 121.82      | 111.27   |
| 14  | B     | 1228 | CLA  | C2D-C1D-ND  | 5.94  | 114.48      | 110.10   |
| 14  | V     | 1501 | CLA  | C2D-C1D-ND  | 5.94  | 114.48      | 110.10   |
| 15  | b     | 1230 | F6C  | C3A-C4A-NA  | 5.94  | 114.48      | 110.10   |
| 14  | H     | 1239 | CLA  | O2D-CGD-CBD | 5.93  | 121.81      | 111.27   |
| 14  | A     | 1109 | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 14  | b     | 1236 | CLA  | O2D-CGD-CBD | 5.93  | 121.81      | 111.27   |
| 15  | B     | 1237 | F6C  | O2A-C1-C2   | 5.93  | 124.22      | 108.64   |
| 14  | B     | 1239 | CLA  | O2D-CGD-CBD | 5.93  | 121.80      | 111.27   |
| 14  | a     | 1126 | CLA  | C2D-C1D-ND  | 5.92  | 114.47      | 110.10   |
| 15  | H     | 1237 | F6C  | O2A-C1-C2   | 5.92  | 124.20      | 108.64   |
| 14  | A     | 1115 | CLA  | C2C-C1C-NC  | 5.92  | 115.52      | 109.97   |
| 15  | b     | 1237 | F6C  | O2A-C1-C2   | 5.92  | 124.19      | 108.64   |
| 14  | G     | 1109 | CLA  | C4A-NA-C1A  | 5.92  | 109.37      | 106.71   |
| 14  | a     | 1137 | CLA  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |
| 14  | a     | 1115 | CLA  | C2C-C1C-NC  | 5.91  | 115.51      | 109.97   |
| 14  | G     | 1111 | CLA  | C2C-C1C-NC  | 5.91  | 115.51      | 109.97   |
| 14  | m     | 1501 | CLA  | C2D-C1D-ND  | 5.91  | 114.46      | 110.10   |
| 14  | G     | 1120 | CLA  | O2D-CGD-CBD | 5.90  | 121.76      | 111.27   |
| 14  | H     | 1224 | CLA  | O2D-CGD-CBD | 5.90  | 121.75      | 111.27   |
| 14  | B     | 1224 | CLA  | O2D-CGD-CBD | 5.89  | 121.74      | 111.27   |
| 14  | b     | 1205 | CLA  | O2A-CGA-O1A | -5.89 | 108.72      | 123.59   |
| 14  | B     | 1205 | CLA  | O2A-CGA-O1A | -5.89 | 108.73      | 123.59   |
| 14  | A     | 1123 | CLA  | C4A-NA-C1A  | 5.89  | 109.35      | 106.71   |
| 15  | G     | 1121 | F6C  | O2D-CGD-CBD | 5.89  | 121.73      | 111.27   |
| 14  | A     | 1120 | CLA  | O2D-CGD-CBD | 5.88  | 121.72      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1126 | CLA  | O2D-CGD-CBD | 5.88  | 121.72      | 111.27   |
| 14  | a     | 1120 | CLA  | O2D-CGD-CBD | 5.88  | 121.72      | 111.27   |
| 15  | A     | 1121 | F6C  | O2D-CGD-CBD | 5.88  | 121.72      | 111.27   |
| 14  | a     | 1109 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 15  | a     | 1121 | F6C  | O2D-CGD-CBD | 5.88  | 121.72      | 111.27   |
| 14  | G     | 1126 | CLA  | C2D-C1D-ND  | 5.88  | 114.44      | 110.10   |
| 14  | H     | 1205 | CLA  | O2A-CGA-O1A | -5.88 | 108.75      | 123.59   |
| 14  | A     | 1109 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 14  | a     | 1102 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 14  | a     | 1111 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 14  | G     | 1109 | CLA  | CHD-C1D-ND  | -5.87 | 119.06      | 124.45   |
| 14  | A     | 1111 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 14  | H     | 1213 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 15  | A     | 1121 | F6C  | CAA-C2A-C1A | -5.87 | 111.94      | 128.11   |
| 14  | G     | 1123 | CLA  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |
| 14  | a     | 1137 | CLA  | C1C-C2C-C3C | -5.87 | 100.79      | 106.96   |
| 14  | b     | 1224 | CLA  | O2D-CGD-CBD | 5.87  | 121.69      | 111.27   |
| 14  | A     | 1126 | CLA  | O2D-CGD-CBD | 5.87  | 121.69      | 111.27   |
| 14  | V     | 1501 | CLA  | C1C-C2C-C3C | -5.86 | 100.79      | 106.96   |
| 14  | G     | 1115 | CLA  | C2C-C1C-NC  | 5.86  | 115.46      | 109.97   |
| 14  | H     | 1201 | CLA  | C2C-C1C-NC  | 5.86  | 115.46      | 109.97   |
| 14  | a     | 1109 | CLA  | C1C-C2C-C3C | -5.86 | 100.80      | 106.96   |
| 14  | A     | 1126 | CLA  | C2D-C1D-ND  | 5.86  | 114.42      | 110.10   |
| 14  | l     | 1502 | CLA  | CHD-C1D-ND  | -5.86 | 119.07      | 124.45   |
| 14  | a     | 1126 | CLA  | O2D-CGD-CBD | 5.85  | 121.67      | 111.27   |
| 15  | G     | 1121 | F6C  | CAA-C2A-C1A | -5.85 | 111.99      | 128.11   |
| 14  | L     | 1502 | CLA  | CHD-C1D-ND  | -5.85 | 119.08      | 124.45   |
| 15  | a     | 1121 | F6C  | CAA-C2A-C1A | -5.85 | 111.99      | 128.11   |
| 14  | G     | 1102 | CLA  | C2C-C1C-NC  | 5.85  | 115.45      | 109.97   |
| 14  | B     | 1213 | CLA  | C2C-C1C-NC  | 5.85  | 115.45      | 109.97   |
| 14  | M     | 1501 | CLA  | C1C-C2C-C3C | -5.85 | 100.81      | 106.96   |
| 14  | b     | 1213 | CLA  | C2C-C1C-NC  | 5.85  | 115.45      | 109.97   |
| 14  | A     | 1102 | CLA  | C2C-C1C-NC  | 5.85  | 115.45      | 109.97   |
| 14  | A     | 1109 | CLA  | C1C-C2C-C3C | -5.85 | 100.81      | 106.96   |
| 15  | H     | 1207 | F6C  | C2D-C1D-ND  | 5.84  | 115.44      | 109.97   |
| 14  | G     | 1104 | CLA  | O2D-CGD-CBD | 5.84  | 121.64      | 111.27   |
| 14  | B     | 1201 | CLA  | C2C-C1C-NC  | 5.84  | 115.44      | 109.97   |
| 14  | A     | 1136 | CLA  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 14  | H     | 1215 | CLA  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 14  | A     | 1137 | CLA  | C1C-C2C-C3C | -5.83 | 100.83      | 106.96   |
| 15  | B     | 1207 | F6C  | C2D-C1D-ND  | 5.83  | 115.44      | 109.97   |
| 14  | G     | 1137 | CLA  | C1C-C2C-C3C | -5.83 | 100.83      | 106.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | m     | 1501 | CLA  | C1C-C2C-C3C | -5.83 | 100.83      | 106.96   |
| 14  | A     | 1104 | CLA  | O2D-CGD-CBD | 5.83  | 121.62      | 111.27   |
| 15  | b     | 1207 | F6C  | C2D-C1D-ND  | 5.83  | 115.43      | 109.97   |
| 14  | H     | 1236 | CLA  | C1C-C2C-C3C | -5.82 | 100.83      | 106.96   |
| 14  | G     | 1109 | CLA  | C1C-C2C-C3C | -5.82 | 100.83      | 106.96   |
| 14  | B     | 1221 | CLA  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 14  | a     | 1104 | CLA  | O2D-CGD-CBD | 5.81  | 121.60      | 111.27   |
| 14  | B     | 1236 | CLA  | C1C-C2C-C3C | -5.81 | 100.85      | 106.96   |
| 14  | B     | 1215 | CLA  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 14  | U     | 1502 | CLA  | CHD-C1D-ND  | -5.81 | 119.12      | 124.45   |
| 14  | b     | 1236 | CLA  | C3D-C2D-C1D | -5.81 | 97.91       | 105.83   |
| 14  | B     | 1236 | CLA  | C3D-C2D-C1D | -5.81 | 97.91       | 105.83   |
| 14  | G     | 1122 | CLA  | O2D-CGD-CBD | 5.80  | 121.58      | 111.27   |
| 14  | H     | 1236 | CLA  | C3D-C2D-C1D | -5.80 | 97.91       | 105.83   |
| 14  | A     | 1122 | CLA  | O2D-CGD-CBD | 5.80  | 121.58      | 111.27   |
| 14  | b     | 1201 | CLA  | C2C-C1C-NC  | 5.80  | 115.41      | 109.97   |
| 14  | b     | 1236 | CLA  | C1C-C2C-C3C | -5.80 | 100.86      | 106.96   |
| 14  | a     | 1122 | CLA  | O2D-CGD-CBD | 5.80  | 121.57      | 111.27   |
| 14  | G     | 1136 | CLA  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |
| 13  | a     | 1011 | CL0  | O2D-CGD-CBD | 5.79  | 121.56      | 111.27   |
| 14  | H     | 1231 | CLA  | CHD-C1D-ND  | -5.79 | 119.14      | 124.45   |
| 14  | B     | 1210 | CLA  | C2C-C1C-NC  | 5.79  | 115.39      | 109.97   |
| 14  | B     | 1231 | CLA  | CHD-C1D-ND  | -5.78 | 119.14      | 124.45   |
| 14  | b     | 1210 | CLA  | C2C-C1C-NC  | 5.78  | 115.39      | 109.97   |
| 14  | B     | 1239 | CLA  | C1C-C2C-C3C | -5.78 | 100.88      | 106.96   |
| 14  | H     | 1239 | CLA  | C1C-C2C-C3C | -5.78 | 100.88      | 106.96   |
| 13  | A     | 1011 | CL0  | O2D-CGD-CBD | 5.78  | 121.54      | 111.27   |
| 14  | b     | 1216 | CLA  | O2A-C1-C2   | 5.78  | 123.82      | 108.64   |
| 14  | b     | 1215 | CLA  | C4A-NA-C1A  | 5.78  | 109.30      | 106.71   |
| 14  | H     | 1227 | CLA  | CHD-C1D-ND  | -5.77 | 119.15      | 124.45   |
| 13  | G     | 1011 | CL0  | O2D-CGD-CBD | 5.77  | 121.53      | 111.27   |
| 14  | b     | 1231 | CLA  | CHD-C1D-ND  | -5.77 | 119.15      | 124.45   |
| 14  | H     | 1210 | CLA  | C2C-C1C-NC  | 5.77  | 115.38      | 109.97   |
| 14  | B     | 1216 | CLA  | O2A-C1-C2   | 5.77  | 123.80      | 108.64   |
| 14  | H     | 1216 | CLA  | O2A-C1-C2   | 5.77  | 123.80      | 108.64   |
| 14  | a     | 1136 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 14  | b     | 1224 | CLA  | O2A-CGA-O1A | -5.77 | 109.03      | 123.59   |
| 14  | b     | 1221 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 14  | b     | 1239 | CLA  | C1C-C2C-C3C | -5.77 | 100.89      | 106.96   |
| 14  | H     | 1221 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 14  | A     | 1103 | CLA  | CHD-C1D-ND  | -5.77 | 119.16      | 124.45   |
| 14  | l     | 1502 | CLA  | C2C-C1C-NC  | 5.76  | 115.37      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1221 | CLA  | O2D-CGD-CBD | 5.76  | 121.50      | 111.27   |
| 14  | B     | 1227 | CLA  | CHD-C1D-ND  | -5.76 | 119.16      | 124.45   |
| 14  | B     | 1221 | CLA  | O2D-CGD-CBD | 5.76  | 121.50      | 111.27   |
| 14  | U     | 1501 | CLA  | C1C-C2C-C3C | -5.76 | 100.91      | 106.96   |
| 14  | b     | 1203 | CLA  | C3D-C2D-C1D | -5.75 | 97.98       | 105.83   |
| 14  | b     | 1227 | CLA  | CHD-C1D-ND  | -5.75 | 119.17      | 124.45   |
| 14  | G     | 1120 | CLA  | C1C-C2C-C3C | -5.75 | 100.91      | 106.96   |
| 14  | G     | 1103 | CLA  | CHD-C1D-ND  | -5.75 | 119.17      | 124.45   |
| 14  | B     | 1214 | CLA  | C2D-C1D-ND  | 5.75  | 114.34      | 110.10   |
| 14  | a     | 1127 | CLA  | C1C-C2C-C3C | -5.75 | 100.91      | 106.96   |
| 14  | B     | 1224 | CLA  | O2A-CGA-O1A | -5.75 | 109.09      | 123.59   |
| 14  | U     | 1502 | CLA  | C2C-C1C-NC  | 5.75  | 115.36      | 109.97   |
| 14  | H     | 1203 | CLA  | C3D-C2D-C1D | -5.75 | 97.99       | 105.83   |
| 14  | L     | 1502 | CLA  | C2C-C1C-NC  | 5.74  | 115.35      | 109.97   |
| 14  | b     | 1226 | CLA  | O2A-CGA-O1A | -5.74 | 109.10      | 123.59   |
| 14  | B     | 1203 | CLA  | C3D-C2D-C1D | -5.74 | 98.00       | 105.83   |
| 14  | B     | 1203 | CLA  | O2A-C1-C2   | 5.74  | 123.72      | 108.64   |
| 14  | H     | 1203 | CLA  | O2A-C1-C2   | 5.74  | 123.71      | 108.64   |
| 14  | b     | 1221 | CLA  | O2D-CGD-CBD | 5.74  | 121.46      | 111.27   |
| 14  | L     | 1501 | CLA  | C1C-C2C-C3C | -5.74 | 100.93      | 106.96   |
| 14  | G     | 1012 | CLA  | CHD-C1D-ND  | -5.73 | 119.18      | 124.45   |
| 14  | H     | 1224 | CLA  | O2A-CGA-O1A | -5.73 | 109.12      | 123.59   |
| 14  | H     | 1214 | CLA  | C2D-C1D-ND  | 5.73  | 114.33      | 110.10   |
| 14  | b     | 1022 | CLA  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 14  | B     | 1226 | CLA  | O2A-CGA-O1A | -5.73 | 109.13      | 123.59   |
| 14  | b     | 1203 | CLA  | O2A-C1-C2   | 5.73  | 123.69      | 108.64   |
| 14  | l     | 1501 | CLA  | C1C-C2C-C3C | -5.73 | 100.93      | 106.96   |
| 14  | b     | 1022 | CLA  | C2C-C1C-NC  | 5.73  | 115.34      | 109.97   |
| 14  | H     | 1226 | CLA  | O2A-CGA-O1A | -5.73 | 109.14      | 123.59   |
| 14  | H     | 1231 | CLA  | C2C-C1C-NC  | 5.72  | 115.33      | 109.97   |
| 14  | a     | 1131 | CLA  | C1C-C2C-C3C | -5.72 | 100.94      | 106.96   |
| 14  | A     | 1012 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 14  | a     | 1103 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 14  | b     | 1214 | CLA  | C2D-C1D-ND  | 5.72  | 114.32      | 110.10   |
| 14  | G     | 1012 | CLA  | C1C-C2C-C3C | -5.72 | 100.95      | 106.96   |
| 14  | G     | 1131 | CLA  | C1C-C2C-C3C | -5.72 | 100.95      | 106.96   |
| 14  | B     | 1022 | CLA  | C2C-C1C-NC  | 5.72  | 115.33      | 109.97   |
| 14  | A     | 1120 | CLA  | C1C-C2C-C3C | -5.71 | 100.95      | 106.96   |
| 14  | A     | 1127 | CLA  | C1C-C2C-C3C | -5.71 | 100.96      | 106.96   |
| 14  | A     | 1131 | CLA  | C1C-C2C-C3C | -5.71 | 100.96      | 106.96   |
| 14  | a     | 1012 | CLA  | CHD-C1D-ND  | -5.71 | 119.21      | 124.45   |
| 14  | b     | 1231 | CLA  | C2C-C1C-NC  | 5.70  | 115.32      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1110 | CLA  | O2D-CGD-CBD | 5.70  | 121.40      | 111.27   |
| 14  | A     | 1110 | CLA  | O2D-CGD-CBD | 5.70  | 121.40      | 111.27   |
| 14  | b     | 1215 | CLA  | CHD-C1D-ND  | -5.70 | 119.22      | 124.45   |
| 14  | G     | 1135 | CLA  | C2D-C1D-ND  | 5.70  | 114.30      | 110.10   |
| 15  | b     | 1230 | F6C  | CAA-C2A-C1A | -5.69 | 112.43      | 128.11   |
| 14  | B     | 1205 | CLA  | CMD-C2D-C1D | 5.69  | 134.75      | 124.71   |
| 14  | A     | 1135 | CLA  | C2D-C1D-ND  | 5.69  | 114.30      | 110.10   |
| 14  | b     | 1221 | CLA  | C1C-C2C-C3C | -5.69 | 100.97      | 106.96   |
| 14  | a     | 1110 | CLA  | O2D-CGD-CBD | 5.69  | 121.38      | 111.27   |
| 14  | A     | 1012 | CLA  | C1C-C2C-C3C | -5.69 | 100.97      | 106.96   |
| 14  | b     | 1205 | CLA  | CMD-C2D-C1D | 5.69  | 134.74      | 124.71   |
| 15  | H     | 1238 | F6C  | O2A-C1-C2   | 5.69  | 123.59      | 108.64   |
| 14  | H     | 1221 | CLA  | C1C-C2C-C3C | -5.69 | 100.98      | 106.96   |
| 14  | b     | 1218 | CLA  | C4A-NA-C1A  | 5.69  | 109.26      | 106.71   |
| 14  | A     | 1112 | CLA  | O2D-CGD-CBD | 5.69  | 121.37      | 111.27   |
| 14  | G     | 1112 | CLA  | C4A-NA-C1A  | 5.69  | 109.26      | 106.71   |
| 14  | B     | 1022 | CLA  | C4A-NA-C1A  | 5.68  | 109.26      | 106.71   |
| 15  | H     | 1230 | F6C  | CAA-C2A-C1A | -5.68 | 112.47      | 128.11   |
| 14  | G     | 1127 | CLA  | C1C-C2C-C3C | -5.68 | 100.99      | 106.96   |
| 15  | B     | 1230 | F6C  | CAA-C2A-C1A | -5.68 | 112.47      | 128.11   |
| 14  | B     | 1215 | CLA  | CHD-C1D-ND  | -5.68 | 119.24      | 124.45   |
| 14  | B     | 1221 | CLA  | C1C-C2C-C3C | -5.68 | 100.99      | 106.96   |
| 14  | a     | 1120 | CLA  | C1C-C2C-C3C | -5.68 | 100.99      | 106.96   |
| 14  | G     | 1112 | CLA  | O2D-CGD-CBD | 5.68  | 121.35      | 111.27   |
| 14  | A     | 1104 | CLA  | CHD-C1D-ND  | -5.68 | 119.24      | 124.45   |
| 14  | a     | 1112 | CLA  | O2D-CGD-CBD | 5.67  | 121.35      | 111.27   |
| 14  | G     | 1104 | CLA  | CHD-C1D-ND  | -5.67 | 119.24      | 124.45   |
| 14  | a     | 1012 | CLA  | C1C-C2C-C3C | -5.67 | 100.99      | 106.96   |
| 14  | B     | 1231 | CLA  | C2C-C1C-NC  | 5.67  | 115.28      | 109.97   |
| 15  | B     | 1238 | F6C  | O2A-C1-C2   | 5.67  | 123.54      | 108.64   |
| 14  | H     | 1205 | CLA  | CMD-C2D-C1D | 5.67  | 134.70      | 124.71   |
| 14  | K     | 1401 | CLA  | C3D-C2D-C1D | -5.67 | 98.10       | 105.83   |
| 14  | a     | 1104 | CLA  | C3D-C2D-C1D | -5.66 | 98.10       | 105.83   |
| 14  | a     | 1117 | CLA  | C2D-C1D-ND  | 5.66  | 114.28      | 110.10   |
| 14  | a     | 1135 | CLA  | C2D-C1D-ND  | 5.66  | 114.28      | 110.10   |
| 14  | a     | 1104 | CLA  | CHD-C1D-ND  | -5.66 | 119.25      | 124.45   |
| 15  | b     | 1238 | F6C  | O2A-C1-C2   | 5.66  | 123.51      | 108.64   |
| 18  | B     | 4005 | BCR  | C24-C23-C22 | -5.66 | 117.68      | 126.23   |
| 14  | T     | 1401 | CLA  | C3D-C2D-C1D | -5.66 | 98.11       | 105.83   |
| 14  | H     | 1226 | CLA  | CHD-C1D-ND  | -5.66 | 119.25      | 124.45   |
| 14  | A     | 1108 | CLA  | O2D-CGD-CBD | 5.66  | 121.32      | 111.27   |
| 14  | A     | 1112 | CLA  | C4A-NA-C1A  | 5.66  | 109.25      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1022 | CLA  | C2C-C1C-NC  | 5.66  | 115.27      | 109.97   |
| 14  | H     | 1240 | CLA  | C1C-C2C-C3C | -5.66 | 101.01      | 106.96   |
| 14  | a     | 1108 | CLA  | O2D-CGD-CBD | 5.65  | 121.31      | 111.27   |
| 14  | b     | 1220 | CLA  | C1C-C2C-C3C | -5.65 | 101.01      | 106.96   |
| 14  | B     | 1235 | CLA  | C4A-NA-C1A  | 5.65  | 109.25      | 106.71   |
| 14  | G     | 1117 | CLA  | C2D-C1D-ND  | 5.65  | 114.27      | 110.10   |
| 14  | k     | 1401 | CLA  | C3D-C2D-C1D | -5.65 | 98.12       | 105.83   |
| 14  | A     | 1117 | CLA  | C2D-C1D-ND  | 5.65  | 114.27      | 110.10   |
| 14  | H     | 1218 | CLA  | C4A-NA-C1A  | 5.65  | 109.25      | 106.71   |
| 14  | A     | 1103 | CLA  | C2D-C1D-ND  | 5.65  | 114.27      | 110.10   |
| 14  | G     | 1108 | CLA  | O2D-CGD-CBD | 5.64  | 121.30      | 111.27   |
| 14  | a     | 1120 | CLA  | C3D-C2D-C1D | -5.64 | 98.13       | 105.83   |
| 14  | a     | 1112 | CLA  | C4A-NA-C1A  | 5.64  | 109.24      | 106.71   |
| 18  | H     | 4005 | BCR  | C24-C23-C22 | -5.64 | 117.71      | 126.23   |
| 14  | G     | 1120 | CLA  | C3D-C2D-C1D | -5.64 | 98.13       | 105.83   |
| 14  | H     | 1226 | CLA  | O2D-CGD-CBD | 5.64  | 121.29      | 111.27   |
| 14  | b     | 1240 | CLA  | O2A-CGA-O1A | -5.64 | 109.36      | 123.59   |
| 14  | B     | 1202 | CLA  | C2C-C1C-NC  | 5.64  | 115.25      | 109.97   |
| 14  | a     | 1125 | CLA  | O2D-CGD-CBD | 5.64  | 121.28      | 111.27   |
| 14  | H     | 1236 | CLA  | C4A-NA-C1A  | 5.64  | 109.24      | 106.71   |
| 14  | B     | 1220 | CLA  | C1C-C2C-C3C | -5.64 | 101.03      | 106.96   |
| 14  | B     | 1218 | CLA  | C4A-NA-C1A  | 5.63  | 109.24      | 106.71   |
| 14  | b     | 1236 | CLA  | C4A-NA-C1A  | 5.63  | 109.24      | 106.71   |
| 14  | a     | 1103 | CLA  | C2D-C1D-ND  | 5.63  | 114.26      | 110.10   |
| 14  | H     | 1240 | CLA  | O2A-CGA-O1A | -5.63 | 109.37      | 123.59   |
| 14  | B     | 1240 | CLA  | O2A-CGA-O1A | -5.63 | 109.38      | 123.59   |
| 14  | G     | 1104 | CLA  | C3D-C2D-C1D | -5.63 | 98.14       | 105.83   |
| 14  | A     | 1120 | CLA  | C3D-C2D-C1D | -5.63 | 98.15       | 105.83   |
| 14  | H     | 1215 | CLA  | CHD-C1D-ND  | -5.63 | 119.28      | 124.45   |
| 14  | G     | 1125 | CLA  | O2D-CGD-CBD | 5.63  | 121.27      | 111.27   |
| 14  | B     | 1226 | CLA  | O2D-CGD-CBD | 5.63  | 121.27      | 111.27   |
| 14  | A     | 1103 | CLA  | C1C-C2C-C3C | -5.63 | 101.04      | 106.96   |
| 14  | G     | 1103 | CLA  | C2D-C1D-ND  | 5.62  | 114.25      | 110.10   |
| 14  | a     | 1132 | CLA  | CHD-C1D-ND  | -5.62 | 119.29      | 124.45   |
| 14  | H     | 1223 | CLA  | C3D-C2D-C1D | -5.62 | 98.16       | 105.83   |
| 14  | B     | 1236 | CLA  | C4A-NA-C1A  | 5.62  | 109.23      | 106.71   |
| 18  | b     | 4005 | BCR  | C24-C23-C22 | -5.62 | 117.74      | 126.23   |
| 14  | H     | 1214 | CLA  | O2D-CGD-CBD | 5.62  | 121.25      | 111.27   |
| 14  | b     | 1240 | CLA  | C1C-C2C-C3C | -5.62 | 101.05      | 106.96   |
| 14  | b     | 1226 | CLA  | O2D-CGD-CBD | 5.62  | 121.25      | 111.27   |
| 14  | b     | 1223 | CLA  | C3D-C2D-C1D | -5.62 | 98.17       | 105.83   |
| 14  | H     | 1202 | CLA  | C2C-C1C-NC  | 5.61  | 115.23      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1104 | CLA  | C3D-C2D-C1D | -5.61 | 98.17       | 105.83   |
| 14  | G     | 1103 | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 13  | A     | 1011 | CL0  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | A     | 1125 | CLA  | O2D-CGD-CBD | 5.61  | 121.24      | 111.27   |
| 14  | B     | 1240 | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | G     | 1102 | CLA  | O2D-CGD-CBD | 5.61  | 121.24      | 111.27   |
| 14  | B     | 1214 | CLA  | O2D-CGD-CBD | 5.61  | 121.23      | 111.27   |
| 18  | m     | 4021 | BCR  | C15-C14-C13 | -5.61 | 119.31      | 127.31   |
| 14  | H     | 1022 | CLA  | C4A-NA-C1A  | 5.61  | 109.23      | 106.71   |
| 13  | a     | 1011 | CL0  | C1C-C2C-C3C | -5.60 | 101.06      | 106.96   |
| 14  | B     | 1208 | CLA  | O2A-CGA-O1A | -5.60 | 109.45      | 123.59   |
| 18  | V     | 4021 | BCR  | C15-C14-C13 | -5.60 | 119.31      | 127.31   |
| 14  | H     | 1220 | CLA  | C1C-C2C-C3C | -5.60 | 101.06      | 106.96   |
| 14  | a     | 1103 | CLA  | C1C-C2C-C3C | -5.60 | 101.06      | 106.96   |
| 14  | b     | 1023 | CLA  | CHD-C1D-ND  | -5.60 | 119.31      | 124.45   |
| 14  | b     | 1208 | CLA  | O2A-CGA-O1A | -5.60 | 109.45      | 123.59   |
| 14  | A     | 1102 | CLA  | O2D-CGD-CBD | 5.60  | 121.22      | 111.27   |
| 14  | H     | 1208 | CLA  | O2A-CGA-O1A | -5.60 | 109.46      | 123.59   |
| 13  | G     | 1011 | CL0  | CMD-C2D-C1D | 5.60  | 134.58      | 124.71   |
| 14  | B     | 1223 | CLA  | C3D-C2D-C1D | -5.60 | 98.19       | 105.83   |
| 14  | b     | 1202 | CLA  | C2C-C1C-NC  | 5.60  | 115.22      | 109.97   |
| 14  | a     | 1102 | CLA  | O2A-C1-C2   | 5.60  | 123.34      | 108.64   |
| 18  | A     | 4001 | BCR  | C7-C8-C9    | -5.59 | 117.78      | 126.23   |
| 14  | b     | 1214 | CLA  | O2D-CGD-CBD | 5.59  | 121.20      | 111.27   |
| 18  | G     | 4001 | BCR  | C7-C8-C9    | -5.59 | 117.79      | 126.23   |
| 13  | A     | 1011 | CL0  | CMD-C2D-C1D | 5.59  | 134.57      | 124.71   |
| 13  | a     | 1011 | CL0  | CMD-C2D-C1D | 5.59  | 134.56      | 124.71   |
| 18  | U     | 4022 | BCR  | C7-C8-C9    | -5.59 | 117.79      | 126.23   |
| 14  | B     | 1226 | CLA  | CHD-C1D-ND  | -5.59 | 119.32      | 124.45   |
| 13  | G     | 1011 | CL0  | C1C-C2C-C3C | -5.59 | 101.08      | 106.96   |
| 14  | b     | 1236 | CLA  | C1D-ND-C4D  | -5.59 | 102.36      | 106.33   |
| 18  | M     | 4021 | BCR  | C15-C14-C13 | -5.59 | 119.33      | 127.31   |
| 14  | a     | 1102 | CLA  | CHD-C1D-ND  | -5.59 | 119.32      | 124.45   |
| 14  | H     | 1203 | CLA  | C4A-NA-C1A  | 5.59  | 109.22      | 106.71   |
| 18  | L     | 4022 | BCR  | C7-C8-C9    | -5.58 | 117.80      | 126.23   |
| 18  | b     | 4009 | BCR  | C24-C23-C22 | -5.58 | 117.80      | 126.23   |
| 14  | H     | 1236 | CLA  | C1D-ND-C4D  | -5.58 | 102.37      | 106.33   |
| 18  | a     | 4001 | BCR  | C7-C8-C9    | -5.58 | 117.80      | 126.23   |
| 14  | a     | 1104 | CLA  | C1D-ND-C4D  | -5.58 | 102.37      | 106.33   |
| 14  | a     | 1102 | CLA  | O2D-CGD-CBD | 5.58  | 121.19      | 111.27   |
| 14  | b     | 1235 | CLA  | C4A-NA-C1A  | 5.58  | 109.22      | 106.71   |
| 14  | B     | 1023 | CLA  | CHD-C1D-ND  | -5.58 | 119.33      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1129 | CLA  | CHD-C1D-ND  | -5.58 | 119.33      | 124.45   |
| 14  | H     | 1023 | CLA  | CHD-C1D-ND  | -5.58 | 119.33      | 124.45   |
| 18  | l     | 4022 | BCR  | C7-C8-C9    | -5.58 | 117.81      | 126.23   |
| 14  | a     | 1109 | CLA  | O2D-CGD-CBD | 5.58  | 121.18      | 111.27   |
| 14  | G     | 1102 | CLA  | CHD-C1D-ND  | -5.57 | 119.33      | 124.45   |
| 14  | A     | 1102 | CLA  | O2A-C1-C2   | 5.57  | 123.27      | 108.64   |
| 14  | A     | 1111 | CLA  | O2D-CGD-CBD | 5.57  | 121.16      | 111.27   |
| 14  | a     | 1132 | CLA  | C1C-C2C-C3C | -5.57 | 101.10      | 106.96   |
| 14  | a     | 1111 | CLA  | O2D-CGD-CBD | 5.57  | 121.16      | 111.27   |
| 14  | A     | 1102 | CLA  | CHD-C1D-ND  | -5.57 | 119.34      | 124.45   |
| 14  | b     | 1023 | CLA  | C3D-C2D-C1D | -5.57 | 98.23       | 105.83   |
| 14  | G     | 1102 | CLA  | O2A-C1-C2   | 5.57  | 123.26      | 108.64   |
| 14  | a     | 1129 | CLA  | CHD-C1D-ND  | -5.56 | 119.34      | 124.45   |
| 14  | b     | 1226 | CLA  | CHD-C1D-ND  | -5.56 | 119.34      | 124.45   |
| 14  | A     | 1104 | CLA  | C1D-ND-C4D  | -5.56 | 102.38      | 106.33   |
| 14  | A     | 1132 | CLA  | CHD-C1D-ND  | -5.56 | 119.34      | 124.45   |
| 14  | G     | 1111 | CLA  | O2D-CGD-CBD | 5.56  | 121.15      | 111.27   |
| 18  | B     | 4009 | BCR  | C24-C23-C22 | -5.56 | 117.83      | 126.23   |
| 14  | H     | 1023 | CLA  | C3D-C2D-C1D | -5.56 | 98.24       | 105.83   |
| 18  | H     | 4010 | BCR  | C20-C19-C18 | 5.56  | 142.03      | 126.42   |
| 14  | b     | 1218 | CLA  | O2D-CGD-CBD | 5.56  | 121.14      | 111.27   |
| 14  | b     | 1214 | CLA  | C1C-C2C-C3C | -5.56 | 101.11      | 106.96   |
| 14  | B     | 1240 | CLA  | CHD-C1D-ND  | -5.56 | 119.35      | 124.45   |
| 14  | A     | 1109 | CLA  | O2D-CGD-CBD | 5.56  | 121.14      | 111.27   |
| 18  | b     | 4010 | BCR  | C20-C19-C18 | 5.56  | 142.02      | 126.42   |
| 18  | B     | 4010 | BCR  | C20-C19-C18 | 5.56  | 142.02      | 126.42   |
| 14  | B     | 1023 | CLA  | C3D-C2D-C1D | -5.56 | 98.25       | 105.83   |
| 14  | G     | 1132 | CLA  | C1C-C2C-C3C | -5.55 | 101.12      | 106.96   |
| 14  | H     | 1215 | CLA  | C1C-C2C-C3C | -5.55 | 101.12      | 106.96   |
| 14  | G     | 1109 | CLA  | O2D-CGD-CBD | 5.55  | 121.14      | 111.27   |
| 14  | b     | 1240 | CLA  | CHD-C1D-ND  | -5.55 | 119.35      | 124.45   |
| 15  | H     | 1237 | F6C  | CMA-C3A-C2A | -5.55 | 111.04      | 126.12   |
| 14  | H     | 1233 | CLA  | C1C-C2C-C3C | -5.55 | 101.12      | 106.96   |
| 14  | G     | 1104 | CLA  | C1D-ND-C4D  | -5.55 | 102.39      | 106.33   |
| 14  | A     | 1013 | CLA  | CMD-C2D-C1D | 5.55  | 134.49      | 124.71   |
| 14  | a     | 1111 | CLA  | C3D-C2D-C1D | -5.55 | 98.26       | 105.83   |
| 14  | A     | 1132 | CLA  | C1C-C2C-C3C | -5.55 | 101.12      | 106.96   |
| 14  | b     | 1233 | CLA  | C1C-C2C-C3C | -5.55 | 101.12      | 106.96   |
| 14  | a     | 1118 | CLA  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 14  | B     | 1218 | CLA  | O2D-CGD-CBD | 5.55  | 121.12      | 111.27   |
| 14  | B     | 1203 | CLA  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 14  | B     | 1236 | CLA  | C1D-ND-C4D  | -5.54 | 102.40      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | b     | 1237 | F6C  | CMA-C3A-C2A | -5.54 | 111.07      | 126.12   |
| 14  | B     | 1211 | CLA  | C2C-C1C-NC  | 5.54  | 115.17      | 109.97   |
| 14  | b     | 1226 | CLA  | C2D-C1D-ND  | 5.54  | 114.19      | 110.10   |
| 14  | H     | 1218 | CLA  | O2D-CGD-CBD | 5.54  | 121.12      | 111.27   |
| 14  | G     | 1111 | CLA  | C3D-C2D-C1D | -5.54 | 98.27       | 105.83   |
| 14  | G     | 1013 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.71   |
| 15  | B     | 1237 | F6C  | CMA-C3A-C2A | -5.54 | 111.07      | 126.12   |
| 14  | B     | 1215 | CLA  | C1C-C2C-C3C | -5.54 | 101.13      | 106.96   |
| 14  | b     | 1201 | CLA  | O2A-CGA-O1A | -5.54 | 109.61      | 123.59   |
| 14  | a     | 1013 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.71   |
| 14  | H     | 1226 | CLA  | C2D-C1D-ND  | 5.54  | 114.19      | 110.10   |
| 14  | B     | 1233 | CLA  | C1C-C2C-C3C | -5.54 | 101.14      | 106.96   |
| 14  | l     | 1503 | CLA  | O2A-C1-C2   | 5.54  | 123.18      | 108.64   |
| 14  | A     | 1111 | CLA  | C3D-C2D-C1D | -5.53 | 98.28       | 105.83   |
| 14  | A     | 1136 | CLA  | O2A-CGA-O1A | -5.53 | 109.63      | 123.59   |
| 14  | B     | 1214 | CLA  | C1C-C2C-C3C | -5.53 | 101.14      | 106.96   |
| 14  | a     | 1136 | CLA  | O2A-CGA-O1A | -5.53 | 109.64      | 123.59   |
| 14  | b     | 1201 | CLA  | CHD-C1D-ND  | -5.53 | 119.37      | 124.45   |
| 14  | b     | 1203 | CLA  | C4A-NA-C1A  | 5.53  | 109.19      | 106.71   |
| 14  | b     | 1215 | CLA  | C1C-C2C-C3C | -5.53 | 101.15      | 106.96   |
| 14  | A     | 1129 | CLA  | CHD-C1D-ND  | -5.53 | 119.38      | 124.45   |
| 14  | A     | 1118 | CLA  | C4A-NA-C1A  | 5.52  | 109.19      | 106.71   |
| 14  | L     | 1503 | CLA  | O2A-C1-C2   | 5.52  | 123.15      | 108.64   |
| 14  | G     | 1136 | CLA  | O2A-CGA-O1A | -5.52 | 109.66      | 123.59   |
| 18  | H     | 4009 | BCR  | C24-C23-C22 | -5.52 | 117.89      | 126.23   |
| 14  | a     | 1117 | CLA  | C1C-C2C-C3C | -5.52 | 101.15      | 106.96   |
| 14  | B     | 1201 | CLA  | O2A-CGA-O1A | -5.52 | 109.67      | 123.59   |
| 14  | G     | 1132 | CLA  | CHD-C1D-ND  | -5.51 | 119.39      | 124.45   |
| 14  | U     | 1503 | CLA  | O2A-C1-C2   | 5.51  | 123.13      | 108.64   |
| 14  | G     | 1135 | CLA  | C1C-C2C-C3C | -5.51 | 101.16      | 106.96   |
| 14  | H     | 1240 | CLA  | CHD-C1D-ND  | -5.51 | 119.39      | 124.45   |
| 14  | A     | 1013 | CLA  | C3D-C2D-C1D | -5.51 | 98.31       | 105.83   |
| 14  | B     | 1226 | CLA  | C2D-C1D-ND  | 5.51  | 114.16      | 110.10   |
| 14  | G     | 1131 | CLA  | C4A-NA-C1A  | 5.51  | 109.18      | 106.71   |
| 14  | H     | 1226 | CLA  | C1C-C2C-C3C | -5.51 | 101.17      | 106.96   |
| 14  | H     | 1201 | CLA  | O2A-CGA-O1A | -5.51 | 109.70      | 123.59   |
| 14  | G     | 1118 | CLA  | C4A-NA-C1A  | 5.51  | 109.18      | 106.71   |
| 14  | b     | 1211 | CLA  | C2C-C1C-NC  | 5.50  | 115.13      | 109.97   |
| 14  | H     | 1211 | CLA  | C2C-C1C-NC  | 5.50  | 115.13      | 109.97   |
| 14  | G     | 1136 | CLA  | C1C-C2C-C3C | -5.50 | 101.17      | 106.96   |
| 14  | A     | 1117 | CLA  | C1C-C2C-C3C | -5.50 | 101.17      | 106.96   |
| 15  | b     | 1237 | F6C  | CMA-C3A-C4A | -5.50 | 115.02      | 124.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1128 | CLA  | C4A-NA-C1A  | 5.50  | 109.18      | 106.71   |
| 14  | a     | 1013 | CLA  | C3D-C2D-C1D | -5.50 | 98.33       | 105.83   |
| 14  | G     | 1108 | CLA  | CHD-C1D-ND  | -5.50 | 119.40      | 124.45   |
| 14  | B     | 1204 | CLA  | C1C-C2C-C3C | -5.50 | 101.18      | 106.96   |
| 14  | A     | 1136 | CLA  | CHD-C1D-ND  | -5.49 | 119.41      | 124.45   |
| 14  | G     | 1115 | CLA  | O2A-CGA-O1A | -5.49 | 109.73      | 123.59   |
| 14  | H     | 1214 | CLA  | C1C-C2C-C3C | -5.49 | 101.18      | 106.96   |
| 14  | G     | 1136 | CLA  | CHD-C1D-ND  | -5.49 | 119.41      | 124.45   |
| 14  | G     | 1117 | CLA  | C1C-C2C-C3C | -5.49 | 101.18      | 106.96   |
| 14  | A     | 1013 | CLA  | C1D-ND-C4D  | -5.49 | 102.44      | 106.33   |
| 14  | H     | 1235 | CLA  | C4A-NA-C1A  | 5.49  | 109.17      | 106.71   |
| 14  | l     | 1502 | CLA  | C4A-NA-C1A  | 5.49  | 109.17      | 106.71   |
| 14  | G     | 1013 | CLA  | C3D-C2D-C1D | -5.49 | 98.34       | 105.83   |
| 14  | a     | 1128 | CLA  | C4A-NA-C1A  | 5.49  | 109.17      | 106.71   |
| 18  | a     | 4005 | BCR  | C28-C27-C26 | -5.49 | 104.28      | 114.08   |
| 14  | a     | 1115 | CLA  | O2A-CGA-O1A | -5.48 | 109.75      | 123.59   |
| 14  | A     | 1128 | CLA  | C4A-NA-C1A  | 5.48  | 109.17      | 106.71   |
| 14  | G     | 1013 | CLA  | C1D-ND-C4D  | -5.48 | 102.44      | 106.33   |
| 14  | U     | 1501 | CLA  | O2A-CGA-O1A | -5.48 | 109.76      | 123.59   |
| 18  | A     | 4005 | BCR  | C28-C27-C26 | -5.48 | 104.29      | 114.08   |
| 18  | G     | 4005 | BCR  | C28-C27-C26 | -5.48 | 104.29      | 114.08   |
| 14  | A     | 1013 | CLA  | O2A-C1-C2   | 5.48  | 123.04      | 108.64   |
| 14  | b     | 1204 | CLA  | C1C-C2C-C3C | -5.48 | 101.20      | 106.96   |
| 14  | A     | 1115 | CLA  | O2A-CGA-O1A | -5.48 | 109.77      | 123.59   |
| 14  | L     | 1501 | CLA  | O2A-CGA-O1A | -5.48 | 109.77      | 123.59   |
| 14  | G     | 1013 | CLA  | O2A-C1-C2   | 5.48  | 123.03      | 108.64   |
| 14  | H     | 1218 | CLA  | C3D-C2D-C1D | -5.48 | 98.36       | 105.83   |
| 14  | l     | 1501 | CLA  | O2A-CGA-O1A | -5.48 | 109.77      | 123.59   |
| 14  | A     | 1113 | CLA  | C1D-ND-C4D  | -5.48 | 102.44      | 106.33   |
| 14  | A     | 1135 | CLA  | C1C-C2C-C3C | -5.48 | 101.20      | 106.96   |
| 14  | H     | 1204 | CLA  | C1C-C2C-C3C | -5.47 | 101.20      | 106.96   |
| 14  | H     | 1225 | CLA  | C1C-C2C-C3C | -5.47 | 101.20      | 106.96   |
| 14  | B     | 1201 | CLA  | CHD-C1D-ND  | -5.47 | 119.42      | 124.45   |
| 15  | B     | 1237 | F6C  | CMA-C3A-C4A | -5.47 | 115.06      | 124.71   |
| 14  | b     | 1218 | CLA  | C3D-C2D-C1D | -5.47 | 98.36       | 105.83   |
| 14  | B     | 1226 | CLA  | C1C-C2C-C3C | -5.47 | 101.20      | 106.96   |
| 14  | a     | 1013 | CLA  | O2A-C1-C2   | 5.47  | 123.02      | 108.64   |
| 14  | A     | 1108 | CLA  | CHD-C1D-ND  | -5.47 | 119.43      | 124.45   |
| 14  | A     | 1136 | CLA  | C1C-C2C-C3C | -5.47 | 101.21      | 106.96   |
| 14  | a     | 1108 | CLA  | CHD-C1D-ND  | -5.47 | 119.43      | 124.45   |
| 14  | G     | 1113 | CLA  | C1D-ND-C4D  | -5.47 | 102.45      | 106.33   |
| 14  | B     | 1218 | CLA  | C3D-C2D-C1D | -5.46 | 98.38       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1105 | CLA  | CHD-C1D-ND  | -5.46 | 119.44      | 124.45   |
| 14  | G     | 1132 | CLA  | C3D-C2D-C1D | -5.46 | 98.38       | 105.83   |
| 14  | b     | 1226 | CLA  | C1C-C2C-C3C | -5.46 | 101.22      | 106.96   |
| 14  | A     | 1131 | CLA  | C4A-NA-C1A  | 5.45  | 109.16      | 106.71   |
| 14  | a     | 1136 | CLA  | CHD-C1D-ND  | -5.45 | 119.44      | 124.45   |
| 14  | a     | 1135 | CLA  | C1C-C2C-C3C | -5.45 | 101.23      | 106.96   |
| 14  | a     | 1113 | CLA  | C1D-ND-C4D  | -5.44 | 102.47      | 106.33   |
| 14  | b     | 1213 | CLA  | O2D-CGD-CBD | 5.44  | 120.94      | 111.27   |
| 14  | G     | 1107 | CLA  | C1C-C2C-C3C | -5.44 | 101.23      | 106.96   |
| 14  | a     | 1107 | CLA  | C1C-C2C-C3C | -5.44 | 101.23      | 106.96   |
| 14  | A     | 1132 | CLA  | C3D-C2D-C1D | -5.44 | 98.40       | 105.83   |
| 14  | H     | 1220 | CLA  | C4A-NA-C1A  | 5.44  | 109.15      | 106.71   |
| 15  | H     | 1237 | F6C  | CMA-C3A-C4A | -5.44 | 115.13      | 124.71   |
| 14  | G     | 1105 | CLA  | C1C-C2C-C3C | -5.44 | 101.24      | 106.96   |
| 14  | A     | 1141 | CLA  | C3D-C2D-C1D | -5.44 | 98.41       | 105.83   |
| 14  | a     | 1132 | CLA  | C3D-C2D-C1D | -5.44 | 98.41       | 105.83   |
| 14  | B     | 1225 | CLA  | C1C-C2C-C3C | -5.44 | 101.24      | 106.96   |
| 14  | G     | 1134 | CLA  | C1C-C2C-C3C | -5.44 | 101.24      | 106.96   |
| 14  | b     | 1225 | CLA  | C1C-C2C-C3C | -5.44 | 101.24      | 106.96   |
| 14  | H     | 1201 | CLA  | CHD-C1D-ND  | -5.44 | 119.46      | 124.45   |
| 14  | a     | 1138 | CLA  | C3D-C2D-C1D | -5.44 | 98.41       | 105.83   |
| 14  | B     | 1213 | CLA  | O2D-CGD-CBD | 5.43  | 120.92      | 111.27   |
| 14  | G     | 1124 | CLA  | C1C-C2C-C3C | -5.43 | 101.24      | 106.96   |
| 14  | a     | 1117 | CLA  | O2A-C1-C2   | 5.43  | 122.91      | 108.64   |
| 14  | a     | 1134 | CLA  | C1C-C2C-C3C | -5.43 | 101.25      | 106.96   |
| 14  | G     | 1105 | CLA  | CHD-C1D-ND  | -5.43 | 119.46      | 124.45   |
| 14  | A     | 1105 | CLA  | C1C-C2C-C3C | -5.43 | 101.25      | 106.96   |
| 14  | a     | 1136 | CLA  | C1C-C2C-C3C | -5.43 | 101.25      | 106.96   |
| 14  | G     | 1136 | CLA  | O2D-CGD-CBD | 5.43  | 120.92      | 111.27   |
| 15  | b     | 1219 | F6C  | C2D-C1D-ND  | 5.43  | 115.06      | 109.97   |
| 14  | A     | 1107 | CLA  | C1C-C2C-C3C | -5.43 | 101.25      | 106.96   |
| 14  | G     | 1141 | CLA  | C3D-C2D-C1D | -5.43 | 98.43       | 105.83   |
| 14  | a     | 1131 | CLA  | C4A-NA-C1A  | 5.43  | 109.14      | 106.71   |
| 14  | B     | 1022 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.71   |
| 14  | H     | 1022 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.71   |
| 14  | a     | 1141 | CLA  | C3D-C2D-C1D | -5.42 | 98.43       | 105.83   |
| 14  | a     | 1013 | CLA  | C1D-ND-C4D  | -5.42 | 102.48      | 106.33   |
| 14  | A     | 1117 | CLA  | O2A-C1-C2   | 5.42  | 122.88      | 108.64   |
| 14  | A     | 1105 | CLA  | CHD-C1D-ND  | -5.42 | 119.47      | 124.45   |
| 14  | A     | 1134 | CLA  | C1C-C2C-C3C | -5.42 | 101.26      | 106.96   |
| 14  | a     | 1105 | CLA  | C1C-C2C-C3C | -5.42 | 101.26      | 106.96   |
| 14  | H     | 1213 | CLA  | O2D-CGD-CBD | 5.42  | 120.89      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1130 | CLA  | CHD-C1D-ND  | -5.41 | 119.48      | 124.45   |
| 14  | G     | 1117 | CLA  | O2A-C1-C2   | 5.41  | 122.86      | 108.64   |
| 14  | A     | 1136 | CLA  | O2D-CGD-CBD | 5.41  | 120.88      | 111.27   |
| 14  | a     | 1114 | CLA  | O2D-CGD-CBD | 5.41  | 120.88      | 111.27   |
| 15  | H     | 1219 | F6C  | C2D-C1D-ND  | 5.41  | 115.04      | 109.97   |
| 14  | G     | 1137 | CLA  | O2A-C1-C2   | 5.41  | 122.85      | 108.64   |
| 14  | A     | 1137 | CLA  | O2A-C1-C2   | 5.41  | 122.85      | 108.64   |
| 14  | a     | 1137 | CLA  | O2A-C1-C2   | 5.41  | 122.84      | 108.64   |
| 14  | a     | 1130 | CLA  | CHD-C1D-ND  | -5.41 | 119.49      | 124.45   |
| 14  | G     | 1114 | CLA  | O2D-CGD-CBD | 5.41  | 120.87      | 111.27   |
| 14  | A     | 1138 | CLA  | C3D-C2D-C1D | -5.41 | 98.45       | 105.83   |
| 14  | B     | 1208 | CLA  | CHD-C1D-ND  | -5.40 | 119.49      | 124.45   |
| 14  | B     | 1227 | CLA  | C1C-C2C-C3C | -5.40 | 101.28      | 106.96   |
| 14  | A     | 1114 | CLA  | O2D-CGD-CBD | 5.40  | 120.86      | 111.27   |
| 14  | H     | 1227 | CLA  | C1C-C2C-C3C | -5.40 | 101.28      | 106.96   |
| 14  | A     | 1124 | CLA  | C1C-C2C-C3C | -5.40 | 101.28      | 106.96   |
| 15  | B     | 1219 | F6C  | C2D-C1D-ND  | 5.40  | 115.03      | 109.97   |
| 14  | b     | 1022 | CLA  | CMD-C2D-C1D | 5.40  | 134.23      | 124.71   |
| 15  | H     | 1237 | F6C  | O2D-CGD-CBD | 5.40  | 120.86      | 111.27   |
| 13  | A     | 1011 | CL0  | C4A-NA-C1A  | 5.40  | 109.13      | 106.71   |
| 14  | A     | 1106 | CLA  | C1C-C2C-C3C | -5.39 | 101.29      | 106.96   |
| 14  | G     | 1138 | CLA  | C3D-C2D-C1D | -5.39 | 98.47       | 105.83   |
| 14  | G     | 1106 | CLA  | C1C-C2C-C3C | -5.39 | 101.29      | 106.96   |
| 14  | b     | 1227 | CLA  | C1C-C2C-C3C | -5.39 | 101.29      | 106.96   |
| 14  | b     | 1227 | CLA  | C3D-C2D-C1D | -5.39 | 98.47       | 105.83   |
| 14  | B     | 1240 | CLA  | O2D-CGD-CBD | 5.39  | 120.85      | 111.27   |
| 14  | G     | 1126 | CLA  | CHD-C1D-ND  | -5.39 | 119.50      | 124.45   |
| 14  | H     | 1208 | CLA  | CHD-C1D-ND  | -5.39 | 119.50      | 124.45   |
| 14  | a     | 1126 | CLA  | CHD-C1D-ND  | -5.39 | 119.50      | 124.45   |
| 14  | B     | 1227 | CLA  | C3D-C2D-C1D | -5.39 | 98.48       | 105.83   |
| 14  | B     | 1217 | CLA  | C1C-C2C-C3C | -5.39 | 101.30      | 106.96   |
| 14  | G     | 1130 | CLA  | O2D-CGD-CBD | 5.38  | 120.84      | 111.27   |
| 14  | H     | 1240 | CLA  | O2D-CGD-CBD | 5.38  | 120.84      | 111.27   |
| 14  | A     | 1109 | CLA  | C3D-C2D-C1D | -5.38 | 98.48       | 105.83   |
| 14  | a     | 1136 | CLA  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |
| 14  | a     | 1106 | CLA  | C1C-C2C-C3C | -5.38 | 101.30      | 106.96   |
| 14  | A     | 1130 | CLA  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |
| 15  | B     | 1237 | F6C  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |
| 14  | a     | 1109 | CLA  | C3D-C2D-C1D | -5.38 | 98.49       | 105.83   |
| 14  | b     | 1240 | CLA  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |
| 15  | b     | 1237 | F6C  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |
| 14  | b     | 1209 | CLA  | O2D-CGD-CBD | 5.38  | 120.83      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | L     | 1502 | CLA  | C4A-NA-C1A  | 5.38  | 109.12      | 106.71   |
| 14  | A     | 1126 | CLA  | CHD-C1D-ND  | -5.38 | 119.51      | 124.45   |
| 14  | H     | 1209 | CLA  | O2D-CGD-CBD | 5.37  | 120.82      | 111.27   |
| 14  | a     | 1130 | CLA  | O2D-CGD-CBD | 5.37  | 120.82      | 111.27   |
| 14  | a     | 1101 | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | G     | 1109 | CLA  | C3D-C2D-C1D | -5.37 | 98.50       | 105.83   |
| 14  | H     | 1227 | CLA  | C3D-C2D-C1D | -5.37 | 98.50       | 105.83   |
| 14  | G     | 1130 | CLA  | CHD-C1D-ND  | -5.37 | 119.52      | 124.45   |
| 14  | H     | 1217 | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | B     | 1209 | CLA  | O2D-CGD-CBD | 5.37  | 120.81      | 111.27   |
| 14  | B     | 1229 | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | B     | 1234 | CLA  | O2D-CGD-CBD | 5.37  | 120.81      | 111.27   |
| 14  | b     | 1229 | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | H     | 1228 | CLA  | CHD-C1D-ND  | -5.37 | 119.52      | 124.45   |
| 14  | a     | 1124 | CLA  | C1C-C2C-C3C | -5.36 | 101.32      | 106.96   |
| 14  | H     | 1229 | CLA  | C1C-C2C-C3C | -5.36 | 101.32      | 106.96   |
| 14  | B     | 1239 | CLA  | C3D-C2D-C1D | -5.36 | 98.51       | 105.83   |
| 15  | b     | 1238 | F6C  | C1A-C2A-C3A | -5.36 | 101.32      | 106.97   |
| 14  | b     | 1217 | CLA  | C1C-C2C-C3C | -5.36 | 101.32      | 106.96   |
| 14  | G     | 1135 | CLA  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 14  | B     | 1235 | CLA  | CHD-C1D-ND  | -5.35 | 119.53      | 124.45   |
| 14  | A     | 1135 | CLA  | O2D-CGD-CBD | 5.35  | 120.78      | 111.27   |
| 14  | G     | 1125 | CLA  | C2C-C1C-NC  | 5.35  | 114.99      | 109.97   |
| 14  | b     | 1239 | CLA  | C3D-C2D-C1D | -5.35 | 98.52       | 105.83   |
| 15  | H     | 1230 | F6C  | C2D-C1D-ND  | 5.35  | 114.99      | 109.97   |
| 15  | b     | 1230 | F6C  | C2D-C1D-ND  | 5.35  | 114.99      | 109.97   |
| 14  | A     | 1101 | CLA  | C1C-C2C-C3C | -5.35 | 101.33      | 106.96   |
| 14  | H     | 1215 | CLA  | C3D-C2D-C1D | -5.35 | 98.53       | 105.83   |
| 14  | a     | 1116 | CLA  | C3D-C2D-C1D | -5.35 | 98.53       | 105.83   |
| 14  | b     | 1235 | CLA  | CHD-C1D-ND  | -5.35 | 119.54      | 124.45   |
| 15  | B     | 1238 | F6C  | C1A-C2A-C3A | -5.35 | 101.34      | 106.97   |
| 14  | A     | 1139 | CLA  | C3D-C2D-C1D | -5.35 | 98.54       | 105.83   |
| 14  | b     | 1208 | CLA  | CHD-C1D-ND  | -5.35 | 119.54      | 124.45   |
| 14  | B     | 1208 | CLA  | C1C-C2C-C3C | -5.35 | 101.34      | 106.96   |
| 14  | b     | 1234 | CLA  | O2D-CGD-CBD | 5.35  | 120.77      | 111.27   |
| 14  | B     | 1220 | CLA  | C4A-NA-C1A  | 5.34  | 109.11      | 106.71   |
| 15  | B     | 1230 | F6C  | C2D-C1D-ND  | 5.34  | 114.98      | 109.97   |
| 14  | G     | 1101 | CLA  | C1C-C2C-C3C | -5.34 | 101.34      | 106.96   |
| 18  | b     | 4004 | BCR  | C20-C19-C18 | 5.34  | 141.43      | 126.42   |
| 14  | H     | 1239 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 14  | H     | 1234 | CLA  | O2D-CGD-CBD | 5.34  | 120.76      | 111.27   |
| 14  | a     | 1131 | CLA  | CHD-C1D-ND  | -5.34 | 119.54      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | H     | 1207 | F6C  | C3D-C2D-C1D | -5.34 | 98.09       | 105.83   |
| 14  | b     | 1215 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 14  | G     | 1139 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 14  | B     | 1234 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 14  | A     | 1124 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 14  | b     | 1208 | CLA  | C1C-C2C-C3C | -5.34 | 101.34      | 106.96   |
| 14  | a     | 1124 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 15  | H     | 1238 | F6C  | C1A-C2A-C3A | -5.34 | 101.35      | 106.97   |
| 14  | G     | 1124 | CLA  | C3D-C2D-C1D | -5.34 | 98.54       | 105.83   |
| 18  | B     | 4004 | BCR  | C20-C19-C18 | 5.34  | 141.41      | 126.42   |
| 15  | b     | 1237 | F6C  | CAA-C2A-C1A | -5.34 | 113.41      | 128.11   |
| 15  | B     | 1207 | F6C  | C3D-C2D-C1D | -5.34 | 98.10       | 105.83   |
| 14  | H     | 1234 | CLA  | C3D-C2D-C1D | -5.34 | 98.55       | 105.83   |
| 14  | A     | 1125 | CLA  | C2C-C1C-NC  | 5.34  | 114.97      | 109.97   |
| 14  | A     | 1126 | CLA  | C1C-C2C-C3C | -5.34 | 101.35      | 106.96   |
| 14  | H     | 1208 | CLA  | C1C-C2C-C3C | -5.34 | 101.35      | 106.96   |
| 14  | a     | 1135 | CLA  | O2D-CGD-CBD | 5.34  | 120.75      | 111.27   |
| 14  | a     | 1129 | CLA  | O2A-CGA-O1A | -5.33 | 110.13      | 123.59   |
| 14  | b     | 1220 | CLA  | C4A-NA-C1A  | 5.33  | 109.10      | 106.71   |
| 14  | b     | 1228 | CLA  | CHD-C1D-ND  | -5.33 | 119.55      | 124.45   |
| 14  | a     | 1126 | CLA  | C1C-C2C-C3C | -5.33 | 101.35      | 106.96   |
| 14  | a     | 1139 | CLA  | C3D-C2D-C1D | -5.33 | 98.55       | 105.83   |
| 14  | G     | 1126 | CLA  | C1C-C2C-C3C | -5.33 | 101.35      | 106.96   |
| 14  | U     | 1502 | CLA  | C4A-NA-C1A  | 5.33  | 109.10      | 106.71   |
| 14  | b     | 1232 | CLA  | C1C-C2C-C3C | -5.33 | 101.35      | 106.96   |
| 14  | G     | 1137 | CLA  | CHD-C1D-ND  | -5.33 | 119.56      | 124.45   |
| 15  | H     | 1237 | F6C  | CAA-C2A-C1A | -5.33 | 113.44      | 128.11   |
| 15  | B     | 1237 | F6C  | CAA-C2A-C1A | -5.33 | 113.44      | 128.11   |
| 14  | B     | 1213 | CLA  | CHD-C1D-ND  | -5.33 | 119.56      | 124.45   |
| 14  | b     | 1216 | CLA  | CHD-C1D-ND  | -5.33 | 119.56      | 124.45   |
| 14  | B     | 1215 | CLA  | C3D-C2D-C1D | -5.32 | 98.56       | 105.83   |
| 18  | H     | 4004 | BCR  | C20-C19-C18 | 5.32  | 141.37      | 126.42   |
| 14  | a     | 1125 | CLA  | C2C-C1C-NC  | 5.32  | 114.96      | 109.97   |
| 14  | A     | 1137 | CLA  | CHD-C1D-ND  | -5.32 | 119.56      | 124.45   |
| 14  | B     | 1232 | CLA  | C1C-C2C-C3C | -5.32 | 101.36      | 106.96   |
| 14  | G     | 1139 | CLA  | C1C-C2C-C3C | -5.32 | 101.36      | 106.96   |
| 14  | A     | 1116 | CLA  | C3D-C2D-C1D | -5.32 | 98.57       | 105.83   |
| 14  | b     | 1234 | CLA  | C3D-C2D-C1D | -5.32 | 98.57       | 105.83   |
| 14  | B     | 1206 | CLA  | C1C-C2C-C3C | -5.32 | 101.36      | 106.96   |
| 14  | H     | 1213 | CLA  | CHD-C1D-ND  | -5.32 | 119.57      | 124.45   |
| 14  | H     | 1235 | CLA  | CHD-C1D-ND  | -5.32 | 119.57      | 124.45   |
| 14  | A     | 1139 | CLA  | C1C-C2C-C3C | -5.31 | 101.37      | 106.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4006 | BCR  | C24-C23-C22 | -5.31 | 118.21      | 126.23   |
| 15  | b     | 1207 | F6C  | C3D-C2D-C1D | -5.31 | 98.14       | 105.83   |
| 18  | A     | 4006 | BCR  | C24-C23-C22 | -5.31 | 118.21      | 126.23   |
| 14  | H     | 1208 | CLA  | C4A-NA-C1A  | 5.31  | 109.09      | 106.71   |
| 14  | b     | 1210 | CLA  | C4A-NA-C1A  | 5.31  | 109.09      | 106.71   |
| 14  | l     | 1501 | CLA  | C4A-NA-C1A  | 5.31  | 109.09      | 106.71   |
| 14  | H     | 1232 | CLA  | C1C-C2C-C3C | -5.31 | 101.38      | 106.96   |
| 14  | b     | 1213 | CLA  | CHD-C1D-ND  | -5.31 | 119.58      | 124.45   |
| 14  | A     | 1140 | CLA  | C1C-C2C-C3C | -5.31 | 101.38      | 106.96   |
| 14  | H     | 1206 | CLA  | C1C-C2C-C3C | -5.31 | 101.38      | 106.96   |
| 14  | a     | 1139 | CLA  | C1C-C2C-C3C | -5.31 | 101.38      | 106.96   |
| 14  | G     | 1138 | CLA  | O2D-CGD-CBD | 5.31  | 120.70      | 111.27   |
| 14  | A     | 1129 | CLA  | O2A-CGA-O1A | -5.31 | 110.20      | 123.59   |
| 14  | b     | 1206 | CLA  | C1C-C2C-C3C | -5.30 | 101.38      | 106.96   |
| 18  | a     | 4006 | BCR  | C24-C23-C22 | -5.30 | 118.22      | 126.23   |
| 14  | G     | 1134 | CLA  | C3D-C2D-C1D | -5.30 | 98.60       | 105.83   |
| 14  | a     | 1137 | CLA  | CHD-C1D-ND  | -5.30 | 119.58      | 124.45   |
| 13  | G     | 1011 | CL0  | C4A-NA-C1A  | 5.30  | 109.09      | 106.71   |
| 15  | B     | 1237 | F6C  | CMD-C2D-C1D | 5.30  | 133.11      | 125.04   |
| 14  | A     | 1138 | CLA  | O2D-CGD-CBD | 5.30  | 120.69      | 111.27   |
| 14  | G     | 1106 | CLA  | C3D-C2D-C1D | -5.30 | 98.60       | 105.83   |
| 14  | b     | 1223 | CLA  | C1C-C2C-C3C | -5.30 | 101.39      | 106.96   |
| 14  | H     | 1022 | CLA  | C3D-C2D-C1D | -5.30 | 98.60       | 105.83   |
| 14  | G     | 1140 | CLA  | C1C-C2C-C3C | -5.30 | 101.39      | 106.96   |
| 15  | H     | 1237 | F6C  | CMD-C2D-C1D | 5.30  | 133.11      | 125.04   |
| 14  | A     | 1131 | CLA  | CHD-C1D-ND  | -5.30 | 119.59      | 124.45   |
| 14  | B     | 1228 | CLA  | CHD-C1D-ND  | -5.30 | 119.59      | 124.45   |
| 14  | B     | 1223 | CLA  | C1C-C2C-C3C | -5.30 | 101.39      | 106.96   |
| 14  | G     | 1136 | CLA  | C3D-C2D-C1D | -5.30 | 98.60       | 105.83   |
| 14  | G     | 1128 | CLA  | C1C-C2C-C3C | -5.29 | 101.39      | 106.96   |
| 14  | B     | 1022 | CLA  | C3D-C2D-C1D | -5.29 | 98.61       | 105.83   |
| 18  | b     | 4004 | BCR  | C7-C8-C9    | -5.29 | 118.24      | 126.23   |
| 14  | G     | 1123 | CLA  | C1C-C2C-C3C | -5.29 | 101.39      | 106.96   |
| 14  | G     | 1129 | CLA  | O2A-CGA-O1A | -5.29 | 110.24      | 123.59   |
| 14  | G     | 1013 | CLA  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 14  | a     | 1138 | CLA  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 14  | a     | 1112 | CLA  | O2A-CGA-O1A | -5.29 | 110.24      | 123.59   |
| 14  | H     | 1223 | CLA  | C1C-C2C-C3C | -5.29 | 101.39      | 106.96   |
| 14  | B     | 1208 | CLA  | C4A-NA-C1A  | 5.29  | 109.08      | 106.71   |
| 14  | A     | 1134 | CLA  | C3D-C2D-C1D | -5.29 | 98.61       | 105.83   |
| 14  | a     | 1134 | CLA  | C3D-C2D-C1D | -5.29 | 98.62       | 105.83   |
| 14  | a     | 1140 | CLA  | C1C-C2C-C3C | -5.29 | 101.40      | 106.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1240 | CLA  | C3D-C2D-C1D | -5.29 | 98.62       | 105.83   |
| 14  | a     | 1013 | CLA  | O2D-CGD-CBD | 5.29  | 120.66      | 111.27   |
| 13  | a     | 1011 | CL0  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |
| 14  | L     | 1501 | CLA  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |
| 14  | A     | 1106 | CLA  | C3D-C2D-C1D | -5.28 | 98.62       | 105.83   |
| 14  | A     | 1013 | CLA  | O2D-CGD-CBD | 5.28  | 120.66      | 111.27   |
| 14  | G     | 1116 | CLA  | C3D-C2D-C1D | -5.28 | 98.62       | 105.83   |
| 14  | B     | 1210 | CLA  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |
| 14  | A     | 1136 | CLA  | C3D-C2D-C1D | -5.28 | 98.62       | 105.83   |
| 14  | A     | 1112 | CLA  | O2A-CGA-O1A | -5.28 | 110.27      | 123.59   |
| 14  | G     | 1112 | CLA  | O2A-CGA-O1A | -5.28 | 110.27      | 123.59   |
| 14  | A     | 1123 | CLA  | C1C-C2C-C3C | -5.28 | 101.41      | 106.96   |
| 14  | a     | 1012 | CLA  | C3D-C2D-C1D | -5.28 | 98.63       | 105.83   |
| 14  | a     | 1136 | CLA  | C3D-C2D-C1D | -5.28 | 98.63       | 105.83   |
| 14  | T     | 1401 | CLA  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |
| 14  | a     | 1106 | CLA  | C3D-C2D-C1D | -5.28 | 98.63       | 105.83   |
| 15  | b     | 1237 | F6C  | CMD-C2D-C1D | 5.27  | 133.07      | 125.04   |
| 14  | A     | 1012 | CLA  | C3D-C2D-C1D | -5.27 | 98.63       | 105.83   |
| 15  | H     | 1219 | F6C  | O2D-CGD-CBD | 5.27  | 120.64      | 111.27   |
| 14  | a     | 1126 | CLA  | O2A-CGA-O1A | -5.27 | 110.29      | 123.59   |
| 15  | B     | 1219 | F6C  | O2D-CGD-CBD | 5.27  | 120.63      | 111.27   |
| 14  | b     | 1240 | CLA  | C3D-C2D-C1D | -5.27 | 98.64       | 105.83   |
| 15  | A     | 1121 | F6C  | C2D-C1D-ND  | 5.27  | 114.91      | 109.97   |
| 14  | a     | 1110 | CLA  | CHD-C1D-ND  | -5.27 | 119.61      | 124.45   |
| 14  | B     | 1216 | CLA  | CHD-C1D-ND  | -5.27 | 119.61      | 124.45   |
| 18  | B     | 4004 | BCR  | C7-C8-C9    | -5.27 | 118.28      | 126.23   |
| 14  | B     | 1023 | CLA  | O2A-CGA-O1A | -5.26 | 110.31      | 123.59   |
| 15  | a     | 1121 | F6C  | C2D-C1D-ND  | 5.26  | 114.90      | 109.97   |
| 14  | H     | 1222 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 14  | b     | 1022 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 14  | A     | 1128 | CLA  | C1C-C2C-C3C | -5.26 | 101.42      | 106.96   |
| 18  | H     | 4004 | BCR  | C7-C8-C9    | -5.26 | 118.29      | 126.23   |
| 14  | K     | 1401 | CLA  | C4A-NA-C1A  | 5.26  | 109.07      | 106.71   |
| 14  | B     | 1210 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 14  | b     | 1220 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 14  | b     | 1023 | CLA  | O2A-CGA-O1A | -5.26 | 110.32      | 123.59   |
| 14  | H     | 1210 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 14  | G     | 1108 | CLA  | C3D-C2D-C1D | -5.26 | 98.66       | 105.83   |
| 14  | H     | 1023 | CLA  | O2A-CGA-O1A | -5.26 | 110.32      | 123.59   |
| 15  | b     | 1219 | F6C  | O2D-CGD-CBD | 5.26  | 120.61      | 111.27   |
| 14  | a     | 1128 | CLA  | C1C-C2C-C3C | -5.25 | 101.43      | 106.96   |
| 14  | G     | 1117 | CLA  | C4A-NA-C1A  | 5.25  | 109.07      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1102 | CLA  | C3D-C2D-C1D | -5.25 | 98.66       | 105.83   |
| 14  | H     | 1220 | CLA  | C3D-C2D-C1D | -5.25 | 98.66       | 105.83   |
| 14  | a     | 1013 | CLA  | O2A-CGA-O1A | -5.25 | 110.34      | 123.59   |
| 14  | a     | 1116 | CLA  | O2D-CGD-CBD | 5.25  | 120.60      | 111.27   |
| 14  | k     | 1401 | CLA  | C4A-NA-C1A  | 5.25  | 109.07      | 106.71   |
| 14  | H     | 1210 | CLA  | CHD-C1D-ND  | -5.25 | 119.63      | 124.45   |
| 14  | b     | 1210 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 14  | H     | 1229 | CLA  | CHD-C1D-ND  | -5.25 | 119.63      | 124.45   |
| 14  | H     | 1224 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 14  | A     | 1108 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 15  | G     | 1121 | F6C  | C2D-C1D-ND  | 5.25  | 114.89      | 109.97   |
| 14  | G     | 1118 | CLA  | O2A-C1-C2   | 5.25  | 122.43      | 108.64   |
| 14  | A     | 1116 | CLA  | O2D-CGD-CBD | 5.25  | 120.59      | 111.27   |
| 14  | B     | 1240 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 14  | G     | 1012 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 14  | B     | 1222 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 14  | b     | 1215 | CLA  | O2D-CGD-CBD | 5.25  | 120.59      | 111.27   |
| 14  | H     | 1210 | CLA  | C4A-NA-C1A  | 5.24  | 109.06      | 106.71   |
| 14  | A     | 1126 | CLA  | O2A-CGA-O1A | -5.24 | 110.36      | 123.59   |
| 14  | a     | 1123 | CLA  | C1C-C2C-C3C | -5.24 | 101.44      | 106.96   |
| 14  | G     | 1116 | CLA  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 14  | U     | 1501 | CLA  | C4A-NA-C1A  | 5.24  | 109.06      | 106.71   |
| 14  | a     | 1108 | CLA  | C3D-C2D-C1D | -5.24 | 98.68       | 105.83   |
| 14  | a     | 1118 | CLA  | O2A-C1-C2   | 5.24  | 122.41      | 108.64   |
| 14  | a     | 1116 | CLA  | CHD-C1D-ND  | -5.24 | 119.64      | 124.45   |
| 14  | A     | 1118 | CLA  | O2A-C1-C2   | 5.24  | 122.41      | 108.64   |
| 14  | A     | 1013 | CLA  | O2A-CGA-O1A | -5.24 | 110.36      | 123.59   |
| 14  | G     | 1126 | CLA  | O2A-CGA-O1A | -5.24 | 110.36      | 123.59   |
| 14  | B     | 1224 | CLA  | C3D-C2D-C1D | -5.24 | 98.68       | 105.83   |
| 14  | G     | 1131 | CLA  | CHD-C1D-ND  | -5.24 | 119.64      | 124.45   |
| 14  | H     | 1215 | CLA  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 14  | b     | 1208 | CLA  | C4A-NA-C1A  | 5.24  | 109.06      | 106.71   |
| 14  | b     | 1210 | CLA  | CHD-C1D-ND  | -5.24 | 119.64      | 124.45   |
| 14  | B     | 1225 | CLA  | O2A-CGA-O1A | -5.24 | 110.38      | 123.59   |
| 14  | A     | 1110 | CLA  | CHD-C1D-ND  | -5.24 | 119.64      | 124.45   |
| 14  | H     | 1225 | CLA  | O2A-CGA-O1A | -5.24 | 110.38      | 123.59   |
| 14  | b     | 1224 | CLA  | C3D-C2D-C1D | -5.23 | 98.69       | 105.83   |
| 14  | B     | 1229 | CLA  | CHD-C1D-ND  | -5.23 | 119.64      | 124.45   |
| 14  | H     | 1222 | CLA  | CHD-C1D-ND  | -5.23 | 119.64      | 124.45   |
| 14  | G     | 1102 | CLA  | C3D-C2D-C1D | -5.23 | 98.69       | 105.83   |
| 14  | H     | 1216 | CLA  | CHD-C1D-ND  | -5.23 | 119.65      | 124.45   |
| 14  | b     | 1222 | CLA  | C3D-C2D-C1D | -5.23 | 98.69       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1141 | CLA  | C4A-NA-C1A  | 5.23  | 109.06      | 106.71   |
| 14  | G     | 1107 | CLA  | O2D-CGD-CBD | 5.23  | 120.56      | 111.27   |
| 14  | G     | 1013 | CLA  | O2A-CGA-O1A | -5.23 | 110.40      | 123.59   |
| 15  | B     | 1219 | F6C  | C1A-C2A-C3A | -5.23 | 101.47      | 106.97   |
| 14  | B     | 1210 | CLA  | CHD-C1D-ND  | -5.23 | 119.65      | 124.45   |
| 14  | B     | 1220 | CLA  | C3D-C2D-C1D | -5.22 | 98.70       | 105.83   |
| 14  | a     | 1127 | CLA  | O2D-CGD-CBD | 5.22  | 120.55      | 111.27   |
| 14  | G     | 1110 | CLA  | CHD-C1D-ND  | -5.22 | 119.65      | 124.45   |
| 14  | B     | 1234 | CLA  | O2A-CGA-O1A | -5.22 | 110.41      | 123.59   |
| 14  | A     | 1127 | CLA  | O2D-CGD-CBD | 5.22  | 120.55      | 111.27   |
| 14  | A     | 1102 | CLA  | C3D-C2D-C1D | -5.22 | 98.70       | 105.83   |
| 14  | A     | 1104 | CLA  | O2A-CGA-O1A | -5.22 | 110.41      | 123.59   |
| 15  | H     | 1219 | F6C  | C1A-C2A-C3A | -5.22 | 101.47      | 106.97   |
| 14  | G     | 1104 | CLA  | O2A-CGA-O1A | -5.22 | 110.41      | 123.59   |
| 14  | k     | 1401 | CLA  | C1D-ND-C4D  | -5.22 | 102.63      | 106.33   |
| 14  | a     | 1141 | CLA  | C4A-NA-C1A  | 5.22  | 109.05      | 106.71   |
| 14  | b     | 1221 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | b     | 1225 | CLA  | O2A-CGA-O1A | -5.22 | 110.42      | 123.59   |
| 14  | G     | 1127 | CLA  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | H     | 1221 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | H     | 1234 | CLA  | O2A-CGA-O1A | -5.22 | 110.42      | 123.59   |
| 14  | A     | 1107 | CLA  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | b     | 1234 | CLA  | O2A-CGA-O1A | -5.22 | 110.42      | 123.59   |
| 14  | A     | 1141 | CLA  | C4A-NA-C1A  | 5.22  | 109.05      | 106.71   |
| 14  | b     | 1213 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | B     | 1215 | CLA  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | B     | 1212 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | a     | 1134 | CLA  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | B     | 1221 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | B     | 1235 | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 14  | a     | 1104 | CLA  | O2A-CGA-O1A | -5.22 | 110.43      | 123.59   |
| 14  | B     | 1213 | CLA  | C3D-C2D-C1D | -5.21 | 98.71       | 105.83   |
| 14  | b     | 1209 | CLA  | C1C-C2C-C3C | -5.21 | 101.47      | 106.96   |
| 15  | b     | 1219 | F6C  | C1A-C2A-C3A | -5.21 | 101.48      | 106.97   |
| 14  | H     | 1213 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | b     | 1222 | CLA  | CHD-C1D-ND  | -5.21 | 119.67      | 124.45   |
| 14  | b     | 1212 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | H     | 1235 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | b     | 1235 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | b     | 1228 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | A     | 1116 | CLA  | CHD-C1D-ND  | -5.21 | 119.67      | 124.45   |
| 14  | b     | 1236 | CLA  | CHD-C1D-ND  | -5.21 | 119.67      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1129 | CLA  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 14  | H     | 1212 | CLA  | C3D-C2D-C1D | -5.21 | 98.73       | 105.83   |
| 14  | b     | 1229 | CLA  | CHD-C1D-ND  | -5.20 | 119.67      | 124.45   |
| 14  | a     | 1107 | CLA  | O2D-CGD-CBD | 5.20  | 120.51      | 111.27   |
| 14  | G     | 1129 | CLA  | C3D-C2D-C1D | -5.20 | 98.73       | 105.83   |
| 14  | K     | 1401 | CLA  | C1D-ND-C4D  | -5.20 | 102.64      | 106.33   |
| 14  | G     | 1134 | CLA  | O2D-CGD-CBD | 5.20  | 120.51      | 111.27   |
| 14  | B     | 1209 | CLA  | C1C-C2C-C3C | -5.20 | 101.49      | 106.96   |
| 14  | G     | 1116 | CLA  | CHD-C1D-ND  | -5.20 | 119.68      | 124.45   |
| 14  | T     | 1401 | CLA  | CHD-C1D-ND  | -5.20 | 119.68      | 124.45   |
| 14  | H     | 1201 | CLA  | C3D-C2D-C1D | -5.20 | 98.74       | 105.83   |
| 14  | G     | 1111 | CLA  | O2A-C1-C2   | 5.20  | 122.29      | 108.64   |
| 14  | b     | 1236 | CLA  | O2A-CGA-O1A | -5.20 | 110.48      | 123.59   |
| 14  | B     | 1231 | CLA  | C4A-NA-C1A  | 5.20  | 109.04      | 106.71   |
| 14  | b     | 1204 | CLA  | C3D-C2D-C1D | -5.20 | 98.74       | 105.83   |
| 14  | a     | 1129 | CLA  | C3D-C2D-C1D | -5.20 | 98.74       | 105.83   |
| 14  | A     | 1111 | CLA  | O2A-C1-C2   | 5.20  | 122.29      | 108.64   |
| 14  | B     | 1236 | CLA  | O2A-CGA-O1A | -5.19 | 110.48      | 123.59   |
| 14  | T     | 1401 | CLA  | C1D-ND-C4D  | -5.19 | 102.65      | 106.33   |
| 14  | A     | 1134 | CLA  | O2D-CGD-CBD | 5.19  | 120.49      | 111.27   |
| 14  | B     | 1201 | CLA  | C3D-C2D-C1D | -5.19 | 98.75       | 105.83   |
| 14  | K     | 1401 | CLA  | O2D-CGD-CBD | 5.19  | 120.49      | 111.27   |
| 14  | H     | 1236 | CLA  | O2A-CGA-O1A | -5.19 | 110.50      | 123.59   |
| 14  | b     | 1201 | CLA  | C3D-C2D-C1D | -5.19 | 98.75       | 105.83   |
| 14  | k     | 1401 | CLA  | O2D-CGD-CBD | 5.19  | 120.49      | 111.27   |
| 14  | H     | 1209 | CLA  | C1C-C2C-C3C | -5.19 | 101.50      | 106.96   |
| 14  | a     | 1111 | CLA  | O2A-C1-C2   | 5.19  | 122.26      | 108.64   |
| 14  | b     | 1205 | CLA  | C1C-C2C-C3C | -5.18 | 101.51      | 106.96   |
| 14  | H     | 1021 | CLA  | CMD-C2D-C1D | 5.18  | 133.85      | 124.71   |
| 14  | B     | 1204 | CLA  | C3D-C2D-C1D | -5.18 | 98.76       | 105.83   |
| 14  | A     | 1012 | CLA  | O2A-CGA-O1A | -5.18 | 110.52      | 123.59   |
| 14  | k     | 1401 | CLA  | CHD-C1D-ND  | -5.18 | 119.70      | 124.45   |
| 14  | B     | 1021 | CLA  | CMD-C2D-C1D | 5.18  | 133.84      | 124.71   |
| 14  | B     | 1236 | CLA  | CHD-C1D-ND  | -5.18 | 119.70      | 124.45   |
| 14  | a     | 1130 | CLA  | C1C-C2C-C3C | -5.17 | 101.52      | 106.96   |
| 14  | b     | 1021 | CLA  | CMD-C2D-C1D | 5.17  | 133.83      | 124.71   |
| 14  | B     | 1222 | CLA  | CHD-C1D-ND  | -5.17 | 119.70      | 124.45   |
| 14  | G     | 1012 | CLA  | O2A-CGA-O1A | -5.17 | 110.53      | 123.59   |
| 14  | H     | 1235 | CLA  | O2A-CGA-O1A | -5.17 | 110.54      | 123.59   |
| 14  | B     | 1205 | CLA  | C1C-C2C-C3C | -5.17 | 101.52      | 106.96   |
| 14  | T     | 1401 | CLA  | O2D-CGD-CBD | 5.17  | 120.46      | 111.27   |
| 14  | U     | 1502 | CLA  | C3D-C2D-C1D | -5.17 | 98.77       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | K     | 1401 | CLA  | CHD-C1D-ND  | -5.17 | 119.70      | 124.45   |
| 14  | a     | 1125 | CLA  | C1D-ND-C4D  | -5.17 | 102.66      | 106.33   |
| 14  | a     | 1125 | CLA  | O2A-C1-C2   | 5.17  | 122.22      | 108.64   |
| 14  | A     | 1130 | CLA  | C1C-C2C-C3C | -5.17 | 101.52      | 106.96   |
| 14  | H     | 1204 | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 14  | a     | 1112 | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 14  | A     | 1117 | CLA  | C4A-NA-C1A  | 5.17  | 109.03      | 106.71   |
| 14  | L     | 1502 | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 14  | B     | 1228 | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 14  | B     | 1203 | CLA  | O2D-CGD-CBD | 5.17  | 120.45      | 111.27   |
| 14  | B     | 1235 | CLA  | O2A-CGA-O1A | -5.17 | 110.55      | 123.59   |
| 14  | a     | 1012 | CLA  | O2A-CGA-O1A | -5.17 | 110.55      | 123.59   |
| 14  | A     | 1137 | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 14  | H     | 1231 | CLA  | C4A-NA-C1A  | 5.16  | 109.03      | 106.71   |
| 14  | A     | 1125 | CLA  | O2A-C1-C2   | 5.16  | 122.21      | 108.64   |
| 14  | G     | 1125 | CLA  | O2A-C1-C2   | 5.16  | 122.21      | 108.64   |
| 14  | b     | 1218 | CLA  | C1D-ND-C4D  | -5.16 | 102.67      | 106.33   |
| 14  | H     | 1203 | CLA  | O2D-CGD-CBD | 5.16  | 120.44      | 111.27   |
| 14  | B     | 1208 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 14  | H     | 1208 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 14  | G     | 1112 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 14  | A     | 1112 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 14  | b     | 1235 | CLA  | O2A-CGA-O1A | -5.16 | 110.58      | 123.59   |
| 14  | H     | 1236 | CLA  | CHD-C1D-ND  | -5.16 | 119.72      | 124.45   |
| 14  | G     | 1137 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 14  | a     | 1137 | CLA  | C3D-C2D-C1D | -5.16 | 98.80       | 105.83   |
| 14  | l     | 1503 | CLA  | C4A-NA-C1A  | 5.15  | 109.02      | 106.71   |
| 14  | G     | 1133 | CLA  | C3D-C2D-C1D | -5.15 | 98.80       | 105.83   |
| 14  | a     | 1117 | CLA  | C3D-C2D-C1D | -5.15 | 98.80       | 105.83   |
| 14  | b     | 1203 | CLA  | O2D-CGD-CBD | 5.15  | 120.42      | 111.27   |
| 14  | H     | 1231 | CLA  | C1C-C2C-C3C | -5.15 | 101.55      | 106.96   |
| 14  | H     | 1208 | CLA  | O2A-CGA-CBA | 5.15  | 128.06      | 111.91   |
| 14  | b     | 1203 | CLA  | CHD-C1D-ND  | -5.14 | 119.73      | 124.45   |
| 14  | b     | 1208 | CLA  | C3D-C2D-C1D | -5.14 | 98.81       | 105.83   |
| 14  | G     | 1130 | CLA  | C1C-C2C-C3C | -5.14 | 101.55      | 106.96   |
| 14  | l     | 1502 | CLA  | C3D-C2D-C1D | -5.14 | 98.81       | 105.83   |
| 14  | H     | 1228 | CLA  | C3D-C2D-C1D | -5.14 | 98.81       | 105.83   |
| 14  | b     | 1231 | CLA  | C1C-C2C-C3C | -5.14 | 101.55      | 106.96   |
| 14  | B     | 1218 | CLA  | C1D-ND-C4D  | -5.14 | 102.68      | 106.33   |
| 14  | A     | 1117 | CLA  | C3D-C2D-C1D | -5.14 | 98.82       | 105.83   |
| 14  | A     | 1133 | CLA  | C3D-C2D-C1D | -5.14 | 98.82       | 105.83   |
| 14  | H     | 1204 | CLA  | C1D-ND-C4D  | -5.14 | 102.69      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | H     | 1219 | F6C  | C3A-C4A-NA  | 5.14  | 113.89      | 110.10   |
| 14  | B     | 1208 | CLA  | O2A-CGA-CBA | 5.14  | 128.02      | 111.91   |
| 14  | H     | 1205 | CLA  | C1C-C2C-C3C | -5.13 | 101.56      | 106.96   |
| 15  | B     | 1219 | F6C  | C3A-C4A-NA  | 5.13  | 113.89      | 110.10   |
| 14  | a     | 1133 | CLA  | C3D-C2D-C1D | -5.13 | 98.83       | 105.83   |
| 14  | a     | 1110 | CLA  | C1C-C2C-C3C | -5.13 | 101.56      | 106.96   |
| 14  | b     | 1224 | CLA  | O2A-C1-C2   | 5.13  | 122.11      | 108.64   |
| 14  | G     | 1117 | CLA  | C3D-C2D-C1D | -5.13 | 98.83       | 105.83   |
| 18  | G     | 4002 | BCR  | C24-C23-C22 | -5.13 | 118.49      | 126.23   |
| 14  | B     | 1224 | CLA  | O2A-C1-C2   | 5.13  | 122.11      | 108.64   |
| 14  | A     | 1119 | CLA  | CHD-C1D-ND  | -5.13 | 119.74      | 124.45   |
| 14  | B     | 1203 | CLA  | CHD-C1D-ND  | -5.13 | 119.74      | 124.45   |
| 14  | H     | 1203 | CLA  | CHD-C1D-ND  | -5.12 | 119.75      | 124.45   |
| 14  | A     | 1113 | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 14  | G     | 1106 | CLA  | CHD-C1D-ND  | -5.12 | 119.75      | 124.45   |
| 14  | a     | 1105 | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 14  | L     | 1503 | CLA  | C4A-NA-C1A  | 5.12  | 109.01      | 106.71   |
| 14  | G     | 1113 | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 14  | H     | 1206 | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 18  | A     | 4002 | BCR  | C24-C23-C22 | -5.12 | 118.50      | 126.23   |
| 14  | H     | 1023 | CLA  | O2A-C1-C2   | 5.12  | 122.09      | 108.64   |
| 14  | A     | 1128 | CLA  | O2A-CGA-O1A | -5.12 | 110.67      | 123.59   |
| 14  | A     | 1105 | CLA  | C3D-C2D-C1D | -5.12 | 98.85       | 105.83   |
| 14  | b     | 1208 | CLA  | O2A-CGA-CBA | 5.12  | 127.97      | 111.91   |
| 14  | B     | 1231 | CLA  | C1C-C2C-C3C | -5.12 | 101.58      | 106.96   |
| 14  | a     | 1107 | CLA  | CHD-C1D-ND  | -5.12 | 119.75      | 124.45   |
| 14  | G     | 1128 | CLA  | O2A-CGA-O1A | -5.12 | 110.68      | 123.59   |
| 14  | a     | 1119 | CLA  | CHD-C1D-ND  | -5.12 | 119.75      | 124.45   |
| 18  | a     | 4002 | BCR  | C24-C23-C22 | -5.12 | 118.50      | 126.23   |
| 14  | b     | 1231 | CLA  | C3D-C2D-C1D | -5.12 | 98.85       | 105.83   |
| 15  | H     | 1230 | F6C  | C1A-C2A-C3A | -5.11 | 101.58      | 106.97   |
| 14  | G     | 1107 | CLA  | CHD-C1D-ND  | -5.11 | 119.75      | 124.45   |
| 14  | G     | 1105 | CLA  | C3D-C2D-C1D | -5.11 | 98.85       | 105.83   |
| 14  | U     | 1503 | CLA  | C4A-NA-C1A  | 5.11  | 109.00      | 106.71   |
| 14  | A     | 1128 | CLA  | O2A-C1-C2   | 5.11  | 122.07      | 108.64   |
| 14  | A     | 1141 | CLA  | C1C-C2C-C3C | -5.11 | 101.58      | 106.96   |
| 14  | a     | 1128 | CLA  | O2A-C1-C2   | 5.11  | 122.07      | 108.64   |
| 14  | A     | 1107 | CLA  | CHD-C1D-ND  | -5.11 | 119.76      | 124.45   |
| 14  | H     | 1224 | CLA  | O2A-C1-C2   | 5.11  | 122.07      | 108.64   |
| 14  | a     | 1106 | CLA  | C4A-NA-C1A  | 5.11  | 109.00      | 106.71   |
| 14  | G     | 1139 | CLA  | CHD-C1D-ND  | -5.11 | 119.76      | 124.45   |
| 14  | a     | 1128 | CLA  | O2A-CGA-O1A | -5.11 | 110.69      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1119 | CLA  | CHD-C1D-ND  | -5.11 | 119.76      | 124.45   |
| 14  | B     | 1231 | CLA  | C3D-C2D-C1D | -5.11 | 98.86       | 105.83   |
| 14  | G     | 1106 | CLA  | C4A-NA-C1A  | 5.11  | 109.00      | 106.71   |
| 14  | B     | 1023 | CLA  | O2A-C1-C2   | 5.11  | 122.06      | 108.64   |
| 14  | A     | 1106 | CLA  | CHD-C1D-ND  | -5.11 | 119.76      | 124.45   |
| 14  | b     | 1231 | CLA  | C4A-NA-C1A  | 5.11  | 109.00      | 106.71   |
| 14  | B     | 1206 | CLA  | C3D-C2D-C1D | -5.11 | 98.86       | 105.83   |
| 14  | A     | 1110 | CLA  | C1C-C2C-C3C | -5.10 | 101.59      | 106.96   |
| 14  | b     | 1204 | CLA  | C1D-ND-C4D  | -5.10 | 102.71      | 106.33   |
| 14  | G     | 1128 | CLA  | C3D-C2D-C1D | -5.10 | 98.87       | 105.83   |
| 14  | b     | 1023 | CLA  | O2A-C1-C2   | 5.10  | 122.04      | 108.64   |
| 14  | A     | 1106 | CLA  | C4A-NA-C1A  | 5.10  | 109.00      | 106.71   |
| 14  | A     | 1125 | CLA  | C1D-ND-C4D  | -5.10 | 102.71      | 106.33   |
| 14  | G     | 1110 | CLA  | C1C-C2C-C3C | -5.10 | 101.59      | 106.96   |
| 14  | b     | 1229 | CLA  | O2A-CGA-O1A | -5.10 | 110.72      | 123.59   |
| 14  | b     | 1023 | CLA  | C1D-ND-C4D  | -5.10 | 102.71      | 106.33   |
| 14  | H     | 1231 | CLA  | C3D-C2D-C1D | -5.10 | 98.87       | 105.83   |
| 14  | B     | 1217 | CLA  | C3D-C2D-C1D | -5.10 | 98.87       | 105.83   |
| 15  | b     | 1230 | F6C  | C1A-C2A-C3A | -5.10 | 101.60      | 106.97   |
| 14  | a     | 1120 | CLA  | C1D-ND-C4D  | -5.10 | 102.71      | 106.33   |
| 14  | a     | 1113 | CLA  | O2D-CGD-CBD | 5.10  | 120.32      | 111.27   |
| 14  | H     | 1220 | CLA  | CHD-C1D-ND  | -5.10 | 119.77      | 124.45   |
| 14  | B     | 1204 | CLA  | C1D-ND-C4D  | -5.10 | 102.72      | 106.33   |
| 14  | H     | 1229 | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 15  | B     | 1230 | F6C  | C1A-C2A-C3A | -5.09 | 101.61      | 106.97   |
| 14  | a     | 1141 | CLA  | C1C-C2C-C3C | -5.09 | 101.60      | 106.96   |
| 14  | G     | 1128 | CLA  | O2A-C1-C2   | 5.09  | 122.02      | 108.64   |
| 14  | a     | 1113 | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 14  | a     | 1117 | CLA  | C4A-NA-C1A  | 5.09  | 109.00      | 106.71   |
| 14  | b     | 1217 | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 14  | b     | 1206 | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 14  | G     | 1125 | CLA  | C1D-ND-C4D  | -5.09 | 102.72      | 106.33   |
| 14  | H     | 1217 | CLA  | C3D-C2D-C1D | -5.09 | 98.89       | 105.83   |
| 14  | H     | 1229 | CLA  | O2A-CGA-O1A | -5.09 | 110.75      | 123.59   |
| 14  | A     | 1119 | CLA  | C3D-C2D-C1D | -5.09 | 98.89       | 105.83   |
| 14  | a     | 1128 | CLA  | C3D-C2D-C1D | -5.09 | 98.89       | 105.83   |
| 14  | A     | 1120 | CLA  | C1D-ND-C4D  | -5.09 | 102.72      | 106.33   |
| 14  | H     | 1233 | CLA  | C3D-C2D-C1D | -5.08 | 98.89       | 105.83   |
| 14  | B     | 1232 | CLA  | C4A-NA-C1A  | 5.08  | 108.99      | 106.71   |
| 14  | A     | 1109 | CLA  | O2A-C1-C2   | 5.08  | 121.99      | 108.64   |
| 14  | A     | 1128 | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 14  | L     | 1501 | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1222 | CLA  | C1C-C2C-C3C | -5.08 | 101.61      | 106.96   |
| 14  | a     | 1139 | CLA  | CHD-C1D-ND  | -5.08 | 119.78      | 124.45   |
| 15  | b     | 1219 | F6C  | C3A-C4A-NA  | 5.08  | 113.85      | 110.10   |
| 14  | a     | 1131 | CLA  | O2A-CGA-O1A | -5.08 | 110.77      | 123.59   |
| 14  | G     | 1109 | CLA  | O2A-C1-C2   | 5.08  | 121.98      | 108.64   |
| 14  | B     | 1226 | CLA  | O2A-CGA-CBA | 5.08  | 127.84      | 111.91   |
| 14  | H     | 1226 | CLA  | O2A-CGA-CBA | 5.08  | 127.84      | 111.91   |
| 14  | U     | 1501 | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 14  | G     | 1119 | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 14  | H     | 1214 | CLA  | CHD-C1D-ND  | -5.08 | 119.79      | 124.45   |
| 14  | B     | 1229 | CLA  | O2A-CGA-O1A | -5.08 | 110.78      | 123.59   |
| 14  | B     | 1232 | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 14  | a     | 1104 | CLA  | O2A-C1-C2   | 5.08  | 121.98      | 108.64   |
| 14  | A     | 1104 | CLA  | O2A-C1-C2   | 5.08  | 121.97      | 108.64   |
| 14  | H     | 1202 | CLA  | C1C-C2C-C3C | -5.08 | 101.62      | 106.96   |
| 14  | A     | 1136 | CLA  | O2A-CGA-CBA | 5.07  | 127.83      | 111.91   |
| 14  | G     | 1136 | CLA  | O2A-CGA-CBA | 5.07  | 127.83      | 111.91   |
| 14  | H     | 1218 | CLA  | C1D-ND-C4D  | -5.07 | 102.73      | 106.33   |
| 14  | B     | 1229 | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 14  | A     | 1118 | CLA  | C1C-C2C-C3C | -5.07 | 101.62      | 106.96   |
| 14  | B     | 1202 | CLA  | C1C-C2C-C3C | -5.07 | 101.62      | 106.96   |
| 14  | B     | 1206 | CLA  | O2D-CGD-CBD | 5.07  | 120.28      | 111.27   |
| 14  | A     | 1139 | CLA  | CHD-C1D-ND  | -5.07 | 119.79      | 124.45   |
| 14  | b     | 1226 | CLA  | O2A-CGA-CBA | 5.07  | 127.82      | 111.91   |
| 14  | b     | 1232 | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 14  | a     | 1130 | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 14  | l     | 1501 | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 14  | a     | 1136 | CLA  | O2A-CGA-CBA | 5.07  | 127.82      | 111.91   |
| 14  | a     | 1109 | CLA  | O2A-C1-C2   | 5.07  | 121.96      | 108.64   |
| 14  | b     | 1232 | CLA  | C4A-NA-C1A  | 5.07  | 108.98      | 106.71   |
| 15  | G     | 1121 | F6C  | C3A-C4A-NA  | 5.07  | 113.84      | 110.10   |
| 14  | a     | 1013 | CLA  | CMB-C2B-C3B | 5.07  | 134.16      | 124.68   |
| 15  | a     | 1121 | F6C  | C3A-C4A-NA  | 5.07  | 113.84      | 110.10   |
| 14  | L     | 1503 | CLA  | C1C-C2C-C3C | -5.07 | 101.63      | 106.96   |
| 14  | b     | 1202 | CLA  | C1C-C2C-C3C | -5.07 | 101.63      | 106.96   |
| 14  | G     | 1013 | CLA  | CHD-C1D-ND  | -5.07 | 119.80      | 124.45   |
| 14  | b     | 1224 | CLA  | CHD-C1D-ND  | -5.07 | 119.80      | 124.45   |
| 14  | B     | 1233 | CLA  | C3D-C2D-C1D | -5.07 | 98.92       | 105.83   |
| 14  | b     | 1229 | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 14  | B     | 1234 | CLA  | C1D-ND-C4D  | -5.06 | 102.74      | 106.33   |
| 14  | A     | 1122 | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 14  | b     | 1234 | CLA  | C1D-ND-C4D  | -5.06 | 102.74      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1206 | CLA  | O2A-CGA-O1A | -5.06 | 110.81      | 123.59   |
| 14  | B     | 1214 | CLA  | CHD-C1D-ND  | -5.06 | 119.80      | 124.45   |
| 14  | G     | 1131 | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 14  | H     | 1206 | CLA  | O2D-CGD-CBD | 5.06  | 120.27      | 111.27   |
| 14  | a     | 1118 | CLA  | C1C-C2C-C3C | -5.06 | 101.63      | 106.96   |
| 14  | A     | 1013 | CLA  | CHD-C1D-ND  | -5.06 | 119.80      | 124.45   |
| 14  | A     | 1113 | CLA  | O2D-CGD-CBD | 5.06  | 120.26      | 111.27   |
| 14  | b     | 1216 | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 14  | H     | 1232 | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 14  | H     | 1216 | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 14  | G     | 1113 | CLA  | O2D-CGD-CBD | 5.06  | 120.26      | 111.27   |
| 14  | A     | 1131 | CLA  | O2A-CGA-O1A | -5.06 | 110.82      | 123.59   |
| 14  | B     | 1232 | CLA  | CHD-C1D-ND  | -5.06 | 119.80      | 124.45   |
| 14  | G     | 1118 | CLA  | C1C-C2C-C3C | -5.06 | 101.64      | 106.96   |
| 14  | a     | 1119 | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 14  | G     | 1120 | CLA  | C1D-ND-C4D  | -5.06 | 102.74      | 106.33   |
| 14  | a     | 1122 | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 14  | U     | 1503 | CLA  | C1C-C2C-C3C | -5.06 | 101.64      | 106.96   |
| 14  | l     | 1503 | CLA  | C1C-C2C-C3C | -5.06 | 101.64      | 106.96   |
| 14  | G     | 1104 | CLA  | O2A-C1-C2   | 5.06  | 121.93      | 108.64   |
| 14  | B     | 1206 | CLA  | O2A-CGA-O1A | -5.06 | 110.83      | 123.59   |
| 14  | A     | 1123 | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 14  | b     | 1220 | CLA  | CHD-C1D-ND  | -5.06 | 119.81      | 124.45   |
| 14  | A     | 1013 | CLA  | CMB-C2B-C3B | 5.06  | 134.14      | 124.68   |
| 18  | m     | 4021 | BCR  | C7-C8-C9    | -5.06 | 118.60      | 126.23   |
| 14  | B     | 1220 | CLA  | CHD-C1D-ND  | -5.05 | 119.81      | 124.45   |
| 14  | b     | 1214 | CLA  | CHD-C1D-ND  | -5.05 | 119.81      | 124.45   |
| 14  | G     | 1105 | CLA  | O2D-CGD-CBD | 5.05  | 120.25      | 111.27   |
| 14  | G     | 1131 | CLA  | O2A-CGA-O1A | -5.05 | 110.84      | 123.59   |
| 14  | A     | 1130 | CLA  | C3D-C2D-C1D | -5.05 | 98.94       | 105.83   |
| 14  | L     | 1501 | CLA  | C1D-ND-C4D  | -5.05 | 102.75      | 106.33   |
| 14  | b     | 1233 | CLA  | O2A-CGA-O1A | -5.05 | 110.71      | 123.30   |
| 14  | B     | 1224 | CLA  | CHD-C1D-ND  | -5.05 | 119.81      | 124.45   |
| 14  | G     | 1122 | CLA  | C3D-C2D-C1D | -5.05 | 98.94       | 105.83   |
| 14  | a     | 1133 | CLA  | O2D-CGD-CBD | 5.05  | 120.24      | 111.27   |
| 14  | H     | 1214 | CLA  | C3D-C2D-C1D | -5.05 | 98.94       | 105.83   |
| 14  | U     | 1501 | CLA  | C1D-ND-C4D  | -5.05 | 102.75      | 106.33   |
| 14  | A     | 1105 | CLA  | O2D-CGD-CBD | 5.05  | 120.23      | 111.27   |
| 14  | b     | 1206 | CLA  | O2D-CGD-CBD | 5.05  | 120.23      | 111.27   |
| 14  | G     | 1141 | CLA  | C1C-C2C-C3C | -5.05 | 101.65      | 106.96   |
| 14  | B     | 1216 | CLA  | C3D-C2D-C1D | -5.05 | 98.95       | 105.83   |
| 14  | V     | 1501 | CLA  | C4A-NA-C1A  | 5.04  | 108.97      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1123 | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 14  | B     | 1222 | CLA  | C1C-C2C-C3C | -5.04 | 101.65      | 106.96   |
| 14  | G     | 1130 | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 14  | b     | 1233 | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 18  | V     | 4021 | BCR  | C7-C8-C9    | -5.04 | 118.61      | 126.23   |
| 14  | H     | 1233 | CLA  | O2A-CGA-O1A | -5.04 | 110.73      | 123.30   |
| 14  | a     | 1106 | CLA  | CHD-C1D-ND  | -5.04 | 119.82      | 124.45   |
| 14  | G     | 1013 | CLA  | CMB-C2B-C3B | 5.04  | 134.11      | 124.68   |
| 14  | H     | 1222 | CLA  | C1C-C2C-C3C | -5.04 | 101.66      | 106.96   |
| 14  | A     | 1140 | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 14  | a     | 1123 | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 14  | H     | 1206 | CLA  | O2A-CGA-O1A | -5.04 | 110.88      | 123.59   |
| 14  | B     | 1214 | CLA  | C3D-C2D-C1D | -5.04 | 98.96       | 105.83   |
| 14  | l     | 1501 | CLA  | C1D-ND-C4D  | -5.04 | 102.76      | 106.33   |
| 14  | H     | 1232 | CLA  | C4A-NA-C1A  | 5.03  | 108.97      | 106.71   |
| 14  | a     | 1129 | CLA  | C1C-C2C-C3C | -5.03 | 101.67      | 106.96   |
| 14  | a     | 1111 | CLA  | CHD-C1D-ND  | -5.03 | 119.83      | 124.45   |
| 14  | A     | 1133 | CLA  | O2D-CGD-CBD | 5.03  | 120.21      | 111.27   |
| 14  | G     | 1133 | CLA  | O2D-CGD-CBD | 5.03  | 120.21      | 111.27   |
| 15  | b     | 1238 | F6C  | O2A-CGA-O1A | -5.03 | 110.89      | 123.59   |
| 18  | M     | 4021 | BCR  | C7-C8-C9    | -5.03 | 118.63      | 126.23   |
| 14  | G     | 1140 | CLA  | C3D-C2D-C1D | -5.03 | 98.97       | 105.83   |
| 14  | b     | 1214 | CLA  | C3D-C2D-C1D | -5.03 | 98.97       | 105.83   |
| 14  | H     | 1234 | CLA  | C1D-ND-C4D  | -5.03 | 102.76      | 106.33   |
| 14  | a     | 1107 | CLA  | C3D-C2D-C1D | -5.03 | 98.97       | 105.83   |
| 14  | G     | 1124 | CLA  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 14  | B     | 1233 | CLA  | O2A-CGA-O1A | -5.03 | 110.77      | 123.30   |
| 14  | a     | 1140 | CLA  | C3D-C2D-C1D | -5.02 | 98.97       | 105.83   |
| 14  | a     | 1105 | CLA  | O2D-CGD-CBD | 5.02  | 120.20      | 111.27   |
| 14  | b     | 1202 | CLA  | CHD-C1D-ND  | -5.02 | 119.84      | 124.45   |
| 15  | B     | 1238 | F6C  | O2A-CGA-O1A | -5.02 | 110.92      | 123.59   |
| 14  | a     | 1105 | CLA  | O2A-CGA-O1A | -5.02 | 110.79      | 123.30   |
| 14  | H     | 1222 | CLA  | O2A-C1-C2   | 5.02  | 121.82      | 108.64   |
| 14  | A     | 1107 | CLA  | C3D-C2D-C1D | -5.02 | 98.98       | 105.83   |
| 14  | B     | 1023 | CLA  | C1D-ND-C4D  | -5.02 | 102.77      | 106.33   |
| 14  | A     | 1124 | CLA  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 14  | G     | 1105 | CLA  | O2A-CGA-O1A | -5.02 | 110.80      | 123.30   |
| 14  | H     | 1224 | CLA  | C4A-NA-C1A  | 5.02  | 108.96      | 106.71   |
| 14  | a     | 1131 | CLA  | C3D-C2D-C1D | -5.02 | 98.99       | 105.83   |
| 14  | a     | 1013 | CLA  | CHD-C1D-ND  | -5.02 | 119.84      | 124.45   |
| 14  | a     | 1124 | CLA  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 14  | B     | 1222 | CLA  | O2A-C1-C2   | 5.01  | 121.81      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1111 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 14  | G     | 1111 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 14  | H     | 1224 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 14  | b     | 1232 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 14  | H     | 1235 | CLA  | C1C-C2C-C3C | -5.01 | 101.69      | 106.96   |
| 15  | A     | 1121 | F6C  | C3A-C4A-NA  | 5.01  | 113.80      | 110.10   |
| 14  | H     | 1023 | CLA  | C1D-ND-C4D  | -5.01 | 102.78      | 106.33   |
| 14  | b     | 1224 | CLA  | O2A-CGA-CBA | 5.01  | 127.63      | 111.91   |
| 14  | A     | 1131 | CLA  | C3D-C2D-C1D | -5.01 | 98.99       | 105.83   |
| 14  | b     | 1222 | CLA  | O2A-C1-C2   | 5.01  | 121.80      | 108.64   |
| 14  | G     | 1106 | CLA  | O2A-CGA-O1A | -5.01 | 110.95      | 123.59   |
| 14  | H     | 1232 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 14  | A     | 1105 | CLA  | O2A-CGA-O1A | -5.01 | 110.81      | 123.30   |
| 14  | a     | 1106 | CLA  | O2A-CGA-O1A | -5.01 | 110.96      | 123.59   |
| 14  | G     | 1107 | CLA  | C3D-C2D-C1D | -5.01 | 99.00       | 105.83   |
| 13  | A     | 1011 | CL0  | O2A-CGA-O1A | -5.01 | 110.96      | 123.59   |
| 13  | a     | 1011 | CL0  | O2A-CGA-O1A | -5.01 | 110.96      | 123.59   |
| 14  | B     | 1235 | CLA  | C1C-C2C-C3C | -5.00 | 101.69      | 106.96   |
| 14  | B     | 1224 | CLA  | O2A-CGA-CBA | 5.00  | 127.61      | 111.91   |
| 14  | H     | 1224 | CLA  | O2A-CGA-CBA | 5.00  | 127.61      | 111.91   |
| 14  | A     | 1106 | CLA  | O2A-CGA-O1A | -5.00 | 110.97      | 123.59   |
| 14  | B     | 1212 | CLA  | C4A-NA-C1A  | 5.00  | 108.95      | 106.71   |
| 14  | A     | 1129 | CLA  | C1C-C2C-C3C | -5.00 | 101.70      | 106.96   |
| 14  | b     | 1236 | CLA  | O2A-C1-C2   | 5.00  | 121.78      | 108.64   |
| 14  | a     | 1114 | CLA  | C3D-C2D-C1D | -5.00 | 99.01       | 105.83   |
| 14  | a     | 1119 | CLA  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 15  | H     | 1238 | F6C  | O2A-CGA-O1A | -5.00 | 110.97      | 123.59   |
| 14  | G     | 1118 | CLA  | C3D-C2D-C1D | -5.00 | 99.01       | 105.83   |
| 14  | m     | 1501 | CLA  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 14  | B     | 1202 | CLA  | CHD-C1D-ND  | -4.99 | 119.86      | 124.45   |
| 14  | a     | 1118 | CLA  | C3D-C2D-C1D | -4.99 | 99.02       | 105.83   |
| 14  | B     | 1231 | CLA  | O2A-C1-C2   | 4.99  | 121.76      | 108.64   |
| 14  | H     | 1211 | CLA  | C1D-ND-C4D  | -4.99 | 102.79      | 106.33   |
| 14  | G     | 1114 | CLA  | C3D-C2D-C1D | -4.99 | 99.02       | 105.83   |
| 13  | G     | 1011 | CL0  | O2A-CGA-O1A | -4.99 | 110.99      | 123.59   |
| 14  | A     | 1119 | CLA  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 14  | B     | 1236 | CLA  | O2A-C1-C2   | 4.99  | 121.75      | 108.64   |
| 14  | G     | 1115 | CLA  | CHD-C1D-ND  | -4.99 | 119.87      | 124.45   |
| 14  | B     | 1211 | CLA  | C1D-ND-C4D  | -4.99 | 102.79      | 106.33   |
| 14  | b     | 1223 | CLA  | O2A-C1-C2   | 4.99  | 121.74      | 108.64   |
| 14  | a     | 1113 | CLA  | C1C-C2C-C3C | -4.99 | 101.71      | 106.96   |
| 14  | b     | 1231 | CLA  | O2A-C1-C2   | 4.99  | 121.74      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1202 | CLA  | CHD-C1D-ND  | -4.99 | 119.87      | 124.45   |
| 14  | H     | 1236 | CLA  | O2A-C1-C2   | 4.99  | 121.74      | 108.64   |
| 14  | B     | 1211 | CLA  | C3D-C2D-C1D | -4.98 | 99.03       | 105.83   |
| 14  | B     | 1225 | CLA  | C4A-NA-C1A  | 4.98  | 108.95      | 106.71   |
| 14  | G     | 1119 | CLA  | O2D-CGD-CBD | 4.98  | 120.12      | 111.27   |
| 14  | H     | 1231 | CLA  | O2A-C1-C2   | 4.98  | 121.73      | 108.64   |
| 14  | A     | 1118 | CLA  | C3D-C2D-C1D | -4.98 | 99.03       | 105.83   |
| 14  | M     | 1501 | CLA  | O2D-CGD-CBD | 4.98  | 120.12      | 111.27   |
| 14  | G     | 1129 | CLA  | C1C-C2C-C3C | -4.98 | 101.72      | 106.96   |
| 14  | G     | 1120 | CLA  | O2A-CGA-O1A | -4.98 | 110.89      | 123.30   |
| 14  | b     | 1225 | CLA  | C4A-NA-C1A  | 4.98  | 108.94      | 106.71   |
| 14  | b     | 1216 | CLA  | C1C-C2C-C3C | -4.98 | 101.72      | 106.96   |
| 14  | A     | 1114 | CLA  | C3D-C2D-C1D | -4.98 | 99.04       | 105.83   |
| 14  | H     | 1213 | CLA  | C4A-NA-C1A  | 4.98  | 108.94      | 106.71   |
| 14  | A     | 1120 | CLA  | O2A-CGA-O1A | -4.98 | 110.89      | 123.30   |
| 14  | m     | 1501 | CLA  | O2A-CGA-O1A | -4.98 | 111.03      | 123.59   |
| 15  | b     | 1238 | F6C  | O2D-CGD-CBD | 4.98  | 120.11      | 111.27   |
| 14  | A     | 1141 | CLA  | CHD-C1D-ND  | -4.97 | 119.88      | 124.45   |
| 14  | b     | 1211 | CLA  | C3D-C2D-C1D | -4.97 | 99.04       | 105.83   |
| 14  | B     | 1223 | CLA  | O2A-C1-C2   | 4.97  | 121.70      | 108.64   |
| 14  | H     | 1223 | CLA  | O2A-C1-C2   | 4.97  | 121.70      | 108.64   |
| 14  | G     | 1113 | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 14  | a     | 1112 | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 15  | B     | 1238 | F6C  | O2D-CGD-CBD | 4.97  | 120.10      | 111.27   |
| 15  | H     | 1238 | F6C  | O2D-CGD-CBD | 4.97  | 120.09      | 111.27   |
| 14  | b     | 1209 | CLA  | O2A-CGA-O1A | -4.97 | 110.92      | 123.30   |
| 14  | A     | 1110 | CLA  | O2A-CGA-O1A | -4.97 | 110.92      | 123.30   |
| 14  | G     | 1112 | CLA  | CHD-C1D-ND  | -4.96 | 119.89      | 124.45   |
| 14  | H     | 1209 | CLA  | O2A-CGA-O1A | -4.96 | 110.93      | 123.30   |
| 14  | V     | 1501 | CLA  | O2D-CGD-CBD | 4.96  | 120.09      | 111.27   |
| 14  | a     | 1110 | CLA  | O2A-CGA-O1A | -4.96 | 110.93      | 123.30   |
| 14  | b     | 1235 | CLA  | C1C-C2C-C3C | -4.96 | 101.74      | 106.96   |
| 14  | H     | 1213 | CLA  | O2A-CGA-O1A | -4.96 | 110.94      | 123.30   |
| 14  | a     | 1128 | CLA  | CHD-C1D-ND  | -4.96 | 119.90      | 124.45   |
| 14  | G     | 1110 | CLA  | O2A-CGA-O1A | -4.96 | 110.94      | 123.30   |
| 14  | B     | 1209 | CLA  | O2A-CGA-O1A | -4.96 | 110.94      | 123.30   |
| 14  | a     | 1120 | CLA  | O2A-CGA-O1A | -4.96 | 110.94      | 123.30   |
| 14  | A     | 1115 | CLA  | CHD-C1D-ND  | -4.96 | 119.90      | 124.45   |
| 14  | a     | 1107 | CLA  | O2A-CGA-O1A | -4.96 | 110.94      | 123.30   |
| 14  | H     | 1233 | CLA  | O2D-CGD-CBD | 4.96  | 120.08      | 111.27   |
| 15  | H     | 1238 | F6C  | C3A-C4A-NA  | 4.96  | 113.76      | 110.10   |
| 14  | B     | 1213 | CLA  | O2A-CGA-O1A | -4.96 | 110.95      | 123.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1233 | CLA  | O2D-CGD-CBD | 4.96  | 120.07      | 111.27   |
| 14  | A     | 1112 | CLA  | CHD-C1D-ND  | -4.96 | 119.90      | 124.45   |
| 14  | A     | 1134 | CLA  | CHD-C1D-ND  | -4.96 | 119.90      | 124.45   |
| 14  | b     | 1213 | CLA  | O2A-CGA-O1A | -4.95 | 110.95      | 123.30   |
| 14  | G     | 1118 | CLA  | CHD-C1D-ND  | -4.95 | 119.90      | 124.45   |
| 14  | A     | 1107 | CLA  | O2A-CGA-O1A | -4.95 | 110.95      | 123.30   |
| 14  | G     | 1107 | CLA  | O2A-CGA-O1A | -4.95 | 110.95      | 123.30   |
| 14  | A     | 1113 | CLA  | C1C-C2C-C3C | -4.95 | 101.75      | 106.96   |
| 15  | b     | 1238 | F6C  | C3A-C4A-NA  | 4.95  | 113.75      | 110.10   |
| 14  | G     | 1112 | CLA  | C1C-C2C-C3C | -4.95 | 101.75      | 106.96   |
| 14  | H     | 1222 | CLA  | O2A-CGA-O1A | -4.95 | 111.09      | 123.59   |
| 14  | B     | 1222 | CLA  | O2A-CGA-O1A | -4.95 | 111.10      | 123.59   |
| 14  | H     | 1205 | CLA  | C1D-ND-C4D  | -4.95 | 102.82      | 106.33   |
| 14  | M     | 1501 | CLA  | O2A-CGA-O1A | -4.95 | 111.11      | 123.59   |
| 14  | A     | 1128 | CLA  | CHD-C1D-ND  | -4.95 | 119.91      | 124.45   |
| 14  | B     | 1216 | CLA  | C1C-C2C-C3C | -4.95 | 101.76      | 106.96   |
| 14  | a     | 1108 | CLA  | C1C-C2C-C3C | -4.95 | 101.76      | 106.96   |
| 14  | b     | 1211 | CLA  | C1D-ND-C4D  | -4.95 | 102.82      | 106.33   |
| 14  | B     | 1233 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 14  | a     | 1141 | CLA  | CHD-C1D-ND  | -4.95 | 119.91      | 124.45   |
| 14  | b     | 1222 | CLA  | O2A-CGA-O1A | -4.95 | 111.11      | 123.59   |
| 14  | G     | 1108 | CLA  | C1C-C2C-C3C | -4.94 | 101.76      | 106.96   |
| 14  | H     | 1216 | CLA  | C1C-C2C-C3C | -4.94 | 101.76      | 106.96   |
| 14  | A     | 1124 | CLA  | CHD-C1D-ND  | -4.94 | 119.91      | 124.45   |
| 14  | G     | 1128 | CLA  | CHD-C1D-ND  | -4.94 | 119.91      | 124.45   |
| 14  | G     | 1141 | CLA  | CHD-C1D-ND  | -4.94 | 119.91      | 124.45   |
| 14  | H     | 1211 | CLA  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 14  | V     | 1501 | CLA  | O2A-CGA-O1A | -4.94 | 111.12      | 123.59   |
| 14  | b     | 1212 | CLA  | O2A-CGA-O1A | -4.94 | 110.99      | 123.30   |
| 14  | G     | 1133 | CLA  | O2A-CGA-O1A | -4.94 | 111.13      | 123.59   |
| 14  | H     | 1212 | CLA  | O2A-CGA-O1A | -4.94 | 110.99      | 123.30   |
| 14  | A     | 1108 | CLA  | C1C-C2C-C3C | -4.94 | 101.77      | 106.96   |
| 14  | H     | 1228 | CLA  | O2A-C1-C2   | 4.94  | 121.61      | 108.64   |
| 14  | B     | 1212 | CLA  | O2A-CGA-O1A | -4.94 | 111.00      | 123.30   |
| 14  | B     | 1224 | CLA  | C4A-NA-C1A  | 4.94  | 108.92      | 106.71   |
| 14  | G     | 1133 | CLA  | CHD-C1D-ND  | -4.93 | 119.92      | 124.45   |
| 14  | L     | 1502 | CLA  | C1D-ND-C4D  | -4.93 | 102.83      | 106.33   |
| 14  | A     | 1140 | CLA  | C4A-NA-C1A  | 4.93  | 108.92      | 106.71   |
| 14  | a     | 1101 | CLA  | C3D-C2D-C1D | -4.93 | 99.10       | 105.83   |
| 14  | H     | 1021 | CLA  | C1C-C2C-C3C | -4.93 | 101.77      | 106.96   |
| 14  | a     | 1112 | CLA  | CHD-C1D-ND  | -4.93 | 119.92      | 124.45   |
| 14  | B     | 1213 | CLA  | C4A-NA-C1A  | 4.93  | 108.92      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | M     | 1501 | CLA  | C4A-NA-C1A  | 4.93  | 108.92      | 106.71   |
| 14  | B     | 1228 | CLA  | O2A-C1-C2   | 4.93  | 121.59      | 108.64   |
| 14  | b     | 1021 | CLA  | C1C-C2C-C3C | -4.93 | 101.77      | 106.96   |
| 14  | A     | 1133 | CLA  | O2A-CGA-O1A | -4.93 | 111.15      | 123.59   |
| 14  | a     | 1126 | CLA  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 14  | H     | 1212 | CLA  | C4A-NA-C1A  | 4.93  | 108.92      | 106.71   |
| 14  | a     | 1133 | CLA  | O2A-CGA-O1A | -4.93 | 111.16      | 123.59   |
| 14  | G     | 1110 | CLA  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 14  | A     | 1101 | CLA  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 14  | a     | 1102 | CLA  | C1C-C2C-C3C | -4.93 | 101.78      | 106.96   |
| 15  | A     | 1121 | F6C  | O2A-CGA-O1A | -4.93 | 111.02      | 123.30   |
| 14  | a     | 1135 | CLA  | CHD-C1D-ND  | -4.93 | 119.93      | 124.45   |
| 14  | G     | 1124 | CLA  | CHD-C1D-ND  | -4.92 | 119.93      | 124.45   |
| 14  | a     | 1129 | CLA  | O2A-C1-C2   | 4.92  | 121.57      | 108.64   |
| 14  | b     | 1212 | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | a     | 1110 | CLA  | C3D-C2D-C1D | -4.92 | 99.11       | 105.83   |
| 14  | B     | 1205 | CLA  | C1D-ND-C4D  | -4.92 | 102.84      | 106.33   |
| 14  | G     | 1116 | CLA  | C1C-C2C-C3C | -4.92 | 101.78      | 106.96   |
| 14  | G     | 1126 | CLA  | C3D-C2D-C1D | -4.92 | 99.12       | 105.83   |
| 14  | A     | 1129 | CLA  | O2A-C1-C2   | 4.92  | 121.56      | 108.64   |
| 14  | G     | 1129 | CLA  | O2A-C1-C2   | 4.92  | 121.56      | 108.64   |
| 14  | A     | 1119 | CLA  | C1C-C2C-C3C | -4.92 | 101.78      | 106.96   |
| 14  | a     | 1134 | CLA  | CHD-C1D-ND  | -4.92 | 119.93      | 124.45   |
| 14  | A     | 1112 | CLA  | C1C-C2C-C3C | -4.92 | 101.79      | 106.96   |
| 14  | a     | 1124 | CLA  | O2A-C1-C2   | 4.92  | 121.56      | 108.64   |
| 14  | A     | 1110 | CLA  | C3D-C2D-C1D | -4.92 | 99.12       | 105.83   |
| 14  | a     | 1140 | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 15  | B     | 1238 | F6C  | C3A-C4A-NA  | 4.91  | 113.73      | 110.10   |
| 14  | G     | 1124 | CLA  | O2A-C1-C2   | 4.91  | 121.55      | 108.64   |
| 14  | B     | 1021 | CLA  | C1C-C2C-C3C | -4.91 | 101.79      | 106.96   |
| 14  | b     | 1235 | CLA  | C1D-ND-C4D  | -4.91 | 102.84      | 106.33   |
| 14  | b     | 1228 | CLA  | O2A-C1-C2   | 4.91  | 121.55      | 108.64   |
| 15  | a     | 1121 | F6C  | O2A-CGA-O1A | -4.91 | 111.05      | 123.30   |
| 14  | a     | 1115 | CLA  | CHD-C1D-ND  | -4.91 | 119.94      | 124.45   |
| 14  | B     | 1231 | CLA  | C1D-ND-C4D  | -4.91 | 102.85      | 106.33   |
| 14  | B     | 1203 | CLA  | O2A-CGA-O1A | -4.91 | 111.20      | 123.59   |
| 15  | G     | 1121 | F6C  | O2A-CGA-O1A | -4.91 | 111.06      | 123.30   |
| 14  | A     | 1124 | CLA  | O2A-C1-C2   | 4.91  | 121.54      | 108.64   |
| 14  | A     | 1126 | CLA  | C3D-C2D-C1D | -4.91 | 99.13       | 105.83   |
| 14  | U     | 1502 | CLA  | C1D-ND-C4D  | -4.91 | 102.85      | 106.33   |
| 14  | G     | 1134 | CLA  | CHD-C1D-ND  | -4.91 | 119.94      | 124.45   |
| 14  | H     | 1203 | CLA  | O2A-CGA-O1A | -4.91 | 111.21      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | l     | 1502 | CLA  | C1D-ND-C4D  | -4.91 | 102.85      | 106.33   |
| 14  | A     | 1116 | CLA  | C1C-C2C-C3C | -4.91 | 101.80      | 106.96   |
| 14  | G     | 1102 | CLA  | C1C-C2C-C3C | -4.90 | 101.80      | 106.96   |
| 14  | A     | 1118 | CLA  | CHD-C1D-ND  | -4.90 | 119.95      | 124.45   |
| 14  | H     | 1227 | CLA  | C4A-NA-C1A  | 4.90  | 108.91      | 106.71   |
| 14  | a     | 1127 | CLA  | O2A-CGA-O1A | -4.90 | 111.23      | 123.59   |
| 14  | b     | 1203 | CLA  | O2A-CGA-O1A | -4.90 | 111.23      | 123.59   |
| 14  | A     | 1102 | CLA  | C1C-C2C-C3C | -4.90 | 101.81      | 106.96   |
| 14  | H     | 1201 | CLA  | C1C-C2C-C3C | -4.90 | 101.81      | 106.96   |
| 14  | G     | 1101 | CLA  | C3D-C2D-C1D | -4.89 | 99.15       | 105.83   |
| 14  | G     | 1119 | CLA  | C1C-C2C-C3C | -4.89 | 101.81      | 106.96   |
| 14  | a     | 1101 | CLA  | C4A-NA-C1A  | 4.89  | 108.91      | 106.71   |
| 14  | B     | 1201 | CLA  | C1C-C2C-C3C | -4.89 | 101.81      | 106.96   |
| 14  | a     | 1116 | CLA  | C1C-C2C-C3C | -4.89 | 101.81      | 106.96   |
| 14  | H     | 1214 | CLA  | O2A-CGA-O1A | -4.89 | 111.26      | 123.59   |
| 14  | B     | 1214 | CLA  | O2A-CGA-O1A | -4.88 | 111.26      | 123.59   |
| 14  | A     | 1113 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 14  | A     | 1135 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 14  | a     | 1124 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 14  | a     | 1115 | CLA  | C1C-C2C-C3C | -4.88 | 101.83      | 106.96   |
| 14  | b     | 1203 | CLA  | C1D-ND-C4D  | -4.88 | 102.87      | 106.33   |
| 14  | b     | 1231 | CLA  | C1D-ND-C4D  | -4.88 | 102.87      | 106.33   |
| 14  | B     | 1235 | CLA  | C1D-ND-C4D  | -4.88 | 102.87      | 106.33   |
| 14  | H     | 1232 | CLA  | O2A-CGA-O1A | -4.88 | 111.14      | 123.30   |
| 14  | a     | 1113 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 14  | G     | 1013 | CLA  | C2C-C1C-NC  | 4.88  | 114.54      | 109.97   |
| 14  | B     | 1203 | CLA  | C1D-ND-C4D  | -4.87 | 102.87      | 106.33   |
| 14  | a     | 1140 | CLA  | O2A-C1-C2   | 4.87  | 121.44      | 108.64   |
| 14  | G     | 1127 | CLA  | O2A-CGA-O1A | -4.87 | 111.29      | 123.59   |
| 18  | B     | 4010 | BCR  | C15-C14-C13 | -4.87 | 120.36      | 127.31   |
| 14  | b     | 1205 | CLA  | C1D-ND-C4D  | -4.87 | 102.87      | 106.33   |
| 14  | a     | 1119 | CLA  | C1C-C2C-C3C | -4.87 | 101.84      | 106.96   |
| 18  | H     | 4010 | BCR  | C15-C14-C13 | -4.87 | 120.36      | 127.31   |
| 14  | b     | 1239 | CLA  | CHD-C1D-ND  | -4.87 | 119.98      | 124.45   |
| 14  | A     | 1127 | CLA  | O2A-CGA-O1A | -4.87 | 111.30      | 123.59   |
| 14  | B     | 1212 | CLA  | O2D-CGD-O1D | -4.87 | 114.32      | 123.84   |
| 14  | A     | 1133 | CLA  | CHD-C1D-ND  | -4.87 | 119.98      | 124.45   |
| 14  | B     | 1232 | CLA  | O2A-CGA-O1A | -4.87 | 111.17      | 123.30   |
| 14  | b     | 1233 | CLA  | C4A-NA-C1A  | 4.87  | 108.89      | 106.71   |
| 14  | G     | 1135 | CLA  | CHD-C1D-ND  | -4.87 | 119.98      | 124.45   |
| 14  | G     | 1140 | CLA  | O2A-C1-C2   | 4.86  | 121.42      | 108.64   |
| 14  | H     | 1205 | CLA  | C3D-C2D-C1D | -4.86 | 99.19       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1224 | CLA  | C1C-C2C-C3C | -4.86 | 101.84      | 106.96   |
| 14  | B     | 1225 | CLA  | CMB-C2B-C3B | 4.86  | 133.78      | 124.68   |
| 14  | A     | 1140 | CLA  | O2A-C1-C2   | 4.86  | 121.42      | 108.64   |
| 14  | G     | 1113 | CLA  | CHD-C1D-ND  | -4.86 | 119.98      | 124.45   |
| 14  | B     | 1227 | CLA  | C4A-NA-C1A  | 4.86  | 108.89      | 106.71   |
| 14  | b     | 1212 | CLA  | O2D-CGD-O1D | -4.86 | 114.33      | 123.84   |
| 14  | b     | 1214 | CLA  | O2A-CGA-O1A | -4.86 | 111.32      | 123.59   |
| 14  | a     | 1136 | CLA  | O2A-C1-C2   | 4.86  | 121.41      | 108.64   |
| 18  | b     | 4010 | BCR  | C15-C14-C13 | -4.86 | 120.37      | 127.31   |
| 14  | A     | 1116 | CLA  | O2A-CGA-O1A | -4.86 | 111.33      | 123.59   |
| 14  | G     | 1139 | CLA  | O2A-CGA-O1A | -4.86 | 111.19      | 123.30   |
| 14  | b     | 1232 | CLA  | O2A-CGA-O1A | -4.86 | 111.19      | 123.30   |
| 14  | H     | 1212 | CLA  | O2D-CGD-O1D | -4.86 | 114.34      | 123.84   |
| 14  | b     | 1201 | CLA  | C1C-C2C-C3C | -4.86 | 101.85      | 106.96   |
| 14  | U     | 1503 | CLA  | O2A-CGA-O1A | -4.85 | 111.34      | 123.59   |
| 14  | G     | 1115 | CLA  | C3D-C2D-C1D | -4.85 | 99.21       | 105.83   |
| 14  | B     | 1205 | CLA  | C3D-C2D-C1D | -4.85 | 99.21       | 105.83   |
| 14  | a     | 1139 | CLA  | O2A-CGA-O1A | -4.85 | 111.20      | 123.30   |
| 14  | G     | 1124 | CLA  | C1D-ND-C4D  | -4.85 | 102.89      | 106.33   |
| 14  | B     | 1239 | CLA  | CHD-C1D-ND  | -4.85 | 120.00      | 124.45   |
| 14  | G     | 1116 | CLA  | O2A-CGA-O1A | -4.85 | 111.35      | 123.59   |
| 14  | B     | 1228 | CLA  | O2A-CGA-O1A | -4.85 | 111.35      | 123.59   |
| 14  | L     | 1503 | CLA  | O2A-CGA-O1A | -4.85 | 111.35      | 123.59   |
| 14  | H     | 1239 | CLA  | CHD-C1D-ND  | -4.85 | 120.00      | 124.45   |
| 14  | H     | 1225 | CLA  | CMB-C2B-C3B | 4.85  | 133.75      | 124.68   |
| 14  | l     | 1503 | CLA  | O2A-CGA-O1A | -4.85 | 111.36      | 123.59   |
| 14  | A     | 1130 | CLA  | CMB-C2B-C3B | 4.85  | 133.75      | 124.68   |
| 14  | b     | 1225 | CLA  | CMB-C2B-C3B | 4.85  | 133.74      | 124.68   |
| 14  | b     | 1205 | CLA  | C3D-C2D-C1D | -4.85 | 99.22       | 105.83   |
| 14  | A     | 1139 | CLA  | O2A-CGA-O1A | -4.84 | 111.22      | 123.30   |
| 14  | A     | 1115 | CLA  | C3D-C2D-C1D | -4.84 | 99.22       | 105.83   |
| 14  | H     | 1225 | CLA  | C4A-NA-C1A  | 4.84  | 108.88      | 106.71   |
| 14  | a     | 1118 | CLA  | CHD-C1D-ND  | -4.84 | 120.00      | 124.45   |
| 14  | a     | 1141 | CLA  | O2A-CGA-O1A | -4.84 | 111.22      | 123.30   |
| 14  | A     | 1136 | CLA  | O2A-C1-C2   | 4.84  | 121.37      | 108.64   |
| 14  | a     | 1116 | CLA  | O2A-CGA-O1A | -4.84 | 111.37      | 123.59   |
| 14  | b     | 1205 | CLA  | O2A-C1-C2   | 4.84  | 121.36      | 108.64   |
| 14  | G     | 1107 | CLA  | C4A-NA-C1A  | 4.84  | 108.88      | 106.71   |
| 14  | m     | 1501 | CLA  | C4A-NA-C1A  | 4.84  | 108.88      | 106.71   |
| 14  | A     | 1115 | CLA  | C1C-C2C-C3C | -4.84 | 101.87      | 106.96   |
| 14  | b     | 1210 | CLA  | O2A-CGA-O1A | -4.84 | 111.38      | 123.59   |
| 14  | B     | 1205 | CLA  | O2A-C1-C2   | 4.84  | 121.36      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1013 | CLA  | C2C-C1C-NC  | 4.84  | 114.51      | 109.97   |
| 14  | a     | 1109 | CLA  | O2A-CGA-O1A | -4.84 | 111.38      | 123.59   |
| 14  | H     | 1228 | CLA  | O2A-CGA-O1A | -4.84 | 111.38      | 123.59   |
| 14  | H     | 1205 | CLA  | O2A-C1-C2   | 4.84  | 121.35      | 108.64   |
| 14  | H     | 1204 | CLA  | O2A-CGA-O1A | -4.84 | 111.39      | 123.59   |
| 14  | G     | 1132 | CLA  | O2A-C1-C2   | 4.84  | 121.34      | 108.64   |
| 14  | a     | 1130 | CLA  | CMB-C2B-C3B | 4.84  | 133.72      | 124.68   |
| 14  | H     | 1231 | CLA  | C1D-ND-C4D  | -4.83 | 102.90      | 106.33   |
| 14  | A     | 1107 | CLA  | C4A-NA-C1A  | 4.83  | 108.88      | 106.71   |
| 14  | U     | 1502 | CLA  | C1C-C2C-C3C | -4.83 | 101.88      | 106.96   |
| 14  | G     | 1136 | CLA  | O2A-C1-C2   | 4.83  | 121.34      | 108.64   |
| 14  | a     | 1133 | CLA  | CHD-C1D-ND  | -4.83 | 120.01      | 124.45   |
| 14  | a     | 1013 | CLA  | C2C-C1C-NC  | 4.83  | 114.50      | 109.97   |
| 14  | G     | 1130 | CLA  | CMB-C2B-C3B | 4.83  | 133.72      | 124.68   |
| 14  | G     | 1109 | CLA  | O2A-CGA-O1A | -4.83 | 111.40      | 123.59   |
| 14  | A     | 1132 | CLA  | O2A-C1-C2   | 4.83  | 121.33      | 108.64   |
| 14  | a     | 1126 | CLA  | C4A-NA-C1A  | 4.83  | 108.88      | 106.71   |
| 14  | B     | 1210 | CLA  | O2A-CGA-O1A | -4.83 | 111.40      | 123.59   |
| 14  | a     | 1114 | CLA  | CHD-C1D-ND  | -4.83 | 120.02      | 124.45   |
| 18  | G     | 4006 | BCR  | C7-C8-C9    | -4.83 | 118.94      | 126.23   |
| 14  | a     | 1115 | CLA  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 14  | A     | 1109 | CLA  | O2A-CGA-O1A | -4.83 | 111.40      | 123.59   |
| 14  | L     | 1502 | CLA  | C1C-C2C-C3C | -4.83 | 101.88      | 106.96   |
| 14  | b     | 1204 | CLA  | O2A-CGA-O1A | -4.83 | 111.41      | 123.59   |
| 14  | b     | 1228 | CLA  | O2D-CGD-CBD | 4.83  | 119.84      | 111.27   |
| 14  | A     | 1141 | CLA  | O2A-CGA-O1A | -4.83 | 111.27      | 123.30   |
| 14  | B     | 1204 | CLA  | O2A-CGA-O1A | -4.83 | 111.41      | 123.59   |
| 14  | b     | 1228 | CLA  | O2A-CGA-O1A | -4.83 | 111.41      | 123.59   |
| 18  | a     | 4006 | BCR  | C7-C8-C9    | -4.83 | 118.94      | 126.23   |
| 14  | l     | 1502 | CLA  | C1C-C2C-C3C | -4.82 | 101.88      | 106.96   |
| 14  | H     | 1210 | CLA  | O2A-CGA-O1A | -4.82 | 111.42      | 123.59   |
| 14  | H     | 1209 | CLA  | CHD-C1D-ND  | -4.82 | 120.02      | 124.45   |
| 14  | G     | 1141 | CLA  | O2A-CGA-O1A | -4.82 | 111.28      | 123.30   |
| 14  | b     | 1216 | CLA  | O2A-CGA-O1A | -4.82 | 111.42      | 123.59   |
| 14  | H     | 1203 | CLA  | C1D-ND-C4D  | -4.82 | 102.91      | 106.33   |
| 14  | A     | 1101 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | a     | 1132 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | H     | 1235 | CLA  | C1D-ND-C4D  | -4.82 | 102.91      | 106.33   |
| 14  | a     | 1132 | CLA  | O2A-C1-C2   | 4.82  | 121.30      | 108.64   |
| 14  | B     | 1228 | CLA  | O2D-CGD-CBD | 4.82  | 119.83      | 111.27   |
| 14  | G     | 1128 | CLA  | CMB-C2B-C3B | 4.82  | 133.69      | 124.68   |
| 14  | A     | 1124 | CLA  | C1D-ND-C4D  | -4.82 | 102.91      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1224 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | b     | 1227 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | B     | 1216 | CLA  | O2A-CGA-O1A | -4.82 | 111.43      | 123.59   |
| 14  | b     | 1233 | CLA  | CHD-C1D-ND  | -4.82 | 120.03      | 124.45   |
| 14  | b     | 1227 | CLA  | O2A-CGA-O1A | -4.82 | 111.30      | 123.30   |
| 14  | a     | 1107 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | a     | 1111 | CLA  | C4A-NA-C1A  | 4.82  | 108.87      | 106.71   |
| 14  | H     | 1216 | CLA  | O2A-CGA-O1A | -4.82 | 111.44      | 123.59   |
| 14  | G     | 1115 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |
| 14  | A     | 1114 | CLA  | CHD-C1D-ND  | -4.82 | 120.03      | 124.45   |
| 14  | G     | 1114 | CLA  | CHD-C1D-ND  | -4.82 | 120.03      | 124.45   |
| 14  | b     | 1201 | CLA  | C1D-ND-C4D  | -4.81 | 102.92      | 106.33   |
| 18  | A     | 4006 | BCR  | C7-C8-C9    | -4.81 | 118.96      | 126.23   |
| 14  | B     | 1225 | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 14  | G     | 1110 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.71   |
| 14  | G     | 1140 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.71   |
| 14  | H     | 1228 | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 14  | a     | 1123 | CLA  | O2A-CGA-O1A | -4.81 | 111.45      | 123.59   |
| 14  | A     | 1126 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.71   |
| 14  | b     | 1213 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.71   |
| 14  | A     | 1111 | CLA  | O2A-CGA-O1A | -4.81 | 111.46      | 123.59   |
| 14  | B     | 1224 | CLA  | C1C-C2C-C3C | -4.81 | 101.90      | 106.96   |
| 14  | G     | 1102 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.71   |
| 14  | H     | 1225 | CLA  | O2D-CGD-CBD | 4.81  | 119.81      | 111.27   |
| 14  | b     | 1225 | CLA  | O2D-CGD-CBD | 4.80  | 119.81      | 111.27   |
| 14  | a     | 1111 | CLA  | O2A-CGA-O1A | -4.80 | 111.47      | 123.59   |
| 14  | H     | 1212 | CLA  | CHD-C1D-ND  | -4.80 | 120.04      | 124.45   |
| 14  | B     | 1227 | CLA  | O2A-CGA-O1A | -4.80 | 111.33      | 123.30   |
| 14  | G     | 1123 | CLA  | O2A-CGA-O1A | -4.80 | 111.48      | 123.59   |
| 14  | V     | 1501 | CLA  | O2A-C1-C2   | 4.80  | 121.25      | 108.64   |
| 14  | G     | 1127 | CLA  | C3D-C2D-C1D | -4.80 | 99.28       | 105.83   |
| 14  | A     | 1123 | CLA  | O2A-CGA-O1A | -4.80 | 111.49      | 123.59   |
| 14  | H     | 1227 | CLA  | O2A-CGA-O1A | -4.80 | 111.35      | 123.30   |
| 14  | A     | 1132 | CLA  | C4A-NA-C1A  | 4.80  | 108.86      | 106.71   |
| 14  | A     | 1112 | CLA  | O2A-C1-C2   | 4.79  | 121.24      | 108.64   |
| 14  | a     | 1112 | CLA  | O2A-C1-C2   | 4.79  | 121.23      | 108.64   |
| 15  | H     | 1230 | F6C  | C3D-C2D-C1D | -4.79 | 98.89       | 105.83   |
| 14  | A     | 1128 | CLA  | CMB-C2B-C3B | 4.79  | 133.64      | 124.68   |
| 14  | B     | 1209 | CLA  | CHD-C1D-ND  | -4.79 | 120.05      | 124.45   |
| 14  | G     | 1111 | CLA  | O2A-CGA-O1A | -4.79 | 111.50      | 123.59   |
| 14  | a     | 1124 | CLA  | C1D-ND-C4D  | -4.79 | 102.93      | 106.33   |
| 14  | G     | 1112 | CLA  | O2A-C1-C2   | 4.79  | 121.22      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1129 | CLA  | C1D-ND-C4D  | -4.79 | 102.93      | 106.33   |
| 14  | A     | 1127 | CLA  | C3D-C2D-C1D | -4.79 | 99.30       | 105.83   |
| 14  | M     | 1501 | CLA  | O2A-C1-C2   | 4.79  | 121.21      | 108.64   |
| 14  | H     | 1233 | CLA  | CHD-C1D-ND  | -4.79 | 120.06      | 124.45   |
| 14  | A     | 1108 | CLA  | O2A-CGA-O1A | -4.79 | 111.37      | 123.30   |
| 14  | G     | 1108 | CLA  | O2A-CGA-O1A | -4.78 | 111.38      | 123.30   |
| 14  | m     | 1501 | CLA  | O2A-C1-C2   | 4.78  | 121.20      | 108.64   |
| 14  | a     | 1127 | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 14  | b     | 1210 | CLA  | C1-C2-C3    | -4.78 | 117.78      | 126.04   |
| 14  | b     | 1209 | CLA  | CHD-C1D-ND  | -4.78 | 120.06      | 124.45   |
| 14  | G     | 1111 | CLA  | C4A-NA-C1A  | 4.78  | 108.86      | 106.71   |
| 14  | a     | 1108 | CLA  | O2A-CGA-O1A | -4.78 | 111.39      | 123.30   |
| 15  | b     | 1230 | F6C  | C3D-C2D-C1D | -4.78 | 98.91       | 105.83   |
| 14  | b     | 1206 | CLA  | CHD-C1D-ND  | -4.78 | 120.06      | 124.45   |
| 14  | a     | 1102 | CLA  | C4A-NA-C1A  | 4.78  | 108.85      | 106.71   |
| 14  | B     | 1212 | CLA  | CHD-C1D-ND  | -4.77 | 120.07      | 124.45   |
| 14  | B     | 1233 | CLA  | CHD-C1D-ND  | -4.77 | 120.07      | 124.45   |
| 14  | G     | 1132 | CLA  | C4A-NA-C1A  | 4.77  | 108.85      | 106.71   |
| 15  | B     | 1230 | F6C  | C3D-C2D-C1D | -4.77 | 98.92       | 105.83   |
| 14  | G     | 1129 | CLA  | C1D-ND-C4D  | -4.77 | 102.94      | 106.33   |
| 14  | G     | 1126 | CLA  | C4A-NA-C1A  | 4.77  | 108.85      | 106.71   |
| 14  | G     | 1135 | CLA  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 14  | K     | 1401 | CLA  | C1C-C2C-C3C | -4.77 | 101.94      | 106.96   |
| 14  | A     | 1110 | CLA  | C4A-NA-C1A  | 4.77  | 108.85      | 106.71   |
| 14  | G     | 1101 | CLA  | C4A-NA-C1A  | 4.77  | 108.85      | 106.71   |
| 14  | B     | 1233 | CLA  | C4A-NA-C1A  | 4.76  | 108.85      | 106.71   |
| 14  | H     | 1210 | CLA  | C1-C2-C3    | -4.76 | 117.80      | 126.04   |
| 14  | b     | 1226 | CLA  | C3D-C2D-C1D | -4.76 | 99.33       | 105.83   |
| 14  | k     | 1401 | CLA  | C1C-C2C-C3C | -4.76 | 101.95      | 106.96   |
| 14  | V     | 1501 | CLA  | C3D-C2D-C1D | -4.76 | 99.33       | 105.83   |
| 14  | H     | 1202 | CLA  | C3D-C2D-C1D | -4.76 | 99.34       | 105.83   |
| 14  | H     | 1213 | CLA  | C1C-C2C-C3C | -4.76 | 101.95      | 106.96   |
| 14  | G     | 1118 | CLA  | O2A-CGA-O1A | -4.76 | 111.58      | 123.59   |
| 14  | T     | 1401 | CLA  | C1C-C2C-C3C | -4.76 | 101.95      | 106.96   |
| 14  | b     | 1224 | CLA  | C1C-C2C-C3C | -4.76 | 101.95      | 106.96   |
| 14  | B     | 1210 | CLA  | C1-C2-C3    | -4.76 | 117.81      | 126.04   |
| 15  | b     | 1230 | F6C  | O2A-CGA-O1A | -4.76 | 111.44      | 123.30   |
| 14  | a     | 1118 | CLA  | O2A-CGA-O1A | -4.76 | 111.59      | 123.59   |
| 15  | H     | 1219 | F6C  | C3D-C2D-C1D | -4.76 | 98.94       | 105.83   |
| 14  | G     | 1101 | CLA  | O2A-CGA-O1A | -4.75 | 111.45      | 123.30   |
| 14  | a     | 1128 | CLA  | CMB-C2B-C3B | 4.75  | 133.57      | 124.68   |
| 14  | A     | 1118 | CLA  | O2A-CGA-O1A | -4.75 | 111.60      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1218 | CLA  | O2A-CGA-O1A | -4.75 | 111.45      | 123.30   |
| 14  | H     | 1223 | CLA  | O2A-CGA-O1A | -4.75 | 111.60      | 123.59   |
| 14  | b     | 1223 | CLA  | O2A-CGA-O1A | -4.75 | 111.60      | 123.59   |
| 14  | T     | 1401 | CLA  | O2A-CGA-O1A | -4.75 | 111.46      | 123.30   |
| 14  | b     | 1239 | CLA  | O2A-C1-C2   | 4.75  | 121.12      | 108.64   |
| 14  | U     | 1503 | CLA  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 15  | b     | 1219 | F6C  | O2A-CGA-O1A | -4.75 | 111.61      | 123.59   |
| 14  | b     | 1213 | CLA  | C1C-C2C-C3C | -4.75 | 101.96      | 106.96   |
| 14  | b     | 1212 | CLA  | CHD-C1D-ND  | -4.75 | 120.09      | 124.45   |
| 14  | H     | 1218 | CLA  | O2A-CGA-O1A | -4.75 | 111.47      | 123.30   |
| 14  | B     | 1223 | CLA  | O2A-CGA-O1A | -4.75 | 111.61      | 123.59   |
| 14  | K     | 1401 | CLA  | O2A-CGA-O1A | -4.74 | 111.47      | 123.30   |
| 14  | A     | 1111 | CLA  | C4A-NA-C1A  | 4.74  | 108.84      | 106.71   |
| 14  | B     | 1202 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 14  | A     | 1012 | CLA  | O2D-CGD-CBD | 4.74  | 119.70      | 111.27   |
| 14  | B     | 1206 | CLA  | CHD-C1D-ND  | -4.74 | 120.09      | 124.45   |
| 14  | A     | 1135 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 14  | G     | 1012 | CLA  | O2D-CGD-CBD | 4.74  | 119.69      | 111.27   |
| 14  | B     | 1217 | CLA  | O2A-CGA-O1A | -4.74 | 111.48      | 123.30   |
| 14  | k     | 1401 | CLA  | O2A-CGA-O1A | -4.74 | 111.48      | 123.30   |
| 15  | H     | 1230 | F6C  | O2A-CGA-O1A | -4.74 | 111.48      | 123.30   |
| 14  | b     | 1202 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 14  | B     | 1239 | CLA  | O2A-C1-C2   | 4.74  | 121.09      | 108.64   |
| 14  | b     | 1234 | CLA  | O2A-C1-C2   | 4.74  | 121.09      | 108.64   |
| 14  | M     | 1501 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 14  | H     | 1217 | CLA  | O2A-CGA-O1A | -4.74 | 111.49      | 123.30   |
| 14  | B     | 1213 | CLA  | C1C-C2C-C3C | -4.74 | 101.97      | 106.96   |
| 15  | B     | 1230 | F6C  | O2A-CGA-O1A | -4.74 | 111.49      | 123.30   |
| 14  | A     | 1101 | CLA  | O2A-CGA-O1A | -4.74 | 111.49      | 123.30   |
| 18  | M     | 4021 | BCR  | C19-C18-C17 | 4.74  | 126.21      | 118.94   |
| 14  | A     | 1129 | CLA  | C1D-ND-C4D  | -4.74 | 102.97      | 106.33   |
| 14  | b     | 1218 | CLA  | O2A-CGA-O1A | -4.74 | 111.49      | 123.30   |
| 14  | G     | 1138 | CLA  | O2A-CGA-O1A | -4.74 | 111.64      | 123.59   |
| 14  | b     | 1021 | CLA  | O2D-CGD-CBD | 4.74  | 119.68      | 111.27   |
| 14  | a     | 1113 | CLA  | O2A-CGA-O1A | -4.74 | 111.50      | 123.30   |
| 14  | B     | 1226 | CLA  | C3D-C2D-C1D | -4.74 | 99.37       | 105.83   |
| 14  | a     | 1012 | CLA  | O2D-CGD-CBD | 4.73  | 119.68      | 111.27   |
| 14  | G     | 1118 | CLA  | C1D-ND-C4D  | -4.73 | 102.97      | 106.33   |
| 15  | B     | 1219 | F6C  | C3D-C2D-C1D | -4.73 | 98.98       | 105.83   |
| 14  | H     | 1239 | CLA  | O2A-C1-C2   | 4.73  | 121.07      | 108.64   |
| 14  | B     | 1201 | CLA  | C1D-ND-C4D  | -4.73 | 102.97      | 106.33   |
| 14  | H     | 1226 | CLA  | C3D-C2D-C1D | -4.73 | 99.37       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | L     | 1503 | CLA  | C3D-C2D-C1D | -4.73 | 99.37       | 105.83   |
| 14  | A     | 1111 | CLA  | C1D-ND-C4D  | -4.73 | 102.97      | 106.33   |
| 15  | b     | 1219 | F6C  | C3D-C2D-C1D | -4.73 | 98.98       | 105.83   |
| 14  | H     | 1021 | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 14  | l     | 1503 | CLA  | C3D-C2D-C1D | -4.73 | 99.38       | 105.83   |
| 18  | m     | 4021 | BCR  | C19-C18-C17 | 4.73  | 126.20      | 118.94   |
| 15  | B     | 1219 | F6C  | O2A-CGA-O1A | -4.73 | 111.66      | 123.59   |
| 14  | a     | 1101 | CLA  | O2A-CGA-O1A | -4.73 | 111.52      | 123.30   |
| 18  | V     | 4021 | BCR  | C19-C18-C17 | 4.72  | 126.19      | 118.94   |
| 14  | b     | 1217 | CLA  | O2A-CGA-O1A | -4.72 | 111.53      | 123.30   |
| 14  | b     | 1220 | CLA  | O2A-C1-C2   | 4.72  | 121.05      | 108.64   |
| 14  | H     | 1206 | CLA  | CHD-C1D-ND  | -4.72 | 120.11      | 124.45   |
| 14  | B     | 1234 | CLA  | O2A-C1-C2   | 4.72  | 121.04      | 108.64   |
| 14  | H     | 1234 | CLA  | O2A-C1-C2   | 4.72  | 121.04      | 108.64   |
| 14  | a     | 1138 | CLA  | O2A-CGA-O1A | -4.72 | 111.69      | 123.59   |
| 18  | L     | 4019 | BCR  | C3-C4-C5    | -4.72 | 105.65      | 114.08   |
| 15  | H     | 1219 | F6C  | O2A-CGA-O1A | -4.72 | 111.69      | 123.59   |
| 14  | G     | 1113 | CLA  | O2A-CGA-O1A | -4.72 | 111.54      | 123.30   |
| 14  | m     | 1501 | CLA  | C3D-C2D-C1D | -4.72 | 99.39       | 105.83   |
| 14  | A     | 1138 | CLA  | O2A-CGA-O1A | -4.72 | 111.69      | 123.59   |
| 14  | a     | 1114 | CLA  | O2A-CGA-O1A | -4.72 | 111.54      | 123.30   |
| 18  | U     | 4019 | BCR  | C3-C4-C5    | -4.72 | 105.66      | 114.08   |
| 14  | a     | 1110 | CLA  | C4A-NA-C1A  | 4.72  | 108.83      | 106.71   |
| 14  | A     | 1113 | CLA  | O2A-CGA-O1A | -4.72 | 111.55      | 123.30   |
| 14  | B     | 1211 | CLA  | O2A-C1-C2   | 4.71  | 121.03      | 108.64   |
| 14  | B     | 1220 | CLA  | O2A-C1-C2   | 4.71  | 121.03      | 108.64   |
| 14  | A     | 1114 | CLA  | O2A-CGA-O1A | -4.71 | 111.55      | 123.30   |
| 14  | B     | 1021 | CLA  | O2D-CGD-CBD | 4.71  | 119.64      | 111.27   |
| 14  | H     | 1211 | CLA  | O2A-C1-C2   | 4.71  | 121.02      | 108.64   |
| 14  | b     | 1211 | CLA  | O2A-C1-C2   | 4.71  | 121.02      | 108.64   |
| 14  | a     | 1013 | CLA  | O2A-CGA-CBA | 4.71  | 126.70      | 111.91   |
| 14  | a     | 1111 | CLA  | C1D-ND-C4D  | -4.71 | 102.99      | 106.33   |
| 14  | H     | 1220 | CLA  | O2A-C1-C2   | 4.71  | 121.01      | 108.64   |
| 14  | G     | 1114 | CLA  | O2A-CGA-O1A | -4.71 | 111.56      | 123.30   |
| 14  | A     | 1013 | CLA  | O2A-CGA-CBA | 4.71  | 126.68      | 111.91   |
| 14  | A     | 1102 | CLA  | C4A-NA-C1A  | 4.70  | 108.82      | 106.71   |
| 14  | B     | 1022 | CLA  | C1C-C2C-C3C | -4.70 | 102.01      | 106.96   |
| 14  | B     | 1228 | CLA  | C1C-C2C-C3C | -4.70 | 102.01      | 106.96   |
| 14  | G     | 1013 | CLA  | O2A-CGA-CBA | 4.70  | 126.66      | 111.91   |
| 14  | a     | 1140 | CLA  | O2A-CGA-O1A | -4.70 | 111.73      | 123.59   |
| 14  | b     | 1228 | CLA  | C1C-C2C-C3C | -4.70 | 102.01      | 106.96   |
| 15  | a     | 1121 | F6C  | C3D-C2D-C1D | -4.70 | 99.02       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1135 | CLA  | C3D-C2D-C1D | -4.70 | 99.42       | 105.83   |
| 14  | B     | 1210 | CLA  | C1D-ND-C4D  | -4.70 | 103.00      | 106.33   |
| 14  | H     | 1233 | CLA  | C4A-NA-C1A  | 4.70  | 108.82      | 106.71   |
| 14  | A     | 1140 | CLA  | O2A-CGA-O1A | -4.70 | 111.74      | 123.59   |
| 14  | H     | 1228 | CLA  | C1C-C2C-C3C | -4.70 | 102.02      | 106.96   |
| 15  | B     | 1207 | F6C  | C4A-C3A-C2A | -4.69 | 100.08      | 106.94   |
| 14  | A     | 1118 | CLA  | C1D-ND-C4D  | -4.69 | 103.00      | 106.33   |
| 14  | b     | 1211 | CLA  | CHD-C1D-ND  | -4.69 | 120.14      | 124.45   |
| 15  | H     | 1207 | F6C  | C4A-C3A-C2A | -4.69 | 100.09      | 106.94   |
| 14  | b     | 1022 | CLA  | C1C-C2C-C3C | -4.69 | 102.02      | 106.96   |
| 14  | G     | 1129 | CLA  | O2D-CGD-O1D | -4.69 | 114.67      | 123.84   |
| 15  | A     | 1121 | F6C  | C3D-C2D-C1D | -4.69 | 99.04       | 105.83   |
| 18  | l     | 4019 | BCR  | C3-C4-C5    | -4.69 | 105.71      | 114.08   |
| 14  | a     | 1129 | CLA  | O2D-CGD-O1D | -4.69 | 114.68      | 123.84   |
| 14  | G     | 1127 | CLA  | O2A-C1-C2   | 4.68  | 120.94      | 108.64   |
| 14  | a     | 1134 | CLA  | O2A-CGA-O1A | -4.68 | 111.62      | 123.30   |
| 14  | G     | 1140 | CLA  | O2A-CGA-O1A | -4.68 | 111.77      | 123.59   |
| 14  | H     | 1022 | CLA  | C1C-C2C-C3C | -4.68 | 102.03      | 106.96   |
| 14  | b     | 1210 | CLA  | C1D-ND-C4D  | -4.68 | 103.01      | 106.33   |
| 14  | b     | 1221 | CLA  | O2A-CGA-O1A | -4.68 | 111.78      | 123.59   |
| 20  | a     | 5003 | LMG  | O7-C10-C11  | 4.68  | 121.59      | 111.50   |
| 15  | b     | 1207 | F6C  | C4A-C3A-C2A | -4.68 | 100.11      | 106.94   |
| 14  | A     | 1129 | CLA  | O2D-CGD-O1D | -4.68 | 114.69      | 123.84   |
| 14  | H     | 1239 | CLA  | O2A-CGA-O1A | -4.68 | 111.79      | 123.59   |
| 14  | G     | 1133 | CLA  | C1D-ND-C4D  | -4.68 | 103.01      | 106.33   |
| 14  | a     | 1127 | CLA  | O2A-C1-C2   | 4.68  | 120.92      | 108.64   |
| 14  | H     | 1201 | CLA  | C1D-ND-C4D  | -4.67 | 103.01      | 106.33   |
| 14  | B     | 1211 | CLA  | CHD-C1D-ND  | -4.67 | 120.16      | 124.45   |
| 14  | A     | 1127 | CLA  | O2A-C1-C2   | 4.67  | 120.92      | 108.64   |
| 14  | H     | 1221 | CLA  | CMB-C2B-C3B | 4.67  | 133.42      | 124.68   |
| 14  | B     | 1239 | CLA  | C4A-NA-C1A  | 4.67  | 108.81      | 106.71   |
| 14  | b     | 1239 | CLA  | C4A-NA-C1A  | 4.67  | 108.81      | 106.71   |
| 14  | B     | 1221 | CLA  | O2A-CGA-O1A | -4.67 | 111.80      | 123.59   |
| 14  | G     | 1111 | CLA  | C1D-ND-C4D  | -4.67 | 103.02      | 106.33   |
| 15  | G     | 1121 | F6C  | C3D-C2D-C1D | -4.67 | 99.07       | 105.83   |
| 14  | a     | 1115 | CLA  | C4A-NA-C1A  | 4.67  | 108.81      | 106.71   |
| 14  | H     | 1211 | CLA  | CHD-C1D-ND  | -4.67 | 120.16      | 124.45   |
| 14  | H     | 1210 | CLA  | C1D-ND-C4D  | -4.67 | 103.02      | 106.33   |
| 14  | b     | 1221 | CLA  | CMB-C2B-C3B | 4.67  | 133.41      | 124.68   |
| 18  | b     | 4004 | BCR  | C19-C18-C17 | 4.67  | 126.10      | 118.94   |
| 14  | b     | 1239 | CLA  | O2A-CGA-O1A | -4.66 | 111.82      | 123.59   |
| 18  | B     | 4004 | BCR  | C19-C18-C17 | 4.66  | 126.10      | 118.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1134 | CLA  | O2A-CGA-O1A | -4.66 | 111.67      | 123.30   |
| 14  | B     | 1209 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 15  | a     | 1121 | F6C  | C1A-C2A-C3A | -4.66 | 102.06      | 106.97   |
| 14  | a     | 1134 | CLA  | C1D-ND-C4D  | -4.66 | 103.02      | 106.33   |
| 14  | G     | 1125 | CLA  | O2A-CGA-O1A | -4.66 | 111.83      | 123.59   |
| 14  | B     | 1239 | CLA  | O2A-CGA-O1A | -4.66 | 111.83      | 123.59   |
| 14  | H     | 1221 | CLA  | O2A-CGA-O1A | -4.66 | 111.83      | 123.59   |
| 14  | B     | 1221 | CLA  | CMB-C2B-C3B | 4.66  | 133.40      | 124.68   |
| 14  | G     | 1122 | CLA  | O2A-CGA-O1A | -4.66 | 111.83      | 123.59   |
| 20  | A     | 5003 | LMG  | O7-C10-C11  | 4.66  | 121.54      | 111.50   |
| 14  | A     | 1122 | CLA  | O2A-CGA-O1A | -4.66 | 111.84      | 123.59   |
| 14  | A     | 1134 | CLA  | O2A-CGA-O1A | -4.66 | 111.69      | 123.30   |
| 14  | A     | 1134 | CLA  | C1D-ND-C4D  | -4.66 | 103.03      | 106.33   |
| 14  | a     | 1132 | CLA  | O2A-CGA-O1A | -4.65 | 111.84      | 123.59   |
| 15  | A     | 1121 | F6C  | C1A-C2A-C3A | -4.65 | 102.07      | 106.97   |
| 14  | a     | 1125 | CLA  | O2A-CGA-O1A | -4.65 | 111.85      | 123.59   |
| 14  | b     | 1209 | CLA  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 14  | H     | 1205 | CLA  | CHD-C1D-ND  | -4.65 | 120.18      | 124.45   |
| 14  | A     | 1132 | CLA  | O2A-CGA-O1A | -4.65 | 111.85      | 123.59   |
| 14  | a     | 1118 | CLA  | C1D-ND-C4D  | -4.65 | 103.03      | 106.33   |
| 14  | A     | 1125 | CLA  | O2A-CGA-O1A | -4.65 | 111.85      | 123.59   |
| 18  | H     | 4004 | BCR  | C19-C18-C17 | 4.65  | 126.08      | 118.94   |
| 13  | G     | 1011 | CL0  | C1D-ND-C4D  | -4.65 | 103.03      | 106.33   |
| 14  | G     | 1132 | CLA  | O2A-CGA-O1A | -4.65 | 111.85      | 123.59   |
| 14  | b     | 1211 | CLA  | O2A-CGA-O1A | -4.65 | 111.86      | 123.59   |
| 14  | H     | 1222 | CLA  | C1D-ND-C4D  | -4.65 | 103.03      | 106.33   |
| 15  | G     | 1121 | F6C  | C1A-C2A-C3A | -4.65 | 102.08      | 106.97   |
| 14  | B     | 1234 | CLA  | C1C-C2C-C3C | -4.65 | 102.07      | 106.96   |
| 14  | H     | 1239 | CLA  | C4A-NA-C1A  | 4.64  | 108.79      | 106.71   |
| 20  | G     | 5003 | LMG  | O7-C10-C11  | 4.64  | 121.51      | 111.50   |
| 14  | a     | 1140 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 14  | a     | 1122 | CLA  | O2A-CGA-O1A | -4.64 | 111.87      | 123.59   |
| 14  | A     | 1140 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 21  | L     | 6101 | LMT  | O5B-C5B-C4B | 4.64  | 118.12      | 109.69   |
| 14  | G     | 1122 | CLA  | O2A-C1-C2   | 4.64  | 120.83      | 108.64   |
| 18  | B     | 4017 | BCR  | C7-C8-C9    | -4.64 | 119.23      | 126.23   |
| 14  | b     | 1205 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 14  | A     | 1103 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 14  | G     | 1134 | CLA  | C1D-ND-C4D  | -4.64 | 103.04      | 106.33   |
| 14  | B     | 1205 | CLA  | CHD-C1D-ND  | -4.63 | 120.19      | 124.45   |
| 13  | A     | 1011 | CL0  | C1D-ND-C4D  | -4.63 | 103.04      | 106.33   |
| 14  | a     | 1105 | CLA  | C1D-ND-C4D  | -4.63 | 103.04      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1209 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 14  | a     | 1103 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 15  | b     | 1207 | F6C  | C4A-NA-C1A  | 4.63  | 109.63      | 106.33   |
| 14  | H     | 1211 | CLA  | O2A-CGA-O1A | -4.63 | 111.91      | 123.59   |
| 14  | B     | 1211 | CLA  | O2A-CGA-O1A | -4.63 | 111.91      | 123.59   |
| 18  | H     | 4017 | BCR  | C7-C8-C9    | -4.63 | 119.24      | 126.23   |
| 18  | b     | 4017 | BCR  | C7-C8-C9    | -4.63 | 119.24      | 126.23   |
| 15  | B     | 1207 | F6C  | O2A-CGA-CBA | 4.63  | 126.43      | 111.91   |
| 14  | G     | 1106 | CLA  | C1D-ND-C4D  | -4.63 | 103.05      | 106.33   |
| 15  | H     | 1207 | F6C  | O2A-CGA-CBA | 4.63  | 126.43      | 111.91   |
| 14  | A     | 1122 | CLA  | O2A-C1-C2   | 4.63  | 120.80      | 108.64   |
| 14  | A     | 1133 | CLA  | C1D-ND-C4D  | -4.63 | 103.05      | 106.33   |
| 14  | b     | 1234 | CLA  | C1C-C2C-C3C | -4.63 | 102.09      | 106.96   |
| 14  | a     | 1122 | CLA  | O2A-C1-C2   | 4.62  | 120.79      | 108.64   |
| 15  | b     | 1207 | F6C  | O2A-CGA-CBA | 4.62  | 126.42      | 111.91   |
| 14  | G     | 1140 | CLA  | CHD-C1D-ND  | -4.62 | 120.21      | 124.45   |
| 14  | H     | 1232 | CLA  | O2D-CGD-CBD | 4.62  | 119.48      | 111.27   |
| 14  | G     | 1103 | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 14  | A     | 1106 | CLA  | C1D-ND-C4D  | -4.62 | 103.05      | 106.33   |
| 14  | H     | 1234 | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 21  | U     | 6101 | LMT  | O5B-C5B-C4B | 4.62  | 118.08      | 109.69   |
| 14  | b     | 1212 | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 21  | l     | 6101 | LMT  | O5B-C5B-C4B | 4.61  | 118.07      | 109.69   |
| 14  | B     | 1232 | CLA  | O2D-CGD-CBD | 4.61  | 119.47      | 111.27   |
| 15  | B     | 1219 | F6C  | O2A-C1-C2   | 4.61  | 120.76      | 108.64   |
| 15  | H     | 1237 | F6C  | C3D-C2D-C1D | -4.61 | 99.15       | 105.83   |
| 14  | B     | 1231 | CLA  | O2A-CGA-O1A | -4.61 | 111.96      | 123.59   |
| 15  | b     | 1219 | F6C  | O2A-C1-C2   | 4.61  | 120.75      | 108.64   |
| 15  | B     | 1237 | F6C  | C3D-C2D-C1D | -4.61 | 99.16       | 105.83   |
| 14  | a     | 1112 | CLA  | O2A-CGA-CBA | 4.61  | 126.37      | 111.91   |
| 14  | B     | 1212 | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 13  | a     | 1011 | CL0  | C1D-ND-C4D  | -4.61 | 103.06      | 106.33   |
| 14  | H     | 1212 | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 15  | H     | 1219 | F6C  | O2A-C1-C2   | 4.60  | 120.73      | 108.64   |
| 14  | G     | 1105 | CLA  | C1D-ND-C4D  | -4.60 | 103.07      | 106.33   |
| 14  | a     | 1106 | CLA  | C1D-ND-C4D  | -4.60 | 103.07      | 106.33   |
| 14  | a     | 1133 | CLA  | C1D-ND-C4D  | -4.60 | 103.07      | 106.33   |
| 14  | H     | 1231 | CLA  | O2A-CGA-O1A | -4.60 | 111.98      | 123.59   |
| 14  | b     | 1232 | CLA  | O2D-CGD-CBD | 4.60  | 119.44      | 111.27   |
| 14  | B     | 1206 | CLA  | O2A-C1-C2   | 4.60  | 120.72      | 108.64   |
| 14  | b     | 1231 | CLA  | O2A-CGA-O1A | -4.60 | 111.99      | 123.59   |
| 14  | b     | 1206 | CLA  | O2A-C1-C2   | 4.60  | 120.71      | 108.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1112 | CLA  | O2A-CGA-CBA | 4.59  | 126.33      | 111.91   |
| 15  | b     | 1237 | F6C  | C3D-C2D-C1D | -4.59 | 99.18       | 105.83   |
| 14  | A     | 1105 | CLA  | C1D-ND-C4D  | -4.59 | 103.07      | 106.33   |
| 14  | H     | 1206 | CLA  | O2A-C1-C2   | 4.59  | 120.70      | 108.64   |
| 14  | A     | 1112 | CLA  | O2A-CGA-CBA | 4.59  | 126.31      | 111.91   |
| 14  | G     | 1124 | CLA  | O2A-CGA-O1A | -4.59 | 112.01      | 123.59   |
| 14  | a     | 1102 | CLA  | C1D-ND-C4D  | -4.59 | 103.08      | 106.33   |
| 15  | H     | 1207 | F6C  | C4A-NA-C1A  | 4.59  | 109.59      | 106.33   |
| 14  | G     | 1115 | CLA  | C4A-NA-C1A  | 4.58  | 108.77      | 106.71   |
| 14  | G     | 1102 | CLA  | O2A-CGA-O1A | -4.58 | 112.03      | 123.59   |
| 14  | A     | 1141 | CLA  | C1D-ND-C4D  | -4.58 | 103.08      | 106.33   |
| 14  | G     | 1117 | CLA  | CHD-C1D-ND  | -4.58 | 120.25      | 124.45   |
| 14  | A     | 1124 | CLA  | O2A-CGA-O1A | -4.58 | 112.04      | 123.59   |
| 15  | H     | 1237 | F6C  | C1A-C2A-C3A | -4.58 | 102.15      | 106.97   |
| 14  | a     | 1124 | CLA  | O2A-CGA-O1A | -4.58 | 112.05      | 123.59   |
| 14  | b     | 1222 | CLA  | C1D-ND-C4D  | -4.57 | 103.09      | 106.33   |
| 14  | A     | 1115 | CLA  | C4A-NA-C1A  | 4.57  | 108.76      | 106.71   |
| 14  | A     | 1107 | CLA  | C1D-ND-C4D  | -4.57 | 103.09      | 106.33   |
| 14  | a     | 1115 | CLA  | O2A-CGA-CBA | 4.57  | 126.25      | 111.91   |
| 14  | G     | 1137 | CLA  | O2A-CGA-O1A | -4.57 | 112.06      | 123.59   |
| 14  | A     | 1102 | CLA  | C1D-ND-C4D  | -4.57 | 103.09      | 106.33   |
| 14  | G     | 1115 | CLA  | O2A-CGA-CBA | 4.57  | 126.24      | 111.91   |
| 14  | a     | 1137 | CLA  | O2A-CGA-O1A | -4.56 | 112.07      | 123.59   |
| 14  | A     | 1115 | CLA  | O2A-CGA-CBA | 4.56  | 126.23      | 111.91   |
| 14  | A     | 1102 | CLA  | O2A-CGA-O1A | -4.56 | 112.07      | 123.59   |
| 14  | G     | 1141 | CLA  | C1D-ND-C4D  | -4.56 | 103.09      | 106.33   |
| 14  | b     | 1211 | CLA  | C4A-NA-C1A  | 4.56  | 108.76      | 106.71   |
| 14  | L     | 1501 | CLA  | CHD-C1D-ND  | -4.56 | 120.26      | 124.45   |
| 14  | B     | 1211 | CLA  | C4A-NA-C1A  | 4.56  | 108.76      | 106.71   |
| 14  | a     | 1116 | CLA  | O2A-C1-C2   | 4.56  | 120.62      | 108.64   |
| 14  | G     | 1107 | CLA  | C1D-ND-C4D  | -4.56 | 103.10      | 106.33   |
| 14  | a     | 1129 | CLA  | O2A-CGA-CBA | 4.56  | 126.21      | 111.91   |
| 15  | b     | 1237 | F6C  | C1A-C2A-C3A | -4.56 | 102.17      | 106.97   |
| 15  | B     | 1237 | F6C  | C1A-C2A-C3A | -4.56 | 102.17      | 106.97   |
| 14  | a     | 1102 | CLA  | O2A-CGA-O1A | -4.56 | 112.09      | 123.59   |
| 14  | A     | 1116 | CLA  | O2A-C1-C2   | 4.56  | 120.61      | 108.64   |
| 14  | G     | 1116 | CLA  | O2A-C1-C2   | 4.56  | 120.61      | 108.64   |
| 14  | a     | 1117 | CLA  | CHD-C1D-ND  | -4.55 | 120.27      | 124.45   |
| 14  | l     | 1501 | CLA  | CHD-C1D-ND  | -4.55 | 120.27      | 124.45   |
| 14  | G     | 1135 | CLA  | O2A-C1-C2   | 4.55  | 120.60      | 108.64   |
| 14  | A     | 1137 | CLA  | O2A-CGA-O1A | -4.55 | 112.11      | 123.59   |
| 14  | H     | 1211 | CLA  | C4A-NA-C1A  | 4.55  | 108.75      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1103 | CLA  | O2A-CGA-O1A | -4.55 | 112.11      | 123.59   |
| 14  | B     | 1222 | CLA  | C1D-ND-C4D  | -4.55 | 103.11      | 106.33   |
| 14  | A     | 1115 | CLA  | O2A-C1-C2   | 4.55  | 120.58      | 108.64   |
| 14  | a     | 1141 | CLA  | C1D-ND-C4D  | -4.54 | 103.11      | 106.33   |
| 14  | A     | 1135 | CLA  | O2A-C1-C2   | 4.54  | 120.58      | 108.64   |
| 14  | A     | 1129 | CLA  | O2A-CGA-CBA | 4.54  | 126.17      | 111.91   |
| 14  | G     | 1115 | CLA  | O2A-C1-C2   | 4.54  | 120.57      | 108.64   |
| 14  | a     | 1135 | CLA  | O2A-C1-C2   | 4.54  | 120.57      | 108.64   |
| 14  | B     | 1021 | CLA  | O2A-CGA-O1A | -4.54 | 112.13      | 123.59   |
| 14  | H     | 1235 | CLA  | O2D-CGD-CBD | 4.54  | 119.34      | 111.27   |
| 14  | G     | 1129 | CLA  | O2A-CGA-CBA | 4.54  | 126.16      | 111.91   |
| 15  | B     | 1207 | F6C  | C4A-NA-C1A  | 4.54  | 109.56      | 106.33   |
| 14  | a     | 1115 | CLA  | O2A-C1-C2   | 4.54  | 120.56      | 108.64   |
| 14  | B     | 1234 | CLA  | CHD-C1D-ND  | -4.54 | 120.28      | 124.45   |
| 14  | b     | 1240 | CLA  | O2A-CGA-CBA | 4.54  | 126.15      | 111.91   |
| 14  | b     | 1021 | CLA  | O2A-CGA-O1A | -4.54 | 112.14      | 123.59   |
| 14  | G     | 1102 | CLA  | C1D-ND-C4D  | -4.54 | 103.11      | 106.33   |
| 14  | a     | 1107 | CLA  | C1D-ND-C4D  | -4.53 | 103.11      | 106.33   |
| 14  | A     | 1103 | CLA  | O2A-CGA-O1A | -4.53 | 112.15      | 123.59   |
| 14  | H     | 1240 | CLA  | O2A-CGA-CBA | 4.53  | 126.14      | 111.91   |
| 14  | a     | 1103 | CLA  | O2A-CGA-O1A | -4.53 | 112.15      | 123.59   |
| 14  | b     | 1235 | CLA  | O2D-CGD-CBD | 4.53  | 119.32      | 111.27   |
| 14  | B     | 1240 | CLA  | O2A-CGA-CBA | 4.53  | 126.13      | 111.91   |
| 14  | A     | 1117 | CLA  | CHD-C1D-ND  | -4.53 | 120.29      | 124.45   |
| 14  | A     | 1122 | CLA  | CHD-C1D-ND  | -4.53 | 120.29      | 124.45   |
| 14  | b     | 1234 | CLA  | CHD-C1D-ND  | -4.53 | 120.29      | 124.45   |
| 14  | H     | 1021 | CLA  | O2A-CGA-O1A | -4.53 | 112.16      | 123.59   |
| 14  | B     | 1235 | CLA  | O2D-CGD-CBD | 4.53  | 119.32      | 111.27   |
| 14  | U     | 1501 | CLA  | CHD-C1D-ND  | -4.53 | 120.29      | 124.45   |
| 14  | a     | 1122 | CLA  | CHD-C1D-ND  | -4.52 | 120.30      | 124.45   |
| 18  | l     | 4022 | BCR  | C24-C23-C22 | -4.52 | 119.40      | 126.23   |
| 14  | H     | 1220 | CLA  | O2A-CGA-O1A | -4.52 | 112.19      | 123.59   |
| 14  | b     | 1220 | CLA  | O2A-CGA-O1A | -4.52 | 112.19      | 123.59   |
| 14  | B     | 1220 | CLA  | O2A-CGA-O1A | -4.52 | 112.19      | 123.59   |
| 18  | L     | 4022 | BCR  | C24-C23-C22 | -4.52 | 119.41      | 126.23   |
| 14  | H     | 1229 | CLA  | C1D-ND-C4D  | -4.52 | 103.13      | 106.33   |
| 14  | A     | 1135 | CLA  | C4A-NA-C1A  | 4.52  | 108.74      | 106.71   |
| 14  | H     | 1022 | CLA  | C1D-ND-C4D  | -4.51 | 103.13      | 106.33   |
| 14  | b     | 1202 | CLA  | C1D-ND-C4D  | -4.51 | 103.13      | 106.33   |
| 18  | H     | 4014 | BCR  | C24-C23-C22 | -4.51 | 119.42      | 126.23   |
| 14  | b     | 1022 | CLA  | C1D-ND-C4D  | -4.51 | 103.13      | 106.33   |
| 14  | H     | 1234 | CLA  | CHD-C1D-ND  | -4.50 | 120.31      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | b     | 4014 | BCR  | C24-C23-C22 | -4.50 | 119.43      | 126.23   |
| 18  | U     | 4022 | BCR  | C24-C23-C22 | -4.50 | 119.43      | 126.23   |
| 18  | B     | 4014 | BCR  | C24-C23-C22 | -4.50 | 119.43      | 126.23   |
| 14  | G     | 1110 | CLA  | C1D-ND-C4D  | -4.49 | 103.14      | 106.33   |
| 14  | G     | 1122 | CLA  | CHD-C1D-ND  | -4.49 | 120.33      | 124.45   |
| 14  | a     | 1101 | CLA  | CHD-C1D-ND  | -4.49 | 120.33      | 124.45   |
| 18  | b     | 4005 | BCR  | C34-C9-C10  | -4.49 | 116.63      | 122.92   |
| 14  | B     | 1226 | CLA  | CMB-C2B-C3B | 4.49  | 133.08      | 124.68   |
| 14  | B     | 1229 | CLA  | C1D-ND-C4D  | -4.49 | 103.14      | 106.33   |
| 14  | b     | 1213 | CLA  | C1D-ND-C4D  | -4.49 | 103.14      | 106.33   |
| 14  | H     | 1202 | CLA  | O2A-CGA-O1A | -4.49 | 112.26      | 123.59   |
| 14  | a     | 1110 | CLA  | C1D-ND-C4D  | -4.49 | 103.15      | 106.33   |
| 14  | B     | 1202 | CLA  | C1D-ND-C4D  | -4.49 | 103.15      | 106.33   |
| 14  | b     | 1226 | CLA  | CMB-C2B-C3B | 4.49  | 133.07      | 124.68   |
| 18  | B     | 4005 | BCR  | C34-C9-C10  | -4.48 | 116.64      | 122.92   |
| 14  | B     | 1022 | CLA  | C1D-ND-C4D  | -4.48 | 103.15      | 106.33   |
| 14  | G     | 1108 | CLA  | C1D-ND-C4D  | -4.48 | 103.15      | 106.33   |
| 14  | B     | 1202 | CLA  | O2A-CGA-O1A | -4.48 | 112.28      | 123.59   |
| 14  | B     | 1213 | CLA  | C1D-ND-C4D  | -4.48 | 103.15      | 106.33   |
| 14  | H     | 1213 | CLA  | C1D-ND-C4D  | -4.48 | 103.15      | 106.33   |
| 14  | b     | 1233 | CLA  | C1D-ND-C4D  | -4.48 | 103.15      | 106.33   |
| 15  | B     | 1237 | F6C  | C4A-NA-C1A  | 4.48  | 109.52      | 106.33   |
| 15  | b     | 1237 | F6C  | C4A-NA-C1A  | 4.48  | 109.52      | 106.33   |
| 14  | A     | 1110 | CLA  | C1D-ND-C4D  | -4.48 | 103.16      | 106.33   |
| 18  | H     | 4005 | BCR  | C34-C9-C10  | -4.47 | 116.66      | 122.92   |
| 14  | a     | 1132 | CLA  | C1D-ND-C4D  | -4.47 | 103.16      | 106.33   |
| 14  | b     | 1202 | CLA  | O2A-CGA-O1A | -4.47 | 112.31      | 123.59   |
| 13  | a     | 1011 | CL0  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 14  | V     | 1501 | CLA  | CHD-C1D-ND  | -4.47 | 120.35      | 124.45   |
| 18  | a     | 4006 | BCR  | C38-C26-C25 | -4.47 | 119.51      | 124.53   |
| 18  | i     | 4018 | BCR  | C24-C23-C22 | -4.47 | 119.49      | 126.23   |
| 21  | H     | 6003 | LMT  | C3'-C4'-C5' | -4.46 | 100.69      | 110.93   |
| 14  | H     | 1227 | CLA  | C1D-ND-C4D  | -4.46 | 103.16      | 106.33   |
| 13  | G     | 1011 | CL0  | C3D-C2D-C1D | -4.46 | 99.74       | 105.83   |
| 14  | H     | 1226 | CLA  | CMB-C2B-C3B | 4.46  | 133.03      | 124.68   |
| 15  | H     | 1237 | F6C  | C4A-NA-C1A  | 4.46  | 109.50      | 106.33   |
| 14  | b     | 1201 | CLA  | O2A-C1-C2   | 4.46  | 120.36      | 108.64   |
| 14  | a     | 1013 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 13  | A     | 1011 | CL0  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 14  | A     | 1108 | CLA  | C1D-ND-C4D  | -4.46 | 103.17      | 106.33   |
| 14  | B     | 1201 | CLA  | O2A-C1-C2   | 4.46  | 120.35      | 108.64   |
| 18  | I     | 4018 | BCR  | C24-C23-C22 | -4.45 | 119.50      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | b     | 6003 | LMT  | C3'-C4'-C5' | -4.45 | 100.72      | 110.93   |
| 14  | a     | 1115 | CLA  | CMB-C2B-C3B | 4.45  | 133.01      | 124.68   |
| 14  | b     | 1229 | CLA  | C1D-ND-C4D  | -4.45 | 103.17      | 106.33   |
| 21  | B     | 6003 | LMT  | C3'-C4'-C5' | -4.45 | 100.72      | 110.93   |
| 14  | m     | 1501 | CLA  | CHD-C1D-ND  | -4.45 | 120.36      | 124.45   |
| 14  | A     | 1101 | CLA  | CHD-C1D-ND  | -4.45 | 120.37      | 124.45   |
| 14  | G     | 1013 | CLA  | C1C-C2C-C3C | -4.45 | 102.28      | 106.96   |
| 14  | G     | 1101 | CLA  | CHD-C1D-ND  | -4.45 | 120.37      | 124.45   |
| 14  | A     | 1013 | CLA  | C1C-C2C-C3C | -4.44 | 102.28      | 106.96   |
| 14  | A     | 1115 | CLA  | CMB-C2B-C3B | 4.44  | 132.99      | 124.68   |
| 14  | M     | 1501 | CLA  | CHD-C1D-ND  | -4.44 | 120.37      | 124.45   |
| 14  | G     | 1113 | CLA  | C4A-NA-C1A  | 4.44  | 108.70      | 106.71   |
| 14  | H     | 1201 | CLA  | O2A-C1-C2   | 4.44  | 120.30      | 108.64   |
| 14  | H     | 1202 | CLA  | C1D-ND-C4D  | -4.44 | 103.18      | 106.33   |
| 14  | H     | 1217 | CLA  | CHD-C1D-ND  | -4.44 | 120.38      | 124.45   |
| 14  | G     | 1135 | CLA  | C4A-NA-C1A  | 4.44  | 108.70      | 106.71   |
| 18  | G     | 4006 | BCR  | C38-C26-C25 | -4.43 | 119.55      | 124.53   |
| 14  | G     | 1115 | CLA  | CMB-C2B-C3B | 4.43  | 132.97      | 124.68   |
| 14  | a     | 1101 | CLA  | C1D-ND-C4D  | -4.43 | 103.19      | 106.33   |
| 18  | a     | 4002 | BCR  | C7-C8-C9    | -4.43 | 119.54      | 126.23   |
| 18  | R     | 4018 | BCR  | C24-C23-C22 | -4.43 | 119.54      | 126.23   |
| 14  | B     | 1233 | CLA  | C1D-ND-C4D  | -4.43 | 103.19      | 106.33   |
| 18  | A     | 4006 | BCR  | C38-C26-C25 | -4.43 | 119.56      | 124.53   |
| 14  | A     | 1132 | CLA  | C1D-ND-C4D  | -4.42 | 103.19      | 106.33   |
| 18  | G     | 4002 | BCR  | C7-C8-C9    | -4.42 | 119.56      | 126.23   |
| 14  | G     | 1139 | CLA  | C1D-ND-C4D  | -4.42 | 103.19      | 106.33   |
| 18  | A     | 4002 | BCR  | C7-C8-C9    | -4.42 | 119.56      | 126.23   |
| 14  | U     | 1503 | CLA  | CHD-C1D-ND  | -4.42 | 120.40      | 124.45   |
| 14  | B     | 1217 | CLA  | CHD-C1D-ND  | -4.41 | 120.40      | 124.45   |
| 14  | H     | 1217 | CLA  | C1D-ND-C4D  | -4.41 | 103.20      | 106.33   |
| 14  | G     | 1132 | CLA  | C1D-ND-C4D  | -4.41 | 103.20      | 106.33   |
| 14  | B     | 1227 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 14  | b     | 1217 | CLA  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 14  | H     | 1223 | CLA  | C4A-NA-C1A  | 4.40  | 108.69      | 106.71   |
| 14  | A     | 1127 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 14  | a     | 1108 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 14  | b     | 1227 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 21  | B     | 6003 | LMT  | O1'-C1'-C2' | 4.40  | 115.17      | 108.30   |
| 14  | L     | 1503 | CLA  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 14  | G     | 1130 | CLA  | O2A-CGA-O1A | -4.40 | 112.49      | 123.59   |
| 18  | A     | 4001 | BCR  | C15-C14-C13 | -4.40 | 121.03      | 127.31   |
| 18  | H     | 4005 | BCR  | C7-C8-C9    | -4.40 | 119.59      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1233 | CLA  | C1D-ND-C4D  | -4.39 | 103.21      | 106.33   |
| 14  | A     | 1113 | CLA  | C4A-NA-C1A  | 4.39  | 108.68      | 106.71   |
| 14  | B     | 1217 | CLA  | C1D-ND-C4D  | -4.39 | 103.22      | 106.33   |
| 18  | b     | 4005 | BCR  | C7-C8-C9    | -4.39 | 119.60      | 126.23   |
| 18  | G     | 4001 | BCR  | C15-C14-C13 | -4.39 | 121.04      | 127.31   |
| 14  | a     | 1130 | CLA  | O2A-CGA-O1A | -4.39 | 112.51      | 123.59   |
| 14  | a     | 1135 | CLA  | C4A-NA-C1A  | 4.39  | 108.68      | 106.71   |
| 18  | a     | 4001 | BCR  | C15-C14-C13 | -4.39 | 121.04      | 127.31   |
| 14  | A     | 1012 | CLA  | O2A-C1-C2   | 4.39  | 120.17      | 108.64   |
| 14  | B     | 1225 | CLA  | C3D-C2D-C1D | -4.39 | 99.84       | 105.83   |
| 14  | a     | 1116 | CLA  | C4A-NA-C1A  | 4.39  | 108.68      | 106.71   |
| 18  | B     | 4005 | BCR  | C7-C8-C9    | -4.39 | 119.61      | 126.23   |
| 14  | a     | 1139 | CLA  | C1D-ND-C4D  | -4.39 | 103.22      | 106.33   |
| 14  | A     | 1130 | CLA  | O2A-CGA-O1A | -4.38 | 112.53      | 123.59   |
| 15  | H     | 1237 | F6C  | C3A-C4A-NA  | 4.38  | 113.33      | 110.10   |
| 14  | b     | 1225 | CLA  | C3D-C2D-C1D | -4.38 | 99.85       | 105.83   |
| 20  | I     | 5006 | LMG  | O7-C10-C11  | 4.38  | 120.95      | 111.50   |
| 21  | H     | 6003 | LMT  | O1'-C1'-C2' | 4.38  | 115.14      | 108.30   |
| 14  | B     | 1223 | CLA  | C4A-NA-C1A  | 4.38  | 108.68      | 106.71   |
| 21  | b     | 6003 | LMT  | O1'-C1'-C2' | 4.38  | 115.14      | 108.30   |
| 14  | A     | 1119 | CLA  | C4A-NA-C1A  | 4.38  | 108.67      | 106.71   |
| 14  | a     | 1113 | CLA  | C4A-NA-C1A  | 4.38  | 108.67      | 106.71   |
| 14  | G     | 1012 | CLA  | O2A-C1-C2   | 4.38  | 120.14      | 108.64   |
| 14  | G     | 1101 | CLA  | C1D-ND-C4D  | -4.38 | 103.23      | 106.33   |
| 14  | a     | 1012 | CLA  | O2A-C1-C2   | 4.38  | 120.13      | 108.64   |
| 14  | a     | 1105 | CLA  | C4A-NA-C1A  | 4.38  | 108.67      | 106.71   |
| 14  | G     | 1127 | CLA  | C1D-ND-C4D  | -4.37 | 103.23      | 106.33   |
| 14  | b     | 1223 | CLA  | C4A-NA-C1A  | 4.37  | 108.67      | 106.71   |
| 20  | R     | 5006 | LMG  | O7-C10-C11  | 4.37  | 120.92      | 111.50   |
| 14  | H     | 1225 | CLA  | C3D-C2D-C1D | -4.37 | 99.86       | 105.83   |
| 14  | A     | 1101 | CLA  | C1D-ND-C4D  | -4.37 | 103.23      | 106.33   |
| 14  | G     | 1119 | CLA  | O2A-CGA-O1A | -4.37 | 112.56      | 123.59   |
| 14  | a     | 1110 | CLA  | CMB-C2B-C3B | 4.37  | 132.85      | 124.68   |
| 20  | i     | 5006 | LMG  | O7-C10-C11  | 4.37  | 120.92      | 111.50   |
| 14  | G     | 1106 | CLA  | O2A-C1-C2   | 4.37  | 120.12      | 108.64   |
| 14  | B     | 1209 | CLA  | C4A-NA-C1A  | 4.37  | 108.67      | 106.71   |
| 14  | G     | 1114 | CLA  | C4A-NA-C1A  | 4.37  | 108.67      | 106.71   |
| 14  | a     | 1119 | CLA  | O2A-CGA-O1A | -4.37 | 112.57      | 123.59   |
| 14  | A     | 1119 | CLA  | O2A-CGA-O1A | -4.37 | 112.57      | 123.59   |
| 14  | A     | 1106 | CLA  | O2A-C1-C2   | 4.37  | 120.11      | 108.64   |
| 15  | H     | 1238 | F6C  | C2D-C1D-ND  | 4.37  | 114.06      | 109.97   |
| 15  | B     | 1238 | F6C  | C2D-C1D-ND  | 4.36  | 114.06      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1110 | CLA  | CMB-C2B-C3B | 4.36  | 132.84      | 124.68   |
| 14  | G     | 1105 | CLA  | C4A-NA-C1A  | 4.36  | 108.67      | 106.71   |
| 14  | A     | 1110 | CLA  | CMB-C2B-C3B | 4.36  | 132.84      | 124.68   |
| 14  | b     | 1217 | CLA  | C1D-ND-C4D  | -4.36 | 103.24      | 106.33   |
| 14  | H     | 1226 | CLA  | O2D-CGD-O1D | -4.36 | 115.31      | 123.84   |
| 14  | a     | 1111 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 15  | b     | 1238 | F6C  | C2D-C1D-ND  | 4.36  | 114.06      | 109.97   |
| 19  | G     | 5002 | LHG  | O7-C7-C8    | 4.36  | 120.89      | 111.50   |
| 14  | a     | 1127 | CLA  | C1D-ND-C4D  | -4.36 | 103.24      | 106.33   |
| 14  | G     | 1111 | CLA  | C1C-C2C-C3C | -4.36 | 102.38      | 106.96   |
| 14  | A     | 1111 | CLA  | C1C-C2C-C3C | -4.36 | 102.38      | 106.96   |
| 14  | a     | 1131 | CLA  | O2A-CGA-CBA | 4.36  | 125.58      | 111.91   |
| 14  | A     | 1139 | CLA  | C1D-ND-C4D  | -4.35 | 103.24      | 106.33   |
| 14  | H     | 1209 | CLA  | C1D-ND-C4D  | -4.35 | 103.24      | 106.33   |
| 14  | G     | 1102 | CLA  | CMB-C2B-C3B | 4.35  | 132.82      | 124.68   |
| 14  | l     | 1503 | CLA  | CHD-C1D-ND  | -4.35 | 120.45      | 124.45   |
| 19  | A     | 5002 | LHG  | O7-C7-C8    | 4.35  | 120.88      | 111.50   |
| 14  | b     | 1204 | CLA  | C4A-NA-C1A  | 4.35  | 108.66      | 106.71   |
| 14  | a     | 1102 | CLA  | CMB-C2B-C3B | 4.35  | 132.82      | 124.68   |
| 14  | B     | 1209 | CLA  | C1D-ND-C4D  | -4.35 | 103.24      | 106.33   |
| 14  | a     | 1106 | CLA  | O2A-C1-C2   | 4.35  | 120.07      | 108.64   |
| 15  | B     | 1237 | F6C  | C3A-C4A-NA  | 4.35  | 113.31      | 110.10   |
| 14  | a     | 1119 | CLA  | CMB-C2B-C3B | 4.35  | 132.82      | 124.68   |
| 14  | a     | 1127 | CLA  | CHD-C1D-ND  | -4.35 | 120.45      | 124.45   |
| 14  | A     | 1102 | CLA  | CMB-C2B-C3B | 4.35  | 132.82      | 124.68   |
| 14  | A     | 1116 | CLA  | C4A-NA-C1A  | 4.35  | 108.66      | 106.71   |
| 14  | A     | 1127 | CLA  | CHD-C1D-ND  | -4.35 | 120.46      | 124.45   |
| 14  | b     | 1226 | CLA  | O2D-CGD-O1D | -4.35 | 115.33      | 123.84   |
| 14  | A     | 1105 | CLA  | C4A-NA-C1A  | 4.35  | 108.66      | 106.71   |
| 14  | A     | 1131 | CLA  | O2A-CGA-CBA | 4.35  | 125.55      | 111.91   |
| 14  | H     | 1209 | CLA  | C4A-NA-C1A  | 4.35  | 108.66      | 106.71   |
| 14  | B     | 1022 | CLA  | O2D-CGD-O1D | -4.35 | 115.34      | 123.84   |
| 14  | b     | 1021 | CLA  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 14  | B     | 1226 | CLA  | O2D-CGD-O1D | -4.34 | 115.34      | 123.84   |
| 14  | a     | 1135 | CLA  | O2A-CGA-O1A | -4.34 | 112.63      | 123.59   |
| 14  | G     | 1131 | CLA  | O2A-CGA-CBA | 4.34  | 125.52      | 111.91   |
| 14  | b     | 1209 | CLA  | C1D-ND-C4D  | -4.34 | 103.25      | 106.33   |
| 14  | a     | 1119 | CLA  | C4A-NA-C1A  | 4.34  | 108.66      | 106.71   |
| 14  | G     | 1135 | CLA  | O2A-CGA-O1A | -4.33 | 112.65      | 123.59   |
| 14  | H     | 1236 | CLA  | O2A-CGA-CBA | 4.33  | 125.51      | 111.91   |
| 14  | B     | 1021 | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 14  | B     | 1236 | CLA  | O2A-CGA-CBA | 4.33  | 125.50      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1119 | CLA  | CMB-C2B-C3B | 4.33  | 132.78      | 124.68   |
| 14  | A     | 1135 | CLA  | O2A-CGA-O1A | -4.33 | 112.66      | 123.59   |
| 18  | H     | 4010 | BCR  | C19-C18-C17 | 4.33  | 125.58      | 118.94   |
| 18  | b     | 4010 | BCR  | C19-C18-C17 | 4.33  | 125.58      | 118.94   |
| 14  | b     | 1236 | CLA  | O2A-CGA-CBA | 4.33  | 125.49      | 111.91   |
| 14  | H     | 1021 | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 14  | G     | 1130 | CLA  | O2A-C1-C2   | 4.33  | 120.01      | 108.64   |
| 14  | B     | 1211 | CLA  | C1C-C2C-C3C | -4.33 | 102.41      | 106.96   |
| 15  | H     | 1207 | F6C  | O2A-C1-C2   | 4.33  | 120.01      | 108.64   |
| 14  | H     | 1022 | CLA  | O2D-CGD-O1D | -4.33 | 115.38      | 123.84   |
| 14  | A     | 1130 | CLA  | O2A-C1-C2   | 4.33  | 120.00      | 108.64   |
| 14  | G     | 1127 | CLA  | CHD-C1D-ND  | -4.33 | 120.48      | 124.45   |
| 18  | m     | 4021 | BCR  | C36-C18-C17 | -4.33 | 116.86      | 122.92   |
| 19  | a     | 5002 | LHG  | O7-C7-C8    | 4.33  | 120.82      | 111.50   |
| 14  | A     | 1119 | CLA  | CMB-C2B-C3B | 4.32  | 132.77      | 124.68   |
| 14  | b     | 1022 | CLA  | O2D-CGD-O1D | -4.32 | 115.39      | 123.84   |
| 14  | a     | 1130 | CLA  | O2A-C1-C2   | 4.32  | 119.99      | 108.64   |
| 14  | a     | 1139 | CLA  | C4A-NA-C1A  | 4.32  | 108.65      | 106.71   |
| 14  | b     | 1211 | CLA  | C1C-C2C-C3C | -4.32 | 102.41      | 106.96   |
| 18  | B     | 4010 | BCR  | C19-C18-C17 | 4.32  | 125.57      | 118.94   |
| 14  | A     | 1114 | CLA  | C4A-NA-C1A  | 4.32  | 108.65      | 106.71   |
| 14  | H     | 1211 | CLA  | C1C-C2C-C3C | -4.32 | 102.42      | 106.96   |
| 18  | M     | 4021 | BCR  | C36-C18-C17 | -4.32 | 116.88      | 122.92   |
| 15  | b     | 1207 | F6C  | O2A-C1-C2   | 4.32  | 119.98      | 108.64   |
| 14  | L     | 1502 | CLA  | O2A-CGA-O1A | -4.31 | 112.70      | 123.59   |
| 15  | B     | 1207 | F6C  | O2A-C1-C2   | 4.31  | 119.97      | 108.64   |
| 14  | G     | 1123 | CLA  | C1D-ND-C4D  | -4.31 | 103.27      | 106.33   |
| 14  | G     | 1139 | CLA  | C4A-NA-C1A  | 4.31  | 108.64      | 106.71   |
| 14  | b     | 1209 | CLA  | C4A-NA-C1A  | 4.31  | 108.64      | 106.71   |
| 14  | l     | 1502 | CLA  | O2A-CGA-O1A | -4.31 | 112.71      | 123.59   |
| 14  | U     | 1502 | CLA  | O2A-CGA-O1A | -4.30 | 112.74      | 123.59   |
| 14  | A     | 1137 | CLA  | C1D-ND-C4D  | -4.30 | 103.28      | 106.33   |
| 18  | V     | 4021 | BCR  | C36-C18-C17 | -4.30 | 116.90      | 122.92   |
| 15  | A     | 1121 | F6C  | C4A-NA-C1A  | 4.29  | 109.39      | 106.33   |
| 14  | B     | 1208 | CLA  | C1D-ND-C4D  | -4.29 | 103.28      | 106.33   |
| 15  | b     | 1237 | F6C  | C3A-C4A-NA  | 4.29  | 113.27      | 110.10   |
| 14  | B     | 1202 | CLA  | O2D-CGD-O1D | -4.29 | 115.45      | 123.84   |
| 14  | a     | 1137 | CLA  | C1D-ND-C4D  | -4.29 | 103.29      | 106.33   |
| 14  | G     | 1116 | CLA  | C4A-NA-C1A  | 4.28  | 108.63      | 106.71   |
| 19  | L     | 5102 | LHG  | O7-C7-C8    | 4.28  | 120.73      | 111.50   |
| 14  | a     | 1123 | CLA  | C1D-ND-C4D  | -4.28 | 103.29      | 106.33   |
| 14  | H     | 1223 | CLA  | CMB-C2B-C3B | 4.28  | 132.69      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1202 | CLA  | O2D-CGD-O1D | -4.28 | 115.47      | 123.84   |
| 19  | U     | 5102 | LHG  | O7-C7-C8    | 4.28  | 120.72      | 111.50   |
| 14  | G     | 1139 | CLA  | O2D-CGD-CBD | 4.28  | 118.87      | 111.27   |
| 15  | G     | 1121 | F6C  | C4A-NA-C1A  | 4.28  | 109.37      | 106.33   |
| 14  | a     | 1139 | CLA  | O2D-CGD-CBD | 4.27  | 118.85      | 111.27   |
| 14  | B     | 1206 | CLA  | C4-C3-C5    | 4.27  | 122.45      | 115.27   |
| 14  | A     | 1139 | CLA  | C4A-NA-C1A  | 4.26  | 108.62      | 106.71   |
| 14  | A     | 1139 | CLA  | O2D-CGD-CBD | 4.26  | 118.84      | 111.27   |
| 14  | b     | 1223 | CLA  | CMB-C2B-C3B | 4.26  | 132.65      | 124.68   |
| 14  | a     | 1135 | CLA  | C1D-ND-C4D  | -4.26 | 103.31      | 106.33   |
| 14  | B     | 1204 | CLA  | C4A-NA-C1A  | 4.26  | 108.62      | 106.71   |
| 15  | H     | 1237 | F6C  | O2A-CGA-O1A | -4.26 | 112.84      | 123.59   |
| 14  | b     | 1224 | CLA  | C1D-ND-C4D  | -4.26 | 103.31      | 106.33   |
| 19  | l     | 5102 | LHG  | O7-C7-C8    | 4.26  | 120.68      | 111.50   |
| 14  | L     | 1503 | CLA  | CAA-C2A-C3A | -4.26 | 101.11      | 112.78   |
| 14  | B     | 1223 | CLA  | CMB-C2B-C3B | 4.26  | 132.65      | 124.68   |
| 14  | G     | 1104 | CLA  | O2A-CGA-CBA | 4.26  | 125.27      | 111.91   |
| 14  | A     | 1123 | CLA  | C1D-ND-C4D  | -4.26 | 103.31      | 106.33   |
| 14  | G     | 1137 | CLA  | C1D-ND-C4D  | -4.26 | 103.31      | 106.33   |
| 14  | l     | 1503 | CLA  | CAA-C2A-C3A | -4.26 | 101.12      | 112.78   |
| 15  | b     | 1237 | F6C  | O2A-CGA-O1A | -4.26 | 112.85      | 123.59   |
| 14  | H     | 1208 | CLA  | C1D-ND-C4D  | -4.26 | 103.31      | 106.33   |
| 15  | B     | 1237 | F6C  | O2A-CGA-O1A | -4.25 | 112.86      | 123.59   |
| 14  | A     | 1104 | CLA  | O2A-CGA-CBA | 4.25  | 125.25      | 111.91   |
| 14  | b     | 1206 | CLA  | C4-C3-C5    | 4.25  | 122.42      | 115.27   |
| 14  | A     | 1116 | CLA  | C1D-ND-C4D  | -4.25 | 103.31      | 106.33   |
| 14  | H     | 1206 | CLA  | C4-C3-C5    | 4.25  | 122.42      | 115.27   |
| 14  | B     | 1224 | CLA  | C1D-ND-C4D  | -4.25 | 103.32      | 106.33   |
| 14  | U     | 1503 | CLA  | CAA-C2A-C3A | -4.25 | 101.15      | 112.78   |
| 14  | b     | 1202 | CLA  | O2D-CGD-O1D | -4.24 | 115.54      | 123.84   |
| 18  | b     | 4010 | BCR  | C36-C18-C17 | -4.24 | 116.98      | 122.92   |
| 14  | a     | 1114 | CLA  | C4A-NA-C1A  | 4.24  | 108.61      | 106.71   |
| 14  | a     | 1104 | CLA  | O2A-CGA-CBA | 4.24  | 125.22      | 111.91   |
| 14  | H     | 1208 | CLA  | CMB-C2B-C3B | 4.24  | 132.61      | 124.68   |
| 14  | G     | 1116 | CLA  | C1D-ND-C4D  | -4.24 | 103.33      | 106.33   |
| 14  | b     | 1021 | CLA  | C1D-ND-C4D  | -4.24 | 103.33      | 106.33   |
| 14  | H     | 1229 | CLA  | O2A-CGA-CBA | 4.24  | 125.20      | 111.91   |
| 14  | B     | 1208 | CLA  | CMB-C2B-C3B | 4.23  | 132.60      | 124.68   |
| 14  | B     | 1023 | CLA  | O2A-CGA-CBA | 4.23  | 125.18      | 111.91   |
| 14  | G     | 1119 | CLA  | C1D-ND-C4D  | -4.23 | 103.33      | 106.33   |
| 14  | H     | 1224 | CLA  | C1D-ND-C4D  | -4.23 | 103.33      | 106.33   |
| 14  | a     | 1134 | CLA  | C4A-NA-C1A  | 4.23  | 108.61      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1202 | CLA  | CMB-C2B-C3B | 4.23  | 132.59      | 124.68   |
| 14  | b     | 1023 | CLA  | O2A-CGA-CBA | 4.23  | 125.17      | 111.91   |
| 14  | B     | 1216 | CLA  | O2D-CGD-CBD | 4.23  | 118.78      | 111.27   |
| 14  | b     | 1205 | CLA  | O2A-CGA-CBA | 4.23  | 125.17      | 111.91   |
| 14  | a     | 1127 | CLA  | CMB-C2B-C3B | 4.23  | 132.58      | 124.68   |
| 14  | b     | 1229 | CLA  | O2A-CGA-CBA | 4.23  | 125.17      | 111.91   |
| 14  | H     | 1216 | CLA  | O2D-CGD-CBD | 4.23  | 118.78      | 111.27   |
| 14  | H     | 1023 | CLA  | O2A-CGA-CBA | 4.22  | 125.17      | 111.91   |
| 14  | b     | 1216 | CLA  | O2D-CGD-CBD | 4.22  | 118.77      | 111.27   |
| 14  | a     | 1116 | CLA  | C1D-ND-C4D  | -4.22 | 103.33      | 106.33   |
| 14  | B     | 1205 | CLA  | O2A-CGA-CBA | 4.22  | 125.16      | 111.91   |
| 14  | b     | 1202 | CLA  | CMB-C2B-C3B | 4.22  | 132.58      | 124.68   |
| 14  | B     | 1229 | CLA  | O2A-CGA-CBA | 4.22  | 125.16      | 111.91   |
| 14  | a     | 1103 | CLA  | O2D-CGD-O1D | -4.22 | 115.58      | 123.84   |
| 14  | B     | 1222 | CLA  | O2A-CGA-CBA | 4.22  | 125.15      | 111.91   |
| 14  | B     | 1021 | CLA  | C1D-ND-C4D  | -4.22 | 103.34      | 106.33   |
| 14  | H     | 1205 | CLA  | O2A-CGA-CBA | 4.22  | 125.14      | 111.91   |
| 14  | H     | 1222 | CLA  | O2A-CGA-CBA | 4.22  | 125.14      | 111.91   |
| 18  | B     | 4010 | BCR  | C36-C18-C17 | -4.22 | 117.02      | 122.92   |
| 14  | b     | 1222 | CLA  | O2A-CGA-CBA | 4.21  | 125.14      | 111.91   |
| 14  | b     | 1208 | CLA  | C1D-ND-C4D  | -4.21 | 103.34      | 106.33   |
| 14  | H     | 1234 | CLA  | O2A-CGA-CBA | 4.21  | 125.13      | 111.91   |
| 14  | H     | 1202 | CLA  | CMB-C2B-C3B | 4.21  | 132.56      | 124.68   |
| 18  | H     | 4010 | BCR  | C36-C18-C17 | -4.21 | 117.02      | 122.92   |
| 14  | b     | 1229 | CLA  | CMB-C2B-C3B | 4.21  | 132.56      | 124.68   |
| 14  | G     | 1117 | CLA  | O2A-CGA-O1A | -4.21 | 112.96      | 123.59   |
| 15  | a     | 1121 | F6C  | C4A-NA-C1A  | 4.21  | 109.33      | 106.33   |
| 14  | b     | 1208 | CLA  | CMB-C2B-C3B | 4.21  | 132.56      | 124.68   |
| 14  | b     | 1216 | CLA  | C1D-ND-C4D  | -4.21 | 103.34      | 106.33   |
| 14  | B     | 1234 | CLA  | O2A-CGA-CBA | 4.21  | 125.12      | 111.91   |
| 14  | G     | 1117 | CLA  | CMB-C2B-C3B | 4.21  | 132.55      | 124.68   |
| 14  | H     | 1021 | CLA  | C1D-ND-C4D  | -4.21 | 103.34      | 106.33   |
| 14  | b     | 1234 | CLA  | O2A-CGA-CBA | 4.21  | 125.11      | 111.91   |
| 14  | G     | 1119 | CLA  | C4A-NA-C1A  | 4.21  | 108.60      | 106.71   |
| 14  | H     | 1204 | CLA  | C4A-NA-C1A  | 4.21  | 108.60      | 106.71   |
| 14  | H     | 1226 | CLA  | C4A-NA-C1A  | 4.21  | 108.60      | 106.71   |
| 14  | A     | 1135 | CLA  | C1D-ND-C4D  | -4.21 | 103.35      | 106.33   |
| 14  | A     | 1127 | CLA  | CMB-C2B-C3B | 4.21  | 132.55      | 124.68   |
| 14  | A     | 1117 | CLA  | O2A-CGA-O1A | -4.20 | 112.98      | 123.59   |
| 14  | G     | 1127 | CLA  | CMB-C2B-C3B | 4.20  | 132.54      | 124.68   |
| 18  | A     | 4004 | BCR  | C28-C27-C26 | -4.20 | 106.57      | 114.08   |
| 14  | G     | 1129 | CLA  | CMB-C2B-C3B | 4.20  | 132.54      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1129 | CLA  | CMB-C2B-C3B | 4.20  | 132.53      | 124.68   |
| 14  | A     | 1128 | CLA  | O2A-CGA-CBA | 4.20  | 125.08      | 111.91   |
| 14  | B     | 1229 | CLA  | CMB-C2B-C3B | 4.20  | 132.53      | 124.68   |
| 14  | A     | 1103 | CLA  | O2D-CGD-O1D | -4.20 | 115.63      | 123.84   |
| 15  | G     | 1121 | F6C  | CMA-C3A-C4A | -4.20 | 117.32      | 124.71   |
| 14  | a     | 1128 | CLA  | O2A-CGA-CBA | 4.20  | 125.07      | 111.91   |
| 14  | B     | 1226 | CLA  | C4A-NA-C1A  | 4.20  | 108.59      | 106.71   |
| 14  | G     | 1103 | CLA  | O2D-CGD-O1D | -4.19 | 115.64      | 123.84   |
| 14  | H     | 1215 | CLA  | O2A-C1-C2   | 4.19  | 119.65      | 108.64   |
| 14  | G     | 1122 | CLA  | C1C-C2C-C3C | -4.19 | 102.55      | 106.96   |
| 15  | a     | 1121 | F6C  | CMA-C3A-C4A | -4.19 | 117.33      | 124.71   |
| 14  | a     | 1117 | CLA  | CMB-C2B-C3B | 4.19  | 132.51      | 124.68   |
| 18  | a     | 4004 | BCR  | C28-C27-C26 | -4.19 | 106.60      | 114.08   |
| 14  | A     | 1117 | CLA  | CMB-C2B-C3B | 4.19  | 132.51      | 124.68   |
| 14  | a     | 1129 | CLA  | CMB-C2B-C3B | 4.19  | 132.51      | 124.68   |
| 14  | G     | 1128 | CLA  | O2A-CGA-CBA | 4.19  | 125.04      | 111.91   |
| 15  | A     | 1121 | F6C  | CMA-C3A-C4A | -4.18 | 117.34      | 124.71   |
| 14  | b     | 1206 | CLA  | C1D-ND-C4D  | -4.18 | 103.36      | 106.33   |
| 18  | G     | 4004 | BCR  | C28-C27-C26 | -4.18 | 106.61      | 114.08   |
| 14  | a     | 1117 | CLA  | O2A-CGA-O1A | -4.18 | 113.04      | 123.59   |
| 14  | G     | 1135 | CLA  | C1D-ND-C4D  | -4.18 | 103.36      | 106.33   |
| 14  | A     | 1134 | CLA  | C4A-NA-C1A  | 4.18  | 108.59      | 106.71   |
| 14  | H     | 1229 | CLA  | CMB-C2B-C3B | 4.18  | 132.50      | 124.68   |
| 14  | B     | 1216 | CLA  | C1D-ND-C4D  | -4.18 | 103.36      | 106.33   |
| 14  | b     | 1215 | CLA  | O2A-C1-C2   | 4.18  | 119.61      | 108.64   |
| 14  | B     | 1215 | CLA  | O2A-C1-C2   | 4.18  | 119.61      | 108.64   |
| 14  | G     | 1123 | CLA  | CHD-C1D-ND  | -4.17 | 120.62      | 124.45   |
| 14  | B     | 1210 | CLA  | O2D-CGD-O1D | -4.17 | 115.68      | 123.84   |
| 14  | B     | 1203 | CLA  | O2A-CGA-CBA | 4.17  | 125.00      | 111.91   |
| 14  | b     | 1203 | CLA  | O2A-CGA-CBA | 4.17  | 125.00      | 111.91   |
| 14  | H     | 1203 | CLA  | O2A-CGA-CBA | 4.17  | 124.99      | 111.91   |
| 14  | B     | 1234 | CLA  | C4A-NA-C1A  | 4.17  | 108.58      | 106.71   |
| 14  | b     | 1226 | CLA  | C4A-NA-C1A  | 4.17  | 108.58      | 106.71   |
| 14  | B     | 1221 | CLA  | O2A-CGA-CBA | 4.16  | 124.98      | 111.91   |
| 14  | B     | 1206 | CLA  | C1D-ND-C4D  | -4.16 | 103.38      | 106.33   |
| 14  | b     | 1223 | CLA  | CHD-C1D-ND  | -4.16 | 120.63      | 124.45   |
| 14  | a     | 1120 | CLA  | CMB-C2B-C3B | 4.16  | 132.46      | 124.68   |
| 14  | b     | 1221 | CLA  | O2A-CGA-CBA | 4.16  | 124.96      | 111.91   |
| 14  | H     | 1203 | CLA  | CAA-C2A-C3A | -4.16 | 101.39      | 112.78   |
| 14  | H     | 1210 | CLA  | O2D-CGD-O1D | -4.16 | 115.71      | 123.84   |
| 14  | b     | 1210 | CLA  | O2D-CGD-O1D | -4.16 | 115.71      | 123.84   |
| 14  | H     | 1221 | CLA  | O2A-CGA-CBA | 4.16  | 124.95      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | l     | 5101 | LHG  | O7-C7-C8    | 4.15  | 120.45      | 111.50   |
| 14  | B     | 1203 | CLA  | CAA-C2A-C3A | -4.15 | 101.41      | 112.78   |
| 14  | A     | 1119 | CLA  | C1D-ND-C4D  | -4.15 | 103.39      | 106.33   |
| 14  | H     | 1223 | CLA  | CHD-C1D-ND  | -4.15 | 120.64      | 124.45   |
| 18  | H     | 4010 | BCR  | C7-C8-C9    | -4.15 | 119.97      | 126.23   |
| 14  | G     | 1120 | CLA  | CMB-C2B-C3B | 4.15  | 132.44      | 124.68   |
| 15  | b     | 1207 | F6C  | O2D-CGD-O1D | -4.15 | 115.73      | 123.84   |
| 14  | A     | 1122 | CLA  | C1C-C2C-C3C | -4.15 | 102.60      | 106.96   |
| 14  | A     | 1120 | CLA  | CMB-C2B-C3B | 4.14  | 132.43      | 124.68   |
| 14  | b     | 1203 | CLA  | CAA-C2A-C3A | -4.14 | 101.43      | 112.78   |
| 14  | G     | 1103 | CLA  | CMB-C2B-C3B | 4.14  | 132.43      | 124.68   |
| 19  | L     | 5101 | LHG  | O7-C7-C8    | 4.14  | 120.43      | 111.50   |
| 14  | a     | 1126 | CLA  | O2A-C1-C2   | 4.14  | 119.52      | 108.64   |
| 14  | a     | 1103 | CLA  | CMB-C2B-C3B | 4.14  | 132.43      | 124.68   |
| 18  | b     | 4009 | BCR  | C7-C8-C9    | -4.14 | 119.98      | 126.23   |
| 14  | b     | 1234 | CLA  | C4A-NA-C1A  | 4.14  | 108.57      | 106.71   |
| 14  | G     | 1115 | CLA  | C1D-ND-C4D  | -4.14 | 103.39      | 106.33   |
| 14  | H     | 1225 | CLA  | O2A-CGA-CBA | 4.14  | 124.89      | 111.91   |
| 14  | A     | 1103 | CLA  | CMB-C2B-C3B | 4.14  | 132.42      | 124.68   |
| 19  | U     | 5101 | LHG  | O7-C7-C8    | 4.14  | 120.41      | 111.50   |
| 14  | A     | 1126 | CLA  | O2A-C1-C2   | 4.13  | 119.50      | 108.64   |
| 15  | B     | 1207 | F6C  | O2D-CGD-O1D | -4.13 | 115.76      | 123.84   |
| 14  | G     | 1136 | CLA  | C1D-ND-C4D  | -4.13 | 103.40      | 106.33   |
| 15  | H     | 1207 | F6C  | O2D-CGD-O1D | -4.13 | 115.76      | 123.84   |
| 14  | B     | 1225 | CLA  | O2A-CGA-CBA | 4.13  | 124.86      | 111.91   |
| 14  | H     | 1201 | CLA  | C1-C2-C3    | -4.13 | 118.90      | 126.04   |
| 14  | L     | 1501 | CLA  | O2D-CGD-O1D | -4.13 | 115.77      | 123.84   |
| 14  | U     | 1501 | CLA  | O2D-CGD-O1D | -4.13 | 115.77      | 123.84   |
| 14  | G     | 1134 | CLA  | C4A-NA-C1A  | 4.13  | 108.56      | 106.71   |
| 14  | B     | 1022 | CLA  | CHD-C1D-ND  | -4.13 | 120.66      | 124.45   |
| 14  | A     | 1136 | CLA  | C1D-ND-C4D  | -4.12 | 103.41      | 106.33   |
| 14  | G     | 1103 | CLA  | C1D-ND-C4D  | -4.12 | 103.41      | 106.33   |
| 18  | B     | 4010 | BCR  | C7-C8-C9    | -4.12 | 120.00      | 126.23   |
| 14  | U     | 1501 | CLA  | O2A-CGA-CBA | 4.12  | 124.84      | 111.91   |
| 14  | a     | 1122 | CLA  | C1C-C2C-C3C | -4.12 | 102.62      | 106.96   |
| 14  | G     | 1126 | CLA  | O2A-C1-C2   | 4.12  | 119.46      | 108.64   |
| 14  | l     | 1501 | CLA  | O2D-CGD-O1D | -4.12 | 115.78      | 123.84   |
| 14  | b     | 1225 | CLA  | O2A-CGA-CBA | 4.12  | 124.83      | 111.91   |
| 14  | B     | 1201 | CLA  | C1-C2-C3    | -4.12 | 118.92      | 126.04   |
| 14  | A     | 1103 | CLA  | C1D-ND-C4D  | -4.12 | 103.41      | 106.33   |
| 14  | G     | 1112 | CLA  | C1D-ND-C4D  | -4.12 | 103.41      | 106.33   |
| 14  | L     | 1501 | CLA  | O2A-CGA-CBA | 4.12  | 124.83      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1211 | CLA  | CMB-C2B-C3B | 4.12  | 132.38      | 124.68   |
| 14  | H     | 1022 | CLA  | CHD-C1D-ND  | -4.12 | 120.67      | 124.45   |
| 14  | A     | 1112 | CLA  | C1D-ND-C4D  | -4.12 | 103.41      | 106.33   |
| 14  | a     | 1012 | CLA  | C4A-NA-C1A  | 4.12  | 108.56      | 106.71   |
| 14  | l     | 1501 | CLA  | O2A-CGA-CBA | 4.12  | 124.83      | 111.91   |
| 14  | H     | 1206 | CLA  | C1D-ND-C4D  | -4.11 | 103.41      | 106.33   |
| 14  | H     | 1211 | CLA  | CMB-C2B-C3B | 4.11  | 132.38      | 124.68   |
| 18  | B     | 4009 | BCR  | C7-C8-C9    | -4.11 | 120.02      | 126.23   |
| 14  | A     | 1123 | CLA  | CHD-C1D-ND  | -4.11 | 120.67      | 124.45   |
| 14  | B     | 1223 | CLA  | CHD-C1D-ND  | -4.11 | 120.67      | 124.45   |
| 18  | H     | 4009 | BCR  | C7-C8-C9    | -4.11 | 120.02      | 126.23   |
| 18  | A     | 4004 | BCR  | C30-C25-C26 | -4.11 | 116.82      | 122.61   |
| 14  | a     | 1112 | CLA  | C1D-ND-C4D  | -4.11 | 103.41      | 106.33   |
| 14  | H     | 1216 | CLA  | C1D-ND-C4D  | -4.11 | 103.42      | 106.33   |
| 14  | H     | 1239 | CLA  | C1-C2-C3    | -4.11 | 118.93      | 126.04   |
| 18  | b     | 4010 | BCR  | C7-C8-C9    | -4.11 | 120.03      | 126.23   |
| 14  | a     | 1115 | CLA  | C1D-ND-C4D  | -4.11 | 103.42      | 106.33   |
| 14  | a     | 1123 | CLA  | CHD-C1D-ND  | -4.11 | 120.68      | 124.45   |
| 15  | B     | 1230 | F6C  | C4A-C3A-C2A | -4.11 | 100.94      | 106.94   |
| 14  | b     | 1201 | CLA  | C1-C2-C3    | -4.11 | 118.94      | 126.04   |
| 14  | a     | 1122 | CLA  | C4-C3-C5    | 4.10  | 122.18      | 115.27   |
| 14  | B     | 1239 | CLA  | C1-C2-C3    | -4.10 | 118.94      | 126.04   |
| 14  | B     | 1211 | CLA  | CMB-C2B-C3B | 4.10  | 132.36      | 124.68   |
| 14  | G     | 1108 | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 14  | a     | 1112 | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 14  | a     | 1108 | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 18  | G     | 4004 | BCR  | C30-C25-C26 | -4.10 | 116.84      | 122.61   |
| 18  | a     | 4002 | BCR  | C34-C9-C10  | -4.10 | 117.19      | 122.92   |
| 14  | b     | 1022 | CLA  | CHD-C1D-ND  | -4.09 | 120.69      | 124.45   |
| 14  | a     | 1119 | CLA  | C1D-ND-C4D  | -4.09 | 103.43      | 106.33   |
| 18  | A     | 4002 | BCR  | C34-C9-C10  | -4.09 | 117.19      | 122.92   |
| 14  | a     | 1136 | CLA  | C1D-ND-C4D  | -4.09 | 103.43      | 106.33   |
| 14  | A     | 1115 | CLA  | C1D-ND-C4D  | -4.09 | 103.43      | 106.33   |
| 14  | A     | 1108 | CLA  | CMB-C2B-C3B | 4.09  | 132.33      | 124.68   |
| 18  | a     | 4004 | BCR  | C30-C25-C26 | -4.09 | 116.85      | 122.61   |
| 18  | G     | 4002 | BCR  | C34-C9-C10  | -4.09 | 117.19      | 122.92   |
| 14  | b     | 1239 | CLA  | C1-C2-C3    | -4.09 | 118.97      | 126.04   |
| 21  | H     | 6003 | LMT  | C1-O1'-C1'  | 4.08  | 120.61      | 113.84   |
| 14  | A     | 1112 | CLA  | CMB-C2B-C3B | 4.08  | 132.32      | 124.68   |
| 14  | A     | 1122 | CLA  | C4-C3-C5    | 4.08  | 122.14      | 115.27   |
| 15  | b     | 1230 | F6C  | C4A-C3A-C2A | -4.08 | 100.98      | 106.94   |
| 15  | H     | 1230 | F6C  | C4A-C3A-C2A | -4.08 | 100.98      | 106.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | I     | 4018 | BCR  | C38-C26-C25 | -4.08 | 119.95      | 124.53   |
| 14  | H     | 1220 | CLA  | C1D-ND-C4D  | -4.08 | 103.44      | 106.33   |
| 18  | R     | 4018 | BCR  | C38-C26-C25 | -4.08 | 119.95      | 124.53   |
| 21  | b     | 6003 | LMT  | C1-O1'-C1'  | 4.08  | 120.60      | 113.84   |
| 14  | A     | 1102 | CLA  | C1-C2-C3    | -4.08 | 120.16      | 126.75   |
| 14  | b     | 1218 | CLA  | CMB-C2B-C3B | 4.07  | 132.30      | 124.68   |
| 14  | b     | 1213 | CLA  | CMB-C2B-C3B | 4.07  | 132.30      | 124.68   |
| 14  | L     | 1503 | CLA  | C1D-ND-C4D  | -4.07 | 103.44      | 106.33   |
| 14  | A     | 1129 | CLA  | C4A-NA-C1A  | 4.07  | 108.54      | 106.71   |
| 21  | B     | 6003 | LMT  | C1-O1'-C1'  | 4.07  | 120.59      | 113.84   |
| 14  | b     | 1225 | CLA  | C1D-ND-C4D  | -4.07 | 103.44      | 106.33   |
| 14  | G     | 1112 | CLA  | CMB-C2B-C3B | 4.07  | 132.29      | 124.68   |
| 14  | G     | 1122 | CLA  | C4-C3-C5    | 4.07  | 122.11      | 115.27   |
| 14  | a     | 1102 | CLA  | C1-C2-C3    | -4.07 | 120.17      | 126.75   |
| 14  | a     | 1103 | CLA  | C1D-ND-C4D  | -4.06 | 103.45      | 106.33   |
| 18  | i     | 4018 | BCR  | C38-C26-C25 | -4.06 | 119.97      | 124.53   |
| 14  | B     | 1206 | CLA  | O2A-CGA-CBA | 4.06  | 124.66      | 111.91   |
| 14  | H     | 1206 | CLA  | O2A-CGA-CBA | 4.06  | 124.65      | 111.91   |
| 14  | b     | 1206 | CLA  | O2A-CGA-CBA | 4.06  | 124.64      | 111.91   |
| 14  | B     | 1225 | CLA  | C1D-ND-C4D  | -4.06 | 103.45      | 106.33   |
| 14  | G     | 1102 | CLA  | C1-C2-C3    | -4.05 | 120.19      | 126.75   |
| 14  | a     | 1129 | CLA  | C4A-NA-C1A  | 4.05  | 108.53      | 106.71   |
| 14  | B     | 1218 | CLA  | CMB-C2B-C3B | 4.05  | 132.26      | 124.68   |
| 14  | H     | 1218 | CLA  | CMB-C2B-C3B | 4.05  | 132.25      | 124.68   |
| 14  | U     | 1503 | CLA  | C1D-ND-C4D  | -4.05 | 103.46      | 106.33   |
| 18  | U     | 4022 | BCR  | C33-C5-C6   | -4.04 | 119.99      | 124.53   |
| 14  | b     | 1221 | CLA  | C1D-ND-C4D  | -4.04 | 103.46      | 106.33   |
| 14  | B     | 1225 | CLA  | CHD-C1D-ND  | -4.04 | 120.74      | 124.45   |
| 14  | B     | 1210 | CLA  | C1C-C2C-C3C | -4.04 | 102.71      | 106.96   |
| 14  | a     | 1135 | CLA  | CMB-C2B-C3B | 4.04  | 132.24      | 124.68   |
| 14  | a     | 1137 | CLA  | O2A-CGA-CBA | 4.04  | 124.58      | 111.91   |
| 14  | B     | 1213 | CLA  | CMB-C2B-C3B | 4.04  | 132.23      | 124.68   |
| 14  | H     | 1225 | CLA  | C1D-ND-C4D  | -4.04 | 103.47      | 106.33   |
| 14  | H     | 1229 | CLA  | C4A-NA-C1A  | 4.04  | 108.52      | 106.71   |
| 14  | G     | 1135 | CLA  | CMB-C2B-C3B | 4.04  | 132.23      | 124.68   |
| 14  | M     | 1501 | CLA  | C1D-ND-C4D  | -4.03 | 103.47      | 106.33   |
| 14  | b     | 1210 | CLA  | C1C-C2C-C3C | -4.03 | 102.72      | 106.96   |
| 14  | A     | 1135 | CLA  | CMB-C2B-C3B | 4.03  | 132.22      | 124.68   |
| 14  | G     | 1133 | CLA  | O2A-CGA-CBA | 4.03  | 124.55      | 111.91   |
| 14  | B     | 1229 | CLA  | C4A-NA-C1A  | 4.03  | 108.52      | 106.71   |
| 14  | a     | 1126 | CLA  | O2A-CGA-CBA | 4.03  | 124.55      | 111.91   |
| 14  | G     | 1137 | CLA  | O2A-CGA-CBA | 4.02  | 124.54      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1234 | CLA  | C4A-NA-C1A  | 4.02  | 108.52      | 106.71   |
| 14  | A     | 1137 | CLA  | O2A-CGA-CBA | 4.02  | 124.53      | 111.91   |
| 18  | L     | 4022 | BCR  | C33-C5-C6   | -4.02 | 120.01      | 124.53   |
| 14  | A     | 1126 | CLA  | O2A-CGA-CBA | 4.02  | 124.53      | 111.91   |
| 14  | G     | 1126 | CLA  | O2A-CGA-CBA | 4.02  | 124.52      | 111.91   |
| 14  | A     | 1012 | CLA  | C4A-NA-C1A  | 4.02  | 108.51      | 106.71   |
| 14  | l     | 1503 | CLA  | C1D-ND-C4D  | -4.02 | 103.48      | 106.33   |
| 14  | A     | 1133 | CLA  | O2A-CGA-CBA | 4.02  | 124.51      | 111.91   |
| 14  | G     | 1114 | CLA  | C1D-ND-C4D  | -4.01 | 103.48      | 106.33   |
| 14  | a     | 1109 | CLA  | C1D-ND-C4D  | -4.01 | 103.48      | 106.33   |
| 15  | B     | 1219 | F6C  | C4A-C3A-C2A | -4.01 | 101.08      | 106.94   |
| 14  | m     | 1501 | CLA  | C1D-ND-C4D  | -4.01 | 103.48      | 106.33   |
| 14  | a     | 1133 | CLA  | O2A-CGA-CBA | 4.01  | 124.49      | 111.91   |
| 14  | H     | 1213 | CLA  | CMB-C2B-C3B | 4.01  | 132.18      | 124.68   |
| 18  | G     | 4002 | BCR  | C38-C26-C25 | -4.01 | 120.03      | 124.53   |
| 14  | b     | 1225 | CLA  | CHD-C1D-ND  | -4.01 | 120.77      | 124.45   |
| 14  | a     | 1114 | CLA  | C1D-ND-C4D  | -4.01 | 103.49      | 106.33   |
| 14  | B     | 1214 | CLA  | O2A-CGA-CBA | 4.01  | 124.48      | 111.91   |
| 18  | l     | 4022 | BCR  | C33-C5-C6   | -4.01 | 120.03      | 124.53   |
| 14  | H     | 1210 | CLA  | C1C-C2C-C3C | -4.01 | 102.75      | 106.96   |
| 18  | b     | 4010 | BCR  | C3-C4-C5    | -4.00 | 106.93      | 114.08   |
| 15  | H     | 1219 | F6C  | C4A-C3A-C2A | -4.00 | 101.09      | 106.94   |
| 14  | b     | 1221 | CLA  | CHD-C1D-ND  | -4.00 | 120.77      | 124.45   |
| 14  | A     | 1116 | CLA  | O2A-CGA-CBA | 4.00  | 124.47      | 111.91   |
| 14  | A     | 1114 | CLA  | C1D-ND-C4D  | -4.00 | 103.49      | 106.33   |
| 15  | H     | 1207 | F6C  | CAA-C2A-C1A | -4.00 | 117.09      | 128.11   |
| 15  | b     | 1219 | F6C  | C4A-C3A-C2A | -4.00 | 101.10      | 106.94   |
| 14  | b     | 1201 | CLA  | CMB-C2B-C3B | 4.00  | 132.16      | 124.68   |
| 14  | G     | 1116 | CLA  | O2A-CGA-CBA | 4.00  | 124.46      | 111.91   |
| 14  | H     | 1214 | CLA  | O2A-CGA-CBA | 4.00  | 124.46      | 111.91   |
| 14  | V     | 1501 | CLA  | C1D-ND-C4D  | -4.00 | 103.50      | 106.33   |
| 14  | B     | 1220 | CLA  | C1D-ND-C4D  | -4.00 | 103.50      | 106.33   |
| 14  | a     | 1116 | CLA  | O2A-CGA-CBA | 4.00  | 124.45      | 111.91   |
| 14  | B     | 1221 | CLA  | C1D-ND-C4D  | -3.99 | 103.50      | 106.33   |
| 14  | G     | 1129 | CLA  | C4A-NA-C1A  | 3.99  | 108.50      | 106.71   |
| 15  | b     | 1207 | F6C  | CAA-C2A-C1A | -3.99 | 117.11      | 128.11   |
| 15  | B     | 1207 | F6C  | CAA-C2A-C1A | -3.99 | 117.11      | 128.11   |
| 14  | H     | 1201 | CLA  | CMB-C2B-C3B | 3.99  | 132.15      | 124.68   |
| 14  | G     | 1012 | CLA  | C4A-NA-C1A  | 3.99  | 108.50      | 106.71   |
| 14  | B     | 1201 | CLA  | CMB-C2B-C3B | 3.99  | 132.15      | 124.68   |
| 18  | a     | 4002 | BCR  | C38-C26-C25 | -3.99 | 120.05      | 124.53   |
| 14  | H     | 1225 | CLA  | CHD-C1D-ND  | -3.99 | 120.79      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1214 | CLA  | O2A-CGA-CBA | 3.98  | 124.41      | 111.91   |
| 18  | B     | 4010 | BCR  | C3-C4-C5    | -3.98 | 106.96      | 114.08   |
| 18  | A     | 4002 | BCR  | C38-C26-C25 | -3.98 | 120.05      | 124.53   |
| 14  | b     | 1215 | CLA  | CMB-C2B-C3B | 3.98  | 132.13      | 124.68   |
| 18  | H     | 4010 | BCR  | C3-C4-C5    | -3.98 | 106.96      | 114.08   |
| 14  | b     | 1221 | CLA  | O2A-C1-C2   | 3.98  | 119.10      | 108.64   |
| 14  | H     | 1221 | CLA  | O2A-C1-C2   | 3.98  | 119.10      | 108.64   |
| 14  | B     | 1221 | CLA  | O2A-C1-C2   | 3.98  | 119.10      | 108.64   |
| 14  | a     | 1126 | CLA  | CMB-C2B-C3B | 3.98  | 132.12      | 124.68   |
| 14  | A     | 1126 | CLA  | CMB-C2B-C3B | 3.98  | 132.12      | 124.68   |
| 14  | H     | 1215 | CLA  | CMB-C2B-C3B | 3.98  | 132.12      | 124.68   |
| 15  | b     | 1238 | F6C  | C3D-C2D-C1D | -3.97 | 100.08      | 105.83   |
| 14  | b     | 1220 | CLA  | C1D-ND-C4D  | -3.97 | 103.51      | 106.33   |
| 14  | B     | 1221 | CLA  | CHD-C1D-ND  | -3.97 | 120.80      | 124.45   |
| 15  | B     | 1238 | F6C  | C3D-C2D-C1D | -3.97 | 100.08      | 105.83   |
| 15  | B     | 1238 | F6C  | C4A-NA-C1A  | 3.97  | 109.15      | 106.33   |
| 14  | G     | 1126 | CLA  | CMB-C2B-C3B | 3.97  | 132.10      | 124.68   |
| 18  | b     | 4005 | BCR  | C33-C5-C6   | -3.97 | 120.07      | 124.53   |
| 15  | b     | 1238 | F6C  | C4A-NA-C1A  | 3.97  | 109.15      | 106.33   |
| 15  | H     | 1238 | F6C  | C3D-C2D-C1D | -3.96 | 100.09      | 105.83   |
| 14  | B     | 1215 | CLA  | CMB-C2B-C3B | 3.96  | 132.09      | 124.68   |
| 14  | A     | 1109 | CLA  | C1D-ND-C4D  | -3.96 | 103.52      | 106.33   |
| 18  | B     | 4005 | BCR  | C33-C5-C6   | -3.96 | 120.08      | 124.53   |
| 14  | V     | 1501 | CLA  | O2A-CGA-CBA | 3.96  | 124.33      | 111.91   |
| 14  | H     | 1221 | CLA  | C1D-ND-C4D  | -3.96 | 103.52      | 106.33   |
| 14  | b     | 1229 | CLA  | C4A-NA-C1A  | 3.96  | 108.48      | 106.71   |
| 14  | m     | 1501 | CLA  | O2A-CGA-CBA | 3.96  | 124.32      | 111.91   |
| 14  | G     | 1125 | CLA  | CHD-C1D-ND  | -3.96 | 120.82      | 124.45   |
| 14  | A     | 1122 | CLA  | C1D-ND-C4D  | -3.95 | 103.53      | 106.33   |
| 14  | M     | 1501 | CLA  | O2A-CGA-CBA | 3.95  | 124.31      | 111.91   |
| 14  | H     | 1228 | CLA  | CMB-C2B-C3B | 3.95  | 132.07      | 124.68   |
| 14  | a     | 1125 | CLA  | CHD-C1D-ND  | -3.95 | 120.83      | 124.45   |
| 14  | a     | 1140 | CLA  | O2A-CGA-CBA | 3.95  | 124.30      | 111.91   |
| 14  | H     | 1221 | CLA  | CHD-C1D-ND  | -3.95 | 120.83      | 124.45   |
| 18  | A     | 4006 | BCR  | C34-C9-C10  | -3.95 | 117.39      | 122.92   |
| 14  | a     | 1125 | CLA  | O2A-CGA-CBA | 3.95  | 124.29      | 111.91   |
| 14  | A     | 1140 | CLA  | O2A-CGA-CBA | 3.94  | 124.28      | 111.91   |
| 14  | H     | 1240 | CLA  | C4A-NA-C1A  | 3.94  | 108.48      | 106.71   |
| 14  | H     | 1222 | CLA  | CMB-C2B-C3B | 3.94  | 132.05      | 124.68   |
| 14  | G     | 1140 | CLA  | O2A-CGA-CBA | 3.94  | 124.28      | 111.91   |
| 14  | G     | 1123 | CLA  | O2A-CGA-CBA | 3.94  | 124.28      | 111.91   |
| 14  | b     | 1228 | CLA  | CMB-C2B-C3B | 3.94  | 132.05      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4006 | BCR  | C34-C9-C10  | -3.94 | 117.41      | 122.92   |
| 14  | B     | 1240 | CLA  | C1D-ND-C4D  | -3.94 | 103.54      | 106.33   |
| 14  | A     | 1125 | CLA  | O2A-CGA-CBA | 3.94  | 124.26      | 111.91   |
| 13  | a     | 1011 | CL0  | O2A-C1-C2   | 3.94  | 118.98      | 108.64   |
| 14  | G     | 1125 | CLA  | O2A-CGA-CBA | 3.94  | 124.26      | 111.91   |
| 14  | b     | 1222 | CLA  | CMB-C2B-C3B | 3.94  | 132.04      | 124.68   |
| 14  | a     | 1122 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 14  | a     | 1123 | CLA  | O2A-CGA-CBA | 3.93  | 124.25      | 111.91   |
| 14  | B     | 1228 | CLA  | CMB-C2B-C3B | 3.93  | 132.04      | 124.68   |
| 14  | H     | 1021 | CLA  | O2D-CGD-O1D | -3.93 | 116.15      | 123.84   |
| 14  | A     | 1123 | CLA  | O2A-CGA-CBA | 3.93  | 124.25      | 111.91   |
| 13  | G     | 1011 | CL0  | O2A-C1-C2   | 3.93  | 118.97      | 108.64   |
| 14  | G     | 1109 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 14  | H     | 1240 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 13  | A     | 1011 | CL0  | O2A-C1-C2   | 3.93  | 118.96      | 108.64   |
| 14  | b     | 1232 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 18  | H     | 4005 | BCR  | C33-C5-C6   | -3.93 | 120.12      | 124.53   |
| 14  | a     | 1138 | CLA  | C1D-ND-C4D  | -3.93 | 103.55      | 106.33   |
| 18  | G     | 4004 | BCR  | C24-C23-C22 | -3.93 | 120.30      | 126.23   |
| 14  | a     | 1111 | CLA  | O2A-CGA-CBA | 3.92  | 124.22      | 111.91   |
| 14  | B     | 1222 | CLA  | CMB-C2B-C3B | 3.92  | 132.02      | 124.68   |
| 14  | A     | 1111 | CLA  | O2A-CGA-CBA | 3.92  | 124.22      | 111.91   |
| 14  | B     | 1232 | CLA  | C1D-ND-C4D  | -3.92 | 103.55      | 106.33   |
| 18  | A     | 4004 | BCR  | C24-C23-C22 | -3.92 | 120.31      | 126.23   |
| 18  | a     | 4006 | BCR  | C34-C9-C10  | -3.92 | 117.43      | 122.92   |
| 18  | a     | 4004 | BCR  | C24-C23-C22 | -3.92 | 120.31      | 126.23   |
| 15  | H     | 1238 | F6C  | C4A-NA-C1A  | 3.92  | 109.12      | 106.33   |
| 14  | A     | 1125 | CLA  | CHD-C1D-ND  | -3.92 | 120.85      | 124.45   |
| 14  | H     | 1023 | CLA  | CAA-C2A-C3A | -3.92 | 102.05      | 112.78   |
| 14  | b     | 1240 | CLA  | C1D-ND-C4D  | -3.92 | 103.55      | 106.33   |
| 14  | G     | 1111 | CLA  | O2A-CGA-CBA | 3.92  | 124.19      | 111.91   |
| 14  | B     | 1021 | CLA  | O2D-CGD-O1D | -3.91 | 116.19      | 123.84   |
| 14  | B     | 1023 | CLA  | CAA-C2A-C3A | -3.91 | 102.07      | 112.78   |
| 14  | G     | 1122 | CLA  | C1D-ND-C4D  | -3.91 | 103.56      | 106.33   |
| 14  | H     | 1224 | CLA  | C4-C3-C5    | 3.91  | 121.85      | 115.27   |
| 14  | b     | 1235 | CLA  | C1-C2-C3    | -3.91 | 119.28      | 126.04   |
| 14  | H     | 1232 | CLA  | C1D-ND-C4D  | -3.90 | 103.56      | 106.33   |
| 14  | b     | 1023 | CLA  | CAA-C2A-C3A | -3.90 | 102.09      | 112.78   |
| 14  | a     | 1130 | CLA  | C4A-NA-C1A  | 3.90  | 108.46      | 106.71   |
| 14  | b     | 1021 | CLA  | O2D-CGD-O1D | -3.90 | 116.22      | 123.84   |
| 14  | B     | 1215 | CLA  | O2A-CGA-CBA | 3.90  | 124.14      | 111.91   |
| 14  | G     | 1108 | CLA  | C4A-NA-C1A  | 3.90  | 108.46      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1215 | CLA  | O2A-CGA-CBA | 3.90  | 124.13      | 111.91   |
| 13  | G     | 1011 | CL0  | CHD-C1D-ND  | -3.89 | 120.88      | 124.45   |
| 14  | B     | 1235 | CLA  | C1-C2-C3    | -3.89 | 119.31      | 126.04   |
| 13  | A     | 1011 | CL0  | CHD-C1D-ND  | -3.89 | 120.88      | 124.45   |
| 14  | a     | 1132 | CLA  | O2D-CGD-O1D | -3.89 | 116.23      | 123.84   |
| 14  | b     | 1215 | CLA  | O2A-CGA-CBA | 3.89  | 124.12      | 111.91   |
| 14  | A     | 1138 | CLA  | C1D-ND-C4D  | -3.89 | 103.57      | 106.33   |
| 14  | A     | 1130 | CLA  | C4A-NA-C1A  | 3.89  | 108.45      | 106.71   |
| 14  | B     | 1210 | CLA  | O2A-CGA-CBA | 3.89  | 124.11      | 111.91   |
| 14  | H     | 1210 | CLA  | O2A-CGA-CBA | 3.89  | 124.11      | 111.91   |
| 14  | b     | 1210 | CLA  | O2A-CGA-CBA | 3.89  | 124.11      | 111.91   |
| 14  | B     | 1224 | CLA  | C4-C3-C5    | 3.89  | 121.81      | 115.27   |
| 14  | B     | 1228 | CLA  | O2A-CGA-CBA | 3.89  | 124.11      | 111.91   |
| 14  | H     | 1235 | CLA  | C1-C2-C3    | -3.88 | 119.33      | 126.04   |
| 14  | H     | 1023 | CLA  | CMB-C2B-C3B | 3.88  | 131.94      | 124.68   |
| 14  | A     | 1132 | CLA  | O2D-CGD-O1D | -3.88 | 116.25      | 123.84   |
| 14  | B     | 1240 | CLA  | C4A-NA-C1A  | 3.88  | 108.45      | 106.71   |
| 15  | b     | 1219 | F6C  | O2A-CGA-CBA | 3.88  | 124.08      | 111.91   |
| 14  | B     | 1023 | CLA  | CMB-C2B-C3B | 3.88  | 131.94      | 124.68   |
| 14  | G     | 1138 | CLA  | C1D-ND-C4D  | -3.88 | 103.58      | 106.33   |
| 14  | H     | 1228 | CLA  | O2A-CGA-CBA | 3.88  | 124.07      | 111.91   |
| 14  | b     | 1023 | CLA  | CMB-C2B-C3B | 3.87  | 131.93      | 124.68   |
| 14  | a     | 1122 | CLA  | O2A-CGA-CBA | 3.87  | 124.07      | 111.91   |
| 14  | G     | 1122 | CLA  | O2A-CGA-CBA | 3.87  | 124.06      | 111.91   |
| 14  | H     | 1201 | CLA  | O2A-CGA-CBA | 3.87  | 124.06      | 111.91   |
| 15  | H     | 1219 | F6C  | O2A-CGA-CBA | 3.87  | 124.06      | 111.91   |
| 14  | b     | 1228 | CLA  | O2A-CGA-CBA | 3.87  | 124.05      | 111.91   |
| 15  | B     | 1219 | F6C  | O2A-CGA-CBA | 3.87  | 124.05      | 111.91   |
| 14  | b     | 1201 | CLA  | O2A-CGA-CBA | 3.87  | 124.05      | 111.91   |
| 14  | A     | 1122 | CLA  | O2A-CGA-CBA | 3.87  | 124.05      | 111.91   |
| 14  | B     | 1022 | CLA  | CMB-C2B-C3B | 3.87  | 131.92      | 124.68   |
| 14  | b     | 1022 | CLA  | CMB-C2B-C3B | 3.87  | 131.92      | 124.68   |
| 14  | b     | 1224 | CLA  | C4-C3-C5    | 3.87  | 121.77      | 115.27   |
| 14  | B     | 1201 | CLA  | O2A-CGA-CBA | 3.86  | 124.03      | 111.91   |
| 18  | V     | 4021 | BCR  | C24-C23-C22 | -3.86 | 120.40      | 126.23   |
| 18  | H     | 4009 | BCR  | C38-C26-C25 | -3.86 | 120.19      | 124.53   |
| 18  | a     | 4004 | BCR  | C33-C5-C6   | -3.86 | 120.19      | 124.53   |
| 14  | H     | 1022 | CLA  | CMB-C2B-C3B | 3.86  | 131.89      | 124.68   |
| 14  | B     | 1206 | CLA  | CMB-C2B-C3B | 3.85  | 131.89      | 124.68   |
| 14  | G     | 1132 | CLA  | O2D-CGD-O1D | -3.85 | 116.30      | 123.84   |
| 14  | G     | 1105 | CLA  | CMB-C2B-C3B | 3.85  | 131.88      | 124.68   |
| 14  | H     | 1232 | CLA  | CMB-C2B-C3B | 3.85  | 131.88      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | m     | 4021 | BCR  | C24-C23-C22 | -3.85 | 120.42      | 126.23   |
| 14  | a     | 1111 | CLA  | C1-C2-C3    | -3.85 | 119.39      | 126.04   |
| 14  | B     | 1232 | CLA  | CMB-C2B-C3B | 3.85  | 131.88      | 124.68   |
| 18  | b     | 4009 | BCR  | C38-C26-C25 | -3.85 | 120.21      | 124.53   |
| 14  | G     | 1130 | CLA  | C4A-NA-C1A  | 3.85  | 108.44      | 106.71   |
| 18  | M     | 4021 | BCR  | C24-C23-C22 | -3.85 | 120.42      | 126.23   |
| 14  | H     | 1223 | CLA  | O2A-CGA-CBA | 3.84  | 123.97      | 111.91   |
| 14  | a     | 1105 | CLA  | CMB-C2B-C3B | 3.84  | 131.87      | 124.68   |
| 14  | B     | 1215 | CLA  | C1D-ND-C4D  | -3.84 | 103.61      | 106.33   |
| 14  | B     | 1223 | CLA  | O2A-CGA-CBA | 3.84  | 123.96      | 111.91   |
| 14  | b     | 1232 | CLA  | CMB-C2B-C3B | 3.84  | 131.86      | 124.68   |
| 14  | H     | 1210 | CLA  | CAC-C3C-C4C | 3.84  | 129.79      | 124.81   |
| 18  | B     | 4009 | BCR  | C38-C26-C25 | -3.84 | 120.22      | 124.53   |
| 18  | G     | 4004 | BCR  | C33-C5-C6   | -3.84 | 120.22      | 124.53   |
| 14  | A     | 1105 | CLA  | CMB-C2B-C3B | 3.84  | 131.85      | 124.68   |
| 15  | b     | 1207 | F6C  | C1A-C2A-C3A | -3.83 | 102.93      | 106.97   |
| 14  | b     | 1206 | CLA  | CMB-C2B-C3B | 3.83  | 131.85      | 124.68   |
| 18  | b     | 4017 | BCR  | C38-C26-C25 | -3.83 | 120.22      | 124.53   |
| 14  | b     | 1223 | CLA  | O2A-CGA-CBA | 3.83  | 123.94      | 111.91   |
| 14  | H     | 1206 | CLA  | CMB-C2B-C3B | 3.83  | 131.84      | 124.68   |
| 18  | a     | 4004 | BCR  | C31-C1-C6   | -3.83 | 104.09      | 110.30   |
| 14  | b     | 1215 | CLA  | C1D-ND-C4D  | -3.83 | 103.61      | 106.33   |
| 14  | H     | 1224 | CLA  | CMB-C2B-C3B | 3.83  | 131.84      | 124.68   |
| 14  | H     | 1201 | CLA  | C4-C3-C5    | 3.83  | 121.71      | 115.27   |
| 14  | A     | 1108 | CLA  | C4A-NA-C1A  | 3.83  | 108.43      | 106.71   |
| 14  | a     | 1108 | CLA  | C4A-NA-C1A  | 3.83  | 108.43      | 106.71   |
| 18  | H     | 4017 | BCR  | C38-C26-C25 | -3.83 | 120.23      | 124.53   |
| 14  | A     | 1111 | CLA  | C1-C2-C3    | -3.83 | 119.42      | 126.04   |
| 14  | A     | 1106 | CLA  | CMB-C2B-C3B | 3.83  | 131.84      | 124.68   |
| 14  | G     | 1106 | CLA  | CMB-C2B-C3B | 3.83  | 131.84      | 124.68   |
| 14  | H     | 1215 | CLA  | C1D-ND-C4D  | -3.82 | 103.62      | 106.33   |
| 14  | a     | 1106 | CLA  | CMB-C2B-C3B | 3.82  | 131.83      | 124.68   |
| 14  | H     | 1205 | CLA  | C3C-C4C-NC  | 3.82  | 114.86      | 110.57   |
| 14  | G     | 1111 | CLA  | C1-C2-C3    | -3.82 | 119.44      | 126.04   |
| 18  | A     | 4004 | BCR  | C33-C5-C6   | -3.82 | 120.24      | 124.53   |
| 18  | I     | 4018 | BCR  | C15-C14-C13 | -3.82 | 121.86      | 127.31   |
| 13  | a     | 1011 | CL0  | CHD-C1D-ND  | -3.82 | 120.94      | 124.45   |
| 14  | B     | 1201 | CLA  | C4-C3-C5    | 3.82  | 121.70      | 115.27   |
| 15  | G     | 1121 | F6C  | C4A-C3A-C2A | -3.82 | 101.36      | 106.94   |
| 15  | B     | 1207 | F6C  | C1A-C2A-C3A | -3.82 | 102.95      | 106.97   |
| 14  | B     | 1224 | CLA  | CMB-C2B-C3B | 3.82  | 131.82      | 124.68   |
| 15  | a     | 1121 | F6C  | C4A-C3A-C2A | -3.81 | 101.37      | 106.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1117 | CLA  | O2D-CGD-O1D | -3.81 | 116.38      | 123.84   |
| 18  | A     | 4004 | BCR  | C31-C1-C6   | -3.81 | 104.11      | 110.30   |
| 14  | b     | 1210 | CLA  | CAC-C3C-C4C | 3.81  | 129.76      | 124.81   |
| 14  | a     | 1117 | CLA  | O2D-CGD-O1D | -3.81 | 116.38      | 123.84   |
| 14  | B     | 1205 | CLA  | C3C-C4C-NC  | 3.81  | 114.85      | 110.57   |
| 14  | b     | 1240 | CLA  | C4A-NA-C1A  | 3.81  | 108.42      | 106.71   |
| 18  | B     | 4017 | BCR  | C38-C26-C25 | -3.81 | 120.25      | 124.53   |
| 14  | b     | 1223 | CLA  | C1D-ND-C4D  | -3.81 | 103.63      | 106.33   |
| 18  | G     | 4004 | BCR  | C31-C1-C6   | -3.81 | 104.12      | 110.30   |
| 14  | A     | 1117 | CLA  | O2D-CGD-O1D | -3.81 | 116.40      | 123.84   |
| 14  | l     | 1502 | CLA  | O2D-CGD-O1D | -3.81 | 116.40      | 123.84   |
| 18  | R     | 4018 | BCR  | C15-C14-C13 | -3.81 | 121.88      | 127.31   |
| 14  | L     | 1502 | CLA  | O2D-CGD-O1D | -3.80 | 116.40      | 123.84   |
| 14  | B     | 1210 | CLA  | CAC-C3C-C4C | 3.80  | 129.74      | 124.81   |
| 14  | H     | 1228 | CLA  | C4A-NA-C1A  | 3.80  | 108.41      | 106.71   |
| 18  | G     | 4006 | BCR  | C33-C5-C6   | -3.80 | 120.26      | 124.53   |
| 14  | G     | 1125 | CLA  | C3C-C4C-NC  | 3.80  | 114.83      | 110.57   |
| 14  | B     | 1228 | CLA  | C4A-NA-C1A  | 3.80  | 108.41      | 106.71   |
| 14  | b     | 1201 | CLA  | C4-C3-C5    | 3.80  | 121.66      | 115.27   |
| 15  | A     | 1121 | F6C  | C4A-C3A-C2A | -3.79 | 101.40      | 106.94   |
| 14  | H     | 1208 | CLA  | O2A-C1-C2   | 3.79  | 118.61      | 108.64   |
| 18  | B     | 4004 | BCR  | C3-C4-C5    | -3.79 | 107.30      | 114.08   |
| 14  | G     | 1103 | CLA  | O2A-CGA-CBA | 3.79  | 123.81      | 111.91   |
| 14  | B     | 1208 | CLA  | O2A-C1-C2   | 3.79  | 118.61      | 108.64   |
| 14  | A     | 1103 | CLA  | O2A-CGA-CBA | 3.79  | 123.81      | 111.91   |
| 14  | B     | 1210 | CLA  | CMB-C2B-C3B | 3.79  | 131.77      | 124.68   |
| 15  | H     | 1207 | F6C  | C1A-C2A-C3A | -3.79 | 102.98      | 106.97   |
| 14  | b     | 1224 | CLA  | CMB-C2B-C3B | 3.79  | 131.77      | 124.68   |
| 18  | H     | 4014 | BCR  | C33-C5-C6   | -3.79 | 120.27      | 124.53   |
| 18  | b     | 4004 | BCR  | C3-C4-C5    | -3.79 | 107.31      | 114.08   |
| 14  | U     | 1502 | CLA  | O2D-CGD-O1D | -3.79 | 116.43      | 123.84   |
| 14  | a     | 1103 | CLA  | O2A-CGA-CBA | 3.79  | 123.79      | 111.91   |
| 14  | b     | 1208 | CLA  | O2A-C1-C2   | 3.79  | 118.59      | 108.64   |
| 18  | B     | 4014 | BCR  | C33-C5-C6   | -3.78 | 120.28      | 124.53   |
| 14  | B     | 1022 | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 14  | A     | 1130 | CLA  | C1D-ND-C4D  | -3.78 | 103.65      | 106.33   |
| 14  | H     | 1223 | CLA  | C1D-ND-C4D  | -3.78 | 103.65      | 106.33   |
| 18  | i     | 4018 | BCR  | C15-C14-C13 | -3.78 | 121.91      | 127.31   |
| 14  | H     | 1022 | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 14  | b     | 1205 | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 18  | R     | 4020 | BCR  | C15-C14-C13 | -3.78 | 121.91      | 127.31   |
| 14  | A     | 1012 | CLA  | O2A-CGA-CBA | 3.78  | 123.77      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1210 | CLA  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 14  | a     | 1012 | CLA  | O2A-CGA-CBA | 3.78  | 123.77      | 111.91   |
| 14  | A     | 1125 | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 18  | b     | 4014 | BCR  | C33-C5-C6   | -3.78 | 120.29      | 124.53   |
| 14  | b     | 1210 | CLA  | CMB-C2B-C3B | 3.78  | 131.74      | 124.68   |
| 16  | B     | 2002 | PQN  | C14-C13-C15 | 3.77  | 121.62      | 115.27   |
| 14  | b     | 1212 | CLA  | CMB-C2B-C3B | 3.77  | 131.73      | 124.68   |
| 16  | b     | 2002 | PQN  | C14-C13-C15 | 3.77  | 121.61      | 115.27   |
| 14  | b     | 1022 | CLA  | C3C-C4C-NC  | 3.77  | 114.80      | 110.57   |
| 18  | H     | 4004 | BCR  | C3-C4-C5    | -3.77 | 107.34      | 114.08   |
| 14  | G     | 1106 | CLA  | O2A-CGA-CBA | 3.77  | 123.74      | 111.91   |
| 14  | H     | 1212 | CLA  | CMB-C2B-C3B | 3.77  | 131.73      | 124.68   |
| 13  | G     | 1011 | CL0  | O2A-CGA-CBA | 3.77  | 123.74      | 111.91   |
| 18  | A     | 4006 | BCR  | C33-C5-C6   | -3.77 | 120.30      | 124.53   |
| 14  | G     | 1012 | CLA  | O2A-CGA-CBA | 3.77  | 123.73      | 111.91   |
| 14  | a     | 1130 | CLA  | C1D-ND-C4D  | -3.77 | 103.66      | 106.33   |
| 13  | a     | 1011 | CL0  | O2A-CGA-CBA | 3.77  | 123.73      | 111.91   |
| 18  | A     | 4004 | BCR  | C7-C8-C9    | -3.77 | 120.54      | 126.23   |
| 13  | A     | 1011 | CL0  | O2A-CGA-CBA | 3.76  | 123.72      | 111.91   |
| 14  | B     | 1212 | CLA  | CMB-C2B-C3B | 3.76  | 131.72      | 124.68   |
| 14  | B     | 1223 | CLA  | C1D-ND-C4D  | -3.76 | 103.66      | 106.33   |
| 18  | I     | 4020 | BCR  | C15-C14-C13 | -3.76 | 121.94      | 127.31   |
| 18  | G     | 4004 | BCR  | C7-C8-C9    | -3.76 | 120.55      | 126.23   |
| 18  | a     | 4006 | BCR  | C33-C5-C6   | -3.76 | 120.30      | 124.53   |
| 15  | G     | 1121 | F6C  | CMA-C3A-C2A | -3.76 | 115.91      | 126.12   |
| 15  | A     | 1121 | F6C  | CMA-C3A-C2A | -3.76 | 115.91      | 126.12   |
| 14  | a     | 1125 | CLA  | C3C-C4C-NC  | 3.76  | 114.79      | 110.57   |
| 14  | a     | 1106 | CLA  | O2A-CGA-CBA | 3.76  | 123.70      | 111.91   |
| 18  | i     | 4020 | BCR  | C15-C14-C13 | -3.76 | 121.95      | 127.31   |
| 15  | a     | 1121 | F6C  | CMA-C3A-C2A | -3.76 | 115.92      | 126.12   |
| 14  | A     | 1106 | CLA  | O2A-CGA-CBA | 3.75  | 123.69      | 111.91   |
| 16  | H     | 2002 | PQN  | C14-C13-C15 | 3.75  | 121.58      | 115.27   |
| 15  | b     | 1238 | F6C  | C1-C2-C3    | -3.75 | 119.56      | 126.04   |
| 18  | a     | 4004 | BCR  | C7-C8-C9    | -3.75 | 120.58      | 126.23   |
| 15  | B     | 1238 | F6C  | C1-C2-C3    | -3.74 | 119.57      | 126.04   |
| 14  | b     | 1228 | CLA  | C1D-ND-C4D  | -3.74 | 103.68      | 106.33   |
| 15  | H     | 1238 | F6C  | C1-C2-C3    | -3.74 | 119.58      | 126.04   |
| 14  | b     | 1228 | CLA  | C4A-NA-C1A  | 3.73  | 108.39      | 106.71   |
| 14  | a     | 1140 | CLA  | C1D-ND-C4D  | -3.73 | 103.68      | 106.33   |
| 14  | B     | 1226 | CLA  | C1-C2-C3    | -3.73 | 119.59      | 126.04   |
| 14  | G     | 1110 | CLA  | O2D-CGD-O1D | -3.73 | 116.55      | 123.84   |
| 14  | A     | 1110 | CLA  | O2D-CGD-O1D | -3.73 | 116.55      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1109 | CLA  | O2A-CGA-CBA | 3.73  | 123.60      | 111.91   |
| 14  | b     | 1226 | CLA  | C1-C2-C3    | -3.72 | 119.60      | 126.04   |
| 14  | H     | 1231 | CLA  | O2D-CGD-O1D | -3.72 | 116.57      | 123.84   |
| 14  | a     | 1131 | CLA  | C1D-ND-C4D  | -3.72 | 103.69      | 106.33   |
| 14  | A     | 1109 | CLA  | O2A-CGA-CBA | 3.71  | 123.57      | 111.91   |
| 14  | G     | 1140 | CLA  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 14  | G     | 1109 | CLA  | O2A-CGA-CBA | 3.71  | 123.55      | 111.91   |
| 14  | H     | 1226 | CLA  | C1-C2-C3    | -3.71 | 119.63      | 126.04   |
| 14  | a     | 1123 | CLA  | CMB-C2B-C3B | 3.71  | 131.62      | 124.68   |
| 14  | b     | 1231 | CLA  | O2D-CGD-O1D | -3.71 | 116.59      | 123.84   |
| 14  | B     | 1231 | CLA  | O2D-CGD-O1D | -3.71 | 116.59      | 123.84   |
| 14  | B     | 1229 | CLA  | O2A-C1-C2   | 3.70  | 118.37      | 108.64   |
| 14  | b     | 1229 | CLA  | O2A-C1-C2   | 3.70  | 118.37      | 108.64   |
| 15  | H     | 1237 | F6C  | O2A-CGA-CBA | 3.70  | 123.53      | 111.91   |
| 14  | A     | 1123 | CLA  | CMB-C2B-C3B | 3.70  | 131.61      | 124.68   |
| 14  | H     | 1229 | CLA  | O2A-C1-C2   | 3.70  | 118.36      | 108.64   |
| 14  | A     | 1118 | CLA  | O2A-CGA-CBA | 3.70  | 123.51      | 111.91   |
| 14  | m     | 1501 | CLA  | C1-C2-C3    | -3.70 | 120.77      | 126.75   |
| 18  | H     | 4004 | BCR  | C36-C18-C17 | -3.70 | 117.75      | 122.92   |
| 14  | G     | 1123 | CLA  | CMB-C2B-C3B | 3.70  | 131.59      | 124.68   |
| 14  | a     | 1110 | CLA  | O2D-CGD-O1D | -3.69 | 116.61      | 123.84   |
| 14  | G     | 1118 | CLA  | O2A-CGA-CBA | 3.69  | 123.50      | 111.91   |
| 14  | a     | 1137 | CLA  | CMB-C2B-C3B | 3.69  | 131.59      | 124.68   |
| 14  | H     | 1228 | CLA  | C1D-ND-C4D  | -3.69 | 103.71      | 106.33   |
| 15  | b     | 1237 | F6C  | O2A-CGA-CBA | 3.69  | 123.50      | 111.91   |
| 14  | A     | 1131 | CLA  | C1D-ND-C4D  | -3.69 | 103.71      | 106.33   |
| 18  | B     | 4004 | BCR  | C36-C18-C17 | -3.69 | 117.75      | 122.92   |
| 14  | a     | 1118 | CLA  | O2A-CGA-CBA | 3.69  | 123.49      | 111.91   |
| 14  | M     | 1501 | CLA  | C1-C2-C3    | -3.69 | 120.78      | 126.75   |
| 18  | b     | 4004 | BCR  | C36-C18-C17 | -3.69 | 117.75      | 122.92   |
| 18  | B     | 4006 | BCR  | C7-C8-C9    | -3.69 | 120.66      | 126.23   |
| 14  | a     | 1012 | CLA  | C1D-ND-C4D  | -3.69 | 103.71      | 106.33   |
| 14  | A     | 1133 | CLA  | C1-C2-C3    | -3.69 | 119.66      | 126.04   |
| 15  | B     | 1237 | F6C  | O2A-CGA-CBA | 3.69  | 123.48      | 111.91   |
| 14  | G     | 1130 | CLA  | C1D-ND-C4D  | -3.69 | 103.72      | 106.33   |
| 14  | G     | 1137 | CLA  | CMB-C2B-C3B | 3.69  | 131.58      | 124.68   |
| 18  | T     | 4001 | BCR  | C34-C9-C10  | -3.69 | 117.76      | 122.92   |
| 14  | a     | 1133 | CLA  | C1-C2-C3    | -3.68 | 119.67      | 126.04   |
| 14  | V     | 1501 | CLA  | C1-C2-C3    | -3.68 | 120.79      | 126.75   |
| 14  | G     | 1115 | CLA  | CBA-CAA-C2A | 3.68  | 124.73      | 113.86   |
| 14  | B     | 1022 | CLA  | O2A-CGA-O1A | -3.68 | 114.30      | 123.59   |
| 14  | b     | 1022 | CLA  | O2A-CGA-O1A | -3.68 | 114.30      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1137 | CLA  | CMB-C2B-C3B | 3.68  | 131.56      | 124.68   |
| 18  | k     | 4001 | BCR  | C34-C9-C10  | -3.68 | 117.77      | 122.92   |
| 14  | a     | 1115 | CLA  | CAA-C2A-C3A | -3.68 | 102.70      | 112.78   |
| 14  | a     | 1127 | CLA  | O2A-CGA-CBA | 3.68  | 123.46      | 111.91   |
| 14  | H     | 1022 | CLA  | O2A-CGA-O1A | -3.68 | 114.31      | 123.59   |
| 14  | A     | 1115 | CLA  | CBA-CAA-C2A | 3.68  | 124.72      | 113.86   |
| 18  | G     | 4004 | BCR  | C27-C26-C25 | -3.68 | 117.39      | 122.73   |
| 19  | U     | 5101 | LHG  | O8-C23-C24  | 3.68  | 123.45      | 111.91   |
| 14  | A     | 1115 | CLA  | CAA-C2A-C3A | -3.68 | 102.71      | 112.78   |
| 14  | A     | 1140 | CLA  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 14  | A     | 1012 | CLA  | C1D-ND-C4D  | -3.67 | 103.72      | 106.33   |
| 18  | H     | 4006 | BCR  | C7-C8-C9    | -3.67 | 120.68      | 126.23   |
| 19  | L     | 5101 | LHG  | O8-C23-C24  | 3.67  | 123.43      | 111.91   |
| 14  | G     | 1115 | CLA  | CAA-C2A-C3A | -3.67 | 102.72      | 112.78   |
| 18  | a     | 4004 | BCR  | C27-C26-C25 | -3.67 | 117.40      | 122.73   |
| 14  | G     | 1133 | CLA  | C1-C2-C3    | -3.67 | 119.69      | 126.04   |
| 14  | G     | 1127 | CLA  | O2A-CGA-CBA | 3.67  | 123.42      | 111.91   |
| 14  | B     | 1212 | CLA  | C1D-ND-C4D  | -3.67 | 103.73      | 106.33   |
| 14  | A     | 1127 | CLA  | O2A-CGA-CBA | 3.67  | 123.42      | 111.91   |
| 14  | a     | 1115 | CLA  | CBA-CAA-C2A | 3.67  | 124.69      | 113.86   |
| 19  | l     | 5101 | LHG  | O8-C23-C24  | 3.67  | 123.42      | 111.91   |
| 15  | b     | 1207 | F6C  | CMA-C3A-C4A | -3.66 | 118.25      | 124.71   |
| 14  | L     | 1503 | CLA  | O2A-CGA-CBA | 3.66  | 123.41      | 111.91   |
| 14  | l     | 1503 | CLA  | O2A-CGA-CBA | 3.66  | 123.41      | 111.91   |
| 15  | b     | 1238 | F6C  | C4A-C3A-C2A | -3.66 | 101.59      | 106.94   |
| 15  | B     | 1238 | F6C  | C4A-C3A-C2A | -3.66 | 101.59      | 106.94   |
| 18  | K     | 4001 | BCR  | C34-C9-C10  | -3.66 | 117.80      | 122.92   |
| 14  | G     | 1136 | CLA  | CMA-C3A-C4A | 3.66  | 121.61      | 111.77   |
| 15  | H     | 1238 | F6C  | C4A-C3A-C2A | -3.66 | 101.60      | 106.94   |
| 14  | U     | 1503 | CLA  | O2A-CGA-CBA | 3.66  | 123.39      | 111.91   |
| 14  | H     | 1235 | CLA  | CMB-C2B-C3B | 3.65  | 131.51      | 124.68   |
| 14  | B     | 1228 | CLA  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |
| 14  | a     | 1125 | CLA  | CMB-C2B-C3B | 3.65  | 131.51      | 124.68   |
| 14  | A     | 1136 | CLA  | CMA-C3A-C4A | 3.65  | 121.59      | 111.77   |
| 18  | A     | 4004 | BCR  | C27-C26-C25 | -3.65 | 117.43      | 122.73   |
| 14  | H     | 1229 | CLA  | C4-C3-C5    | 3.65  | 121.41      | 115.27   |
| 15  | B     | 1207 | F6C  | CMA-C3A-C4A | -3.65 | 118.28      | 124.71   |
| 18  | b     | 4006 | BCR  | C7-C8-C9    | -3.65 | 120.72      | 126.23   |
| 14  | G     | 1012 | CLA  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |
| 14  | B     | 1229 | CLA  | C4-C3-C5    | 3.65  | 121.40      | 115.27   |
| 14  | B     | 1204 | CLA  | O2D-CGD-O1D | -3.65 | 116.71      | 123.84   |
| 14  | H     | 1204 | CLA  | O2D-CGD-O1D | -3.65 | 116.71      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1136 | CLA  | CMA-C3A-C4A | 3.65  | 121.57      | 111.77   |
| 13  | a     | 1011 | CL0  | O2D-CGD-O1D | -3.64 | 116.71      | 123.84   |
| 14  | G     | 1012 | CLA  | CAA-C2A-C3A | -3.64 | 102.80      | 112.78   |
| 14  | b     | 1229 | CLA  | C4-C3-C5    | 3.64  | 121.40      | 115.27   |
| 15  | H     | 1207 | F6C  | CMA-C3A-C4A | -3.64 | 118.29      | 124.71   |
| 13  | A     | 1011 | CL0  | O2D-CGD-O1D | -3.64 | 116.72      | 123.84   |
| 14  | H     | 1212 | CLA  | C1D-ND-C4D  | -3.64 | 103.75      | 106.33   |
| 14  | A     | 1012 | CLA  | CAA-C2A-C3A | -3.64 | 102.81      | 112.78   |
| 14  | b     | 1204 | CLA  | O2D-CGD-O1D | -3.64 | 116.72      | 123.84   |
| 14  | a     | 1012 | CLA  | CAA-C2A-C3A | -3.64 | 102.81      | 112.78   |
| 14  | a     | 1129 | CLA  | C1-C2-C3    | -3.64 | 120.87      | 126.75   |
| 14  | G     | 1131 | CLA  | C1D-ND-C4D  | -3.63 | 103.75      | 106.33   |
| 14  | B     | 1235 | CLA  | CMB-C2B-C3B | 3.63  | 131.48      | 124.68   |
| 14  | b     | 1235 | CLA  | CMB-C2B-C3B | 3.63  | 131.48      | 124.68   |
| 13  | G     | 1011 | CL0  | O2D-CGD-O1D | -3.63 | 116.74      | 123.84   |
| 14  | b     | 1021 | CLA  | CAA-C2A-C3A | -3.63 | 102.85      | 112.78   |
| 14  | H     | 1021 | CLA  | CAA-C2A-C3A | -3.62 | 102.85      | 112.78   |
| 14  | A     | 1125 | CLA  | CMB-C2B-C3B | 3.62  | 131.46      | 124.68   |
| 14  | G     | 1128 | CLA  | CMB-C2B-C1B | -3.62 | 122.90      | 128.46   |
| 14  | a     | 1135 | CLA  | O2A-CGA-CBA | 3.62  | 123.27      | 111.91   |
| 18  | A     | 4004 | BCR  | C3-C4-C5    | -3.62 | 107.61      | 114.08   |
| 14  | G     | 1129 | CLA  | C1-C2-C3    | -3.62 | 120.89      | 126.75   |
| 18  | a     | 4004 | BCR  | C3-C4-C5    | -3.62 | 107.62      | 114.08   |
| 14  | B     | 1021 | CLA  | CAA-C2A-C3A | -3.62 | 102.87      | 112.78   |
| 14  | A     | 1135 | CLA  | O2A-CGA-CBA | 3.62  | 123.26      | 111.91   |
| 14  | G     | 1132 | CLA  | O2A-CGA-CBA | 3.62  | 123.26      | 111.91   |
| 18  | G     | 4004 | BCR  | C3-C4-C5    | -3.61 | 107.63      | 114.08   |
| 18  | R     | 4018 | BCR  | C33-C5-C6   | -3.61 | 120.47      | 124.53   |
| 14  | G     | 1135 | CLA  | O2A-CGA-CBA | 3.61  | 123.24      | 111.91   |
| 14  | G     | 1125 | CLA  | CMB-C2B-C3B | 3.61  | 131.43      | 124.68   |
| 14  | A     | 1129 | CLA  | C1-C2-C3    | -3.61 | 120.92      | 126.75   |
| 14  | G     | 1125 | CLA  | C1C-C2C-C3C | -3.61 | 103.17      | 106.96   |
| 14  | A     | 1132 | CLA  | O2A-CGA-CBA | 3.61  | 123.22      | 111.91   |
| 14  | A     | 1128 | CLA  | CMB-C2B-C1B | -3.61 | 122.92      | 128.46   |
| 14  | H     | 1216 | CLA  | O2A-CGA-CBA | 3.61  | 123.22      | 111.91   |
| 14  | G     | 1125 | CLA  | OBD-CAD-C3D | -3.60 | 119.84      | 128.52   |
| 14  | B     | 1216 | CLA  | O2A-CGA-CBA | 3.60  | 123.22      | 111.91   |
| 14  | b     | 1216 | CLA  | O2A-CGA-CBA | 3.60  | 123.22      | 111.91   |
| 14  | a     | 1125 | CLA  | OBD-CAD-C3D | -3.60 | 119.85      | 128.52   |
| 18  | a     | 4003 | BCR  | C7-C8-C9    | -3.60 | 120.79      | 126.23   |
| 14  | b     | 1212 | CLA  | C1D-ND-C4D  | -3.60 | 103.78      | 106.33   |
| 14  | a     | 1127 | CLA  | C1-C2-C3    | -3.60 | 119.82      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 4003 | BCR  | C7-C8-C9    | -3.60 | 120.80      | 126.23   |
| 14  | a     | 1125 | CLA  | C1C-C2C-C3C | -3.60 | 103.17      | 106.96   |
| 14  | A     | 1125 | CLA  | C1C-C2C-C3C | -3.60 | 103.18      | 106.96   |
| 14  | A     | 1125 | CLA  | OBD-CAD-C3D | -3.60 | 119.87      | 128.52   |
| 18  | I     | 4018 | BCR  | C33-C5-C6   | -3.59 | 120.49      | 124.53   |
| 14  | a     | 1138 | CLA  | CAA-C2A-C3A | -3.59 | 102.94      | 112.78   |
| 14  | a     | 1128 | CLA  | CMB-C2B-C1B | -3.59 | 122.95      | 128.46   |
| 14  | a     | 1132 | CLA  | O2A-CGA-CBA | 3.59  | 123.17      | 111.91   |
| 14  | B     | 1201 | CLA  | CMC-C2C-C1C | 3.59  | 130.50      | 125.04   |
| 14  | H     | 1201 | CLA  | CMC-C2C-C1C | 3.59  | 130.50      | 125.04   |
| 14  | H     | 1222 | CLA  | CAA-CBA-CGA | -3.59 | 102.78      | 113.25   |
| 14  | a     | 1123 | CLA  | CMA-C3A-C4A | 3.58  | 121.41      | 111.77   |
| 14  | G     | 1138 | CLA  | CAA-C2A-C3A | -3.58 | 102.96      | 112.78   |
| 14  | l     | 1503 | CLA  | O2D-CGD-O1D | -3.58 | 116.84      | 123.84   |
| 14  | A     | 1138 | CLA  | CAA-C2A-C3A | -3.58 | 102.97      | 112.78   |
| 14  | a     | 1103 | CLA  | O2A-C1-C2   | 3.58  | 118.04      | 108.64   |
| 14  | A     | 1103 | CLA  | O2A-C1-C2   | 3.58  | 118.04      | 108.64   |
| 14  | G     | 1104 | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 18  | G     | 4003 | BCR  | C7-C8-C9    | -3.58 | 120.83      | 126.23   |
| 14  | A     | 1104 | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 14  | A     | 1127 | CLA  | C1-C2-C3    | -3.57 | 119.86      | 126.04   |
| 14  | A     | 1123 | CLA  | CMA-C3A-C4A | 3.57  | 121.38      | 111.77   |
| 14  | G     | 1123 | CLA  | CMA-C3A-C4A | 3.57  | 121.38      | 111.77   |
| 14  | U     | 1503 | CLA  | O2D-CGD-O1D | -3.57 | 116.86      | 123.84   |
| 19  | G     | 5001 | LHG  | O7-C7-C8    | 3.57  | 119.19      | 111.50   |
| 14  | G     | 1103 | CLA  | O2A-C1-C2   | 3.57  | 118.01      | 108.64   |
| 14  | L     | 1503 | CLA  | O2D-CGD-O1D | -3.57 | 116.86      | 123.84   |
| 14  | a     | 1104 | CLA  | CMB-C2B-C3B | 3.57  | 131.35      | 124.68   |
| 14  | b     | 1022 | CLA  | C4-C3-C5    | 3.57  | 121.27      | 115.27   |
| 14  | b     | 1201 | CLA  | CMC-C2C-C1C | 3.57  | 130.47      | 125.04   |
| 14  | B     | 1222 | CLA  | CAA-CBA-CGA | -3.57 | 102.83      | 113.25   |
| 14  | B     | 1022 | CLA  | C4-C3-C5    | 3.56  | 121.27      | 115.27   |
| 19  | A     | 5001 | LHG  | O7-C7-C8    | 3.56  | 119.18      | 111.50   |
| 18  | G     | 4006 | BCR  | C3-C4-C5    | -3.56 | 107.72      | 114.08   |
| 18  | i     | 4018 | BCR  | C7-C8-C9    | -3.56 | 120.86      | 126.23   |
| 19  | a     | 5001 | LHG  | O7-C7-C8    | 3.56  | 119.17      | 111.50   |
| 14  | G     | 1127 | CLA  | C1-C2-C3    | -3.56 | 119.89      | 126.04   |
| 18  | R     | 4018 | BCR  | C7-C8-C9    | -3.56 | 120.86      | 126.23   |
| 15  | H     | 1230 | F6C  | O2D-CGD-O1D | -3.55 | 116.89      | 123.84   |
| 14  | B     | 1215 | CLA  | O2A-CGA-O1A | -3.55 | 114.62      | 123.59   |
| 14  | b     | 1222 | CLA  | CAA-CBA-CGA | -3.55 | 102.87      | 113.25   |
| 18  | I     | 4018 | BCR  | C7-C8-C9    | -3.55 | 120.87      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | i     | 4018 | BCR  | C33-C5-C6   | -3.55 | 120.54      | 124.53   |
| 14  | a     | 1124 | CLA  | CMA-C3A-C4A | 3.55  | 121.32      | 111.77   |
| 14  | G     | 1124 | CLA  | CMA-C3A-C4A | 3.55  | 121.31      | 111.77   |
| 14  | H     | 1022 | CLA  | C4-C3-C5    | 3.55  | 121.24      | 115.27   |
| 14  | b     | 1215 | CLA  | O2A-CGA-O1A | -3.55 | 114.64      | 123.59   |
| 14  | G     | 1131 | CLA  | C1-C2-C3    | -3.54 | 119.92      | 126.04   |
| 14  | A     | 1124 | CLA  | CMA-C3A-C4A | 3.54  | 121.29      | 111.77   |
| 14  | H     | 1215 | CLA  | O2A-CGA-O1A | -3.54 | 114.66      | 123.59   |
| 14  | b     | 1240 | CLA  | CMB-C2B-C3B | 3.53  | 131.29      | 124.68   |
| 18  | A     | 4006 | BCR  | C3-C4-C5    | -3.53 | 107.77      | 114.08   |
| 14  | A     | 1132 | CLA  | CAA-C2A-C3A | -3.53 | 103.12      | 112.78   |
| 18  | a     | 4006 | BCR  | C3-C4-C5    | -3.53 | 107.78      | 114.08   |
| 15  | B     | 1238 | F6C  | CMA-C3A-C4A | -3.53 | 118.50      | 124.71   |
| 15  | H     | 1238 | F6C  | CMA-C3A-C4A | -3.53 | 118.50      | 124.71   |
| 14  | a     | 1132 | CLA  | CAA-C2A-C3A | -3.53 | 103.12      | 112.78   |
| 14  | G     | 1135 | CLA  | C1-C2-C3    | -3.52 | 121.05      | 126.75   |
| 18  | M     | 4021 | BCR  | C33-C5-C6   | -3.52 | 120.57      | 124.53   |
| 14  | G     | 1132 | CLA  | CAA-C2A-C3A | -3.52 | 103.13      | 112.78   |
| 15  | B     | 1230 | F6C  | O2D-CGD-O1D | -3.52 | 116.95      | 123.84   |
| 14  | B     | 1239 | CLA  | O2A-CGA-CBA | 3.52  | 122.96      | 111.91   |
| 14  | H     | 1239 | CLA  | O2A-CGA-CBA | 3.52  | 122.95      | 111.91   |
| 14  | A     | 1124 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 18  | m     | 4021 | BCR  | C33-C5-C6   | -3.52 | 120.58      | 124.53   |
| 14  | b     | 1239 | CLA  | O2A-CGA-CBA | 3.52  | 122.95      | 111.91   |
| 14  | a     | 1111 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 15  | b     | 1230 | F6C  | O2D-CGD-O1D | -3.52 | 116.96      | 123.84   |
| 14  | G     | 1138 | CLA  | O2A-CGA-CBA | 3.51  | 122.94      | 111.91   |
| 14  | A     | 1135 | CLA  | C1-C2-C3    | -3.51 | 121.07      | 126.75   |
| 18  | V     | 4021 | BCR  | C33-C5-C6   | -3.51 | 120.58      | 124.53   |
| 14  | A     | 1111 | CLA  | CMB-C2B-C3B | 3.51  | 131.25      | 124.68   |
| 14  | a     | 1131 | CLA  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 14  | H     | 1240 | CLA  | CMB-C2B-C3B | 3.51  | 131.24      | 124.68   |
| 18  | G     | 4002 | BCR  | C3-C4-C5    | -3.51 | 107.81      | 114.08   |
| 15  | b     | 1238 | F6C  | CMA-C3A-C4A | -3.51 | 118.53      | 124.71   |
| 14  | a     | 1135 | CLA  | C1-C2-C3    | -3.51 | 121.08      | 126.75   |
| 14  | B     | 1240 | CLA  | CMB-C2B-C3B | 3.51  | 131.24      | 124.68   |
| 15  | b     | 1237 | F6C  | C1-C2-C3    | -3.51 | 119.98      | 126.04   |
| 14  | A     | 1131 | CLA  | C1-C2-C3    | -3.51 | 119.98      | 126.04   |
| 14  | a     | 1013 | CLA  | O2D-CGD-O1D | -3.50 | 116.99      | 123.84   |
| 15  | B     | 1237 | F6C  | C1-C2-C3    | -3.50 | 119.98      | 126.04   |
| 14  | A     | 1013 | CLA  | O2D-CGD-O1D | -3.50 | 116.99      | 123.84   |
| 14  | G     | 1124 | CLA  | CMB-C2B-C3B | 3.50  | 131.23      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1124 | CLA  | CMB-C2B-C3B | 3.50  | 131.23      | 124.68   |
| 14  | A     | 1138 | CLA  | O2A-CGA-CBA | 3.50  | 122.88      | 111.91   |
| 14  | H     | 1209 | CLA  | O2D-CGD-O1D | -3.50 | 117.00      | 123.84   |
| 14  | a     | 1107 | CLA  | O2A-CGA-CBA | 3.49  | 125.25      | 114.03   |
| 14  | G     | 1013 | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 14  | a     | 1138 | CLA  | O2A-CGA-CBA | 3.49  | 122.87      | 111.91   |
| 14  | G     | 1107 | CLA  | O2A-CGA-CBA | 3.49  | 125.25      | 114.03   |
| 14  | a     | 1138 | CLA  | O2A-C1-C2   | 3.49  | 117.81      | 108.64   |
| 14  | b     | 1205 | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 14  | G     | 1111 | CLA  | CMB-C2B-C3B | 3.49  | 131.21      | 124.68   |
| 14  | U     | 1502 | CLA  | C1-C2-C3    | -3.49 | 120.00      | 126.04   |
| 18  | A     | 4002 | BCR  | C3-C4-C5    | -3.49 | 107.84      | 114.08   |
| 15  | H     | 1237 | F6C  | C4A-C3A-C2A | -3.49 | 101.84      | 106.94   |
| 14  | B     | 1209 | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 14  | A     | 1138 | CLA  | O2A-C1-C2   | 3.49  | 117.81      | 108.64   |
| 18  | a     | 4002 | BCR  | C3-C4-C5    | -3.49 | 107.84      | 114.08   |
| 14  | H     | 1023 | CLA  | C4C-C3C-C2C | -3.49 | 101.81      | 106.90   |
| 15  | H     | 1207 | F6C  | C4-C3-C2    | -3.49 | 114.73      | 123.68   |
| 14  | l     | 1502 | CLA  | C1-C2-C3    | -3.49 | 120.01      | 126.04   |
| 15  | H     | 1237 | F6C  | C1-C2-C3    | -3.49 | 120.01      | 126.04   |
| 20  | H     | 5002 | LMG  | O7-C10-C11  | 3.49  | 119.01      | 111.50   |
| 14  | G     | 1138 | CLA  | O2A-C1-C2   | 3.49  | 117.80      | 108.64   |
| 14  | B     | 1023 | CLA  | C4C-C3C-C2C | -3.49 | 101.82      | 106.90   |
| 18  | L     | 4022 | BCR  | C33-C5-C4   | 3.49  | 120.31      | 113.62   |
| 15  | B     | 1237 | F6C  | C4A-C3A-C2A | -3.49 | 101.85      | 106.94   |
| 14  | A     | 1107 | CLA  | O2A-CGA-CBA | 3.48  | 125.23      | 114.03   |
| 18  | U     | 4022 | BCR  | C33-C5-C4   | 3.48  | 120.31      | 113.62   |
| 14  | b     | 1227 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 14  | G     | 1118 | CLA  | C4-C3-C5    | 3.48  | 121.13      | 115.27   |
| 14  | B     | 1227 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 14  | b     | 1209 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 14  | a     | 1109 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 14  | L     | 1502 | CLA  | C1-C2-C3    | -3.48 | 120.03      | 126.04   |
| 14  | H     | 1202 | CLA  | O2A-CGA-CBA | 3.48  | 122.82      | 111.91   |
| 14  | H     | 1021 | CLA  | CAA-CBA-CGA | -3.48 | 103.09      | 113.25   |
| 14  | B     | 1223 | CLA  | C3C-C4C-NC  | 3.48  | 114.47      | 110.57   |
| 14  | H     | 1223 | CLA  | C3C-C4C-NC  | 3.48  | 114.47      | 110.57   |
| 14  | B     | 1202 | CLA  | O2A-CGA-CBA | 3.48  | 122.82      | 111.91   |
| 14  | G     | 1102 | CLA  | O2A-CGA-CBA | 3.48  | 122.82      | 111.91   |
| 14  | A     | 1122 | CLA  | CAC-C3C-C4C | 3.48  | 129.32      | 124.81   |
| 14  | a     | 1122 | CLA  | CAC-C3C-C4C | 3.48  | 129.32      | 124.81   |
| 20  | b     | 5002 | LMG  | O7-C10-C11  | 3.48  | 118.99      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1223 | CLA  | C3C-C4C-NC  | 3.48  | 114.47      | 110.57   |
| 14  | B     | 1021 | CLA  | CAA-CBA-CGA | -3.48 | 103.10      | 113.25   |
| 15  | b     | 1207 | F6C  | C4-C3-C2    | -3.47 | 114.77      | 123.68   |
| 14  | a     | 1118 | CLA  | C4-C3-C5    | 3.47  | 121.11      | 115.27   |
| 14  | B     | 1023 | CLA  | O2D-CGD-CBD | 3.47  | 117.44      | 111.27   |
| 15  | b     | 1237 | F6C  | C4A-C3A-C2A | -3.47 | 101.87      | 106.94   |
| 14  | H     | 1205 | CLA  | O2D-CGD-O1D | -3.47 | 117.05      | 123.84   |
| 14  | b     | 1021 | CLA  | CAA-CBA-CGA | -3.47 | 103.11      | 113.25   |
| 14  | A     | 1109 | CLA  | O2D-CGD-O1D | -3.47 | 117.05      | 123.84   |
| 18  | l     | 4022 | BCR  | C33-C5-C4   | 3.47  | 120.28      | 113.62   |
| 14  | G     | 1122 | CLA  | CAC-C3C-C4C | 3.47  | 129.31      | 124.81   |
| 14  | a     | 1138 | CLA  | CMC-C2C-C1C | 3.47  | 130.32      | 125.04   |
| 14  | b     | 1023 | CLA  | O2D-CGD-CBD | 3.47  | 117.43      | 111.27   |
| 14  | A     | 1118 | CLA  | C4-C3-C5    | 3.47  | 121.11      | 115.27   |
| 14  | H     | 1023 | CLA  | O2D-CGD-CBD | 3.47  | 117.43      | 111.27   |
| 15  | b     | 1230 | F6C  | CMA-C3A-C4A | -3.47 | 118.60      | 124.71   |
| 15  | B     | 1207 | F6C  | C4-C3-C2    | -3.47 | 114.78      | 123.68   |
| 14  | B     | 1205 | CLA  | O2D-CGD-O1D | -3.47 | 117.06      | 123.84   |
| 14  | b     | 1201 | CLA  | O2D-CGD-O1D | -3.47 | 117.06      | 123.84   |
| 14  | G     | 1109 | CLA  | O2D-CGD-O1D | -3.47 | 117.06      | 123.84   |
| 14  | b     | 1202 | CLA  | O2A-CGA-CBA | 3.46  | 122.78      | 111.91   |
| 14  | A     | 1102 | CLA  | O2A-CGA-CBA | 3.46  | 122.78      | 111.91   |
| 18  | U     | 4019 | BCR  | C28-C27-C26 | -3.46 | 107.89      | 114.08   |
| 20  | B     | 5002 | LMG  | O7-C10-C11  | 3.46  | 118.96      | 111.50   |
| 14  | B     | 1201 | CLA  | O2D-CGD-O1D | -3.46 | 117.07      | 123.84   |
| 14  | H     | 1227 | CLA  | O2D-CGD-O1D | -3.46 | 117.07      | 123.84   |
| 14  | a     | 1102 | CLA  | O2A-CGA-CBA | 3.46  | 122.76      | 111.91   |
| 14  | b     | 1023 | CLA  | C4C-C3C-C2C | -3.46 | 101.86      | 106.90   |
| 18  | H     | 4014 | BCR  | C30-C25-C26 | -3.46 | 117.74      | 122.61   |
| 14  | A     | 1138 | CLA  | CMC-C2C-C1C | 3.46  | 130.30      | 125.04   |
| 14  | H     | 1201 | CLA  | O2D-CGD-O1D | -3.46 | 117.08      | 123.84   |
| 15  | B     | 1230 | F6C  | CMA-C3A-C4A | -3.46 | 118.62      | 124.71   |
| 14  | a     | 1141 | CLA  | O2D-CGD-O1D | -3.45 | 117.08      | 123.84   |
| 15  | H     | 1230 | F6C  | CMA-C3A-C4A | -3.45 | 118.63      | 124.71   |
| 14  | H     | 1220 | CLA  | O2D-CGD-O1D | -3.45 | 117.09      | 123.84   |
| 14  | H     | 1231 | CLA  | CMC-C2C-C1C | 3.45  | 130.29      | 125.04   |
| 14  | G     | 1130 | CLA  | O2A-CGA-CBA | 3.45  | 122.73      | 111.91   |
| 18  | L     | 4019 | BCR  | C28-C27-C26 | -3.44 | 107.93      | 114.08   |
| 14  | B     | 1220 | CLA  | O2D-CGD-O1D | -3.44 | 117.10      | 123.84   |
| 14  | G     | 1137 | CLA  | O2D-CGD-O1D | -3.44 | 117.10      | 123.84   |
| 14  | a     | 1137 | CLA  | O2D-CGD-O1D | -3.44 | 117.10      | 123.84   |
| 21  | l     | 6101 | LMT  | C3'-C4'-C5' | -3.44 | 103.03      | 110.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4003 | BCR  | C28-C27-C26 | -3.44 | 107.93      | 114.08   |
| 14  | G     | 1141 | CLA  | O2D-CGD-O1D | -3.44 | 117.11      | 123.84   |
| 18  | B     | 4014 | BCR  | C30-C25-C26 | -3.44 | 117.77      | 122.61   |
| 14  | A     | 1141 | CLA  | O2D-CGD-O1D | -3.44 | 117.11      | 123.84   |
| 18  | I     | 4019 | BCR  | C28-C27-C26 | -3.44 | 107.94      | 114.08   |
| 21  | U     | 6101 | LMT  | C3'-C4'-C5' | -3.44 | 103.04      | 110.93   |
| 14  | A     | 1130 | CLA  | O2A-CGA-CBA | 3.44  | 122.70      | 111.91   |
| 14  | b     | 1231 | CLA  | CMC-C2C-C1C | 3.44  | 130.27      | 125.04   |
| 14  | G     | 1138 | CLA  | CMC-C2C-C1C | 3.44  | 130.27      | 125.04   |
| 14  | a     | 1130 | CLA  | O2A-CGA-CBA | 3.44  | 122.69      | 111.91   |
| 18  | A     | 4003 | BCR  | C28-C27-C26 | -3.44 | 107.94      | 114.08   |
| 21  | L     | 6101 | LMT  | C3'-C4'-C5' | -3.43 | 103.06      | 110.93   |
| 14  | H     | 1204 | CLA  | O2A-CGA-CBA | 3.43  | 122.67      | 111.91   |
| 14  | B     | 1234 | CLA  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 14  | b     | 1220 | CLA  | O2D-CGD-O1D | -3.43 | 117.13      | 123.84   |
| 14  | b     | 1204 | CLA  | O2A-CGA-CBA | 3.43  | 122.67      | 111.91   |
| 18  | b     | 4014 | BCR  | C30-C25-C26 | -3.43 | 117.78      | 122.61   |
| 14  | A     | 1137 | CLA  | O2D-CGD-O1D | -3.43 | 117.13      | 123.84   |
| 18  | H     | 4006 | BCR  | C24-C23-C22 | -3.43 | 121.06      | 126.23   |
| 14  | H     | 1234 | CLA  | C3C-C4C-NC  | 3.43  | 114.41      | 110.57   |
| 14  | B     | 1204 | CLA  | O2A-CGA-CBA | 3.43  | 122.66      | 111.91   |
| 14  | G     | 1125 | CLA  | O2D-CGD-O1D | -3.42 | 117.14      | 123.84   |
| 14  | b     | 1203 | CLA  | C1-C2-C3    | -3.42 | 120.12      | 126.04   |
| 14  | H     | 1220 | CLA  | O2A-CGA-CBA | 3.42  | 122.65      | 111.91   |
| 14  | a     | 1126 | CLA  | C1D-ND-C4D  | -3.42 | 103.90      | 106.33   |
| 18  | H     | 4006 | BCR  | C3-C4-C5    | -3.42 | 107.97      | 114.08   |
| 14  | H     | 1224 | CLA  | C1-O2A-CGA  | 3.42  | 125.42      | 116.44   |
| 14  | B     | 1214 | CLA  | C1D-ND-C4D  | -3.42 | 103.91      | 106.33   |
| 14  | B     | 1220 | CLA  | O2A-CGA-CBA | 3.42  | 122.64      | 111.91   |
| 18  | b     | 4006 | BCR  | C24-C23-C22 | -3.42 | 121.07      | 126.23   |
| 14  | B     | 1231 | CLA  | CMC-C2C-C1C | 3.42  | 130.25      | 125.04   |
| 14  | B     | 1224 | CLA  | C1-O2A-CGA  | 3.42  | 125.41      | 116.44   |
| 14  | b     | 1021 | CLA  | C4-C3-C5    | 3.42  | 121.02      | 115.27   |
| 14  | H     | 1226 | CLA  | C1-O2A-CGA  | 3.42  | 125.41      | 116.44   |
| 14  | B     | 1226 | CLA  | C1-O2A-CGA  | 3.42  | 125.41      | 116.44   |
| 14  | b     | 1226 | CLA  | C1-O2A-CGA  | 3.41  | 125.40      | 116.44   |
| 14  | b     | 1220 | CLA  | O2A-CGA-CBA | 3.41  | 122.62      | 111.91   |
| 18  | a     | 4003 | BCR  | C28-C27-C26 | -3.41 | 107.99      | 114.08   |
| 18  | B     | 4006 | BCR  | C24-C23-C22 | -3.41 | 121.08      | 126.23   |
| 14  | b     | 1234 | CLA  | C3C-C4C-NC  | 3.41  | 114.40      | 110.57   |
| 14  | G     | 1128 | CLA  | O2D-CGD-O1D | -3.41 | 117.17      | 123.84   |
| 18  | b     | 4006 | BCR  | C3-C4-C5    | -3.41 | 107.99      | 114.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1128 | CLA  | O2D-CGD-O1D | -3.41 | 117.18      | 123.84   |
| 18  | B     | 4006 | BCR  | C3-C4-C5    | -3.41 | 107.99      | 114.08   |
| 14  | b     | 1224 | CLA  | C1-O2A-CGA  | 3.41  | 125.38      | 116.44   |
| 14  | A     | 1126 | CLA  | C1D-ND-C4D  | -3.41 | 103.92      | 106.33   |
| 14  | G     | 1126 | CLA  | C1D-ND-C4D  | -3.41 | 103.92      | 106.33   |
| 18  | a     | 4005 | BCR  | C33-C5-C6   | -3.40 | 120.71      | 124.53   |
| 14  | b     | 1233 | CLA  | O2A-CGA-CBA | 3.40  | 124.96      | 114.03   |
| 14  | b     | 1214 | CLA  | C1D-ND-C4D  | -3.40 | 103.92      | 106.33   |
| 14  | H     | 1233 | CLA  | O2A-CGA-CBA | 3.40  | 124.95      | 114.03   |
| 14  | b     | 1021 | CLA  | CHD-C1D-ND  | -3.40 | 121.33      | 124.45   |
| 14  | G     | 1116 | CLA  | CMB-C2B-C3B | 3.40  | 131.04      | 124.68   |
| 14  | B     | 1203 | CLA  | C1-C2-C3    | -3.40 | 120.16      | 126.04   |
| 14  | A     | 1125 | CLA  | O2D-CGD-O1D | -3.40 | 117.20      | 123.84   |
| 14  | B     | 1233 | CLA  | O2A-CGA-CBA | 3.39  | 124.93      | 114.03   |
| 14  | B     | 1021 | CLA  | C4-C3-C5    | 3.39  | 120.98      | 115.27   |
| 14  | a     | 1125 | CLA  | O2D-CGD-O1D | -3.39 | 117.20      | 123.84   |
| 14  | A     | 1116 | CLA  | CMB-C2B-C3B | 3.39  | 131.02      | 124.68   |
| 14  | a     | 1123 | CLA  | O2D-CGD-O1D | -3.39 | 117.22      | 123.84   |
| 14  | H     | 1203 | CLA  | C1-C2-C3    | -3.38 | 120.19      | 126.04   |
| 14  | B     | 1021 | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 14  | H     | 1021 | CLA  | C4-C3-C5    | 3.38  | 120.96      | 115.27   |
| 14  | b     | 1239 | CLA  | C1D-ND-C4D  | -3.38 | 103.93      | 106.33   |
| 14  | a     | 1128 | CLA  | O2D-CGD-O1D | -3.38 | 117.23      | 123.84   |
| 18  | G     | 4005 | BCR  | C33-C5-C6   | -3.38 | 120.73      | 124.53   |
| 14  | b     | 1220 | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 14  | H     | 1214 | CLA  | C1D-ND-C4D  | -3.38 | 103.94      | 106.33   |
| 14  | b     | 1023 | CLA  | C4-C3-C5    | 3.37  | 120.95      | 115.27   |
| 14  | B     | 1220 | CLA  | CMB-C2B-C3B | 3.37  | 130.99      | 124.68   |
| 14  | a     | 1116 | CLA  | CMB-C2B-C3B | 3.37  | 130.98      | 124.68   |
| 18  | A     | 4005 | BCR  | C33-C5-C6   | -3.37 | 120.75      | 124.53   |
| 14  | a     | 1124 | CLA  | O2A-CGA-CBA | 3.36  | 122.46      | 111.91   |
| 14  | H     | 1220 | CLA  | CMB-C2B-C3B | 3.36  | 130.97      | 124.68   |
| 14  | a     | 1135 | CLA  | CAC-C3C-C4C | 3.36  | 129.17      | 124.81   |
| 14  | A     | 1123 | CLA  | O2D-CGD-O1D | -3.36 | 117.27      | 123.84   |
| 14  | H     | 1021 | CLA  | CHD-C1D-ND  | -3.36 | 121.36      | 124.45   |
| 14  | A     | 1124 | CLA  | O2A-CGA-CBA | 3.36  | 122.45      | 111.91   |
| 14  | G     | 1123 | CLA  | O2D-CGD-O1D | -3.36 | 117.27      | 123.84   |
| 18  | l     | 4022 | BCR  | C36-C18-C17 | -3.36 | 118.22      | 122.92   |
| 14  | G     | 1124 | CLA  | O2A-CGA-CBA | 3.36  | 122.45      | 111.91   |
| 14  | B     | 1023 | CLA  | C4-C3-C5    | 3.36  | 120.92      | 115.27   |
| 21  | l     | 6002 | LMT  | C3'-C4'-C5' | -3.36 | 103.23      | 110.93   |
| 14  | A     | 1135 | CLA  | CAC-C3C-C4C | 3.35  | 129.16      | 124.81   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1117 | CLA  | O2A-CGA-CBA | 3.35  | 122.43      | 111.91   |
| 18  | b     | 4009 | BCR  | C15-C14-C13 | -3.35 | 122.52      | 127.31   |
| 14  | G     | 1117 | CLA  | O2A-CGA-CBA | 3.35  | 122.43      | 111.91   |
| 14  | a     | 1117 | CLA  | O2A-CGA-CBA | 3.35  | 122.43      | 111.91   |
| 14  | H     | 1023 | CLA  | C4-C3-C5    | 3.35  | 120.90      | 115.27   |
| 18  | H     | 4010 | BCR  | C34-C9-C10  | -3.35 | 118.23      | 122.92   |
| 14  | B     | 1239 | CLA  | C1D-ND-C4D  | -3.35 | 103.96      | 106.33   |
| 21  | L     | 6002 | LMT  | C3'-C4'-C5' | -3.35 | 103.25      | 110.93   |
| 15  | B     | 1238 | F6C  | O2A-CGA-CBA | 3.35  | 122.41      | 111.91   |
| 14  | b     | 1202 | CLA  | O2A-C1-C2   | 3.35  | 117.43      | 108.64   |
| 14  | G     | 1135 | CLA  | CAC-C3C-C4C | 3.35  | 129.15      | 124.81   |
| 18  | a     | 4006 | BCR  | C37-C22-C21 | -3.34 | 118.24      | 122.92   |
| 15  | b     | 1238 | F6C  | O2A-CGA-CBA | 3.34  | 122.40      | 111.91   |
| 14  | H     | 1239 | CLA  | C1D-ND-C4D  | -3.34 | 103.96      | 106.33   |
| 18  | B     | 4010 | BCR  | C34-C9-C10  | -3.34 | 118.24      | 122.92   |
| 18  | L     | 4022 | BCR  | C36-C18-C17 | -3.34 | 118.25      | 122.92   |
| 14  | k     | 1401 | CLA  | CAC-C3C-C4C | 3.34  | 129.14      | 124.81   |
| 14  | a     | 1115 | CLA  | C4-C3-C5    | 3.34  | 120.89      | 115.27   |
| 18  | U     | 4022 | BCR  | C36-C18-C17 | -3.34 | 118.25      | 122.92   |
| 15  | H     | 1238 | F6C  | O2A-CGA-CBA | 3.34  | 122.38      | 111.91   |
| 21  | U     | 6002 | LMT  | C3'-C4'-C5' | -3.34 | 103.28      | 110.93   |
| 14  | K     | 1401 | CLA  | CAC-C3C-C4C | 3.34  | 129.14      | 124.81   |
| 14  | B     | 1202 | CLA  | O2A-C1-C2   | 3.34  | 117.40      | 108.64   |
| 14  | B     | 1235 | CLA  | O2A-CGA-CBA | 3.33  | 122.37      | 111.91   |
| 15  | H     | 1237 | F6C  | O2D-CGD-O1D | -3.33 | 117.32      | 123.84   |
| 15  | H     | 1219 | F6C  | C3D-C4D-ND  | 3.33  | 115.04      | 110.17   |
| 14  | T     | 1401 | CLA  | CAC-C3C-C4C | 3.33  | 129.13      | 124.81   |
| 14  | G     | 1115 | CLA  | OBD-CAD-C3D | -3.33 | 120.50      | 128.52   |
| 14  | b     | 1236 | CLA  | C3C-C4C-NC  | 3.33  | 114.31      | 110.57   |
| 14  | A     | 1115 | CLA  | OBD-CAD-C3D | -3.33 | 120.51      | 128.52   |
| 15  | b     | 1219 | F6C  | C3D-C4D-ND  | 3.33  | 115.04      | 110.17   |
| 14  | a     | 1116 | CLA  | C4-C3-C5    | 3.33  | 120.87      | 115.27   |
| 15  | B     | 1237 | F6C  | O2D-CGD-O1D | -3.33 | 117.33      | 123.84   |
| 14  | H     | 1202 | CLA  | O2A-C1-C2   | 3.33  | 117.37      | 108.64   |
| 14  | H     | 1235 | CLA  | O2A-CGA-CBA | 3.32  | 122.34      | 111.91   |
| 18  | b     | 4010 | BCR  | C34-C9-C10  | -3.32 | 118.27      | 122.92   |
| 14  | b     | 1211 | CLA  | O2A-CGA-CBA | 3.32  | 122.33      | 111.91   |
| 14  | b     | 1235 | CLA  | O2A-CGA-CBA | 3.32  | 122.33      | 111.91   |
| 18  | b     | 4010 | BCR  | C24-C23-C22 | -3.32 | 121.22      | 126.23   |
| 14  | b     | 1021 | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 18  | B     | 4009 | BCR  | C15-C14-C13 | -3.32 | 122.57      | 127.31   |
| 13  | a     | 1011 | CL0  | C3C-C4C-NC  | 3.32  | 114.29      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1128 | CLA  | C1D-ND-C4D  | -3.32 | 103.98      | 106.33   |
| 15  | B     | 1219 | F6C  | C3D-C4D-ND  | 3.32  | 115.02      | 110.17   |
| 15  | b     | 1237 | F6C  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 14  | H     | 1211 | CLA  | O2A-CGA-CBA | 3.32  | 122.32      | 111.91   |
| 14  | B     | 1211 | CLA  | O2A-CGA-CBA | 3.31  | 122.31      | 111.91   |
| 18  | H     | 4004 | BCR  | C15-C14-C13 | -3.31 | 122.58      | 127.31   |
| 14  | A     | 1116 | CLA  | C4-C3-C5    | 3.31  | 120.85      | 115.27   |
| 14  | A     | 1115 | CLA  | C4-C3-C5    | 3.31  | 120.84      | 115.27   |
| 14  | B     | 1021 | CLA  | CMB-C2B-C3B | 3.31  | 130.88      | 124.68   |
| 13  | G     | 1011 | CL0  | CMA-C3A-C2A | -3.31 | 100.47      | 113.83   |
| 18  | A     | 4006 | BCR  | C37-C22-C21 | -3.31 | 118.29      | 122.92   |
| 13  | a     | 1011 | CL0  | CMA-C3A-C2A | -3.31 | 100.47      | 113.83   |
| 14  | a     | 1115 | CLA  | OBD-CAD-C3D | -3.31 | 120.56      | 128.52   |
| 14  | a     | 1124 | CLA  | C1-C2-C3    | -3.31 | 120.32      | 126.04   |
| 14  | G     | 1116 | CLA  | C4-C3-C5    | 3.31  | 120.84      | 115.27   |
| 18  | a     | 4005 | BCR  | C27-C26-C25 | -3.31 | 117.93      | 122.73   |
| 18  | H     | 4010 | BCR  | C24-C23-C22 | -3.31 | 121.24      | 126.23   |
| 15  | B     | 1207 | F6C  | CHB-C4A-C3A | -3.30 | 118.55      | 125.48   |
| 14  | B     | 1216 | CLA  | C4A-NA-C1A  | 3.30  | 108.19      | 106.71   |
| 18  | B     | 4010 | BCR  | C24-C23-C22 | -3.30 | 121.24      | 126.23   |
| 15  | b     | 1207 | F6C  | CHB-C4A-C3A | -3.30 | 118.55      | 125.48   |
| 18  | A     | 4005 | BCR  | C27-C26-C25 | -3.30 | 117.94      | 122.73   |
| 13  | A     | 1011 | CL0  | CMA-C3A-C2A | -3.30 | 100.51      | 113.83   |
| 18  | B     | 4004 | BCR  | C15-C14-C13 | -3.30 | 122.60      | 127.31   |
| 14  | G     | 1105 | CLA  | O2A-CGA-CBA | 3.30  | 124.64      | 114.03   |
| 14  | A     | 1124 | CLA  | C1-C2-C3    | -3.30 | 120.34      | 126.04   |
| 14  | H     | 1021 | CLA  | CMB-C2B-C3B | 3.30  | 130.85      | 124.68   |
| 14  | G     | 1124 | CLA  | C1-C2-C3    | -3.30 | 120.34      | 126.04   |
| 14  | a     | 1105 | CLA  | O2A-CGA-CBA | 3.30  | 124.63      | 114.03   |
| 14  | G     | 1111 | CLA  | CAC-C3C-C4C | 3.30  | 129.09      | 124.81   |
| 14  | A     | 1105 | CLA  | O2A-CGA-CBA | 3.30  | 124.62      | 114.03   |
| 14  | G     | 1115 | CLA  | C4-C3-C5    | 3.30  | 120.82      | 115.27   |
| 14  | b     | 1208 | CLA  | C1-O2A-CGA  | 3.30  | 125.09      | 116.44   |
| 18  | H     | 4009 | BCR  | C15-C14-C13 | -3.29 | 122.61      | 127.31   |
| 18  | G     | 4006 | BCR  | C37-C22-C21 | -3.29 | 118.31      | 122.92   |
| 14  | H     | 1236 | CLA  | C3C-C4C-NC  | 3.29  | 114.26      | 110.57   |
| 15  | H     | 1207 | F6C  | CHB-C4A-C3A | -3.29 | 118.58      | 125.48   |
| 14  | a     | 1109 | CLA  | C4-C3-C5    | 3.29  | 120.81      | 115.27   |
| 14  | A     | 1109 | CLA  | C4-C3-C5    | 3.29  | 120.81      | 115.27   |
| 14  | B     | 1208 | CLA  | C1-O2A-CGA  | 3.29  | 125.07      | 116.44   |
| 13  | a     | 1011 | CL0  | CAA-C2A-C3A | -3.29 | 103.77      | 112.78   |
| 14  | G     | 1136 | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1208 | CLA  | C1-O2A-CGA  | 3.29  | 125.07      | 116.44   |
| 13  | A     | 1011 | CL0  | C3C-C4C-NC  | 3.29  | 114.26      | 110.57   |
| 14  | B     | 1236 | CLA  | C3C-C4C-NC  | 3.29  | 114.26      | 110.57   |
| 15  | H     | 1219 | F6C  | C4A-NA-C1A  | 3.29  | 108.67      | 106.33   |
| 13  | G     | 1011 | CL0  | CAA-C2A-C3A | -3.29 | 103.78      | 112.78   |
| 13  | A     | 1011 | CL0  | CAA-C2A-C3A | -3.29 | 103.78      | 112.78   |
| 14  | G     | 1109 | CLA  | C4-C3-C5    | 3.28  | 120.80      | 115.27   |
| 18  | G     | 4005 | BCR  | C27-C26-C25 | -3.28 | 117.97      | 122.73   |
| 18  | H     | 4009 | BCR  | C38-C26-C27 | 3.28  | 119.92      | 113.62   |
| 14  | A     | 1136 | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 18  | b     | 4004 | BCR  | C15-C14-C13 | -3.28 | 122.63      | 127.31   |
| 13  | G     | 1011 | CL0  | C3C-C4C-NC  | 3.27  | 114.24      | 110.57   |
| 14  | H     | 1021 | CLA  | C3C-C4C-NC  | 3.27  | 114.24      | 110.57   |
| 14  | A     | 1102 | CLA  | CMC-C2C-C1C | 3.27  | 130.02      | 125.04   |
| 14  | a     | 1102 | CLA  | CMC-C2C-C1C | 3.27  | 130.02      | 125.04   |
| 14  | H     | 1022 | CLA  | OBD-CAD-C3D | -3.27 | 120.66      | 128.52   |
| 18  | B     | 4009 | BCR  | C38-C26-C27 | 3.26  | 119.89      | 113.62   |
| 14  | a     | 1136 | CLA  | O2D-CGD-O1D | -3.26 | 117.46      | 123.84   |
| 14  | a     | 1107 | CLA  | CMB-C2B-C3B | 3.26  | 130.78      | 124.68   |
| 14  | B     | 1211 | CLA  | CMC-C2C-C1C | 3.26  | 130.01      | 125.04   |
| 14  | b     | 1022 | CLA  | OBD-CAD-C3D | -3.26 | 120.67      | 128.52   |
| 14  | A     | 1111 | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.81   |
| 14  | a     | 1111 | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.81   |
| 18  | U     | 4019 | BCR  | C7-C8-C9    | -3.26 | 121.31      | 126.23   |
| 14  | G     | 1116 | CLA  | CMC-C2C-C1C | 3.26  | 130.00      | 125.04   |
| 14  | b     | 1216 | CLA  | C4A-NA-C1A  | 3.26  | 108.17      | 106.71   |
| 14  | H     | 1236 | CLA  | O2D-CGD-O1D | -3.26 | 117.47      | 123.84   |
| 14  | A     | 1116 | CLA  | CMC-C2C-C1C | 3.25  | 130.00      | 125.04   |
| 14  | G     | 1102 | CLA  | CMC-C2C-C1C | 3.25  | 130.00      | 125.04   |
| 14  | G     | 1107 | CLA  | CMB-C2B-C3B | 3.25  | 130.77      | 124.68   |
| 14  | a     | 1134 | CLA  | CMB-C2B-C3B | 3.25  | 130.77      | 124.68   |
| 14  | b     | 1202 | CLA  | C1-O2A-CGA  | 3.25  | 124.98      | 116.44   |
| 14  | B     | 1021 | CLA  | C3C-C4C-NC  | 3.25  | 114.22      | 110.57   |
| 14  | B     | 1202 | CLA  | C1-O2A-CGA  | 3.25  | 124.98      | 116.44   |
| 14  | B     | 1022 | CLA  | OBD-CAD-C3D | -3.25 | 120.69      | 128.52   |
| 18  | H     | 4009 | BCR  | C3-C4-C5    | -3.25 | 108.27      | 114.08   |
| 14  | B     | 1236 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 14  | b     | 1236 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 14  | A     | 1107 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 15  | H     | 1207 | F6C  | C4-C3-C5    | 3.25  | 120.74      | 115.27   |
| 15  | B     | 1219 | F6C  | C4A-NA-C1A  | 3.25  | 108.64      | 106.33   |
| 14  | H     | 1202 | CLA  | C1-O2A-CGA  | 3.25  | 124.97      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1101 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 14  | a     | 1135 | CLA  | CMD-C2D-C3D | -3.25 | 120.14      | 127.61   |
| 14  | b     | 1211 | CLA  | CMC-C2C-C1C | 3.25  | 129.99      | 125.04   |
| 14  | G     | 1134 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 14  | b     | 1022 | CLA  | C4-C3-C2    | -3.25 | 115.35      | 123.68   |
| 14  | A     | 1101 | CLA  | O2D-CGD-O1D | -3.25 | 117.49      | 123.84   |
| 18  | b     | 4009 | BCR  | C38-C26-C27 | 3.25  | 119.85      | 113.62   |
| 14  | A     | 1134 | CLA  | CMB-C2B-C3B | 3.25  | 130.75      | 124.68   |
| 14  | a     | 1101 | CLA  | O2D-CGD-O1D | -3.25 | 117.49      | 123.84   |
| 14  | A     | 1128 | CLA  | C1D-ND-C4D  | -3.24 | 104.03      | 106.33   |
| 14  | B     | 1022 | CLA  | C4-C3-C2    | -3.24 | 115.36      | 123.68   |
| 14  | a     | 1140 | CLA  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 14  | a     | 1135 | CLA  | C4D-C3D-CAD | 3.24  | 111.92      | 108.10   |
| 15  | b     | 1219 | F6C  | C4A-NA-C1A  | 3.24  | 108.64      | 106.33   |
| 18  | B     | 4009 | BCR  | C3-C4-C5    | -3.24 | 108.29      | 114.08   |
| 18  | l     | 4019 | BCR  | C7-C8-C9    | -3.24 | 121.34      | 126.23   |
| 14  | A     | 1135 | CLA  | CMD-C2D-C3D | -3.24 | 120.16      | 127.61   |
| 18  | H     | 4006 | BCR  | C38-C26-C25 | -3.24 | 120.89      | 124.53   |
| 14  | A     | 1140 | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 14  | H     | 1211 | CLA  | CMC-C2C-C1C | 3.24  | 129.97      | 125.04   |
| 14  | H     | 1223 | CLA  | C1-C2-C3    | -3.24 | 120.45      | 126.04   |
| 14  | H     | 1231 | CLA  | O2A-CGA-CBA | 3.24  | 122.06      | 111.91   |
| 14  | a     | 1116 | CLA  | CMC-C2C-C1C | 3.23  | 129.97      | 125.04   |
| 15  | B     | 1207 | F6C  | C4-C3-C5    | 3.23  | 120.71      | 115.27   |
| 18  | L     | 4019 | BCR  | C7-C8-C9    | -3.23 | 121.35      | 126.23   |
| 14  | a     | 1128 | CLA  | C1D-ND-C4D  | -3.23 | 104.04      | 106.33   |
| 18  | i     | 4020 | BCR  | C23-C22-C21 | -3.23 | 113.98      | 118.94   |
| 15  | b     | 1207 | F6C  | C4-C3-C5    | 3.23  | 120.71      | 115.27   |
| 14  | B     | 1231 | CLA  | O2A-CGA-CBA | 3.23  | 122.04      | 111.91   |
| 14  | G     | 1135 | CLA  | CMD-C2D-C3D | -3.23 | 120.19      | 127.61   |
| 14  | G     | 1120 | CLA  | O2A-CGA-CBA | 3.23  | 124.40      | 114.03   |
| 14  | A     | 1106 | CLA  | O2D-CGD-O1D | -3.23 | 117.53      | 123.84   |
| 14  | a     | 1114 | CLA  | O2A-CGA-CBA | 3.23  | 124.40      | 114.03   |
| 14  | H     | 1022 | CLA  | C4-C3-C2    | -3.23 | 115.40      | 123.68   |
| 14  | b     | 1231 | CLA  | O2A-CGA-CBA | 3.23  | 122.03      | 111.91   |
| 14  | G     | 1140 | CLA  | O2D-CGD-O1D | -3.22 | 117.53      | 123.84   |
| 18  | H     | 4009 | BCR  | C33-C5-C6   | -3.22 | 120.91      | 124.53   |
| 14  | A     | 1114 | CLA  | O2A-CGA-CBA | 3.22  | 124.39      | 114.03   |
| 18  | I     | 4020 | BCR  | C23-C22-C21 | -3.22 | 114.00      | 118.94   |
| 14  | A     | 1135 | CLA  | C4D-C3D-CAD | 3.22  | 111.89      | 108.10   |
| 14  | B     | 1223 | CLA  | C1-C2-C3    | -3.22 | 120.47      | 126.04   |
| 14  | A     | 1120 | CLA  | O2A-CGA-CBA | 3.22  | 124.38      | 114.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | R     | 4020 | BCR  | C23-C22-C21 | -3.22 | 114.00      | 118.94   |
| 14  | G     | 1135 | CLA  | C4D-C3D-CAD | 3.22  | 111.89      | 108.10   |
| 14  | a     | 1106 | CLA  | O2D-CGD-O1D | -3.22 | 117.54      | 123.84   |
| 14  | B     | 1212 | CLA  | CMA-C3A-C4A | 3.22  | 120.42      | 111.77   |
| 14  | b     | 1212 | CLA  | CMA-C3A-C4A | 3.22  | 120.42      | 111.77   |
| 18  | b     | 4009 | BCR  | C3-C4-C5    | -3.22 | 108.33      | 114.08   |
| 14  | G     | 1114 | CLA  | O2A-CGA-CBA | 3.22  | 124.37      | 114.03   |
| 14  | G     | 1106 | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 14  | B     | 1204 | CLA  | CMC-C2C-C1C | 3.22  | 129.94      | 125.04   |
| 14  | H     | 1212 | CLA  | CMA-C3A-C4A | 3.22  | 120.41      | 111.77   |
| 14  | a     | 1120 | CLA  | O2A-CGA-CBA | 3.21  | 124.36      | 114.03   |
| 14  | b     | 1021 | CLA  | C3C-C4C-NC  | 3.21  | 114.17      | 110.57   |
| 14  | H     | 1221 | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 14  | b     | 1223 | CLA  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 14  | B     | 1204 | CLA  | O2A-C1-C2   | 3.21  | 117.07      | 108.64   |
| 14  | H     | 1204 | CLA  | O2A-C1-C2   | 3.21  | 117.07      | 108.64   |
| 18  | B     | 4009 | BCR  | C33-C5-C6   | -3.21 | 120.92      | 124.53   |
| 14  | G     | 1126 | CLA  | C4-C3-C5    | 3.21  | 120.67      | 115.27   |
| 14  | B     | 1221 | CLA  | CMA-C3A-C2A | 3.21  | 126.77      | 113.83   |
| 14  | b     | 1204 | CLA  | O2A-C1-C2   | 3.21  | 117.06      | 108.64   |
| 14  | H     | 1221 | CLA  | CMA-C3A-C2A | 3.21  | 126.76      | 113.83   |
| 18  | A     | 4005 | BCR  | C15-C14-C13 | -3.20 | 122.74      | 127.31   |
| 14  | H     | 1204 | CLA  | CMC-C2C-C1C | 3.20  | 129.92      | 125.04   |
| 14  | b     | 1221 | CLA  | CMA-C3A-C2A | 3.20  | 126.74      | 113.83   |
| 14  | a     | 1111 | CLA  | CMC-C2C-C1C | 3.20  | 129.91      | 125.04   |
| 14  | a     | 1139 | CLA  | O2A-CGA-CBA | 3.20  | 124.31      | 114.03   |
| 14  | A     | 1111 | CLA  | CMC-C2C-C1C | 3.20  | 129.91      | 125.04   |
| 14  | L     | 1503 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 14  | G     | 1139 | CLA  | O2A-CGA-CBA | 3.20  | 124.30      | 114.03   |
| 14  | A     | 1139 | CLA  | O2A-CGA-CBA | 3.20  | 124.30      | 114.03   |
| 18  | B     | 4006 | BCR  | C38-C26-C25 | -3.20 | 120.94      | 124.53   |
| 14  | a     | 1123 | CLA  | C3C-C4C-NC  | 3.19  | 114.15      | 110.57   |
| 14  | b     | 1213 | CLA  | CAA-C2A-C3A | -3.19 | 104.03      | 112.78   |
| 18  | l     | 4022 | BCR  | C19-C18-C17 | 3.19  | 123.84      | 118.94   |
| 18  | G     | 4005 | BCR  | C15-C14-C13 | -3.19 | 122.76      | 127.31   |
| 14  | G     | 1111 | CLA  | CMC-C2C-C1C | 3.19  | 129.90      | 125.04   |
| 14  | a     | 1126 | CLA  | C4-C3-C5    | 3.19  | 120.64      | 115.27   |
| 14  | a     | 1130 | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 14  | b     | 1204 | CLA  | CMC-C2C-C1C | 3.19  | 129.89      | 125.04   |
| 14  | H     | 1213 | CLA  | CAA-C2A-C3A | -3.19 | 104.05      | 112.78   |
| 14  | l     | 1503 | CLA  | CMB-C2B-C3B | 3.19  | 130.64      | 124.68   |
| 14  | B     | 1213 | CLA  | CAA-C2A-C3A | -3.19 | 104.06      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1130 | CLA  | O2D-CGD-O1D | -3.18 | 117.61      | 123.84   |
| 16  | a     | 2001 | PQN  | C14-C13-C15 | 3.18  | 120.62      | 115.27   |
| 14  | A     | 1130 | CLA  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 14  | A     | 1126 | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 14  | a     | 1140 | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 14  | b     | 1221 | CLA  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 14  | B     | 1221 | CLA  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 18  | b     | 4009 | BCR  | C33-C5-C6   | -3.18 | 120.96      | 124.53   |
| 14  | U     | 1503 | CLA  | CMB-C2B-C3B | 3.18  | 130.62      | 124.68   |
| 18  | a     | 4005 | BCR  | C15-C14-C13 | -3.17 | 122.78      | 127.31   |
| 14  | H     | 1206 | CLA  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 14  | L     | 1503 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 18  | L     | 4022 | BCR  | C19-C18-C17 | 3.17  | 123.81      | 118.94   |
| 14  | b     | 1225 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 14  | b     | 1022 | CLA  | CMC-C2C-C1C | 3.17  | 129.87      | 125.04   |
| 14  | H     | 1216 | CLA  | C4A-NA-C1A  | 3.17  | 108.13      | 106.71   |
| 14  | H     | 1225 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 18  | b     | 4006 | BCR  | C38-C26-C25 | -3.17 | 120.97      | 124.53   |
| 14  | A     | 1137 | CLA  | C1-C2-C3    | -3.17 | 121.62      | 126.75   |
| 14  | G     | 1140 | CLA  | C4-C3-C5    | 3.17  | 120.60      | 115.27   |
| 14  | B     | 1227 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 14  | G     | 1137 | CLA  | C1-C2-C3    | -3.17 | 121.62      | 126.75   |
| 18  | U     | 4022 | BCR  | C19-C18-C17 | 3.17  | 123.81      | 118.94   |
| 14  | G     | 1125 | CLA  | C4C-C3C-C2C | -3.17 | 102.28      | 106.90   |
| 14  | A     | 1123 | CLA  | C3C-C4C-NC  | 3.17  | 114.12      | 110.57   |
| 15  | b     | 1230 | F6C  | C4A-NA-C1A  | 3.17  | 108.58      | 106.33   |
| 14  | U     | 1503 | CLA  | C1-C2-C3    | -3.16 | 120.57      | 126.04   |
| 14  | M     | 1501 | CLA  | CMA-C3A-C4A | 3.16  | 120.28      | 111.77   |
| 14  | b     | 1227 | CLA  | CMB-C2B-C3B | 3.16  | 130.60      | 124.68   |
| 14  | T     | 1401 | CLA  | O2A-CGA-CBA | 3.16  | 124.19      | 114.03   |
| 14  | b     | 1206 | CLA  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |
| 14  | H     | 1227 | CLA  | CMB-C2B-C3B | 3.16  | 130.59      | 124.68   |
| 14  | B     | 1214 | CLA  | CMB-C2B-C3B | 3.16  | 130.59      | 124.68   |
| 14  | G     | 1116 | CLA  | C1-C2-C3    | -3.16 | 120.58      | 126.04   |
| 16  | A     | 2001 | PQN  | C14-C13-C15 | 3.16  | 120.59      | 115.27   |
| 14  | H     | 1235 | CLA  | C1-O2A-CGA  | 3.16  | 124.73      | 116.44   |
| 14  | H     | 1222 | CLA  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |
| 14  | B     | 1225 | CLA  | C1-C2-C3    | -3.16 | 120.58      | 126.04   |
| 14  | a     | 1110 | CLA  | O2A-CGA-CBA | 3.16  | 124.18      | 114.03   |
| 14  | G     | 1104 | CLA  | C1-C2-C3    | -3.16 | 120.58      | 126.04   |
| 18  | a     | 4004 | BCR  | C15-C14-C13 | -3.16 | 122.80      | 127.31   |
| 14  | B     | 1206 | CLA  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | V     | 1501 | CLA  | CMA-C3A-C4A | 3.16  | 120.26      | 111.77   |
| 14  | B     | 1222 | CLA  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 14  | l     | 1503 | CLA  | C1-C2-C3    | -3.16 | 120.58      | 126.04   |
| 14  | B     | 1235 | CLA  | C1-O2A-CGA  | 3.16  | 124.72      | 116.44   |
| 14  | H     | 1022 | CLA  | CMC-C2C-C1C | 3.16  | 129.84      | 125.04   |
| 18  | i     | 4020 | BCR  | C38-C26-C25 | -3.15 | 120.99      | 124.53   |
| 16  | G     | 2001 | PQN  | C14-C13-C15 | 3.15  | 120.58      | 115.27   |
| 14  | G     | 1123 | CLA  | CMC-C2C-C1C | 3.15  | 129.84      | 125.04   |
| 14  | b     | 1222 | CLA  | O2D-CGD-O1D | -3.15 | 117.67      | 123.84   |
| 14  | A     | 1116 | CLA  | C1-C2-C3    | -3.15 | 120.59      | 126.04   |
| 14  | B     | 1022 | CLA  | CMC-C2C-C1C | 3.15  | 129.84      | 125.04   |
| 14  | A     | 1110 | CLA  | O2A-CGA-CBA | 3.15  | 124.16      | 114.03   |
| 14  | k     | 1401 | CLA  | O2A-CGA-CBA | 3.15  | 124.15      | 114.03   |
| 14  | A     | 1125 | CLA  | C4C-C3C-C2C | -3.15 | 102.31      | 106.90   |
| 14  | G     | 1123 | CLA  | C3C-C4C-NC  | 3.15  | 114.10      | 110.57   |
| 14  | K     | 1401 | CLA  | O2A-CGA-CBA | 3.15  | 124.15      | 114.03   |
| 18  | G     | 4001 | BCR  | C33-C5-C6   | -3.15 | 120.99      | 124.53   |
| 14  | b     | 1214 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 14  | H     | 1210 | CLA  | C3C-C4C-NC  | 3.15  | 114.10      | 110.57   |
| 14  | b     | 1235 | CLA  | C1-O2A-CGA  | 3.14  | 124.69      | 116.44   |
| 14  | A     | 1140 | CLA  | C4-C3-C5    | 3.14  | 120.56      | 115.27   |
| 14  | m     | 1501 | CLA  | CMA-C3A-C4A | 3.14  | 120.22      | 111.77   |
| 14  | b     | 1214 | CLA  | C4A-NA-C1A  | 3.14  | 108.12      | 106.71   |
| 14  | b     | 1208 | CLA  | O2D-CGD-O1D | -3.14 | 117.69      | 123.84   |
| 14  | G     | 1110 | CLA  | O2A-CGA-CBA | 3.14  | 124.12      | 114.03   |
| 14  | H     | 1214 | CLA  | CMB-C2B-C3B | 3.14  | 130.55      | 124.68   |
| 14  | a     | 1137 | CLA  | C1-C2-C3    | -3.14 | 121.68      | 126.75   |
| 14  | a     | 1125 | CLA  | C4C-C3C-C2C | -3.14 | 102.33      | 106.90   |
| 15  | H     | 1230 | F6C  | C4A-NA-C1A  | 3.13  | 108.56      | 106.33   |
| 14  | A     | 1123 | CLA  | CMC-C2C-C1C | 3.13  | 129.81      | 125.04   |
| 14  | a     | 1123 | CLA  | CMC-C2C-C1C | 3.13  | 129.81      | 125.04   |
| 14  | a     | 1104 | CLA  | C1-C2-C3    | -3.13 | 120.62      | 126.04   |
| 14  | a     | 1116 | CLA  | C1-C2-C3    | -3.13 | 120.62      | 126.04   |
| 15  | B     | 1230 | F6C  | C4A-NA-C1A  | 3.13  | 108.56      | 106.33   |
| 14  | H     | 1203 | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 14  | a     | 1113 | CLA  | O2A-CGA-CBA | 3.13  | 124.09      | 114.03   |
| 14  | b     | 1239 | CLA  | O2D-CGD-O1D | -3.13 | 117.72      | 123.84   |
| 14  | G     | 1125 | CLA  | C1-C2-C3    | -3.13 | 120.63      | 126.04   |
| 18  | U     | 4019 | BCR  | C34-C9-C8   | 3.13  | 123.00      | 118.08   |
| 14  | A     | 1113 | CLA  | O2A-CGA-CBA | 3.13  | 124.07      | 114.03   |
| 18  | l     | 4019 | BCR  | C34-C9-C8   | 3.13  | 123.00      | 118.08   |
| 14  | L     | 1502 | CLA  | O2A-CGA-CBA | 3.12  | 121.71      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 4004 | BCR  | C15-C14-C13 | -3.12 | 122.85      | 127.31   |
| 14  | A     | 1104 | CLA  | C1-C2-C3    | -3.12 | 120.64      | 126.04   |
| 18  | b     | 4006 | BCR  | C36-C18-C17 | -3.12 | 118.55      | 122.92   |
| 14  | l     | 1502 | CLA  | O2A-CGA-CBA | 3.12  | 121.71      | 111.91   |
| 18  | G     | 4004 | BCR  | C15-C14-C13 | -3.12 | 122.85      | 127.31   |
| 14  | a     | 1141 | CLA  | O2A-CGA-CBA | 3.12  | 124.06      | 114.03   |
| 14  | B     | 1203 | CLA  | CMB-C2B-C3B | 3.12  | 130.52      | 124.68   |
| 14  | G     | 1113 | CLA  | O2A-CGA-CBA | 3.12  | 124.06      | 114.03   |
| 14  | b     | 1203 | CLA  | CMB-C2B-C3B | 3.12  | 130.52      | 124.68   |
| 14  | b     | 1218 | CLA  | O2A-CGA-CBA | 3.12  | 124.05      | 114.03   |
| 14  | B     | 1208 | CLA  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 14  | U     | 1502 | CLA  | O2A-CGA-CBA | 3.12  | 121.69      | 111.91   |
| 14  | B     | 1218 | CLA  | O2A-CGA-CBA | 3.12  | 124.05      | 114.03   |
| 14  | L     | 1502 | CLA  | CMB-C2B-C3B | 3.12  | 130.51      | 124.68   |
| 18  | A     | 4001 | BCR  | C33-C5-C6   | -3.12 | 121.03      | 124.53   |
| 18  | G     | 4001 | BCR  | C24-C23-C22 | -3.12 | 121.53      | 126.23   |
| 18  | a     | 4005 | BCR  | C38-C26-C27 | 3.11  | 119.60      | 113.62   |
| 14  | b     | 1216 | CLA  | CMB-C2B-C3B | 3.11  | 130.50      | 124.68   |
| 18  | L     | 4019 | BCR  | C34-C9-C8   | 3.11  | 122.98      | 118.08   |
| 14  | a     | 1125 | CLA  | C1-C2-C3    | -3.11 | 120.66      | 126.04   |
| 14  | H     | 1216 | CLA  | CMB-C2B-C3B | 3.11  | 130.50      | 124.68   |
| 14  | l     | 1502 | CLA  | CMB-C2B-C3B | 3.11  | 130.50      | 124.68   |
| 15  | H     | 1237 | F6C  | CAA-CBA-CGA | -3.11 | 104.38      | 113.43   |
| 14  | H     | 1208 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 15  | B     | 1237 | F6C  | CAA-CBA-CGA | -3.11 | 104.39      | 113.43   |
| 15  | H     | 1230 | F6C  | C3D-C4D-ND  | 3.11  | 114.72      | 110.17   |
| 14  | H     | 1218 | CLA  | O2A-CGA-CBA | 3.11  | 124.02      | 114.03   |
| 14  | b     | 1210 | CLA  | C3C-C4C-NC  | 3.11  | 114.06      | 110.57   |
| 18  | A     | 4001 | BCR  | C24-C23-C22 | -3.11 | 121.54      | 126.23   |
| 14  | H     | 1229 | CLA  | CAA-C2A-C3A | -3.11 | 104.27      | 112.78   |
| 18  | A     | 4005 | BCR  | C38-C26-C27 | 3.11  | 119.58      | 113.62   |
| 14  | G     | 1107 | CLA  | C3C-C4C-NC  | 3.11  | 114.06      | 110.57   |
| 14  | A     | 1141 | CLA  | O2A-CGA-CBA | 3.11  | 124.01      | 114.03   |
| 14  | U     | 1502 | CLA  | CMB-C2B-C3B | 3.11  | 130.49      | 124.68   |
| 14  | G     | 1141 | CLA  | O2A-CGA-CBA | 3.10  | 124.00      | 114.03   |
| 18  | H     | 4006 | BCR  | C36-C18-C17 | -3.10 | 118.58      | 122.92   |
| 14  | H     | 1213 | CLA  | CMC-C2C-C1C | 3.10  | 129.76      | 125.04   |
| 14  | B     | 1211 | CLA  | CAC-C3C-C4C | 3.10  | 128.84      | 124.81   |
| 14  | b     | 1213 | CLA  | CMC-C2C-C1C | 3.10  | 129.76      | 125.04   |
| 14  | A     | 1125 | CLA  | C1-C2-C3    | -3.10 | 120.68      | 126.04   |
| 14  | A     | 1107 | CLA  | C3C-C4C-NC  | 3.10  | 114.05      | 110.57   |
| 14  | a     | 1119 | CLA  | C1-C2-C3    | -3.10 | 120.68      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4005 | BCR  | C38-C26-C27 | 3.10  | 119.57      | 113.62   |
| 18  | B     | 4006 | BCR  | C36-C18-C17 | -3.10 | 118.58      | 122.92   |
| 15  | b     | 1237 | F6C  | CAA-CBA-CGA | -3.10 | 104.42      | 113.43   |
| 14  | B     | 1229 | CLA  | CAA-C2A-C3A | -3.10 | 104.29      | 112.78   |
| 18  | I     | 4020 | BCR  | C38-C26-C25 | -3.10 | 121.05      | 124.53   |
| 21  | H     | 6004 | LMT  | O5'-C1'-C2' | -3.10 | 103.80      | 110.35   |
| 14  | H     | 1220 | CLA  | CMA-C3A-C4A | 3.10  | 120.09      | 111.77   |
| 14  | A     | 1119 | CLA  | C1-C2-C3    | -3.10 | 120.69      | 126.04   |
| 18  | H     | 4004 | BCR  | C24-C23-C22 | -3.09 | 121.56      | 126.23   |
| 21  | B     | 6004 | LMT  | O5'-C1'-C2' | -3.09 | 103.80      | 110.35   |
| 14  | B     | 1216 | CLA  | CMB-C2B-C3B | 3.09  | 130.47      | 124.68   |
| 14  | G     | 1119 | CLA  | C1-C2-C3    | -3.09 | 120.69      | 126.04   |
| 14  | a     | 1107 | CLA  | C3C-C4C-NC  | 3.09  | 114.04      | 110.57   |
| 14  | b     | 1220 | CLA  | CMA-C3A-C4A | 3.09  | 120.08      | 111.77   |
| 21  | b     | 6004 | LMT  | O5'-C1'-C2' | -3.09 | 103.80      | 110.35   |
| 14  | H     | 1212 | CLA  | O2A-CGA-CBA | 3.09  | 123.96      | 114.03   |
| 14  | H     | 1224 | CLA  | O1D-CGD-CBD | -3.09 | 118.16      | 124.48   |
| 14  | a     | 1115 | CLA  | CMC-C2C-C1C | 3.09  | 129.75      | 125.04   |
| 14  | H     | 1211 | CLA  | CAC-C3C-C4C | 3.09  | 128.82      | 124.81   |
| 14  | B     | 1210 | CLA  | C3C-C4C-NC  | 3.09  | 114.04      | 110.57   |
| 14  | G     | 1139 | CLA  | CMC-C2C-C1C | 3.09  | 129.74      | 125.04   |
| 14  | B     | 1239 | CLA  | O2D-CGD-O1D | -3.09 | 117.80      | 123.84   |
| 14  | T     | 1401 | CLA  | C3C-C4C-NC  | 3.09  | 114.03      | 110.57   |
| 14  | B     | 1214 | CLA  | C4A-NA-C1A  | 3.09  | 108.09      | 106.71   |
| 14  | b     | 1212 | CLA  | O2A-CGA-CBA | 3.09  | 123.95      | 114.03   |
| 14  | B     | 1213 | CLA  | CMC-C2C-C1C | 3.09  | 129.74      | 125.04   |
| 14  | b     | 1229 | CLA  | CAA-C2A-C3A | -3.09 | 104.33      | 112.78   |
| 14  | A     | 1139 | CLA  | CMC-C2C-C1C | 3.08  | 129.74      | 125.04   |
| 13  | a     | 1011 | CL0  | CMB-C2B-C3B | 3.08  | 130.45      | 124.68   |
| 14  | B     | 1212 | CLA  | O2A-CGA-CBA | 3.08  | 123.93      | 114.03   |
| 15  | G     | 1121 | F6C  | O2A-CGA-CBA | 3.08  | 123.93      | 114.03   |
| 14  | B     | 1220 | CLA  | CMA-C3A-C4A | 3.08  | 120.06      | 111.77   |
| 14  | k     | 1401 | CLA  | C3C-C4C-NC  | 3.08  | 114.03      | 110.57   |
| 14  | a     | 1118 | CLA  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 18  | R     | 4020 | BCR  | C38-C26-C25 | -3.08 | 121.07      | 124.53   |
| 14  | a     | 1139 | CLA  | CMC-C2C-C1C | 3.08  | 129.73      | 125.04   |
| 14  | A     | 1132 | CLA  | CMC-C2C-C1C | 3.08  | 129.73      | 125.04   |
| 15  | A     | 1121 | F6C  | O2A-CGA-CBA | 3.08  | 123.92      | 114.03   |
| 14  | K     | 1401 | CLA  | C3C-C4C-NC  | 3.08  | 114.02      | 110.57   |
| 14  | b     | 1210 | CLA  | C6-C5-C3    | -3.08 | 105.39      | 113.45   |
| 18  | a     | 4001 | BCR  | C33-C5-C6   | -3.08 | 121.07      | 124.53   |
| 15  | B     | 1230 | F6C  | C3D-C4D-ND  | 3.07  | 114.67      | 110.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | b     | 4004 | BCR  | C24-C23-C22 | -3.07 | 121.59      | 126.23   |
| 14  | H     | 1239 | CLA  | O2D-CGD-O1D | -3.07 | 117.83      | 123.84   |
| 14  | G     | 1104 | CLA  | CMC-C2C-C1C | 3.07  | 129.72      | 125.04   |
| 15  | B     | 1230 | F6C  | O2A-CGA-CBA | 3.07  | 123.90      | 114.03   |
| 14  | a     | 1132 | CLA  | CMC-C2C-C1C | 3.07  | 129.72      | 125.04   |
| 14  | A     | 1137 | CLA  | CAA-CBA-CGA | -3.07 | 104.28      | 113.25   |
| 15  | H     | 1230 | F6C  | O2A-CGA-CBA | 3.07  | 123.90      | 114.03   |
| 15  | b     | 1230 | F6C  | O2A-CGA-CBA | 3.07  | 123.90      | 114.03   |
| 14  | G     | 1130 | CLA  | CAA-C2A-C3A | -3.07 | 104.37      | 112.78   |
| 14  | b     | 1211 | CLA  | CAC-C3C-C4C | 3.07  | 128.79      | 124.81   |
| 14  | G     | 1137 | CLA  | CAA-CBA-CGA | -3.07 | 104.28      | 113.25   |
| 14  | B     | 1210 | CLA  | C6-C5-C3    | -3.07 | 105.41      | 113.45   |
| 15  | H     | 1230 | F6C  | CHB-C4A-C3A | -3.07 | 119.04      | 125.48   |
| 18  | a     | 4001 | BCR  | C24-C23-C22 | -3.07 | 121.60      | 126.23   |
| 15  | B     | 1230 | F6C  | CHB-C4A-C3A | -3.07 | 119.04      | 125.48   |
| 14  | G     | 1118 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 18  | B     | 4004 | BCR  | C24-C23-C22 | -3.07 | 121.60      | 126.23   |
| 14  | B     | 1224 | CLA  | O1D-CGD-CBD | -3.07 | 118.21      | 124.48   |
| 14  | A     | 1118 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 14  | B     | 1205 | CLA  | OBD-CAD-C3D | -3.07 | 121.14      | 128.52   |
| 14  | H     | 1205 | CLA  | OBD-CAD-C3D | -3.07 | 121.14      | 128.52   |
| 14  | A     | 1130 | CLA  | CAA-C2A-C3A | -3.06 | 104.39      | 112.78   |
| 15  | a     | 1121 | F6C  | O2A-CGA-CBA | 3.06  | 123.88      | 114.03   |
| 14  | b     | 1205 | CLA  | OBD-CAD-C3D | -3.06 | 121.15      | 128.52   |
| 14  | A     | 1128 | CLA  | C4-C3-C5    | 3.06  | 120.42      | 115.27   |
| 14  | H     | 1210 | CLA  | C6-C5-C3    | -3.06 | 105.42      | 113.45   |
| 14  | a     | 1134 | CLA  | O2A-CGA-CBA | 3.06  | 123.87      | 114.03   |
| 13  | A     | 1011 | CL0  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 15  | b     | 1230 | F6C  | CHB-C4A-C3A | -3.06 | 119.06      | 125.48   |
| 14  | a     | 1134 | CLA  | CMC-C2C-C1C | 3.06  | 129.70      | 125.04   |
| 14  | A     | 1115 | CLA  | CMC-C2C-C1C | 3.06  | 129.70      | 125.04   |
| 14  | a     | 1130 | CLA  | CAA-C2A-C3A | -3.06 | 104.41      | 112.78   |
| 14  | a     | 1137 | CLA  | CAA-CBA-CGA | -3.06 | 104.32      | 113.25   |
| 14  | B     | 1223 | CLA  | O2D-CGD-O1D | -3.06 | 117.86      | 123.84   |
| 14  | b     | 1226 | CLA  | CMB-C2B-C1B | -3.06 | 123.77      | 128.46   |
| 18  | H     | 4010 | BCR  | C34-C9-C8   | 3.06  | 122.89      | 118.08   |
| 14  | G     | 1132 | CLA  | CMC-C2C-C1C | 3.05  | 129.69      | 125.04   |
| 14  | H     | 1214 | CLA  | C4A-NA-C1A  | 3.05  | 108.08      | 106.71   |
| 14  | a     | 1128 | CLA  | C4-C3-C5    | 3.05  | 120.41      | 115.27   |
| 18  | G     | 4005 | BCR  | C35-C13-C12 | 3.05  | 122.89      | 118.08   |
| 14  | H     | 1217 | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 15  | G     | 1121 | F6C  | CMC-C2C-C3C | 3.05  | 130.69      | 124.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1134 | CLA  | O2A-CGA-CBA | 3.05  | 123.83      | 114.03   |
| 14  | H     | 1223 | CLA  | O2D-CGD-O1D | -3.05 | 117.88      | 123.84   |
| 13  | a     | 1011 | CL0  | C1-C2-C3    | -3.05 | 120.77      | 126.04   |
| 14  | A     | 1104 | CLA  | CMC-C2C-C1C | 3.05  | 129.68      | 125.04   |
| 14  | a     | 1104 | CLA  | CMC-C2C-C1C | 3.05  | 129.68      | 125.04   |
| 14  | A     | 1126 | CLA  | O1D-CGD-CBD | -3.05 | 118.25      | 124.48   |
| 18  | b     | 4010 | BCR  | C34-C9-C8   | 3.05  | 122.88      | 118.08   |
| 14  | B     | 1224 | CLA  | C3C-C4C-NC  | 3.05  | 113.99      | 110.57   |
| 14  | H     | 1204 | CLA  | C3D-C4D-ND  | 3.05  | 115.17      | 110.24   |
| 14  | G     | 1126 | CLA  | O1D-CGD-CBD | -3.04 | 118.25      | 124.48   |
| 14  | a     | 1127 | CLA  | C3C-C4C-NC  | 3.04  | 113.98      | 110.57   |
| 13  | G     | 1011 | CL0  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 14  | A     | 1134 | CLA  | O2A-CGA-CBA | 3.04  | 123.81      | 114.03   |
| 14  | b     | 1224 | CLA  | O1D-CGD-CBD | -3.04 | 118.26      | 124.48   |
| 15  | a     | 1121 | F6C  | CMC-C2C-C3C | 3.04  | 130.68      | 124.94   |
| 15  | b     | 1230 | F6C  | C3D-C4D-ND  | 3.04  | 114.62      | 110.17   |
| 18  | B     | 4010 | BCR  | C34-C9-C8   | 3.04  | 122.87      | 118.08   |
| 18  | G     | 4006 | BCR  | C30-C25-C24 | 3.04  | 124.38      | 115.78   |
| 14  | b     | 1217 | CLA  | O2D-CGD-O1D | -3.04 | 117.89      | 123.84   |
| 14  | a     | 1126 | CLA  | O1D-CGD-CBD | -3.04 | 118.26      | 124.48   |
| 14  | a     | 1138 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 14  | a     | 1111 | CLA  | CAA-C2A-C3A | -3.04 | 104.45      | 112.78   |
| 18  | A     | 4005 | BCR  | C35-C13-C12 | 3.04  | 122.87      | 118.08   |
| 14  | B     | 1217 | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 14  | H     | 1232 | CLA  | O2A-CGA-CBA | 3.04  | 123.79      | 114.03   |
| 14  | H     | 1215 | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 14  | b     | 1215 | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 14  | B     | 1232 | CLA  | O2A-CGA-CBA | 3.04  | 123.78      | 114.03   |
| 14  | b     | 1232 | CLA  | O2A-CGA-CBA | 3.04  | 123.78      | 114.03   |
| 15  | A     | 1121 | F6C  | CMC-C2C-C3C | 3.03  | 130.66      | 124.94   |
| 18  | A     | 4006 | BCR  | C30-C25-C24 | 3.03  | 124.36      | 115.78   |
| 14  | G     | 1134 | CLA  | CMC-C2C-C1C | 3.03  | 129.66      | 125.04   |
| 14  | A     | 1138 | CLA  | CMB-C2B-C3B | 3.03  | 130.35      | 124.68   |
| 14  | B     | 1226 | CLA  | CMB-C2B-C1B | -3.03 | 123.80      | 128.46   |
| 18  | a     | 4006 | BCR  | C30-C25-C24 | 3.03  | 124.36      | 115.78   |
| 14  | G     | 1128 | CLA  | C4-C3-C5    | 3.03  | 120.37      | 115.27   |
| 14  | A     | 1119 | CLA  | C1-O2A-CGA  | 3.03  | 124.40      | 116.44   |
| 14  | a     | 1115 | CLA  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 14  | A     | 1111 | CLA  | CAA-C2A-C3A | -3.03 | 104.47      | 112.78   |
| 14  | a     | 1119 | CLA  | C1-O2A-CGA  | 3.03  | 124.40      | 116.44   |
| 14  | b     | 1204 | CLA  | C3D-C4D-ND  | 3.03  | 115.14      | 110.24   |
| 14  | H     | 1204 | CLA  | C1-O2A-CGA  | 3.03  | 124.40      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | b     | 1219 | F6C  | C1-C2-C3    | -3.03 | 120.80      | 126.04   |
| 14  | G     | 1115 | CLA  | CMC-C2C-C1C | 3.03  | 129.66      | 125.04   |
| 14  | B     | 1239 | CLA  | CAC-C3C-C2C | 3.03  | 132.71      | 127.53   |
| 14  | b     | 1224 | CLA  | C3C-C4C-NC  | 3.03  | 113.97      | 110.57   |
| 16  | G     | 2001 | PQN  | C2M-C2-C3   | -3.03 | 119.46      | 124.40   |
| 13  | A     | 1011 | CL0  | C1-C2-C3    | -3.03 | 120.80      | 126.04   |
| 14  | b     | 1223 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | G     | 1119 | CLA  | C1-O2A-CGA  | 3.03  | 124.39      | 116.44   |
| 14  | H     | 1226 | CLA  | CMB-C2B-C1B | -3.03 | 123.81      | 128.46   |
| 13  | G     | 1011 | CL0  | C1-C2-C3    | -3.03 | 120.81      | 126.04   |
| 14  | A     | 1113 | CLA  | C3D-C4D-ND  | 3.03  | 115.14      | 110.24   |
| 14  | H     | 1239 | CLA  | CAC-C3C-C2C | 3.03  | 132.71      | 127.53   |
| 14  | b     | 1211 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | A     | 1134 | CLA  | CMC-C2C-C1C | 3.03  | 129.65      | 125.04   |
| 14  | B     | 1215 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 15  | B     | 1219 | F6C  | C1-C2-C3    | -3.03 | 120.81      | 126.04   |
| 14  | G     | 1140 | CLA  | C3C-C4C-NC  | 3.03  | 113.96      | 110.57   |
| 15  | b     | 1219 | F6C  | CMA-C3A-C4A | -3.03 | 119.38      | 124.71   |
| 15  | H     | 1219 | F6C  | C1-C2-C3    | -3.03 | 120.81      | 126.04   |
| 14  | B     | 1204 | CLA  | C3D-C4D-ND  | 3.02  | 115.13      | 110.24   |
| 14  | H     | 1211 | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 14  | b     | 1239 | CLA  | CAC-C3C-C2C | 3.02  | 132.70      | 127.53   |
| 14  | b     | 1204 | CLA  | C1-O2A-CGA  | 3.02  | 124.37      | 116.44   |
| 14  | G     | 1119 | CLA  | O2A-CGA-CBA | 3.02  | 121.39      | 111.91   |
| 14  | G     | 1111 | CLA  | CAA-C2A-C3A | -3.02 | 104.50      | 112.78   |
| 14  | G     | 1101 | CLA  | O2A-CGA-CBA | 3.02  | 123.74      | 114.03   |
| 14  | A     | 1115 | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 15  | B     | 1219 | F6C  | CMA-C3A-C4A | -3.02 | 119.39      | 124.71   |
| 14  | B     | 1211 | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 18  | B     | 4006 | BCR  | C33-C5-C6   | -3.02 | 121.14      | 124.53   |
| 14  | B     | 1204 | CLA  | C1-O2A-CGA  | 3.02  | 124.36      | 116.44   |
| 14  | a     | 1113 | CLA  | C3D-C4D-ND  | 3.02  | 115.12      | 110.24   |
| 14  | A     | 1101 | CLA  | O2A-CGA-CBA | 3.02  | 123.73      | 114.03   |
| 14  | G     | 1138 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 14  | G     | 1012 | CLA  | C4-C3-C5    | 3.02  | 120.35      | 115.27   |
| 18  | a     | 4005 | BCR  | C35-C13-C12 | 3.02  | 122.83      | 118.08   |
| 14  | G     | 1115 | CLA  | O2D-CGD-O1D | -3.01 | 117.94      | 123.84   |
| 14  | G     | 1113 | CLA  | C3D-C4D-ND  | 3.01  | 115.11      | 110.24   |
| 18  | A     | 4003 | BCR  | C3-C4-C5    | -3.01 | 108.69      | 114.08   |
| 14  | b     | 1233 | CLA  | CMA-C3A-C4A | 3.01  | 119.87      | 111.77   |
| 14  | G     | 1111 | CLA  | C3C-C4C-NC  | 3.01  | 113.95      | 110.57   |
| 18  | b     | 4006 | BCR  | C33-C5-C6   | -3.01 | 121.14      | 124.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1101 | CLA  | O2A-CGA-CBA | 3.01  | 123.71      | 114.03   |
| 15  | H     | 1219 | F6C  | CMA-C3A-C4A | -3.01 | 119.41      | 124.71   |
| 14  | A     | 1119 | CLA  | O2A-CGA-CBA | 3.01  | 121.36      | 111.91   |
| 14  | G     | 1127 | CLA  | C3C-C4C-NC  | 3.01  | 113.95      | 110.57   |
| 18  | A     | 4002 | BCR  | C37-C22-C21 | -3.01 | 118.71      | 122.92   |
| 14  | H     | 1233 | CLA  | CMA-C3A-C4A | 3.01  | 119.86      | 111.77   |
| 18  | G     | 4002 | BCR  | C36-C18-C17 | -3.01 | 118.71      | 122.92   |
| 18  | a     | 4003 | BCR  | C3-C4-C5    | -3.01 | 108.71      | 114.08   |
| 14  | B     | 1233 | CLA  | CMA-C3A-C4A | 3.01  | 119.85      | 111.77   |
| 18  | b     | 4005 | BCR  | C36-C18-C17 | -3.01 | 118.71      | 122.92   |
| 18  | b     | 4014 | BCR  | C33-C5-C4   | 3.01  | 119.39      | 113.62   |
| 18  | B     | 4014 | BCR  | C33-C5-C4   | 3.00  | 119.39      | 113.62   |
| 14  | a     | 1012 | CLA  | C4-C3-C5    | 3.00  | 120.32      | 115.27   |
| 18  | G     | 4002 | BCR  | C37-C22-C21 | -3.00 | 118.72      | 122.92   |
| 21  | a     | 6003 | LMT  | C3'-C4'-C5' | -3.00 | 104.04      | 110.93   |
| 14  | H     | 1232 | CLA  | CMA-C3A-C4A | 3.00  | 119.84      | 111.77   |
| 14  | H     | 1227 | CLA  | C3C-C4C-NC  | 3.00  | 113.94      | 110.57   |
| 14  | a     | 1111 | CLA  | C3C-C4C-NC  | 3.00  | 113.94      | 110.57   |
| 14  | a     | 1119 | CLA  | O2A-CGA-CBA | 3.00  | 121.32      | 111.91   |
| 14  | b     | 1232 | CLA  | CMA-C3A-C4A | 3.00  | 119.84      | 111.77   |
| 14  | A     | 1111 | CLA  | C3C-C4C-NC  | 3.00  | 113.94      | 110.57   |
| 14  | A     | 1012 | CLA  | C4-C3-C5    | 3.00  | 120.32      | 115.27   |
| 14  | A     | 1127 | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 14  | H     | 1224 | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 18  | H     | 4014 | BCR  | C33-C5-C4   | 3.00  | 119.37      | 113.62   |
| 18  | b     | 4005 | BCR  | C38-C26-C25 | -3.00 | 121.16      | 124.53   |
| 16  | a     | 2001 | PQN  | C2M-C2-C3   | -3.00 | 119.51      | 124.40   |
| 14  | A     | 1140 | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 16  | A     | 2001 | PQN  | C2M-C2-C3   | -2.99 | 119.51      | 124.40   |
| 18  | H     | 4006 | BCR  | C33-C5-C6   | -2.99 | 121.17      | 124.53   |
| 14  | B     | 1232 | CLA  | CMA-C3A-C4A | 2.99  | 119.82      | 111.77   |
| 21  | A     | 6003 | LMT  | C3'-C4'-C5' | -2.99 | 104.06      | 110.93   |
| 14  | G     | 1131 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | G     | 1012 | CLA  | CMC-C2C-C1C | 2.99  | 129.60      | 125.04   |
| 18  | G     | 4003 | BCR  | C3-C4-C5    | -2.99 | 108.73      | 114.08   |
| 14  | G     | 1113 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | a     | 1113 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 18  | B     | 4017 | BCR  | C24-C23-C22 | -2.99 | 121.71      | 126.23   |
| 14  | A     | 1113 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | a     | 1131 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | G     | 1141 | CLA  | CMA-C3A-C4A | 2.99  | 119.81      | 111.77   |
| 14  | A     | 1131 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | B     | 4005 | BCR  | C38-C26-C25 | -2.99 | 121.17      | 124.53   |
| 18  | b     | 4014 | BCR  | C36-C18-C17 | -2.99 | 118.74      | 122.92   |
| 14  | a     | 1133 | CLA  | CMB-C2B-C3B | 2.99  | 130.27      | 124.68   |
| 21  | G     | 6003 | LMT  | C3'-C4'-C5' | -2.99 | 104.08      | 110.93   |
| 14  | A     | 1141 | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 14  | a     | 1141 | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 14  | B     | 1221 | CLA  | C3C-C4C-NC  | 2.99  | 113.92      | 110.57   |
| 14  | B     | 1227 | CLA  | C3C-C4C-NC  | 2.98  | 113.92      | 110.57   |
| 14  | b     | 1239 | CLA  | C3C-C4C-NC  | 2.98  | 113.92      | 110.57   |
| 14  | H     | 1218 | CLA  | CMC-C2C-C1C | 2.98  | 129.58      | 125.04   |
| 14  | b     | 1227 | CLA  | O2A-CGA-CBA | 2.98  | 123.61      | 114.03   |
| 14  | A     | 1012 | CLA  | CMC-C2C-C1C | 2.98  | 129.58      | 125.04   |
| 20  | G     | 5003 | LMG  | O8-C28-C29  | 2.98  | 121.27      | 111.91   |
| 14  | H     | 1221 | CLA  | C3C-C4C-NC  | 2.98  | 113.91      | 110.57   |
| 14  | b     | 1218 | CLA  | CMC-C2C-C1C | 2.98  | 129.58      | 125.04   |
| 14  | a     | 1103 | CLA  | CHB-C4A-NA  | 2.98  | 128.63      | 124.51   |
| 20  | a     | 5003 | LMG  | O8-C28-C29  | 2.98  | 121.26      | 111.91   |
| 14  | a     | 1140 | CLA  | C3C-C4C-NC  | 2.98  | 113.91      | 110.57   |
| 20  | A     | 5003 | LMG  | O8-C28-C29  | 2.98  | 121.26      | 111.91   |
| 18  | H     | 4017 | BCR  | C24-C23-C22 | -2.98 | 121.73      | 126.23   |
| 14  | A     | 1133 | CLA  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 14  | B     | 1227 | CLA  | O2A-CGA-CBA | 2.98  | 123.60      | 114.03   |
| 18  | B     | 4005 | BCR  | C36-C18-C17 | -2.98 | 118.75      | 122.92   |
| 14  | a     | 1108 | CLA  | O2A-CGA-CBA | 2.98  | 123.59      | 114.03   |
| 14  | b     | 1229 | CLA  | O2D-CGD-O1D | -2.98 | 118.02      | 123.84   |
| 18  | H     | 4005 | BCR  | C38-C26-C25 | -2.98 | 121.19      | 124.53   |
| 21  | i     | 6001 | LMT  | C3'-C4'-C5' | -2.98 | 104.10      | 110.93   |
| 14  | a     | 1012 | CLA  | CMC-C2C-C1C | 2.97  | 129.57      | 125.04   |
| 18  | A     | 4002 | BCR  | C36-C18-C17 | -2.97 | 118.76      | 122.92   |
| 18  | a     | 4002 | BCR  | C37-C22-C21 | -2.97 | 118.76      | 122.92   |
| 14  | H     | 1227 | CLA  | O2A-CGA-CBA | 2.97  | 123.58      | 114.03   |
| 14  | A     | 1108 | CLA  | O2A-CGA-CBA | 2.97  | 123.58      | 114.03   |
| 14  | b     | 1217 | CLA  | C3C-C4C-NC  | 2.97  | 113.90      | 110.57   |
| 14  | G     | 1133 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 14  | B     | 1229 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 14  | H     | 1229 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 21  | R     | 6001 | LMT  | C3'-C4'-C5' | -2.97 | 104.12      | 110.93   |
| 14  | A     | 1120 | CLA  | CMC-C2C-C1C | 2.97  | 129.56      | 125.04   |
| 14  | B     | 1218 | CLA  | CMC-C2C-C1C | 2.97  | 129.56      | 125.04   |
| 14  | G     | 1103 | CLA  | CAA-C2A-C3A | -2.97 | 104.65      | 112.78   |
| 14  | G     | 1120 | CLA  | CMC-C2C-C1C | 2.97  | 129.56      | 125.04   |
| 21  | I     | 6001 | LMT  | C3'-C4'-C5' | -2.97 | 104.13      | 110.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1118 | CLA  | C3C-C4C-NC  | 2.97  | 113.90      | 110.57   |
| 14  | V     | 1501 | CLA  | C4D-C3D-CAD | 2.97  | 111.59      | 108.10   |
| 18  | a     | 4002 | BCR  | C36-C18-C17 | -2.96 | 118.77      | 122.92   |
| 14  | a     | 1103 | CLA  | CAA-C2A-C3A | -2.96 | 104.66      | 112.78   |
| 14  | b     | 1225 | CLA  | C3C-C4C-NC  | 2.96  | 113.89      | 110.57   |
| 18  | b     | 4017 | BCR  | C24-C23-C22 | -2.96 | 121.76      | 126.23   |
| 14  | G     | 1103 | CLA  | CHB-C4A-NA  | 2.96  | 128.61      | 124.51   |
| 18  | H     | 4005 | BCR  | C36-C18-C17 | -2.96 | 118.78      | 122.92   |
| 18  | G     | 4005 | BCR  | C34-C9-C8   | 2.96  | 122.74      | 118.08   |
| 14  | a     | 1120 | CLA  | CMC-C2C-C1C | 2.96  | 129.55      | 125.04   |
| 14  | H     | 1217 | CLA  | C3C-C4C-NC  | 2.96  | 113.89      | 110.57   |
| 14  | G     | 1134 | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 14  | G     | 1108 | CLA  | O2A-CGA-CBA | 2.96  | 123.53      | 114.03   |
| 15  | b     | 1237 | F6C  | C3D-C4D-ND  | 2.96  | 114.49      | 110.17   |
| 18  | A     | 4005 | BCR  | C34-C9-C8   | 2.95  | 122.73      | 118.08   |
| 14  | b     | 1221 | CLA  | C3C-C4C-NC  | 2.95  | 113.88      | 110.57   |
| 14  | B     | 1202 | CLA  | CHB-C4A-NA  | 2.95  | 128.60      | 124.51   |
| 14  | a     | 1134 | CLA  | O2D-CGD-O1D | -2.95 | 118.06      | 123.84   |
| 14  | A     | 1103 | CLA  | CAA-C2A-C3A | -2.95 | 104.69      | 112.78   |
| 14  | a     | 1123 | CLA  | C1-C2-C3    | -2.95 | 120.94      | 126.04   |
| 14  | b     | 1239 | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 15  | B     | 1237 | F6C  | C3D-C4D-ND  | 2.95  | 114.48      | 110.17   |
| 18  | B     | 4014 | BCR  | C36-C18-C17 | -2.95 | 118.79      | 122.92   |
| 18  | H     | 4014 | BCR  | C36-C18-C17 | -2.95 | 118.79      | 122.92   |
| 14  | B     | 1239 | CLA  | C3C-C4C-NC  | 2.95  | 113.88      | 110.57   |
| 14  | G     | 1118 | CLA  | O2D-CGD-O1D | -2.95 | 118.07      | 123.84   |
| 14  | G     | 1106 | CLA  | C1-C2-C3    | -2.95 | 120.94      | 126.04   |
| 14  | A     | 1134 | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 14  | A     | 1103 | CLA  | CHB-C4A-NA  | 2.95  | 128.59      | 124.51   |
| 18  | a     | 4002 | BCR  | C28-C27-C26 | -2.95 | 108.82      | 114.08   |
| 14  | G     | 1101 | CLA  | C3C-C4C-NC  | 2.95  | 113.87      | 110.57   |
| 14  | M     | 1501 | CLA  | C4D-C3D-CAD | 2.94  | 111.57      | 108.10   |
| 14  | H     | 1216 | CLA  | CAA-C2A-C3A | -2.94 | 104.71      | 112.78   |
| 14  | a     | 1106 | CLA  | C1-C2-C3    | -2.94 | 120.95      | 126.04   |
| 14  | G     | 1123 | CLA  | C1-C2-C3    | -2.94 | 120.95      | 126.04   |
| 14  | A     | 1117 | CLA  | C1-C2-C3    | -2.94 | 120.95      | 126.04   |
| 14  | G     | 1117 | CLA  | C1-C2-C3    | -2.94 | 120.95      | 126.04   |
| 14  | a     | 1109 | CLA  | CMA-C3A-C4A | 2.94  | 119.68      | 111.77   |
| 18  | A     | 4002 | BCR  | C28-C27-C26 | -2.94 | 108.83      | 114.08   |
| 14  | A     | 1106 | CLA  | C1-C2-C3    | -2.94 | 120.96      | 126.04   |
| 14  | A     | 1125 | CLA  | CAA-C2A-C3A | -2.94 | 104.73      | 112.78   |
| 14  | a     | 1118 | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | R     | 4020 | BCR  | C34-C9-C8   | 2.94  | 122.71      | 118.08   |
| 14  | A     | 1118 | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 14  | B     | 1239 | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 18  | a     | 4005 | BCR  | C34-C9-C8   | 2.94  | 122.70      | 118.08   |
| 14  | b     | 1227 | CLA  | C3C-C4C-NC  | 2.93  | 113.86      | 110.57   |
| 14  | a     | 1106 | CLA  | CMC-C2C-C1C | 2.93  | 129.51      | 125.04   |
| 15  | B     | 1238 | F6C  | C3D-C4D-ND  | 2.93  | 114.46      | 110.17   |
| 14  | A     | 1109 | CLA  | CMA-C3A-C4A | 2.93  | 119.66      | 111.77   |
| 14  | b     | 1216 | CLA  | CAA-C2A-C3A | -2.93 | 104.75      | 112.78   |
| 14  | b     | 1209 | CLA  | O2A-CGA-CBA | 2.93  | 123.45      | 114.03   |
| 14  | a     | 1125 | CLA  | CAA-C2A-C3A | -2.93 | 104.75      | 112.78   |
| 14  | H     | 1234 | CLA  | C1-O2A-CGA  | 2.93  | 124.13      | 116.44   |
| 14  | G     | 1132 | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 14  | B     | 1216 | CLA  | CAA-C2A-C3A | -2.93 | 104.75      | 112.78   |
| 14  | B     | 1234 | CLA  | C1-O2A-CGA  | 2.93  | 124.13      | 116.44   |
| 15  | H     | 1237 | F6C  | C3D-C4D-ND  | 2.93  | 114.45      | 110.17   |
| 14  | a     | 1129 | CLA  | C3C-C4C-NC  | 2.93  | 113.86      | 110.57   |
| 14  | H     | 1239 | CLA  | C3C-C4C-NC  | 2.93  | 113.85      | 110.57   |
| 14  | A     | 1123 | CLA  | C1-C2-C3    | -2.93 | 120.98      | 126.04   |
| 14  | B     | 1221 | CLA  | CMC-C2C-C1C | 2.93  | 129.50      | 125.04   |
| 15  | a     | 1121 | F6C  | CHD-C1D-ND  | -2.93 | 119.76      | 124.20   |
| 14  | A     | 1106 | CLA  | CMC-C2C-C1C | 2.93  | 129.49      | 125.04   |
| 14  | G     | 1106 | CLA  | CMC-C2C-C1C | 2.93  | 129.49      | 125.04   |
| 14  | b     | 1216 | CLA  | C1-O2A-CGA  | 2.92  | 124.12      | 116.44   |
| 14  | B     | 1217 | CLA  | C3C-C4C-NC  | 2.92  | 113.85      | 110.57   |
| 18  | I     | 4020 | BCR  | C34-C9-C8   | 2.92  | 122.69      | 118.08   |
| 14  | B     | 1209 | CLA  | O2A-CGA-CBA | 2.92  | 123.42      | 114.03   |
| 14  | G     | 1125 | CLA  | CAA-C2A-C3A | -2.92 | 104.77      | 112.78   |
| 14  | A     | 1118 | CLA  | C3C-C4C-NC  | 2.92  | 113.85      | 110.57   |
| 15  | b     | 1238 | F6C  | C3D-C4D-ND  | 2.92  | 114.44      | 110.17   |
| 14  | b     | 1234 | CLA  | C1-O2A-CGA  | 2.92  | 124.11      | 116.44   |
| 14  | A     | 1129 | CLA  | C3C-C4C-NC  | 2.92  | 113.85      | 110.57   |
| 14  | H     | 1202 | CLA  | CHB-C4A-NA  | 2.92  | 128.55      | 124.51   |
| 14  | B     | 1216 | CLA  | C1-O2A-CGA  | 2.92  | 124.11      | 116.44   |
| 14  | H     | 1221 | CLA  | CMC-C2C-C1C | 2.92  | 129.49      | 125.04   |
| 14  | G     | 1124 | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 14  | a     | 1101 | CLA  | C3C-C4C-NC  | 2.92  | 113.85      | 110.57   |
| 14  | H     | 1226 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.33   |
| 14  | A     | 1132 | CLA  | CMB-C2B-C3B | 2.92  | 130.14      | 124.68   |
| 14  | H     | 1205 | CLA  | CAA-C2A-C3A | -2.92 | 104.79      | 112.78   |
| 14  | B     | 1210 | CLA  | CMC-C2C-C1C | 2.92  | 129.48      | 125.04   |
| 14  | A     | 1124 | CLA  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1223 | CLA  | OBD-CAD-C3D | -2.92 | 121.50      | 128.52   |
| 14  | B     | 1225 | CLA  | C3C-C4C-NC  | 2.92  | 113.84      | 110.57   |
| 15  | b     | 1207 | F6C  | CMC-C2C-C3C | 2.92  | 130.44      | 124.94   |
| 14  | b     | 1221 | CLA  | CMC-C2C-C1C | 2.91  | 129.48      | 125.04   |
| 14  | B     | 1205 | CLA  | CAA-C2A-C3A | -2.91 | 104.80      | 112.78   |
| 14  | b     | 1202 | CLA  | CHB-C4A-NA  | 2.91  | 128.54      | 124.51   |
| 18  | G     | 4002 | BCR  | C28-C27-C26 | -2.91 | 108.87      | 114.08   |
| 14  | H     | 1216 | CLA  | C1-O2A-CGA  | 2.91  | 124.09      | 116.44   |
| 14  | B     | 1223 | CLA  | OBD-CAD-C3D | -2.91 | 121.51      | 128.52   |
| 14  | a     | 1117 | CLA  | C1-C2-C3    | -2.91 | 121.00      | 126.04   |
| 15  | A     | 1121 | F6C  | CHD-C1D-ND  | -2.91 | 119.78      | 124.20   |
| 15  | a     | 1121 | F6C  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 15  | B     | 1207 | F6C  | CMC-C2C-C3C | 2.91  | 130.43      | 124.94   |
| 15  | H     | 1207 | F6C  | CMC-C2C-C3C | 2.91  | 130.43      | 124.94   |
| 14  | L     | 1502 | CLA  | C3D-C4D-ND  | 2.91  | 114.95      | 110.24   |
| 14  | H     | 1209 | CLA  | O2A-CGA-CBA | 2.91  | 123.39      | 114.03   |
| 15  | H     | 1237 | F6C  | C4-C3-C5    | 2.91  | 120.17      | 115.27   |
| 14  | G     | 1109 | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 14  | b     | 1205 | CLA  | CAA-C2A-C3A | -2.91 | 104.81      | 112.78   |
| 15  | b     | 1230 | F6C  | CHD-C1D-ND  | -2.91 | 119.79      | 124.20   |
| 14  | H     | 1222 | CLA  | CAA-C2A-C3A | -2.91 | 104.81      | 112.78   |
| 14  | m     | 1501 | CLA  | C4D-C3D-CAD | 2.91  | 111.52      | 108.10   |
| 14  | H     | 1239 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 14  | A     | 1135 | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 14  | G     | 1135 | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 15  | G     | 1121 | F6C  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 14  | a     | 1118 | CLA  | C3C-C4C-NC  | 2.91  | 113.83      | 110.57   |
| 18  | i     | 4020 | BCR  | C34-C9-C8   | 2.90  | 122.65      | 118.08   |
| 14  | G     | 1129 | CLA  | C3C-C4C-NC  | 2.90  | 113.83      | 110.57   |
| 14  | a     | 1132 | CLA  | CMB-C2B-C3B | 2.90  | 130.11      | 124.68   |
| 14  | A     | 1101 | CLA  | C3C-C4C-NC  | 2.90  | 113.83      | 110.57   |
| 14  | a     | 1124 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 15  | G     | 1121 | F6C  | CHD-C1D-ND  | -2.90 | 119.80      | 124.20   |
| 14  | H     | 1223 | CLA  | OBD-CAD-C3D | -2.90 | 121.54      | 128.52   |
| 15  | A     | 1121 | F6C  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 14  | b     | 1222 | CLA  | CAA-C2A-C3A | -2.90 | 104.84      | 112.78   |
| 14  | H     | 1211 | CLA  | C3C-C4C-NC  | 2.90  | 113.82      | 110.57   |
| 14  | B     | 1222 | CLA  | CAA-C2A-C3A | -2.90 | 104.84      | 112.78   |
| 14  | G     | 1134 | CLA  | C3C-C4C-NC  | 2.90  | 113.82      | 110.57   |
| 14  | H     | 1225 | CLA  | C3C-C4C-NC  | 2.90  | 113.82      | 110.57   |
| 14  | U     | 1502 | CLA  | C3D-C4D-ND  | 2.90  | 114.92      | 110.24   |
| 14  | a     | 1135 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1230 | F6C  | CHD-C1D-ND  | -2.89 | 119.81      | 124.20   |
| 15  | b     | 1237 | F6C  | C4-C3-C5    | 2.89  | 120.14      | 115.27   |
| 15  | H     | 1238 | F6C  | C3D-C4D-ND  | 2.89  | 114.40      | 110.17   |
| 18  | a     | 4006 | BCR  | C33-C5-C4   | 2.89  | 119.17      | 113.62   |
| 14  | b     | 1210 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 15  | B     | 1237 | F6C  | C4-C3-C5    | 2.89  | 120.14      | 115.27   |
| 14  | B     | 1211 | CLA  | C3C-C4C-NC  | 2.89  | 113.81      | 110.57   |
| 14  | G     | 1107 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 15  | a     | 1121 | F6C  | C3D-C4D-ND  | 2.88  | 114.39      | 110.17   |
| 18  | G     | 4004 | BCR  | C38-C26-C27 | 2.88  | 119.16      | 113.62   |
| 18  | V     | 4021 | BCR  | C37-C22-C21 | -2.88 | 118.89      | 122.92   |
| 14  | A     | 1139 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 18  | A     | 4006 | BCR  | C33-C5-C4   | 2.88  | 119.15      | 113.62   |
| 14  | a     | 1139 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 15  | A     | 1121 | F6C  | C3D-C4D-ND  | 2.88  | 114.38      | 110.17   |
| 14  | l     | 1502 | CLA  | C3D-C4D-ND  | 2.88  | 114.90      | 110.24   |
| 18  | H     | 4004 | BCR  | C2-C1-C6    | 2.88  | 114.92      | 110.48   |
| 14  | H     | 1210 | CLA  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 14  | a     | 1107 | CLA  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 15  | G     | 1121 | F6C  | C3D-C4D-ND  | 2.88  | 114.38      | 110.17   |
| 18  | A     | 4005 | BCR  | C7-C8-C9    | -2.88 | 121.89      | 126.23   |
| 18  | G     | 4006 | BCR  | C33-C5-C4   | 2.88  | 119.15      | 113.62   |
| 14  | H     | 1023 | CLA  | CHD-C4C-NC  | -2.88 | 119.67      | 124.20   |
| 14  | A     | 1134 | CLA  | CMA-C3A-C4A | 2.88  | 119.51      | 111.77   |
| 14  | a     | 1118 | CLA  | CAA-C2A-C3A | -2.88 | 104.90      | 112.78   |
| 18  | m     | 4021 | BCR  | C37-C22-C21 | -2.88 | 118.89      | 122.92   |
| 14  | b     | 1023 | CLA  | C1C-C2C-C3C | -2.88 | 103.93      | 106.96   |
| 14  | a     | 1013 | CLA  | C3C-C4C-NC  | 2.88  | 113.80      | 110.57   |
| 14  | H     | 1201 | CLA  | C3C-C4C-NC  | 2.88  | 113.80      | 110.57   |
| 14  | G     | 1134 | CLA  | CMA-C3A-C4A | 2.87  | 119.50      | 111.77   |
| 21  | b     | 6003 | LMT  | O5B-C1B-C2B | 2.87  | 116.43      | 110.35   |
| 15  | G     | 1121 | F6C  | CHB-C4A-C3A | -2.87 | 119.45      | 125.48   |
| 14  | G     | 1139 | CLA  | CMB-C2B-C3B | 2.87  | 130.06      | 124.68   |
| 18  | l     | 4022 | BCR  | C1-C6-C5    | -2.87 | 118.56      | 122.61   |
| 18  | M     | 4021 | BCR  | C37-C22-C21 | -2.87 | 118.90      | 122.92   |
| 14  | A     | 1134 | CLA  | C3C-C4C-NC  | 2.87  | 113.79      | 110.57   |
| 14  | a     | 1105 | CLA  | CAA-C2A-C3A | -2.87 | 104.91      | 112.78   |
| 21  | B     | 6003 | LMT  | O5B-C1B-C2B | 2.87  | 116.43      | 110.35   |
| 18  | B     | 4004 | BCR  | C2-C1-C6    | 2.87  | 114.90      | 110.48   |
| 15  | a     | 1121 | F6C  | CHB-C4A-C3A | -2.87 | 119.46      | 125.48   |
| 21  | H     | 6003 | LMT  | O5B-C1B-C2B | 2.87  | 116.42      | 110.35   |
| 14  | b     | 1201 | CLA  | C3C-C4C-NC  | 2.87  | 113.79      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1226 | CLA  | C1D-ND-C4D  | -2.87 | 104.30      | 106.33   |
| 14  | A     | 1107 | CLA  | CMC-C2C-C1C | 2.87  | 129.41      | 125.04   |
| 14  | b     | 1211 | CLA  | C3C-C4C-NC  | 2.87  | 113.79      | 110.57   |
| 18  | A     | 4004 | BCR  | C38-C26-C27 | 2.87  | 119.13      | 113.62   |
| 18  | U     | 4022 | BCR  | C1-C6-C5    | -2.87 | 118.58      | 122.61   |
| 14  | B     | 1023 | CLA  | CHD-C4C-NC  | -2.87 | 119.69      | 124.20   |
| 14  | G     | 1013 | CLA  | C3C-C4C-NC  | 2.87  | 113.78      | 110.57   |
| 14  | G     | 1105 | CLA  | CAA-C2A-C3A | -2.87 | 104.93      | 112.78   |
| 18  | b     | 4004 | BCR  | C2-C1-C6    | 2.87  | 114.89      | 110.48   |
| 14  | B     | 1236 | CLA  | CMC-C2C-C1C | 2.86  | 129.40      | 125.04   |
| 14  | G     | 1118 | CLA  | CAA-C2A-C3A | -2.86 | 104.93      | 112.78   |
| 14  | A     | 1108 | CLA  | C3C-C4C-NC  | 2.86  | 113.78      | 110.57   |
| 15  | A     | 1121 | F6C  | CHB-C4A-C3A | -2.86 | 119.47      | 125.48   |
| 14  | k     | 1401 | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 14  | A     | 1118 | CLA  | CAA-C2A-C3A | -2.86 | 104.94      | 112.78   |
| 15  | b     | 1219 | F6C  | CHA-C1A-C2A | -2.86 | 122.08      | 129.84   |
| 14  | A     | 1105 | CLA  | CAA-C2A-C3A | -2.86 | 104.94      | 112.78   |
| 14  | H     | 1236 | CLA  | CMC-C2C-C1C | 2.86  | 129.40      | 125.04   |
| 14  | a     | 1108 | CLA  | C3C-C4C-NC  | 2.86  | 113.78      | 110.57   |
| 14  | b     | 1239 | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 18  | G     | 4005 | BCR  | C7-C8-C9    | -2.86 | 121.91      | 126.23   |
| 18  | L     | 4022 | BCR  | C1-C6-C5    | -2.86 | 118.58      | 122.61   |
| 14  | H     | 1213 | CLA  | O2A-CGA-CBA | 2.86  | 123.22      | 114.03   |
| 14  | G     | 1136 | CLA  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |
| 18  | a     | 4005 | BCR  | C7-C8-C9    | -2.86 | 121.91      | 126.23   |
| 14  | a     | 1134 | CLA  | CMA-C3A-C4A | 2.86  | 119.46      | 111.77   |
| 18  | a     | 4004 | BCR  | C38-C26-C27 | 2.86  | 119.11      | 113.62   |
| 15  | B     | 1219 | F6C  | CHA-C1A-C2A | -2.86 | 122.09      | 129.84   |
| 14  | B     | 1213 | CLA  | O2A-CGA-CBA | 2.86  | 123.21      | 114.03   |
| 14  | A     | 1013 | CLA  | C3C-C4C-NC  | 2.86  | 113.78      | 110.57   |
| 14  | H     | 1229 | CLA  | CMC-C2C-C1C | 2.86  | 129.39      | 125.04   |
| 14  | B     | 1023 | CLA  | C1C-C2C-C3C | -2.86 | 103.95      | 106.96   |
| 14  | G     | 1013 | CLA  | C1-C2-C3    | -2.86 | 121.10      | 126.04   |
| 14  | V     | 1501 | CLA  | CAA-C2A-C3A | -2.86 | 104.95      | 112.78   |
| 14  | B     | 1239 | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 14  | B     | 1201 | CLA  | C3C-C4C-NC  | 2.86  | 113.77      | 110.57   |
| 14  | a     | 1119 | CLA  | C3C-C4C-NC  | 2.86  | 113.77      | 110.57   |
| 14  | A     | 1136 | CLA  | CMB-C2B-C3B | 2.85  | 130.02      | 124.68   |
| 14  | m     | 1501 | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |
| 14  | G     | 1108 | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |
| 14  | G     | 1133 | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |
| 14  | V     | 1501 | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | H     | 1219 | F6C  | CHA-C1A-C2A | -2.85 | 122.11      | 129.84   |
| 14  | b     | 1023 | CLA  | CAC-C3C-C2C | -2.85 | 122.66      | 127.53   |
| 14  | K     | 1401 | CLA  | CMA-C3A-C4A | 2.85  | 119.43      | 111.77   |
| 14  | b     | 1228 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 14  | b     | 1213 | CLA  | O2A-CGA-CBA | 2.85  | 123.18      | 114.03   |
| 14  | H     | 1023 | CLA  | C1C-C2C-C3C | -2.85 | 103.96      | 106.96   |
| 14  | m     | 1501 | CLA  | CAA-C2A-C3A | -2.85 | 104.98      | 112.78   |
| 14  | M     | 1501 | CLA  | CAA-C2A-C3A | -2.85 | 104.98      | 112.78   |
| 14  | B     | 1229 | CLA  | CMC-C2C-C1C | 2.85  | 129.38      | 125.04   |
| 14  | b     | 1236 | CLA  | CMC-C2C-C1C | 2.85  | 129.38      | 125.04   |
| 14  | a     | 1134 | CLA  | C3C-C4C-NC  | 2.85  | 113.76      | 110.57   |
| 14  | a     | 1013 | CLA  | C1-C2-C3    | -2.85 | 121.12      | 126.04   |
| 15  | H     | 1230 | F6C  | CHD-C1D-ND  | -2.85 | 119.88      | 124.20   |
| 14  | T     | 1401 | CLA  | CMA-C3A-C4A | 2.85  | 119.42      | 111.77   |
| 14  | H     | 1239 | CLA  | C4-C3-C5    | 2.85  | 120.06      | 115.27   |
| 14  | A     | 1133 | CLA  | C3C-C4C-NC  | 2.85  | 113.76      | 110.57   |
| 18  | b     | 4009 | BCR  | C33-C5-C4   | 2.84  | 119.08      | 113.62   |
| 14  | B     | 1021 | CLA  | O2A-CGA-CBA | 2.84  | 120.83      | 111.91   |
| 18  | a     | 4004 | BCR  | C37-C22-C21 | -2.84 | 118.94      | 122.92   |
| 14  | G     | 1120 | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 14  | b     | 1023 | CLA  | CHD-C4C-NC  | -2.84 | 119.73      | 124.20   |
| 14  | a     | 1114 | CLA  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 15  | b     | 1238 | F6C  | CHB-C4A-C3A | -2.84 | 119.52      | 125.48   |
| 14  | B     | 1228 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 14  | H     | 1021 | CLA  | O2A-CGA-CBA | 2.84  | 120.81      | 111.91   |
| 18  | a     | 4003 | BCR  | C37-C22-C23 | 2.84  | 122.55      | 118.08   |
| 14  | H     | 1215 | CLA  | C4-C3-C5    | 2.84  | 120.04      | 115.27   |
| 14  | l     | 1501 | CLA  | O2A-C1-C2   | 2.84  | 116.09      | 108.64   |
| 14  | B     | 1215 | CLA  | C4-C3-C5    | 2.84  | 120.04      | 115.27   |
| 14  | a     | 1136 | CLA  | CMB-C2B-C3B | 2.83  | 129.98      | 124.68   |
| 14  | a     | 1111 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | H     | 1228 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | a     | 1103 | CLA  | CMD-C2D-C3D | -2.83 | 121.10      | 127.61   |
| 14  | A     | 1109 | CLA  | CMB-C2B-C3B | 2.83  | 129.98      | 124.68   |
| 14  | b     | 1215 | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 14  | b     | 1021 | CLA  | O2A-CGA-CBA | 2.83  | 120.79      | 111.91   |
| 19  | A     | 5001 | LHG  | O8-C23-C24  | 2.83  | 120.79      | 111.91   |
| 14  | A     | 1114 | CLA  | CMB-C2B-C3B | 2.83  | 129.97      | 124.68   |
| 14  | G     | 1141 | CLA  | C3C-C4C-NC  | 2.83  | 113.75      | 110.57   |
| 18  | B     | 4009 | BCR  | C33-C5-C4   | 2.83  | 119.05      | 113.62   |
| 14  | B     | 1023 | CLA  | CAC-C3C-C2C | -2.83 | 122.69      | 127.53   |
| 19  | G     | 5001 | LHG  | O8-C23-C24  | 2.83  | 120.78      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | H     | 1237 | F6C  | CHB-C4A-C3A | -2.83 | 119.55      | 125.48   |
| 14  | M     | 1501 | CLA  | C3C-C4C-NC  | 2.83  | 113.74      | 110.57   |
| 18  | A     | 4003 | BCR  | C37-C22-C23 | 2.83  | 122.53      | 118.08   |
| 14  | b     | 1229 | CLA  | CMC-C2C-C1C | 2.83  | 129.34      | 125.04   |
| 14  | A     | 1013 | CLA  | C4-C3-C5    | 2.83  | 120.02      | 115.27   |
| 14  | U     | 1501 | CLA  | C3D-C4D-ND  | 2.83  | 114.81      | 110.24   |
| 14  | U     | 1501 | CLA  | O2A-C1-C2   | 2.83  | 116.06      | 108.64   |
| 19  | a     | 5001 | LHG  | O8-C23-C24  | 2.82  | 120.77      | 111.91   |
| 14  | a     | 1141 | CLA  | C3C-C4C-NC  | 2.82  | 113.74      | 110.57   |
| 18  | T     | 4001 | BCR  | C33-C5-C6   | -2.82 | 121.36      | 124.53   |
| 18  | G     | 4004 | BCR  | C37-C22-C21 | -2.82 | 118.97      | 122.92   |
| 14  | a     | 1103 | CLA  | C4-C3-C5    | 2.82  | 120.02      | 115.27   |
| 15  | B     | 1237 | F6C  | CHB-C4A-C3A | -2.82 | 119.56      | 125.48   |
| 18  | k     | 4001 | BCR  | C33-C5-C6   | -2.82 | 121.36      | 124.53   |
| 14  | A     | 1013 | CLA  | C1-C2-C3    | -2.82 | 121.16      | 126.04   |
| 14  | A     | 1119 | CLA  | C3C-C4C-NC  | 2.82  | 113.74      | 110.57   |
| 14  | A     | 1141 | CLA  | C3C-C4C-NC  | 2.82  | 113.74      | 110.57   |
| 14  | L     | 1501 | CLA  | O2A-C1-C2   | 2.82  | 116.05      | 108.64   |
| 15  | B     | 1238 | F6C  | CHB-C4A-C3A | -2.82 | 119.56      | 125.48   |
| 14  | A     | 1120 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 18  | i     | 4020 | BCR  | C23-C24-C25 | -2.82 | 119.28      | 127.20   |
| 14  | a     | 1109 | CLA  | CMB-C2B-C3B | 2.82  | 129.96      | 124.68   |
| 14  | B     | 1202 | CLA  | C4D-C3D-CAD | 2.82  | 111.42      | 108.10   |
| 14  | B     | 1214 | CLA  | OBD-CAD-C3D | -2.82 | 121.73      | 128.52   |
| 18  | a     | 4005 | BCR  | C36-C18-C17 | -2.82 | 118.97      | 122.92   |
| 14  | H     | 1234 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 14  | G     | 1013 | CLA  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 14  | G     | 1114 | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 20  | H     | 5002 | LMG  | O1-C1-C2    | 2.82  | 112.70      | 108.30   |
| 14  | G     | 1109 | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 14  | A     | 1104 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 14  | G     | 1103 | CLA  | CMD-C2D-C3D | -2.82 | 121.14      | 127.61   |
| 18  | i     | 4020 | BCR  | C37-C22-C23 | 2.82  | 122.51      | 118.08   |
| 14  | G     | 1128 | CLA  | C1-C2-C3    | -2.82 | 121.17      | 126.04   |
| 18  | I     | 4020 | BCR  | C23-C24-C25 | -2.82 | 119.29      | 127.20   |
| 14  | A     | 1111 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 18  | H     | 4009 | BCR  | C33-C5-C4   | 2.81  | 119.02      | 113.62   |
| 14  | a     | 1104 | CLA  | O2D-CGD-O1D | -2.81 | 118.33      | 123.84   |
| 14  | H     | 1023 | CLA  | CAC-C3C-C2C | -2.81 | 122.72      | 127.53   |
| 14  | a     | 1112 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 15  | H     | 1238 | F6C  | CHB-C4A-C3A | -2.81 | 119.58      | 125.48   |
| 14  | B     | 1234 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1127 | CLA  | CMC-C2C-C1C | 2.81  | 129.32      | 125.04   |
| 14  | L     | 1501 | CLA  | C3D-C4D-ND  | 2.81  | 114.78      | 110.24   |
| 14  | V     | 1501 | CLA  | CMC-C2C-C1C | 2.81  | 129.32      | 125.04   |
| 18  | A     | 4004 | BCR  | C37-C22-C21 | -2.81 | 118.99      | 122.92   |
| 15  | b     | 1237 | F6C  | CHB-C4A-C3A | -2.81 | 119.59      | 125.48   |
| 18  | G     | 4005 | BCR  | C36-C18-C17 | -2.81 | 118.99      | 122.92   |
| 14  | H     | 1202 | CLA  | C4D-C3D-CAD | 2.81  | 111.41      | 108.10   |
| 14  | b     | 1226 | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.33   |
| 14  | H     | 1214 | CLA  | OBD-CAD-C3D | -2.81 | 121.76      | 128.52   |
| 14  | A     | 1103 | CLA  | CMD-C2D-C3D | -2.81 | 121.16      | 127.61   |
| 14  | A     | 1103 | CLA  | C4-C3-C5    | 2.81  | 119.99      | 115.27   |
| 14  | b     | 1213 | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.81   |
| 14  | a     | 1120 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 14  | G     | 1103 | CLA  | C4-C3-C5    | 2.81  | 119.99      | 115.27   |
| 14  | G     | 1119 | CLA  | C3C-C4C-NC  | 2.81  | 113.72      | 110.57   |
| 14  | b     | 1232 | CLA  | C4D-C3D-CAD | 2.80  | 111.40      | 108.10   |
| 14  | b     | 1213 | CLA  | O2D-CGD-O1D | -2.80 | 118.35      | 123.84   |
| 18  | R     | 4020 | BCR  | C23-C24-C25 | -2.80 | 119.33      | 127.20   |
| 14  | A     | 1127 | CLA  | CMC-C2C-C1C | 2.80  | 129.31      | 125.04   |
| 14  | G     | 1012 | CLA  | C1-C2-C3    | -2.80 | 121.19      | 126.04   |
| 18  | A     | 4005 | BCR  | C36-C18-C17 | -2.80 | 119.00      | 122.92   |
| 14  | M     | 1501 | CLA  | CMC-C2C-C1C | 2.80  | 129.31      | 125.04   |
| 14  | H     | 1021 | CLA  | CMA-C3A-C2A | -2.80 | 102.52      | 113.83   |
| 18  | K     | 4001 | BCR  | C33-C5-C6   | -2.80 | 121.38      | 124.53   |
| 14  | A     | 1112 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 14  | G     | 1104 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 14  | H     | 1223 | CLA  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 14  | b     | 1021 | CLA  | CMA-C3A-C2A | -2.80 | 102.53      | 113.83   |
| 14  | B     | 1223 | CLA  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 18  | K     | 4001 | BCR  | C19-C18-C17 | 2.80  | 123.24      | 118.94   |
| 14  | a     | 1013 | CLA  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 14  | B     | 1021 | CLA  | CMA-C3A-C2A | -2.80 | 102.53      | 113.83   |
| 14  | G     | 1112 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 18  | G     | 4003 | BCR  | C37-C22-C23 | 2.80  | 122.49      | 118.08   |
| 14  | l     | 1501 | CLA  | C3D-C4D-ND  | 2.80  | 114.77      | 110.24   |
| 18  | k     | 4001 | BCR  | C19-C18-C17 | 2.80  | 123.23      | 118.94   |
| 14  | b     | 1214 | CLA  | OBD-CAD-C3D | -2.80 | 121.79      | 128.52   |
| 14  | B     | 1204 | CLA  | CAC-C3C-C4C | 2.80  | 128.44      | 124.81   |
| 14  | a     | 1133 | CLA  | C3C-C4C-NC  | 2.80  | 113.71      | 110.57   |
| 14  | G     | 1107 | CLA  | CMA-C3A-C4A | 2.80  | 119.29      | 111.77   |
| 14  | H     | 1206 | CLA  | C1-C2-C3    | -2.79 | 121.21      | 126.04   |
| 20  | B     | 5002 | LMG  | O1-C1-C2    | 2.79  | 112.67      | 108.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1012 | CLA  | C1-C2-C3    | -2.79 | 121.21      | 126.04   |
| 14  | m     | 1501 | CLA  | CMC-C2C-C1C | 2.79  | 129.29      | 125.04   |
| 14  | b     | 1235 | CLA  | C3D-C4D-ND  | 2.79  | 114.76      | 110.24   |
| 14  | G     | 1111 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 14  | A     | 1107 | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 14  | b     | 1202 | CLA  | C4D-C3D-CAD | 2.79  | 111.38      | 108.10   |
| 14  | b     | 1234 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 14  | G     | 1103 | CLA  | C3D-C4D-ND  | 2.79  | 114.75      | 110.24   |
| 18  | I     | 4020 | BCR  | C37-C22-C23 | 2.79  | 122.47      | 118.08   |
| 14  | G     | 1113 | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 14  | b     | 1223 | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 14  | b     | 1222 | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 20  | b     | 5002 | LMG  | O1-C1-C2    | 2.79  | 112.65      | 108.30   |
| 14  | b     | 1206 | CLA  | C1-C2-C3    | -2.79 | 121.22      | 126.04   |
| 14  | A     | 1012 | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 18  | l     | 4022 | BCR  | C3-C4-C5    | -2.78 | 109.11      | 114.08   |
| 18  | U     | 4022 | BCR  | C3-C4-C5    | -2.78 | 109.11      | 114.08   |
| 14  | b     | 1234 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 14  | H     | 1204 | CLA  | CAC-C3C-C4C | 2.78  | 128.42      | 124.81   |
| 14  | B     | 1232 | CLA  | C4D-C3D-CAD | 2.78  | 111.38      | 108.10   |
| 14  | A     | 1012 | CLA  | C1-C2-C3    | -2.78 | 121.23      | 126.04   |
| 14  | G     | 1113 | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | G     | 1127 | CLA  | CMC-C2C-C1C | 2.78  | 129.27      | 125.04   |
| 14  | A     | 1103 | CLA  | C3D-C4D-ND  | 2.78  | 114.74      | 110.24   |
| 14  | A     | 1128 | CLA  | C1-C2-C3    | -2.78 | 121.23      | 126.04   |
| 14  | G     | 1116 | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | G     | 1124 | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | G     | 1133 | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 14  | a     | 1012 | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 14  | G     | 1012 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 14  | B     | 1206 | CLA  | C1-C2-C3    | -2.78 | 121.24      | 126.04   |
| 14  | a     | 1107 | CLA  | CMA-C3A-C4A | 2.78  | 119.24      | 111.77   |
| 14  | B     | 1213 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 14  | b     | 1229 | CLA  | CMA-C3A-C4A | 2.78  | 119.24      | 111.77   |
| 14  | H     | 1213 | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.81   |
| 14  | H     | 1022 | CLA  | O2A-C1-C2   | 2.78  | 115.93      | 108.64   |
| 14  | A     | 1113 | CLA  | CMA-C3A-C4A | 2.78  | 119.23      | 111.77   |
| 14  | H     | 1221 | CLA  | C1-O2A-CGA  | 2.78  | 123.72      | 116.44   |
| 14  | B     | 1222 | CLA  | C4-C3-C5    | 2.77  | 119.94      | 115.27   |
| 14  | a     | 1116 | CLA  | C3C-C4C-NC  | 2.77  | 113.68      | 110.57   |
| 18  | H     | 4017 | BCR  | C33-C5-C6   | -2.77 | 121.41      | 124.53   |
| 14  | b     | 1212 | CLA  | CAA-C2A-C3A | -2.77 | 105.18      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1222 | CLA  | C4-C3-C5    | 2.77  | 119.94      | 115.27   |
| 14  | H     | 1234 | CLA  | C4-C3-C5    | 2.77  | 119.94      | 115.27   |
| 18  | L     | 4022 | BCR  | C3-C4-C5    | -2.77 | 109.13      | 114.08   |
| 14  | H     | 1212 | CLA  | CAA-C2A-C3A | -2.77 | 105.19      | 112.78   |
| 18  | L     | 4019 | BCR  | C32-C1-C6   | -2.77 | 105.80      | 110.30   |
| 14  | H     | 1232 | CLA  | C4D-C3D-CAD | 2.77  | 111.36      | 108.10   |
| 14  | b     | 1203 | CLA  | C3C-C4C-NC  | 2.77  | 113.68      | 110.57   |
| 14  | H     | 1235 | CLA  | C3D-C4D-ND  | 2.77  | 114.72      | 110.24   |
| 14  | B     | 1212 | CLA  | CAA-C2A-C3A | -2.77 | 105.19      | 112.78   |
| 14  | H     | 1235 | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 14  | B     | 1234 | CLA  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 14  | B     | 1235 | CLA  | C3D-C4D-ND  | 2.77  | 114.72      | 110.24   |
| 14  | a     | 1103 | CLA  | C3D-C4D-ND  | 2.77  | 114.72      | 110.24   |
| 18  | T     | 4001 | BCR  | C19-C18-C17 | 2.77  | 123.19      | 118.94   |
| 15  | b     | 1237 | F6C  | CHB-C4A-NA  | 2.77  | 127.00      | 124.45   |
| 14  | A     | 1012 | CLA  | CMB-C2B-C3B | 2.77  | 129.86      | 124.68   |
| 14  | a     | 1128 | CLA  | C1-C2-C3    | -2.77 | 121.26      | 126.04   |
| 20  | i     | 5006 | LMG  | O8-C28-C29  | 2.77  | 120.59      | 111.91   |
| 14  | B     | 1229 | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 14  | a     | 1113 | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 14  | A     | 1133 | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 20  | I     | 5006 | LMG  | O8-C28-C29  | 2.77  | 120.59      | 111.91   |
| 14  | A     | 1113 | CLA  | C3C-C4C-NC  | 2.77  | 113.67      | 110.57   |
| 18  | B     | 4017 | BCR  | C33-C5-C6   | -2.77 | 121.42      | 124.53   |
| 15  | b     | 1219 | F6C  | CHD-C1D-ND  | -2.77 | 120.01      | 124.20   |
| 14  | A     | 1116 | CLA  | C3C-C4C-NC  | 2.77  | 113.67      | 110.57   |
| 20  | R     | 5006 | LMG  | O8-C28-C29  | 2.77  | 120.58      | 111.91   |
| 14  | B     | 1235 | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 14  | a     | 1133 | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 14  | A     | 1013 | CLA  | CHB-C4A-NA  | 2.76  | 128.34      | 124.51   |
| 14  | G     | 1013 | CLA  | CHB-C4A-NA  | 2.76  | 128.34      | 124.51   |
| 18  | U     | 4019 | BCR  | C32-C1-C6   | -2.76 | 105.82      | 110.30   |
| 18  | a     | 4006 | BCR  | C31-C1-C6   | -2.76 | 105.82      | 110.30   |
| 15  | b     | 1238 | F6C  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 18  | a     | 4003 | BCR  | C33-C5-C6   | -2.76 | 121.43      | 124.53   |
| 18  | b     | 4017 | BCR  | C15-C14-C13 | -2.76 | 123.37      | 127.31   |
| 14  | b     | 1221 | CLA  | C1-O2A-CGA  | 2.76  | 123.69      | 116.44   |
| 14  | b     | 1204 | CLA  | CAC-C3C-C4C | 2.76  | 128.39      | 124.81   |
| 14  | B     | 1022 | CLA  | O2A-C1-C2   | 2.76  | 115.89      | 108.64   |
| 16  | a     | 2001 | PQN  | C11-C12-C13 | -2.76 | 122.20      | 126.79   |
| 14  | H     | 1211 | CLA  | C3D-C4D-ND  | 2.76  | 114.70      | 110.24   |
| 16  | A     | 2001 | PQN  | C11-C12-C13 | -2.76 | 122.20      | 126.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | H     | 4017 | BCR  | C15-C14-C13 | -2.76 | 123.37      | 127.31   |
| 14  | b     | 1201 | CLA  | C4D-C3D-CAD | 2.76  | 111.35      | 108.10   |
| 18  | R     | 4020 | BCR  | C37-C22-C23 | 2.76  | 122.42      | 118.08   |
| 14  | B     | 1221 | CLA  | C1-O2A-CGA  | 2.76  | 123.68      | 116.44   |
| 15  | H     | 1230 | F6C  | CMC-C2C-C3C | 2.76  | 130.14      | 124.94   |
| 14  | b     | 1022 | CLA  | O2A-C1-C2   | 2.76  | 115.88      | 108.64   |
| 14  | b     | 1226 | CLA  | C4-C3-C5    | 2.76  | 119.91      | 115.27   |
| 14  | G     | 1102 | CLA  | O2D-CGD-O1D | -2.76 | 118.45      | 123.84   |
| 14  | H     | 1201 | CLA  | C4D-C3D-CAD | 2.76  | 111.34      | 108.10   |
| 14  | a     | 1106 | CLA  | C3C-C4C-NC  | 2.76  | 113.66      | 110.57   |
| 16  | G     | 2001 | PQN  | C11-C12-C13 | -2.76 | 122.20      | 126.79   |
| 14  | G     | 1118 | CLA  | CMC-C2C-C1C | 2.76  | 129.24      | 125.04   |
| 14  | a     | 1013 | CLA  | CHB-C4A-NA  | 2.76  | 128.32      | 124.51   |
| 14  | H     | 1213 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 14  | H     | 1232 | CLA  | CMC-C2C-C1C | 2.75  | 129.23      | 125.04   |
| 14  | B     | 1213 | CLA  | CAC-C3C-C4C | 2.75  | 128.38      | 124.81   |
| 14  | A     | 1102 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 14  | b     | 1235 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 14  | b     | 1235 | CLA  | C4-C3-C5    | 2.75  | 119.90      | 115.27   |
| 13  | G     | 1011 | CL0  | C3D-C4D-ND  | 2.75  | 114.69      | 110.24   |
| 14  | H     | 1229 | CLA  | CMA-C3A-C4A | 2.75  | 119.17      | 111.77   |
| 14  | A     | 1124 | CLA  | C3C-C4C-NC  | 2.75  | 113.66      | 110.57   |
| 15  | b     | 1219 | F6C  | O2D-CGD-O1D | -2.75 | 118.46      | 123.84   |
| 18  | A     | 4006 | BCR  | C31-C1-C6   | -2.75 | 105.84      | 110.30   |
| 15  | B     | 1237 | F6C  | CHB-C4A-NA  | 2.75  | 126.98      | 124.45   |
| 18  | b     | 4017 | BCR  | C33-C5-C6   | -2.75 | 121.44      | 124.53   |
| 15  | B     | 1230 | F6C  | CMC-C2C-C3C | 2.75  | 130.13      | 124.94   |
| 18  | I     | 4018 | BCR  | C37-C22-C21 | -2.75 | 119.07      | 122.92   |
| 14  | l     | 1503 | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 13  | A     | 1011 | CL0  | C3D-C4D-ND  | 2.75  | 114.68      | 110.24   |
| 14  | H     | 1228 | CLA  | CAA-C2A-C3A | -2.75 | 105.25      | 112.78   |
| 18  | l     | 4019 | BCR  | C12-C13-C14 | -2.75 | 114.72      | 118.94   |
| 14  | G     | 1111 | CLA  | CMA-C3A-C4A | 2.75  | 119.16      | 111.77   |
| 18  | A     | 4003 | BCR  | C33-C5-C6   | -2.75 | 121.44      | 124.53   |
| 14  | A     | 1106 | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 18  | l     | 4019 | BCR  | C32-C1-C6   | -2.75 | 105.84      | 110.30   |
| 14  | a     | 1117 | CLA  | CAC-C3C-C4C | 2.75  | 128.37      | 124.81   |
| 13  | a     | 1011 | CL0  | C3D-C4D-ND  | 2.75  | 114.68      | 110.24   |
| 14  | a     | 1111 | CLA  | CMA-C3A-C4A | 2.75  | 119.16      | 111.77   |
| 15  | b     | 1230 | F6C  | CMC-C2C-C3C | 2.75  | 130.12      | 124.94   |
| 14  | b     | 1222 | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 18  | B     | 4017 | BCR  | C15-C14-C13 | -2.75 | 123.39      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1102 | CLA  | O2D-CGD-O1D | -2.75 | 118.47      | 123.84   |
| 14  | b     | 1231 | CLA  | C3D-C4D-ND  | 2.74  | 114.68      | 110.24   |
| 14  | b     | 1232 | CLA  | CMC-C2C-C1C | 2.74  | 129.22      | 125.04   |
| 14  | a     | 1012 | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 14  | B     | 1211 | CLA  | C3D-C4D-ND  | 2.74  | 114.68      | 110.24   |
| 14  | A     | 1118 | CLA  | CMC-C2C-C1C | 2.74  | 129.22      | 125.04   |
| 15  | H     | 1219 | F6C  | O2D-CGD-O1D | -2.74 | 118.47      | 123.84   |
| 14  | B     | 1228 | CLA  | CAA-C2A-C3A | -2.74 | 105.27      | 112.78   |
| 15  | B     | 1219 | F6C  | CHD-C1D-ND  | -2.74 | 120.04      | 124.20   |
| 15  | B     | 1219 | F6C  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 18  | G     | 4006 | BCR  | C31-C1-C6   | -2.74 | 105.85      | 110.30   |
| 14  | B     | 1232 | CLA  | CMC-C2C-C1C | 2.74  | 129.21      | 125.04   |
| 18  | i     | 4018 | BCR  | C37-C22-C21 | -2.74 | 119.09      | 122.92   |
| 14  | G     | 1106 | CLA  | C3C-C4C-NC  | 2.74  | 113.64      | 110.57   |
| 14  | G     | 1122 | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 14  | A     | 1111 | CLA  | CMA-C3A-C4A | 2.74  | 119.13      | 111.77   |
| 14  | b     | 1214 | CLA  | CMC-C2C-C1C | 2.74  | 129.21      | 125.04   |
| 14  | a     | 1012 | CLA  | C3C-C4C-NC  | 2.74  | 113.64      | 110.57   |
| 14  | G     | 1012 | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 14  | H     | 1222 | CLA  | C3C-C4C-NC  | 2.73  | 113.64      | 110.57   |
| 14  | a     | 1124 | CLA  | C3C-C4C-NC  | 2.73  | 113.64      | 110.57   |
| 14  | B     | 1214 | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 14  | L     | 1503 | CLA  | C3C-C4C-NC  | 2.73  | 113.64      | 110.57   |
| 14  | H     | 1202 | CLA  | C1-C2-C3    | -2.73 | 121.31      | 126.04   |
| 14  | B     | 1226 | CLA  | C4-C3-C5    | 2.73  | 119.87      | 115.27   |
| 14  | A     | 1013 | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 14  | b     | 1228 | CLA  | CAA-C2A-C3A | -2.73 | 105.30      | 112.78   |
| 14  | a     | 1013 | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 15  | B     | 1238 | F6C  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 14  | B     | 1235 | CLA  | C4-C3-C5    | 2.73  | 119.87      | 115.27   |
| 14  | a     | 1113 | CLA  | C3C-C4C-NC  | 2.73  | 113.64      | 110.57   |
| 14  | A     | 1113 | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 14  | G     | 1113 | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 18  | H     | 4009 | BCR  | C37-C22-C21 | -2.73 | 119.10      | 122.92   |
| 14  | B     | 1201 | CLA  | C4D-C3D-CAD | 2.73  | 111.31      | 108.10   |
| 15  | H     | 1237 | F6C  | CHB-C4A-NA  | 2.73  | 126.96      | 124.45   |
| 14  | H     | 1235 | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 14  | A     | 1122 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 14  | G     | 1013 | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 14  | B     | 1222 | CLA  | C3C-C4C-NC  | 2.73  | 113.63      | 110.57   |
| 14  | b     | 1211 | CLA  | C3D-C4D-ND  | 2.73  | 114.65      | 110.24   |
| 14  | K     | 1401 | CLA  | C4D-C3D-CAD | 2.73  | 111.31      | 108.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1226 | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 14  | a     | 1140 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 14  | B     | 1203 | CLA  | C3C-C4C-NC  | 2.73  | 113.63      | 110.57   |
| 14  | B     | 1202 | CLA  | C1-C2-C3    | -2.73 | 121.33      | 126.04   |
| 14  | a     | 1138 | CLA  | CMA-C3A-C4A | 2.73  | 119.10      | 111.77   |
| 14  | a     | 1122 | CLA  | O2D-CGD-O1D | -2.72 | 118.51      | 123.84   |
| 14  | H     | 1231 | CLA  | CMD-C2D-C3D | -2.72 | 121.35      | 127.61   |
| 14  | A     | 1138 | CLA  | CMA-C3A-C4A | 2.72  | 119.09      | 111.77   |
| 18  | B     | 4009 | BCR  | C37-C22-C21 | -2.72 | 119.11      | 122.92   |
| 18  | L     | 4019 | BCR  | C12-C13-C14 | -2.72 | 114.76      | 118.94   |
| 14  | G     | 1120 | CLA  | CMA-C3A-C4A | 2.72  | 119.09      | 111.77   |
| 14  | A     | 1139 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 14  | H     | 1209 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 15  | H     | 1219 | F6C  | CHD-C1D-ND  | -2.72 | 120.08      | 124.20   |
| 14  | a     | 1118 | CLA  | CMC-C2C-C1C | 2.72  | 129.18      | 125.04   |
| 18  | G     | 4003 | BCR  | C33-C5-C6   | -2.72 | 121.47      | 124.53   |
| 15  | H     | 1238 | F6C  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | G     | 1138 | CLA  | CMA-C3A-C4A | 2.72  | 119.08      | 111.77   |
| 14  | a     | 1127 | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | B     | 1231 | CLA  | C3D-C4D-ND  | 2.72  | 114.64      | 110.24   |
| 14  | H     | 1203 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 14  | T     | 1401 | CLA  | C4D-C3D-CAD | 2.72  | 111.30      | 108.10   |
| 14  | a     | 1120 | CLA  | CMA-C3A-C4A | 2.72  | 119.08      | 111.77   |
| 14  | G     | 1139 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 14  | b     | 1206 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 14  | G     | 1114 | CLA  | O2D-CGD-O1D | -2.72 | 118.53      | 123.84   |
| 14  | B     | 1231 | CLA  | CMD-C2D-C3D | -2.72 | 121.37      | 127.61   |
| 14  | A     | 1120 | CLA  | CMA-C3A-C4A | 2.72  | 119.07      | 111.77   |
| 18  | H     | 4009 | BCR  | C1-C6-C5    | -2.72 | 118.79      | 122.61   |
| 14  | G     | 1122 | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 14  | A     | 1012 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 14  | B     | 1209 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 14  | A     | 1117 | CLA  | CAC-C3C-C4C | 2.71  | 128.33      | 124.81   |
| 14  | G     | 1105 | CLA  | CMC-C2C-C1C | 2.71  | 129.17      | 125.04   |
| 14  | a     | 1105 | CLA  | CMC-C2C-C1C | 2.71  | 129.17      | 125.04   |
| 14  | a     | 1128 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 21  | b     | 6002 | LMT  | C1'-O5'-C5' | -2.71 | 108.36      | 113.69   |
| 14  | b     | 1202 | CLA  | C1-C2-C3    | -2.71 | 121.35      | 126.04   |
| 14  | G     | 1108 | CLA  | CMA-C3A-C4A | 2.71  | 119.06      | 111.77   |
| 14  | a     | 1108 | CLA  | CMA-C3A-C4A | 2.71  | 119.06      | 111.77   |
| 14  | G     | 1117 | CLA  | CAC-C3C-C4C | 2.71  | 128.33      | 124.81   |
| 14  | G     | 1012 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1233 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 14  | a     | 1122 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 14  | B     | 1216 | CLA  | C3D-C4D-ND  | 2.71  | 114.62      | 110.24   |
| 15  | H     | 1219 | F6C  | CHB-C4A-C3A | -2.71 | 119.80      | 125.48   |
| 14  | G     | 1140 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 14  | a     | 1113 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 14  | k     | 1401 | CLA  | C4D-C3D-CAD | 2.71  | 111.29      | 108.10   |
| 14  | b     | 1231 | CLA  | CMD-C2D-C3D | -2.71 | 121.38      | 127.61   |
| 18  | R     | 4018 | BCR  | C37-C22-C21 | -2.71 | 119.13      | 122.92   |
| 18  | U     | 4019 | BCR  | C12-C13-C14 | -2.71 | 114.79      | 118.94   |
| 18  | a     | 4003 | BCR  | C15-C14-C13 | -2.71 | 123.45      | 127.31   |
| 14  | A     | 1140 | CLA  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 14  | b     | 1209 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 14  | G     | 1108 | CLA  | C3D-C4D-ND  | 2.71  | 114.61      | 110.24   |
| 14  | G     | 1107 | CLA  | O2D-CGD-O1D | -2.71 | 118.55      | 123.84   |
| 14  | M     | 1501 | CLA  | CMD-C2D-C3D | -2.71 | 121.39      | 127.61   |
| 14  | A     | 1107 | CLA  | O2D-CGD-O1D | -2.70 | 118.55      | 123.84   |
| 14  | A     | 1108 | CLA  | CMA-C3A-C4A | 2.70  | 119.04      | 111.77   |
| 18  | G     | 4002 | BCR  | C19-C18-C17 | 2.70  | 123.09      | 118.94   |
| 14  | A     | 1108 | CLA  | C3D-C4D-ND  | 2.70  | 114.61      | 110.24   |
| 14  | A     | 1128 | CLA  | C3C-C4C-NC  | 2.70  | 113.60      | 110.57   |
| 14  | A     | 1105 | CLA  | CMC-C2C-C1C | 2.70  | 129.16      | 125.04   |
| 14  | m     | 1501 | CLA  | CMD-C2D-C3D | -2.70 | 121.40      | 127.61   |
| 14  | A     | 1114 | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 14  | B     | 1209 | CLA  | C3D-C4D-ND  | 2.70  | 114.61      | 110.24   |
| 14  | A     | 1122 | CLA  | C3C-C4C-NC  | 2.70  | 113.60      | 110.57   |
| 14  | a     | 1131 | CLA  | CMC-C2C-C1C | 2.70  | 129.15      | 125.04   |
| 14  | A     | 1101 | CLA  | C4D-C3D-CAD | 2.70  | 111.28      | 108.10   |
| 18  | A     | 4003 | BCR  | C15-C14-C13 | -2.70 | 123.46      | 127.31   |
| 14  | H     | 1208 | CLA  | CAA-CBA-CGA | -2.70 | 105.37      | 113.25   |
| 15  | B     | 1219 | F6C  | CHB-C4A-C3A | -2.70 | 119.82      | 125.48   |
| 14  | A     | 1127 | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 14  | H     | 1209 | CLA  | C3D-C4D-ND  | 2.70  | 114.60      | 110.24   |
| 14  | G     | 1128 | CLA  | C3C-C4C-NC  | 2.70  | 113.60      | 110.57   |
| 21  | H     | 6002 | LMT  | C1'-O5'-C5' | -2.70 | 108.39      | 113.69   |
| 14  | b     | 1208 | CLA  | CAA-CBA-CGA | -2.70 | 105.37      | 113.25   |
| 14  | G     | 1138 | CLA  | CBA-CAA-C2A | 2.70  | 121.82      | 113.86   |
| 14  | B     | 1208 | CLA  | CAA-CBA-CGA | -2.70 | 105.38      | 113.25   |
| 14  | U     | 1503 | CLA  | C3C-C4C-NC  | 2.70  | 113.59      | 110.57   |
| 14  | H     | 1229 | CLA  | C3D-C4D-ND  | 2.70  | 114.60      | 110.24   |
| 14  | b     | 1209 | CLA  | C3D-C4D-ND  | 2.69  | 114.60      | 110.24   |
| 21  | B     | 6002 | LMT  | C1'-O5'-C5' | -2.69 | 108.40      | 113.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1126 | CLA  | CAA-C2A-C3A | -2.69 | 105.40      | 112.78   |
| 14  | G     | 1101 | CLA  | C4D-C3D-CAD | 2.69  | 111.27      | 108.10   |
| 14  | G     | 1105 | CLA  | C3D-C4D-ND  | 2.69  | 114.59      | 110.24   |
| 14  | a     | 1138 | CLA  | CBA-CAA-C2A | 2.69  | 121.81      | 113.86   |
| 18  | B     | 4006 | BCR  | C34-C9-C10  | -2.69 | 119.15      | 122.92   |
| 14  | a     | 1101 | CLA  | CMA-C3A-C4A | 2.69  | 119.01      | 111.77   |
| 18  | B     | 4009 | BCR  | C1-C6-C5    | -2.69 | 118.82      | 122.61   |
| 14  | A     | 1138 | CLA  | CBA-CAA-C2A | 2.69  | 121.81      | 113.86   |
| 18  | a     | 4002 | BCR  | C19-C18-C17 | 2.69  | 123.07      | 118.94   |
| 14  | H     | 1206 | CLA  | C3C-C4C-NC  | 2.69  | 113.59      | 110.57   |
| 14  | H     | 1231 | CLA  | C3D-C4D-ND  | 2.69  | 114.59      | 110.24   |
| 14  | b     | 1218 | CLA  | C3D-C4D-ND  | 2.69  | 114.59      | 110.24   |
| 14  | H     | 1220 | CLA  | C1-C2-C3    | -2.69 | 121.39      | 126.04   |
| 14  | b     | 1216 | CLA  | C3D-C4D-ND  | 2.69  | 114.59      | 110.24   |
| 18  | G     | 4003 | BCR  | C15-C14-C13 | -2.69 | 123.47      | 127.31   |
| 14  | A     | 1105 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | a     | 1107 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | b     | 1201 | CLA  | C3D-C4D-ND  | 2.69  | 114.59      | 110.24   |
| 14  | a     | 1114 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | a     | 1116 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | A     | 1105 | CLA  | C3C-C4C-NC  | 2.69  | 113.58      | 110.57   |
| 14  | B     | 1225 | CLA  | O2D-CGD-O1D | -2.69 | 118.59      | 123.84   |
| 14  | B     | 1218 | CLA  | C3D-C4D-ND  | 2.69  | 114.58      | 110.24   |
| 14  | G     | 1101 | CLA  | CMA-C3A-C4A | 2.69  | 118.99      | 111.77   |
| 14  | B     | 1023 | CLA  | CHC-C1C-C2C | -2.69 | 119.29      | 126.72   |
| 14  | b     | 1233 | CLA  | C3C-C4C-NC  | 2.69  | 113.58      | 110.57   |
| 14  | H     | 1214 | CLA  | CMC-C2C-C1C | 2.69  | 129.13      | 125.04   |
| 14  | a     | 1104 | CLA  | C3D-C4D-ND  | 2.68  | 114.58      | 110.24   |
| 18  | b     | 4006 | BCR  | C34-C9-C10  | -2.68 | 119.16      | 122.92   |
| 14  | B     | 1233 | CLA  | C3C-C4C-NC  | 2.68  | 113.58      | 110.57   |
| 14  | G     | 1105 | CLA  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 14  | b     | 1023 | CLA  | CHC-C1C-C2C | -2.68 | 119.30      | 126.72   |
| 14  | a     | 1101 | CLA  | CMC-C2C-C1C | 2.68  | 129.13      | 125.04   |
| 14  | a     | 1118 | CLA  | C3D-C4D-ND  | 2.68  | 114.58      | 110.24   |
| 18  | A     | 4005 | BCR  | C34-C9-C10  | -2.68 | 119.17      | 122.92   |
| 14  | A     | 1116 | CLA  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 14  | A     | 1101 | CLA  | CMA-C3A-C4A | 2.68  | 118.98      | 111.77   |
| 18  | k     | 4001 | BCR  | C35-C13-C12 | 2.68  | 122.30      | 118.08   |
| 18  | H     | 4006 | BCR  | C34-C9-C10  | -2.68 | 119.17      | 122.92   |
| 14  | a     | 1105 | CLA  | C3D-C4D-ND  | 2.68  | 114.58      | 110.24   |
| 15  | H     | 1219 | F6C  | C4-C3-C5    | 2.68  | 119.78      | 115.27   |
| 14  | B     | 1229 | CLA  | C3D-C4D-ND  | 2.68  | 114.57      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1116 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 14  | H     | 1216 | CLA  | C3D-C4D-ND  | 2.68  | 114.57      | 110.24   |
| 14  | G     | 1127 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 18  | a     | 4005 | BCR  | C34-C9-C10  | -2.68 | 119.17      | 122.92   |
| 14  | H     | 1023 | CLA  | CHC-C1C-C2C | -2.68 | 119.31      | 126.72   |
| 14  | A     | 1108 | CLA  | CAA-C2A-C3A | -2.68 | 105.44      | 112.78   |
| 18  | b     | 4009 | BCR  | C37-C22-C21 | -2.68 | 119.17      | 122.92   |
| 14  | A     | 1104 | CLA  | C3D-C4D-ND  | 2.68  | 114.57      | 110.24   |
| 18  | T     | 4001 | BCR  | C36-C18-C17 | -2.68 | 119.17      | 122.92   |
| 14  | H     | 1226 | CLA  | CMC-C2C-C3C | 2.68  | 133.39      | 126.12   |
| 14  | A     | 1105 | CLA  | C3D-C4D-ND  | 2.68  | 114.57      | 110.24   |
| 14  | V     | 1501 | CLA  | CMD-C2D-C3D | -2.68 | 121.45      | 127.61   |
| 14  | A     | 1131 | CLA  | CMC-C2C-C1C | 2.68  | 129.12      | 125.04   |
| 18  | K     | 4001 | BCR  | C36-C18-C17 | -2.68 | 119.17      | 122.92   |
| 14  | A     | 1126 | CLA  | CAA-C2A-C3A | -2.68 | 105.45      | 112.78   |
| 14  | a     | 1108 | CLA  | CAA-C2A-C3A | -2.68 | 105.45      | 112.78   |
| 14  | a     | 1108 | CLA  | C3D-C4D-ND  | 2.68  | 114.57      | 110.24   |
| 14  | H     | 1217 | CLA  | O2A-CGA-CBA | 2.68  | 122.63      | 114.03   |
| 14  | B     | 1206 | CLA  | C3C-C4C-NC  | 2.68  | 113.57      | 110.57   |
| 14  | G     | 1131 | CLA  | CMC-C2C-C1C | 2.67  | 129.11      | 125.04   |
| 14  | B     | 1214 | CLA  | CMA-C3A-C4A | 2.67  | 118.96      | 111.77   |
| 14  | a     | 1106 | CLA  | C4-C3-C5    | 2.67  | 119.77      | 115.27   |
| 14  | A     | 1118 | CLA  | C3D-C4D-ND  | 2.67  | 114.56      | 110.24   |
| 14  | l     | 1501 | CLA  | CMA-C3A-C4A | 2.67  | 118.96      | 111.77   |
| 14  | G     | 1106 | CLA  | C4-C3-C5    | 2.67  | 119.77      | 115.27   |
| 14  | a     | 1139 | CLA  | C3C-C4C-NC  | 2.67  | 113.57      | 110.57   |
| 14  | A     | 1101 | CLA  | CMC-C2C-C1C | 2.67  | 129.11      | 125.04   |
| 18  | a     | 4004 | BCR  | C34-C9-C8   | 2.67  | 122.29      | 118.08   |
| 14  | b     | 1229 | CLA  | C3D-C4D-ND  | 2.67  | 114.56      | 110.24   |
| 18  | A     | 4002 | BCR  | C19-C18-C17 | 2.67  | 123.04      | 118.94   |
| 14  | b     | 1225 | CLA  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 14  | G     | 1118 | CLA  | C3D-C4D-ND  | 2.67  | 114.56      | 110.24   |
| 14  | G     | 1126 | CLA  | CAA-C2A-C3A | -2.67 | 105.46      | 112.78   |
| 15  | b     | 1219 | F6C  | CHB-C4A-C3A | -2.67 | 119.88      | 125.48   |
| 14  | B     | 1226 | CLA  | CMC-C2C-C3C | 2.67  | 133.37      | 126.12   |
| 14  | A     | 1102 | CLA  | C3C-C4C-NC  | 2.67  | 113.56      | 110.57   |
| 18  | b     | 4005 | BCR  | C19-C18-C17 | 2.67  | 123.04      | 118.94   |
| 18  | A     | 4004 | BCR  | C34-C9-C8   | 2.67  | 122.28      | 118.08   |
| 14  | a     | 1109 | CLA  | C4D-C3D-CAD | 2.67  | 111.24      | 108.10   |
| 18  | H     | 4005 | BCR  | C33-C5-C4   | 2.67  | 118.74      | 113.62   |
| 14  | H     | 1225 | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 14  | a     | 1105 | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1217 | CLA  | O2A-CGA-CBA | 2.67  | 122.60      | 114.03   |
| 14  | a     | 1134 | CLA  | C4D-C3D-CAD | 2.67  | 111.24      | 108.10   |
| 14  | U     | 1501 | CLA  | CMB-C2B-C3B | 2.67  | 129.66      | 124.68   |
| 18  | B     | 4005 | BCR  | C33-C5-C4   | 2.67  | 118.74      | 113.62   |
| 15  | B     | 1219 | F6C  | C4-C3-C5    | 2.66  | 119.75      | 115.27   |
| 14  | b     | 1214 | CLA  | CMA-C3A-C4A | 2.66  | 118.93      | 111.77   |
| 14  | B     | 1220 | CLA  | C1-C2-C3    | -2.66 | 121.44      | 126.04   |
| 18  | b     | 4009 | BCR  | C1-C6-C5    | -2.66 | 118.86      | 122.61   |
| 14  | a     | 1101 | CLA  | C4D-C3D-CAD | 2.66  | 111.24      | 108.10   |
| 14  | b     | 1226 | CLA  | CMC-C2C-C3C | 2.66  | 133.35      | 126.12   |
| 14  | b     | 1213 | CLA  | C3C-C4C-NC  | 2.66  | 113.56      | 110.57   |
| 14  | G     | 1102 | CLA  | C3C-C4C-NC  | 2.66  | 113.56      | 110.57   |
| 14  | L     | 1501 | CLA  | CMA-C3A-C4A | 2.66  | 118.93      | 111.77   |
| 14  | G     | 1112 | CLA  | CAA-CBA-CGA | -2.66 | 105.47      | 113.25   |
| 14  | A     | 1137 | CLA  | C3C-C4C-NC  | 2.66  | 113.56      | 110.57   |
| 14  | A     | 1106 | CLA  | C4-C3-C5    | 2.66  | 119.75      | 115.27   |
| 14  | A     | 1112 | CLA  | CAA-CBA-CGA | -2.66 | 105.48      | 113.25   |
| 14  | G     | 1108 | CLA  | CAA-C2A-C3A | -2.66 | 105.50      | 112.78   |
| 14  | B     | 1201 | CLA  | C3D-C4D-ND  | 2.66  | 114.54      | 110.24   |
| 18  | G     | 4005 | BCR  | C34-C9-C10  | -2.66 | 119.20      | 122.92   |
| 18  | T     | 4001 | BCR  | C35-C13-C12 | 2.66  | 122.27      | 118.08   |
| 14  | U     | 1501 | CLA  | CMA-C3A-C4A | 2.66  | 118.92      | 111.77   |
| 18  | K     | 4001 | BCR  | C35-C13-C12 | 2.66  | 122.26      | 118.08   |
| 14  | G     | 1104 | CLA  | C3D-C4D-ND  | 2.66  | 114.54      | 110.24   |
| 14  | H     | 1218 | CLA  | C3D-C4D-ND  | 2.66  | 114.54      | 110.24   |
| 18  | B     | 4005 | BCR  | C19-C18-C17 | 2.66  | 123.02      | 118.94   |
| 14  | a     | 1105 | CLA  | C3C-C4C-NC  | 2.66  | 113.55      | 110.57   |
| 21  | A     | 6002 | LMT  | O1'-C1'-C2' | 2.66  | 112.45      | 108.30   |
| 14  | H     | 1201 | CLA  | C3D-C4D-ND  | 2.66  | 114.53      | 110.24   |
| 14  | a     | 1112 | CLA  | CAA-CBA-CGA | -2.66 | 105.49      | 113.25   |
| 14  | H     | 1203 | CLA  | O2D-CGD-O1D | -2.66 | 118.65      | 123.84   |
| 14  | H     | 1214 | CLA  | CMA-C3A-C4A | 2.65  | 118.91      | 111.77   |
| 14  | b     | 1211 | CLA  | CAA-C2A-C3A | -2.65 | 105.51      | 112.78   |
| 14  | b     | 1217 | CLA  | O2A-CGA-CBA | 2.65  | 122.56      | 114.03   |
| 14  | G     | 1101 | CLA  | CMC-C2C-C1C | 2.65  | 129.08      | 125.04   |
| 14  | G     | 1125 | CLA  | CHD-C4C-C3C | -2.65 | 120.94      | 124.84   |
| 14  | G     | 1013 | CLA  | C3D-C4D-ND  | 2.65  | 114.53      | 110.24   |
| 18  | k     | 4001 | BCR  | C36-C18-C17 | -2.65 | 119.21      | 122.92   |
| 14  | L     | 1501 | CLA  | CMB-C2B-C3B | 2.65  | 129.64      | 124.68   |
| 14  | l     | 1501 | CLA  | CMB-C2B-C3B | 2.65  | 129.64      | 124.68   |
| 14  | A     | 1013 | CLA  | C3D-C4D-ND  | 2.65  | 114.53      | 110.24   |
| 14  | G     | 1105 | CLA  | C3C-C4C-NC  | 2.65  | 113.54      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | l     | 6002 | LMT  | C3B-C4B-C5B | -2.65 | 105.51      | 110.24   |
| 18  | a     | 4002 | BCR  | C38-C26-C27 | 2.65  | 118.70      | 113.62   |
| 18  | G     | 4004 | BCR  | C34-C9-C8   | 2.65  | 122.25      | 118.08   |
| 21  | G     | 6002 | LMT  | O1'-C1'-C2' | 2.65  | 112.44      | 108.30   |
| 14  | b     | 1217 | CLA  | CMC-C2C-C1C | 2.65  | 129.07      | 125.04   |
| 14  | G     | 1137 | CLA  | C3C-C4C-NC  | 2.65  | 113.54      | 110.57   |
| 14  | G     | 1126 | CLA  | C3C-C4C-NC  | 2.65  | 113.54      | 110.57   |
| 21  | L     | 6002 | LMT  | C3B-C4B-C5B | -2.64 | 105.52      | 110.24   |
| 14  | b     | 1220 | CLA  | C1-C2-C3    | -2.64 | 121.47      | 126.04   |
| 14  | B     | 1203 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 21  | l     | 6101 | LMT  | C1B-O5B-C5B | 2.64  | 118.88      | 113.69   |
| 14  | b     | 1203 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 14  | B     | 1211 | CLA  | CAA-C2A-C3A | -2.64 | 105.54      | 112.78   |
| 14  | G     | 1110 | CLA  | C3C-C4C-NC  | 2.64  | 113.53      | 110.57   |
| 14  | L     | 1503 | CLA  | C3D-C4D-ND  | 2.64  | 114.51      | 110.24   |
| 14  | G     | 1105 | CLA  | CMD-C2D-C3D | -2.64 | 121.54      | 127.61   |
| 14  | b     | 1239 | CLA  | CMC-C2C-C3C | 2.64  | 133.29      | 126.12   |
| 14  | H     | 1213 | CLA  | C3C-C4C-NC  | 2.64  | 113.53      | 110.57   |
| 18  | b     | 4005 | BCR  | C33-C5-C4   | 2.64  | 118.69      | 113.62   |
| 18  | L     | 4019 | BCR  | C8-C9-C10   | -2.64 | 114.89      | 118.94   |
| 18  | l     | 4019 | BCR  | C8-C9-C10   | -2.64 | 114.89      | 118.94   |
| 14  | B     | 1217 | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 14  | A     | 1105 | CLA  | CMD-C2D-C3D | -2.64 | 121.54      | 127.61   |
| 14  | a     | 1137 | CLA  | C3C-C4C-NC  | 2.64  | 113.53      | 110.57   |
| 18  | H     | 4014 | BCR  | C37-C22-C21 | -2.64 | 119.23      | 122.92   |
| 14  | a     | 1129 | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 21  | a     | 6002 | LMT  | O1'-C1'-C2' | 2.64  | 112.42      | 108.30   |
| 14  | G     | 1012 | CLA  | OBD-CAD-C3D | -2.64 | 122.17      | 128.52   |
| 14  | H     | 1211 | CLA  | CAA-C2A-C3A | -2.64 | 105.56      | 112.78   |
| 18  | G     | 4002 | BCR  | C38-C26-C27 | 2.64  | 118.68      | 113.62   |
| 14  | A     | 1125 | CLA  | CHD-C4C-C3C | -2.64 | 120.96      | 124.84   |
| 14  | H     | 1239 | CLA  | CMC-C2C-C3C | 2.64  | 133.28      | 126.12   |
| 14  | B     | 1239 | CLA  | CMC-C2C-C3C | 2.64  | 133.28      | 126.12   |
| 14  | a     | 1105 | CLA  | CMD-C2D-C3D | -2.64 | 121.55      | 127.61   |
| 14  | b     | 1227 | CLA  | CMC-C2C-C1C | 2.64  | 129.05      | 125.04   |
| 15  | b     | 1219 | F6C  | C4-C3-C5    | 2.64  | 119.71      | 115.27   |
| 14  | a     | 1012 | CLA  | C6-C5-C3    | -2.64 | 106.54      | 113.45   |
| 21  | A     | 6002 | LMT  | O5B-C5B-C4B | 2.64  | 114.48      | 109.69   |
| 14  | A     | 1117 | CLA  | CBA-CAA-C2A | 2.64  | 121.64      | 113.86   |
| 18  | I     | 4020 | BCR  | C36-C18-C17 | -2.64 | 119.23      | 122.92   |
| 14  | a     | 1125 | CLA  | CHD-C4C-C3C | -2.64 | 120.97      | 124.84   |
| 14  | G     | 1119 | CLA  | C3D-C4D-ND  | 2.64  | 114.50      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1117 | CLA  | CBA-CAA-C2A | 2.64  | 121.64      | 113.86   |
| 14  | G     | 1012 | CLA  | C6-C5-C3    | -2.63 | 106.55      | 113.45   |
| 14  | A     | 1012 | CLA  | OBD-CAD-C3D | -2.63 | 122.18      | 128.52   |
| 21  | U     | 6101 | LMT  | C1B-O5B-C5B | 2.63  | 118.86      | 113.69   |
| 14  | G     | 1117 | CLA  | CBA-CAA-C2A | 2.63  | 121.64      | 113.86   |
| 14  | H     | 1227 | CLA  | CMC-C2C-C1C | 2.63  | 129.05      | 125.04   |
| 14  | a     | 1115 | CLA  | C3D-C4D-ND  | 2.63  | 114.50      | 110.24   |
| 18  | l     | 4019 | BCR  | C27-C26-C25 | -2.63 | 118.91      | 122.73   |
| 14  | B     | 1227 | CLA  | CMC-C2C-C1C | 2.63  | 129.05      | 125.04   |
| 14  | H     | 1204 | CLA  | CMB-C2B-C3B | 2.63  | 129.60      | 124.68   |
| 14  | A     | 1012 | CLA  | C6-C5-C3    | -2.63 | 106.56      | 113.45   |
| 18  | b     | 4014 | BCR  | C37-C22-C21 | -2.63 | 119.24      | 122.92   |
| 14  | a     | 1102 | CLA  | C3C-C4C-NC  | 2.63  | 113.52      | 110.57   |
| 14  | A     | 1109 | CLA  | C4D-C3D-CAD | 2.63  | 111.19      | 108.10   |
| 14  | H     | 1202 | CLA  | CMC-C2C-C1C | 2.63  | 129.04      | 125.04   |
| 14  | A     | 1113 | CLA  | CAA-C2A-C3A | -2.63 | 105.58      | 112.78   |
| 18  | A     | 4002 | BCR  | C38-C26-C27 | 2.63  | 118.67      | 113.62   |
| 14  | H     | 1209 | CLA  | CAA-C2A-C3A | -2.63 | 105.58      | 112.78   |
| 14  | B     | 1204 | CLA  | CMB-C2B-C3B | 2.63  | 129.59      | 124.68   |
| 14  | A     | 1134 | CLA  | C4D-C3D-CAD | 2.63  | 111.19      | 108.10   |
| 18  | H     | 4005 | BCR  | C19-C18-C17 | 2.63  | 122.97      | 118.94   |
| 18  | b     | 4014 | BCR  | C19-C18-C17 | 2.63  | 122.97      | 118.94   |
| 14  | A     | 1110 | CLA  | C3C-C4C-NC  | 2.63  | 113.52      | 110.57   |
| 14  | A     | 1129 | CLA  | CMC-C2C-C1C | 2.63  | 129.04      | 125.04   |
| 14  | b     | 1210 | CLA  | C3D-C4D-ND  | 2.63  | 114.49      | 110.24   |
| 21  | U     | 6002 | LMT  | C3B-C4B-C5B | -2.63 | 105.56      | 110.24   |
| 14  | a     | 1013 | CLA  | C3D-C4D-ND  | 2.63  | 114.48      | 110.24   |
| 14  | l     | 1503 | CLA  | C3D-C4D-ND  | 2.63  | 114.48      | 110.24   |
| 14  | G     | 1138 | CLA  | CED-O2D-CGD | 2.62  | 121.87      | 115.94   |
| 14  | A     | 1136 | CLA  | CMC-C2C-C1C | 2.62  | 129.04      | 125.04   |
| 14  | b     | 1222 | CLA  | CAA-C2A-C1A | -2.62 | 103.38      | 111.97   |
| 14  | B     | 1209 | CLA  | CAA-C2A-C3A | -2.62 | 105.59      | 112.78   |
| 14  | H     | 1222 | CLA  | CAA-C2A-C1A | -2.62 | 103.38      | 111.97   |
| 14  | U     | 1501 | CLA  | C3C-C4C-NC  | 2.62  | 113.51      | 110.57   |
| 14  | B     | 1222 | CLA  | CAA-C2A-C1A | -2.62 | 103.38      | 111.97   |
| 14  | G     | 1129 | CLA  | CMC-C2C-C1C | 2.62  | 129.03      | 125.04   |
| 14  | G     | 1113 | CLA  | CAA-C2A-C3A | -2.62 | 105.60      | 112.78   |
| 14  | a     | 1012 | CLA  | OBD-CAD-C3D | -2.62 | 122.21      | 128.52   |
| 14  | G     | 1109 | CLA  | C4D-C3D-CAD | 2.62  | 111.19      | 108.10   |
| 14  | B     | 1210 | CLA  | C3D-C4D-ND  | 2.62  | 114.48      | 110.24   |
| 14  | U     | 1503 | CLA  | C3D-C4D-ND  | 2.62  | 114.48      | 110.24   |
| 14  | H     | 1236 | CLA  | CHD-C4C-C3C | -2.62 | 120.99      | 124.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | L     | 6101 | LMT  | C1B-O5B-C5B | 2.62  | 118.83      | 113.69   |
| 14  | G     | 1134 | CLA  | C4D-C3D-CAD | 2.62  | 111.18      | 108.10   |
| 14  | B     | 1021 | CLA  | O2A-C1-C2   | 2.62  | 115.52      | 108.64   |
| 14  | G     | 1110 | CLA  | C3D-C4D-ND  | 2.62  | 114.47      | 110.24   |
| 14  | H     | 1210 | CLA  | C3D-C4D-ND  | 2.62  | 114.47      | 110.24   |
| 18  | L     | 4019 | BCR  | C27-C26-C25 | -2.62 | 118.93      | 122.73   |
| 14  | a     | 1113 | CLA  | CAA-C2A-C3A | -2.62 | 105.61      | 112.78   |
| 18  | a     | 4003 | BCR  | C34-C9-C10  | -2.62 | 119.26      | 122.92   |
| 14  | L     | 1501 | CLA  | C3C-C4C-NC  | 2.62  | 113.50      | 110.57   |
| 14  | a     | 1110 | CLA  | C3D-C4D-ND  | 2.62  | 114.47      | 110.24   |
| 14  | A     | 1138 | CLA  | CED-O2D-CGD | 2.62  | 121.85      | 115.94   |
| 21  | a     | 6002 | LMT  | O5B-C5B-C4B | 2.62  | 114.44      | 109.69   |
| 14  | b     | 1209 | CLA  | CAA-C2A-C3A | -2.61 | 105.62      | 112.78   |
| 14  | A     | 1115 | CLA  | C3C-C4C-NC  | 2.61  | 113.50      | 110.57   |
| 18  | U     | 4019 | BCR  | C27-C26-C25 | -2.61 | 118.94      | 122.73   |
| 14  | b     | 1204 | CLA  | CMB-C2B-C3B | 2.61  | 129.57      | 124.68   |
| 14  | B     | 1202 | CLA  | CMC-C2C-C1C | 2.61  | 129.02      | 125.04   |
| 18  | a     | 4001 | BCR  | C36-C18-C17 | -2.61 | 119.26      | 122.92   |
| 18  | L     | 4019 | BCR  | C29-C30-C25 | 2.61  | 114.50      | 110.48   |
| 18  | U     | 4019 | BCR  | C29-C30-C25 | 2.61  | 114.50      | 110.48   |
| 14  | b     | 1236 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 14  | a     | 1112 | CLA  | C3C-C4C-NC  | 2.61  | 113.50      | 110.57   |
| 18  | R     | 4020 | BCR  | C36-C18-C17 | -2.61 | 119.27      | 122.92   |
| 14  | B     | 1236 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 18  | i     | 4020 | BCR  | C36-C18-C17 | -2.61 | 119.27      | 122.92   |
| 14  | A     | 1110 | CLA  | C3D-C4D-ND  | 2.61  | 114.46      | 110.24   |
| 18  | l     | 4019 | BCR  | C29-C30-C25 | 2.61  | 114.50      | 110.48   |
| 18  | B     | 4014 | BCR  | C37-C22-C21 | -2.61 | 119.27      | 122.92   |
| 14  | B     | 1213 | CLA  | C3C-C4C-NC  | 2.61  | 113.50      | 110.57   |
| 14  | H     | 1021 | CLA  | O2A-C1-C2   | 2.61  | 115.49      | 108.64   |
| 14  | b     | 1021 | CLA  | O2A-C1-C2   | 2.61  | 115.49      | 108.64   |
| 14  | a     | 1138 | CLA  | CED-O2D-CGD | 2.61  | 121.84      | 115.94   |
| 14  | G     | 1119 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 14  | b     | 1240 | CLA  | CED-O2D-CGD | 2.61  | 121.84      | 115.94   |
| 21  | G     | 6004 | LMT  | C1'-O5'-C5' | -2.61 | 108.57      | 113.69   |
| 14  | H     | 1217 | CLA  | CMC-C2C-C1C | 2.61  | 129.01      | 125.04   |
| 18  | i     | 4018 | BCR  | C38-C26-C27 | 2.61  | 118.62      | 113.62   |
| 18  | U     | 4019 | BCR  | C8-C9-C10   | -2.61 | 114.94      | 118.94   |
| 14  | G     | 1115 | CLA  | C3D-C4D-ND  | 2.61  | 114.45      | 110.24   |
| 14  | a     | 1117 | CLA  | C1D-ND-C4D  | -2.61 | 104.48      | 106.33   |
| 14  | H     | 1235 | CLA  | C3C-C4C-NC  | 2.61  | 113.49      | 110.57   |
| 14  | b     | 1202 | CLA  | CMC-C2C-C1C | 2.61  | 129.01      | 125.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | l     | 4019 | BCR  | C33-C5-C4   | 2.61  | 118.62      | 113.62   |
| 14  | a     | 1119 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 14  | B     | 1021 | CLA  | C1-O2A-CGA  | 2.60  | 123.28      | 116.44   |
| 21  | G     | 6002 | LMT  | O5B-C5B-C4B | 2.60  | 114.42      | 109.69   |
| 21  | L     | 6101 | LMT  | C4B-C3B-C2B | 2.60  | 115.37      | 110.82   |
| 14  | A     | 1102 | CLA  | C3D-C4D-ND  | 2.60  | 114.45      | 110.24   |
| 14  | A     | 1119 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 18  | I     | 4018 | BCR  | C38-C26-C27 | 2.60  | 118.62      | 113.62   |
| 18  | A     | 4003 | BCR  | C34-C9-C10  | -2.60 | 119.28      | 122.92   |
| 14  | B     | 1235 | CLA  | C3C-C4C-NC  | 2.60  | 113.49      | 110.57   |
| 14  | b     | 1236 | CLA  | CHD-C4C-C3C | -2.60 | 121.02      | 124.84   |
| 14  | A     | 1126 | CLA  | C3C-C4C-NC  | 2.60  | 113.49      | 110.57   |
| 14  | a     | 1136 | CLA  | CMC-C2C-C1C | 2.60  | 129.00      | 125.04   |
| 18  | T     | 4001 | BCR  | C24-C23-C22 | -2.60 | 122.30      | 126.23   |
| 14  | G     | 1112 | CLA  | C3C-C4C-NC  | 2.60  | 113.49      | 110.57   |
| 14  | G     | 1136 | CLA  | CMC-C2C-C1C | 2.60  | 129.00      | 125.04   |
| 18  | A     | 4003 | BCR  | C24-C23-C22 | -2.60 | 122.31      | 126.23   |
| 14  | A     | 1115 | CLA  | C3D-C4D-ND  | 2.60  | 114.44      | 110.24   |
| 14  | A     | 1119 | CLA  | C3D-C4D-ND  | 2.60  | 114.44      | 110.24   |
| 18  | a     | 4003 | BCR  | C24-C23-C22 | -2.60 | 122.31      | 126.23   |
| 14  | G     | 1115 | CLA  | C3C-C4C-NC  | 2.60  | 113.48      | 110.57   |
| 21  | l     | 6101 | LMT  | C4B-C3B-C2B | 2.60  | 115.36      | 110.82   |
| 14  | A     | 1117 | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.33   |
| 14  | a     | 1106 | CLA  | O1D-CGD-CBD | -2.60 | 119.17      | 124.48   |
| 14  | a     | 1119 | CLA  | C3D-C4D-ND  | 2.60  | 114.44      | 110.24   |
| 14  | B     | 1240 | CLA  | CED-O2D-CGD | 2.60  | 121.81      | 115.94   |
| 18  | R     | 4018 | BCR  | C38-C26-C27 | 2.59  | 118.60      | 113.62   |
| 14  | a     | 1141 | CLA  | CMC-C2C-C1C | 2.59  | 128.99      | 125.04   |
| 18  | B     | 4014 | BCR  | C19-C18-C17 | 2.59  | 122.92      | 118.94   |
| 18  | A     | 4001 | BCR  | C36-C18-C17 | -2.59 | 119.29      | 122.92   |
| 14  | A     | 1112 | CLA  | C3C-C4C-NC  | 2.59  | 113.48      | 110.57   |
| 14  | a     | 1110 | CLA  | C3C-C4C-NC  | 2.59  | 113.48      | 110.57   |
| 14  | G     | 1141 | CLA  | CMB-C2B-C3B | 2.59  | 129.53      | 124.68   |
| 14  | H     | 1021 | CLA  | C1-O2A-CGA  | 2.59  | 123.25      | 116.44   |
| 18  | K     | 4001 | BCR  | C24-C23-C22 | -2.59 | 122.32      | 126.23   |
| 14  | b     | 1021 | CLA  | C1-O2A-CGA  | 2.59  | 123.25      | 116.44   |
| 14  | B     | 1236 | CLA  | CHD-C4C-C3C | -2.59 | 121.03      | 124.84   |
| 14  | U     | 1501 | CLA  | CMC-C2C-C1C | 2.59  | 128.99      | 125.04   |
| 14  | H     | 1240 | CLA  | CED-O2D-CGD | 2.59  | 121.80      | 115.94   |
| 18  | G     | 4003 | BCR  | C24-C23-C22 | -2.59 | 122.32      | 126.23   |
| 14  | H     | 1236 | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 14  | b     | 1235 | CLA  | C3C-C4C-NC  | 2.59  | 113.48      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1126 | CLA  | C3C-C4C-NC  | 2.59  | 113.48      | 110.57   |
| 14  | G     | 1106 | CLA  | O1D-CGD-CBD | -2.59 | 119.19      | 124.48   |
| 18  | H     | 4017 | BCR  | C34-C9-C10  | -2.59 | 119.30      | 122.92   |
| 14  | B     | 1220 | CLA  | C3C-C4C-NC  | 2.59  | 113.47      | 110.57   |
| 18  | L     | 4019 | BCR  | C33-C5-C4   | 2.59  | 118.58      | 113.62   |
| 14  | A     | 1141 | CLA  | CMC-C2C-C1C | 2.59  | 128.98      | 125.04   |
| 18  | k     | 4001 | BCR  | C24-C23-C22 | -2.58 | 122.33      | 126.23   |
| 21  | A     | 6004 | LMT  | C1'-O5'-C5' | -2.58 | 108.62      | 113.69   |
| 14  | b     | 1203 | CLA  | CMC-C2C-C1C | 2.58  | 128.97      | 125.04   |
| 14  | l     | 1501 | CLA  | C3C-C4C-NC  | 2.58  | 113.47      | 110.57   |
| 21  | a     | 6002 | LMT  | C1'-O5'-C5' | -2.58 | 108.62      | 113.69   |
| 14  | a     | 1102 | CLA  | C3D-C4D-ND  | 2.58  | 114.41      | 110.24   |
| 18  | U     | 4019 | BCR  | C33-C5-C4   | 2.58  | 118.58      | 113.62   |
| 20  | i     | 5006 | LMG  | O6-C5-C6    | 2.58  | 112.85      | 106.44   |
| 15  | b     | 1219 | F6C  | OMB-CMB-C2B | -2.58 | 119.85      | 125.69   |
| 18  | G     | 4001 | BCR  | C36-C18-C17 | -2.58 | 119.31      | 122.92   |
| 14  | b     | 1234 | CLA  | C3D-C4D-ND  | 2.58  | 114.41      | 110.24   |
| 14  | a     | 1115 | CLA  | C3C-C4C-NC  | 2.58  | 113.46      | 110.57   |
| 18  | H     | 4014 | BCR  | C19-C18-C17 | 2.58  | 122.90      | 118.94   |
| 18  | A     | 4006 | BCR  | C24-C25-C26 | -2.58 | 115.22      | 121.46   |
| 14  | a     | 1135 | CLA  | C3D-C4D-ND  | 2.58  | 114.41      | 110.24   |
| 14  | G     | 1107 | CLA  | C4D-C3D-CAD | 2.58  | 111.13      | 108.10   |
| 21  | U     | 6101 | LMT  | C4B-C3B-C2B | 2.58  | 115.32      | 110.82   |
| 21  | a     | 6004 | LMT  | C1'-O5'-C5' | -2.58 | 108.63      | 113.69   |
| 14  | L     | 1501 | CLA  | CMC-C2C-C1C | 2.58  | 128.96      | 125.04   |
| 14  | H     | 1203 | CLA  | CMC-C2C-C1C | 2.58  | 128.96      | 125.04   |
| 20  | I     | 5006 | LMG  | O6-C5-C6    | 2.58  | 112.84      | 106.44   |
| 14  | B     | 1208 | CLA  | C4-C3-C5    | 2.58  | 119.60      | 115.27   |
| 14  | A     | 1106 | CLA  | O1D-CGD-CBD | -2.58 | 119.22      | 124.48   |
| 14  | B     | 1021 | CLA  | C3D-C4D-ND  | 2.57  | 114.40      | 110.24   |
| 14  | G     | 1102 | CLA  | C3D-C4D-ND  | 2.57  | 114.40      | 110.24   |
| 14  | B     | 1203 | CLA  | CMC-C2C-C1C | 2.57  | 128.96      | 125.04   |
| 14  | B     | 1234 | CLA  | C3D-C4D-ND  | 2.57  | 114.40      | 110.24   |
| 14  | H     | 1208 | CLA  | C3C-C4C-NC  | 2.57  | 113.46      | 110.57   |
| 14  | b     | 1231 | CLA  | C4D-C3D-CAD | 2.57  | 111.13      | 108.10   |
| 14  | b     | 1220 | CLA  | C3C-C4C-NC  | 2.57  | 113.45      | 110.57   |
| 18  | B     | 4017 | BCR  | C34-C9-C10  | -2.57 | 119.32      | 122.92   |
| 21  | A     | 6002 | LMT  | C1'-O5'-C5' | -2.57 | 108.64      | 113.69   |
| 14  | H     | 1023 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 21  | G     | 6002 | LMT  | C1'-O5'-C5' | -2.57 | 108.64      | 113.69   |
| 18  | A     | 4002 | BCR  | C23-C22-C21 | 2.57  | 122.89      | 118.94   |
| 14  | H     | 1021 | CLA  | C3D-C4D-ND  | 2.57  | 114.39      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | a     | 4006 | BCR  | C24-C25-C26 | -2.57 | 115.24      | 121.46   |
| 18  | G     | 4002 | BCR  | C23-C22-C21 | 2.57  | 122.88      | 118.94   |
| 14  | b     | 1023 | CLA  | CHB-C4A-NA  | 2.57  | 128.06      | 124.51   |
| 14  | k     | 1401 | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 14  | a     | 1132 | CLA  | C3C-C4C-NC  | 2.57  | 113.45      | 110.57   |
| 18  | G     | 4006 | BCR  | C24-C25-C26 | -2.57 | 115.24      | 121.46   |
| 18  | G     | 4003 | BCR  | C34-C9-C10  | -2.57 | 119.33      | 122.92   |
| 14  | b     | 1021 | CLA  | C3D-C4D-ND  | 2.57  | 114.39      | 110.24   |
| 14  | b     | 1208 | CLA  | C3C-C4C-NC  | 2.57  | 113.45      | 110.57   |
| 15  | B     | 1219 | F6C  | OMB-CMB-C2B | -2.57 | 119.88      | 125.69   |
| 14  | a     | 1104 | CLA  | C4D-C3D-CAD | 2.57  | 111.12      | 108.10   |
| 14  | B     | 1202 | CLA  | C3D-C4D-ND  | 2.57  | 114.39      | 110.24   |
| 14  | H     | 1234 | CLA  | C3D-C4D-ND  | 2.57  | 114.39      | 110.24   |
| 14  | B     | 1023 | CLA  | CHB-C4A-NA  | 2.57  | 128.06      | 124.51   |
| 20  | R     | 5006 | LMG  | O6-C5-C6    | 2.57  | 112.81      | 106.44   |
| 14  | H     | 1208 | CLA  | C4-C3-C5    | 2.57  | 119.59      | 115.27   |
| 14  | l     | 1502 | CLA  | CMC-C2C-C1C | 2.57  | 128.95      | 125.04   |
| 14  | l     | 1501 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | B     | 1208 | CLA  | C3C-C4C-NC  | 2.56  | 113.45      | 110.57   |
| 14  | G     | 1132 | CLA  | C3C-C4C-NC  | 2.56  | 113.45      | 110.57   |
| 14  | G     | 1141 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | G     | 1124 | CLA  | C4-C3-C5    | 2.56  | 119.58      | 115.27   |
| 14  | A     | 1132 | CLA  | C3C-C4C-NC  | 2.56  | 113.44      | 110.57   |
| 14  | H     | 1220 | CLA  | C3C-C4C-NC  | 2.56  | 113.44      | 110.57   |
| 14  | B     | 1205 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | A     | 1103 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 18  | A     | 4004 | BCR  | C36-C18-C17 | -2.56 | 119.33      | 122.92   |
| 18  | b     | 4017 | BCR  | C34-C9-C10  | -2.56 | 119.33      | 122.92   |
| 14  | A     | 1117 | CLA  | CMA-C3A-C4A | 2.56  | 118.66      | 111.77   |
| 14  | G     | 1117 | CLA  | CMA-C3A-C4A | 2.56  | 118.66      | 111.77   |
| 14  | a     | 1113 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | A     | 1141 | CLA  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 14  | G     | 1101 | CLA  | CAA-C2A-C3A | -2.56 | 105.77      | 112.78   |
| 14  | a     | 1124 | CLA  | C4-C3-C5    | 2.56  | 119.58      | 115.27   |
| 18  | G     | 4004 | BCR  | C36-C18-C17 | -2.56 | 119.34      | 122.92   |
| 14  | a     | 1103 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | H     | 1210 | CLA  | C4C-C3C-C2C | -2.56 | 103.17      | 106.90   |
| 14  | a     | 1101 | CLA  | CAA-C2A-C3A | -2.56 | 105.78      | 112.78   |
| 14  | H     | 1202 | CLA  | C3D-C4D-ND  | 2.56  | 114.37      | 110.24   |
| 14  | a     | 1123 | CLA  | C1-O2A-CGA  | 2.56  | 123.15      | 116.44   |
| 14  | G     | 1103 | CLA  | CMC-C2C-C1C | 2.56  | 128.93      | 125.04   |
| 14  | b     | 1232 | CLA  | CMD-C2D-C3D | -2.56 | 121.73      | 127.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1116 | CLA  | CAC-C3C-C4C | 2.55  | 128.12      | 124.81   |
| 14  | a     | 1141 | CLA  | CMB-C2B-C3B | 2.55  | 129.46      | 124.68   |
| 14  | H     | 1232 | CLA  | CMD-C2D-C3D | -2.55 | 121.74      | 127.61   |
| 18  | a     | 4002 | BCR  | C23-C22-C21 | 2.55  | 122.86      | 118.94   |
| 14  | A     | 1101 | CLA  | CAA-C2A-C3A | -2.55 | 105.78      | 112.78   |
| 14  | G     | 1104 | CLA  | CAA-C2A-C3A | -2.55 | 105.79      | 112.78   |
| 14  | A     | 1124 | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 14  | H     | 1211 | CLA  | C4D-C3D-CAD | 2.55  | 111.10      | 108.10   |
| 14  | G     | 1107 | CLA  | C3D-C4D-ND  | 2.55  | 114.37      | 110.24   |
| 19  | l     | 5102 | LHG  | O8-C23-C24  | 2.55  | 119.91      | 111.91   |
| 14  | a     | 1117 | CLA  | CMA-C3A-C4A | 2.55  | 118.63      | 111.77   |
| 14  | b     | 1208 | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 14  | G     | 1117 | CLA  | C1D-ND-C4D  | -2.55 | 104.52      | 106.33   |
| 14  | A     | 1104 | CLA  | C4D-C3D-CAD | 2.55  | 111.10      | 108.10   |
| 14  | G     | 1113 | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 14  | G     | 1103 | CLA  | CAC-C3C-C4C | 2.55  | 128.12      | 124.81   |
| 15  | H     | 1219 | F6C  | OMB-CMB-C2B | -2.55 | 119.92      | 125.69   |
| 14  | T     | 1401 | CLA  | CMB-C2B-C3B | 2.55  | 129.45      | 124.68   |
| 14  | U     | 1502 | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 14  | b     | 1202 | CLA  | C3D-C4D-ND  | 2.55  | 114.36      | 110.24   |
| 15  | b     | 1207 | F6C  | CHB-C4A-NA  | 2.55  | 126.80      | 124.45   |
| 16  | b     | 2002 | PQN  | C11-C12-C13 | -2.55 | 122.55      | 126.79   |
| 18  | a     | 4004 | BCR  | C36-C18-C17 | -2.55 | 119.35      | 122.92   |
| 14  | A     | 1113 | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 14  | K     | 1401 | CLA  | CMB-C2B-C3B | 2.55  | 129.45      | 124.68   |
| 14  | a     | 1132 | CLA  | C1-C2-C3    | -2.55 | 121.64      | 126.04   |
| 14  | a     | 1103 | CLA  | CAC-C3C-C4C | 2.55  | 128.12      | 124.81   |
| 19  | L     | 5102 | LHG  | O8-C23-C24  | 2.55  | 119.90      | 111.91   |
| 19  | U     | 5102 | LHG  | O8-C23-C24  | 2.55  | 119.90      | 111.91   |
| 14  | H     | 1236 | CLA  | C1-C2-C3    | -2.55 | 121.64      | 126.04   |
| 14  | A     | 1103 | CLA  | CAC-C3C-C4C | 2.55  | 128.11      | 124.81   |
| 14  | A     | 1107 | CLA  | C4D-C3D-CAD | 2.55  | 111.10      | 108.10   |
| 14  | G     | 1136 | CLA  | C4-C3-C5    | 2.55  | 119.55      | 115.27   |
| 18  | H     | 4005 | BCR  | C37-C22-C21 | -2.55 | 119.36      | 122.92   |
| 14  | a     | 1116 | CLA  | CAC-C3C-C4C | 2.55  | 128.11      | 124.81   |
| 14  | b     | 1210 | CLA  | C4C-C3C-C2C | -2.54 | 103.19      | 106.90   |
| 14  | a     | 1115 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 14  | B     | 1236 | CLA  | C1-C2-C3    | -2.54 | 121.64      | 126.04   |
| 16  | B     | 2002 | PQN  | C11-C12-C13 | -2.54 | 122.56      | 126.79   |
| 16  | H     | 2002 | PQN  | C11-C12-C13 | -2.54 | 122.56      | 126.79   |
| 14  | b     | 1205 | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 14  | A     | 1107 | CLA  | C3D-C4D-ND  | 2.54  | 114.35      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1211 | CLA  | C4D-C3D-CAD | 2.54  | 111.09      | 108.10   |
| 14  | G     | 1123 | CLA  | C1-O2A-CGA  | 2.54  | 123.11      | 116.44   |
| 14  | H     | 1205 | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 14  | A     | 1123 | CLA  | C1-O2A-CGA  | 2.54  | 123.11      | 116.44   |
| 14  | L     | 1502 | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 14  | H     | 1224 | CLA  | CAA-C2A-C3A | -2.54 | 105.82      | 112.78   |
| 14  | I     | 1502 | CLA  | C4-C3-C5    | 2.54  | 119.54      | 115.27   |
| 14  | B     | 1209 | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 14  | A     | 1135 | CLA  | C3D-C4D-ND  | 2.54  | 114.34      | 110.24   |
| 14  | G     | 1132 | CLA  | C1-C2-C3    | -2.54 | 121.65      | 126.04   |
| 14  | A     | 1115 | CLA  | O1D-CGD-CBD | -2.54 | 119.29      | 124.48   |
| 14  | B     | 1232 | CLA  | CMD-C2D-C3D | -2.54 | 121.78      | 127.61   |
| 14  | b     | 1224 | CLA  | CAA-C2A-C3A | -2.54 | 105.83      | 112.78   |
| 14  | b     | 1209 | CLA  | CMC-C2C-C1C | 2.54  | 128.90      | 125.04   |
| 14  | b     | 1225 | CLA  | C3D-C4D-ND  | 2.54  | 114.34      | 110.24   |
| 14  | G     | 1115 | CLA  | O1D-CGD-CBD | -2.54 | 119.29      | 124.48   |
| 14  | B     | 1210 | CLA  | C4C-C3C-C2C | -2.54 | 103.20      | 106.90   |
| 14  | B     | 1224 | CLA  | CAA-C2A-C3A | -2.54 | 105.83      | 112.78   |
| 14  | A     | 1104 | CLA  | CAA-C2A-C3A | -2.54 | 105.83      | 112.78   |
| 14  | G     | 1109 | CLA  | CMD-C2D-C3D | -2.54 | 121.78      | 127.61   |
| 14  | A     | 1132 | CLA  | C1-C2-C3    | -2.54 | 121.66      | 126.04   |
| 18  | H     | 4017 | BCR  | C23-C24-C25 | -2.54 | 120.08      | 127.20   |
| 14  | H     | 1225 | CLA  | C3D-C4D-ND  | 2.53  | 114.34      | 110.24   |
| 14  | b     | 1213 | CLA  | C3D-C4D-ND  | 2.53  | 114.34      | 110.24   |
| 18  | U     | 4022 | BCR  | C35-C13-C12 | 2.53  | 122.07      | 118.08   |
| 14  | G     | 1133 | CLA  | C3D-C4D-ND  | 2.53  | 114.34      | 110.24   |
| 14  | A     | 1116 | CLA  | CAC-C3C-C4C | 2.53  | 128.10      | 124.81   |
| 18  | B     | 4017 | BCR  | C23-C24-C25 | -2.53 | 120.09      | 127.20   |
| 14  | H     | 1222 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | H     | 1235 | CLA  | C4D-C3D-CAD | 2.53  | 111.08      | 108.10   |
| 14  | A     | 1130 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | b     | 1220 | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 14  | G     | 1105 | CLA  | C4D-C3D-CAD | 2.53  | 111.08      | 108.10   |
| 14  | A     | 1109 | CLA  | CMD-C2D-C3D | -2.53 | 121.79      | 127.61   |
| 14  | G     | 1135 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 18  | b     | 4017 | BCR  | C23-C24-C25 | -2.53 | 120.09      | 127.20   |
| 18  | L     | 4022 | BCR  | C35-C13-C12 | 2.53  | 122.06      | 118.08   |
| 14  | a     | 1130 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | b     | 1217 | CLA  | C4D-C3D-CAD | 2.53  | 111.08      | 108.10   |
| 14  | b     | 1229 | CLA  | C3C-C4C-NC  | 2.53  | 113.41      | 110.57   |
| 14  | H     | 1213 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | a     | 1109 | CLA  | C1-C2-C3    | -2.53 | 121.67      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1104 | CLA  | C4D-C3D-CAD | 2.53  | 111.08      | 108.10   |
| 14  | B     | 1213 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | a     | 1133 | CLA  | C3D-C4D-ND  | 2.53  | 114.33      | 110.24   |
| 14  | A     | 1136 | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 14  | L     | 1502 | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 18  | B     | 4005 | BCR  | C37-C22-C21 | -2.53 | 119.38      | 122.92   |
| 14  | b     | 1235 | CLA  | C4D-C3D-CAD | 2.53  | 111.08      | 108.10   |
| 14  | b     | 1021 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 14  | B     | 1228 | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.81   |
| 14  | H     | 1209 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 14  | b     | 1226 | CLA  | CAA-C2A-C3A | -2.53 | 105.86      | 112.78   |
| 14  | H     | 1021 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 14  | G     | 1132 | CLA  | O1D-CGD-CBD | -2.53 | 119.31      | 124.48   |
| 14  | b     | 1211 | CLA  | C4D-C3D-CAD | 2.53  | 111.07      | 108.10   |
| 14  | a     | 1128 | CLA  | CAA-C2A-C3A | -2.53 | 105.86      | 112.78   |
| 18  | L     | 4022 | BCR  | C34-C9-C10  | -2.53 | 119.38      | 122.92   |
| 14  | a     | 1104 | CLA  | CAA-C2A-C3A | -2.53 | 105.86      | 112.78   |
| 14  | B     | 1235 | CLA  | OBD-CAD-C3D | -2.53 | 122.44      | 128.52   |
| 14  | B     | 1215 | CLA  | CMA-C3A-C4A | 2.53  | 118.56      | 111.77   |
| 14  | B     | 1229 | CLA  | C3C-C4C-NC  | 2.53  | 113.40      | 110.57   |
| 14  | b     | 1228 | CLA  | CAC-C3C-C4C | 2.52  | 128.09      | 124.81   |
| 18  | A     | 4003 | BCR  | C23-C24-C25 | -2.52 | 120.11      | 127.20   |
| 18  | l     | 4022 | BCR  | C34-C9-C10  | -2.52 | 119.39      | 122.92   |
| 14  | b     | 1215 | CLA  | CMA-C3A-C4A | 2.52  | 118.56      | 111.77   |
| 14  | a     | 1124 | CLA  | C3D-C4D-ND  | 2.52  | 114.32      | 110.24   |
| 14  | B     | 1231 | CLA  | C4D-C3D-CAD | 2.52  | 111.07      | 108.10   |
| 18  | A     | 4002 | BCR  | C30-C25-C24 | 2.52  | 122.91      | 115.78   |
| 18  | a     | 4003 | BCR  | C23-C24-C25 | -2.52 | 120.12      | 127.20   |
| 14  | U     | 1502 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |
| 14  | l     | 1501 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |
| 18  | G     | 4003 | BCR  | C33-C5-C4   | 2.52  | 118.46      | 113.62   |
| 18  | G     | 4002 | BCR  | C30-C25-C24 | 2.52  | 122.91      | 115.78   |
| 18  | a     | 4005 | BCR  | C19-C18-C17 | 2.52  | 122.81      | 118.94   |
| 14  | a     | 1131 | CLA  | C3C-C4C-NC  | 2.52  | 113.40      | 110.57   |
| 14  | A     | 1133 | CLA  | C3D-C4D-ND  | 2.52  | 114.32      | 110.24   |
| 18  | G     | 4003 | BCR  | C23-C24-C25 | -2.52 | 120.12      | 127.20   |
| 14  | b     | 1236 | CLA  | C1-C2-C3    | -2.52 | 121.68      | 126.04   |
| 14  | H     | 1218 | CLA  | O2D-CGD-O1D | -2.52 | 118.91      | 123.84   |
| 14  | H     | 1228 | CLA  | CAC-C3C-C4C | 2.52  | 128.08      | 124.81   |
| 14  | a     | 1117 | CLA  | C3B-C4B-NB  | 2.52  | 112.47      | 109.21   |
| 14  | A     | 1112 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |
| 14  | B     | 1220 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1215 | CLA  | CMA-C3A-C4A | 2.52  | 118.54      | 111.77   |
| 14  | H     | 1220 | CLA  | CAA-C2A-C3A | -2.52 | 105.88      | 112.78   |
| 14  | a     | 1138 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |
| 14  | b     | 1228 | CLA  | C1-C2-C3    | -2.52 | 121.69      | 126.04   |
| 14  | B     | 1226 | CLA  | CAA-C2A-C3A | -2.52 | 105.88      | 112.78   |
| 18  | l     | 4022 | BCR  | C35-C13-C12 | 2.52  | 122.04      | 118.08   |
| 14  | L     | 1501 | CLA  | C4-C3-C5    | 2.52  | 119.51      | 115.27   |
| 14  | A     | 1109 | CLA  | C1-C2-C3    | -2.52 | 121.69      | 126.04   |
| 14  | H     | 1234 | CLA  | C4C-C3C-C2C | -2.52 | 103.23      | 106.90   |
| 14  | H     | 1235 | CLA  | OBD-CAD-C3D | -2.52 | 122.46      | 128.52   |
| 14  | b     | 1220 | CLA  | CMC-C2C-C1C | 2.52  | 128.87      | 125.04   |
| 14  | A     | 1138 | CLA  | C4-C3-C5    | 2.52  | 119.50      | 115.27   |
| 14  | B     | 1021 | CLA  | CMC-C2C-C1C | 2.52  | 128.87      | 125.04   |
| 13  | a     | 1011 | CL0  | C1-O2A-CGA  | 2.52  | 123.05      | 116.44   |
| 14  | a     | 1107 | CLA  | C4D-C3D-CAD | 2.52  | 111.06      | 108.10   |
| 14  | G     | 1130 | CLA  | C3D-C4D-ND  | 2.52  | 114.31      | 110.24   |
| 14  | A     | 1131 | CLA  | C3C-C4C-NC  | 2.52  | 113.39      | 110.57   |
| 14  | H     | 1229 | CLA  | C3C-C4C-NC  | 2.52  | 113.39      | 110.57   |
| 14  | a     | 1109 | CLA  | CMD-C2D-C3D | -2.51 | 121.83      | 127.61   |
| 14  | A     | 1128 | CLA  | CAA-C2A-C3A | -2.51 | 105.89      | 112.78   |
| 14  | b     | 1235 | CLA  | OBD-CAD-C3D | -2.51 | 122.47      | 128.52   |
| 14  | H     | 1220 | CLA  | C4-C3-C5    | 2.51  | 119.50      | 115.27   |
| 14  | a     | 1136 | CLA  | C4-C3-C5    | 2.51  | 119.50      | 115.27   |
| 18  | a     | 4002 | BCR  | C30-C25-C24 | 2.51  | 122.89      | 115.78   |
| 18  | a     | 4003 | BCR  | C33-C5-C4   | 2.51  | 118.44      | 113.62   |
| 14  | a     | 1116 | CLA  | CAA-CBA-CGA | -2.51 | 105.91      | 113.25   |
| 14  | G     | 1109 | CLA  | C1-C2-C3    | -2.51 | 121.70      | 126.04   |
| 14  | A     | 1139 | CLA  | CMA-C3A-C4A | 2.51  | 118.53      | 111.77   |
| 18  | U     | 4022 | BCR  | C34-C9-C10  | -2.51 | 119.40      | 122.92   |
| 14  | b     | 1222 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | H     | 1226 | CLA  | CAA-C2A-C3A | -2.51 | 105.90      | 112.78   |
| 14  | B     | 1225 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | G     | 1139 | CLA  | CMA-C3A-C4A | 2.51  | 118.52      | 111.77   |
| 14  | G     | 1101 | CLA  | CMB-C2B-C3B | 2.51  | 129.38      | 124.68   |
| 14  | A     | 1129 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | G     | 1128 | CLA  | CAA-C2A-C3A | -2.51 | 105.91      | 112.78   |
| 14  | a     | 1012 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | a     | 1107 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | a     | 1129 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 14  | b     | 1233 | CLA  | C3D-C4D-ND  | 2.51  | 114.30      | 110.24   |
| 15  | B     | 1207 | F6C  | CHB-C4A-NA  | 2.51  | 126.76      | 124.45   |
| 14  | a     | 1139 | CLA  | CMA-C3A-C4A | 2.51  | 118.51      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1105 | CLA  | C4D-C3D-CAD | 2.51  | 111.05      | 108.10   |
| 14  | a     | 1108 | CLA  | CMC-C2C-C1C | 2.51  | 128.86      | 125.04   |
| 14  | B     | 1208 | CLA  | C3D-C4D-ND  | 2.51  | 114.29      | 110.24   |
| 18  | A     | 4003 | BCR  | C33-C5-C4   | 2.51  | 118.43      | 113.62   |
| 14  | G     | 1124 | CLA  | C3D-C4D-ND  | 2.51  | 114.29      | 110.24   |
| 14  | U     | 1501 | CLA  | C4-C3-C5    | 2.51  | 119.49      | 115.27   |
| 14  | A     | 1108 | CLA  | CMC-C2C-C1C | 2.51  | 128.86      | 125.04   |
| 14  | H     | 1208 | CLA  | C3D-C4D-ND  | 2.51  | 114.29      | 110.24   |
| 14  | A     | 1132 | CLA  | O1D-CGD-CBD | -2.51 | 119.36      | 124.48   |
| 14  | A     | 1117 | CLA  | C3B-C4B-NB  | 2.51  | 112.45      | 109.21   |
| 14  | A     | 1124 | CLA  | C3D-C4D-ND  | 2.51  | 114.29      | 110.24   |
| 14  | H     | 1231 | CLA  | C4D-C3D-CAD | 2.51  | 111.05      | 108.10   |
| 14  | B     | 1220 | CLA  | CAA-C2A-C3A | -2.51 | 105.92      | 112.78   |
| 14  | H     | 1232 | CLA  | CAC-C3C-C4C | 2.50  | 128.06      | 124.81   |
| 14  | G     | 1116 | CLA  | CAA-CBA-CGA | -2.50 | 105.94      | 113.25   |
| 14  | B     | 1205 | CLA  | CBA-CAA-C2A | 2.50  | 121.25      | 113.86   |
| 15  | H     | 1207 | F6C  | CHB-C4A-NA  | 2.50  | 126.75      | 124.45   |
| 14  | a     | 1105 | CLA  | C4D-C3D-CAD | 2.50  | 111.05      | 108.10   |
| 14  | a     | 1115 | CLA  | C4D-C3D-CAD | 2.50  | 111.05      | 108.10   |
| 14  | B     | 1234 | CLA  | C4C-C3C-C2C | -2.50 | 103.25      | 106.90   |
| 18  | b     | 4005 | BCR  | C37-C22-C21 | -2.50 | 119.42      | 122.92   |
| 14  | a     | 1112 | CLA  | C4-C3-C5    | 2.50  | 119.48      | 115.27   |
| 18  | A     | 4005 | BCR  | C19-C18-C17 | 2.50  | 122.78      | 118.94   |
| 14  | B     | 1233 | CLA  | C3D-C4D-ND  | 2.50  | 114.29      | 110.24   |
| 14  | G     | 1129 | CLA  | C3D-C4D-ND  | 2.50  | 114.29      | 110.24   |
| 14  | a     | 1137 | CLA  | C3D-C4D-ND  | 2.50  | 114.29      | 110.24   |
| 14  | B     | 1218 | CLA  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 14  | b     | 1232 | CLA  | CAC-C3C-C4C | 2.50  | 128.06      | 124.81   |
| 14  | B     | 1220 | CLA  | CMC-C2C-C1C | 2.50  | 128.85      | 125.04   |
| 14  | B     | 1217 | CLA  | C4D-C3D-CAD | 2.50  | 111.05      | 108.10   |
| 14  | A     | 1116 | CLA  | CAA-CBA-CGA | -2.50 | 105.94      | 113.25   |
| 14  | a     | 1132 | CLA  | O1D-CGD-CBD | -2.50 | 119.37      | 124.48   |
| 14  | B     | 1222 | CLA  | C3D-C4D-ND  | 2.50  | 114.28      | 110.24   |
| 14  | a     | 1132 | CLA  | C3D-C4D-ND  | 2.50  | 114.28      | 110.24   |
| 15  | b     | 1219 | F6C  | CMC-C2C-C3C | 2.50  | 129.66      | 124.94   |
| 13  | G     | 1011 | CL0  | C1-O2A-CGA  | 2.50  | 123.00      | 116.44   |
| 14  | H     | 1205 | CLA  | CBA-CAA-C2A | 2.50  | 121.24      | 113.86   |
| 14  | K     | 1401 | CLA  | C3D-C4D-ND  | 2.50  | 114.28      | 110.24   |
| 14  | B     | 1228 | CLA  | C1-C2-C3    | -2.50 | 121.72      | 126.04   |
| 18  | m     | 4021 | BCR  | C30-C25-C26 | -2.50 | 119.09      | 122.61   |
| 14  | b     | 1205 | CLA  | CBA-CAA-C2A | 2.50  | 121.24      | 113.86   |
| 14  | b     | 1234 | CLA  | C4C-C3C-C2C | -2.50 | 103.26      | 106.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1112 | CLA  | C4-C3-C5    | 2.50  | 119.47      | 115.27   |
| 14  | k     | 1401 | CLA  | C3D-C4D-ND  | 2.50  | 114.28      | 110.24   |
| 14  | a     | 1138 | CLA  | CAC-C3C-C4C | 2.50  | 128.05      | 124.81   |
| 13  | A     | 1011 | CL0  | C1-O2A-CGA  | 2.50  | 122.99      | 116.44   |
| 14  | B     | 1232 | CLA  | CAC-C3C-C4C | 2.50  | 128.05      | 124.81   |
| 14  | B     | 1235 | CLA  | C4D-C3D-CAD | 2.50  | 111.04      | 108.10   |
| 14  | G     | 1115 | CLA  | C4D-C3D-CAD | 2.50  | 111.04      | 108.10   |
| 14  | H     | 1233 | CLA  | C3D-C4D-ND  | 2.50  | 114.27      | 110.24   |
| 14  | G     | 1131 | CLA  | CMB-C2B-C3B | 2.49  | 129.35      | 124.68   |
| 14  | G     | 1131 | CLA  | C3C-C4C-NC  | 2.49  | 113.37      | 110.57   |
| 15  | b     | 1238 | F6C  | CMA-C3A-C2A | -2.49 | 119.34      | 126.12   |
| 14  | A     | 1115 | CLA  | C4D-C3D-CAD | 2.49  | 111.04      | 108.10   |
| 14  | G     | 1138 | CLA  | C4-C3-C5    | 2.49  | 119.47      | 115.27   |
| 14  | G     | 1138 | CLA  | CAC-C3C-C4C | 2.49  | 128.05      | 124.81   |
| 14  | A     | 1012 | CLA  | C3D-C4D-ND  | 2.49  | 114.27      | 110.24   |
| 14  | T     | 1401 | CLA  | C3D-C4D-ND  | 2.49  | 114.27      | 110.24   |
| 14  | H     | 1235 | CLA  | CMA-C3A-C4A | 2.49  | 118.47      | 111.77   |
| 14  | a     | 1115 | CLA  | C4-C3-C2    | -2.49 | 117.28      | 123.68   |
| 14  | b     | 1220 | CLA  | CAA-C2A-C3A | -2.49 | 105.95      | 112.78   |
| 14  | A     | 1127 | CLA  | C3D-C4D-ND  | 2.49  | 114.27      | 110.24   |
| 14  | G     | 1122 | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 14  | G     | 1114 | CLA  | C3D-C4D-ND  | 2.49  | 114.27      | 110.24   |
| 14  | H     | 1228 | CLA  | C1-C2-C3    | -2.49 | 121.73      | 126.04   |
| 14  | b     | 1218 | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 18  | B     | 4009 | BCR  | C36-C18-C17 | -2.49 | 119.43      | 122.92   |
| 14  | B     | 1235 | CLA  | CMA-C3A-C4A | 2.49  | 118.47      | 111.77   |
| 14  | b     | 1235 | CLA  | CMA-C3A-C4A | 2.49  | 118.47      | 111.77   |
| 18  | V     | 4021 | BCR  | C30-C25-C26 | -2.49 | 119.11      | 122.61   |
| 14  | H     | 1224 | CLA  | C1-C2-C3    | -2.49 | 121.74      | 126.04   |
| 18  | H     | 4009 | BCR  | C36-C18-C17 | -2.49 | 119.44      | 122.92   |
| 14  | G     | 1101 | CLA  | CMD-C2D-C3D | -2.49 | 121.89      | 127.61   |
| 14  | G     | 1108 | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 14  | a     | 1108 | CLA  | O1D-CGD-CBD | -2.49 | 119.39      | 124.48   |
| 14  | H     | 1214 | CLA  | CAA-C2A-C3A | -2.49 | 105.97      | 112.78   |
| 21  | b     | 6003 | LMT  | O5'-C1'-O1' | -2.49 | 104.08      | 109.97   |
| 14  | A     | 1127 | CLA  | C4-C3-C5    | 2.49  | 119.45      | 115.27   |
| 14  | a     | 1131 | CLA  | CMB-C2B-C3B | 2.49  | 129.33      | 124.68   |
| 15  | B     | 1219 | F6C  | CMC-C2C-C3C | 2.49  | 129.63      | 124.94   |
| 14  | G     | 1117 | CLA  | C3B-C4B-NB  | 2.49  | 112.42      | 109.21   |
| 14  | H     | 1217 | CLA  | C4D-C3D-CAD | 2.49  | 111.03      | 108.10   |
| 18  | G     | 4005 | BCR  | C19-C18-C17 | 2.48  | 122.75      | 118.94   |
| 14  | A     | 1114 | CLA  | C3D-C4D-ND  | 2.48  | 114.26      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1138 | CLA  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 18  | M     | 4021 | BCR  | C30-C25-C26 | -2.48 | 119.11      | 122.61   |
| 14  | b     | 1214 | CLA  | CAA-C2A-C3A | -2.48 | 105.98      | 112.78   |
| 14  | G     | 1138 | CLA  | O2D-CGD-O1D | -2.48 | 118.98      | 123.84   |
| 14  | a     | 1134 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 14  | A     | 1138 | CLA  | O2D-CGD-O1D | -2.48 | 118.98      | 123.84   |
| 15  | H     | 1219 | F6C  | CMC-C2C-C3C | 2.48  | 129.62      | 124.94   |
| 14  | B     | 1214 | CLA  | CAA-C2A-C3A | -2.48 | 105.98      | 112.78   |
| 14  | b     | 1224 | CLA  | C1-C2-C3    | -2.48 | 121.75      | 126.04   |
| 18  | b     | 4009 | BCR  | C36-C18-C17 | -2.48 | 119.45      | 122.92   |
| 14  | G     | 1111 | CLA  | CAA-CBA-CGA | -2.48 | 106.00      | 113.25   |
| 14  | A     | 1132 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 14  | a     | 1138 | CLA  | O2D-CGD-O1D | -2.48 | 118.99      | 123.84   |
| 14  | A     | 1108 | CLA  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 14  | G     | 1108 | CLA  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 14  | A     | 1137 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 14  | G     | 1012 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 14  | b     | 1208 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 15  | B     | 1238 | F6C  | CMA-C3A-C2A | -2.48 | 119.39      | 126.12   |
| 14  | A     | 1122 | CLA  | CMB-C2B-C3B | 2.48  | 129.31      | 124.68   |
| 14  | A     | 1131 | CLA  | CMB-C2B-C3B | 2.48  | 129.31      | 124.68   |
| 14  | H     | 1220 | CLA  | CMC-C2C-C1C | 2.48  | 128.81      | 125.04   |
| 14  | G     | 1137 | CLA  | C3D-C4D-ND  | 2.48  | 114.25      | 110.24   |
| 14  | a     | 1111 | CLA  | CAA-CBA-CGA | -2.48 | 106.02      | 113.25   |
| 14  | A     | 1101 | CLA  | CMB-C2B-C3B | 2.48  | 129.31      | 124.68   |
| 21  | B     | 6003 | LMT  | O5'-C1'-O1' | -2.48 | 104.11      | 109.97   |
| 14  | A     | 1111 | CLA  | CAA-CBA-CGA | -2.47 | 106.02      | 113.25   |
| 14  | H     | 1023 | CLA  | CBC-CAC-C3C | 2.47  | 119.25      | 112.43   |
| 14  | G     | 1127 | CLA  | C3D-C4D-ND  | 2.47  | 114.24      | 110.24   |
| 14  | a     | 1122 | CLA  | CMB-C2B-C3B | 2.47  | 129.31      | 124.68   |
| 14  | A     | 1115 | CLA  | C4-C3-C2    | -2.47 | 117.33      | 123.68   |
| 14  | G     | 1132 | CLA  | C3D-C4D-ND  | 2.47  | 114.24      | 110.24   |
| 15  | A     | 1121 | F6C  | CHB-C4A-NA  | 2.47  | 126.72      | 124.45   |
| 14  | G     | 1136 | CLA  | C3C-C4C-NC  | 2.47  | 113.34      | 110.57   |
| 14  | H     | 1224 | CLA  | C4-C3-C2    | -2.47 | 117.34      | 123.68   |
| 15  | b     | 1238 | F6C  | CHB-C4A-NA  | 2.47  | 126.72      | 124.45   |
| 14  | a     | 1101 | CLA  | CMD-C2D-C3D | -2.47 | 121.93      | 127.61   |
| 14  | a     | 1117 | CLA  | CHC-C1C-C2C | -2.47 | 119.89      | 126.72   |
| 14  | a     | 1139 | CLA  | C4D-C3D-CAD | 2.47  | 111.01      | 108.10   |
| 14  | H     | 1226 | CLA  | CHC-C1C-C2C | -2.47 | 119.89      | 126.72   |
| 14  | H     | 1217 | CLA  | CMA-C3A-C4A | 2.47  | 118.40      | 111.77   |
| 18  | K     | 4001 | BCR  | C3-C4-C5    | -2.47 | 109.67      | 114.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1114 | CLA  | CMD-C2D-C3D | -2.47 | 121.94      | 127.61   |
| 14  | G     | 1127 | CLA  | C4-C3-C5    | 2.47  | 119.42      | 115.27   |
| 14  | G     | 1115 | CLA  | C4-C3-C2    | -2.47 | 117.35      | 123.68   |
| 15  | H     | 1238 | F6C  | CMA-C3A-C2A | -2.47 | 119.42      | 126.12   |
| 14  | B     | 1023 | CLA  | CBC-CAC-C3C | 2.47  | 119.23      | 112.43   |
| 18  | T     | 4001 | BCR  | C3-C4-C5    | -2.47 | 109.67      | 114.08   |
| 21  | b     | 6001 | LMT  | C3'-C4'-C5' | -2.47 | 105.27      | 110.93   |
| 14  | A     | 1101 | CLA  | CMD-C2D-C3D | -2.46 | 121.94      | 127.61   |
| 14  | H     | 1212 | CLA  | CAC-C3C-C4C | 2.46  | 128.01      | 124.81   |
| 18  | H     | 4017 | BCR  | C35-C13-C12 | 2.46  | 121.96      | 118.08   |
| 14  | B     | 1224 | CLA  | C1-C2-C3    | -2.46 | 121.78      | 126.04   |
| 14  | a     | 1127 | CLA  | C4-C3-C5    | 2.46  | 119.42      | 115.27   |
| 14  | a     | 1101 | CLA  | CMB-C2B-C3B | 2.46  | 129.29      | 124.68   |
| 14  | a     | 1138 | CLA  | C1-O2A-CGA  | 2.46  | 122.91      | 116.44   |
| 14  | B     | 1206 | CLA  | CMC-C2C-C3C | 2.46  | 132.80      | 126.12   |
| 14  | a     | 1127 | CLA  | C3D-C4D-ND  | 2.46  | 114.22      | 110.24   |
| 14  | H     | 1234 | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 21  | H     | 6003 | LMT  | O5'-C1'-O1' | -2.46 | 104.14      | 109.97   |
| 18  | B     | 4017 | BCR  | C35-C13-C12 | 2.46  | 121.95      | 118.08   |
| 14  | G     | 1130 | CLA  | C3C-C4C-NC  | 2.46  | 113.33      | 110.57   |
| 14  | A     | 1114 | CLA  | CMD-C2D-C3D | -2.46 | 121.95      | 127.61   |
| 21  | B     | 6001 | LMT  | C3'-C4'-C5' | -2.46 | 105.28      | 110.93   |
| 18  | L     | 4019 | BCR  | C35-C13-C12 | 2.46  | 121.95      | 118.08   |
| 14  | A     | 1134 | CLA  | C3D-C4D-ND  | 2.46  | 114.22      | 110.24   |
| 14  | A     | 1117 | CLA  | CHC-C1C-C2C | -2.46 | 119.92      | 126.72   |
| 14  | B     | 1226 | CLA  | CHC-C1C-C2C | -2.46 | 119.92      | 126.72   |
| 14  | H     | 1215 | CLA  | CMC-C2C-C1C | 2.46  | 128.78      | 125.04   |
| 15  | B     | 1238 | F6C  | CHB-C4A-NA  | 2.46  | 126.71      | 124.45   |
| 14  | G     | 1128 | CLA  | CMC-C2C-C3C | 2.46  | 132.79      | 126.12   |
| 14  | b     | 1023 | CLA  | CBC-CAC-C3C | 2.46  | 119.21      | 112.43   |
| 18  | H     | 4009 | BCR  | C1-C6-C7    | 2.46  | 122.73      | 115.78   |
| 14  | G     | 1117 | CLA  | CHC-C1C-C2C | -2.46 | 119.93      | 126.72   |
| 14  | b     | 1226 | CLA  | CHC-C1C-C2C | -2.46 | 119.93      | 126.72   |
| 18  | a     | 4006 | BCR  | C35-C13-C12 | 2.46  | 121.95      | 118.08   |
| 21  | H     | 6001 | LMT  | C3'-C4'-C5' | -2.46 | 105.30      | 110.93   |
| 14  | B     | 1212 | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 13  | a     | 1011 | CL0  | C4-C3-C5    | 2.46  | 119.40      | 115.27   |
| 14  | G     | 1134 | CLA  | C3D-C4D-ND  | 2.46  | 114.21      | 110.24   |
| 14  | b     | 1206 | CLA  | CMC-C2C-C3C | 2.45  | 132.78      | 126.12   |
| 14  | B     | 1217 | CLA  | CMA-C3A-C4A | 2.45  | 118.37      | 111.77   |
| 18  | k     | 4001 | BCR  | C3-C4-C5    | -2.45 | 109.69      | 114.08   |
| 15  | B     | 1230 | F6C  | CHA-C1A-C2A | -2.45 | 123.19      | 129.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1136 | CLA  | C3C-C4C-NC  | 2.45  | 113.32      | 110.57   |
| 14  | a     | 1114 | CLA  | C3D-C4D-ND  | 2.45  | 114.20      | 110.24   |
| 14  | B     | 1235 | CLA  | CMC-C2C-C1C | 2.45  | 128.77      | 125.04   |
| 15  | G     | 1121 | F6C  | CHB-C4A-NA  | 2.45  | 126.71      | 124.45   |
| 18  | l     | 4019 | BCR  | C35-C13-C12 | 2.45  | 121.94      | 118.08   |
| 14  | b     | 1224 | CLA  | C4-C3-C2    | -2.45 | 117.39      | 123.68   |
| 14  | b     | 1235 | CLA  | CMC-C2C-C1C | 2.45  | 128.77      | 125.04   |
| 14  | G     | 1106 | CLA  | C3D-C4D-ND  | 2.45  | 114.20      | 110.24   |
| 14  | b     | 1205 | CLA  | C4D-C3D-CAD | 2.45  | 110.98      | 108.10   |
| 14  | H     | 1206 | CLA  | CMC-C2C-C3C | 2.45  | 132.77      | 126.12   |
| 14  | b     | 1215 | CLA  | C1-C2-C3    | -2.45 | 121.81      | 126.04   |
| 14  | B     | 1224 | CLA  | C4-C3-C2    | -2.45 | 117.39      | 123.68   |
| 14  | b     | 1217 | CLA  | CMA-C3A-C4A | 2.45  | 118.35      | 111.77   |
| 14  | G     | 1138 | CLA  | C1-O2A-CGA  | 2.45  | 122.87      | 116.44   |
| 14  | B     | 1210 | CLA  | C1-O2A-CGA  | 2.45  | 122.87      | 116.44   |
| 14  | A     | 1138 | CLA  | C1-O2A-CGA  | 2.45  | 122.86      | 116.44   |
| 14  | b     | 1210 | CLA  | C1-O2A-CGA  | 2.45  | 122.86      | 116.44   |
| 14  | A     | 1141 | CLA  | C4D-C3D-CAD | 2.45  | 110.98      | 108.10   |
| 14  | l     | 1501 | CLA  | C1-O2A-CGA  | 2.45  | 122.86      | 116.44   |
| 14  | B     | 1215 | CLA  | CMC-C2C-C1C | 2.45  | 128.76      | 125.04   |
| 14  | A     | 1128 | CLA  | CMC-C2C-C3C | 2.45  | 132.76      | 126.12   |
| 14  | a     | 1114 | CLA  | CMD-C2D-C3D | -2.45 | 121.99      | 127.61   |
| 14  | m     | 1501 | CLA  | C5-C3-C4    | 2.45  | 120.00      | 114.60   |
| 15  | a     | 1121 | F6C  | CHB-C4A-NA  | 2.45  | 126.70      | 124.45   |
| 14  | A     | 1136 | CLA  | C3D-C4D-ND  | 2.44  | 114.19      | 110.24   |
| 18  | B     | 4009 | BCR  | C1-C6-C7    | 2.44  | 122.69      | 115.78   |
| 14  | a     | 1128 | CLA  | CMC-C2C-C3C | 2.44  | 132.75      | 126.12   |
| 14  | H     | 1220 | CLA  | C3D-C4D-ND  | 2.44  | 114.19      | 110.24   |
| 14  | B     | 1234 | CLA  | CAC-C3C-C4C | 2.44  | 127.98      | 124.81   |
| 14  | G     | 1118 | CLA  | C1-C2-C3    | -2.44 | 121.82      | 126.04   |
| 18  | b     | 4017 | BCR  | C35-C13-C12 | 2.44  | 121.92      | 118.08   |
| 14  | A     | 1139 | CLA  | C4D-C3D-CAD | 2.44  | 110.97      | 108.10   |
| 15  | H     | 1230 | F6C  | CHA-C1A-C2A | -2.44 | 123.22      | 129.84   |
| 14  | a     | 1103 | CLA  | C1-O2A-CGA  | 2.44  | 122.85      | 116.44   |
| 14  | V     | 1501 | CLA  | C5-C3-C4    | 2.44  | 120.00      | 114.60   |
| 15  | H     | 1237 | F6C  | CHA-C1A-C2A | -2.44 | 123.22      | 129.84   |
| 14  | a     | 1136 | CLA  | C3D-C4D-ND  | 2.44  | 114.19      | 110.24   |
| 14  | G     | 1139 | CLA  | C4D-C3D-CAD | 2.44  | 110.97      | 108.10   |
| 14  | M     | 1501 | CLA  | C5-C3-C4    | 2.44  | 119.99      | 114.60   |
| 15  | b     | 1230 | F6C  | CHA-C1A-C2A | -2.44 | 123.22      | 129.84   |
| 14  | U     | 1501 | CLA  | C1-O2A-CGA  | 2.44  | 122.84      | 116.44   |
| 14  | H     | 1235 | CLA  | CMC-C2C-C1C | 2.44  | 128.75      | 125.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1202 | CLA  | C11-C12-C13 | -2.44 | 108.04      | 115.92   |
| 14  | L     | 1501 | CLA  | C1-O2A-CGA  | 2.44  | 122.84      | 116.44   |
| 14  | A     | 1103 | CLA  | C1-O2A-CGA  | 2.44  | 122.84      | 116.44   |
| 21  | a     | 6002 | LMT  | O1B-C4'-C5' | -2.44 | 102.77      | 109.45   |
| 14  | A     | 1106 | CLA  | C3D-C4D-ND  | 2.44  | 114.18      | 110.24   |
| 14  | A     | 1130 | CLA  | C3C-C4C-NC  | 2.44  | 113.30      | 110.57   |
| 20  | b     | 5002 | LMG  | O8-C28-C29  | 2.44  | 119.55      | 111.91   |
| 14  | a     | 1106 | CLA  | C3D-C4D-ND  | 2.44  | 114.18      | 110.24   |
| 14  | H     | 1227 | CLA  | CMD-C2D-C3D | -2.44 | 122.01      | 127.61   |
| 18  | b     | 4009 | BCR  | C1-C6-C7    | 2.43  | 122.67      | 115.78   |
| 14  | G     | 1136 | CLA  | C3D-C4D-ND  | 2.43  | 114.18      | 110.24   |
| 14  | B     | 1215 | CLA  | C1-C2-C3    | -2.43 | 121.83      | 126.04   |
| 14  | b     | 1212 | CLA  | CAC-C3C-C4C | 2.43  | 127.97      | 124.81   |
| 20  | B     | 5002 | LMG  | O8-C28-C29  | 2.43  | 119.54      | 111.91   |
| 14  | B     | 1228 | CLA  | OBD-CAD-C3D | -2.43 | 122.67      | 128.52   |
| 14  | H     | 1210 | CLA  | C1-O2A-CGA  | 2.43  | 122.83      | 116.44   |
| 14  | G     | 1103 | CLA  | C1-O2A-CGA  | 2.43  | 122.83      | 116.44   |
| 18  | U     | 4019 | BCR  | C35-C13-C12 | 2.43  | 121.91      | 118.08   |
| 18  | A     | 4001 | BCR  | C34-C9-C10  | -2.43 | 119.52      | 122.92   |
| 14  | U     | 1503 | CLA  | CMA-C3A-C4A | 2.43  | 118.31      | 111.77   |
| 14  | A     | 1120 | CLA  | C3D-C4D-ND  | 2.43  | 114.17      | 110.24   |
| 21  | m     | 6000 | LMT  | C3'-C4'-C5' | -2.43 | 105.35      | 110.93   |
| 21  | A     | 6002 | LMT  | O1B-C4'-C5' | -2.43 | 102.79      | 109.45   |
| 15  | b     | 1237 | F6C  | CHA-C1A-C2A | -2.43 | 123.25      | 129.84   |
| 14  | H     | 1228 | CLA  | OBD-CAD-C3D | -2.43 | 122.67      | 128.52   |
| 18  | a     | 4001 | BCR  | C34-C9-C10  | -2.43 | 119.52      | 122.92   |
| 14  | B     | 1227 | CLA  | CMD-C2D-C3D | -2.43 | 122.02      | 127.61   |
| 13  | A     | 1011 | CL0  | C4-C3-C5    | 2.43  | 119.36      | 115.27   |
| 18  | A     | 4006 | BCR  | C35-C13-C12 | 2.43  | 121.90      | 118.08   |
| 20  | H     | 5002 | LMG  | O8-C28-C29  | 2.43  | 119.53      | 111.91   |
| 14  | a     | 1130 | CLA  | C3C-C4C-NC  | 2.43  | 113.29      | 110.57   |
| 15  | B     | 1237 | F6C  | CHA-C1A-C2A | -2.43 | 123.25      | 129.84   |
| 14  | H     | 1206 | CLA  | CHC-C1C-C2C | -2.43 | 120.01      | 126.72   |
| 14  | B     | 1205 | CLA  | C4D-C3D-CAD | 2.43  | 110.96      | 108.10   |
| 14  | B     | 1217 | CLA  | CMB-C2B-C3B | 2.43  | 129.22      | 124.68   |
| 14  | H     | 1218 | CLA  | C3C-C4C-NC  | 2.43  | 113.29      | 110.57   |
| 14  | b     | 1228 | CLA  | OBD-CAD-C3D | -2.43 | 122.68      | 128.52   |
| 14  | A     | 1108 | CLA  | O2D-CGD-O1D | -2.43 | 119.09      | 123.84   |
| 14  | l     | 1503 | CLA  | CMA-C3A-C4A | 2.43  | 118.29      | 111.77   |
| 14  | A     | 1118 | CLA  | C1-C2-C3    | -2.42 | 121.85      | 126.04   |
| 14  | L     | 1503 | CLA  | CMA-C3A-C4A | 2.42  | 118.29      | 111.77   |
| 21  | M     | 6000 | LMT  | C3'-C4'-C5' | -2.42 | 105.37      | 110.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1012 | CLA  | C11-C12-C13 | -2.42 | 108.08      | 115.92   |
| 14  | a     | 1012 | CLA  | C11-C12-C13 | -2.42 | 108.08      | 115.92   |
| 14  | b     | 1206 | CLA  | C3D-C4D-ND  | 2.42  | 114.16      | 110.24   |
| 15  | B     | 1238 | F6C  | CHA-C1A-C2A | -2.42 | 123.27      | 129.84   |
| 14  | k     | 1401 | CLA  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 14  | G     | 1116 | CLA  | C3D-C4D-ND  | 2.42  | 114.16      | 110.24   |
| 14  | b     | 1234 | CLA  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 14  | b     | 1215 | CLA  | CMC-C2C-C1C | 2.42  | 128.73      | 125.04   |
| 18  | B     | 4004 | BCR  | C37-C22-C21 | -2.42 | 119.53      | 122.92   |
| 21  | V     | 6000 | LMT  | C3'-C4'-C5' | -2.42 | 105.37      | 110.93   |
| 14  | b     | 1202 | CLA  | C11-C12-C13 | -2.42 | 108.09      | 115.92   |
| 14  | a     | 1126 | CLA  | CMC-C2C-C1C | 2.42  | 128.73      | 125.04   |
| 14  | B     | 1202 | CLA  | C11-C12-C13 | -2.42 | 108.09      | 115.92   |
| 14  | U     | 1503 | CLA  | C4-C3-C5    | 2.42  | 119.34      | 115.27   |
| 14  | G     | 1123 | CLA  | C4D-C3D-CAD | 2.42  | 110.95      | 108.10   |
| 14  | A     | 1012 | CLA  | C11-C12-C13 | -2.42 | 108.09      | 115.92   |
| 14  | B     | 1206 | CLA  | C3D-C4D-ND  | 2.42  | 114.15      | 110.24   |
| 18  | G     | 4002 | BCR  | C33-C5-C6   | -2.42 | 121.81      | 124.53   |
| 21  | G     | 6002 | LMT  | O1B-C4'-C5' | -2.42 | 102.82      | 109.45   |
| 15  | H     | 1238 | F6C  | CHA-C1A-C2A | -2.42 | 123.28      | 129.84   |
| 15  | b     | 1238 | F6C  | CHA-C1A-C2A | -2.42 | 123.28      | 129.84   |
| 14  | T     | 1401 | CLA  | OBD-CAD-C3D | -2.42 | 122.70      | 128.52   |
| 14  | b     | 1227 | CLA  | CMD-C2D-C3D | -2.42 | 122.05      | 127.61   |
| 18  | H     | 4004 | BCR  | C37-C22-C21 | -2.42 | 119.54      | 122.92   |
| 14  | k     | 1401 | CLA  | OBD-CAD-C3D | -2.42 | 122.70      | 128.52   |
| 14  | H     | 1214 | CLA  | C4-C3-C5    | 2.42  | 119.34      | 115.27   |
| 14  | a     | 1118 | CLA  | C1-C2-C3    | -2.42 | 121.86      | 126.04   |
| 14  | A     | 1117 | CLA  | C1-O2A-CGA  | 2.42  | 122.78      | 116.44   |
| 14  | G     | 1117 | CLA  | C1-O2A-CGA  | 2.42  | 122.78      | 116.44   |
| 14  | G     | 1108 | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 14  | a     | 1108 | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 14  | H     | 1217 | CLA  | CMB-C2B-C3B | 2.42  | 129.20      | 124.68   |
| 14  | H     | 1214 | CLA  | O1D-CGD-CBD | -2.42 | 119.54      | 124.48   |
| 14  | b     | 1214 | CLA  | O1D-CGD-CBD | -2.41 | 119.54      | 124.48   |
| 14  | H     | 1215 | CLA  | C1-C2-C3    | -2.41 | 121.87      | 126.04   |
| 14  | B     | 1220 | CLA  | C3D-C4D-ND  | 2.41  | 114.14      | 110.24   |
| 14  | a     | 1120 | CLA  | C3D-C4D-ND  | 2.41  | 114.14      | 110.24   |
| 14  | A     | 1116 | CLA  | C3D-C4D-ND  | 2.41  | 114.14      | 110.24   |
| 14  | B     | 1206 | CLA  | CHC-C1C-C2C | -2.41 | 120.05      | 126.72   |
| 18  | a     | 4003 | BCR  | C36-C18-C17 | -2.41 | 119.54      | 122.92   |
| 14  | G     | 1114 | CLA  | CMA-C3A-C4A | 2.41  | 118.26      | 111.77   |
| 14  | a     | 1136 | CLA  | C3C-C4C-NC  | 2.41  | 113.28      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1233 | CLA  | CMD-C2D-C3D | -2.41 | 122.07      | 127.61   |
| 14  | a     | 1117 | CLA  | C1-O2A-CGA  | 2.41  | 122.77      | 116.44   |
| 14  | B     | 1214 | CLA  | C4-C3-C5    | 2.41  | 119.33      | 115.27   |
| 15  | B     | 1238 | F6C  | CMD-C2D-C3D | -2.41 | 122.07      | 127.61   |
| 14  | b     | 1206 | CLA  | CAA-C2A-C3A | -2.41 | 106.18      | 112.78   |
| 18  | G     | 4001 | BCR  | C34-C9-C10  | -2.41 | 119.55      | 122.92   |
| 14  | b     | 1023 | CLA  | C3D-C4D-ND  | 2.41  | 114.14      | 110.24   |
| 14  | b     | 1214 | CLA  | C4-C3-C5    | 2.41  | 119.33      | 115.27   |
| 14  | H     | 1205 | CLA  | C4D-C3D-CAD | 2.41  | 110.94      | 108.10   |
| 14  | K     | 1401 | CLA  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 14  | K     | 1401 | CLA  | OBD-CAD-C3D | -2.41 | 122.72      | 128.52   |
| 18  | a     | 4002 | BCR  | C33-C5-C6   | -2.41 | 121.82      | 124.53   |
| 14  | A     | 1123 | CLA  | C4D-C3D-CAD | 2.41  | 110.94      | 108.10   |
| 14  | G     | 1120 | CLA  | C3D-C4D-ND  | 2.41  | 114.13      | 110.24   |
| 15  | H     | 1238 | F6C  | CMD-C2D-C3D | -2.41 | 122.07      | 127.61   |
| 14  | b     | 1206 | CLA  | CHC-C1C-C2C | -2.41 | 120.06      | 126.72   |
| 14  | b     | 1217 | CLA  | CMB-C2B-C3B | 2.41  | 129.18      | 124.68   |
| 14  | B     | 1214 | CLA  | O1D-CGD-CBD | -2.41 | 119.56      | 124.48   |
| 18  | b     | 4004 | BCR  | C37-C22-C21 | -2.41 | 119.55      | 122.92   |
| 14  | b     | 1023 | CLA  | CMC-C2C-C3C | 2.41  | 132.65      | 126.12   |
| 14  | a     | 1119 | CLA  | CED-O2D-CGD | 2.41  | 121.38      | 115.94   |
| 15  | H     | 1207 | F6C  | C3D-C4D-ND  | 2.40  | 113.69      | 110.17   |
| 14  | G     | 1141 | CLA  | C4D-C3D-CAD | 2.40  | 110.93      | 108.10   |
| 14  | T     | 1401 | CLA  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 14  | H     | 1206 | CLA  | C3D-C4D-ND  | 2.40  | 114.13      | 110.24   |
| 14  | A     | 1114 | CLA  | CMA-C3A-C4A | 2.40  | 118.23      | 111.77   |
| 14  | b     | 1233 | CLA  | CMD-C2D-C3D | -2.40 | 122.08      | 127.61   |
| 14  | b     | 1228 | CLA  | C3D-C4D-ND  | 2.40  | 114.13      | 110.24   |
| 19  | U     | 5101 | LHG  | C5-O7-C7    | -2.40 | 111.87      | 117.79   |
| 15  | b     | 1238 | F6C  | CED-O2D-CGD | 2.40  | 121.37      | 115.94   |
| 14  | B     | 1023 | CLA  | CMC-C2C-C3C | 2.40  | 132.64      | 126.12   |
| 14  | H     | 1023 | CLA  | CMC-C2C-C3C | 2.40  | 132.64      | 126.12   |
| 15  | b     | 1238 | F6C  | CMD-C2D-C3D | -2.40 | 122.09      | 127.61   |
| 14  | G     | 1106 | CLA  | C4D-C3D-CAD | 2.40  | 110.93      | 108.10   |
| 14  | a     | 1122 | CLA  | C1-C2-C3    | -2.40 | 121.89      | 126.04   |
| 14  | G     | 1103 | CLA  | CAA-CBA-CGA | -2.40 | 106.24      | 113.25   |
| 15  | H     | 1238 | F6C  | CHB-C4A-NA  | 2.40  | 126.66      | 124.45   |
| 14  | B     | 1231 | CLA  | C4-C3-C5    | 2.40  | 119.31      | 115.27   |
| 14  | B     | 1233 | CLA  | CMD-C2D-C3D | -2.40 | 122.09      | 127.61   |
| 14  | B     | 1206 | CLA  | CAA-C2A-C3A | -2.40 | 106.21      | 112.78   |
| 14  | H     | 1021 | CLA  | C1-C2-C3    | -2.40 | 121.89      | 126.04   |
| 14  | a     | 1101 | CLA  | O1D-CGD-CBD | -2.40 | 119.58      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4006 | BCR  | C35-C13-C12 | 2.40  | 121.86      | 118.08   |
| 18  | A     | 4003 | BCR  | C36-C18-C17 | -2.40 | 119.56      | 122.92   |
| 14  | B     | 1218 | CLA  | C3C-C4C-NC  | 2.40  | 113.26      | 110.57   |
| 14  | a     | 1141 | CLA  | C4D-C3D-CAD | 2.40  | 110.92      | 108.10   |
| 14  | A     | 1119 | CLA  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 18  | l     | 4019 | BCR  | C33-C5-C6   | -2.40 | 121.83      | 124.53   |
| 14  | a     | 1116 | CLA  | C3D-C4D-ND  | 2.40  | 114.12      | 110.24   |
| 13  | G     | 1011 | CL0  | C4-C3-C5    | 2.40  | 119.30      | 115.27   |
| 14  | b     | 1231 | CLA  | C4-C3-C5    | 2.40  | 119.30      | 115.27   |
| 14  | A     | 1101 | CLA  | O1D-CGD-CBD | -2.40 | 119.58      | 124.48   |
| 14  | b     | 1220 | CLA  | C3D-C4D-ND  | 2.40  | 114.11      | 110.24   |
| 14  | H     | 1236 | CLA  | C3D-C4D-ND  | 2.40  | 114.11      | 110.24   |
| 14  | H     | 1211 | CLA  | C4-C3-C5    | 2.40  | 119.30      | 115.27   |
| 14  | A     | 1126 | CLA  | CMC-C2C-C1C | 2.40  | 128.69      | 125.04   |
| 18  | U     | 4019 | BCR  | C8-C7-C6    | -2.40 | 120.47      | 127.20   |
| 14  | B     | 1204 | CLA  | OBD-CAD-C3D | -2.39 | 122.76      | 128.52   |
| 14  | B     | 1023 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 14  | b     | 1236 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 14  | l     | 1502 | CLA  | C3C-C4C-NC  | 2.39  | 113.26      | 110.57   |
| 14  | A     | 1103 | CLA  | CAA-CBA-CGA | -2.39 | 106.26      | 113.25   |
| 18  | B     | 4009 | BCR  | C35-C13-C12 | 2.39  | 121.85      | 118.08   |
| 14  | a     | 1130 | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 14  | H     | 1224 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 14  | A     | 1122 | CLA  | C1-C2-C3    | -2.39 | 121.90      | 126.04   |
| 18  | T     | 4001 | BCR  | C8-C9-C10   | 2.39  | 122.61      | 118.94   |
| 14  | b     | 1233 | CLA  | C4D-C3D-CAD | 2.39  | 110.92      | 108.10   |
| 14  | b     | 1022 | CLA  | O2A-CGA-CBA | 2.39  | 119.42      | 111.91   |
| 14  | B     | 1226 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 14  | B     | 1205 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 15  | B     | 1207 | F6C  | C3D-C4D-ND  | 2.39  | 113.67      | 110.17   |
| 16  | G     | 2001 | PQN  | C2M-C2-C1   | 2.39  | 120.23      | 116.27   |
| 14  | B     | 1236 | CLA  | C3D-C4D-ND  | 2.39  | 114.11      | 110.24   |
| 18  | A     | 4002 | BCR  | C33-C5-C6   | -2.39 | 121.84      | 124.53   |
| 14  | G     | 1122 | CLA  | C1-C2-C3    | -2.39 | 121.91      | 126.04   |
| 14  | B     | 1022 | CLA  | O2A-CGA-CBA | 2.39  | 119.41      | 111.91   |
| 14  | B     | 1228 | CLA  | C3D-C4D-ND  | 2.39  | 114.10      | 110.24   |
| 14  | H     | 1205 | CLA  | CHD-C4C-C3C | -2.39 | 121.33      | 124.84   |
| 14  | B     | 1222 | CLA  | CMA-C3A-C4A | 2.39  | 118.20      | 111.77   |
| 14  | H     | 1206 | CLA  | CAA-C2A-C3A | -2.39 | 106.23      | 112.78   |
| 15  | b     | 1238 | F6C  | OMB-CMB-C2B | -2.39 | 120.28      | 125.69   |
| 14  | G     | 1101 | CLA  | O1D-CGD-CBD | -2.39 | 119.59      | 124.48   |
| 14  | A     | 1106 | CLA  | CAA-C2A-C3A | -2.39 | 106.24      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | H     | 4009 | BCR  | C35-C13-C12 | 2.39  | 121.84      | 118.08   |
| 14  | b     | 1021 | CLA  | C6-C5-C3    | -2.39 | 107.19      | 113.45   |
| 15  | B     | 1238 | F6C  | OMB-CMB-C2B | -2.39 | 120.29      | 125.69   |
| 14  | H     | 1022 | CLA  | O2A-CGA-CBA | 2.39  | 119.40      | 111.91   |
| 18  | L     | 4019 | BCR  | C8-C7-C6    | -2.39 | 120.50      | 127.20   |
| 14  | B     | 1021 | CLA  | C1-C2-C3    | -2.39 | 121.91      | 126.04   |
| 14  | a     | 1114 | CLA  | CMA-C3A-C4A | 2.39  | 118.19      | 111.77   |
| 14  | G     | 1101 | CLA  | C3D-C4D-ND  | 2.39  | 114.10      | 110.24   |
| 18  | l     | 4019 | BCR  | C8-C7-C6    | -2.39 | 120.50      | 127.20   |
| 14  | B     | 1211 | CLA  | C4-C3-C5    | 2.39  | 119.29      | 115.27   |
| 14  | H     | 1205 | CLA  | C3D-C4D-ND  | 2.39  | 114.10      | 110.24   |
| 14  | L     | 1503 | CLA  | C4-C3-C5    | 2.39  | 119.28      | 115.27   |
| 14  | a     | 1103 | CLA  | CAA-CBA-CGA | -2.39 | 106.28      | 113.25   |
| 14  | G     | 1106 | CLA  | CAA-C2A-C3A | -2.39 | 106.25      | 112.78   |
| 18  | b     | 4009 | BCR  | C35-C13-C12 | 2.39  | 121.83      | 118.08   |
| 14  | H     | 1023 | CLA  | C3D-C4D-ND  | 2.38  | 114.09      | 110.24   |
| 14  | H     | 1233 | CLA  | C4D-C3D-CAD | 2.38  | 110.91      | 108.10   |
| 14  | H     | 1226 | CLA  | C3D-C4D-ND  | 2.38  | 114.09      | 110.24   |
| 14  | H     | 1208 | CLA  | CAA-C2A-C3A | -2.38 | 106.25      | 112.78   |
| 14  | H     | 1222 | CLA  | CMA-C3A-C4A | 2.38  | 118.18      | 111.77   |
| 19  | L     | 5101 | LHG  | C5-O7-C7    | -2.38 | 111.92      | 117.79   |
| 15  | B     | 1238 | F6C  | CED-O2D-CGD | 2.38  | 121.33      | 115.94   |
| 14  | H     | 1204 | CLA  | OBD-CAD-C3D | -2.38 | 122.79      | 128.52   |
| 14  | A     | 1130 | CLA  | C4-C3-C5    | 2.38  | 119.28      | 115.27   |
| 14  | G     | 1135 | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 14  | a     | 1135 | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 16  | a     | 2001 | PQN  | C2M-C2-C1   | 2.38  | 120.22      | 116.27   |
| 14  | H     | 1209 | CLA  | C4D-C3D-CAD | 2.38  | 110.90      | 108.10   |
| 14  | b     | 1021 | CLA  | C1-C2-C3    | -2.38 | 121.92      | 126.04   |
| 18  | k     | 4001 | BCR  | C8-C9-C10   | 2.38  | 122.59      | 118.94   |
| 14  | G     | 1130 | CLA  | C4-C3-C5    | 2.38  | 119.28      | 115.27   |
| 14  | b     | 1222 | CLA  | CMA-C3A-C4A | 2.38  | 118.17      | 111.77   |
| 14  | L     | 1502 | CLA  | C1-O2A-CGA  | 2.38  | 122.69      | 116.44   |
| 14  | H     | 1231 | CLA  | C4-C3-C5    | 2.38  | 119.28      | 115.27   |
| 19  | l     | 5101 | LHG  | C5-O7-C7    | -2.38 | 111.93      | 117.79   |
| 14  | B     | 1021 | CLA  | C6-C5-C3    | -2.38 | 107.22      | 113.45   |
| 14  | A     | 1129 | CLA  | C5-C3-C4    | 2.38  | 119.86      | 114.60   |
| 15  | A     | 1121 | F6C  | OMB-CMB-C2B | -2.38 | 120.31      | 125.69   |
| 15  | G     | 1121 | F6C  | OMB-CMB-C2B | -2.38 | 120.31      | 125.69   |
| 14  | b     | 1211 | CLA  | C4-C3-C5    | 2.38  | 119.27      | 115.27   |
| 14  | A     | 1135 | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 14  | b     | 1218 | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1205 | CLA  | C3D-C4D-ND  | 2.38  | 114.08      | 110.24   |
| 14  | H     | 1228 | CLA  | C3D-C4D-ND  | 2.38  | 114.08      | 110.24   |
| 16  | A     | 2001 | PQN  | C2M-C2-C1   | 2.38  | 120.21      | 116.27   |
| 14  | G     | 1119 | CLA  | CED-O2D-CGD | 2.38  | 121.31      | 115.94   |
| 14  | a     | 1106 | CLA  | CAA-C2A-C3A | -2.38 | 106.27      | 112.78   |
| 14  | b     | 1208 | CLA  | CAA-C2A-C3A | -2.38 | 106.27      | 112.78   |
| 14  | H     | 1225 | CLA  | CMB-C2B-C1B | -2.38 | 124.81      | 128.46   |
| 14  | b     | 1210 | CLA  | O1D-CGD-CBD | -2.38 | 119.62      | 124.48   |
| 15  | H     | 1238 | F6C  | CED-O2D-CGD | 2.38  | 121.31      | 115.94   |
| 14  | b     | 1204 | CLA  | OBD-CAD-C3D | -2.38 | 122.80      | 128.52   |
| 18  | l     | 4019 | BCR  | C36-C18-C17 | -2.37 | 119.60      | 122.92   |
| 15  | b     | 1237 | F6C  | OMB-CMB-C2B | -2.37 | 120.32      | 125.69   |
| 14  | B     | 1209 | CLA  | C4D-C3D-CAD | 2.37  | 110.89      | 108.10   |
| 15  | b     | 1207 | F6C  | CHD-C1D-ND  | -2.37 | 120.60      | 124.20   |
| 14  | B     | 1224 | CLA  | C3D-C4D-ND  | 2.37  | 114.08      | 110.24   |
| 14  | A     | 1101 | CLA  | C3D-C4D-ND  | 2.37  | 114.08      | 110.24   |
| 14  | A     | 1131 | CLA  | C3D-C4D-ND  | 2.37  | 114.08      | 110.24   |
| 14  | M     | 1501 | CLA  | C3D-C4D-ND  | 2.37  | 114.08      | 110.24   |
| 15  | b     | 1207 | F6C  | C3D-C4D-ND  | 2.37  | 113.64      | 110.17   |
| 14  | b     | 1214 | CLA  | CAC-C3C-C4C | 2.37  | 127.89      | 124.81   |
| 18  | B     | 4004 | BCR  | C33-C5-C6   | -2.37 | 121.86      | 124.53   |
| 14  | H     | 1214 | CLA  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 14  | B     | 1208 | CLA  | CAA-C2A-C3A | -2.37 | 106.28      | 112.78   |
| 14  | A     | 1111 | CLA  | C3D-C4D-ND  | 2.37  | 114.07      | 110.24   |
| 14  | B     | 1240 | CLA  | O1D-CGD-CBD | -2.37 | 119.63      | 124.48   |
| 14  | H     | 1021 | CLA  | C6-C5-C3    | -2.37 | 107.24      | 113.45   |
| 18  | b     | 4014 | BCR  | C8-C7-C6    | -2.37 | 120.55      | 127.20   |
| 18  | G     | 4003 | BCR  | C36-C18-C17 | -2.37 | 119.60      | 122.92   |
| 21  | b     | 6004 | LMT  | O5'-C5'-C4' | 2.37  | 114.75      | 109.75   |
| 15  | b     | 1207 | F6C  | OBD-CAD-C3D | -2.37 | 122.82      | 128.52   |
| 14  | H     | 1210 | CLA  | O1D-CGD-CBD | -2.37 | 119.64      | 124.48   |
| 14  | B     | 1204 | CLA  | C4-C3-C5    | 2.37  | 119.26      | 115.27   |
| 14  | l     | 1503 | CLA  | C4-C3-C5    | 2.37  | 119.26      | 115.27   |
| 15  | a     | 1121 | F6C  | OMB-CMB-C2B | -2.37 | 120.33      | 125.69   |
| 15  | H     | 1219 | F6C  | CMD-C2D-C3D | -2.37 | 122.17      | 127.61   |
| 14  | G     | 1122 | CLA  | CMA-C3A-C4A | 2.37  | 118.14      | 111.77   |
| 14  | B     | 1214 | CLA  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 18  | H     | 4014 | BCR  | C8-C7-C6    | -2.37 | 120.55      | 127.20   |
| 15  | B     | 1219 | F6C  | CMD-C2D-C3D | -2.37 | 122.17      | 127.61   |
| 14  | U     | 1502 | CLA  | C3C-C4C-NC  | 2.37  | 113.23      | 110.57   |
| 18  | U     | 4019 | BCR  | C36-C18-C17 | -2.37 | 119.61      | 122.92   |
| 18  | B     | 4014 | BCR  | C8-C7-C6    | -2.37 | 120.56      | 127.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | l     | 1502 | CLA  | CAA-C2A-C3A | -2.37 | 106.30      | 112.78   |
| 18  | H     | 4014 | BCR  | C35-C13-C12 | 2.37  | 121.81      | 118.08   |
| 14  | m     | 1501 | CLA  | C3D-C4D-ND  | 2.37  | 114.06      | 110.24   |
| 14  | G     | 1126 | CLA  | CMC-C2C-C1C | 2.37  | 128.64      | 125.04   |
| 18  | a     | 4002 | BCR  | C35-C13-C14 | -2.37 | 119.61      | 122.92   |
| 14  | a     | 1129 | CLA  | C5-C3-C4    | 2.37  | 119.83      | 114.60   |
| 14  | U     | 1502 | CLA  | C1-O2A-CGA  | 2.37  | 122.65      | 116.44   |
| 18  | K     | 4001 | BCR  | C8-C9-C10   | 2.36  | 122.57      | 118.94   |
| 15  | H     | 1238 | F6C  | OMB-CMB-C2B | -2.36 | 120.34      | 125.69   |
| 14  | b     | 1226 | CLA  | C3D-C4D-ND  | 2.36  | 114.06      | 110.24   |
| 14  | B     | 1205 | CLA  | CHD-C4C-C3C | -2.36 | 121.36      | 124.84   |
| 15  | H     | 1237 | F6C  | OMB-CMB-C2B | -2.36 | 120.34      | 125.69   |
| 18  | L     | 4019 | BCR  | C33-C5-C6   | -2.36 | 121.87      | 124.53   |
| 14  | B     | 1210 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 21  | G     | 6001 | LMT  | O5'-C5'-C6' | 2.36  | 112.31      | 106.44   |
| 14  | H     | 1204 | CLA  | C4-C3-C5    | 2.36  | 119.25      | 115.27   |
| 18  | A     | 4005 | BCR  | C37-C22-C21 | -2.36 | 119.61      | 122.92   |
| 15  | B     | 1237 | F6C  | OMB-CMB-C2B | -2.36 | 120.35      | 125.69   |
| 14  | M     | 1501 | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 14  | l     | 1502 | CLA  | C1-O2A-CGA  | 2.36  | 122.64      | 116.44   |
| 14  | B     | 1233 | CLA  | C4D-C3D-CAD | 2.36  | 110.88      | 108.10   |
| 14  | L     | 1502 | CLA  | C3C-C4C-NC  | 2.36  | 113.22      | 110.57   |
| 14  | B     | 1225 | CLA  | CMB-C2B-C1B | -2.36 | 124.83      | 128.46   |
| 14  | a     | 1125 | CLA  | CAC-C3C-C2C | 2.36  | 131.57      | 127.53   |
| 14  | b     | 1209 | CLA  | C4D-C3D-CAD | 2.36  | 110.88      | 108.10   |
| 14  | U     | 1502 | CLA  | CAA-C2A-C3A | -2.36 | 106.31      | 112.78   |
| 14  | G     | 1111 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 14  | b     | 1224 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 14  | H     | 1229 | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 14  | b     | 1240 | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 14  | H     | 1213 | CLA  | C4D-C3D-CAD | 2.36  | 110.88      | 108.10   |
| 14  | a     | 1123 | CLA  | C4D-C3D-CAD | 2.36  | 110.88      | 108.10   |
| 14  | A     | 1125 | CLA  | CAC-C3C-C2C | 2.36  | 131.56      | 127.53   |
| 14  | G     | 1129 | CLA  | C5-C3-C4    | 2.36  | 119.81      | 114.60   |
| 14  | L     | 1502 | CLA  | CAA-C2A-C3A | -2.36 | 106.32      | 112.78   |
| 14  | V     | 1501 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 18  | L     | 4019 | BCR  | C36-C18-C17 | -2.36 | 119.62      | 122.92   |
| 18  | B     | 4014 | BCR  | C35-C13-C12 | 2.36  | 121.79      | 118.08   |
| 14  | H     | 1240 | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 14  | G     | 1131 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 14  | a     | 1101 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 14  | a     | 1131 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1207 | F6C  | OBD-CAD-C3D | -2.36 | 122.85      | 128.52   |
| 15  | b     | 1219 | F6C  | CMD-C2D-C3D | -2.36 | 122.19      | 127.61   |
| 14  | m     | 1501 | CLA  | O2D-CGD-O1D | -2.36 | 119.23      | 123.84   |
| 14  | B     | 1227 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 14  | b     | 1227 | CLA  | C3D-C4D-ND  | 2.36  | 114.05      | 110.24   |
| 21  | G     | 6001 | LMT  | O5'-C5'-C4' | 2.36  | 114.72      | 109.75   |
| 18  | G     | 4005 | BCR  | C37-C22-C21 | -2.36 | 119.62      | 122.92   |
| 15  | H     | 1207 | F6C  | CHD-C1D-ND  | -2.36 | 120.63      | 124.20   |
| 21  | A     | 6001 | LMT  | O5'-C5'-C6' | 2.35  | 112.29      | 106.44   |
| 14  | B     | 1214 | CLA  | CAC-C3C-C4C | 2.35  | 127.86      | 124.81   |
| 18  | H     | 4004 | BCR  | C33-C5-C6   | -2.35 | 121.88      | 124.53   |
| 18  | b     | 4004 | BCR  | C33-C5-C6   | -2.35 | 121.88      | 124.53   |
| 14  | a     | 1111 | CLA  | C3D-C4D-ND  | 2.35  | 114.05      | 110.24   |
| 14  | b     | 1204 | CLA  | C4-C3-C5    | 2.35  | 119.23      | 115.27   |
| 14  | G     | 1125 | CLA  | CAC-C3C-C2C | 2.35  | 131.56      | 127.53   |
| 14  | H     | 1227 | CLA  | C3D-C4D-ND  | 2.35  | 114.05      | 110.24   |
| 14  | b     | 1204 | CLA  | C4D-C3D-CAD | 2.35  | 110.87      | 108.10   |
| 18  | a     | 4005 | BCR  | C37-C22-C21 | -2.35 | 119.63      | 122.92   |
| 14  | B     | 1234 | CLA  | CMB-C2B-C3B | 2.35  | 129.08      | 124.68   |
| 15  | H     | 1207 | F6C  | OBD-CAD-C3D | -2.35 | 122.86      | 128.52   |
| 14  | H     | 1204 | CLA  | C4D-C3D-CAD | 2.35  | 110.87      | 108.10   |
| 21  | a     | 6001 | LMT  | O5'-C5'-C6' | 2.35  | 112.28      | 106.44   |
| 14  | b     | 1225 | CLA  | CMB-C2B-C1B | -2.35 | 124.85      | 128.46   |
| 14  | A     | 1112 | CLA  | C3D-C4D-ND  | 2.35  | 114.04      | 110.24   |
| 14  | G     | 1112 | CLA  | C3D-C4D-ND  | 2.35  | 114.04      | 110.24   |
| 14  | B     | 1214 | CLA  | C3D-C4D-ND  | 2.35  | 114.04      | 110.24   |
| 14  | A     | 1106 | CLA  | C4D-C3D-CAD | 2.35  | 110.87      | 108.10   |
| 15  | B     | 1207 | F6C  | CHD-C1D-ND  | -2.35 | 120.64      | 124.20   |
| 15  | b     | 1207 | F6C  | C11-C10-C8  | -2.35 | 108.32      | 115.92   |
| 14  | b     | 1232 | CLA  | C3C-C4C-NC  | 2.35  | 113.21      | 110.57   |
| 14  | B     | 1213 | CLA  | C4D-C3D-CAD | 2.35  | 110.86      | 108.10   |
| 14  | b     | 1213 | CLA  | C4D-C3D-CAD | 2.35  | 110.86      | 108.10   |
| 14  | H     | 1239 | CLA  | C6-C5-C3    | -2.35 | 107.30      | 113.45   |
| 14  | b     | 1239 | CLA  | C6-C5-C3    | -2.35 | 107.30      | 113.45   |
| 18  | G     | 4002 | BCR  | C35-C13-C14 | -2.35 | 119.63      | 122.92   |
| 14  | H     | 1234 | CLA  | CMB-C2B-C3B | 2.35  | 129.07      | 124.68   |
| 14  | V     | 1501 | CLA  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 21  | B     | 6004 | LMT  | O5'-C5'-C4' | 2.35  | 114.70      | 109.75   |
| 14  | H     | 1240 | CLA  | C3D-C4D-ND  | 2.35  | 114.03      | 110.24   |
| 14  | A     | 1122 | CLA  | CMA-C3A-C4A | 2.35  | 118.08      | 111.77   |
| 14  | b     | 1234 | CLA  | CMB-C2B-C3B | 2.35  | 129.07      | 124.68   |
| 14  | b     | 1214 | CLA  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1139 | CLA  | C3D-C4D-ND  | 2.35  | 114.03      | 110.24   |
| 14  | a     | 1118 | CLA  | O1D-CGD-CBD | -2.35 | 119.69      | 124.48   |
| 19  | A     | 5002 | LHG  | O4-P-O5     | 2.35  | 119.86      | 110.68   |
| 18  | M     | 4021 | BCR  | C3-C4-C5    | -2.34 | 109.89      | 114.08   |
| 18  | U     | 4019 | BCR  | C33-C5-C6   | -2.34 | 121.89      | 124.53   |
| 14  | H     | 1214 | CLA  | C3D-C4D-ND  | 2.34  | 114.03      | 110.24   |
| 21  | A     | 6001 | LMT  | O5'-C5'-C4' | 2.34  | 114.69      | 109.75   |
| 18  | k     | 4001 | BCR  | C15-C14-C13 | -2.34 | 123.97      | 127.31   |
| 15  | B     | 1207 | F6C  | C11-C10-C8  | -2.34 | 108.35      | 115.92   |
| 14  | b     | 1229 | CLA  | CMD-C2D-C3D | -2.34 | 122.23      | 127.61   |
| 14  | A     | 1126 | CLA  | C3D-C4D-ND  | 2.34  | 114.03      | 110.24   |
| 14  | G     | 1139 | CLA  | C3D-C4D-ND  | 2.34  | 114.03      | 110.24   |
| 14  | B     | 1239 | CLA  | C6-C5-C3    | -2.34 | 107.31      | 113.45   |
| 19  | G     | 5002 | LHG  | O4-P-O5     | 2.34  | 119.85      | 110.68   |
| 19  | a     | 5002 | LHG  | O4-P-O5     | 2.34  | 119.85      | 110.68   |
| 14  | a     | 1106 | CLA  | C4D-C3D-CAD | 2.34  | 110.86      | 108.10   |
| 14  | H     | 1232 | CLA  | C3C-C4C-NC  | 2.34  | 113.20      | 110.57   |
| 21  | b     | 6004 | LMT  | C2'-C3'-C4' | 2.34  | 115.03      | 109.68   |
| 18  | A     | 4002 | BCR  | C35-C13-C14 | -2.34 | 119.64      | 122.92   |
| 14  | a     | 1112 | CLA  | C3D-C4D-ND  | 2.34  | 114.02      | 110.24   |
| 14  | b     | 1214 | CLA  | C3D-C4D-ND  | 2.34  | 114.02      | 110.24   |
| 14  | A     | 1134 | CLA  | CMD-C2D-C3D | -2.34 | 122.23      | 127.61   |
| 14  | G     | 1134 | CLA  | CMD-C2D-C3D | -2.34 | 122.23      | 127.61   |
| 14  | H     | 1214 | CLA  | CAC-C3C-C4C | 2.34  | 127.85      | 124.81   |
| 15  | H     | 1207 | F6C  | C11-C10-C8  | -2.34 | 108.36      | 115.92   |
| 14  | b     | 1236 | CLA  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 14  | A     | 1138 | CLA  | C3D-C4D-ND  | 2.34  | 114.02      | 110.24   |
| 14  | G     | 1138 | CLA  | C3D-C4D-ND  | 2.34  | 114.02      | 110.24   |
| 14  | a     | 1130 | CLA  | CMB-C2B-C1B | -2.34 | 124.87      | 128.46   |
| 14  | b     | 1023 | CLA  | CMA-C3A-C4A | 2.34  | 118.06      | 111.77   |
| 14  | G     | 1130 | CLA  | CMB-C2B-C1B | -2.34 | 124.87      | 128.46   |
| 14  | B     | 1204 | CLA  | C4D-C3D-CAD | 2.34  | 110.85      | 108.10   |
| 21  | a     | 6001 | LMT  | O5'-C5'-C4' | 2.34  | 114.68      | 109.75   |
| 14  | A     | 1130 | CLA  | CMB-C2B-C1B | -2.34 | 124.87      | 128.46   |
| 14  | G     | 1110 | CLA  | CMC-C2C-C1C | 2.34  | 128.60      | 125.04   |
| 14  | A     | 1128 | CLA  | CHC-C1C-C2C | -2.34 | 120.26      | 126.72   |
| 18  | b     | 4014 | BCR  | C35-C13-C12 | 2.33  | 121.76      | 118.08   |
| 21  | H     | 6004 | LMT  | C2'-C3'-C4' | 2.33  | 115.01      | 109.68   |
| 14  | B     | 1229 | CLA  | O1D-CGD-CBD | -2.33 | 119.71      | 124.48   |
| 18  | K     | 4001 | BCR  | C15-C14-C13 | -2.33 | 123.98      | 127.31   |
| 14  | a     | 1138 | CLA  | C3D-C4D-ND  | 2.33  | 114.01      | 110.24   |
| 14  | G     | 1126 | CLA  | C3D-C4D-ND  | 2.33  | 114.01      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1240 | CLA  | CMC-C2C-C1C | 2.33  | 128.59      | 125.04   |
| 14  | a     | 1122 | CLA  | CMA-C3A-C4A | 2.33  | 118.04      | 111.77   |
| 14  | G     | 1128 | CLA  | CHC-C1C-C2C | -2.33 | 120.27      | 126.72   |
| 14  | a     | 1128 | CLA  | CHC-C1C-C2C | -2.33 | 120.27      | 126.72   |
| 18  | B     | 4009 | BCR  | C19-C18-C17 | 2.33  | 122.52      | 118.94   |
| 14  | H     | 1214 | CLA  | C4D-C3D-CAD | 2.33  | 110.84      | 108.10   |
| 14  | H     | 1229 | CLA  | CMD-C2D-C3D | -2.33 | 122.25      | 127.61   |
| 14  | b     | 1228 | CLA  | CMD-C2D-C3D | -2.33 | 122.25      | 127.61   |
| 14  | a     | 1115 | CLA  | CMA-C3A-C4A | 2.33  | 118.04      | 111.77   |
| 14  | B     | 1023 | CLA  | CAA-C2A-C1A | -2.33 | 104.34      | 111.97   |
| 14  | B     | 1229 | CLA  | CMD-C2D-C3D | -2.33 | 122.25      | 127.61   |
| 21  | H     | 6004 | LMT  | O5'-C5'-C4' | 2.33  | 114.67      | 109.75   |
| 15  | b     | 1238 | F6C  | CHD-C1D-ND  | -2.33 | 120.67      | 124.20   |
| 18  | b     | 4010 | BCR  | C33-C5-C4   | 2.33  | 118.09      | 113.62   |
| 15  | H     | 1238 | F6C  | CHD-C1D-ND  | -2.33 | 120.67      | 124.20   |
| 21  | B     | 6004 | LMT  | C2'-C3'-C4' | 2.33  | 115.00      | 109.68   |
| 14  | B     | 1023 | CLA  | C3C-C4C-NC  | 2.33  | 113.18      | 110.57   |
| 14  | b     | 1023 | CLA  | CAA-C2A-C1A | -2.33 | 104.34      | 111.97   |
| 18  | b     | 4009 | BCR  | C19-C18-C17 | 2.33  | 122.51      | 118.94   |
| 14  | B     | 1240 | CLA  | C3D-C4D-ND  | 2.33  | 114.00      | 110.24   |
| 14  | H     | 1023 | CLA  | CAA-C2A-C1A | -2.33 | 104.35      | 111.97   |
| 14  | a     | 1134 | CLA  | CMD-C2D-C3D | -2.33 | 122.26      | 127.61   |
| 14  | b     | 1221 | CLA  | CHA-C1A-NA  | -2.33 | 121.07      | 126.40   |
| 14  | H     | 1236 | CLA  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 14  | b     | 1214 | CLA  | C3C-C4C-NC  | 2.33  | 113.18      | 110.57   |
| 14  | B     | 1228 | CLA  | CMD-C2D-C3D | -2.33 | 122.27      | 127.61   |
| 14  | B     | 1023 | CLA  | CMA-C3A-C4A | 2.33  | 118.02      | 111.77   |
| 14  | H     | 1023 | CLA  | C3C-C4C-NC  | 2.32  | 113.18      | 110.57   |
| 14  | H     | 1228 | CLA  | CMD-C2D-C3D | -2.32 | 122.27      | 127.61   |
| 19  | L     | 5101 | LHG  | O8-C23-O10  | -2.32 | 117.73      | 123.59   |
| 14  | B     | 1236 | CLA  | CMB-C2B-C3B | 2.32  | 129.02      | 124.68   |
| 14  | G     | 1123 | CLA  | C3D-C4D-ND  | 2.32  | 114.00      | 110.24   |
| 19  | U     | 5101 | LHG  | O8-C23-O10  | -2.32 | 117.73      | 123.59   |
| 18  | V     | 4021 | BCR  | C3-C4-C5    | -2.32 | 109.93      | 114.08   |
| 14  | B     | 1204 | CLA  | CAA-C2A-C3A | -2.32 | 106.42      | 112.78   |
| 14  | A     | 1115 | CLA  | CMA-C3A-C4A | 2.32  | 118.01      | 111.77   |
| 14  | H     | 1240 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 14  | B     | 1232 | CLA  | C3C-C4C-NC  | 2.32  | 113.17      | 110.57   |
| 14  | A     | 1139 | CLA  | C3D-C4D-ND  | 2.32  | 113.99      | 110.24   |
| 14  | b     | 1205 | CLA  | CHD-C4C-C3C | -2.32 | 121.43      | 124.84   |
| 14  | a     | 1126 | CLA  | C3D-C4D-ND  | 2.32  | 113.99      | 110.24   |
| 14  | A     | 1118 | CLA  | O1D-CGD-CBD | -2.32 | 119.74      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1229 | CLA  | O1D-CGD-CBD | -2.32 | 119.74      | 124.48   |
| 14  | b     | 1232 | CLA  | C3D-C4D-ND  | 2.32  | 113.99      | 110.24   |
| 14  | H     | 1221 | CLA  | CHA-C1A-NA  | -2.32 | 121.09      | 126.40   |
| 18  | B     | 4010 | BCR  | C33-C5-C4   | 2.32  | 118.07      | 113.62   |
| 18  | m     | 4021 | BCR  | C3-C4-C5    | -2.32 | 109.94      | 114.08   |
| 14  | B     | 1240 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 14  | H     | 1023 | CLA  | CMA-C3A-C4A | 2.32  | 118.00      | 111.77   |
| 14  | H     | 1231 | CLA  | CMB-C2B-C3B | 2.32  | 129.01      | 124.68   |
| 14  | B     | 1221 | CLA  | CHA-C1A-NA  | -2.32 | 121.09      | 126.40   |
| 14  | a     | 1110 | CLA  | C4D-C3D-CAD | 2.32  | 110.83      | 108.10   |
| 18  | H     | 4009 | BCR  | C19-C18-C17 | 2.32  | 122.49      | 118.94   |
| 14  | H     | 1209 | CLA  | CMB-C2B-C3B | 2.32  | 129.01      | 124.68   |
| 14  | A     | 1123 | CLA  | C3D-C4D-ND  | 2.32  | 113.98      | 110.24   |
| 14  | G     | 1115 | CLA  | CAC-C3C-C4C | 2.32  | 127.81      | 124.81   |
| 18  | T     | 4001 | BCR  | C15-C14-C13 | -2.31 | 124.01      | 127.31   |
| 15  | B     | 1238 | F6C  | CHD-C1D-ND  | -2.31 | 120.69      | 124.20   |
| 14  | b     | 1240 | CLA  | C3D-C4D-ND  | 2.31  | 113.98      | 110.24   |
| 14  | B     | 1214 | CLA  | C3C-C4C-NC  | 2.31  | 113.16      | 110.57   |
| 14  | A     | 1110 | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 14  | b     | 1214 | CLA  | C4D-C3D-CAD | 2.31  | 110.82      | 108.10   |
| 14  | B     | 1201 | CLA  | CMD-C2D-C3D | -2.31 | 122.30      | 127.61   |
| 14  | b     | 1211 | CLA  | O1D-CGD-CBD | -2.31 | 119.75      | 124.48   |
| 14  | b     | 1204 | CLA  | CAA-C2A-C3A | -2.31 | 106.45      | 112.78   |
| 14  | G     | 1117 | CLA  | CAA-C2A-C1A | -2.31 | 104.40      | 111.97   |
| 14  | a     | 1115 | CLA  | CAC-C3C-C4C | 2.31  | 127.81      | 124.81   |
| 14  | H     | 1204 | CLA  | CAA-C2A-C3A | -2.31 | 106.45      | 112.78   |
| 18  | H     | 4010 | BCR  | C33-C5-C4   | 2.31  | 118.05      | 113.62   |
| 14  | a     | 1117 | CLA  | CAA-C2A-C1A | -2.31 | 104.41      | 111.97   |
| 14  | A     | 1115 | CLA  | CAC-C3C-C4C | 2.31  | 127.81      | 124.81   |
| 14  | G     | 1132 | CLA  | C1-O2A-CGA  | 2.31  | 122.50      | 116.44   |
| 14  | b     | 1231 | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 19  | l     | 5101 | LHG  | O8-C23-O10  | -2.31 | 117.77      | 123.59   |
| 14  | b     | 1022 | CLA  | C4C-C3C-C2C | -2.31 | 103.53      | 106.90   |
| 14  | A     | 1110 | CLA  | C4D-C3D-CAD | 2.31  | 110.82      | 108.10   |
| 14  | G     | 1115 | CLA  | CMA-C3A-C4A | 2.31  | 117.97      | 111.77   |
| 14  | H     | 1233 | CLA  | O2D-CGD-O1D | -2.31 | 119.33      | 123.84   |
| 21  | a     | 6001 | LMT  | C1'-O5'-C5' | 2.31  | 118.22      | 113.69   |
| 14  | A     | 1132 | CLA  | C1-O2A-CGA  | 2.31  | 122.49      | 116.44   |
| 14  | b     | 1201 | CLA  | CMD-C2D-C3D | -2.31 | 122.31      | 127.61   |
| 14  | H     | 1201 | CLA  | CMD-C2D-C3D | -2.31 | 122.31      | 127.61   |
| 14  | A     | 1117 | CLA  | CAA-C2A-C1A | -2.30 | 104.42      | 111.97   |
| 14  | B     | 1214 | CLA  | C4D-C3D-CAD | 2.30  | 110.81      | 108.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1231 | CLA  | CMB-C2B-C3B | 2.30  | 128.99      | 124.68   |
| 18  | I     | 4020 | BCR  | C35-C13-C12 | 2.30  | 121.71      | 118.08   |
| 14  | B     | 1209 | CLA  | CMB-C2B-C3B | 2.30  | 128.99      | 124.68   |
| 14  | a     | 1110 | CLA  | CMC-C2C-C1C | 2.30  | 128.55      | 125.04   |
| 14  | b     | 1212 | CLA  | CHC-C1C-C2C | -2.30 | 120.35      | 126.72   |
| 14  | H     | 1022 | CLA  | C4C-C3C-C2C | -2.30 | 103.54      | 106.90   |
| 14  | H     | 1212 | CLA  | CHC-C1C-C2C | -2.30 | 120.36      | 126.72   |
| 14  | a     | 1123 | CLA  | C3D-C4D-ND  | 2.30  | 113.96      | 110.24   |
| 14  | H     | 1214 | CLA  | C3C-C4C-NC  | 2.30  | 113.15      | 110.57   |
| 21  | A     | 6001 | LMT  | C1'-O5'-C5' | 2.30  | 118.20      | 113.69   |
| 14  | A     | 1122 | CLA  | C4C-C3C-C2C | -2.30 | 103.55      | 106.90   |
| 14  | a     | 1122 | CLA  | C4C-C3C-C2C | -2.30 | 103.55      | 106.90   |
| 21  | G     | 6001 | LMT  | C1'-O5'-C5' | 2.30  | 118.20      | 113.69   |
| 14  | H     | 1215 | CLA  | C3D-C4D-ND  | 2.30  | 113.95      | 110.24   |
| 14  | B     | 1202 | CLA  | CMD-C2D-C3D | -2.30 | 122.33      | 127.61   |
| 14  | a     | 1132 | CLA  | C1-O2A-CGA  | 2.30  | 122.47      | 116.44   |
| 14  | b     | 1209 | CLA  | CMB-C2B-C3B | 2.30  | 128.97      | 124.68   |
| 14  | B     | 1211 | CLA  | O1D-CGD-CBD | -2.30 | 119.78      | 124.48   |
| 14  | B     | 1022 | CLA  | C4C-C3C-C2C | -2.30 | 103.55      | 106.90   |
| 14  | B     | 1212 | CLA  | CHC-C1C-C2C | -2.30 | 120.37      | 126.72   |
| 14  | A     | 1013 | CLA  | CBA-CAA-C2A | 2.30  | 120.64      | 113.86   |
| 14  | b     | 1023 | CLA  | C3C-C4C-NC  | 2.30  | 113.15      | 110.57   |
| 14  | H     | 1211 | CLA  | O1D-CGD-CBD | -2.30 | 119.79      | 124.48   |
| 14  | G     | 1118 | CLA  | O1D-CGD-CBD | -2.29 | 119.79      | 124.48   |
| 14  | B     | 1235 | CLA  | CAA-C2A-C3A | -2.29 | 106.50      | 112.78   |
| 14  | B     | 1215 | CLA  | C3D-C4D-ND  | 2.29  | 113.95      | 110.24   |
| 14  | A     | 1112 | CLA  | C4D-C3D-CAD | 2.29  | 110.80      | 108.10   |
| 14  | b     | 1213 | CLA  | CMD-C2D-C3D | -2.29 | 122.34      | 127.61   |
| 14  | H     | 1220 | CLA  | C4-C3-C2    | -2.29 | 117.80      | 123.68   |
| 18  | i     | 4020 | BCR  | C35-C13-C12 | 2.29  | 121.69      | 118.08   |
| 14  | a     | 1118 | CLA  | C4D-C3D-CAD | 2.29  | 110.80      | 108.10   |
| 14  | H     | 1209 | CLA  | CAC-C3C-C4C | 2.29  | 127.78      | 124.81   |
| 18  | a     | 4004 | BCR  | C33-C5-C4   | 2.29  | 118.01      | 113.62   |
| 18  | R     | 4020 | BCR  | C35-C13-C12 | 2.29  | 121.68      | 118.08   |
| 14  | H     | 1202 | CLA  | CMD-C2D-C3D | -2.29 | 122.35      | 127.61   |
| 14  | H     | 1213 | CLA  | CMD-C2D-C3D | -2.29 | 122.35      | 127.61   |
| 14  | G     | 1013 | CLA  | CBA-CAA-C2A | 2.29  | 120.62      | 113.86   |
| 14  | H     | 1232 | CLA  | C3D-C4D-ND  | 2.29  | 113.94      | 110.24   |
| 14  | a     | 1013 | CLA  | CBA-CAA-C2A | 2.29  | 120.62      | 113.86   |
| 14  | T     | 1401 | CLA  | C4C-C3C-C2C | -2.29 | 103.56      | 106.90   |
| 14  | a     | 1102 | CLA  | CMD-C2D-C3D | -2.29 | 122.35      | 127.61   |
| 14  | b     | 1235 | CLA  | CAA-C2A-C3A | -2.29 | 106.51      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1214 | CLA  | CMD-C2D-C3D | -2.29 | 122.35      | 127.61   |
| 14  | a     | 1114 | CLA  | CHC-C1C-C2C | -2.29 | 120.40      | 126.72   |
| 14  | B     | 1233 | CLA  | O2D-CGD-O1D | -2.29 | 119.37      | 123.84   |
| 14  | b     | 1218 | CLA  | C4D-C3D-CAD | 2.29  | 110.79      | 108.10   |
| 14  | B     | 1232 | CLA  | C3D-C4D-ND  | 2.29  | 113.93      | 110.24   |
| 18  | l     | 4022 | BCR  | C1-C6-C7    | 2.28  | 122.24      | 115.78   |
| 14  | a     | 1112 | CLA  | C4D-C3D-CAD | 2.28  | 110.79      | 108.10   |
| 14  | b     | 1209 | CLA  | CAC-C3C-C4C | 2.28  | 127.77      | 124.81   |
| 14  | b     | 1221 | CLA  | C4-C3-C2    | -2.28 | 117.82      | 123.68   |
| 14  | H     | 1235 | CLA  | CAA-C2A-C3A | -2.28 | 106.53      | 112.78   |
| 14  | G     | 1122 | CLA  | C4C-C3C-C2C | -2.28 | 103.57      | 106.90   |
| 14  | G     | 1114 | CLA  | CHC-C1C-C2C | -2.28 | 120.41      | 126.72   |
| 14  | B     | 1208 | CLA  | CMC-C2C-C1C | 2.28  | 128.52      | 125.04   |
| 14  | B     | 1213 | CLA  | CMD-C2D-C3D | -2.28 | 122.36      | 127.61   |
| 14  | A     | 1102 | CLA  | CMD-C2D-C3D | -2.28 | 122.36      | 127.61   |
| 18  | G     | 4004 | BCR  | C33-C5-C4   | 2.28  | 118.00      | 113.62   |
| 15  | b     | 1207 | F6C  | C1-C2-C3    | -2.28 | 122.10      | 126.04   |
| 14  | a     | 1122 | CLA  | C3D-C4D-ND  | 2.28  | 113.93      | 110.24   |
| 14  | b     | 1217 | CLA  | C3D-C4D-ND  | 2.28  | 113.93      | 110.24   |
| 14  | A     | 1114 | CLA  | CHC-C1C-C2C | -2.28 | 120.41      | 126.72   |
| 14  | b     | 1214 | CLA  | CMD-C2D-C3D | -2.28 | 122.37      | 127.61   |
| 14  | B     | 1240 | CLA  | CMD-C2D-C3D | -2.28 | 122.37      | 127.61   |
| 14  | k     | 1401 | CLA  | C4C-C3C-C2C | -2.28 | 103.57      | 106.90   |
| 14  | a     | 1140 | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 14  | G     | 1102 | CLA  | CMD-C2D-C3D | -2.28 | 122.37      | 127.61   |
| 14  | A     | 1135 | CLA  | C5-C3-C4    | 2.28  | 119.64      | 114.60   |
| 14  | G     | 1135 | CLA  | C5-C3-C4    | 2.28  | 119.64      | 114.60   |
| 14  | B     | 1220 | CLA  | C4-C3-C2    | -2.28 | 117.83      | 123.68   |
| 14  | b     | 1202 | CLA  | CMD-C2D-C3D | -2.28 | 122.37      | 127.61   |
| 14  | B     | 1221 | CLA  | C4-C3-C2    | -2.28 | 117.83      | 123.68   |
| 14  | B     | 1202 | CLA  | C4-C3-C5    | 2.28  | 119.10      | 115.27   |
| 14  | b     | 1222 | CLA  | C4-C3-C2    | -2.28 | 117.83      | 123.68   |
| 14  | H     | 1224 | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 14  | K     | 1401 | CLA  | C4C-C3C-C2C | -2.28 | 103.58      | 106.90   |
| 15  | B     | 1237 | F6C  | CED-O2D-CGD | 2.28  | 121.09      | 115.94   |
| 14  | H     | 1221 | CLA  | C4-C3-C2    | -2.28 | 117.84      | 123.68   |
| 14  | A     | 1102 | CLA  | C4D-C3D-CAD | 2.28  | 110.78      | 108.10   |
| 14  | H     | 1214 | CLA  | CMD-C2D-C3D | -2.28 | 122.38      | 127.61   |
| 14  | b     | 1215 | CLA  | C3D-C4D-ND  | 2.28  | 113.92      | 110.24   |
| 14  | A     | 1140 | CLA  | CMC-C2C-C1C | 2.28  | 128.50      | 125.04   |
| 18  | k     | 4001 | BCR  | C30-C25-C26 | -2.28 | 119.41      | 122.61   |
| 14  | A     | 1122 | CLA  | C3D-C4D-ND  | 2.28  | 113.92      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1112 | CLA  | C4D-C3D-CAD | 2.28  | 110.78      | 108.10   |
| 14  | b     | 1220 | CLA  | C4-C3-C2    | -2.28 | 117.84      | 123.68   |
| 15  | H     | 1207 | F6C  | C1-C2-C3    | -2.28 | 122.11      | 126.04   |
| 14  | G     | 1110 | CLA  | C4D-C3D-CAD | 2.27  | 110.78      | 108.10   |
| 14  | H     | 1202 | CLA  | C3C-C4C-NC  | 2.27  | 113.12      | 110.57   |
| 14  | b     | 1202 | CLA  | C4-C3-C5    | 2.27  | 119.10      | 115.27   |
| 15  | B     | 1207 | F6C  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 14  | b     | 1240 | CLA  | CMD-C2D-C3D | -2.27 | 122.38      | 127.61   |
| 14  | G     | 1118 | CLA  | C4D-C3D-CAD | 2.27  | 110.78      | 108.10   |
| 14  | B     | 1211 | CLA  | C4C-C3C-C2C | -2.27 | 103.58      | 106.90   |
| 15  | H     | 1237 | F6C  | CED-O2D-CGD | 2.27  | 121.08      | 115.94   |
| 18  | U     | 4022 | BCR  | C1-C6-C7    | 2.27  | 122.21      | 115.78   |
| 14  | b     | 1224 | CLA  | C4C-C3C-C2C | -2.27 | 103.58      | 106.90   |
| 18  | A     | 4004 | BCR  | C33-C5-C4   | 2.27  | 117.98      | 113.62   |
| 14  | H     | 1240 | CLA  | C1-O2A-CGA  | 2.27  | 122.40      | 116.44   |
| 14  | H     | 1222 | CLA  | C4-C3-C2    | -2.27 | 117.85      | 123.68   |
| 14  | G     | 1138 | CLA  | CMD-C2D-C3D | -2.27 | 122.39      | 127.61   |
| 14  | G     | 1114 | CLA  | C4D-C3D-CAD | 2.27  | 110.77      | 108.10   |
| 18  | K     | 4001 | BCR  | C30-C25-C26 | -2.27 | 119.42      | 122.61   |
| 14  | A     | 1141 | CLA  | C3D-C4D-ND  | 2.27  | 113.91      | 110.24   |
| 14  | b     | 1233 | CLA  | O2D-CGD-O1D | -2.27 | 119.40      | 123.84   |
| 15  | b     | 1237 | F6C  | CED-O2D-CGD | 2.27  | 121.07      | 115.94   |
| 14  | b     | 1208 | CLA  | CMC-C2C-C1C | 2.27  | 128.50      | 125.04   |
| 18  | L     | 4022 | BCR  | C1-C6-C7    | 2.27  | 122.20      | 115.78   |
| 14  | H     | 1202 | CLA  | C4-C3-C5    | 2.27  | 119.09      | 115.27   |
| 21  | U     | 6002 | LMT  | O1B-C1B-C2B | 2.27  | 113.98      | 108.10   |
| 18  | B     | 4006 | BCR  | C33-C5-C4   | 2.27  | 117.97      | 113.62   |
| 14  | G     | 1111 | CLA  | C4D-C3D-CAD | 2.27  | 110.77      | 108.10   |
| 18  | T     | 4001 | BCR  | C30-C25-C26 | -2.27 | 119.42      | 122.61   |
| 21  | R     | 6001 | LMT  | C1'-O5'-C5' | -2.27 | 109.24      | 113.69   |
| 14  | b     | 1223 | CLA  | C4C-C3C-C2C | -2.27 | 103.59      | 106.90   |
| 14  | A     | 1133 | CLA  | CMC-C2C-C1C | 2.27  | 128.49      | 125.04   |
| 14  | b     | 1212 | CLA  | CMD-C2D-C3D | -2.27 | 122.40      | 127.61   |
| 14  | b     | 1217 | CLA  | O1D-CGD-CBD | -2.27 | 119.85      | 124.48   |
| 14  | H     | 1208 | CLA  | CMC-C2C-C1C | 2.27  | 128.49      | 125.04   |
| 14  | B     | 1240 | CLA  | C1-O2A-CGA  | 2.27  | 122.39      | 116.44   |
| 14  | B     | 1223 | CLA  | C4C-C3C-C2C | -2.27 | 103.59      | 106.90   |
| 14  | a     | 1135 | CLA  | C5-C3-C4    | 2.27  | 119.61      | 114.60   |
| 14  | G     | 1133 | CLA  | CMC-C2C-C1C | 2.27  | 128.49      | 125.04   |
| 14  | B     | 1222 | CLA  | C4-C3-C2    | -2.26 | 117.87      | 123.68   |
| 14  | B     | 1224 | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 14  | B     | 1218 | CLA  | C4D-C3D-CAD | 2.26  | 110.77      | 108.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | l     | 6002 | LMT  | O1B-C1B-C2B | 2.26  | 113.97      | 108.10   |
| 18  | b     | 4006 | BCR  | C33-C5-C4   | 2.26  | 117.97      | 113.62   |
| 14  | A     | 1114 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 14  | a     | 1102 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 14  | a     | 1133 | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 14  | G     | 1102 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 14  | H     | 1218 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 14  | b     | 1228 | CLA  | C3C-C4C-NC  | 2.26  | 113.11      | 110.57   |
| 14  | G     | 1111 | CLA  | C4C-C3C-C2C | -2.26 | 103.60      | 106.90   |
| 14  | a     | 1111 | CLA  | C4C-C3C-C2C | -2.26 | 103.60      | 106.90   |
| 14  | H     | 1240 | CLA  | CMD-C2D-C3D | -2.26 | 122.41      | 127.61   |
| 14  | B     | 1228 | CLA  | C3C-C4C-NC  | 2.26  | 113.11      | 110.57   |
| 14  | A     | 1118 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 14  | H     | 1229 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 21  | a     | 6001 | LMT  | O1'-C1'-C2' | 2.26  | 111.83      | 108.30   |
| 18  | H     | 4004 | BCR  | C34-C9-C10  | -2.26 | 119.76      | 122.92   |
| 14  | A     | 1103 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 15  | H     | 1237 | F6C  | CMC-C2C-C3C | 2.26  | 129.20      | 124.94   |
| 18  | l     | 4019 | BCR  | C23-C24-C25 | -2.26 | 120.86      | 127.20   |
| 14  | B     | 1209 | CLA  | CAC-C3C-C4C | 2.26  | 127.74      | 124.81   |
| 14  | b     | 1211 | CLA  | C4C-C3C-C2C | -2.26 | 103.61      | 106.90   |
| 14  | B     | 1217 | CLA  | O1D-CGD-CBD | -2.26 | 119.86      | 124.48   |
| 14  | a     | 1111 | CLA  | C4D-C3D-CAD | 2.26  | 110.76      | 108.10   |
| 20  | G     | 5003 | LMG  | O8-C28-O10  | -2.26 | 117.90      | 123.59   |
| 20  | a     | 5003 | LMG  | O8-C28-O10  | -2.26 | 117.90      | 123.59   |
| 14  | G     | 1122 | CLA  | C3D-C4D-ND  | 2.26  | 113.89      | 110.24   |
| 14  | H     | 1217 | CLA  | O1D-CGD-CBD | -2.26 | 119.87      | 124.48   |
| 14  | G     | 1106 | CLA  | CMA-C3A-C4A | 2.26  | 117.84      | 111.77   |
| 14  | B     | 1217 | CLA  | C3D-C4D-ND  | 2.26  | 113.89      | 110.24   |
| 20  | A     | 5003 | LMG  | O8-C28-O10  | -2.25 | 117.90      | 123.59   |
| 21  | I     | 6001 | LMT  | C1'-O5'-C5' | -2.25 | 109.26      | 113.69   |
| 21  | L     | 6002 | LMT  | O1B-C1B-C2B | 2.25  | 113.94      | 108.10   |
| 14  | B     | 1224 | CLA  | C4C-C3C-C2C | -2.25 | 103.61      | 106.90   |
| 14  | B     | 1212 | CLA  | CMD-C2D-C3D | -2.25 | 122.43      | 127.61   |
| 14  | H     | 1221 | CLA  | C4-C3-C5    | 2.25  | 119.06      | 115.27   |
| 14  | H     | 1223 | CLA  | C1-O2A-CGA  | 2.25  | 122.36      | 116.44   |
| 14  | H     | 1211 | CLA  | C4C-C3C-C2C | -2.25 | 103.61      | 106.90   |
| 14  | A     | 1138 | CLA  | CMD-C2D-C3D | -2.25 | 122.43      | 127.61   |
| 18  | B     | 4004 | BCR  | C34-C9-C10  | -2.25 | 119.77      | 122.92   |
| 14  | H     | 1223 | CLA  | C4C-C3C-C2C | -2.25 | 103.61      | 106.90   |
| 14  | b     | 1221 | CLA  | C4-C3-C5    | 2.25  | 119.06      | 115.27   |
| 14  | G     | 1141 | CLA  | C3D-C4D-ND  | 2.25  | 113.88      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1240 | CLA  | C1-O2A-CGA  | 2.25  | 122.35      | 116.44   |
| 14  | b     | 1224 | CLA  | CMC-C2C-C1C | 2.25  | 128.47      | 125.04   |
| 15  | b     | 1237 | F6C  | CMC-C2C-C3C | 2.25  | 129.19      | 124.94   |
| 14  | H     | 1228 | CLA  | C3C-C4C-NC  | 2.25  | 113.09      | 110.57   |
| 13  | G     | 1011 | CL0  | C2A-C3A-C4A | 2.25  | 105.50      | 101.87   |
| 21  | i     | 6001 | LMT  | C1'-O5'-C5' | -2.25 | 109.27      | 113.69   |
| 14  | H     | 1021 | CLA  | C11-C10-C8  | -2.25 | 108.65      | 115.92   |
| 14  | G     | 1124 | CLA  | CMC-C2C-C1C | 2.25  | 128.46      | 125.04   |
| 14  | l     | 1501 | CLA  | OBD-CAD-C3D | -2.25 | 123.11      | 128.52   |
| 14  | H     | 1217 | CLA  | C3D-C4D-ND  | 2.25  | 113.88      | 110.24   |
| 21  | A     | 6001 | LMT  | O1'-C1'-C2' | 2.25  | 111.81      | 108.30   |
| 18  | L     | 4019 | BCR  | C23-C24-C25 | -2.25 | 120.89      | 127.20   |
| 14  | A     | 1106 | CLA  | CMA-C3A-C4A | 2.25  | 117.81      | 111.77   |
| 14  | B     | 1229 | CLA  | C4D-C3D-CAD | 2.25  | 110.75      | 108.10   |
| 14  | A     | 1117 | CLA  | CAA-C2A-C3A | -2.25 | 106.62      | 112.78   |
| 14  | G     | 1117 | CLA  | CAA-C2A-C3A | -2.25 | 106.62      | 112.78   |
| 14  | G     | 1140 | CLA  | CMC-C2C-C1C | 2.25  | 128.46      | 125.04   |
| 14  | a     | 1141 | CLA  | C3D-C4D-ND  | 2.25  | 113.87      | 110.24   |
| 14  | B     | 1021 | CLA  | C11-C10-C8  | -2.25 | 108.66      | 115.92   |
| 14  | A     | 1111 | CLA  | C4D-C3D-CAD | 2.25  | 110.74      | 108.10   |
| 14  | b     | 1218 | CLA  | O1D-CGD-CBD | -2.25 | 119.89      | 124.48   |
| 14  | A     | 1111 | CLA  | C4C-C3C-C2C | -2.25 | 103.62      | 106.90   |
| 14  | B     | 1223 | CLA  | C1-O2A-CGA  | 2.25  | 122.33      | 116.44   |
| 14  | U     | 1501 | CLA  | OBD-CAD-C3D | -2.25 | 123.12      | 128.52   |
| 14  | b     | 1229 | CLA  | C4D-C3D-CAD | 2.24  | 110.74      | 108.10   |
| 15  | H     | 1238 | F6C  | CMC-C2C-C3C | 2.24  | 129.17      | 124.94   |
| 14  | H     | 1212 | CLA  | CMD-C2D-C3D | -2.24 | 122.45      | 127.61   |
| 14  | B     | 1216 | CLA  | C3C-C4C-NC  | 2.24  | 113.09      | 110.57   |
| 14  | G     | 1120 | CLA  | C4D-C3D-CAD | 2.24  | 110.74      | 108.10   |
| 14  | b     | 1021 | CLA  | C11-C10-C8  | -2.24 | 108.67      | 115.92   |
| 18  | U     | 4019 | BCR  | C23-C24-C25 | -2.24 | 120.91      | 127.20   |
| 14  | B     | 1221 | CLA  | C4-C3-C5    | 2.24  | 119.04      | 115.27   |
| 14  | G     | 1103 | CLA  | C4D-C3D-CAD | 2.24  | 110.74      | 108.10   |
| 18  | H     | 4006 | BCR  | C33-C5-C4   | 2.24  | 117.92      | 113.62   |
| 18  | l     | 4019 | BCR  | C24-C23-C22 | -2.24 | 122.85      | 126.23   |
| 14  | a     | 1106 | CLA  | CMA-C3A-C4A | 2.24  | 117.80      | 111.77   |
| 18  | l     | 4022 | BCR  | C37-C22-C21 | -2.24 | 119.78      | 122.92   |
| 14  | B     | 1202 | CLA  | C3C-C4C-NC  | 2.24  | 113.08      | 110.57   |
| 14  | L     | 1501 | CLA  | OBD-CAD-C3D | -2.24 | 123.13      | 128.52   |
| 14  | a     | 1117 | CLA  | CAA-C2A-C3A | -2.24 | 106.65      | 112.78   |
| 15  | B     | 1237 | F6C  | CMC-C2C-C3C | 2.24  | 129.16      | 124.94   |
| 14  | A     | 1120 | CLA  | C4D-C3D-CAD | 2.24  | 110.73      | 108.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1227 | CLA  | C4D-C3D-CAD | 2.24  | 110.73      | 108.10   |
| 14  | a     | 1103 | CLA  | C4D-C3D-CAD | 2.24  | 110.73      | 108.10   |
| 14  | G     | 1129 | CLA  | CAA-C2A-C3A | -2.24 | 106.65      | 112.78   |
| 14  | B     | 1204 | CLA  | C3C-C4C-NC  | 2.24  | 113.08      | 110.57   |
| 14  | a     | 1108 | CLA  | CED-O2D-CGD | 2.24  | 121.00      | 115.94   |
| 14  | H     | 1022 | CLA  | C3D-C4D-ND  | 2.24  | 113.86      | 110.24   |
| 14  | b     | 1233 | CLA  | CMC-C2C-C1C | 2.24  | 128.44      | 125.04   |
| 14  | H     | 1201 | CLA  | C4-C3-C2    | -2.24 | 117.94      | 123.68   |
| 14  | a     | 1122 | CLA  | O1D-CGD-CBD | -2.24 | 119.91      | 124.48   |
| 14  | b     | 1216 | CLA  | C3C-C4C-NC  | 2.24  | 113.08      | 110.57   |
| 14  | A     | 1112 | CLA  | CMD-C2D-C3D | -2.24 | 122.47      | 127.61   |
| 15  | B     | 1219 | F6C  | CMA-C3A-C2A | -2.23 | 120.05      | 126.12   |
| 14  | b     | 1223 | CLA  | C1-O2A-CGA  | 2.23  | 122.31      | 116.44   |
| 14  | H     | 1205 | CLA  | C4C-C3C-C2C | -2.23 | 103.64      | 106.90   |
| 18  | i     | 4020 | BCR  | C33-C5-C6   | -2.23 | 122.02      | 124.53   |
| 14  | G     | 1135 | CLA  | CHC-C1C-C2C | -2.23 | 120.54      | 126.72   |
| 18  | b     | 4004 | BCR  | C34-C9-C10  | -2.23 | 119.79      | 122.92   |
| 18  | L     | 4019 | BCR  | C24-C23-C22 | -2.23 | 122.86      | 126.23   |
| 14  | A     | 1122 | CLA  | O1D-CGD-CBD | -2.23 | 119.91      | 124.48   |
| 14  | b     | 1228 | CLA  | CHC-C1C-C2C | -2.23 | 120.54      | 126.72   |
| 14  | k     | 1401 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 14  | b     | 1227 | CLA  | C4D-C3D-CAD | 2.23  | 110.73      | 108.10   |
| 15  | H     | 1219 | F6C  | CMA-C3A-C2A | -2.23 | 120.06      | 126.12   |
| 14  | G     | 1112 | CLA  | CMD-C2D-C3D | -2.23 | 122.48      | 127.61   |
| 14  | a     | 1112 | CLA  | CMD-C2D-C3D | -2.23 | 122.48      | 127.61   |
| 14  | A     | 1129 | CLA  | CAA-C2A-C3A | -2.23 | 106.66      | 112.78   |
| 14  | B     | 1201 | CLA  | C4-C3-C2    | -2.23 | 117.95      | 123.68   |
| 14  | B     | 1228 | CLA  | C4-C3-C5    | 2.23  | 119.03      | 115.27   |
| 14  | a     | 1138 | CLA  | CMD-C2D-C3D | -2.23 | 122.48      | 127.61   |
| 14  | K     | 1401 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 14  | B     | 1228 | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 21  | G     | 6001 | LMT  | O1'-C1'-C2' | 2.23  | 111.79      | 108.30   |
| 14  | T     | 1401 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 14  | a     | 1140 | CLA  | C3D-C4D-ND  | 2.23  | 113.85      | 110.24   |
| 14  | A     | 1102 | CLA  | C5-C3-C4    | 2.23  | 119.53      | 114.60   |
| 14  | H     | 1228 | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 14  | a     | 1102 | CLA  | C5-C3-C4    | 2.23  | 119.53      | 114.60   |
| 14  | A     | 1128 | CLA  | C4C-C3C-C2C | -2.23 | 103.65      | 106.90   |
| 14  | a     | 1128 | CLA  | C4C-C3C-C2C | -2.23 | 103.65      | 106.90   |
| 14  | G     | 1122 | CLA  | O1D-CGD-CBD | -2.23 | 119.92      | 124.48   |
| 15  | b     | 1219 | F6C  | CMA-C3A-C2A | -2.23 | 120.07      | 126.12   |
| 14  | a     | 1120 | CLA  | O1D-CGD-CBD | -2.23 | 119.93      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1114 | CLA  | C3C-C4C-NC  | 2.23  | 113.07      | 110.57   |
| 14  | H     | 1233 | CLA  | CMC-C2C-C1C | 2.23  | 128.43      | 125.04   |
| 14  | B     | 1218 | CLA  | O1D-CGD-CBD | -2.23 | 119.93      | 124.48   |
| 14  | G     | 1129 | CLA  | CMD-C2D-C3D | -2.23 | 122.49      | 127.61   |
| 15  | B     | 1238 | F6C  | CMC-C2C-C3C | 2.23  | 129.14      | 124.94   |
| 13  | A     | 1011 | CL0  | C2A-C3A-C4A | 2.23  | 105.47      | 101.87   |
| 14  | A     | 1129 | CLA  | CMD-C2D-C3D | -2.22 | 122.50      | 127.61   |
| 14  | a     | 1129 | CLA  | CMD-C2D-C3D | -2.22 | 122.50      | 127.61   |
| 14  | A     | 1113 | CLA  | C4D-C3D-CAD | 2.22  | 110.72      | 108.10   |
| 14  | A     | 1135 | CLA  | CHC-C1C-C2C | -2.22 | 120.57      | 126.72   |
| 14  | b     | 1201 | CLA  | C4-C3-C2    | -2.22 | 117.97      | 123.68   |
| 14  | b     | 1022 | CLA  | C3D-C4D-ND  | 2.22  | 113.83      | 110.24   |
| 20  | i     | 5006 | LMG  | C8-O7-C10   | -2.22 | 112.32      | 117.79   |
| 14  | a     | 1114 | CLA  | C4D-C3D-CAD | 2.22  | 110.71      | 108.10   |
| 14  | a     | 1129 | CLA  | CAA-C2A-C3A | -2.22 | 106.70      | 112.78   |
| 20  | R     | 5006 | LMG  | C8-O7-C10   | -2.22 | 112.32      | 117.79   |
| 14  | H     | 1216 | CLA  | C3C-C4C-NC  | 2.22  | 113.06      | 110.57   |
| 14  | A     | 1108 | CLA  | CED-O2D-CGD | 2.22  | 120.96      | 115.94   |
| 13  | a     | 1011 | CL0  | C2A-C3A-C4A | 2.22  | 105.45      | 101.87   |
| 18  | L     | 4022 | BCR  | C37-C22-C21 | -2.22 | 119.81      | 122.92   |
| 14  | H     | 1240 | CLA  | O2D-CGD-O1D | -2.22 | 119.50      | 123.84   |
| 14  | b     | 1234 | CLA  | CAA-C2A-C3A | -2.22 | 106.70      | 112.78   |
| 18  | b     | 4014 | BCR  | C34-C9-C8   | 2.22  | 121.57      | 118.08   |
| 14  | H     | 1234 | CLA  | CAA-C2A-C3A | -2.22 | 106.71      | 112.78   |
| 14  | A     | 1119 | CLA  | CMC-C2C-C1C | 2.22  | 128.41      | 125.04   |
| 14  | H     | 1228 | CLA  | C4-C3-C5    | 2.22  | 119.00      | 115.27   |
| 14  | A     | 1124 | CLA  | CMC-C2C-C1C | 2.22  | 128.41      | 125.04   |
| 18  | U     | 4022 | BCR  | C37-C22-C21 | -2.22 | 119.82      | 122.92   |
| 14  | G     | 1108 | CLA  | CED-O2D-CGD | 2.21  | 120.95      | 115.94   |
| 14  | A     | 1109 | CLA  | OBD-CAD-C3D | -2.21 | 123.19      | 128.52   |
| 14  | H     | 1232 | CLA  | O2D-CGD-O1D | -2.21 | 119.51      | 123.84   |
| 14  | H     | 1224 | CLA  | C4C-C3C-C2C | -2.21 | 103.67      | 106.90   |
| 14  | B     | 1234 | CLA  | CAA-C2A-C3A | -2.21 | 106.72      | 112.78   |
| 14  | A     | 1129 | CLA  | O1D-CGD-CBD | -2.21 | 119.95      | 124.48   |
| 14  | G     | 1102 | CLA  | C5-C3-C4    | 2.21  | 119.49      | 114.60   |
| 18  | l     | 4019 | BCR  | C37-C22-C21 | -2.21 | 119.82      | 122.92   |
| 20  | I     | 5006 | LMG  | C8-O7-C10   | -2.21 | 112.34      | 117.79   |
| 14  | a     | 1124 | CLA  | CMC-C2C-C1C | 2.21  | 128.41      | 125.04   |
| 18  | B     | 4014 | BCR  | C34-C9-C8   | 2.21  | 121.56      | 118.08   |
| 14  | b     | 1239 | CLA  | CAA-CBA-CGA | -2.21 | 106.79      | 113.25   |
| 14  | A     | 1120 | CLA  | O1D-CGD-CBD | -2.21 | 119.96      | 124.48   |
| 13  | A     | 1011 | CL0  | CMC-C2C-C1C | 2.21  | 128.41      | 125.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 1240 | CLA  | O2D-CGD-O1D | -2.21 | 119.51      | 123.84   |
| 14  | H     | 1208 | CLA  | CMA-C3A-C4A | 2.21  | 117.72      | 111.77   |
| 14  | B     | 1022 | CLA  | C3D-C4D-ND  | 2.21  | 113.82      | 110.24   |
| 14  | B     | 1205 | CLA  | C4C-C3C-C2C | -2.21 | 103.67      | 106.90   |
| 18  | H     | 4014 | BCR  | C34-C9-C8   | 2.21  | 121.56      | 118.08   |
| 14  | G     | 1109 | CLA  | OBD-CAD-C3D | -2.21 | 123.20      | 128.52   |
| 14  | G     | 1120 | CLA  | O1D-CGD-CBD | -2.21 | 119.96      | 124.48   |
| 14  | a     | 1104 | CLA  | C3C-C4C-NC  | 2.21  | 113.05      | 110.57   |
| 18  | U     | 4019 | BCR  | C24-C23-C22 | -2.21 | 122.89      | 126.23   |
| 14  | B     | 1232 | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 14  | A     | 1114 | CLA  | C3C-C4C-NC  | 2.21  | 113.05      | 110.57   |
| 14  | B     | 1203 | CLA  | C3D-C4D-ND  | 2.21  | 113.81      | 110.24   |
| 14  | B     | 1233 | CLA  | CMC-C2C-C1C | 2.21  | 128.41      | 125.04   |
| 18  | V     | 4021 | BCR  | C38-C26-C25 | -2.21 | 122.05      | 124.53   |
| 14  | b     | 1228 | CLA  | C4-C3-C5    | 2.21  | 118.99      | 115.27   |
| 14  | a     | 1139 | CLA  | CMD-C2D-C3D | -2.21 | 122.53      | 127.61   |
| 13  | a     | 1011 | CL0  | CMC-C2C-C1C | 2.21  | 128.40      | 125.04   |
| 14  | A     | 1139 | CLA  | CMD-C2D-C3D | -2.21 | 122.53      | 127.61   |
| 15  | b     | 1238 | F6C  | CMC-C2C-C3C | 2.21  | 129.10      | 124.94   |
| 14  | B     | 1240 | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 14  | B     | 1239 | CLA  | CAA-CBA-CGA | -2.21 | 106.80      | 113.25   |
| 21  | L     | 6002 | LMT  | C6'-C5'-C4' | 2.21  | 119.75      | 113.33   |
| 14  | A     | 1140 | CLA  | C3D-C4D-ND  | 2.21  | 113.81      | 110.24   |
| 14  | H     | 1218 | CLA  | O1D-CGD-CBD | -2.21 | 119.97      | 124.48   |
| 14  | a     | 1105 | CLA  | CMA-C3A-C4A | 2.21  | 117.70      | 111.77   |
| 14  | a     | 1114 | CLA  | C3C-C4C-NC  | 2.21  | 113.05      | 110.57   |
| 14  | b     | 1232 | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 21  | U     | 6002 | LMT  | C6'-C5'-C4' | 2.21  | 119.75      | 113.33   |
| 14  | H     | 1204 | CLA  | C3C-C4C-NC  | 2.21  | 113.05      | 110.57   |
| 14  | G     | 1113 | CLA  | C4D-C3D-CAD | 2.21  | 110.70      | 108.10   |
| 18  | R     | 4020 | BCR  | C33-C5-C6   | -2.21 | 122.05      | 124.53   |
| 14  | a     | 1120 | CLA  | C4D-C3D-CAD | 2.21  | 110.69      | 108.10   |
| 14  | b     | 1204 | CLA  | C3C-C4C-NC  | 2.21  | 113.04      | 110.57   |
| 14  | a     | 1104 | CLA  | C4-C3-C5    | 2.20  | 118.98      | 115.27   |
| 14  | a     | 1135 | CLA  | CHC-C1C-C2C | -2.20 | 120.62      | 126.72   |
| 18  | U     | 4019 | BCR  | C4-C5-C6    | -2.20 | 119.53      | 122.73   |
| 14  | b     | 1202 | CLA  | C3C-C4C-NC  | 2.20  | 113.04      | 110.57   |
| 14  | G     | 1140 | CLA  | C3D-C4D-ND  | 2.20  | 113.80      | 110.24   |
| 14  | G     | 1104 | CLA  | C3C-C4C-NC  | 2.20  | 113.04      | 110.57   |
| 14  | a     | 1129 | CLA  | O1D-CGD-CBD | -2.20 | 119.98      | 124.48   |
| 14  | a     | 1137 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 14  | b     | 1223 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1227 | CLA  | C4D-C3D-CAD | 2.20  | 110.69      | 108.10   |
| 18  | a     | 4005 | BCR  | C30-C25-C26 | -2.20 | 119.51      | 122.61   |
| 14  | A     | 1140 | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 14  | G     | 1140 | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 14  | G     | 1128 | CLA  | C4C-C3C-C2C | -2.20 | 103.69      | 106.90   |
| 18  | I     | 4020 | BCR  | C33-C5-C6   | -2.20 | 122.06      | 124.53   |
| 13  | G     | 1011 | CL0  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 14  | a     | 1119 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 14  | B     | 1223 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 14  | H     | 1203 | CLA  | C4-C3-C5    | 2.20  | 118.97      | 115.27   |
| 14  | a     | 1140 | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 18  | U     | 4019 | BCR  | C37-C22-C21 | -2.20 | 119.84      | 122.92   |
| 14  | G     | 1119 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 21  | l     | 6002 | LMT  | C6'-C5'-C4' | 2.20  | 119.72      | 113.33   |
| 18  | L     | 4019 | BCR  | C4-C5-C6    | -2.20 | 119.54      | 122.73   |
| 14  | A     | 1105 | CLA  | CMA-C3A-C4A | 2.20  | 117.68      | 111.77   |
| 14  | B     | 1208 | CLA  | CMA-C3A-C4A | 2.20  | 117.68      | 111.77   |
| 14  | H     | 1022 | CLA  | CHD-C4C-C3C | -2.20 | 121.61      | 124.84   |
| 14  | H     | 1239 | CLA  | CAA-CBA-CGA | -2.20 | 106.84      | 113.25   |
| 18  | l     | 4019 | BCR  | C4-C5-C6    | -2.20 | 119.54      | 122.73   |
| 14  | G     | 1133 | CLA  | C4D-C3D-CAD | 2.19  | 110.68      | 108.10   |
| 18  | A     | 4005 | BCR  | C30-C25-C26 | -2.19 | 119.52      | 122.61   |
| 14  | B     | 1234 | CLA  | CMC-C2C-C1C | 2.19  | 128.38      | 125.04   |
| 18  | L     | 4019 | BCR  | C37-C22-C21 | -2.19 | 119.85      | 122.92   |
| 14  | A     | 1104 | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 14  | B     | 1215 | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 14  | b     | 1203 | CLA  | C3D-C4D-ND  | 2.19  | 113.79      | 110.24   |
| 14  | b     | 1203 | CLA  | C4-C3-C5    | 2.19  | 118.96      | 115.27   |
| 14  | G     | 1105 | CLA  | CMA-C3A-C4A | 2.19  | 117.67      | 111.77   |
| 15  | a     | 1121 | F6C  | CHA-C1A-C2A | -2.19 | 123.89      | 129.84   |
| 14  | b     | 1215 | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 14  | a     | 1109 | CLA  | OBD-CAD-C3D | -2.19 | 123.24      | 128.52   |
| 14  | G     | 1104 | CLA  | O1D-CGD-CBD | -2.19 | 120.00      | 124.48   |
| 14  | G     | 1139 | CLA  | CMD-C2D-C3D | -2.19 | 122.57      | 127.61   |
| 15  | a     | 1121 | F6C  | CMD-C2D-C3D | -2.19 | 122.57      | 127.61   |
| 14  | G     | 1104 | CLA  | C4-C3-C5    | 2.19  | 118.96      | 115.27   |
| 15  | A     | 1121 | F6C  | CHA-C1A-C2A | -2.19 | 123.90      | 129.84   |
| 14  | b     | 1210 | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 14  | a     | 1126 | CLA  | CMD-C2D-C3D | -2.19 | 122.57      | 127.61   |
| 15  | b     | 1237 | F6C  | C4-C3-C2    | -2.19 | 118.06      | 123.68   |
| 14  | H     | 1234 | CLA  | CMC-C2C-C1C | 2.19  | 128.38      | 125.04   |
| 18  | b     | 4010 | BCR  | C4-C5-C6    | -2.19 | 119.55      | 122.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1129 | CLA  | O1D-CGD-CBD | -2.19 | 120.00      | 124.48   |
| 15  | G     | 1121 | F6C  | CHA-C1A-C2A | -2.19 | 123.90      | 129.84   |
| 14  | H     | 1203 | CLA  | C3D-C4D-ND  | 2.19  | 113.78      | 110.24   |
| 15  | G     | 1121 | F6C  | CMD-C2D-C3D | -2.19 | 122.58      | 127.61   |
| 15  | A     | 1121 | F6C  | CMD-C2D-C3D | -2.19 | 122.58      | 127.61   |
| 14  | b     | 1208 | CLA  | CMA-C3A-C4A | 2.19  | 117.65      | 111.77   |
| 14  | B     | 1022 | CLA  | CHD-C4C-C3C | -2.19 | 121.62      | 124.84   |
| 14  | b     | 1022 | CLA  | CHD-C4C-C3C | -2.19 | 121.63      | 124.84   |
| 14  | H     | 1022 | CLA  | C4D-C3D-CAD | 2.19  | 110.67      | 108.10   |
| 14  | B     | 1203 | CLA  | C4-C3-C5    | 2.19  | 118.95      | 115.27   |
| 14  | A     | 1104 | CLA  | C4-C3-C5    | 2.18  | 118.95      | 115.27   |
| 14  | a     | 1113 | CLA  | C4D-C3D-CAD | 2.18  | 110.67      | 108.10   |
| 14  | a     | 1109 | CLA  | C3D-C4D-ND  | 2.18  | 113.77      | 110.24   |
| 18  | G     | 4005 | BCR  | C30-C25-C26 | -2.18 | 119.54      | 122.61   |
| 14  | B     | 1201 | CLA  | CMA-C3A-C4A | 2.18  | 117.64      | 111.77   |
| 14  | b     | 1234 | CLA  | CMC-C2C-C1C | 2.18  | 128.36      | 125.04   |
| 14  | B     | 1210 | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 15  | B     | 1237 | F6C  | C4-C3-C2    | -2.18 | 118.08      | 123.68   |
| 18  | M     | 4021 | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |
| 15  | H     | 1237 | F6C  | C4-C3-C2    | -2.18 | 118.08      | 123.68   |
| 14  | b     | 1205 | CLA  | C4C-C3C-C2C | -2.18 | 103.72      | 106.90   |
| 14  | A     | 1110 | CLA  | CMD-C2D-C3D | -2.18 | 122.60      | 127.61   |
| 15  | a     | 1121 | F6C  | CBC-CAC-C3C | -2.18 | 106.72      | 112.27   |
| 14  | G     | 1137 | CLA  | CMC-C2C-C1C | 2.18  | 128.36      | 125.04   |
| 14  | A     | 1141 | CLA  | CAC-C3C-C4C | 2.18  | 127.64      | 124.81   |
| 14  | G     | 1110 | CLA  | CMD-C2D-C3D | -2.18 | 122.60      | 127.61   |
| 18  | A     | 4003 | BCR  | C34-C9-C8   | 2.18  | 121.51      | 118.08   |
| 14  | H     | 1201 | CLA  | CMA-C3A-C4A | 2.18  | 117.62      | 111.77   |
| 14  | a     | 1130 | CLA  | C1-C2-C3    | -2.18 | 122.28      | 126.04   |
| 14  | b     | 1201 | CLA  | CMA-C3A-C4A | 2.18  | 117.62      | 111.77   |
| 14  | a     | 1110 | CLA  | CMD-C2D-C3D | -2.18 | 122.61      | 127.61   |
| 18  | a     | 4003 | BCR  | C34-C9-C8   | 2.18  | 121.51      | 118.08   |
| 14  | A     | 1137 | CLA  | CMC-C2C-C1C | 2.18  | 128.35      | 125.04   |
| 14  | H     | 1223 | CLA  | CMC-C2C-C1C | 2.18  | 128.35      | 125.04   |
| 18  | H     | 4010 | BCR  | C4-C5-C6    | -2.18 | 119.57      | 122.73   |
| 14  | A     | 1126 | CLA  | CMD-C2D-C3D | -2.17 | 122.61      | 127.61   |
| 14  | b     | 1203 | CLA  | CBC-CAC-C3C | -2.17 | 106.44      | 112.43   |
| 14  | H     | 1240 | CLA  | C3C-C4C-NC  | 2.17  | 113.01      | 110.57   |
| 18  | B     | 4010 | BCR  | C4-C5-C6    | -2.17 | 119.58      | 122.73   |
| 14  | H     | 1236 | CLA  | C4D-C3D-CAD | 2.17  | 110.66      | 108.10   |
| 15  | A     | 1121 | F6C  | CBC-CAC-C3C | -2.17 | 106.73      | 112.27   |
| 18  | m     | 4021 | BCR  | C38-C26-C25 | -2.17 | 122.09      | 124.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 1208 | CLA  | CMD-C2D-C3D | -2.17 | 122.62      | 127.61   |
| 14  | b     | 1240 | CLA  | C3C-C4C-NC  | 2.17  | 113.01      | 110.57   |
| 14  | A     | 1130 | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 14  | b     | 1208 | CLA  | CMD-C2D-C3D | -2.17 | 122.62      | 127.61   |
| 14  | H     | 1208 | CLA  | C4D-C3D-CAD | 2.17  | 110.65      | 108.10   |
| 14  | a     | 1141 | CLA  | CAC-C3C-C4C | 2.17  | 127.62      | 124.81   |
| 15  | H     | 1230 | F6C  | CHB-C4A-NA  | 2.17  | 126.45      | 124.45   |
| 14  | A     | 1102 | CLA  | CMA-C3A-C4A | 2.17  | 117.60      | 111.77   |
| 14  | b     | 1211 | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 14  | A     | 1104 | CLA  | O1D-CGD-CBD | -2.17 | 120.05      | 124.48   |
| 14  | H     | 1208 | CLA  | CMD-C2D-C3D | -2.17 | 122.63      | 127.61   |
| 20  | I     | 5006 | LMG  | O7-C10-O9   | -2.17 | 118.46      | 123.70   |
| 20  | H     | 5002 | LMG  | C8-O7-C10   | -2.17 | 112.45      | 117.79   |
| 14  | G     | 1130 | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 14  | L     | 1503 | CLA  | C4C-C3C-C2C | -2.17 | 103.74      | 106.90   |
| 14  | a     | 1102 | CLA  | CMA-C3A-C4A | 2.17  | 117.60      | 111.77   |
| 14  | B     | 1022 | CLA  | C4D-C3D-CAD | 2.17  | 110.65      | 108.10   |
| 14  | a     | 1124 | CLA  | C4D-C3D-CAD | 2.17  | 110.65      | 108.10   |
| 14  | H     | 1215 | CLA  | C3C-C4C-NC  | 2.17  | 113.00      | 110.57   |
| 14  | G     | 1141 | CLA  | CAC-C3C-C4C | 2.17  | 127.62      | 124.81   |
| 14  | A     | 1125 | CLA  | C4-C3-C5    | 2.17  | 118.91      | 115.27   |
| 14  | B     | 1210 | CLA  | CMA-C3A-C4A | 2.17  | 117.59      | 111.77   |
| 14  | B     | 1203 | CLA  | CBC-CAC-C3C | -2.17 | 106.46      | 112.43   |
| 15  | b     | 1230 | F6C  | CHB-C4A-NA  | 2.16  | 126.44      | 124.45   |
| 14  | G     | 1136 | CLA  | C1-C2-C3    | -2.16 | 122.30      | 126.04   |
| 14  | B     | 1212 | CLA  | C3D-C4D-ND  | 2.16  | 113.74      | 110.24   |
| 14  | H     | 1210 | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 14  | B     | 1236 | CLA  | C4D-C3D-CAD | 2.16  | 110.65      | 108.10   |
| 14  | a     | 1127 | CLA  | CAA-CBA-CGA | -2.16 | 106.93      | 113.25   |
| 14  | A     | 1133 | CLA  | C4D-C3D-CAD | 2.16  | 110.64      | 108.10   |
| 15  | G     | 1121 | F6C  | CBC-CAC-C3C | -2.16 | 106.76      | 112.27   |
| 14  | b     | 1210 | CLA  | CMA-C3A-C4A | 2.16  | 117.58      | 111.77   |
| 14  | m     | 1501 | CLA  | CED-O2D-CGD | 2.16  | 120.83      | 115.94   |
| 18  | H     | 4004 | BCR  | C33-C5-C4   | 2.16  | 117.77      | 113.62   |
| 18  | G     | 4002 | BCR  | C31-C1-C6   | -2.16 | 106.79      | 110.30   |
| 14  | G     | 1102 | CLA  | CMA-C3A-C4A | 2.16  | 117.58      | 111.77   |
| 14  | G     | 1128 | CLA  | C3D-C4D-ND  | 2.16  | 113.73      | 110.24   |
| 14  | G     | 1127 | CLA  | CAA-CBA-CGA | -2.16 | 106.94      | 113.25   |
| 14  | a     | 1104 | CLA  | O1D-CGD-CBD | -2.16 | 120.06      | 124.48   |
| 14  | a     | 1123 | CLA  | O1D-CGD-CBD | -2.16 | 120.06      | 124.48   |
| 14  | b     | 1222 | CLA  | O1D-CGD-CBD | -2.16 | 120.06      | 124.48   |
| 14  | G     | 1106 | CLA  | CMD-C2D-C3D | -2.16 | 122.64      | 127.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | b     | 4005 | BCR  | C23-C22-C21 | 2.16  | 122.25      | 118.94   |
| 21  | b     | 6003 | LMT  | C4B-C3B-C2B | 2.16  | 114.59      | 110.82   |
| 18  | G     | 4003 | BCR  | C34-C9-C8   | 2.16  | 121.48      | 118.08   |
| 18  | k     | 4001 | BCR  | C37-C22-C23 | 2.16  | 121.48      | 118.08   |
| 14  | H     | 1212 | CLA  | C3D-C4D-ND  | 2.16  | 113.73      | 110.24   |
| 14  | A     | 1127 | CLA  | CAA-CBA-CGA | -2.16 | 106.94      | 113.25   |
| 14  | G     | 1125 | CLA  | C4-C3-C5    | 2.16  | 118.90      | 115.27   |
| 20  | B     | 5002 | LMG  | C8-O7-C10   | -2.16 | 112.48      | 117.79   |
| 14  | A     | 1107 | CLA  | CMD-C2D-C3D | -2.16 | 122.65      | 127.61   |
| 14  | U     | 1503 | CLA  | C4C-C3C-C2C | -2.16 | 103.75      | 106.90   |
| 14  | a     | 1012 | CLA  | C6-C7-C8    | -2.16 | 108.95      | 115.92   |
| 14  | G     | 1126 | CLA  | CMD-C2D-C3D | -2.16 | 122.65      | 127.61   |
| 15  | B     | 1230 | F6C  | CHB-C4A-NA  | 2.16  | 126.44      | 124.45   |
| 14  | A     | 1012 | CLA  | C6-C7-C8    | -2.15 | 108.95      | 115.92   |
| 14  | a     | 1106 | CLA  | CAA-C2A-C1A | -2.15 | 104.91      | 111.97   |
| 14  | B     | 1208 | CLA  | C4D-C3D-CAD | 2.15  | 110.64      | 108.10   |
| 20  | R     | 5006 | LMG  | O7-C10-O9   | -2.15 | 118.50      | 123.70   |
| 14  | b     | 1212 | CLA  | C3D-C4D-ND  | 2.15  | 113.72      | 110.24   |
| 14  | M     | 1501 | CLA  | CED-O2D-CGD | 2.15  | 120.81      | 115.94   |
| 14  | A     | 1109 | CLA  | C3D-C4D-ND  | 2.15  | 113.72      | 110.24   |
| 14  | b     | 1216 | CLA  | CAC-C3C-C4C | 2.15  | 127.60      | 124.81   |
| 18  | A     | 4002 | BCR  | C31-C1-C6   | -2.15 | 106.81      | 110.30   |
| 14  | A     | 1123 | CLA  | O1D-CGD-CBD | -2.15 | 120.08      | 124.48   |
| 14  | H     | 1203 | CLA  | CBC-CAC-C3C | -2.15 | 106.50      | 112.43   |
| 14  | b     | 1239 | CLA  | C4C-C3C-C2C | -2.15 | 103.76      | 106.90   |
| 14  | G     | 1107 | CLA  | CMD-C2D-C3D | -2.15 | 122.67      | 127.61   |
| 14  | a     | 1125 | CLA  | C4-C3-C5    | 2.15  | 118.89      | 115.27   |
| 14  | G     | 1012 | CLA  | C6-C7-C8    | -2.15 | 108.97      | 115.92   |
| 14  | b     | 1208 | CLA  | C1-C2-C3    | -2.15 | 122.32      | 126.04   |
| 14  | H     | 1231 | CLA  | CHB-C4A-NA  | 2.15  | 127.48      | 124.51   |
| 14  | b     | 1216 | CLA  | CHC-C1C-C2C | -2.15 | 120.78      | 126.72   |
| 14  | H     | 1227 | CLA  | CAC-C3C-C4C | 2.15  | 127.60      | 124.81   |
| 14  | a     | 1133 | CLA  | C4D-C3D-CAD | 2.15  | 110.63      | 108.10   |
| 14  | H     | 1210 | CLA  | CMA-C3A-C4A | 2.15  | 117.55      | 111.77   |
| 18  | H     | 4014 | BCR  | C1-C6-C5    | -2.15 | 119.59      | 122.61   |
| 14  | A     | 1136 | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 14  | B     | 1222 | CLA  | O1D-CGD-CBD | -2.15 | 120.09      | 124.48   |
| 18  | B     | 4004 | BCR  | C33-C5-C4   | 2.15  | 117.74      | 113.62   |
| 18  | K     | 4001 | BCR  | C37-C22-C23 | 2.15  | 121.46      | 118.08   |
| 14  | B     | 1214 | CLA  | C1-O2A-CGA  | 2.15  | 122.08      | 116.44   |
| 14  | B     | 1240 | CLA  | C3C-C4C-NC  | 2.15  | 112.98      | 110.57   |
| 14  | b     | 1206 | CLA  | CMB-C2B-C1B | -2.15 | 125.16      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1123 | CLA  | O1D-CGD-CBD | -2.15 | 120.09      | 124.48   |
| 21  | l     | 6002 | LMT  | C1'-O5'-C5' | -2.15 | 109.47      | 113.69   |
| 14  | H     | 1211 | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 15  | b     | 1237 | F6C  | OBD-CAD-C3D | -2.15 | 123.35      | 128.52   |
| 14  | B     | 1211 | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 15  | H     | 1237 | F6C  | OBD-CAD-C3D | -2.15 | 123.36      | 128.52   |
| 14  | G     | 1140 | CLA  | CMA-C3A-C4A | 2.15  | 117.54      | 111.77   |
| 20  | i     | 5006 | LMG  | O7-C10-O9   | -2.15 | 118.52      | 123.70   |
| 14  | B     | 1221 | CLA  | CHB-C4A-NA  | 2.15  | 127.48      | 124.51   |
| 14  | B     | 1021 | CLA  | C4C-C3C-C2C | -2.15 | 103.77      | 106.90   |
| 21  | H     | 6003 | LMT  | C1B-O5B-C5B | 2.15  | 117.90      | 113.69   |
| 14  | H     | 1239 | CLA  | CHC-C1C-C2C | -2.15 | 120.79      | 126.72   |
| 15  | B     | 1237 | F6C  | OBD-CAD-C3D | -2.15 | 123.36      | 128.52   |
| 15  | B     | 1238 | F6C  | C4-C3-C5    | 2.14  | 118.88      | 115.27   |
| 14  | l     | 1503 | CLA  | C4C-C3C-C2C | -2.14 | 103.77      | 106.90   |
| 14  | B     | 1206 | CLA  | CMB-C2B-C1B | -2.14 | 125.17      | 128.46   |
| 14  | a     | 1135 | CLA  | OBD-CAD-C3D | -2.14 | 123.36      | 128.52   |
| 14  | a     | 1107 | CLA  | CMD-C2D-C3D | -2.14 | 122.68      | 127.61   |
| 14  | B     | 1239 | CLA  | CHC-C1C-C2C | -2.14 | 120.79      | 126.72   |
| 14  | A     | 1106 | CLA  | CAA-C2A-C1A | -2.14 | 104.95      | 111.97   |
| 14  | b     | 1217 | CLA  | CHD-C4C-C3C | -2.14 | 121.69      | 124.84   |
| 20  | b     | 5002 | LMG  | C8-O7-C10   | -2.14 | 112.52      | 117.79   |
| 18  | b     | 4005 | BCR  | C8-C9-C10   | 2.14  | 122.23      | 118.94   |
| 14  | G     | 1122 | CLA  | CMC-C2C-C1C | 2.14  | 128.30      | 125.04   |
| 14  | G     | 1135 | CLA  | CMC-C2C-C1C | 2.14  | 128.30      | 125.04   |
| 14  | b     | 1228 | CLA  | C4D-C3D-CAD | 2.14  | 110.62      | 108.10   |
| 14  | H     | 1222 | CLA  | O1D-CGD-CBD | -2.14 | 120.10      | 124.48   |
| 14  | B     | 1227 | CLA  | CAC-C3C-C4C | 2.14  | 127.59      | 124.81   |
| 21  | B     | 6003 | LMT  | C4B-C3B-C2B | 2.14  | 114.56      | 110.82   |
| 18  | a     | 4003 | BCR  | C35-C13-C14 | -2.14 | 119.92      | 122.92   |
| 18  | B     | 4005 | BCR  | C8-C9-C10   | 2.14  | 122.23      | 118.94   |
| 18  | H     | 4005 | BCR  | C23-C22-C21 | 2.14  | 122.23      | 118.94   |
| 14  | B     | 1239 | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 14  | b     | 1214 | CLA  | C1-O2A-CGA  | 2.14  | 122.06      | 116.44   |
| 21  | L     | 6002 | LMT  | C1'-O5'-C5' | -2.14 | 109.49      | 113.69   |
| 14  | A     | 1129 | CLA  | C4D-C3D-CAD | 2.14  | 110.62      | 108.10   |
| 14  | G     | 1106 | CLA  | CAA-C2A-C1A | -2.14 | 104.96      | 111.97   |
| 14  | A     | 1106 | CLA  | CMD-C2D-C3D | -2.14 | 122.69      | 127.61   |
| 18  | a     | 4004 | BCR  | C34-C9-C10  | -2.14 | 119.93      | 122.92   |
| 18  | b     | 4004 | BCR  | C35-C13-C14 | -2.14 | 119.93      | 122.92   |
| 18  | B     | 4005 | BCR  | C23-C22-C21 | 2.14  | 122.22      | 118.94   |
| 14  | H     | 1214 | CLA  | C1-O2A-CGA  | 2.14  | 122.06      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1131 | CLA  | C1-O2A-CGA  | 2.14  | 122.06      | 116.44   |
| 14  | B     | 1231 | CLA  | CHB-C4A-NA  | 2.14  | 127.47      | 124.51   |
| 14  | B     | 1223 | CLA  | CAA-C2A-C3A | -2.14 | 106.92      | 112.78   |
| 14  | B     | 1023 | CLA  | C1-C2-C3    | -2.14 | 122.34      | 126.04   |
| 15  | G     | 1121 | F6C  | O1D-CGD-CBD | -2.14 | 120.11      | 124.48   |
| 14  | G     | 1013 | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 14  | a     | 1137 | CLA  | CMD-C2D-C3D | -2.14 | 122.69      | 127.61   |
| 15  | b     | 1238 | F6C  | C4-C3-C5    | 2.14  | 118.87      | 115.27   |
| 14  | b     | 1236 | CLA  | C4D-C3D-CAD | 2.14  | 110.62      | 108.10   |
| 14  | H     | 1223 | CLA  | CAA-C2A-C3A | -2.14 | 106.92      | 112.78   |
| 15  | A     | 1121 | F6C  | O1D-CGD-CBD | -2.14 | 120.11      | 124.48   |
| 15  | H     | 1238 | F6C  | C4-C3-C5    | 2.14  | 118.87      | 115.27   |
| 14  | V     | 1501 | CLA  | CED-O2D-CGD | 2.14  | 120.77      | 115.94   |
| 14  | G     | 1109 | CLA  | C3D-C4D-ND  | 2.14  | 113.69      | 110.24   |
| 14  | A     | 1124 | CLA  | C4D-C3D-CAD | 2.14  | 110.61      | 108.10   |
| 21  | U     | 6002 | LMT  | C1'-O5'-C5' | -2.14 | 109.49      | 113.69   |
| 14  | G     | 1131 | CLA  | C1-O2A-CGA  | 2.14  | 122.05      | 116.44   |
| 14  | B     | 1216 | CLA  | CHC-C1C-C2C | -2.14 | 120.81      | 126.72   |
| 21  | H     | 6003 | LMT  | C4B-C3B-C2B | 2.14  | 114.55      | 110.82   |
| 14  | H     | 1206 | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 14  | H     | 1239 | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 14  | B     | 1205 | CLA  | C1-C2-C3    | -2.14 | 122.35      | 126.04   |
| 14  | G     | 1110 | CLA  | CAA-C2A-C3A | -2.14 | 106.93      | 112.78   |
| 14  | G     | 1124 | CLA  | C4D-C3D-CAD | 2.14  | 110.61      | 108.10   |
| 14  | b     | 1223 | CLA  | CAA-C2A-C3A | -2.14 | 106.93      | 112.78   |
| 14  | A     | 1135 | CLA  | CMC-C2C-C1C | 2.14  | 128.29      | 125.04   |
| 14  | H     | 1216 | CLA  | CHC-C1C-C2C | -2.14 | 120.82      | 126.72   |
| 14  | A     | 1104 | CLA  | CMD-C2D-C3D | -2.13 | 122.70      | 127.61   |
| 14  | a     | 1132 | CLA  | C16-C15-C13 | -2.13 | 109.02      | 115.92   |
| 14  | b     | 1022 | CLA  | C4D-C3D-CAD | 2.13  | 110.61      | 108.10   |
| 14  | G     | 1137 | CLA  | CMD-C2D-C3D | -2.13 | 122.70      | 127.61   |
| 14  | A     | 1128 | CLA  | C3D-C4D-ND  | 2.13  | 113.69      | 110.24   |
| 14  | H     | 1217 | CLA  | CHD-C4C-C3C | -2.13 | 121.70      | 124.84   |
| 14  | b     | 1023 | CLA  | C1-C2-C3    | -2.13 | 122.35      | 126.04   |
| 18  | T     | 4001 | BCR  | C37-C22-C23 | 2.13  | 121.44      | 118.08   |
| 14  | A     | 1140 | CLA  | CMA-C3A-C4A | 2.13  | 117.51      | 111.77   |
| 18  | B     | 4004 | BCR  | C35-C13-C14 | -2.13 | 119.93      | 122.92   |
| 14  | A     | 1132 | CLA  | C16-C15-C13 | -2.13 | 109.02      | 115.92   |
| 14  | a     | 1106 | CLA  | CMD-C2D-C3D | -2.13 | 122.71      | 127.61   |
| 18  | A     | 4004 | BCR  | C34-C9-C10  | -2.13 | 119.94      | 122.92   |
| 18  | G     | 4003 | BCR  | C35-C13-C14 | -2.13 | 119.94      | 122.92   |
| 14  | A     | 1131 | CLA  | C1-O2A-CGA  | 2.13  | 122.04      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | b     | 4004 | BCR  | C33-C5-C4   | 2.13  | 117.71      | 113.62   |
| 18  | a     | 4002 | BCR  | C31-C1-C6   | -2.13 | 106.84      | 110.30   |
| 14  | A     | 1137 | CLA  | CMD-C2D-C3D | -2.13 | 122.71      | 127.61   |
| 14  | A     | 1122 | CLA  | CMC-C2C-C1C | 2.13  | 128.29      | 125.04   |
| 14  | G     | 1104 | CLA  | CMD-C2D-C3D | -2.13 | 122.71      | 127.61   |
| 21  | B     | 6003 | LMT  | C1B-O5B-C5B | 2.13  | 117.87      | 113.69   |
| 14  | U     | 1503 | CLA  | CHC-C1C-C2C | -2.13 | 120.83      | 126.72   |
| 14  | G     | 1101 | CLA  | CAC-C3C-C4C | 2.13  | 127.58      | 124.81   |
| 18  | A     | 4003 | BCR  | C35-C13-C14 | -2.13 | 119.94      | 122.92   |
| 14  | a     | 1136 | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 14  | B     | 1216 | CLA  | CAC-C3C-C4C | 2.13  | 127.57      | 124.81   |
| 14  | G     | 1117 | CLA  | CMD-C2D-C3D | -2.13 | 122.72      | 127.61   |
| 14  | a     | 1129 | CLA  | C4D-C3D-CAD | 2.13  | 110.61      | 108.10   |
| 14  | b     | 1208 | CLA  | C4D-C3D-CAD | 2.13  | 110.61      | 108.10   |
| 14  | b     | 1227 | CLA  | CAC-C3C-C4C | 2.13  | 127.57      | 124.81   |
| 14  | A     | 1135 | CLA  | OBD-CAD-C3D | -2.13 | 123.40      | 128.52   |
| 14  | A     | 1013 | CLA  | C4C-C3C-C2C | -2.13 | 103.79      | 106.90   |
| 14  | b     | 1021 | CLA  | C4C-C3C-C2C | -2.13 | 103.79      | 106.90   |
| 14  | A     | 1117 | CLA  | CMD-C2D-C3D | -2.13 | 122.72      | 127.61   |
| 14  | H     | 1212 | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 14  | A     | 1131 | CLA  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 14  | b     | 1239 | CLA  | CHC-C1C-C2C | -2.13 | 120.84      | 126.72   |
| 14  | H     | 1205 | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 18  | A     | 4003 | BCR  | C23-C22-C21 | -2.13 | 115.68      | 118.94   |
| 18  | B     | 4014 | BCR  | C1-C6-C5    | -2.13 | 119.62      | 122.61   |
| 14  | B     | 1208 | CLA  | C1-C2-C3    | -2.13 | 122.37      | 126.04   |
| 18  | H     | 4005 | BCR  | C8-C9-C10   | 2.13  | 122.20      | 118.94   |
| 14  | a     | 1135 | CLA  | CMC-C2C-C1C | 2.13  | 128.28      | 125.04   |
| 15  | a     | 1121 | F6C  | O1D-CGD-CBD | -2.13 | 120.14      | 124.48   |
| 14  | B     | 1228 | CLA  | C4D-C3D-CAD | 2.13  | 110.60      | 108.10   |
| 14  | G     | 1132 | CLA  | C16-C15-C13 | -2.13 | 109.05      | 115.92   |
| 14  | H     | 1021 | CLA  | C4C-C3C-C2C | -2.12 | 103.80      | 106.90   |
| 14  | a     | 1116 | CLA  | CMA-C3A-C4A | 2.12  | 117.48      | 111.77   |
| 14  | a     | 1140 | CLA  | CMA-C3A-C4A | 2.12  | 117.48      | 111.77   |
| 14  | H     | 1208 | CLA  | C1-C2-C3    | -2.12 | 122.37      | 126.04   |
| 18  | a     | 4003 | BCR  | C23-C22-C21 | -2.12 | 115.68      | 118.94   |
| 14  | a     | 1122 | CLA  | C4D-C3D-CAD | 2.12  | 110.60      | 108.10   |
| 14  | b     | 1209 | CLA  | CMD-C2D-C3D | -2.12 | 122.73      | 127.61   |
| 14  | L     | 1503 | CLA  | CHC-C1C-C2C | -2.12 | 120.85      | 126.72   |
| 14  | A     | 1110 | CLA  | CAA-C2A-C3A | -2.12 | 106.97      | 112.78   |
| 14  | b     | 1205 | CLA  | C1-C2-C3    | -2.12 | 122.37      | 126.04   |
| 18  | H     | 4004 | BCR  | C35-C13-C14 | -2.12 | 119.95      | 122.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1209 | CLA  | CMD-C2D-C3D | -2.12 | 122.73      | 127.61   |
| 14  | H     | 1218 | CLA  | CMD-C2D-C3D | -2.12 | 122.73      | 127.61   |
| 14  | H     | 1221 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 14  | G     | 1129 | CLA  | C4D-C3D-CAD | 2.12  | 110.59      | 108.10   |
| 14  | b     | 1234 | CLA  | C4D-C3D-CAD | 2.12  | 110.59      | 108.10   |
| 14  | a     | 1123 | CLA  | OBD-CAD-C3D | -2.12 | 123.42      | 128.52   |
| 14  | G     | 1113 | CLA  | CMD-C2D-C3D | -2.12 | 122.74      | 127.61   |
| 14  | a     | 1013 | CLA  | C4C-C3C-C2C | -2.12 | 103.81      | 106.90   |
| 18  | G     | 4003 | BCR  | C23-C22-C21 | -2.12 | 115.69      | 118.94   |
| 14  | B     | 1217 | CLA  | CHD-C4C-C3C | -2.12 | 121.72      | 124.84   |
| 14  | H     | 1023 | CLA  | C1-C2-C3    | -2.12 | 122.38      | 126.04   |
| 14  | G     | 1135 | CLA  | OBD-CAD-C3D | -2.12 | 123.42      | 128.52   |
| 18  | G     | 4004 | BCR  | C34-C9-C10  | -2.12 | 119.95      | 122.92   |
| 14  | a     | 1113 | CLA  | CMD-C2D-C3D | -2.12 | 122.74      | 127.61   |
| 21  | b     | 6003 | LMT  | C1B-O5B-C5B | 2.12  | 117.85      | 113.69   |
| 14  | A     | 1113 | CLA  | CMD-C2D-C3D | -2.12 | 122.74      | 127.61   |
| 14  | b     | 1221 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 14  | a     | 1109 | CLA  | CHC-C1C-C2C | -2.12 | 120.87      | 126.72   |
| 14  | A     | 1117 | CLA  | C4D-C3D-CAD | 2.12  | 110.59      | 108.10   |
| 14  | G     | 1129 | CLA  | C4C-C3C-C2C | -2.12 | 103.81      | 106.90   |
| 14  | G     | 1116 | CLA  | CMA-C3A-C4A | 2.12  | 117.46      | 111.77   |
| 14  | A     | 1122 | CLA  | C4D-C3D-CAD | 2.12  | 110.59      | 108.10   |
| 14  | H     | 1228 | CLA  | C4D-C3D-CAD | 2.12  | 110.59      | 108.10   |
| 14  | A     | 1109 | CLA  | CHC-C1C-C2C | -2.12 | 120.87      | 126.72   |
| 18  | l     | 4019 | BCR  | C15-C14-C13 | -2.12 | 124.29      | 127.31   |
| 15  | b     | 1230 | F6C  | CMD-C2D-C3D | -2.11 | 122.75      | 127.61   |
| 18  | R     | 4020 | BCR  | C7-C8-C9    | -2.11 | 123.04      | 126.23   |
| 15  | B     | 1230 | F6C  | CMD-C2D-C3D | -2.11 | 122.75      | 127.61   |
| 14  | B     | 1234 | CLA  | C4D-C3D-CAD | 2.11  | 110.59      | 108.10   |
| 13  | a     | 1011 | CL0  | C6-C5-C3    | -2.11 | 107.91      | 113.45   |
| 14  | a     | 1131 | CLA  | O1D-CGD-CBD | -2.11 | 120.16      | 124.48   |
| 14  | a     | 1110 | CLA  | CAA-C2A-C3A | -2.11 | 106.99      | 112.78   |
| 14  | G     | 1131 | CLA  | O1D-CGD-CBD | -2.11 | 120.16      | 124.48   |
| 14  | a     | 1117 | CLA  | CMD-C2D-C3D | -2.11 | 122.75      | 127.61   |
| 14  | a     | 1128 | CLA  | C3D-C4D-ND  | 2.11  | 113.66      | 110.24   |
| 14  | B     | 1228 | CLA  | CMC-C2C-C3C | 2.11  | 131.85      | 126.12   |
| 14  | H     | 1216 | CLA  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 14  | B     | 1228 | CLA  | C4C-C3C-C2C | -2.11 | 103.82      | 106.90   |
| 15  | H     | 1230 | F6C  | CMD-C2D-C3D | -2.11 | 122.76      | 127.61   |
| 14  | l     | 1503 | CLA  | CHC-C1C-C2C | -2.11 | 120.88      | 126.72   |
| 14  | a     | 1122 | CLA  | CMC-C2C-C1C | 2.11  | 128.25      | 125.04   |
| 14  | A     | 1116 | CLA  | CMA-C3A-C4A | 2.11  | 117.44      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | k     | 1401 | CLA  | CMD-C2D-C3D | -2.11 | 122.76      | 127.61   |
| 14  | H     | 1206 | CLA  | CMB-C2B-C1B | -2.11 | 125.22      | 128.46   |
| 14  | H     | 1228 | CLA  | C4C-C3C-C2C | -2.11 | 103.82      | 106.90   |
| 14  | b     | 1236 | CLA  | CAC-C3C-C2C | 2.11  | 131.13      | 127.53   |
| 14  | H     | 1201 | CLA  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 14  | b     | 1228 | CLA  | C4C-C3C-C2C | -2.11 | 103.83      | 106.90   |
| 14  | G     | 1117 | CLA  | C4D-C3D-CAD | 2.11  | 110.58      | 108.10   |
| 14  | b     | 1223 | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 14  | G     | 1123 | CLA  | OBD-CAD-C3D | -2.11 | 123.45      | 128.52   |
| 14  | b     | 1228 | CLA  | CMC-C2C-C3C | 2.11  | 131.84      | 126.12   |
| 14  | B     | 1235 | CLA  | CBA-CAA-C2A | 2.11  | 120.08      | 113.86   |
| 14  | A     | 1138 | CLA  | CHC-C1C-C2C | -2.11 | 120.90      | 126.72   |
| 14  | G     | 1109 | CLA  | CHC-C1C-C2C | -2.11 | 120.90      | 126.72   |
| 14  | H     | 1228 | CLA  | CMC-C2C-C3C | 2.11  | 131.83      | 126.12   |
| 14  | H     | 1234 | CLA  | C4D-C3D-CAD | 2.11  | 110.58      | 108.10   |
| 14  | A     | 1101 | CLA  | CAC-C3C-C4C | 2.11  | 127.54      | 124.81   |
| 14  | b     | 1239 | CLA  | C3D-C4D-ND  | 2.11  | 113.64      | 110.24   |
| 18  | I     | 4020 | BCR  | C7-C8-C9    | -2.11 | 123.05      | 126.23   |
| 14  | B     | 1209 | CLA  | CMD-C2D-C3D | -2.10 | 122.77      | 127.61   |
| 14  | a     | 1130 | CLA  | OBD-CAD-C3D | -2.10 | 123.45      | 128.52   |
| 14  | T     | 1401 | CLA  | CMD-C2D-C3D | -2.10 | 122.77      | 127.61   |
| 14  | a     | 1104 | CLA  | CMD-C2D-C3D | -2.10 | 122.77      | 127.61   |
| 14  | a     | 1109 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 18  | i     | 4020 | BCR  | C7-C8-C9    | -2.10 | 123.06      | 126.23   |
| 14  | b     | 1206 | CLA  | C4C-C3C-C2C | -2.10 | 103.83      | 106.90   |
| 14  | a     | 1138 | CLA  | CHC-C1C-C2C | -2.10 | 120.90      | 126.72   |
| 18  | L     | 4022 | BCR  | C4-C5-C6    | -2.10 | 119.68      | 122.73   |
| 14  | H     | 1022 | CLA  | CHA-C1A-NA  | -2.10 | 121.58      | 126.40   |
| 14  | b     | 1201 | CLA  | CAC-C3C-C4C | 2.10  | 127.54      | 124.81   |
| 14  | G     | 1130 | CLA  | OBD-CAD-C3D | -2.10 | 123.46      | 128.52   |
| 14  | b     | 1221 | CLA  | C3D-C4D-ND  | 2.10  | 113.64      | 110.24   |
| 14  | A     | 1123 | CLA  | OBD-CAD-C3D | -2.10 | 123.47      | 128.52   |
| 14  | A     | 1103 | CLA  | CAA-C2A-C1A | -2.10 | 105.09      | 111.97   |
| 14  | B     | 1206 | CLA  | C4C-C3C-C2C | -2.10 | 103.84      | 106.90   |
| 18  | b     | 4014 | BCR  | C1-C6-C5    | -2.10 | 119.66      | 122.61   |
| 14  | B     | 1212 | CLA  | C3C-C4C-NC  | 2.10  | 112.92      | 110.57   |
| 14  | A     | 1129 | CLA  | C4C-C3C-C2C | -2.10 | 103.84      | 106.90   |
| 18  | b     | 4010 | BCR  | C31-C1-C6   | -2.10 | 106.89      | 110.30   |
| 14  | H     | 1203 | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 14  | b     | 1235 | CLA  | CMD-C2D-C3D | -2.10 | 122.79      | 127.61   |
| 14  | H     | 1212 | CLA  | CMC-C2C-C3C | 2.10  | 131.81      | 126.12   |
| 14  | G     | 1103 | CLA  | CAA-C2A-C1A | -2.10 | 105.10      | 111.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 1122 | CLA  | C4D-C3D-CAD | 2.10  | 110.57      | 108.10   |
| 14  | a     | 1103 | CLA  | CAA-C2A-C1A | -2.10 | 105.10      | 111.97   |
| 14  | G     | 1138 | CLA  | CHC-C1C-C2C | -2.10 | 120.92      | 126.72   |
| 14  | B     | 1236 | CLA  | CAC-C3C-C2C | 2.10  | 131.12      | 127.53   |
| 18  | A     | 4003 | BCR  | C38-C26-C27 | 2.10  | 117.64      | 113.62   |
| 14  | B     | 1218 | CLA  | CMD-C2D-C3D | -2.10 | 122.79      | 127.61   |
| 14  | b     | 1218 | CLA  | CED-O2D-CGD | 2.10  | 120.68      | 115.94   |
| 18  | l     | 4022 | BCR  | C4-C5-C6    | -2.10 | 119.69      | 122.73   |
| 18  | a     | 4006 | BCR  | C12-C13-C14 | -2.10 | 115.72      | 118.94   |
| 14  | H     | 1216 | CLA  | CMD-C2D-C3D | -2.10 | 122.79      | 127.61   |
| 14  | b     | 1218 | CLA  | CMD-C2D-C3D | -2.10 | 122.79      | 127.61   |
| 18  | B     | 4010 | BCR  | C31-C1-C6   | -2.10 | 106.90      | 110.30   |
| 18  | H     | 4010 | BCR  | C31-C1-C6   | -2.10 | 106.90      | 110.30   |
| 14  | H     | 1235 | CLA  | CMD-C2D-C3D | -2.10 | 122.79      | 127.61   |
| 14  | B     | 1223 | CLA  | O1D-CGD-CBD | -2.10 | 120.20      | 124.48   |
| 14  | b     | 1239 | CLA  | CAA-C2A-C3A | -2.09 | 107.04      | 112.78   |
| 14  | H     | 1223 | CLA  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 14  | H     | 1235 | CLA  | CBA-CAA-C2A | 2.09  | 120.05      | 113.86   |
| 13  | A     | 1011 | CL0  | C6-C5-C3    | -2.09 | 107.96      | 113.45   |
| 14  | K     | 1401 | CLA  | CMD-C2D-C3D | -2.09 | 122.80      | 127.61   |
| 14  | b     | 1226 | CLA  | CAA-CBA-CGA | -2.09 | 107.14      | 113.25   |
| 14  | b     | 1203 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.51   |
| 14  | B     | 1235 | CLA  | CMD-C2D-C3D | -2.09 | 122.80      | 127.61   |
| 14  | B     | 1239 | CLA  | CAA-C2A-C3A | -2.09 | 107.05      | 112.78   |
| 14  | b     | 1231 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.51   |
| 14  | b     | 1233 | CLA  | CHC-C1C-C2C | -2.09 | 120.94      | 126.72   |
| 14  | G     | 1104 | CLA  | CHD-C4C-C3C | -2.09 | 121.77      | 124.84   |
| 14  | b     | 1235 | CLA  | CBA-CAA-C2A | 2.09  | 120.04      | 113.86   |
| 14  | H     | 1234 | CLA  | C1-C2-C3    | -2.09 | 122.42      | 126.04   |
| 18  | b     | 4017 | BCR  | C36-C18-C17 | -2.09 | 119.99      | 122.92   |
| 14  | H     | 1021 | CLA  | C4D-C3D-CAD | 2.09  | 110.56      | 108.10   |
| 14  | B     | 1226 | CLA  | CAA-CBA-CGA | -2.09 | 107.14      | 113.25   |
| 14  | H     | 1218 | CLA  | CED-O2D-CGD | 2.09  | 120.67      | 115.94   |
| 14  | H     | 1239 | CLA  | CAA-C2A-C3A | -2.09 | 107.05      | 112.78   |
| 14  | a     | 1012 | CLA  | C1-O2A-CGA  | 2.09  | 121.93      | 116.44   |
| 14  | B     | 1201 | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.81   |
| 14  | A     | 1130 | CLA  | OBD-CAD-C3D | -2.09 | 123.49      | 128.52   |
| 18  | a     | 4003 | BCR  | C38-C26-C27 | 2.09  | 117.63      | 113.62   |
| 14  | H     | 1239 | CLA  | C3D-C4D-ND  | 2.09  | 113.62      | 110.24   |
| 14  | a     | 1129 | CLA  | C4C-C3C-C2C | -2.09 | 103.85      | 106.90   |
| 13  | G     | 1011 | CL0  | C6-C5-C3    | -2.09 | 107.98      | 113.45   |
| 14  | b     | 1212 | CLA  | CMC-C2C-C3C | 2.09  | 131.79      | 126.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 1214 | CLA  | CED-O2D-CGD | 2.09  | 120.66      | 115.94   |
| 14  | H     | 1226 | CLA  | CAA-CBA-CGA | -2.09 | 107.15      | 113.25   |
| 14  | B     | 1212 | CLA  | CMC-C2C-C3C | 2.09  | 131.78      | 126.12   |
| 14  | A     | 1109 | CLA  | CMC-C2C-C1C | 2.09  | 128.22      | 125.04   |
| 14  | H     | 1236 | CLA  | CAC-C3C-C2C | 2.09  | 131.10      | 127.53   |
| 18  | a     | 4001 | BCR  | C37-C22-C21 | -2.09 | 120.00      | 122.92   |
| 18  | U     | 4022 | BCR  | C4-C5-C6    | -2.08 | 119.70      | 122.73   |
| 14  | a     | 1125 | CLA  | C1-O2A-CGA  | 2.08  | 121.91      | 116.44   |
| 18  | A     | 4006 | BCR  | C12-C13-C14 | -2.08 | 115.74      | 118.94   |
| 14  | B     | 1223 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 18  | b     | 4017 | BCR  | C37-C22-C23 | 2.08  | 121.36      | 118.08   |
| 14  | b     | 1223 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 14  | a     | 1101 | CLA  | CAC-C3C-C4C | 2.08  | 127.51      | 124.81   |
| 14  | B     | 1212 | CLA  | C4C-C3C-C2C | -2.08 | 103.86      | 106.90   |
| 14  | H     | 1212 | CLA  | C4C-C3C-C2C | -2.08 | 103.86      | 106.90   |
| 14  | a     | 1134 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 18  | G     | 4003 | BCR  | C38-C26-C27 | 2.08  | 117.61      | 113.62   |
| 14  | H     | 1201 | CLA  | O1D-CGD-CBD | -2.08 | 120.22      | 124.48   |
| 14  | B     | 1214 | CLA  | CED-O2D-CGD | 2.08  | 120.64      | 115.94   |
| 18  | G     | 4001 | BCR  | C37-C22-C21 | -2.08 | 120.01      | 122.92   |
| 14  | H     | 1223 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 14  | b     | 1022 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 14  | B     | 1233 | CLA  | CHC-C1C-C2C | -2.08 | 120.97      | 126.72   |
| 18  | B     | 4004 | BCR  | C30-C25-C26 | -2.08 | 119.68      | 122.61   |
| 14  | A     | 1103 | CLA  | CHC-C1C-C2C | -2.08 | 120.97      | 126.72   |
| 14  | B     | 1216 | CLA  | CMD-C2D-C3D | -2.08 | 122.83      | 127.61   |
| 14  | B     | 1218 | CLA  | CED-O2D-CGD | 2.08  | 120.64      | 115.94   |
| 14  | A     | 1012 | CLA  | C1-O2A-CGA  | 2.08  | 121.90      | 116.44   |
| 14  | L     | 1503 | CLA  | CAA-C2A-C1A | -2.08 | 105.16      | 111.97   |
| 18  | k     | 4001 | BCR  | C33-C5-C4   | 2.08  | 117.61      | 113.62   |
| 14  | A     | 1139 | CLA  | CHA-C1A-NA  | -2.08 | 121.64      | 126.40   |
| 18  | B     | 4017 | BCR  | C37-C22-C23 | 2.08  | 121.35      | 118.08   |
| 14  | H     | 1233 | CLA  | CHC-C1C-C2C | -2.08 | 120.98      | 126.72   |
| 18  | L     | 4019 | BCR  | C15-C14-C13 | -2.08 | 124.35      | 127.31   |
| 14  | G     | 1134 | CLA  | CHA-C1A-NA  | -2.08 | 121.64      | 126.40   |
| 14  | G     | 1117 | CLA  | O1D-CGD-CBD | -2.08 | 120.23      | 124.48   |
| 14  | A     | 1139 | CLA  | CAC-C3C-C4C | 2.08  | 127.50      | 124.81   |
| 14  | G     | 1139 | CLA  | CAC-C3C-C4C | 2.08  | 127.50      | 124.81   |
| 14  | a     | 1127 | CLA  | CMA-C3A-C4A | 2.08  | 117.35      | 111.77   |
| 14  | B     | 1201 | CLA  | O1D-CGD-CBD | -2.08 | 120.24      | 124.48   |
| 20  | B     | 5002 | LMG  | O6-C5-C6    | 2.08  | 111.60      | 106.44   |
| 14  | G     | 1012 | CLA  | C1-O2A-CGA  | 2.08  | 121.89      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1136 | CLA  | C4D-C3D-CAD | 2.08  | 110.54      | 108.10   |
| 14  | b     | 1240 | CLA  | CHC-C1C-C2C | -2.08 | 120.98      | 126.72   |
| 14  | B     | 1022 | CLA  | CHA-C1A-NA  | -2.07 | 121.65      | 126.40   |
| 14  | a     | 1103 | CLA  | CHC-C1C-C2C | -2.07 | 120.98      | 126.72   |
| 20  | H     | 5002 | LMG  | O6-C5-C6    | 2.07  | 111.59      | 106.44   |
| 14  | B     | 1234 | CLA  | C1-C2-C3    | -2.07 | 122.45      | 126.04   |
| 14  | l     | 1503 | CLA  | CAA-C2A-C1A | -2.07 | 105.18      | 111.97   |
| 18  | H     | 4004 | BCR  | C30-C25-C26 | -2.07 | 119.69      | 122.61   |
| 20  | b     | 5002 | LMG  | O6-C5-C6    | 2.07  | 111.59      | 106.44   |
| 14  | B     | 1203 | CLA  | CHB-C4A-NA  | 2.07  | 127.38      | 124.51   |
| 14  | U     | 1503 | CLA  | CAA-C2A-C1A | -2.07 | 105.18      | 111.97   |
| 14  | b     | 1214 | CLA  | CAA-CBA-CGA | -2.07 | 107.19      | 113.25   |
| 14  | G     | 1137 | CLA  | C5-C3-C4    | 2.07  | 119.18      | 114.60   |
| 14  | G     | 1103 | CLA  | CHC-C1C-C2C | -2.07 | 120.99      | 126.72   |
| 18  | i     | 4020 | BCR  | C31-C1-C6   | -2.07 | 106.94      | 110.30   |
| 13  | a     | 1011 | CL0  | C4C-C3C-C2C | -2.07 | 103.88      | 106.90   |
| 14  | A     | 1108 | CLA  | C4C-C3C-C2C | -2.07 | 103.88      | 106.90   |
| 14  | B     | 1221 | CLA  | C3D-C4D-ND  | 2.07  | 113.59      | 110.24   |
| 14  | B     | 1239 | CLA  | C3D-C4D-ND  | 2.07  | 113.59      | 110.24   |
| 14  | B     | 1240 | CLA  | CHC-C1C-C2C | -2.07 | 120.99      | 126.72   |
| 14  | A     | 1123 | CLA  | CHD-C4C-C3C | -2.07 | 121.80      | 124.84   |
| 14  | A     | 1120 | CLA  | C3C-C4C-NC  | 2.07  | 112.89      | 110.57   |
| 20  | G     | 5003 | LMG  | C4-C3-C2    | 2.07  | 114.44      | 110.82   |
| 14  | H     | 1240 | CLA  | CHC-C1C-C2C | -2.07 | 120.99      | 126.72   |
| 14  | a     | 1139 | CLA  | CAC-C3C-C4C | 2.07  | 127.50      | 124.81   |
| 14  | a     | 1123 | CLA  | CHD-C4C-C3C | -2.07 | 121.80      | 124.84   |
| 14  | G     | 1125 | CLA  | C1-O2A-CGA  | 2.07  | 121.88      | 116.44   |
| 18  | H     | 4017 | BCR  | C34-C9-C8   | 2.07  | 121.34      | 118.08   |
| 18  | b     | 4004 | BCR  | C30-C25-C26 | -2.07 | 119.70      | 122.61   |
| 14  | a     | 1137 | CLA  | CHC-C1C-C2C | -2.07 | 121.00      | 126.72   |
| 14  | a     | 1117 | CLA  | O1D-CGD-CBD | -2.07 | 120.25      | 124.48   |
| 14  | H     | 1224 | CLA  | C4D-C3D-CAD | 2.07  | 110.53      | 108.10   |
| 14  | a     | 1117 | CLA  | C4D-C3D-CAD | 2.07  | 110.53      | 108.10   |
| 14  | b     | 1021 | CLA  | C4D-C3D-CAD | 2.07  | 110.53      | 108.10   |
| 20  | a     | 5003 | LMG  | C4-C3-C2    | 2.07  | 114.43      | 110.82   |
| 14  | A     | 1104 | CLA  | CHD-C4C-C3C | -2.07 | 121.80      | 124.84   |
| 18  | a     | 4006 | BCR  | C38-C26-C27 | 2.07  | 117.59      | 113.62   |
| 14  | A     | 1125 | CLA  | C1-O2A-CGA  | 2.07  | 121.87      | 116.44   |
| 14  | A     | 1129 | CLA  | CAA-CBA-CGA | -2.07 | 107.21      | 113.25   |
| 14  | A     | 1127 | CLA  | CMA-C3A-C4A | 2.07  | 117.33      | 111.77   |
| 18  | A     | 4003 | BCR  | C38-C26-C25 | -2.07 | 122.21      | 124.53   |
| 14  | b     | 1212 | CLA  | C3C-C4C-NC  | 2.07  | 112.89      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | G     | 4001 | BCR  | C28-C27-C26 | -2.07 | 110.39      | 114.08   |
| 14  | a     | 1107 | CLA  | CAA-CBA-CGA | -2.07 | 107.02      | 112.51   |
| 14  | b     | 1216 | CLA  | CMD-C2D-C3D | -2.07 | 122.86      | 127.61   |
| 14  | B     | 1021 | CLA  | C4D-C3D-CAD | 2.07  | 110.53      | 108.10   |
| 18  | B     | 4017 | BCR  | C36-C18-C17 | -2.07 | 120.03      | 122.92   |
| 14  | b     | 1212 | CLA  | C4C-C3C-C2C | -2.07 | 103.89      | 106.90   |
| 18  | H     | 4017 | BCR  | C36-C18-C17 | -2.07 | 120.03      | 122.92   |
| 14  | a     | 1139 | CLA  | CHA-C1A-NA  | -2.07 | 121.67      | 126.40   |
| 18  | U     | 4019 | BCR  | C15-C14-C13 | -2.06 | 124.36      | 127.31   |
| 14  | G     | 1129 | CLA  | CAA-CBA-CGA | -2.06 | 107.22      | 113.25   |
| 14  | G     | 1109 | CLA  | CMC-C2C-C1C | 2.06  | 128.18      | 125.04   |
| 15  | H     | 1230 | F6C  | CMA-C3A-C2A | -2.06 | 120.51      | 126.12   |
| 15  | b     | 1230 | F6C  | CMA-C3A-C2A | -2.06 | 120.51      | 126.12   |
| 14  | G     | 1139 | CLA  | CHA-C1A-NA  | -2.06 | 121.67      | 126.40   |
| 14  | a     | 1129 | CLA  | CAA-CBA-CGA | -2.06 | 107.22      | 113.25   |
| 14  | b     | 1214 | CLA  | CED-O2D-CGD | 2.06  | 120.60      | 115.94   |
| 14  | B     | 1239 | CLA  | CHA-C4D-ND  | 2.06  | 136.81      | 132.50   |
| 14  | a     | 1137 | CLA  | C5-C3-C4    | 2.06  | 119.16      | 114.60   |
| 15  | B     | 1230 | F6C  | CMA-C3A-C2A | -2.06 | 120.52      | 126.12   |
| 14  | H     | 1214 | CLA  | CAA-CBA-CGA | -2.06 | 107.22      | 113.25   |
| 14  | B     | 1218 | CLA  | CHB-C4A-NA  | 2.06  | 127.36      | 124.51   |
| 18  | K     | 4001 | BCR  | C33-C5-C4   | 2.06  | 117.58      | 113.62   |
| 14  | A     | 1112 | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 18  | B     | 4017 | BCR  | C34-C9-C8   | 2.06  | 121.33      | 118.08   |
| 14  | a     | 1119 | CLA  | C4C-C3C-C2C | -2.06 | 103.89      | 106.90   |
| 14  | B     | 1208 | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 14  | G     | 1127 | CLA  | CMA-C3A-C4A | 2.06  | 117.31      | 111.77   |
| 13  | G     | 1011 | CL0  | C4C-C3C-C2C | -2.06 | 103.89      | 106.90   |
| 18  | G     | 4006 | BCR  | C12-C13-C14 | -2.06 | 115.78      | 118.94   |
| 14  | H     | 1239 | CLA  | CHA-C4D-ND  | 2.06  | 136.81      | 132.50   |
| 14  | A     | 1134 | CLA  | CHA-C1A-NA  | -2.06 | 121.68      | 126.40   |
| 14  | a     | 1131 | CLA  | CMD-C2D-C3D | -2.06 | 122.88      | 127.61   |
| 14  | a     | 1108 | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.90   |
| 18  | A     | 4001 | BCR  | C28-C27-C26 | -2.06 | 110.40      | 114.08   |
| 18  | a     | 4001 | BCR  | C28-C27-C26 | -2.06 | 110.40      | 114.08   |
| 14  | A     | 1107 | CLA  | CAA-CBA-CGA | -2.06 | 107.05      | 112.51   |
| 14  | A     | 1137 | CLA  | C5-C3-C4    | 2.06  | 119.15      | 114.60   |
| 18  | G     | 4003 | BCR  | C38-C26-C25 | -2.06 | 122.22      | 124.53   |
| 14  | G     | 1137 | CLA  | CHC-C1C-C2C | -2.06 | 121.03      | 126.72   |
| 14  | a     | 1117 | CLA  | C4-C3-C5    | 2.06  | 118.73      | 115.27   |
| 14  | A     | 1137 | CLA  | CHC-C1C-C2C | -2.06 | 121.03      | 126.72   |
| 14  | B     | 1214 | CLA  | CAA-CBA-CGA | -2.06 | 107.24      | 113.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 1117 | CLA  | CMC-C2C-C3C | 2.06  | 131.70      | 126.12   |
| 18  | I     | 4020 | BCR  | C31-C1-C6   | -2.06 | 106.96      | 110.30   |
| 14  | b     | 1218 | CLA  | CHB-C4A-NA  | 2.06  | 127.36      | 124.51   |
| 14  | A     | 1117 | CLA  | CMC-C2C-C3C | 2.06  | 131.70      | 126.12   |
| 14  | G     | 1136 | CLA  | C4D-C3D-CAD | 2.06  | 110.52      | 108.10   |
| 14  | H     | 1221 | CLA  | C3D-C4D-ND  | 2.06  | 113.56      | 110.24   |
| 14  | B     | 1222 | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.90   |
| 14  | H     | 1211 | CLA  | CMD-C2D-C3D | -2.06 | 122.89      | 127.61   |
| 18  | R     | 4020 | BCR  | C31-C1-C6   | -2.05 | 106.97      | 110.30   |
| 14  | G     | 1112 | CLA  | O1D-CGD-CBD | -2.05 | 120.28      | 124.48   |
| 14  | b     | 1208 | CLA  | O1D-CGD-CBD | -2.05 | 120.28      | 124.48   |
| 13  | A     | 1011 | CL0  | C4C-C3C-C2C | -2.05 | 103.90      | 106.90   |
| 19  | I     | 5102 | LHG  | C5-O7-C7    | -2.05 | 112.74      | 117.79   |
| 14  | G     | 1108 | CLA  | C4C-C3C-C2C | -2.05 | 103.91      | 106.90   |
| 18  | b     | 4017 | BCR  | C34-C9-C8   | 2.05  | 121.31      | 118.08   |
| 20  | A     | 5003 | LMG  | C4-C3-C2    | 2.05  | 114.41      | 110.82   |
| 14  | A     | 1117 | CLA  | O1D-CGD-CBD | -2.05 | 120.28      | 124.48   |
| 14  | H     | 1208 | CLA  | O1D-CGD-CBD | -2.05 | 120.28      | 124.48   |
| 14  | A     | 1117 | CLA  | C4-C3-C5    | 2.05  | 118.72      | 115.27   |
| 18  | A     | 4006 | BCR  | C38-C26-C27 | 2.05  | 117.56      | 113.62   |
| 18  | G     | 4006 | BCR  | C38-C26-C27 | 2.05  | 117.56      | 113.62   |
| 18  | H     | 4006 | BCR  | C35-C13-C12 | 2.05  | 121.31      | 118.08   |
| 14  | H     | 1218 | CLA  | CHB-C4A-NA  | 2.05  | 127.35      | 124.51   |
| 19  | L     | 5102 | LHG  | C5-O7-C7    | -2.05 | 112.74      | 117.79   |
| 18  | T     | 4001 | BCR  | C33-C5-C4   | 2.05  | 117.56      | 113.62   |
| 14  | B     | 1233 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 18  | a     | 4003 | BCR  | C38-C26-C25 | -2.05 | 122.22      | 124.53   |
| 14  | A     | 1131 | CLA  | CMD-C2D-C3D | -2.05 | 122.90      | 127.61   |
| 14  | B     | 1239 | CLA  | CMD-C2D-C3D | -2.05 | 122.90      | 127.61   |
| 14  | b     | 1239 | CLA  | CMD-C2D-C3D | -2.05 | 122.90      | 127.61   |
| 18  | b     | 4006 | BCR  | C35-C13-C12 | 2.05  | 121.31      | 118.08   |
| 14  | a     | 1141 | CLA  | CMD-C2D-C3D | -2.05 | 122.90      | 127.61   |
| 18  | A     | 4001 | BCR  | C37-C22-C21 | -2.05 | 120.05      | 122.92   |
| 14  | B     | 1223 | CLA  | CMA-C3A-C4A | 2.05  | 117.28      | 111.77   |
| 14  | G     | 1107 | CLA  | CAA-CBA-CGA | -2.05 | 107.07      | 112.51   |
| 14  | b     | 1234 | CLA  | C1-C2-C3    | -2.05 | 122.50      | 126.04   |
| 18  | a     | 4004 | BCR  | C23-C22-C21 | 2.05  | 122.08      | 118.94   |
| 15  | b     | 1230 | F6C  | OMB-CMB-C2B | -2.05 | 121.06      | 125.69   |
| 14  | b     | 1223 | CLA  | CMA-C3A-C4A | 2.05  | 117.28      | 111.77   |
| 14  | b     | 1201 | CLA  | O1D-CGD-CBD | -2.05 | 120.30      | 124.48   |
| 14  | H     | 1222 | CLA  | C4C-C3C-C2C | -2.05 | 103.92      | 106.90   |
| 14  | G     | 1123 | CLA  | CHD-C4C-C3C | -2.05 | 121.83      | 124.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1136 | CLA  | CAA-C2A-C3A | -2.04 | 107.18      | 112.78   |
| 14  | H     | 1239 | CLA  | CMD-C2D-C3D | -2.04 | 122.91      | 127.61   |
| 14  | a     | 1104 | CLA  | CHD-C4C-C3C | -2.04 | 121.83      | 124.84   |
| 14  | A     | 1133 | CLA  | CHC-C1C-C2C | -2.04 | 121.07      | 126.72   |
| 14  | b     | 1239 | CLA  | CHA-C4D-ND  | 2.04  | 136.78      | 132.50   |
| 14  | b     | 1023 | CLA  | C3B-C4B-NB  | 2.04  | 111.85      | 109.21   |
| 14  | G     | 1117 | CLA  | C4-C3-C5    | 2.04  | 118.71      | 115.27   |
| 14  | B     | 1231 | CLA  | C3C-C4C-NC  | 2.04  | 112.86      | 110.57   |
| 19  | U     | 5102 | LHG  | C5-O7-C7    | -2.04 | 112.76      | 117.79   |
| 14  | B     | 1236 | CLA  | CAA-C2A-C3A | -2.04 | 107.19      | 112.78   |
| 14  | B     | 1211 | CLA  | CMD-C2D-C3D | -2.04 | 122.92      | 127.61   |
| 14  | G     | 1117 | CLA  | CMC-C2C-C3C | 2.04  | 131.66      | 126.12   |
| 14  | H     | 1231 | CLA  | C3C-C4C-NC  | 2.04  | 112.86      | 110.57   |
| 14  | a     | 1120 | CLA  | C3C-C4C-NC  | 2.04  | 112.86      | 110.57   |
| 14  | b     | 1233 | CLA  | CAC-C3C-C4C | 2.04  | 127.46      | 124.81   |
| 14  | a     | 1112 | CLA  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 18  | B     | 4006 | BCR  | C35-C13-C12 | 2.04  | 121.29      | 118.08   |
| 14  | H     | 1205 | CLA  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 14  | a     | 1136 | CLA  | CAA-C2A-C3A | -2.04 | 107.19      | 112.78   |
| 15  | H     | 1230 | F6C  | OMB-CMB-C2B | -2.04 | 121.08      | 125.69   |
| 21  | H     | 6004 | LMT  | O1B-C4'-C5' | -2.04 | 103.86      | 109.45   |
| 14  | H     | 1223 | CLA  | CMA-C3A-C4A | 2.04  | 117.25      | 111.77   |
| 14  | G     | 1136 | CLA  | CAA-C2A-C3A | -2.04 | 107.20      | 112.78   |
| 18  | H     | 4017 | BCR  | C37-C22-C23 | 2.04  | 121.29      | 118.08   |
| 14  | G     | 1102 | CLA  | C1-O2A-CGA  | 2.04  | 121.79      | 116.44   |
| 14  | H     | 1216 | CLA  | C4-C3-C5    | 2.04  | 118.70      | 115.27   |
| 14  | G     | 1102 | CLA  | O1D-CGD-CBD | -2.04 | 120.32      | 124.48   |
| 15  | B     | 1230 | F6C  | OMB-CMB-C2B | -2.04 | 121.08      | 125.69   |
| 14  | G     | 1133 | CLA  | CHC-C1C-C2C | -2.04 | 121.09      | 126.72   |
| 14  | b     | 1211 | CLA  | CMD-C2D-C3D | -2.04 | 122.93      | 127.61   |
| 14  | a     | 1133 | CLA  | CHC-C1C-C2C | -2.04 | 121.09      | 126.72   |
| 14  | G     | 1131 | CLA  | CMD-C2D-C3D | -2.04 | 122.93      | 127.61   |
| 14  | B     | 1216 | CLA  | C4-C3-C5    | 2.04  | 118.69      | 115.27   |
| 14  | V     | 1501 | CLA  | CHC-C1C-C2C | -2.04 | 121.09      | 126.72   |
| 14  | H     | 1023 | CLA  | C3B-C4B-NB  | 2.04  | 111.84      | 109.21   |
| 14  | G     | 1138 | CLA  | O1D-CGD-CBD | -2.03 | 120.32      | 124.48   |
| 14  | b     | 1236 | CLA  | CAA-C2A-C3A | -2.03 | 107.21      | 112.78   |
| 14  | a     | 1107 | CLA  | CAA-C2A-C3A | -2.03 | 107.21      | 112.78   |
| 14  | B     | 1205 | CLA  | O1D-CGD-CBD | -2.03 | 120.32      | 124.48   |
| 14  | H     | 1206 | CLA  | C4D-C3D-CAD | 2.03  | 110.49      | 108.10   |
| 14  | a     | 1136 | CLA  | C4D-C3D-CAD | 2.03  | 110.49      | 108.10   |
| 14  | H     | 1233 | CLA  | CAC-C3C-C4C | 2.03  | 127.45      | 124.81   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 1132 | CLA  | CMD-C2D-C3D | -2.03 | 122.94      | 127.61   |
| 14  | a     | 1132 | CLA  | CMD-C2D-C3D | -2.03 | 122.94      | 127.61   |
| 14  | A     | 1102 | CLA  | O1D-CGD-CBD | -2.03 | 120.33      | 124.48   |
| 14  | G     | 1120 | CLA  | C3C-C4C-NC  | 2.03  | 112.85      | 110.57   |
| 14  | b     | 1226 | CLA  | C3B-C4B-NB  | 2.03  | 111.84      | 109.21   |
| 21  | A     | 6004 | LMT  | C3'-C4'-C5' | -2.03 | 106.61      | 110.24   |
| 14  | M     | 1501 | CLA  | CHC-C1C-C2C | -2.03 | 121.10      | 126.72   |
| 14  | b     | 1206 | CLA  | C4D-C3D-CAD | 2.03  | 110.49      | 108.10   |
| 14  | A     | 1112 | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 14  | A     | 1138 | CLA  | O1D-CGD-CBD | -2.03 | 120.33      | 124.48   |
| 14  | G     | 1141 | CLA  | CMD-C2D-C3D | -2.03 | 122.94      | 127.61   |
| 14  | m     | 1501 | CLA  | CHC-C1C-C2C | -2.03 | 121.11      | 126.72   |
| 14  | B     | 1023 | CLA  | O2D-CGD-O1D | -2.03 | 119.87      | 123.84   |
| 14  | A     | 1119 | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 21  | B     | 6004 | LMT  | O1B-C4'-C5' | -2.03 | 103.89      | 109.45   |
| 14  | G     | 1113 | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 18  | H     | 4010 | BCR  | C37-C22-C21 | -2.03 | 120.08      | 122.92   |
| 14  | b     | 1222 | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 14  | G     | 1132 | CLA  | CMD-C2D-C3D | -2.03 | 122.95      | 127.61   |
| 14  | H     | 1236 | CLA  | CAA-C2A-C3A | -2.03 | 107.23      | 112.78   |
| 21  | a     | 6004 | LMT  | C3'-C4'-C5' | -2.03 | 106.62      | 110.24   |
| 14  | A     | 1102 | CLA  | C1-O2A-CGA  | 2.03  | 121.76      | 116.44   |
| 14  | U     | 1501 | CLA  | CMD-C2D-C3D | -2.03 | 122.95      | 127.61   |
| 14  | L     | 1501 | CLA  | CMD-C2D-C3D | -2.03 | 122.95      | 127.61   |
| 14  | H     | 1223 | CLA  | C4D-C3D-CAD | 2.03  | 110.48      | 108.10   |
| 20  | b     | 5002 | LMG  | O2-C2-C3    | -2.03 | 105.67      | 110.35   |
| 14  | a     | 1138 | CLA  | O1D-CGD-CBD | -2.02 | 120.34      | 124.48   |
| 21  | l     | 6002 | LMT  | O1'-C1'-C2' | 2.02  | 111.46      | 108.30   |
| 14  | A     | 1141 | CLA  | CMD-C2D-C3D | -2.02 | 122.96      | 127.61   |
| 14  | a     | 1116 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 20  | H     | 5002 | LMG  | O2-C2-C3    | -2.02 | 105.67      | 110.35   |
| 14  | a     | 1102 | CLA  | O1D-CGD-CBD | -2.02 | 120.34      | 124.48   |
| 14  | b     | 1225 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 14  | G     | 1119 | CLA  | C4C-C3C-C2C | -2.02 | 103.95      | 106.90   |
| 18  | b     | 4010 | BCR  | C37-C22-C21 | -2.02 | 120.09      | 122.92   |
| 14  | b     | 1205 | CLA  | O1D-CGD-CBD | -2.02 | 120.34      | 124.48   |
| 14  | l     | 1501 | CLA  | CMD-C2D-C3D | -2.02 | 122.96      | 127.61   |
| 14  | G     | 1141 | CLA  | O1D-CGD-CBD | -2.02 | 120.35      | 124.48   |
| 14  | A     | 1140 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 14  | B     | 1206 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 14  | B     | 1224 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 15  | H     | 1219 | F6C  | CHB-C4A-NA  | 2.02  | 126.31      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 4004 | BCR  | C23-C22-C21 | 2.02  | 122.04      | 118.94   |
| 14  | G     | 1112 | CLA  | C4C-C3C-C2C | -2.02 | 103.95      | 106.90   |
| 14  | A     | 1107 | CLA  | CAA-C2A-C3A | -2.02 | 107.24      | 112.78   |
| 14  | B     | 1226 | CLA  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 14  | a     | 1140 | CLA  | C4D-C3D-CAD | 2.02  | 110.48      | 108.10   |
| 14  | A     | 1113 | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 14  | U     | 1501 | CLA  | CHC-C1C-C2C | -2.02 | 121.14      | 126.72   |
| 18  | I     | 4020 | BCR  | C32-C1-C6   | 2.02  | 113.57      | 110.30   |
| 21  | U     | 6002 | LMT  | O1'-C1'-C2' | 2.02  | 111.45      | 108.30   |
| 14  | G     | 1107 | CLA  | CAA-C2A-C3A | -2.02 | 107.25      | 112.78   |
| 14  | A     | 1108 | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 14  | B     | 1223 | CLA  | C4D-C3D-CAD | 2.02  | 110.47      | 108.10   |
| 20  | B     | 5002 | LMG  | O2-C2-C3    | -2.02 | 105.68      | 110.35   |
| 21  | b     | 6004 | LMT  | O1B-C4'-C5' | -2.02 | 103.92      | 109.45   |
| 18  | i     | 4020 | BCR  | C32-C1-C6   | 2.02  | 113.57      | 110.30   |
| 14  | a     | 1102 | CLA  | C1-O2A-CGA  | 2.02  | 121.74      | 116.44   |
| 14  | G     | 1135 | CLA  | CHA-C4D-ND  | 2.02  | 136.72      | 132.50   |
| 14  | B     | 1023 | CLA  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 14  | H     | 1226 | CLA  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 14  | H     | 1239 | CLA  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 18  | a     | 4006 | BCR  | C23-C22-C21 | 2.02  | 122.04      | 118.94   |
| 14  | G     | 1117 | CLA  | CHA-C4D-ND  | 2.02  | 136.72      | 132.50   |
| 18  | R     | 4020 | BCR  | C32-C1-C6   | 2.02  | 113.57      | 110.30   |
| 18  | B     | 4010 | BCR  | C37-C22-C21 | -2.02 | 120.10      | 122.92   |
| 14  | b     | 1023 | CLA  | O2D-CGD-O1D | -2.02 | 119.90      | 123.84   |
| 14  | B     | 1225 | CLA  | C4D-C3D-CAD | 2.02  | 110.47      | 108.10   |
| 21  | G     | 6004 | LMT  | C3'-C4'-C5' | -2.01 | 106.64      | 110.24   |
| 14  | a     | 1108 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 14  | a     | 1112 | CLA  | C4C-C3C-C2C | -2.01 | 103.96      | 106.90   |
| 14  | A     | 1141 | CLA  | O1D-CGD-CBD | -2.01 | 120.36      | 124.48   |
| 14  | l     | 1501 | CLA  | CHC-C1C-C2C | -2.01 | 121.15      | 126.72   |
| 15  | b     | 1207 | F6C  | CMA-C3A-C2A | -2.01 | 120.66      | 126.12   |
| 14  | b     | 1216 | CLA  | C4-C3-C5    | 2.01  | 118.65      | 115.27   |
| 21  | L     | 6002 | LMT  | O1'-C1'-C2' | 2.01  | 111.44      | 108.30   |
| 14  | A     | 1135 | CLA  | CHA-C4D-ND  | 2.01  | 136.70      | 132.50   |
| 18  | G     | 4004 | BCR  | C23-C22-C21 | 2.01  | 122.02      | 118.94   |
| 14  | b     | 1231 | CLA  | C3C-C4C-NC  | 2.01  | 112.82      | 110.57   |
| 14  | L     | 1501 | CLA  | CHC-C1C-C2C | -2.01 | 121.17      | 126.72   |
| 14  | b     | 1222 | CLA  | C1-C2-C3    | -2.01 | 122.57      | 126.04   |
| 14  | A     | 1111 | CLA  | CMD-C2D-C3D | -2.01 | 122.99      | 127.61   |
| 21  | G     | 6001 | LMT  | O5B-C5B-C6B | 2.01  | 111.43      | 106.44   |
| 14  | a     | 1141 | CLA  | O1D-CGD-CBD | -2.01 | 120.38      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1207 | F6C  | CMA-C3A-C2A | -2.01 | 120.67      | 126.12   |
| 21  | B     | 6001 | LMT  | C1'-O5'-C5' | -2.01 | 109.75      | 113.69   |
| 21  | A     | 6001 | LMT  | O5B-C5B-C6B | 2.01  | 111.42      | 106.44   |
| 21  | b     | 6001 | LMT  | C1'-O5'-C5' | -2.01 | 109.75      | 113.69   |
| 14  | a     | 1131 | CLA  | C4-C3-C5    | 2.01  | 118.64      | 115.27   |
| 21  | a     | 6001 | LMT  | O5B-C5B-C6B | 2.01  | 111.42      | 106.44   |
| 14  | b     | 1223 | CLA  | CHA-C4D-ND  | 2.01  | 136.69      | 132.50   |
| 14  | K     | 1401 | CLA  | O1D-CGD-CBD | -2.01 | 120.38      | 124.48   |
| 14  | G     | 1122 | CLA  | CHC-C1C-C2C | -2.00 | 121.18      | 126.72   |
| 14  | H     | 1225 | CLA  | CMC-C2C-C1C | 2.00  | 128.09      | 125.04   |
| 18  | A     | 4006 | BCR  | C23-C22-C21 | 2.00  | 122.02      | 118.94   |
| 14  | H     | 1023 | CLA  | O2D-CGD-O1D | -2.00 | 119.92      | 123.84   |
| 21  | l     | 6002 | LMT  | O5B-C5B-C6B | 2.00  | 111.42      | 106.44   |
| 21  | U     | 6002 | LMT  | O5B-C5B-C6B | 2.00  | 111.41      | 106.44   |
| 21  | L     | 6002 | LMT  | O5B-C5B-C6B | 2.00  | 111.41      | 106.44   |
| 14  | G     | 1111 | CLA  | CMD-C2D-C3D | -2.00 | 123.01      | 127.61   |

All (264) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 13  | A     | 1011 | CL0  | NA   |
| 13  | A     | 1011 | CL0  | NC   |
| 13  | A     | 1011 | CL0  | ND   |
| 13  | G     | 1011 | CL0  | NA   |
| 13  | G     | 1011 | CL0  | NC   |
| 13  | G     | 1011 | CL0  | ND   |
| 13  | a     | 1011 | CL0  | NA   |
| 13  | a     | 1011 | CL0  | NC   |
| 13  | a     | 1011 | CL0  | ND   |
| 14  | A     | 1012 | CLA  | ND   |
| 14  | A     | 1013 | CLA  | ND   |
| 14  | A     | 1101 | CLA  | ND   |
| 14  | A     | 1102 | CLA  | ND   |
| 14  | A     | 1103 | CLA  | ND   |
| 14  | A     | 1104 | CLA  | ND   |
| 14  | A     | 1105 | CLA  | ND   |
| 14  | A     | 1106 | CLA  | ND   |
| 14  | A     | 1107 | CLA  | ND   |
| 14  | A     | 1108 | CLA  | ND   |
| 14  | A     | 1109 | CLA  | ND   |
| 14  | A     | 1110 | CLA  | ND   |
| 14  | A     | 1111 | CLA  | ND   |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | A            | 1112       | CLA         | ND          |
| 14         | A            | 1113       | CLA         | ND          |
| 14         | A            | 1114       | CLA         | ND          |
| 14         | A            | 1115       | CLA         | ND          |
| 14         | A            | 1116       | CLA         | ND          |
| 14         | A            | 1117       | CLA         | ND          |
| 14         | A            | 1118       | CLA         | ND          |
| 14         | A            | 1119       | CLA         | ND          |
| 14         | A            | 1120       | CLA         | ND          |
| 14         | A            | 1122       | CLA         | ND          |
| 14         | A            | 1123       | CLA         | ND          |
| 14         | A            | 1124       | CLA         | ND          |
| 14         | A            | 1125       | CLA         | ND          |
| 14         | A            | 1126       | CLA         | ND          |
| 14         | A            | 1127       | CLA         | ND          |
| 14         | A            | 1128       | CLA         | ND          |
| 14         | A            | 1129       | CLA         | ND          |
| 14         | A            | 1130       | CLA         | ND          |
| 14         | A            | 1131       | CLA         | ND          |
| 14         | A            | 1132       | CLA         | ND          |
| 14         | A            | 1133       | CLA         | ND          |
| 14         | A            | 1134       | CLA         | ND          |
| 14         | A            | 1135       | CLA         | ND          |
| 14         | A            | 1136       | CLA         | ND          |
| 14         | A            | 1137       | CLA         | ND          |
| 14         | A            | 1138       | CLA         | ND          |
| 14         | A            | 1139       | CLA         | ND          |
| 14         | A            | 1140       | CLA         | ND          |
| 14         | A            | 1141       | CLA         | ND          |
| 14         | B            | 1021       | CLA         | ND          |
| 14         | B            | 1022       | CLA         | ND          |
| 14         | B            | 1023       | CLA         | ND          |
| 14         | B            | 1201       | CLA         | ND          |
| 14         | B            | 1202       | CLA         | ND          |
| 14         | B            | 1203       | CLA         | ND          |
| 14         | B            | 1204       | CLA         | ND          |
| 14         | B            | 1205       | CLA         | ND          |
| 14         | B            | 1206       | CLA         | ND          |
| 14         | B            | 1208       | CLA         | ND          |
| 14         | B            | 1209       | CLA         | ND          |
| 14         | B            | 1210       | CLA         | ND          |
| 14         | B            | 1211       | CLA         | ND          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | B            | 1212       | CLA         | ND          |
| 14         | B            | 1213       | CLA         | ND          |
| 14         | B            | 1214       | CLA         | ND          |
| 14         | B            | 1215       | CLA         | ND          |
| 14         | B            | 1216       | CLA         | ND          |
| 14         | B            | 1217       | CLA         | ND          |
| 14         | B            | 1218       | CLA         | ND          |
| 14         | B            | 1220       | CLA         | ND          |
| 14         | B            | 1221       | CLA         | ND          |
| 14         | B            | 1222       | CLA         | ND          |
| 14         | B            | 1223       | CLA         | ND          |
| 14         | B            | 1224       | CLA         | ND          |
| 14         | B            | 1225       | CLA         | ND          |
| 14         | B            | 1226       | CLA         | ND          |
| 14         | B            | 1227       | CLA         | ND          |
| 14         | B            | 1228       | CLA         | ND          |
| 14         | B            | 1229       | CLA         | ND          |
| 14         | B            | 1231       | CLA         | ND          |
| 14         | B            | 1232       | CLA         | ND          |
| 14         | B            | 1233       | CLA         | ND          |
| 14         | B            | 1234       | CLA         | ND          |
| 14         | B            | 1235       | CLA         | ND          |
| 14         | B            | 1236       | CLA         | ND          |
| 14         | B            | 1239       | CLA         | ND          |
| 14         | B            | 1240       | CLA         | ND          |
| 14         | K            | 1401       | CLA         | ND          |
| 14         | L            | 1501       | CLA         | ND          |
| 14         | L            | 1502       | CLA         | ND          |
| 14         | L            | 1503       | CLA         | ND          |
| 14         | M            | 1501       | CLA         | ND          |
| 14         | G            | 1012       | CLA         | ND          |
| 14         | G            | 1013       | CLA         | ND          |
| 14         | G            | 1101       | CLA         | ND          |
| 14         | G            | 1102       | CLA         | ND          |
| 14         | G            | 1103       | CLA         | ND          |
| 14         | G            | 1104       | CLA         | ND          |
| 14         | G            | 1105       | CLA         | ND          |
| 14         | G            | 1106       | CLA         | ND          |
| 14         | G            | 1107       | CLA         | ND          |
| 14         | G            | 1108       | CLA         | ND          |
| 14         | G            | 1109       | CLA         | ND          |
| 14         | G            | 1110       | CLA         | ND          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | G            | 1111       | CLA         | ND          |
| 14         | G            | 1112       | CLA         | ND          |
| 14         | G            | 1113       | CLA         | ND          |
| 14         | G            | 1114       | CLA         | ND          |
| 14         | G            | 1115       | CLA         | ND          |
| 14         | G            | 1116       | CLA         | ND          |
| 14         | G            | 1117       | CLA         | ND          |
| 14         | G            | 1118       | CLA         | ND          |
| 14         | G            | 1119       | CLA         | ND          |
| 14         | G            | 1120       | CLA         | ND          |
| 14         | G            | 1122       | CLA         | ND          |
| 14         | G            | 1123       | CLA         | ND          |
| 14         | G            | 1124       | CLA         | ND          |
| 14         | G            | 1125       | CLA         | ND          |
| 14         | G            | 1126       | CLA         | ND          |
| 14         | G            | 1127       | CLA         | ND          |
| 14         | G            | 1128       | CLA         | ND          |
| 14         | G            | 1129       | CLA         | ND          |
| 14         | G            | 1130       | CLA         | ND          |
| 14         | G            | 1131       | CLA         | ND          |
| 14         | G            | 1132       | CLA         | ND          |
| 14         | G            | 1133       | CLA         | ND          |
| 14         | G            | 1134       | CLA         | ND          |
| 14         | G            | 1135       | CLA         | ND          |
| 14         | G            | 1136       | CLA         | ND          |
| 14         | G            | 1137       | CLA         | ND          |
| 14         | G            | 1138       | CLA         | ND          |
| 14         | G            | 1139       | CLA         | ND          |
| 14         | G            | 1140       | CLA         | ND          |
| 14         | G            | 1141       | CLA         | ND          |
| 14         | H            | 1021       | CLA         | ND          |
| 14         | H            | 1022       | CLA         | ND          |
| 14         | H            | 1023       | CLA         | ND          |
| 14         | H            | 1201       | CLA         | ND          |
| 14         | H            | 1202       | CLA         | ND          |
| 14         | H            | 1203       | CLA         | ND          |
| 14         | H            | 1204       | CLA         | ND          |
| 14         | H            | 1205       | CLA         | ND          |
| 14         | H            | 1206       | CLA         | ND          |
| 14         | H            | 1208       | CLA         | ND          |
| 14         | H            | 1209       | CLA         | ND          |
| 14         | H            | 1210       | CLA         | ND          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | H            | 1211       | CLA         | ND          |
| 14         | H            | 1212       | CLA         | ND          |
| 14         | H            | 1213       | CLA         | ND          |
| 14         | H            | 1214       | CLA         | ND          |
| 14         | H            | 1215       | CLA         | ND          |
| 14         | H            | 1216       | CLA         | ND          |
| 14         | H            | 1217       | CLA         | ND          |
| 14         | H            | 1218       | CLA         | ND          |
| 14         | H            | 1220       | CLA         | ND          |
| 14         | H            | 1221       | CLA         | ND          |
| 14         | H            | 1222       | CLA         | ND          |
| 14         | H            | 1223       | CLA         | ND          |
| 14         | H            | 1224       | CLA         | ND          |
| 14         | H            | 1225       | CLA         | ND          |
| 14         | H            | 1226       | CLA         | ND          |
| 14         | H            | 1227       | CLA         | ND          |
| 14         | H            | 1228       | CLA         | ND          |
| 14         | H            | 1229       | CLA         | ND          |
| 14         | H            | 1231       | CLA         | ND          |
| 14         | H            | 1232       | CLA         | ND          |
| 14         | H            | 1233       | CLA         | ND          |
| 14         | H            | 1234       | CLA         | ND          |
| 14         | H            | 1235       | CLA         | ND          |
| 14         | H            | 1236       | CLA         | ND          |
| 14         | H            | 1239       | CLA         | ND          |
| 14         | H            | 1240       | CLA         | ND          |
| 14         | T            | 1401       | CLA         | ND          |
| 14         | U            | 1501       | CLA         | ND          |
| 14         | U            | 1502       | CLA         | ND          |
| 14         | U            | 1503       | CLA         | ND          |
| 14         | V            | 1501       | CLA         | ND          |
| 14         | a            | 1012       | CLA         | ND          |
| 14         | a            | 1013       | CLA         | ND          |
| 14         | a            | 1101       | CLA         | ND          |
| 14         | a            | 1102       | CLA         | ND          |
| 14         | a            | 1103       | CLA         | ND          |
| 14         | a            | 1104       | CLA         | ND          |
| 14         | a            | 1105       | CLA         | ND          |
| 14         | a            | 1106       | CLA         | ND          |
| 14         | a            | 1107       | CLA         | ND          |
| 14         | a            | 1108       | CLA         | ND          |
| 14         | a            | 1109       | CLA         | ND          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 14         | a            | 1110       | CLA         | ND          |
| 14         | a            | 1111       | CLA         | ND          |
| 14         | a            | 1112       | CLA         | ND          |
| 14         | a            | 1113       | CLA         | ND          |
| 14         | a            | 1114       | CLA         | ND          |
| 14         | a            | 1115       | CLA         | ND          |
| 14         | a            | 1116       | CLA         | ND          |
| 14         | a            | 1117       | CLA         | ND          |
| 14         | a            | 1118       | CLA         | ND          |
| 14         | a            | 1119       | CLA         | ND          |
| 14         | a            | 1120       | CLA         | ND          |
| 14         | a            | 1122       | CLA         | ND          |
| 14         | a            | 1123       | CLA         | ND          |
| 14         | a            | 1124       | CLA         | ND          |
| 14         | a            | 1125       | CLA         | ND          |
| 14         | a            | 1126       | CLA         | ND          |
| 14         | a            | 1127       | CLA         | ND          |
| 14         | a            | 1128       | CLA         | ND          |
| 14         | a            | 1129       | CLA         | ND          |
| 14         | a            | 1130       | CLA         | ND          |
| 14         | a            | 1131       | CLA         | ND          |
| 14         | a            | 1132       | CLA         | ND          |
| 14         | a            | 1133       | CLA         | ND          |
| 14         | a            | 1134       | CLA         | ND          |
| 14         | a            | 1135       | CLA         | ND          |
| 14         | a            | 1136       | CLA         | ND          |
| 14         | a            | 1137       | CLA         | ND          |
| 14         | a            | 1138       | CLA         | ND          |
| 14         | a            | 1139       | CLA         | ND          |
| 14         | a            | 1140       | CLA         | ND          |
| 14         | a            | 1141       | CLA         | ND          |
| 14         | b            | 1021       | CLA         | ND          |
| 14         | b            | 1022       | CLA         | ND          |
| 14         | b            | 1023       | CLA         | ND          |
| 14         | b            | 1201       | CLA         | ND          |
| 14         | b            | 1202       | CLA         | ND          |
| 14         | b            | 1203       | CLA         | ND          |
| 14         | b            | 1204       | CLA         | ND          |
| 14         | b            | 1205       | CLA         | ND          |
| 14         | b            | 1206       | CLA         | ND          |
| 14         | b            | 1208       | CLA         | ND          |
| 14         | b            | 1209       | CLA         | ND          |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | b     | 1210 | CLA  | ND   |
| 14  | b     | 1211 | CLA  | ND   |
| 14  | b     | 1212 | CLA  | ND   |
| 14  | b     | 1213 | CLA  | ND   |
| 14  | b     | 1214 | CLA  | ND   |
| 14  | b     | 1215 | CLA  | ND   |
| 14  | b     | 1216 | CLA  | ND   |
| 14  | b     | 1217 | CLA  | ND   |
| 14  | b     | 1218 | CLA  | ND   |
| 14  | b     | 1220 | CLA  | ND   |
| 14  | b     | 1221 | CLA  | ND   |
| 14  | b     | 1222 | CLA  | ND   |
| 14  | b     | 1223 | CLA  | ND   |
| 14  | b     | 1224 | CLA  | ND   |
| 14  | b     | 1225 | CLA  | ND   |
| 14  | b     | 1226 | CLA  | ND   |
| 14  | b     | 1227 | CLA  | ND   |
| 14  | b     | 1228 | CLA  | ND   |
| 14  | b     | 1229 | CLA  | ND   |
| 14  | b     | 1231 | CLA  | ND   |
| 14  | b     | 1232 | CLA  | ND   |
| 14  | b     | 1233 | CLA  | ND   |
| 14  | b     | 1234 | CLA  | ND   |
| 14  | b     | 1235 | CLA  | ND   |
| 14  | b     | 1236 | CLA  | ND   |
| 14  | b     | 1239 | CLA  | ND   |
| 14  | b     | 1240 | CLA  | ND   |
| 14  | k     | 1401 | CLA  | ND   |
| 14  | l     | 1501 | CLA  | ND   |
| 14  | l     | 1502 | CLA  | ND   |
| 14  | l     | 1503 | CLA  | ND   |
| 14  | m     | 1501 | CLA  | ND   |

All (4777) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1013 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1013 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1103 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1103 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1103 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1103 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1106 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1107 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1108 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1108 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1109 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1111 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1111 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1112 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1112 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1113 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1115 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1115 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1116 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1116 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1117 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1117 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1118 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1118 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1118 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1119 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1119 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1119 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1120 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1122 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1122 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1122 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1122 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1123 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1124 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1124 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1125 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1125 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1125 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1125 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1127 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1127 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1128 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1128 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1128 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1130 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1131 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1131 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1132 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1132 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1134 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1134 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1135 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1138 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1138 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1138 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1138 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1139 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1139 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1139 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1140 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1140 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1140 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1141 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1141 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1141 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1021 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1022 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1023 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1023 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1202 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1202 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1202 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1202 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 1203 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1205 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1206 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1206 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1206 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1208 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1208 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1209 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1209 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1210 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1210 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1215 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1217 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1217 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1220 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1221 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1221 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1221 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1221 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1223 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1224 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1225 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1225 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1226 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1228 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1229 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1229 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1229 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1229 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1232 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1233 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1233 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1233 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1235 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1235 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1236 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1236 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1236 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1240 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1240 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1240 | CLA  | O2A-C1-C2-C3    |
| 14  | K     | 1401 | CLA  | C1A-C2A-CAA-CBA |
| 14  | K     | 1401 | CLA  | C3A-C2A-CAA-CBA |
| 14  | L     | 1503 | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 1503 | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 1503 | CLA  | O1A-CGA-O2A-C1  |
| 14  | M     | 1501 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1013 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1013 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1103 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1103 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1103 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1103 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1106 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1107 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1108 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1108 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1109 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1111 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1111 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1112 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1112 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1113 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1115 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1115 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1116 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1116 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1117 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1117 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1118 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1118 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1118 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1119 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1119 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1120 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1122 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1122 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1122 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1122 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1123 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1124 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1124 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1125 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1125 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1125 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1125 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1127 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1127 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1128 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1128 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1128 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1130 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1131 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1131 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1132 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1132 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1134 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1134 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1135 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1138 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1138 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1138 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1138 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1139 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1139 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1139 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1140 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1140 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1140 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1141 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1141 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1141 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1021 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1022 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1023 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1023 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1202 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1202 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1202 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1202 | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 1203 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1205 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1206 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1206 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1206 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1208 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1208 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1209 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1209 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1210 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1210 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1213 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1215 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1217 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1217 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1220 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1221 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1221 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1221 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1221 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1223 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1224 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1225 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1225 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1226 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1228 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1229 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1229 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1229 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1229 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1232 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1233 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1233 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1233 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1235 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1235 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1236 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1236 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1236 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1240 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1240 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1240 | CLA  | O2A-C1-C2-C3    |
| 14  | T     | 1401 | CLA  | C1A-C2A-CAA-CBA |
| 14  | T     | 1401 | CLA  | C3A-C2A-CAA-CBA |
| 14  | U     | 1503 | CLA  | C1A-C2A-CAA-CBA |
| 14  | U     | 1503 | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1503 | CLA  | O1A-CGA-O2A-C1  |
| 14  | V     | 1501 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1013 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1013 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1103 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1103 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1103 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1103 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1106 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1107 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1108 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1108 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1109 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1111 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1111 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1112 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1112 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1113 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1115 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1115 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1116 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1116 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1117 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1117 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1118 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1118 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1118 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1119 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1119 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1120 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1122 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1122 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1122 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1122 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1123 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1124 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1124 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1125 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1125 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1125 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1125 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1127 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1127 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1128 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1128 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1128 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1130 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1131 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1131 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1132 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1132 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1134 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1134 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1135 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1138 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1138 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1138 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1138 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1139 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1139 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1139 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1140 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1140 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1140 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1141 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1141 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1141 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1021 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1022 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1023 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1023 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1202 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1202 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1202 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1202 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 1203 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1205 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1206 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1206 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1206 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1208 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1208 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1209 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1209 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1210 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1210 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1215 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1217 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1217 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1220 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1221 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1221 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1221 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1221 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1223 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1224 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1225 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1225 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1226 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1228 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1229 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1229 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1229 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1229 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1232 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1233 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1233 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1233 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1235 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1235 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1236 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1236 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1236 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1240 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1240 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1240 | CLA  | O2A-C1-C2-C3    |
| 14  | k     | 1401 | CLA  | C1A-C2A-CAA-CBA |
| 14  | k     | 1401 | CLA  | C3A-C2A-CAA-CBA |
| 14  | l     | 1503 | CLA  | C1A-C2A-CAA-CBA |
| 14  | l     | 1503 | CLA  | CBA-CGA-O2A-C1  |
| 14  | l     | 1503 | CLA  | O1A-CGA-O2A-C1  |
| 14  | m     | 1501 | CLA  | CBD-CGD-O2D-CED |
| 15  | A     | 1121 | F6C  | C2A-CAA-CBA-CGA |
| 15  | A     | 1121 | F6C  | C3A-C2A-CAA-CBA |
| 15  | A     | 1121 | F6C  | C2B-C3B-CAB-CBB |
| 15  | A     | 1121 | F6C  | C4B-C3B-CAB-CBB |
| 15  | A     | 1121 | F6C  | C1B-C2B-CMB-OMB |
| 15  | A     | 1121 | F6C  | C3B-C2B-CMB-OMB |
| 15  | B     | 1207 | F6C  | C4-C3-C5-C6     |
| 15  | B     | 1219 | F6C  | C1B-C2B-CMB-OMB |
| 15  | B     | 1219 | F6C  | C2-C3-C5-C6     |
| 15  | B     | 1219 | F6C  | C4-C3-C5-C6     |
| 15  | B     | 1230 | F6C  | CHA-CBD-CGD-O1D |
| 15  | B     | 1230 | F6C  | CHA-CBD-CGD-O2D |
| 15  | B     | 1230 | F6C  | C3B-C2B-CMB-OMB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1237 | F6C  | C2B-C3B-CAB-CBB |
| 15  | B     | 1237 | F6C  | O1A-CGA-O2A-C1  |
| 15  | B     | 1238 | F6C  | C1B-C2B-CMB-OMB |
| 15  | B     | 1238 | F6C  | C3B-C2B-CMB-OMB |
| 15  | G     | 1121 | F6C  | C2A-CAA-CBA-CGA |
| 15  | G     | 1121 | F6C  | C3A-C2A-CAA-CBA |
| 15  | G     | 1121 | F6C  | C2B-C3B-CAB-CBB |
| 15  | G     | 1121 | F6C  | C4B-C3B-CAB-CBB |
| 15  | G     | 1121 | F6C  | C1B-C2B-CMB-OMB |
| 15  | G     | 1121 | F6C  | C3B-C2B-CMB-OMB |
| 15  | H     | 1207 | F6C  | C4-C3-C5-C6     |
| 15  | H     | 1219 | F6C  | C1B-C2B-CMB-OMB |
| 15  | H     | 1219 | F6C  | C2-C3-C5-C6     |
| 15  | H     | 1219 | F6C  | C4-C3-C5-C6     |
| 15  | H     | 1230 | F6C  | CHA-CBD-CGD-O1D |
| 15  | H     | 1230 | F6C  | CHA-CBD-CGD-O2D |
| 15  | H     | 1230 | F6C  | C3B-C2B-CMB-OMB |
| 15  | H     | 1237 | F6C  | C2B-C3B-CAB-CBB |
| 15  | H     | 1237 | F6C  | O1A-CGA-O2A-C1  |
| 15  | H     | 1238 | F6C  | C1B-C2B-CMB-OMB |
| 15  | H     | 1238 | F6C  | C3B-C2B-CMB-OMB |
| 15  | a     | 1121 | F6C  | C2A-CAA-CBA-CGA |
| 15  | a     | 1121 | F6C  | C3A-C2A-CAA-CBA |
| 15  | a     | 1121 | F6C  | C2B-C3B-CAB-CBB |
| 15  | a     | 1121 | F6C  | C4B-C3B-CAB-CBB |
| 15  | a     | 1121 | F6C  | C1B-C2B-CMB-OMB |
| 15  | a     | 1121 | F6C  | C3B-C2B-CMB-OMB |
| 15  | b     | 1207 | F6C  | C4-C3-C5-C6     |
| 15  | b     | 1219 | F6C  | C1B-C2B-CMB-OMB |
| 15  | b     | 1219 | F6C  | C2-C3-C5-C6     |
| 15  | b     | 1219 | F6C  | C4-C3-C5-C6     |
| 15  | b     | 1230 | F6C  | CHA-CBD-CGD-O1D |
| 15  | b     | 1230 | F6C  | CHA-CBD-CGD-O2D |
| 15  | b     | 1230 | F6C  | C3B-C2B-CMB-OMB |
| 15  | b     | 1237 | F6C  | C2B-C3B-CAB-CBB |
| 15  | b     | 1237 | F6C  | O1A-CGA-O2A-C1  |
| 15  | b     | 1238 | F6C  | C1B-C2B-CMB-OMB |
| 15  | b     | 1238 | F6C  | C3B-C2B-CMB-OMB |
| 18  | A     | 4001 | BCR  | C11-C10-C9-C8   |
| 18  | A     | 4001 | BCR  | C11-C10-C9-C34  |
| 18  | A     | 4001 | BCR  | C15-C16-C17-C18 |
| 18  | A     | 4001 | BCR  | C17-C18-C19-C20 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 18         | A            | 4001       | BCR         | C36-C18-C19-C20 |
| 18         | A            | 4002       | BCR         | C11-C10-C9-C8   |
| 18         | A            | 4002       | BCR         | C11-C10-C9-C34  |
| 18         | A            | 4002       | BCR         | C9-C10-C11-C12  |
| 18         | A            | 4002       | BCR         | C10-C11-C12-C13 |
| 18         | A            | 4002       | BCR         | C15-C16-C17-C18 |
| 18         | A            | 4002       | BCR         | C21-C22-C23-C24 |
| 18         | A            | 4002       | BCR         | C37-C22-C23-C24 |
| 18         | A            | 4002       | BCR         | C23-C24-C25-C30 |
| 18         | A            | 4003       | BCR         | C11-C10-C9-C8   |
| 18         | A            | 4003       | BCR         | C11-C10-C9-C34  |
| 18         | A            | 4004       | BCR         | C11-C10-C9-C8   |
| 18         | A            | 4004       | BCR         | C11-C10-C9-C34  |
| 18         | A            | 4005       | BCR         | C7-C8-C9-C10    |
| 18         | A            | 4005       | BCR         | C7-C8-C9-C34    |
| 18         | A            | 4005       | BCR         | C11-C10-C9-C8   |
| 18         | A            | 4005       | BCR         | C11-C10-C9-C34  |
| 18         | A            | 4006       | BCR         | C7-C8-C9-C10    |
| 18         | A            | 4006       | BCR         | C7-C8-C9-C34    |
| 18         | A            | 4006       | BCR         | C11-C10-C9-C8   |
| 18         | A            | 4006       | BCR         | C11-C10-C9-C34  |
| 18         | A            | 4006       | BCR         | C36-C18-C19-C20 |
| 18         | B            | 4004       | BCR         | C11-C10-C9-C8   |
| 18         | B            | 4004       | BCR         | C11-C10-C9-C34  |
| 18         | B            | 4004       | BCR         | C10-C11-C12-C13 |
| 18         | B            | 4004       | BCR         | C21-C22-C23-C24 |
| 18         | B            | 4004       | BCR         | C37-C22-C23-C24 |
| 18         | B            | 4004       | BCR         | C23-C24-C25-C30 |
| 18         | B            | 4005       | BCR         | C11-C10-C9-C8   |
| 18         | B            | 4005       | BCR         | C11-C10-C9-C34  |
| 18         | B            | 4005       | BCR         | C21-C22-C23-C24 |
| 18         | B            | 4005       | BCR         | C37-C22-C23-C24 |
| 18         | B            | 4006       | BCR         | C7-C8-C9-C10    |
| 18         | B            | 4006       | BCR         | C7-C8-C9-C34    |
| 18         | B            | 4006       | BCR         | C10-C11-C12-C13 |
| 18         | B            | 4006       | BCR         | C11-C12-C13-C14 |
| 18         | B            | 4006       | BCR         | C11-C12-C13-C35 |
| 18         | B            | 4009       | BCR         | C5-C6-C7-C8     |
| 18         | B            | 4010       | BCR         | C23-C24-C25-C30 |
| 18         | B            | 4014       | BCR         | C17-C18-C19-C20 |
| 18         | B            | 4014       | BCR         | C36-C18-C19-C20 |
| 18         | B            | 4014       | BCR         | C37-C22-C23-C24 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 18         | B            | 4017       | BCR         | C7-C8-C9-C10    |
| 18         | B            | 4017       | BCR         | C7-C8-C9-C34    |
| 18         | B            | 4017       | BCR         | C11-C10-C9-C8   |
| 18         | B            | 4017       | BCR         | C11-C10-C9-C34  |
| 18         | B            | 4017       | BCR         | C10-C11-C12-C13 |
| 18         | B            | 4017       | BCR         | C18-C19-C20-C21 |
| 18         | B            | 4017       | BCR         | C19-C20-C21-C22 |
| 18         | B            | 4017       | BCR         | C21-C22-C23-C24 |
| 18         | B            | 4017       | BCR         | C37-C22-C23-C24 |
| 18         | I            | 4018       | BCR         | C1-C6-C7-C8     |
| 18         | I            | 4018       | BCR         | C7-C8-C9-C34    |
| 18         | I            | 4018       | BCR         | C11-C10-C9-C8   |
| 18         | I            | 4018       | BCR         | C11-C10-C9-C34  |
| 18         | I            | 4018       | BCR         | C10-C11-C12-C13 |
| 18         | I            | 4018       | BCR         | C15-C16-C17-C18 |
| 18         | I            | 4020       | BCR         | C10-C11-C12-C13 |
| 18         | K            | 4001       | BCR         | C7-C8-C9-C10    |
| 18         | K            | 4001       | BCR         | C7-C8-C9-C34    |
| 18         | K            | 4001       | BCR         | C11-C10-C9-C8   |
| 18         | K            | 4001       | BCR         | C11-C10-C9-C34  |
| 18         | K            | 4001       | BCR         | C10-C11-C12-C13 |
| 18         | K            | 4001       | BCR         | C23-C24-C25-C30 |
| 18         | L            | 4019       | BCR         | C1-C6-C7-C8     |
| 18         | L            | 4019       | BCR         | C21-C22-C23-C24 |
| 18         | L            | 4019       | BCR         | C37-C22-C23-C24 |
| 18         | L            | 4022       | BCR         | C7-C8-C9-C10    |
| 18         | L            | 4022       | BCR         | C7-C8-C9-C34    |
| 18         | L            | 4022       | BCR         | C11-C10-C9-C8   |
| 18         | L            | 4022       | BCR         | C11-C10-C9-C34  |
| 18         | L            | 4022       | BCR         | C11-C12-C13-C14 |
| 18         | L            | 4022       | BCR         | C11-C12-C13-C35 |
| 18         | M            | 4021       | BCR         | C11-C10-C9-C8   |
| 18         | M            | 4021       | BCR         | C11-C10-C9-C34  |
| 18         | M            | 4021       | BCR         | C10-C11-C12-C13 |
| 18         | M            | 4021       | BCR         | C17-C18-C19-C20 |
| 18         | M            | 4021       | BCR         | C36-C18-C19-C20 |
| 18         | G            | 4001       | BCR         | C11-C10-C9-C8   |
| 18         | G            | 4001       | BCR         | C11-C10-C9-C34  |
| 18         | G            | 4001       | BCR         | C15-C16-C17-C18 |
| 18         | G            | 4001       | BCR         | C17-C18-C19-C20 |
| 18         | G            | 4001       | BCR         | C36-C18-C19-C20 |
| 18         | G            | 4002       | BCR         | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | G     | 4002 | BCR  | C11-C10-C9-C34  |
| 18  | G     | 4002 | BCR  | C9-C10-C11-C12  |
| 18  | G     | 4002 | BCR  | C10-C11-C12-C13 |
| 18  | G     | 4002 | BCR  | C15-C16-C17-C18 |
| 18  | G     | 4002 | BCR  | C21-C22-C23-C24 |
| 18  | G     | 4002 | BCR  | C37-C22-C23-C24 |
| 18  | G     | 4002 | BCR  | C23-C24-C25-C30 |
| 18  | G     | 4003 | BCR  | C11-C10-C9-C8   |
| 18  | G     | 4003 | BCR  | C11-C10-C9-C34  |
| 18  | G     | 4004 | BCR  | C11-C10-C9-C8   |
| 18  | G     | 4004 | BCR  | C11-C10-C9-C34  |
| 18  | G     | 4005 | BCR  | C7-C8-C9-C10    |
| 18  | G     | 4005 | BCR  | C7-C8-C9-C34    |
| 18  | G     | 4005 | BCR  | C11-C10-C9-C8   |
| 18  | G     | 4005 | BCR  | C11-C10-C9-C34  |
| 18  | G     | 4006 | BCR  | C7-C8-C9-C10    |
| 18  | G     | 4006 | BCR  | C7-C8-C9-C34    |
| 18  | G     | 4006 | BCR  | C11-C10-C9-C8   |
| 18  | G     | 4006 | BCR  | C11-C10-C9-C34  |
| 18  | G     | 4006 | BCR  | C36-C18-C19-C20 |
| 18  | H     | 4004 | BCR  | C11-C10-C9-C8   |
| 18  | H     | 4004 | BCR  | C11-C10-C9-C34  |
| 18  | H     | 4004 | BCR  | C10-C11-C12-C13 |
| 18  | H     | 4004 | BCR  | C21-C22-C23-C24 |
| 18  | H     | 4004 | BCR  | C37-C22-C23-C24 |
| 18  | H     | 4004 | BCR  | C23-C24-C25-C30 |
| 18  | H     | 4005 | BCR  | C11-C10-C9-C8   |
| 18  | H     | 4005 | BCR  | C11-C10-C9-C34  |
| 18  | H     | 4005 | BCR  | C21-C22-C23-C24 |
| 18  | H     | 4005 | BCR  | C37-C22-C23-C24 |
| 18  | H     | 4006 | BCR  | C7-C8-C9-C10    |
| 18  | H     | 4006 | BCR  | C7-C8-C9-C34    |
| 18  | H     | 4006 | BCR  | C10-C11-C12-C13 |
| 18  | H     | 4006 | BCR  | C11-C12-C13-C14 |
| 18  | H     | 4006 | BCR  | C11-C12-C13-C35 |
| 18  | H     | 4009 | BCR  | C5-C6-C7-C8     |
| 18  | H     | 4010 | BCR  | C23-C24-C25-C30 |
| 18  | H     | 4014 | BCR  | C17-C18-C19-C20 |
| 18  | H     | 4014 | BCR  | C36-C18-C19-C20 |
| 18  | H     | 4014 | BCR  | C37-C22-C23-C24 |
| 18  | H     | 4017 | BCR  | C7-C8-C9-C10    |
| 18  | H     | 4017 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | H     | 4017 | BCR  | C11-C10-C9-C8   |
| 18  | H     | 4017 | BCR  | C11-C10-C9-C34  |
| 18  | H     | 4017 | BCR  | C10-C11-C12-C13 |
| 18  | H     | 4017 | BCR  | C18-C19-C20-C21 |
| 18  | H     | 4017 | BCR  | C19-C20-C21-C22 |
| 18  | H     | 4017 | BCR  | C21-C22-C23-C24 |
| 18  | H     | 4017 | BCR  | C37-C22-C23-C24 |
| 18  | R     | 4018 | BCR  | C1-C6-C7-C8     |
| 18  | R     | 4018 | BCR  | C7-C8-C9-C34    |
| 18  | R     | 4018 | BCR  | C11-C10-C9-C8   |
| 18  | R     | 4018 | BCR  | C11-C10-C9-C34  |
| 18  | R     | 4018 | BCR  | C10-C11-C12-C13 |
| 18  | R     | 4018 | BCR  | C15-C16-C17-C18 |
| 18  | R     | 4020 | BCR  | C10-C11-C12-C13 |
| 18  | T     | 4001 | BCR  | C7-C8-C9-C10    |
| 18  | T     | 4001 | BCR  | C7-C8-C9-C34    |
| 18  | T     | 4001 | BCR  | C11-C10-C9-C8   |
| 18  | T     | 4001 | BCR  | C11-C10-C9-C34  |
| 18  | T     | 4001 | BCR  | C10-C11-C12-C13 |
| 18  | T     | 4001 | BCR  | C23-C24-C25-C30 |
| 18  | U     | 4019 | BCR  | C1-C6-C7-C8     |
| 18  | U     | 4019 | BCR  | C21-C22-C23-C24 |
| 18  | U     | 4019 | BCR  | C37-C22-C23-C24 |
| 18  | U     | 4022 | BCR  | C7-C8-C9-C10    |
| 18  | U     | 4022 | BCR  | C7-C8-C9-C34    |
| 18  | U     | 4022 | BCR  | C11-C10-C9-C8   |
| 18  | U     | 4022 | BCR  | C11-C10-C9-C34  |
| 18  | U     | 4022 | BCR  | C11-C12-C13-C14 |
| 18  | U     | 4022 | BCR  | C11-C12-C13-C35 |
| 18  | V     | 4021 | BCR  | C11-C10-C9-C8   |
| 18  | V     | 4021 | BCR  | C11-C10-C9-C34  |
| 18  | V     | 4021 | BCR  | C10-C11-C12-C13 |
| 18  | V     | 4021 | BCR  | C17-C18-C19-C20 |
| 18  | V     | 4021 | BCR  | C36-C18-C19-C20 |
| 18  | a     | 4001 | BCR  | C11-C10-C9-C8   |
| 18  | a     | 4001 | BCR  | C11-C10-C9-C34  |
| 18  | a     | 4001 | BCR  | C15-C16-C17-C18 |
| 18  | a     | 4001 | BCR  | C17-C18-C19-C20 |
| 18  | a     | 4001 | BCR  | C36-C18-C19-C20 |
| 18  | a     | 4002 | BCR  | C11-C10-C9-C8   |
| 18  | a     | 4002 | BCR  | C11-C10-C9-C34  |
| 18  | a     | 4002 | BCR  | C9-C10-C11-C12  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 18         | a            | 4002       | BCR         | C10-C11-C12-C13 |
| 18         | a            | 4002       | BCR         | C15-C16-C17-C18 |
| 18         | a            | 4002       | BCR         | C21-C22-C23-C24 |
| 18         | a            | 4002       | BCR         | C37-C22-C23-C24 |
| 18         | a            | 4002       | BCR         | C23-C24-C25-C30 |
| 18         | a            | 4003       | BCR         | C11-C10-C9-C8   |
| 18         | a            | 4003       | BCR         | C11-C10-C9-C34  |
| 18         | a            | 4004       | BCR         | C11-C10-C9-C8   |
| 18         | a            | 4004       | BCR         | C11-C10-C9-C34  |
| 18         | a            | 4005       | BCR         | C7-C8-C9-C10    |
| 18         | a            | 4005       | BCR         | C7-C8-C9-C34    |
| 18         | a            | 4005       | BCR         | C11-C10-C9-C8   |
| 18         | a            | 4005       | BCR         | C11-C10-C9-C34  |
| 18         | a            | 4006       | BCR         | C7-C8-C9-C10    |
| 18         | a            | 4006       | BCR         | C7-C8-C9-C34    |
| 18         | a            | 4006       | BCR         | C11-C10-C9-C8   |
| 18         | a            | 4006       | BCR         | C11-C10-C9-C34  |
| 18         | a            | 4006       | BCR         | C36-C18-C19-C20 |
| 18         | b            | 4004       | BCR         | C11-C10-C9-C8   |
| 18         | b            | 4004       | BCR         | C11-C10-C9-C34  |
| 18         | b            | 4004       | BCR         | C10-C11-C12-C13 |
| 18         | b            | 4004       | BCR         | C21-C22-C23-C24 |
| 18         | b            | 4004       | BCR         | C37-C22-C23-C24 |
| 18         | b            | 4004       | BCR         | C23-C24-C25-C30 |
| 18         | b            | 4005       | BCR         | C11-C10-C9-C8   |
| 18         | b            | 4005       | BCR         | C11-C10-C9-C34  |
| 18         | b            | 4005       | BCR         | C21-C22-C23-C24 |
| 18         | b            | 4005       | BCR         | C37-C22-C23-C24 |
| 18         | b            | 4006       | BCR         | C7-C8-C9-C10    |
| 18         | b            | 4006       | BCR         | C7-C8-C9-C34    |
| 18         | b            | 4006       | BCR         | C10-C11-C12-C13 |
| 18         | b            | 4006       | BCR         | C11-C12-C13-C14 |
| 18         | b            | 4006       | BCR         | C11-C12-C13-C35 |
| 18         | b            | 4009       | BCR         | C5-C6-C7-C8     |
| 18         | b            | 4010       | BCR         | C23-C24-C25-C30 |
| 18         | b            | 4014       | BCR         | C17-C18-C19-C20 |
| 18         | b            | 4014       | BCR         | C36-C18-C19-C20 |
| 18         | b            | 4014       | BCR         | C37-C22-C23-C24 |
| 18         | b            | 4017       | BCR         | C7-C8-C9-C10    |
| 18         | b            | 4017       | BCR         | C7-C8-C9-C34    |
| 18         | b            | 4017       | BCR         | C11-C10-C9-C8   |
| 18         | b            | 4017       | BCR         | C11-C10-C9-C34  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | b     | 4017 | BCR  | C10-C11-C12-C13 |
| 18  | b     | 4017 | BCR  | C18-C19-C20-C21 |
| 18  | b     | 4017 | BCR  | C19-C20-C21-C22 |
| 18  | b     | 4017 | BCR  | C21-C22-C23-C24 |
| 18  | b     | 4017 | BCR  | C37-C22-C23-C24 |
| 18  | i     | 4018 | BCR  | C1-C6-C7-C8     |
| 18  | i     | 4018 | BCR  | C7-C8-C9-C34    |
| 18  | i     | 4018 | BCR  | C11-C10-C9-C8   |
| 18  | i     | 4018 | BCR  | C11-C10-C9-C34  |
| 18  | i     | 4018 | BCR  | C10-C11-C12-C13 |
| 18  | i     | 4018 | BCR  | C15-C16-C17-C18 |
| 18  | i     | 4020 | BCR  | C10-C11-C12-C13 |
| 18  | k     | 4001 | BCR  | C7-C8-C9-C10    |
| 18  | k     | 4001 | BCR  | C7-C8-C9-C34    |
| 18  | k     | 4001 | BCR  | C11-C10-C9-C8   |
| 18  | k     | 4001 | BCR  | C11-C10-C9-C34  |
| 18  | k     | 4001 | BCR  | C10-C11-C12-C13 |
| 18  | k     | 4001 | BCR  | C23-C24-C25-C30 |
| 18  | l     | 4019 | BCR  | C1-C6-C7-C8     |
| 18  | l     | 4019 | BCR  | C21-C22-C23-C24 |
| 18  | l     | 4019 | BCR  | C37-C22-C23-C24 |
| 18  | l     | 4022 | BCR  | C7-C8-C9-C10    |
| 18  | l     | 4022 | BCR  | C7-C8-C9-C34    |
| 18  | l     | 4022 | BCR  | C11-C10-C9-C8   |
| 18  | l     | 4022 | BCR  | C11-C10-C9-C34  |
| 18  | l     | 4022 | BCR  | C11-C12-C13-C14 |
| 18  | l     | 4022 | BCR  | C11-C12-C13-C35 |
| 18  | m     | 4021 | BCR  | C11-C10-C9-C8   |
| 18  | m     | 4021 | BCR  | C11-C10-C9-C34  |
| 18  | m     | 4021 | BCR  | C10-C11-C12-C13 |
| 18  | m     | 4021 | BCR  | C17-C18-C19-C20 |
| 18  | m     | 4021 | BCR  | C36-C18-C19-C20 |
| 19  | A     | 5001 | LHG  | C3-O3-P-O5      |
| 19  | A     | 5001 | LHG  | C3-O3-P-O6      |
| 19  | A     | 5001 | LHG  | C4-O6-P-O4      |
| 19  | A     | 5002 | LHG  | C4-O6-P-O3      |
| 19  | A     | 5002 | LHG  | C4-O6-P-O4      |
| 19  | A     | 5002 | LHG  | O6-C4-C5-O7     |
| 19  | A     | 5002 | LHG  | C8-C7-O7-C5     |
| 19  | L     | 5101 | LHG  | O6-C4-C5-C6     |
| 19  | L     | 5101 | LHG  | O6-C4-C5-O7     |
| 19  | L     | 5102 | LHG  | O1-C1-C2-C3     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | L     | 5102 | LHG  | C1-C2-C3-O3     |
| 19  | L     | 5102 | LHG  | O2-C2-C3-O3     |
| 19  | G     | 5001 | LHG  | C3-O3-P-O5      |
| 19  | G     | 5001 | LHG  | C3-O3-P-O6      |
| 19  | G     | 5001 | LHG  | C4-O6-P-O4      |
| 19  | G     | 5002 | LHG  | C4-O6-P-O3      |
| 19  | G     | 5002 | LHG  | C4-O6-P-O4      |
| 19  | G     | 5002 | LHG  | O6-C4-C5-O7     |
| 19  | G     | 5002 | LHG  | C8-C7-O7-C5     |
| 19  | U     | 5101 | LHG  | O6-C4-C5-C6     |
| 19  | U     | 5101 | LHG  | O6-C4-C5-O7     |
| 19  | U     | 5102 | LHG  | O1-C1-C2-C3     |
| 19  | U     | 5102 | LHG  | C1-C2-C3-O3     |
| 19  | U     | 5102 | LHG  | O2-C2-C3-O3     |
| 19  | a     | 5001 | LHG  | C3-O3-P-O5      |
| 19  | a     | 5001 | LHG  | C3-O3-P-O6      |
| 19  | a     | 5001 | LHG  | C4-O6-P-O4      |
| 19  | a     | 5002 | LHG  | C4-O6-P-O3      |
| 19  | a     | 5002 | LHG  | C4-O6-P-O4      |
| 19  | a     | 5002 | LHG  | O6-C4-C5-O7     |
| 19  | a     | 5002 | LHG  | C8-C7-O7-C5     |
| 19  | l     | 5101 | LHG  | O6-C4-C5-C6     |
| 19  | l     | 5101 | LHG  | O6-C4-C5-O7     |
| 19  | l     | 5102 | LHG  | O1-C1-C2-C3     |
| 19  | l     | 5102 | LHG  | C1-C2-C3-O3     |
| 19  | l     | 5102 | LHG  | O2-C2-C3-O3     |
| 20  | B     | 5002 | LMG  | O6-C1-O1-C7     |
| 20  | B     | 5002 | LMG  | C11-C10-O7-C8   |
| 20  | B     | 5002 | LMG  | O10-C28-O8-C9   |
| 20  | B     | 5002 | LMG  | C29-C28-O8-C9   |
| 20  | H     | 5002 | LMG  | O6-C1-O1-C7     |
| 20  | H     | 5002 | LMG  | C11-C10-O7-C8   |
| 20  | H     | 5002 | LMG  | O10-C28-O8-C9   |
| 20  | H     | 5002 | LMG  | C29-C28-O8-C9   |
| 20  | b     | 5002 | LMG  | O6-C1-O1-C7     |
| 20  | b     | 5002 | LMG  | C11-C10-O7-C8   |
| 20  | b     | 5002 | LMG  | O10-C28-O8-C9   |
| 20  | b     | 5002 | LMG  | C29-C28-O8-C9   |
| 21  | A     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 21  | A     | 6002 | LMT  | O5B-C1B-O1B-C4' |
| 21  | A     | 6004 | LMT  | C2-C1-O1'-C1'   |
| 21  | B     | 6001 | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | B     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 21  | B     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 21  | B     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 21  | B     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 21  | L     | 6101 | LMT  | C2-C1-O1'-C1'   |
| 21  | G     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 21  | G     | 6002 | LMT  | O5B-C1B-O1B-C4' |
| 21  | G     | 6004 | LMT  | C2-C1-O1'-C1'   |
| 21  | H     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | H     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 21  | H     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 21  | H     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 21  | H     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 21  | U     | 6101 | LMT  | C2-C1-O1'-C1'   |
| 21  | a     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 21  | a     | 6002 | LMT  | O5B-C1B-O1B-C4' |
| 21  | a     | 6004 | LMT  | C2-C1-O1'-C1'   |
| 21  | b     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | b     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 21  | b     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 21  | b     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 21  | b     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 21  | l     | 6101 | LMT  | C2-C1-O1'-C1'   |
| 14  | B     | 1023 | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 1023 | CLA  | C2C-C3C-CAC-CBC |
| 14  | b     | 1023 | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 1023 | CLA  | C4C-C3C-CAC-CBC |
| 14  | H     | 1023 | CLA  | C4C-C3C-CAC-CBC |
| 14  | b     | 1023 | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 1108 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1119 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1134 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1139 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1108 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1119 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1134 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1139 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1108 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1119 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1134 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1139 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1101 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1114 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1117 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1119 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1120 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1122 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1132 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1134 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1138 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1208 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1214 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1218 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1224 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1226 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1227 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1234 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1235 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1236 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1239 | CLA  | CBD-CGD-O2D-CED |
| 14  | K     | 1401 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1101 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1114 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1117 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1119 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1120 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1122 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1132 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1134 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1138 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1208 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1214 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1218 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1224 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1226 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1227 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1234 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1235 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1236 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1239 | CLA  | CBD-CGD-O2D-CED |
| 14  | T     | 1401 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1101 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1114 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1117 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1119 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1120 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1122 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1132 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1134 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1138 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1208 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1214 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1218 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1224 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1226 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1227 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1234 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1235 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1236 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1239 | CLA  | CBD-CGD-O2D-CED |
| 14  | k     | 1401 | CLA  | CBD-CGD-O2D-CED |
| 15  | A     | 1121 | F6C  | CBD-CGD-O2D-CED |
| 15  | B     | 1230 | F6C  | CBD-CGD-O2D-CED |
| 15  | G     | 1121 | F6C  | CBD-CGD-O2D-CED |
| 15  | H     | 1230 | F6C  | CBD-CGD-O2D-CED |
| 15  | a     | 1121 | F6C  | CBD-CGD-O2D-CED |
| 15  | b     | 1230 | F6C  | CBD-CGD-O2D-CED |
| 14  | A     | 1103 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1128 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1220 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1222 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1224 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1240 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1103 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1128 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1220 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1222 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1224 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1240 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1103 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1128 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1220 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1222 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1224 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1240 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1107 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1112 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1122 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1112 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1122 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1107 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1112 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1122 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1239 | CLA  | C4C-C3C-CAC-CBC |
| 14  | H     | 1239 | CLA  | C4C-C3C-CAC-CBC |
| 14  | b     | 1239 | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 1131 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1135 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1107 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1131 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1135 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1131 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1135 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1203 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1206 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1224 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1240 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1203 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1206 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1224 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1240 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1203 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1206 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1224 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1240 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1012 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1102 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1105 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1106 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1109 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1111 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1116 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1126 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1127 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1130 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1201 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1215 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1223 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1228 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1231 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1012 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1102 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1105 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1106 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1109 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1111 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1116 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1126 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1127 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1130 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1201 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1215 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1223 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1228 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1231 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1012 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1102 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1105 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1106 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1109 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1111 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1116 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1126 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1127 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1130 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1201 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1215 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1223 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1228 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1231 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1118 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1133 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1135 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1138 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1203 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1210 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1118 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1133 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1135 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1138 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1203 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1210 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1118 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1133 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1135 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1138 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1203 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1210 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 5003 | LMG  | O10-C28-O8-C9   |
| 20  | I     | 5006 | LMG  | O10-C28-O8-C9   |
| 20  | G     | 5003 | LMG  | O10-C28-O8-C9   |
| 20  | R     | 5006 | LMG  | O10-C28-O8-C9   |
| 20  | a     | 5003 | LMG  | O10-C28-O8-C9   |
| 20  | i     | 5006 | LMG  | O10-C28-O8-C9   |
| 14  | B     | 1021 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1229 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1232 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1233 | CLA  | O1D-CGD-O2D-CED |
| 14  | M     | 1501 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1021 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1229 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1232 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1233 | CLA  | O1D-CGD-O2D-CED |
| 14  | V     | 1501 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1021 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1229 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1232 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1233 | CLA  | O1D-CGD-O2D-CED |
| 14  | m     | 1501 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1114 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1140 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1202 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1140 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1202 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1140 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1202 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1114 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1114 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 5002 | LHG  | O9-C7-O7-C5     |
| 19  | G     | 5002 | LHG  | O9-C7-O7-C5     |
| 19  | a     | 5002 | LHG  | O9-C7-O7-C5     |
| 20  | B     | 5002 | LMG  | O9-C10-O7-C8    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | H     | 5002 | LMG  | O9-C10-O7-C8    |
| 20  | b     | 5002 | LMG  | O9-C10-O7-C8    |
| 14  | B     | 1239 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1239 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1239 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1112 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1116 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1136 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1138 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1201 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1205 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1216 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1231 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1236 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1112 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1116 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1136 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1138 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1201 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1205 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1216 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1231 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1236 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1112 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1116 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1136 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1138 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1201 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1205 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1216 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1231 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1236 | CLA  | C3-C5-C6-C7     |
| 15  | B     | 1238 | F6C  | C3-C5-C6-C7     |
| 15  | H     | 1238 | F6C  | C3-C5-C6-C7     |
| 15  | b     | 1238 | F6C  | C3-C5-C6-C7     |
| 16  | B     | 2002 | PQN  | C13-C15-C16-C17 |
| 16  | H     | 2002 | PQN  | C13-C15-C16-C17 |
| 16  | b     | 2002 | PQN  | C13-C15-C16-C17 |
| 14  | A     | 1103 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1117 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1128 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1210 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1214 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1222 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1229 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1103 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1117 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1128 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1210 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1214 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1222 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1229 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1103 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1117 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1128 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1210 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1214 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1222 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1229 | CLA  | CBA-CGA-O2A-C1  |
| 15  | B     | 1237 | F6C  | CBA-CGA-O2A-C1  |
| 15  | H     | 1237 | F6C  | CBA-CGA-O2A-C1  |
| 15  | b     | 1237 | F6C  | CBA-CGA-O2A-C1  |
| 20  | A     | 5003 | LMG  | C29-C28-O8-C9   |
| 20  | I     | 5006 | LMG  | C29-C28-O8-C9   |
| 20  | G     | 5003 | LMG  | C29-C28-O8-C9   |
| 20  | R     | 5006 | LMG  | C29-C28-O8-C9   |
| 20  | a     | 5003 | LMG  | C29-C28-O8-C9   |
| 20  | i     | 5006 | LMG  | C29-C28-O8-C9   |
| 14  | B     | 1239 | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 1239 | CLA  | C2C-C3C-CAC-CBC |
| 14  | b     | 1239 | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 1115 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1115 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1115 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1133 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1141 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1133 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1141 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1133 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1141 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1022 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1022 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1022 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1126 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1226 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1126 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1226 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1126 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1226 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1109 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1109 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1109 | CLA  | C2-C3-C5-C6     |
| 15  | B     | 1207 | F6C  | C2-C3-C5-C6     |
| 15  | H     | 1207 | F6C  | C2-C3-C5-C6     |
| 15  | b     | 1207 | F6C  | C2-C3-C5-C6     |
| 14  | B     | 1205 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1212 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1205 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1212 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1205 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1212 | CLA  | CBD-CGD-O2D-CED |
| 15  | B     | 1237 | F6C  | CBD-CGD-O2D-CED |
| 15  | H     | 1237 | F6C  | CBD-CGD-O2D-CED |
| 15  | b     | 1237 | F6C  | CBD-CGD-O2D-CED |
| 14  | A     | 1106 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1116 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1127 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1134 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1220 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1221 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1225 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1236 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1106 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1116 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1119 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1127 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1134 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1221 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1225 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1236 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1106 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1116 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1119 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1127 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1134 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1220 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1221 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1225 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1236 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1129 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1129 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1129 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 5003 | LMG  | C35-C36-C37-C38 |
| 20  | B     | 5002 | LMG  | C17-C18-C19-C20 |
| 20  | G     | 5003 | LMG  | C35-C36-C37-C38 |
| 20  | H     | 5002 | LMG  | C17-C18-C19-C20 |
| 20  | a     | 5003 | LMG  | C35-C36-C37-C38 |
| 20  | b     | 5002 | LMG  | C17-C18-C19-C20 |
| 14  | A     | 1104 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1124 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1208 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1239 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1104 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1124 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1208 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1239 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1104 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1124 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1208 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1239 | CLA  | C3-C5-C6-C7     |
| 15  | B     | 1207 | F6C  | C3-C5-C6-C7     |
| 15  | H     | 1207 | F6C  | C3-C5-C6-C7     |
| 15  | b     | 1207 | F6C  | C3-C5-C6-C7     |
| 14  | A     | 1118 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1122 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1129 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1133 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1135 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1138 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1202 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1226 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1236 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1239 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1118 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1122 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1129 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1133 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1135 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1138 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1202 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1226 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1236 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1239 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1118 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1122 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1129 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1133 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1135 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1138 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1202 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1226 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1236 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1239 | CLA  | CBA-CGA-O2A-C1  |
| 21  | L     | 6002 | LMT  | C4B-C5B-C6B-O6B |
| 21  | U     | 6002 | LMT  | C4B-C5B-C6B-O6B |
| 21  | l     | 6002 | LMT  | C4B-C5B-C6B-O6B |
| 15  | B     | 1207 | F6C  | C1A-C2A-CAA-CBA |
| 15  | B     | 1230 | F6C  | C1A-C2A-CAA-CBA |
| 15  | H     | 1207 | F6C  | C1A-C2A-CAA-CBA |
| 15  | H     | 1230 | F6C  | C1A-C2A-CAA-CBA |
| 15  | b     | 1207 | F6C  | C1A-C2A-CAA-CBA |
| 15  | b     | 1230 | F6C  | C1A-C2A-CAA-CBA |
| 14  | B     | 1216 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 1225 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1216 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1225 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1216 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1225 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1101 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1120 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1138 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1208 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1227 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1239 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1101 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1120 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1138 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1208 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1227 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1239 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1101 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1120 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1208 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1227 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1239 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 6004 | LMT  | O5B-C5B-C6B-O6B |
| 21  | H     | 6004 | LMT  | O5B-C5B-C6B-O6B |
| 21  | b     | 6004 | LMT  | O5B-C5B-C6B-O6B |
| 14  | A     | 1122 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1211 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1226 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1236 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1122 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1211 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1226 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1236 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1122 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1211 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1226 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1236 | CLA  | O1A-CGA-O2A-C1  |
| 14  | K     | 1401 | CLA  | O1D-CGD-O2D-CED |
| 14  | T     | 1401 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1138 | CLA  | O1D-CGD-O2D-CED |
| 14  | k     | 1401 | CLA  | O1D-CGD-O2D-CED |
| 15  | B     | 1230 | F6C  | O1D-CGD-O2D-CED |
| 15  | H     | 1230 | F6C  | O1D-CGD-O2D-CED |
| 15  | b     | 1230 | F6C  | O1D-CGD-O2D-CED |
| 18  | A     | 4003 | BCR  | C9-C10-C11-C12  |
| 18  | B     | 4017 | BCR  | C9-C10-C11-C12  |
| 18  | G     | 4002 | BCR  | C13-C14-C15-C16 |
| 18  | G     | 4003 | BCR  | C9-C10-C11-C12  |
| 18  | H     | 4017 | BCR  | C9-C10-C11-C12  |
| 18  | b     | 4017 | BCR  | C9-C10-C11-C12  |
| 21  | I     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 21  | R     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 21  | i     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 14  | B     | 1204 | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 1503 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1204 | CLA  | CBD-CGD-O2D-CED |
| 14  | U     | 1503 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1204 | CLA  | CBD-CGD-O2D-CED |
| 14  | l     | 1503 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1132 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1218 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1236 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1132 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1218 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1236 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1132 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1218 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1236 | CLA  | O1D-CGD-O2D-CED |
| 15  | A     | 1121 | F6C  | O1D-CGD-O2D-CED |
| 15  | G     | 1121 | F6C  | O1D-CGD-O2D-CED |
| 15  | a     | 1121 | F6C  | O1D-CGD-O2D-CED |
| 19  | A     | 5001 | LHG  | O2-C2-C3-O3     |
| 19  | G     | 5001 | LHG  | O2-C2-C3-O3     |
| 19  | a     | 5001 | LHG  | O2-C2-C3-O3     |
| 14  | A     | 1140 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1022 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1140 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1022 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1140 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1022 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1130 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1022 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1211 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1215 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1130 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1022 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1211 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1215 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1130 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1022 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1211 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1215 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1117 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1214 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1229 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1117 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1214 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1229 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1117 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1214 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1229 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1235 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1235 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1235 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1220 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1220 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1220 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1130 | CLA  | O1A-CGA-O2A-C1  |
| 19  | A     | 5001 | LHG  | C11-C12-C13-C14 |
| 19  | G     | 5001 | LHG  | C11-C12-C13-C14 |
| 19  | a     | 5001 | LHG  | C11-C12-C13-C14 |
| 21  | L     | 6101 | LMT  | O5B-C5B-C6B-O6B |
| 21  | L     | 6101 | LMT  | O5'-C5'-C6'-O6' |
| 21  | U     | 6101 | LMT  | O5B-C5B-C6B-O6B |
| 21  | U     | 6101 | LMT  | O5'-C5'-C6'-O6' |
| 21  | l     | 6101 | LMT  | O5B-C5B-C6B-O6B |
| 21  | l     | 6101 | LMT  | O5'-C5'-C6'-O6' |
| 14  | A     | 1136 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1136 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1136 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1115 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1202 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1206 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1224 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1115 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1202 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1206 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1224 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1115 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1202 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1206 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1224 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1109 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1109 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1109 | CLA  | CBA-CGA-O2A-C1  |
| 21  | L     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 21  | U     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 21  | l     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 21  | B     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 21  | H     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 21  | b     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 14  | A     | 1130 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1130 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1237 | F6C  | C2A-CAA-CBA-CGA |
| 15  | B     | 1238 | F6C  | C2A-CAA-CBA-CGA |
| 15  | H     | 1237 | F6C  | C2A-CAA-CBA-CGA |
| 15  | H     | 1238 | F6C  | C2A-CAA-CBA-CGA |
| 15  | b     | 1237 | F6C  | C2A-CAA-CBA-CGA |
| 15  | b     | 1238 | F6C  | C2A-CAA-CBA-CGA |
| 21  | I     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 21  | R     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 21  | i     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 14  | A     | 1115 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1136 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1201 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1203 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1224 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1229 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1115 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1136 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1201 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1203 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1224 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1229 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1115 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1136 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1201 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1203 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1224 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1229 | CLA  | C4-C3-C5-C6     |
| 21  | G     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 21  | a     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 14  | A     | 1115 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1118 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1136 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1201 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1203 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1224 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1229 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1115 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1118 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1136 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1201 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1203 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1224 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1229 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1115 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1118 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1136 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1201 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1203 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1224 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1229 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1113 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1122 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1213 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1217 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1113 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1122 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1213 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1217 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1220 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1113 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1122 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1213 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1217 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1117 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1214 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1226 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1234 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1117 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1214 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1226 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1234 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1117 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1214 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1226 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1234 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 21  | H     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 21  | b     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 14  | B     | 1202 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1202 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1202 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 20  | A     | 5003 | LMG  | O6-C1-O1-C7     |
| 20  | G     | 5003 | LMG  | O6-C1-O1-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | a     | 5003 | LMG  | O6-C1-O1-C7     |
| 21  | A     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | A     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 21  | G     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | G     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 21  | a     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | a     | 6004 | LMT  | O5'-C1'-O1'-C1  |
| 14  | A     | 1111 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1111 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1111 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1104 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1104 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1104 | CLA  | CBA-CGA-O2A-C1  |
| 21  | L     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | M     | 6000 | LMT  | O5'-C5'-C6'-O6' |
| 21  | U     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | V     | 6000 | LMT  | O5'-C5'-C6'-O6' |
| 21  | l     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | m     | 6000 | LMT  | O5'-C5'-C6'-O6' |
| 21  | A     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 21  | G     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 21  | a     | 6003 | LMT  | C4B-C5B-C6B-O6B |
| 15  | B     | 1219 | F6C  | C1A-C2A-CAA-CBA |
| 15  | H     | 1219 | F6C  | C1A-C2A-CAA-CBA |
| 15  | b     | 1219 | F6C  | C1A-C2A-CAA-CBA |
| 14  | A     | 1127 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1224 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1228 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1127 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1224 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1228 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1116 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1127 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1228 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1215 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1215 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1215 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1116 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1126 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1215 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1116 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1126 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1215 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1215 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1224 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1111 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1126 | CLA  | O1D-CGD-O2D-CED |
| 21  | L     | 6101 | LMT  | C4B-C5B-C6B-O6B |
| 21  | U     | 6101 | LMT  | C4B-C5B-C6B-O6B |
| 21  | l     | 6101 | LMT  | C4B-C5B-C6B-O6B |
| 14  | A     | 1109 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1109 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1109 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1102 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1106 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1111 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1223 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1102 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1106 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1223 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1102 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1106 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1111 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1223 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1116 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1123 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1201 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1216 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1116 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1123 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1201 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1216 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1116 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1123 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1201 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1216 | CLA  | CBA-CGA-O2A-C1  |
| 15  | B     | 1219 | F6C  | CBA-CGA-O2A-C1  |
| 15  | H     | 1219 | F6C  | CBA-CGA-O2A-C1  |
| 15  | b     | 1219 | F6C  | CBA-CGA-O2A-C1  |
| 15  | B     | 1219 | F6C  | CBD-CGD-O2D-CED |
| 15  | H     | 1219 | F6C  | CBD-CGD-O2D-CED |
| 15  | b     | 1219 | F6C  | CBD-CGD-O2D-CED |
| 18  | A     | 4002 | BCR  | C13-C14-C15-C16 |
| 18  | a     | 4002 | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 4003 | BCR  | C9-C10-C11-C12  |
| 14  | B     | 1226 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1226 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1226 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 6004 | LMT  | C4B-C5B-C6B-O6B |
| 21  | H     | 6004 | LMT  | C4B-C5B-C6B-O6B |
| 21  | b     | 6004 | LMT  | C4B-C5B-C6B-O6B |
| 14  | B     | 1021 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1221 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1021 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1221 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1021 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1221 | CLA  | C5-C6-C7-C8     |
| 16  | A     | 2001 | PQN  | C25-C26-C27-C28 |
| 16  | G     | 2001 | PQN  | C25-C26-C27-C28 |
| 16  | a     | 2001 | PQN  | C25-C26-C27-C28 |
| 14  | B     | 1231 | CLA  | O1D-CGD-O2D-CED |
| 20  | B     | 5002 | LMG  | C2-C1-O1-C7     |
| 20  | H     | 5002 | LMG  | C2-C1-O1-C7     |
| 20  | b     | 5002 | LMG  | C2-C1-O1-C7     |
| 21  | A     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 21  | G     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 21  | a     | 6004 | LMT  | C2'-C1'-O1'-C1  |
| 19  | A     | 5002 | LHG  | O7-C5-C6-O8     |
| 19  | G     | 5002 | LHG  | O7-C5-C6-O8     |
| 19  | a     | 5002 | LHG  | O7-C5-C6-O8     |
| 14  | A     | 1123 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1201 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1216 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1123 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1201 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1216 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1123 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1201 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1216 | CLA  | O1A-CGA-O2A-C1  |
| 21  | I     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 21  | R     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 21  | i     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 14  | A     | 1126 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1226 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1126 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1226 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1126 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1226 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1104 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1117 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1123 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1126 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1201 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1203 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1216 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1220 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1221 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1222 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1224 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1234 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1240 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1104 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1117 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1123 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1126 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1201 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1203 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1216 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1220 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1221 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1222 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1224 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1234 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1240 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1104 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1117 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1123 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1126 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1201 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1203 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1216 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1220 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1221 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1222 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1224 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1234 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1240 | CLA  | C11-C12-C13-C14 |
| 15  | B     | 1207 | F6C  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1237 | F6C  | C6-C7-C8-C9     |
| 15  | B     | 1237 | F6C  | C11-C10-C8-C9   |
| 15  | B     | 1237 | F6C  | C11-C12-C13-C14 |
| 15  | H     | 1207 | F6C  | C14-C13-C15-C16 |
| 15  | H     | 1237 | F6C  | C6-C7-C8-C9     |
| 15  | H     | 1237 | F6C  | C11-C10-C8-C9   |
| 15  | H     | 1237 | F6C  | C11-C12-C13-C14 |
| 15  | b     | 1207 | F6C  | C14-C13-C15-C16 |
| 15  | b     | 1237 | F6C  | C6-C7-C8-C9     |
| 15  | b     | 1237 | F6C  | C11-C10-C8-C9   |
| 15  | b     | 1237 | F6C  | C11-C12-C13-C14 |
| 16  | A     | 2001 | PQN  | C19-C18-C20-C21 |
| 16  | A     | 2001 | PQN  | C21-C22-C23-C24 |
| 16  | G     | 2001 | PQN  | C19-C18-C20-C21 |
| 16  | G     | 2001 | PQN  | C21-C22-C23-C24 |
| 16  | a     | 2001 | PQN  | C19-C18-C20-C21 |
| 16  | a     | 2001 | PQN  | C21-C22-C23-C24 |
| 14  | A     | 1012 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1012 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1231 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1012 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1231 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1104 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1104 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1104 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1131 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1131 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1131 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 4001 | BCR  | C7-C8-C9-C34    |
| 18  | A     | 4004 | BCR  | C37-C22-C23-C24 |
| 18  | A     | 4005 | BCR  | C37-C22-C23-C24 |
| 18  | A     | 4006 | BCR  | C37-C22-C23-C24 |
| 18  | B     | 4004 | BCR  | C7-C8-C9-C34    |
| 18  | B     | 4005 | BCR  | C11-C12-C13-C35 |
| 18  | B     | 4006 | BCR  | C37-C22-C23-C24 |
| 18  | K     | 4001 | BCR  | C11-C12-C13-C35 |
| 18  | K     | 4001 | BCR  | C36-C18-C19-C20 |
| 18  | L     | 4019 | BCR  | C7-C8-C9-C34    |
| 18  | M     | 4021 | BCR  | C7-C8-C9-C34    |
| 18  | G     | 4001 | BCR  | C7-C8-C9-C34    |
| 18  | G     | 4004 | BCR  | C37-C22-C23-C24 |
| 18  | G     | 4005 | BCR  | C37-C22-C23-C24 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 18         | G            | 4006       | BCR         | C37-C22-C23-C24 |
| 18         | H            | 4004       | BCR         | C7-C8-C9-C34    |
| 18         | H            | 4005       | BCR         | C11-C12-C13-C35 |
| 18         | H            | 4006       | BCR         | C37-C22-C23-C24 |
| 18         | T            | 4001       | BCR         | C11-C12-C13-C35 |
| 18         | T            | 4001       | BCR         | C36-C18-C19-C20 |
| 18         | U            | 4019       | BCR         | C7-C8-C9-C34    |
| 18         | V            | 4021       | BCR         | C7-C8-C9-C34    |
| 18         | a            | 4001       | BCR         | C7-C8-C9-C34    |
| 18         | a            | 4004       | BCR         | C37-C22-C23-C24 |
| 18         | a            | 4005       | BCR         | C37-C22-C23-C24 |
| 18         | a            | 4006       | BCR         | C37-C22-C23-C24 |
| 18         | b            | 4004       | BCR         | C7-C8-C9-C34    |
| 18         | b            | 4005       | BCR         | C11-C12-C13-C35 |
| 18         | b            | 4006       | BCR         | C37-C22-C23-C24 |
| 18         | k            | 4001       | BCR         | C11-C12-C13-C35 |
| 18         | k            | 4001       | BCR         | C36-C18-C19-C20 |
| 18         | l            | 4019       | BCR         | C7-C8-C9-C34    |
| 18         | m            | 4021       | BCR         | C7-C8-C9-C34    |
| 18         | A            | 4001       | BCR         | C7-C8-C9-C10    |
| 18         | A            | 4004       | BCR         | C21-C22-C23-C24 |
| 18         | A            | 4005       | BCR         | C21-C22-C23-C24 |
| 18         | A            | 4006       | BCR         | C21-C22-C23-C24 |
| 18         | B            | 4004       | BCR         | C7-C8-C9-C10    |
| 18         | B            | 4006       | BCR         | C21-C22-C23-C24 |
| 18         | I            | 4018       | BCR         | C7-C8-C9-C10    |
| 18         | K            | 4001       | BCR         | C11-C12-C13-C14 |
| 18         | L            | 4019       | BCR         | C7-C8-C9-C10    |
| 18         | M            | 4021       | BCR         | C7-C8-C9-C10    |
| 18         | G            | 4001       | BCR         | C7-C8-C9-C10    |
| 18         | G            | 4004       | BCR         | C21-C22-C23-C24 |
| 18         | G            | 4005       | BCR         | C21-C22-C23-C24 |
| 18         | G            | 4006       | BCR         | C21-C22-C23-C24 |
| 18         | H            | 4004       | BCR         | C7-C8-C9-C10    |
| 18         | H            | 4006       | BCR         | C21-C22-C23-C24 |
| 18         | R            | 4018       | BCR         | C7-C8-C9-C10    |
| 18         | T            | 4001       | BCR         | C11-C12-C13-C14 |
| 18         | U            | 4019       | BCR         | C7-C8-C9-C10    |
| 18         | V            | 4021       | BCR         | C7-C8-C9-C10    |
| 18         | a            | 4001       | BCR         | C7-C8-C9-C10    |
| 18         | a            | 4004       | BCR         | C21-C22-C23-C24 |
| 18         | a            | 4005       | BCR         | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 4006 | BCR  | C21-C22-C23-C24 |
| 18  | b     | 4004 | BCR  | C7-C8-C9-C10    |
| 18  | b     | 4006 | BCR  | C21-C22-C23-C24 |
| 18  | i     | 4018 | BCR  | C7-C8-C9-C10    |
| 18  | k     | 4001 | BCR  | C11-C12-C13-C14 |
| 18  | l     | 4019 | BCR  | C7-C8-C9-C10    |
| 18  | m     | 4021 | BCR  | C7-C8-C9-C10    |
| 15  | B     | 1219 | F6C  | O1A-CGA-O2A-C1  |
| 15  | H     | 1219 | F6C  | O1A-CGA-O2A-C1  |
| 15  | b     | 1219 | F6C  | O1A-CGA-O2A-C1  |
| 14  | B     | 1021 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1216 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1239 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1123 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1021 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1216 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1220 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1239 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1021 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1216 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1239 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1105 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1130 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1105 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1105 | CLA  | O1D-CGD-O2D-CED |
| 20  | I     | 5006 | LMG  | O6-C5-C6-O5     |
| 20  | R     | 5006 | LMG  | O6-C5-C6-O5     |
| 20  | i     | 5006 | LMG  | O6-C5-C6-O5     |
| 21  | B     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 21  | H     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 21  | b     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 21  | I     | 6001 | LMT  | C4'-C5'-C6'-O6' |
| 21  | R     | 6001 | LMT  | C4'-C5'-C6'-O6' |
| 21  | i     | 6001 | LMT  | C4'-C5'-C6'-O6' |
| 14  | G     | 1130 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1130 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1112 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1131 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1234 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1112 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1131 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1234 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1112 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1131 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1234 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1104 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1123 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1126 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1128 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1133 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1133 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1140 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1205 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1211 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1220 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1220 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1224 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1234 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1234 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1104 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1125 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1126 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1128 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1133 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1133 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1140 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1205 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1211 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1220 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1224 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1234 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1234 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 1104 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1123 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1126 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1128 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1133 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1133 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1140 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1205 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1211 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1220 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1220 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1224 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1234 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1234 | CLA  | C15-C16-C17-C18 |
| 15  | B     | 1207 | F6C  | C13-C15-C16-C17 |
| 15  | B     | 1237 | F6C  | C8-C10-C11-C12  |
| 15  | H     | 1207 | F6C  | C13-C15-C16-C17 |
| 15  | H     | 1237 | F6C  | C8-C10-C11-C12  |
| 15  | b     | 1207 | F6C  | C13-C15-C16-C17 |
| 15  | b     | 1237 | F6C  | C8-C10-C11-C12  |
| 16  | A     | 2001 | PQN  | C18-C20-C21-C22 |
| 16  | G     | 2001 | PQN  | C18-C20-C21-C22 |
| 16  | a     | 2001 | PQN  | C18-C20-C21-C22 |
| 21  | A     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 21  | A     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 21  | G     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 21  | G     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 21  | a     | 6001 | LMT  | O5'-C5'-C6'-O6' |
| 21  | a     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 19  | A     | 5002 | LHG  | C23-C24-C25-C26 |
| 19  | G     | 5002 | LHG  | C23-C24-C25-C26 |
| 19  | a     | 5002 | LHG  | C23-C24-C25-C26 |
| 14  | B     | 1201 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1201 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1201 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1109 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1119 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1123 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1125 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1208 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1215 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1221 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1224 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1229 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1235 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1109 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1119 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1123 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1208 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1215 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1221 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1224 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1229 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1235 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1109 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1119 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1123 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1125 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1208 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1215 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1221 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1224 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1229 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1235 | CLA  | C10-C11-C12-C13 |
| 15  | B     | 1237 | F6C  | C13-C15-C16-C17 |
| 15  | H     | 1237 | F6C  | C13-C15-C16-C17 |
| 15  | b     | 1237 | F6C  | C13-C15-C16-C17 |
| 19  | L     | 5101 | LHG  | C7-C8-C9-C10    |
| 19  | U     | 5101 | LHG  | C7-C8-C9-C10    |
| 19  | l     | 5101 | LHG  | C7-C8-C9-C10    |
| 20  | B     | 5002 | LMG  | C10-C11-C12-C13 |
| 20  | I     | 5006 | LMG  | C10-C11-C12-C13 |
| 20  | H     | 5002 | LMG  | C10-C11-C12-C13 |
| 20  | R     | 5006 | LMG  | C10-C11-C12-C13 |
| 20  | b     | 5002 | LMG  | C10-C11-C12-C13 |
| 20  | i     | 5006 | LMG  | C10-C11-C12-C13 |
| 14  | A     | 1127 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1222 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1127 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1222 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1127 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1222 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1106 | CLA  | CBA-CGA-O2A-C1  |
| 14  | M     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1106 | CLA  | CBA-CGA-O2A-C1  |
| 14  | V     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1106 | CLA  | CBA-CGA-O2A-C1  |
| 14  | m     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | H     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | b     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 14  | A     | 1128 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1136 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1140 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1128 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1136 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1140 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1128 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1136 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1140 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1109 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1122 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1109 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1122 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1109 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1122 | CLA  | C5-C6-C7-C8     |
| 19  | A     | 5001 | LHG  | C23-C24-C25-C26 |
| 19  | G     | 5001 | LHG  | C23-C24-C25-C26 |
| 19  | a     | 5001 | LHG  | C23-C24-C25-C26 |
| 14  | B     | 1222 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1222 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 1222 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 1109 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1109 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1109 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1140 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1140 | CLA  | O1D-CGD-O2D-CED |
| 13  | A     | 1011 | CL0  | C11-C12-C13-C15 |
| 13  | G     | 1011 | CL0  | C11-C12-C13-C15 |
| 13  | a     | 1011 | CL0  | C11-C12-C13-C15 |
| 14  | A     | 1104 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 1117 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 1136 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1206 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1206 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1206 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1223 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1104 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 1117 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1136 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1206 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1206 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1206 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1223 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1104 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 1117 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1136 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1206 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1206 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1206 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1223 | CLA  | C6-C7-C8-C10    |
| 15  | B     | 1207 | F6C  | C6-C7-C8-C10    |
| 15  | H     | 1207 | F6C  | C6-C7-C8-C10    |
| 15  | b     | 1207 | F6C  | C6-C7-C8-C10    |
| 14  | A     | 1104 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1116 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1104 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1116 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1104 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1116 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 6003 | LMT  | O1'-C1-C2-C3    |
| 21  | G     | 6003 | LMT  | O1'-C1-C2-C3    |
| 21  | a     | 6003 | LMT  | O1'-C1-C2-C3    |
| 18  | K     | 4001 | BCR  | C9-C10-C11-C12  |
| 18  | T     | 4001 | BCR  | C9-C10-C11-C12  |
| 18  | k     | 4001 | BCR  | C9-C10-C11-C12  |
| 14  | A     | 1111 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1133 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1135 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1111 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1133 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1135 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1111 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1133 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1135 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1109 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1109 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1109 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1140 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1106 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1201 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1216 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1231 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1239 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1106 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1201 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1216 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1231 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1239 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1106 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1201 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1210 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1216 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1231 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1239 | CLA  | C13-C15-C16-C17 |
| 15  | B     | 1207 | F6C  | C15-C16-C17-C18 |
| 16  | A     | 2001 | PQN  | C15-C16-C17-C18 |
| 16  | G     | 2001 | PQN  | C15-C16-C17-C18 |
| 16  | a     | 2001 | PQN  | C15-C16-C17-C18 |
| 19  | L     | 5101 | LHG  | C11-C10-C9-C8   |
| 19  | U     | 5101 | LHG  | C11-C10-C9-C8   |
| 19  | l     | 5101 | LHG  | C11-C10-C9-C8   |
| 21  | A     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 21  | G     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 21  | a     | 6004 | LMT  | O5'-C5'-C6'-O6' |
| 14  | B     | 1210 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1210 | CLA  | C10-C11-C12-C13 |
| 15  | H     | 1207 | F6C  | C15-C16-C17-C18 |
| 15  | b     | 1207 | F6C  | C15-C16-C17-C18 |
| 14  | A     | 1133 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1133 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1133 | CLA  | O1D-CGD-O2D-CED |
| 21  | M     | 6000 | LMT  | O1'-C1-C2-C3    |
| 21  | V     | 6000 | LMT  | O1'-C1-C2-C3    |
| 21  | m     | 6000 | LMT  | O1'-C1-C2-C3    |
| 18  | A     | 4005 | BCR  | C10-C11-C12-C13 |
| 18  | A     | 4006 | BCR  | C10-C11-C12-C13 |
| 18  | B     | 4014 | BCR  | C10-C11-C12-C13 |
| 18  | L     | 4019 | BCR  | C18-C19-C20-C21 |
| 18  | G     | 4005 | BCR  | C10-C11-C12-C13 |
| 18  | G     | 4006 | BCR  | C10-C11-C12-C13 |
| 18  | U     | 4019 | BCR  | C18-C19-C20-C21 |
| 18  | a     | 4005 | BCR  | C10-C11-C12-C13 |
| 18  | a     | 4006 | BCR  | C10-C11-C12-C13 |
| 18  | b     | 4014 | BCR  | C10-C11-C12-C13 |
| 18  | l     | 4019 | BCR  | C18-C19-C20-C21 |
| 14  | b     | 1212 | CLA  | O1D-CGD-O2D-CED |
| 21  | A     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | G     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 21  | a     | 6002 | LMT  | O5'-C5'-C6'-O6' |
| 14  | A     | 1104 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1115 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1117 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1104 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1115 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1117 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1104 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1115 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1117 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1212 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1212 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1112 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1112 | CLA  | O1A-CGA-O2A-C1  |
| 21  | L     | 6001 | LMT  | O1'-C1-C2-C3    |
| 21  | U     | 6001 | LMT  | O1'-C1-C2-C3    |
| 21  | l     | 6001 | LMT  | O1'-C1-C2-C3    |
| 14  | A     | 1104 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 1117 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1119 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1205 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1208 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1211 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1211 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1222 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1234 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1240 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1104 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1117 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1119 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1205 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1208 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1211 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1211 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1222 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1234 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1240 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1104 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 1117 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1119 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1205 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1208 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1211 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1211 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1211 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1222 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1234 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1240 | CLA  | C5-C6-C7-C8     |
| 15  | B     | 1219 | F6C  | C5-C6-C7-C8     |
| 15  | H     | 1219 | F6C  | C5-C6-C7-C8     |
| 15  | b     | 1219 | F6C  | C5-C6-C7-C8     |
| 21  | L     | 6101 | LMT  | O1'-C1-C2-C3    |
| 21  | U     | 6101 | LMT  | O1'-C1-C2-C3    |
| 21  | l     | 6101 | LMT  | O1'-C1-C2-C3    |
| 21  | A     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 21  | G     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 21  | a     | 6003 | LMT  | O5B-C5B-C6B-O6B |
| 14  | B     | 1202 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1202 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1202 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1131 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1131 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1112 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1131 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1225 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1225 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1103 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1211 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1216 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1226 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1229 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1103 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1211 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1216 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1226 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1229 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1103 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1216 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1226 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1229 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 5001 | LHG  | C4-O6-P-O3      |
| 19  | L     | 5102 | LHG  | C3-O3-P-O6      |
| 19  | G     | 5001 | LHG  | C4-O6-P-O3      |
| 19  | U     | 5102 | LHG  | C3-O3-P-O6      |
| 19  | a     | 5001 | LHG  | C4-O6-P-O3      |
| 19  | l     | 5102 | LHG  | C3-O3-P-O6      |
| 14  | H     | 1225 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1237 | F6C  | O1D-CGD-O2D-CED |
| 15  | H     | 1237 | F6C  | O1D-CGD-O2D-CED |
| 15  | b     | 1237 | F6C  | O1D-CGD-O2D-CED |
| 14  | B     | 1022 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1022 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1022 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1234 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1234 | CLA  | O1A-CGA-O2A-C1  |
| 21  | I     | 6001 | LMT  | O1'-C1-C2-C3    |
| 21  | R     | 6001 | LMT  | O1'-C1-C2-C3    |
| 21  | i     | 6001 | LMT  | O1'-C1-C2-C3    |
| 14  | B     | 1214 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1214 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1214 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1234 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1140 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1228 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1140 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1228 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1140 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1228 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1111 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1111 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1111 | CLA  | C11-C12-C13-C14 |
| 21  | L     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 21  | U     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 21  | l     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 19  | L     | 5101 | LHG  | C8-C7-O7-C5     |
| 19  | U     | 5101 | LHG  | C8-C7-O7-C5     |
| 19  | l     | 5101 | LHG  | C8-C7-O7-C5     |
| 18  | L     | 4019 | BCR  | C11-C10-C9-C34  |
| 18  | U     | 4019 | BCR  | C11-C10-C9-C34  |
| 18  | l     | 4019 | BCR  | C11-C10-C9-C34  |
| 19  | A     | 5001 | LHG  | C11-C10-C9-C8   |
| 19  | L     | 5102 | LHG  | C13-C14-C15-C16 |
| 19  | G     | 5001 | LHG  | C11-C10-C9-C8   |
| 19  | U     | 5102 | LHG  | C13-C14-C15-C16 |
| 19  | a     | 5001 | LHG  | C11-C10-C9-C8   |
| 19  | l     | 5102 | LHG  | C13-C14-C15-C16 |
| 21  | I     | 6001 | LMT  | C6-C7-C8-C9     |
| 21  | i     | 6001 | LMT  | C6-C7-C8-C9     |
| 14  | A     | 1141 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1204 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1141 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1204 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1141 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1204 | CLA  | O1D-CGD-O2D-CED |
| 13  | A     | 1011 | CL0  | C16-C17-C18-C20 |
| 13  | G     | 1011 | CL0  | C16-C17-C18-C20 |
| 13  | a     | 1011 | CL0  | C16-C17-C18-C20 |
| 14  | G     | 1117 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1117 | CLA  | C16-C17-C18-C19 |
| 19  | l     | 5102 | LHG  | C12-C13-C14-C15 |
| 21  | R     | 6001 | LMT  | C6-C7-C8-C9     |
| 19  | L     | 5101 | LHG  | O9-C7-O7-C5     |
| 19  | U     | 5101 | LHG  | O9-C7-O7-C5     |
| 19  | l     | 5101 | LHG  | O9-C7-O7-C5     |
| 14  | B     | 1240 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1240 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1240 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 5002 | LHG  | C28-C29-C30-C31 |
| 19  | L     | 5102 | LHG  | C11-C12-C13-C14 |
| 19  | L     | 5102 | LHG  | C12-C13-C14-C15 |
| 19  | G     | 5002 | LHG  | C28-C29-C30-C31 |
| 19  | U     | 5102 | LHG  | C11-C12-C13-C14 |
| 19  | U     | 5102 | LHG  | C12-C13-C14-C15 |
| 19  | a     | 5002 | LHG  | C28-C29-C30-C31 |
| 19  | l     | 5102 | LHG  | C11-C12-C13-C14 |
| 19  | L     | 5101 | LHG  | C26-C27-C28-C29 |
| 19  | U     | 5101 | LHG  | C26-C27-C28-C29 |
| 14  | A     | 1117 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1117 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1117 | CLA  | C13-C15-C16-C17 |
| 19  | l     | 5101 | LHG  | C26-C27-C28-C29 |
| 18  | I     | 4020 | BCR  | C11-C10-C9-C8   |
| 18  | L     | 4019 | BCR  | C11-C10-C9-C8   |
| 18  | R     | 4020 | BCR  | C11-C10-C9-C8   |
| 18  | U     | 4019 | BCR  | C11-C10-C9-C8   |
| 18  | i     | 4020 | BCR  | C11-C10-C9-C8   |
| 18  | l     | 4019 | BCR  | C11-C10-C9-C8   |
| 14  | B     | 1231 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1231 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1231 | CLA  | CBA-CGA-O2A-C1  |
| 16  | A     | 2001 | PQN  | C20-C21-C22-C23 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 16  | G     | 2001 | PQN  | C20-C21-C22-C23 |
| 16  | a     | 2001 | PQN  | C20-C21-C22-C23 |
| 14  | M     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 14  | V     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 14  | m     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1117 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 1118 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1201 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1211 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1225 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1235 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1240 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1118 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1201 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1211 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1221 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1225 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1235 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1240 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1118 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1201 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1211 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1225 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1235 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1240 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1205 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1205 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1205 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1240 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1240 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1240 | CLA  | C4-C3-C5-C6     |
| 19  | L     | 5102 | LHG  | C26-C27-C28-C29 |
| 19  | U     | 5102 | LHG  | C26-C27-C28-C29 |
| 19  | l     | 5102 | LHG  | C26-C27-C28-C29 |
| 20  | A     | 5003 | LMG  | C29-C30-C31-C32 |
| 20  | A     | 5003 | LMG  | C30-C31-C32-C33 |
| 20  | G     | 5003 | LMG  | C29-C30-C31-C32 |
| 20  | a     | 5003 | LMG  | C29-C30-C31-C32 |
| 20  | a     | 5003 | LMG  | C30-C31-C32-C33 |
| 14  | A     | 1109 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1023 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1202 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1215 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1109 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1023 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1202 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1215 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1109 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1023 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1202 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1215 | CLA  | C6-C7-C8-C9     |
| 19  | A     | 5002 | LHG  | C33-C34-C35-C36 |
| 19  | G     | 5002 | LHG  | C33-C34-C35-C36 |
| 19  | a     | 5002 | LHG  | C33-C34-C35-C36 |
| 20  | G     | 5003 | LMG  | C30-C31-C32-C33 |
| 14  | A     | 1012 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1132 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1214 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1012 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1132 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1214 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1012 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1132 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1214 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1106 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1106 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1106 | CLA  | O1A-CGA-O2A-C1  |
| 19  | A     | 5001 | LHG  | O1-C1-C2-C3     |
| 19  | G     | 5001 | LHG  | O1-C1-C2-C3     |
| 19  | a     | 5001 | LHG  | O1-C1-C2-C3     |
| 18  | A     | 4006 | BCR  | C17-C18-C19-C20 |
| 18  | B     | 4014 | BCR  | C21-C22-C23-C24 |
| 18  | G     | 4006 | BCR  | C17-C18-C19-C20 |
| 18  | H     | 4014 | BCR  | C21-C22-C23-C24 |
| 18  | b     | 4014 | BCR  | C21-C22-C23-C24 |
| 20  | I     | 5006 | LMG  | O9-C10-O7-C8    |
| 20  | R     | 5006 | LMG  | O9-C10-O7-C8    |
| 20  | i     | 5006 | LMG  | O9-C10-O7-C8    |
| 14  | A     | 1138 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1223 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1138 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1223 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1138 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1223 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | I     | 5006 | LMG  | C11-C10-O7-C8   |
| 20  | R     | 5006 | LMG  | C11-C10-O7-C8   |
| 20  | i     | 5006 | LMG  | C11-C10-O7-C8   |
| 19  | L     | 5102 | LHG  | C7-C8-C9-C10    |
| 19  | U     | 5102 | LHG  | C7-C8-C9-C10    |
| 19  | l     | 5102 | LHG  | C7-C8-C9-C10    |
| 14  | L     | 1503 | CLA  | O1D-CGD-O2D-CED |
| 14  | U     | 1503 | CLA  | O1D-CGD-O2D-CED |
| 14  | l     | 1503 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 5002 | LHG  | C13-C14-C15-C16 |
| 19  | G     | 5002 | LHG  | C13-C14-C15-C16 |
| 19  | a     | 5002 | LHG  | C13-C14-C15-C16 |
| 21  | M     | 6000 | LMT  | C3-C4-C5-C6     |
| 21  | V     | 6000 | LMT  | C3-C4-C5-C6     |
| 21  | m     | 6000 | LMT  | C3-C4-C5-C6     |
| 13  | A     | 1011 | CL0  | C16-C17-C18-C19 |
| 13  | G     | 1011 | CL0  | C16-C17-C18-C19 |
| 13  | a     | 1011 | CL0  | C16-C17-C18-C19 |
| 14  | A     | 1112 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1112 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1211 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1221 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1221 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1224 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1112 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1112 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1211 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1221 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1224 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1112 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1112 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1211 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1221 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1221 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1224 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 1127 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1225 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1127 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1225 | CLA  | C5-C6-C7-C8     |
| 14  | U     | 1501 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1220 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1225 | CLA  | C5-C6-C7-C8     |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 19         | A            | 5001       | LHG         | C29-C30-C31-C32 |
| 19         | G            | 5001       | LHG         | C29-C30-C31-C32 |
| 19         | a            | 5001       | LHG         | C29-C30-C31-C32 |
| 14         | B            | 1206       | CLA         | C5-C6-C7-C8     |
| 14         | B            | 1220       | CLA         | C15-C16-C17-C18 |
| 14         | L            | 1501       | CLA         | C10-C11-C12-C13 |
| 14         | H            | 1206       | CLA         | C5-C6-C7-C8     |
| 14         | H            | 1220       | CLA         | C15-C16-C17-C18 |
| 14         | a            | 1127       | CLA         | C13-C15-C16-C17 |
| 14         | b            | 1206       | CLA         | C5-C6-C7-C8     |
| 14         | l            | 1501       | CLA         | C10-C11-C12-C13 |
| 21         | B            | 6001       | LMT         | C4-C5-C6-C7     |
| 21         | H            | 6001       | LMT         | C4-C5-C6-C7     |
| 21         | b            | 6001       | LMT         | C4-C5-C6-C7     |
| 14         | B            | 1228       | CLA         | C3-C5-C6-C7     |
| 14         | H            | 1228       | CLA         | C3-C5-C6-C7     |
| 14         | b            | 1228       | CLA         | C3-C5-C6-C7     |
| 14         | L            | 1502       | CLA         | CBA-CGA-O2A-C1  |
| 14         | U            | 1502       | CLA         | CBA-CGA-O2A-C1  |
| 14         | l            | 1502       | CLA         | CBA-CGA-O2A-C1  |
| 14         | H            | 1216       | CLA         | O1D-CGD-O2D-CED |
| 14         | b            | 1216       | CLA         | O1D-CGD-O2D-CED |
| 14         | A            | 1012       | CLA         | C3A-C2A-CAA-CBA |
| 14         | A            | 1103       | CLA         | C3A-C2A-CAA-CBA |
| 14         | A            | 1112       | CLA         | C3A-C2A-CAA-CBA |
| 14         | A            | 1115       | CLA         | C3A-C2A-CAA-CBA |
| 14         | B            | 1236       | CLA         | C3A-C2A-CAA-CBA |
| 14         | G            | 1012       | CLA         | C3A-C2A-CAA-CBA |
| 14         | G            | 1103       | CLA         | C3A-C2A-CAA-CBA |
| 14         | G            | 1112       | CLA         | C3A-C2A-CAA-CBA |
| 14         | G            | 1115       | CLA         | C3A-C2A-CAA-CBA |
| 14         | H            | 1236       | CLA         | C3A-C2A-CAA-CBA |
| 14         | a            | 1012       | CLA         | C3A-C2A-CAA-CBA |
| 14         | a            | 1103       | CLA         | C3A-C2A-CAA-CBA |
| 14         | a            | 1112       | CLA         | C3A-C2A-CAA-CBA |
| 14         | a            | 1115       | CLA         | C3A-C2A-CAA-CBA |
| 14         | b            | 1236       | CLA         | C3A-C2A-CAA-CBA |
| 18         | A            | 4006       | BCR         | C19-C20-C21-C22 |
| 18         | G            | 4006       | BCR         | C19-C20-C21-C22 |
| 18         | a            | 4006       | BCR         | C19-C20-C21-C22 |
| 14         | B            | 1216       | CLA         | O1D-CGD-O2D-CED |
| 14         | B            | 1201       | CLA         | C16-C17-C18-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1204 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1225 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1226 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1201 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1204 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1225 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1226 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1201 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1204 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1225 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1226 | CLA  | C16-C17-C18-C20 |
| 21  | I     | 6001 | LMT  | C5-C6-C7-C8     |
| 21  | R     | 6001 | LMT  | C5-C6-C7-C8     |
| 21  | i     | 6001 | LMT  | C5-C6-C7-C8     |
| 14  | B     | 1214 | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 1231 | CLA  | O2A-C1-C2-C3    |
| 14  | H     | 1214 | CLA  | O2A-C1-C2-C3    |
| 14  | H     | 1231 | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 1214 | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 1231 | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 1240 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1240 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1240 | CLA  | C2-C3-C5-C6     |
| 19  | A     | 5001 | LHG  | C8-C7-O7-C5     |
| 19  | G     | 5001 | LHG  | C8-C7-O7-C5     |
| 19  | a     | 5001 | LHG  | C8-C7-O7-C5     |
| 14  | A     | 1120 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1120 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1120 | CLA  | C2A-CAA-CBA-CGA |
| 19  | L     | 5102 | LHG  | O1-C1-C2-O2     |
| 19  | U     | 5102 | LHG  | O1-C1-C2-O2     |
| 19  | l     | 5102 | LHG  | O1-C1-C2-O2     |
| 19  | L     | 5102 | LHG  | C28-C29-C30-C31 |
| 19  | U     | 5102 | LHG  | C28-C29-C30-C31 |
| 19  | l     | 5102 | LHG  | C28-C29-C30-C31 |
| 14  | A     | 1111 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1111 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1111 | CLA  | C11-C12-C13-C15 |
| 20  | B     | 5002 | LMG  | C12-C13-C14-C15 |
| 20  | H     | 5002 | LMG  | C12-C13-C14-C15 |
| 20  | b     | 5002 | LMG  | C12-C13-C14-C15 |
| 19  | A     | 5001 | LHG  | O9-C7-O7-C5     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | G     | 5001 | LHG  | O9-C7-O7-C5     |
| 19  | a     | 5001 | LHG  | O9-C7-O7-C5     |
| 21  | A     | 6004 | LMT  | C1-C2-C3-C4     |
| 21  | G     | 6004 | LMT  | C1-C2-C3-C4     |
| 21  | a     | 6004 | LMT  | C1-C2-C3-C4     |
| 14  | B     | 1210 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1228 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1239 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1210 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1228 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1239 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1210 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1228 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1239 | CLA  | C2-C1-O2A-CGA   |
| 20  | A     | 5003 | LMG  | C36-C37-C38-C39 |
| 20  | I     | 5006 | LMG  | C11-C12-C13-C14 |
| 20  | G     | 5003 | LMG  | C36-C37-C38-C39 |
| 20  | R     | 5006 | LMG  | C11-C12-C13-C14 |
| 20  | a     | 5003 | LMG  | C36-C37-C38-C39 |
| 20  | i     | 5006 | LMG  | C11-C12-C13-C14 |
| 14  | B     | 1231 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1236 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1231 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1236 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1231 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1236 | CLA  | C5-C6-C7-C8     |
| 15  | B     | 1207 | F6C  | C5-C6-C7-C8     |
| 15  | H     | 1207 | F6C  | C5-C6-C7-C8     |
| 15  | b     | 1207 | F6C  | C5-C6-C7-C8     |
| 16  | B     | 2002 | PQN  | C25-C26-C27-C28 |
| 16  | H     | 2002 | PQN  | C25-C26-C27-C28 |
| 16  | b     | 2002 | PQN  | C25-C26-C27-C28 |
| 18  | A     | 4001 | BCR  | C1-C6-C7-C8     |
| 18  | A     | 4001 | BCR  | C5-C6-C7-C8     |
| 18  | A     | 4002 | BCR  | C23-C24-C25-C26 |
| 18  | A     | 4003 | BCR  | C1-C6-C7-C8     |
| 18  | A     | 4003 | BCR  | C5-C6-C7-C8     |
| 18  | A     | 4005 | BCR  | C1-C6-C7-C8     |
| 18  | A     | 4005 | BCR  | C5-C6-C7-C8     |
| 18  | A     | 4006 | BCR  | C23-C24-C25-C26 |
| 18  | A     | 4006 | BCR  | C23-C24-C25-C30 |
| 18  | B     | 4004 | BCR  | C23-C24-C25-C26 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 18         | B            | 4006       | BCR         | C1-C6-C7-C8     |
| 18         | B            | 4006       | BCR         | C5-C6-C7-C8     |
| 18         | B            | 4006       | BCR         | C23-C24-C25-C26 |
| 18         | B            | 4006       | BCR         | C23-C24-C25-C30 |
| 18         | B            | 4009       | BCR         | C1-C6-C7-C8     |
| 18         | B            | 4010       | BCR         | C23-C24-C25-C26 |
| 18         | B            | 4017       | BCR         | C1-C6-C7-C8     |
| 18         | B            | 4017       | BCR         | C5-C6-C7-C8     |
| 18         | B            | 4017       | BCR         | C23-C24-C25-C26 |
| 18         | B            | 4017       | BCR         | C23-C24-C25-C30 |
| 18         | I            | 4018       | BCR         | C5-C6-C7-C8     |
| 18         | I            | 4020       | BCR         | C23-C24-C25-C26 |
| 18         | I            | 4020       | BCR         | C23-C24-C25-C30 |
| 18         | K            | 4001       | BCR         | C1-C6-C7-C8     |
| 18         | K            | 4001       | BCR         | C5-C6-C7-C8     |
| 18         | K            | 4001       | BCR         | C23-C24-C25-C26 |
| 18         | L            | 4019       | BCR         | C5-C6-C7-C8     |
| 18         | M            | 4021       | BCR         | C5-C6-C7-C8     |
| 18         | M            | 4021       | BCR         | C23-C24-C25-C26 |
| 18         | M            | 4021       | BCR         | C23-C24-C25-C30 |
| 18         | G            | 4001       | BCR         | C1-C6-C7-C8     |
| 18         | G            | 4001       | BCR         | C5-C6-C7-C8     |
| 18         | G            | 4002       | BCR         | C23-C24-C25-C26 |
| 18         | G            | 4003       | BCR         | C1-C6-C7-C8     |
| 18         | G            | 4003       | BCR         | C5-C6-C7-C8     |
| 18         | G            | 4005       | BCR         | C1-C6-C7-C8     |
| 18         | G            | 4005       | BCR         | C5-C6-C7-C8     |
| 18         | G            | 4006       | BCR         | C23-C24-C25-C26 |
| 18         | G            | 4006       | BCR         | C23-C24-C25-C30 |
| 18         | H            | 4004       | BCR         | C23-C24-C25-C26 |
| 18         | H            | 4006       | BCR         | C1-C6-C7-C8     |
| 18         | H            | 4006       | BCR         | C5-C6-C7-C8     |
| 18         | H            | 4006       | BCR         | C23-C24-C25-C26 |
| 18         | H            | 4006       | BCR         | C23-C24-C25-C30 |
| 18         | H            | 4009       | BCR         | C1-C6-C7-C8     |
| 18         | H            | 4010       | BCR         | C23-C24-C25-C26 |
| 18         | H            | 4017       | BCR         | C1-C6-C7-C8     |
| 18         | H            | 4017       | BCR         | C5-C6-C7-C8     |
| 18         | H            | 4017       | BCR         | C23-C24-C25-C26 |
| 18         | H            | 4017       | BCR         | C23-C24-C25-C30 |
| 18         | R            | 4018       | BCR         | C5-C6-C7-C8     |
| 18         | R            | 4020       | BCR         | C23-C24-C25-C26 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | R     | 4020 | BCR  | C23-C24-C25-C30 |
| 18  | T     | 4001 | BCR  | C1-C6-C7-C8     |
| 18  | T     | 4001 | BCR  | C5-C6-C7-C8     |
| 18  | T     | 4001 | BCR  | C23-C24-C25-C26 |
| 18  | U     | 4019 | BCR  | C5-C6-C7-C8     |
| 18  | V     | 4021 | BCR  | C5-C6-C7-C8     |
| 18  | V     | 4021 | BCR  | C23-C24-C25-C26 |
| 18  | V     | 4021 | BCR  | C23-C24-C25-C30 |
| 18  | a     | 4001 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4001 | BCR  | C5-C6-C7-C8     |
| 18  | a     | 4001 | BCR  | C23-C24-C25-C26 |
| 18  | a     | 4002 | BCR  | C23-C24-C25-C26 |
| 18  | a     | 4003 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4003 | BCR  | C5-C6-C7-C8     |
| 18  | a     | 4005 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4005 | BCR  | C5-C6-C7-C8     |
| 18  | a     | 4006 | BCR  | C23-C24-C25-C26 |
| 18  | a     | 4006 | BCR  | C23-C24-C25-C30 |
| 18  | b     | 4004 | BCR  | C23-C24-C25-C26 |
| 18  | b     | 4006 | BCR  | C1-C6-C7-C8     |
| 18  | b     | 4006 | BCR  | C5-C6-C7-C8     |
| 18  | b     | 4006 | BCR  | C23-C24-C25-C26 |
| 18  | b     | 4006 | BCR  | C23-C24-C25-C30 |
| 18  | b     | 4009 | BCR  | C1-C6-C7-C8     |
| 18  | b     | 4010 | BCR  | C23-C24-C25-C26 |
| 18  | b     | 4017 | BCR  | C1-C6-C7-C8     |
| 18  | b     | 4017 | BCR  | C5-C6-C7-C8     |
| 18  | b     | 4017 | BCR  | C23-C24-C25-C26 |
| 18  | b     | 4017 | BCR  | C23-C24-C25-C30 |
| 18  | i     | 4018 | BCR  | C5-C6-C7-C8     |
| 18  | i     | 4020 | BCR  | C23-C24-C25-C26 |
| 18  | i     | 4020 | BCR  | C23-C24-C25-C30 |
| 18  | k     | 4001 | BCR  | C1-C6-C7-C8     |
| 18  | k     | 4001 | BCR  | C5-C6-C7-C8     |
| 18  | k     | 4001 | BCR  | C23-C24-C25-C26 |
| 18  | l     | 4019 | BCR  | C5-C6-C7-C8     |
| 18  | m     | 4021 | BCR  | C5-C6-C7-C8     |
| 18  | m     | 4021 | BCR  | C23-C24-C25-C26 |
| 18  | m     | 4021 | BCR  | C23-C24-C25-C30 |
| 14  | A     | 1115 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1115 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1115 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1136 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1021 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1203 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1226 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1136 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1021 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1203 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1226 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1136 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1021 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1203 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1226 | CLA  | C13-C15-C16-C17 |
| 19  | G     | 5002 | LHG  | C18-C19-C20-C21 |
| 19  | a     | 5002 | LHG  | C18-C19-C20-C21 |
| 14  | B     | 1205 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1205 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1205 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 5002 | LHG  | C18-C19-C20-C21 |
| 21  | I     | 6001 | LMT  | C4-C5-C6-C7     |
| 21  | R     | 6001 | LMT  | C4-C5-C6-C7     |
| 21  | i     | 6001 | LMT  | C4-C5-C6-C7     |
| 14  | A     | 1112 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1225 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1112 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1225 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1112 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1225 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1109 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1112 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1021 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1023 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1202 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1203 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1206 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1221 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1222 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1224 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1225 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1234 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1109 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1112 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1021 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1023 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1202 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1203 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1206 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1221 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1222 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1224 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1225 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1234 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1109 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1112 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1021 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1023 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1202 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1203 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1206 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1221 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1222 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1224 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1225 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1234 | CLA  | C6-C7-C8-C10    |
| 16  | A     | 2001 | PQN  | C17-C18-C20-C21 |
| 16  | G     | 2001 | PQN  | C17-C18-C20-C21 |
| 16  | a     | 2001 | PQN  | C17-C18-C20-C21 |
| 14  | B     | 1231 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1231 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1231 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1104 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1104 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1104 | CLA  | C13-C15-C16-C17 |
| 16  | B     | 2002 | PQN  | C15-C16-C17-C18 |
| 16  | H     | 2002 | PQN  | C15-C16-C17-C18 |
| 16  | b     | 2002 | PQN  | C15-C16-C17-C18 |
| 15  | B     | 1237 | F6C  | C1A-C2A-CAA-CBA |
| 15  | H     | 1237 | F6C  | C1A-C2A-CAA-CBA |
| 15  | b     | 1237 | F6C  | C1A-C2A-CAA-CBA |
| 14  | A     | 1116 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1235 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1116 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1235 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1116 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1235 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | A     | 5002 | LHG  | C7-C8-C9-C10    |
| 19  | G     | 5002 | LHG  | C7-C8-C9-C10    |
| 19  | a     | 5002 | LHG  | C7-C8-C9-C10    |
| 14  | A     | 1126 | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1126 | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1126 | CLA  | CBA-CGA-O2A-C1  |
| 14  | l     | 1501 | CLA  | CBA-CGA-O2A-C1  |
| 15  | B     | 1238 | F6C  | CBA-CGA-O2A-C1  |
| 15  | H     | 1238 | F6C  | CBA-CGA-O2A-C1  |
| 15  | b     | 1238 | F6C  | CBA-CGA-O2A-C1  |
| 19  | A     | 5002 | LHG  | C24-C23-O8-C6   |
| 19  | G     | 5002 | LHG  | C24-C23-O8-C6   |
| 19  | a     | 5002 | LHG  | C24-C23-O8-C6   |
| 14  | B     | 1023 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1224 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1023 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1224 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1023 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1224 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1225 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1225 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1225 | CLA  | C15-C16-C17-C18 |
| 20  | B     | 5002 | LMG  | C33-C34-C35-C36 |
| 20  | H     | 5002 | LMG  | C33-C34-C35-C36 |
| 20  | b     | 5002 | LMG  | C33-C34-C35-C36 |
| 15  | B     | 1207 | F6C  | C2B-C3B-CAB-CBB |
| 15  | H     | 1207 | F6C  | C2B-C3B-CAB-CBB |
| 15  | b     | 1207 | F6C  | C2B-C3B-CAB-CBB |
| 21  | L     | 6002 | LMT  | C4'-C5'-C6'-O6' |
| 21  | U     | 6002 | LMT  | C4'-C5'-C6'-O6' |
| 21  | B     | 6004 | LMT  | C1-C2-C3-C4     |
| 21  | H     | 6004 | LMT  | C1-C2-C3-C4     |
| 21  | b     | 6004 | LMT  | C1-C2-C3-C4     |
| 14  | B     | 1215 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1215 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1215 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1140 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1140 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1140 | CLA  | CBA-CGA-O2A-C1  |
| 21  | l     | 6002 | LMT  | C4'-C5'-C6'-O6' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1012 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1012 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 1012 | CLA  | C15-C16-C17-C18 |
| 20  | A     | 5003 | LMG  | C12-C13-C14-C15 |
| 20  | G     | 5003 | LMG  | C12-C13-C14-C15 |
| 20  | a     | 5003 | LMG  | C12-C13-C14-C15 |
| 21  | B     | 6001 | LMT  | C7-C8-C9-C10    |
| 21  | b     | 6001 | LMT  | C7-C8-C9-C10    |
| 18  | A     | 4003 | BCR  | C18-C19-C20-C21 |
| 18  | A     | 4004 | BCR  | C18-C19-C20-C21 |
| 18  | G     | 4003 | BCR  | C18-C19-C20-C21 |
| 18  | G     | 4004 | BCR  | C18-C19-C20-C21 |
| 18  | H     | 4014 | BCR  | C10-C11-C12-C13 |
| 18  | a     | 4003 | BCR  | C18-C19-C20-C21 |
| 18  | a     | 4004 | BCR  | C18-C19-C20-C21 |
| 21  | H     | 6001 | LMT  | C7-C8-C9-C10    |
| 15  | B     | 1207 | F6C  | C4B-C3B-CAB-CBB |
| 15  | B     | 1237 | F6C  | C4B-C3B-CAB-CBB |
| 15  | H     | 1207 | F6C  | C4B-C3B-CAB-CBB |
| 15  | H     | 1237 | F6C  | C4B-C3B-CAB-CBB |
| 15  | b     | 1207 | F6C  | C4B-C3B-CAB-CBB |
| 15  | b     | 1237 | F6C  | C4B-C3B-CAB-CBB |
| 14  | A     | 1113 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1113 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1113 | CLA  | CBD-CGD-O2D-CED |
| 14  | l     | 1502 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1220 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1220 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1220 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1220 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1220 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1220 | CLA  | O1D-CGD-O2D-CED |
| 20  | I     | 5006 | LMG  | C2-C1-O1-C7     |
| 20  | R     | 5006 | LMG  | C2-C1-O1-C7     |
| 20  | i     | 5006 | LMG  | C2-C1-O1-C7     |
| 19  | L     | 5101 | LHG  | O7-C5-C6-O8     |
| 19  | U     | 5101 | LHG  | O7-C5-C6-O8     |
| 19  | l     | 5101 | LHG  | O7-C5-C6-O8     |
| 19  | L     | 5102 | LHG  | C24-C23-O8-C6   |
| 19  | U     | 5102 | LHG  | C24-C23-O8-C6   |
| 19  | l     | 5102 | LHG  | C24-C23-O8-C6   |
| 14  | L     | 1502 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | U     | 1502 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1117 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1117 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1117 | CLA  | C16-C17-C18-C20 |
| 16  | B     | 2002 | PQN  | C20-C21-C22-C23 |
| 16  | H     | 2002 | PQN  | C20-C21-C22-C23 |
| 16  | b     | 2002 | PQN  | C20-C21-C22-C23 |
| 14  | A     | 1125 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1125 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1125 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1125 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1125 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1205 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1125 | CLA  | C2-C3-C5-C6     |
| 21  | A     | 6002 | LMT  | C1-C2-C3-C4     |
| 21  | G     | 6002 | LMT  | C1-C2-C3-C4     |
| 13  | A     | 1011 | CL0  | C11-C12-C13-C14 |
| 13  | G     | 1011 | CL0  | C11-C12-C13-C14 |
| 13  | a     | 1011 | CL0  | C11-C12-C13-C14 |
| 14  | A     | 1117 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1133 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1021 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1206 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1206 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1216 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1221 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1223 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1239 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1117 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1133 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1021 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1206 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1206 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1216 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1221 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1223 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1239 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1117 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1133 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1021 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1206 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1206 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1216 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1221 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1223 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1239 | CLA  | C14-C13-C15-C16 |
| 19  | A     | 5002 | LHG  | C31-C32-C33-C34 |
| 19  | G     | 5002 | LHG  | C31-C32-C33-C34 |
| 19  | a     | 5002 | LHG  | C31-C32-C33-C34 |
| 14  | A     | 1110 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1125 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1212 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1110 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1125 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1212 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1110 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1125 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1212 | CLA  | C2A-CAA-CBA-CGA |
| 21  | a     | 6002 | LMT  | C1-C2-C3-C4     |
| 19  | A     | 5001 | LHG  | C25-C26-C27-C28 |
| 19  | G     | 5001 | LHG  | C25-C26-C27-C28 |
| 19  | a     | 5001 | LHG  | C25-C26-C27-C28 |
| 21  | A     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 21  | G     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 21  | a     | 6002 | LMT  | O5B-C5B-C6B-O6B |
| 15  | B     | 1238 | F6C  | C1A-C2A-CAA-CBA |
| 15  | H     | 1238 | F6C  | C1A-C2A-CAA-CBA |
| 15  | b     | 1238 | F6C  | C1A-C2A-CAA-CBA |
| 18  | B     | 4009 | BCR  | C7-C8-C9-C34    |
| 18  | H     | 4009 | BCR  | C7-C8-C9-C34    |
| 18  | b     | 4009 | BCR  | C7-C8-C9-C34    |
| 14  | A     | 1116 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1228 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1116 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1228 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1116 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1228 | CLA  | C5-C6-C7-C8     |
| 19  | A     | 5002 | LHG  | C34-C35-C36-C37 |
| 19  | G     | 5002 | LHG  | C34-C35-C36-C37 |
| 19  | a     | 5002 | LHG  | C34-C35-C36-C37 |
| 18  | B     | 4009 | BCR  | C7-C8-C9-C10    |
| 18  | H     | 4009 | BCR  | C7-C8-C9-C10    |
| 18  | a     | 4006 | BCR  | C17-C18-C19-C20 |
| 18  | b     | 4009 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1115 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1115 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1115 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1102 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1105 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1106 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1107 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1108 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1113 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1120 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1132 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1022 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1202 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1211 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1212 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1213 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1215 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1216 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1222 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1233 | CLA  | C1A-C2A-CAA-CBA |
| 14  | M     | 1501 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1102 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1105 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1106 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1107 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1108 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1113 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1120 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1132 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1022 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1202 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1211 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1212 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1215 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1216 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1222 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1233 | CLA  | C1A-C2A-CAA-CBA |
| 14  | V     | 1501 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1102 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1105 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1106 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1107 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1108 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1113 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1120 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1132 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1022 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1202 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1211 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1212 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1213 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1215 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1216 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1222 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1233 | CLA  | C1A-C2A-CAA-CBA |
| 14  | m     | 1501 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1130 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1240 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 1130 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1240 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1130 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1240 | CLA  | C16-C17-C18-C19 |
| 20  | A     | 5003 | LMG  | O9-C10-O7-C8    |
| 20  | G     | 5003 | LMG  | O9-C10-O7-C8    |
| 20  | a     | 5003 | LMG  | O9-C10-O7-C8    |
| 20  | A     | 5003 | LMG  | C11-C10-O7-C8   |
| 20  | G     | 5003 | LMG  | C11-C10-O7-C8   |
| 20  | a     | 5003 | LMG  | C11-C10-O7-C8   |
| 18  | B     | 4004 | BCR  | C19-C20-C21-C22 |
| 18  | H     | 4004 | BCR  | C19-C20-C21-C22 |
| 18  | b     | 4004 | BCR  | C19-C20-C21-C22 |
| 14  | A     | 1136 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1136 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1136 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1136 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 1136 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1136 | CLA  | C15-C16-C17-C18 |
| 21  | M     | 6000 | LMT  | O5B-C5B-C6B-O6B |
| 14  | A     | 1117 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1117 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1117 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1136 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1136 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1136 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | I     | 6001 | LMT  | C1-C2-C3-C4     |
| 21  | R     | 6001 | LMT  | C1-C2-C3-C4     |
| 21  | i     | 6001 | LMT  | C1-C2-C3-C4     |
| 14  | B     | 1234 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1234 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1234 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1136 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1136 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1136 | CLA  | CBA-CGA-O2A-C1  |
| 21  | V     | 6000 | LMT  | O5B-C5B-C6B-O6B |
| 21  | m     | 6000 | LMT  | O5B-C5B-C6B-O6B |
| 19  | A     | 5002 | LHG  | O6-C4-C5-C6     |
| 19  | G     | 5002 | LHG  | O6-C4-C5-C6     |
| 19  | a     | 5002 | LHG  | O6-C4-C5-C6     |
| 19  | L     | 5102 | LHG  | C35-C36-C37-C38 |
| 19  | l     | 5102 | LHG  | C35-C36-C37-C38 |
| 19  | U     | 5102 | LHG  | C35-C36-C37-C38 |
| 14  | A     | 1116 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1116 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1116 | CLA  | C6-C7-C8-C10    |
| 15  | B     | 1219 | F6C  | O1D-CGD-O2D-CED |
| 15  | b     | 1219 | F6C  | O1D-CGD-O2D-CED |
| 14  | B     | 1205 | CLA  | C4-C3-C5-C6     |
| 14  | L     | 1503 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1205 | CLA  | C4-C3-C5-C6     |
| 14  | U     | 1503 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1205 | CLA  | C4-C3-C5-C6     |
| 14  | l     | 1503 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1205 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1205 | CLA  | C2-C3-C5-C6     |
| 20  | A     | 5003 | LMG  | C13-C14-C15-C16 |
| 20  | G     | 5003 | LMG  | C13-C14-C15-C16 |
| 20  | a     | 5003 | LMG  | C13-C14-C15-C16 |
| 14  | A     | 1119 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1119 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1119 | CLA  | C10-C11-C12-C13 |
| 19  | A     | 5002 | LHG  | O10-C23-O8-C6   |
| 19  | G     | 5002 | LHG  | O10-C23-O8-C6   |
| 19  | a     | 5002 | LHG  | O10-C23-O8-C6   |
| 15  | H     | 1219 | F6C  | O1D-CGD-O2D-CED |
| 14  | A     | 1013 | CLA  | C3-C5-C6-C7     |
| 19  | A     | 5001 | LHG  | C4-C5-C6-O8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | L     | 5101 | LHG  | C4-C5-C6-O8     |
| 19  | G     | 5001 | LHG  | C4-C5-C6-O8     |
| 19  | U     | 5101 | LHG  | C4-C5-C6-O8     |
| 19  | a     | 5001 | LHG  | C4-C5-C6-O8     |
| 19  | l     | 5101 | LHG  | C4-C5-C6-O8     |
| 14  | B     | 1202 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1234 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1235 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1202 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1234 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1235 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1234 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 1235 | CLA  | C5-C6-C7-C8     |
| 21  | U     | 6001 | LMT  | C9-C10-C11-C12  |
| 14  | L     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 14  | U     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 21  | L     | 6001 | LMT  | C9-C10-C11-C12  |
| 21  | l     | 6001 | LMT  | C9-C10-C11-C12  |
| 14  | b     | 1202 | CLA  | C15-C16-C17-C18 |
| 19  | L     | 5102 | LHG  | C11-C10-C9-C8   |
| 19  | U     | 5102 | LHG  | C11-C10-C9-C8   |
| 19  | l     | 5102 | LHG  | C11-C10-C9-C8   |
| 21  | L     | 6001 | LMT  | C3-C4-C5-C6     |
| 21  | l     | 6001 | LMT  | C3-C4-C5-C6     |
| 14  | l     | 1501 | CLA  | O1A-CGA-O2A-C1  |
| 21  | U     | 6001 | LMT  | C3-C4-C5-C6     |
| 14  | B     | 1229 | CLA  | C3-C5-C6-C7     |
| 14  | L     | 1503 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1013 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1229 | CLA  | C3-C5-C6-C7     |
| 14  | U     | 1503 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1013 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1229 | CLA  | C3-C5-C6-C7     |
| 14  | l     | 1503 | CLA  | C3-C5-C6-C7     |
| 19  | A     | 5001 | LHG  | C13-C14-C15-C16 |
| 19  | G     | 5001 | LHG  | C13-C14-C15-C16 |
| 19  | a     | 5001 | LHG  | C13-C14-C15-C16 |
| 21  | A     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 21  | G     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 21  | a     | 6001 | LMT  | C4B-C5B-C6B-O6B |
| 14  | A     | 1140 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1140 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | B     | 6003 | LMT  | C2B-C1B-O1B-C4' |
| 21  | H     | 6003 | LMT  | C2B-C1B-O1B-C4' |
| 21  | b     | 6003 | LMT  | C2B-C1B-O1B-C4' |
| 20  | A     | 5003 | LMG  | O6-C5-C6-O5     |
| 20  | G     | 5003 | LMG  | O6-C5-C6-O5     |
| 20  | a     | 5003 | LMG  | O6-C5-C6-O5     |
| 14  | B     | 1236 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1236 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1236 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1140 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1119 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 1119 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1119 | CLA  | C16-C17-C18-C19 |
| 21  | B     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 21  | H     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 21  | b     | 6003 | LMT  | O5'-C5'-C6'-O6' |
| 19  | U     | 5101 | LHG  | C11-C12-C13-C14 |
| 19  | L     | 5101 | LHG  | C11-C12-C13-C14 |
| 19  | L     | 5101 | LHG  | C28-C29-C30-C31 |
| 19  | U     | 5101 | LHG  | C28-C29-C30-C31 |
| 19  | l     | 5101 | LHG  | C11-C12-C13-C14 |
| 19  | l     | 5101 | LHG  | C28-C29-C30-C31 |
| 14  | A     | 1129 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1129 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1129 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1216 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1216 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1216 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1104 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1104 | CLA  | O1D-CGD-O2D-CED |
| 19  | L     | 5102 | LHG  | C34-C35-C36-C37 |
| 19  | G     | 5001 | LHG  | C14-C15-C16-C17 |
| 19  | U     | 5102 | LHG  | C34-C35-C36-C37 |
| 19  | l     | 5102 | LHG  | C34-C35-C36-C37 |
| 14  | G     | 1104 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1204 | CLA  | C15-C16-C17-C18 |
| 14  | L     | 1502 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1204 | CLA  | C15-C16-C17-C18 |
| 14  | U     | 1502 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1204 | CLA  | C15-C16-C17-C18 |
| 14  | l     | 1502 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 5001 | LHG  | C14-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | a     | 5001 | LHG  | C14-C15-C16-C17 |
| 21  | L     | 6001 | LMT  | C4-C5-C6-C7     |
| 21  | U     | 6001 | LMT  | C4-C5-C6-C7     |
| 14  | A     | 1013 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1021 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1235 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1013 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1021 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1235 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1013 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1021 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1235 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1140 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1140 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1126 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1126 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1126 | CLA  | C11-C12-C13-C15 |
| 21  | l     | 6001 | LMT  | C4-C5-C6-C7     |
| 14  | B     | 1210 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1210 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1210 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1126 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1126 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1126 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1111 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1111 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1128 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1235 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1111 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1128 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1206 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1235 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1111 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1111 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1128 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1235 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1140 | CLA  | CAA-CBA-CGA-O2A |
| 21  | L     | 6101 | LMT  | C4'-C5'-C6'-O6' |
| 21  | U     | 6101 | LMT  | C4'-C5'-C6'-O6' |
| 21  | l     | 6101 | LMT  | C4'-C5'-C6'-O6' |
| 14  | B     | 1206 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1111 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1206 | CLA  | C13-C15-C16-C17 |
| 15  | B     | 1207 | F6C  | C8-C10-C11-C12  |
| 15  | H     | 1207 | F6C  | C8-C10-C11-C12  |
| 15  | b     | 1207 | F6C  | C8-C10-C11-C12  |
| 14  | B     | 1235 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1235 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1235 | CLA  | O1A-CGA-O2A-C1  |
| 15  | B     | 1238 | F6C  | O1A-CGA-O2A-C1  |
| 15  | H     | 1238 | F6C  | O1A-CGA-O2A-C1  |
| 15  | b     | 1238 | F6C  | O1A-CGA-O2A-C1  |
| 14  | G     | 1119 | CLA  | C16-C17-C18-C20 |
| 21  | L     | 6101 | LMT  | C1-C2-C3-C4     |
| 21  | U     | 6101 | LMT  | C1-C2-C3-C4     |
| 21  | l     | 6101 | LMT  | C1-C2-C3-C4     |
| 14  | A     | 1133 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1133 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1133 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 5002 | LHG  | C25-C26-C27-C28 |
| 14  | A     | 1115 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 1117 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1128 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1133 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1133 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1208 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1211 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1216 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1216 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1231 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1240 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1115 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1117 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1128 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1133 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1133 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1208 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1211 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1216 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1216 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1231 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1240 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1115 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1117 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1128 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1133 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1133 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1208 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1211 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1216 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1216 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1231 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1240 | CLA  | C11-C12-C13-C15 |
| 15  | B     | 1237 | F6C  | C11-C12-C13-C15 |
| 15  | H     | 1237 | F6C  | C11-C12-C13-C15 |
| 15  | b     | 1237 | F6C  | C11-C12-C13-C15 |
| 19  | A     | 5002 | LHG  | C25-C26-C27-C28 |
| 19  | G     | 5002 | LHG  | C25-C26-C27-C28 |
| 20  | i     | 5006 | LMG  | C31-C32-C33-C34 |
| 21  | B     | 6001 | LMT  | C3-C4-C5-C6     |
| 21  | H     | 6001 | LMT  | C3-C4-C5-C6     |
| 21  | b     | 6001 | LMT  | C3-C4-C5-C6     |
| 14  | A     | 1104 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 1115 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1128 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1131 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1133 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1203 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1206 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1208 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1211 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1224 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1224 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1231 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1239 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1104 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1115 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1128 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1131 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1133 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1203 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1206 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1208 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1211 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1224 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1224 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1231 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1239 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1104 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1115 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1128 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1131 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1133 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1203 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1206 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1208 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1211 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1224 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1224 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1231 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1239 | CLA  | C11-C10-C8-C9   |
| 15  | B     | 1207 | F6C  | C6-C7-C8-C9     |
| 15  | H     | 1207 | F6C  | C6-C7-C8-C9     |
| 15  | b     | 1207 | F6C  | C6-C7-C8-C9     |
| 18  | b     | 4006 | BCR  | C9-C10-C11-C12  |
| 20  | I     | 5006 | LMG  | C31-C32-C33-C34 |
| 20  | R     | 5006 | LMG  | C31-C32-C33-C34 |
| 14  | A     | 1119 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1119 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1119 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 1214 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1214 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1214 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1136 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1136 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1136 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1119 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1222 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 1224 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1222 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1224 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1119 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1222 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1224 | CLA  | C16-C17-C18-C19 |
| 19  | L     | 5102 | LHG  | C33-C34-C35-C36 |
| 19  | U     | 5102 | LHG  | C33-C34-C35-C36 |
| 19  | l     | 5102 | LHG  | C33-C34-C35-C36 |
| 20  | b     | 5002 | LMG  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | B     | 5002 | LMG  | C19-C20-C21-C22 |
| 19  | A     | 5001 | LHG  | C1-C2-C3-O3     |
| 19  | G     | 5001 | LHG  | C1-C2-C3-O3     |
| 19  | a     | 5001 | LHG  | C1-C2-C3-O3     |
| 14  | B     | 1225 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1225 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1225 | CLA  | CBA-CGA-O2A-C1  |
| 20  | H     | 5002 | LMG  | C19-C20-C21-C22 |
| 14  | B     | 1211 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1211 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1211 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 5001 | LHG  | C9-C10-C11-C12  |
| 14  | L     | 1503 | CLA  | C10-C11-C12-C13 |
| 14  | U     | 1503 | CLA  | C10-C11-C12-C13 |
| 14  | l     | 1503 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1222 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 5001 | LHG  | C9-C10-C11-C12  |
| 19  | G     | 5001 | LHG  | C9-C10-C11-C12  |
| 14  | A     | 1131 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1131 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1131 | CLA  | C4-C3-C5-C6     |
| 15  | B     | 1237 | F6C  | C4-C3-C5-C6     |
| 15  | H     | 1237 | F6C  | C4-C3-C5-C6     |
| 15  | b     | 1237 | F6C  | C4-C3-C5-C6     |
| 14  | L     | 1503 | CLA  | C2-C3-C5-C6     |
| 14  | U     | 1503 | CLA  | C2-C3-C5-C6     |
| 14  | l     | 1503 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1222 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 1222 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 6003 | LMT  | C5-C6-C7-C8     |
| 21  | H     | 6003 | LMT  | C5-C6-C7-C8     |
| 21  | b     | 6003 | LMT  | C5-C6-C7-C8     |
| 14  | A     | 1102 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1119 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1127 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1133 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1140 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1227 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1231 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1233 | CLA  | C3A-C2A-CAA-CBA |
| 14  | L     | 1503 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1102 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1119 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1127 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1133 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1140 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1227 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1231 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1233 | CLA  | C3A-C2A-CAA-CBA |
| 14  | U     | 1503 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1102 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1119 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1127 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1133 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1140 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1227 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1231 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1233 | CLA  | C3A-C2A-CAA-CBA |
| 14  | l     | 1503 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1125 | CLA  | C8-C10-C11-C12  |
| 18  | B     | 4006 | BCR  | C9-C10-C11-C12  |
| 18  | K     | 4001 | BCR  | C19-C20-C21-C22 |
| 18  | H     | 4006 | BCR  | C9-C10-C11-C12  |
| 18  | T     | 4001 | BCR  | C19-C20-C21-C22 |
| 18  | k     | 4001 | BCR  | C19-C20-C21-C22 |
| 21  | A     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 21  | G     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 21  | a     | 6001 | LMT  | C2-C1-O1'-C1'   |
| 14  | A     | 1125 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1125 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1125 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1125 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1125 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 1226 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1228 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1226 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1228 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1226 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1228 | CLA  | C6-C7-C8-C10    |
| 19  | A     | 5002 | LHG  | C4-C5-C6-O8     |
| 19  | G     | 5002 | LHG  | C4-C5-C6-O8     |
| 19  | a     | 5002 | LHG  | C4-C5-C6-O8     |
| 19  | l     | 5102 | LHG  | O10-C23-O8-C6   |
| 20  | b     | 5002 | LMG  | C32-C33-C34-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1238 | F6C  | C3A-C2A-CAA-CBA |
| 15  | H     | 1238 | F6C  | C3A-C2A-CAA-CBA |
| 15  | b     | 1238 | F6C  | C3A-C2A-CAA-CBA |
| 20  | B     | 5002 | LMG  | C32-C33-C34-C35 |
| 20  | H     | 5002 | LMG  | C32-C33-C34-C35 |
| 19  | L     | 5102 | LHG  | O10-C23-O8-C6   |
| 19  | U     | 5102 | LHG  | O10-C23-O8-C6   |
| 14  | a     | 1012 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1111 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1111 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1111 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1012 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1012 | CLA  | C13-C15-C16-C17 |
| 15  | B     | 1207 | F6C  | C3B-C2B-CMB-OMB |
| 15  | B     | 1219 | F6C  | C3B-C2B-CMB-OMB |
| 15  | H     | 1207 | F6C  | C3B-C2B-CMB-OMB |
| 15  | H     | 1219 | F6C  | C3B-C2B-CMB-OMB |
| 15  | b     | 1207 | F6C  | C3B-C2B-CMB-OMB |
| 15  | b     | 1219 | F6C  | C3B-C2B-CMB-OMB |
| 14  | A     | 1109 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1109 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1109 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1021 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1021 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1021 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1118 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1126 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1204 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1118 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1126 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1204 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1118 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1126 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1204 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 1119 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1119 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1119 | CLA  | O1A-CGA-O2A-C1  |
| 19  | A     | 5001 | LHG  | O7-C5-C6-O8     |
| 19  | G     | 5001 | LHG  | O7-C5-C6-O8     |
| 19  | a     | 5001 | LHG  | O7-C5-C6-O8     |
| 13  | G     | 1011 | CL0  | C5-C6-C7-C8     |
| 13  | a     | 1011 | CL0  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1206 | CLA  | C10-C11-C12-C13 |
| 14  | K     | 1401 | CLA  | C2C-C3C-CAC-CBC |
| 14  | T     | 1401 | CLA  | C2C-C3C-CAC-CBC |
| 18  | A     | 4003 | BCR  | C19-C20-C21-C22 |
| 18  | G     | 4003 | BCR  | C19-C20-C21-C22 |
| 18  | a     | 4003 | BCR  | C19-C20-C21-C22 |
| 20  | I     | 5006 | LMG  | O6-C1-O1-C7     |
| 20  | R     | 5006 | LMG  | O6-C1-O1-C7     |
| 20  | i     | 5006 | LMG  | O6-C1-O1-C7     |
| 21  | A     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 21  | G     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 21  | a     | 6003 | LMT  | O5'-C1'-O1'-C1  |
| 13  | A     | 1011 | CL0  | C5-C6-C7-C8     |
| 14  | B     | 1206 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1206 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1109 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1111 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1133 | CLA  | C2-C1-O2A-CGA   |
| 14  | M     | 1501 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1109 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1111 | CLA  | C2-C1-O2A-CGA   |
| 14  | V     | 1501 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1109 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1111 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1133 | CLA  | C2-C1-O2A-CGA   |
| 14  | m     | 1501 | CLA  | C2-C1-O2A-CGA   |
| 15  | B     | 1237 | F6C  | C2-C1-O2A-CGA   |
| 15  | H     | 1237 | F6C  | C2-C1-O2A-CGA   |
| 15  | b     | 1237 | F6C  | C2-C1-O2A-CGA   |
| 14  | A     | 1131 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1131 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1131 | CLA  | C2-C3-C5-C6     |
| 19  | L     | 5102 | LHG  | C27-C28-C29-C30 |
| 21  | B     | 6004 | LMT  | C5'-C4'-O1B-C1B |
| 21  | H     | 6004 | LMT  | C5'-C4'-O1B-C1B |
| 21  | b     | 6004 | LMT  | C5'-C4'-O1B-C1B |
| 14  | A     | 1104 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1115 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 1104 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1115 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1104 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1115 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1201 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1226 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1234 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1201 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1226 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1234 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1201 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1226 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1234 | CLA  | C11-C12-C13-C14 |
| 14  | k     | 1401 | CLA  | C2C-C3C-CAC-CBC |
| 19  | U     | 5102 | LHG  | C27-C28-C29-C30 |
| 19  | l     | 5102 | LHG  | C27-C28-C29-C30 |
| 14  | A     | 1103 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1103 | CLA  | CBD-CGD-O2D-CED |
| 21  | B     | 6001 | LMT  | C6-C7-C8-C9     |
| 21  | H     | 6001 | LMT  | C6-C7-C8-C9     |
| 21  | b     | 6001 | LMT  | C6-C7-C8-C9     |
| 14  | B     | 1201 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1201 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1201 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 1130 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1130 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1130 | CLA  | C6-C7-C8-C10    |
| 15  | B     | 1219 | F6C  | C6-C7-C8-C9     |
| 15  | H     | 1219 | F6C  | C6-C7-C8-C9     |
| 15  | b     | 1219 | F6C  | C6-C7-C8-C9     |
| 18  | A     | 4001 | BCR  | C23-C24-C25-C26 |
| 18  | A     | 4001 | BCR  | C23-C24-C25-C30 |
| 18  | A     | 4004 | BCR  | C23-C24-C25-C26 |
| 18  | A     | 4004 | BCR  | C23-C24-C25-C30 |
| 18  | M     | 4021 | BCR  | C1-C6-C7-C8     |
| 18  | G     | 4001 | BCR  | C23-C24-C25-C26 |
| 18  | G     | 4001 | BCR  | C23-C24-C25-C30 |
| 18  | G     | 4004 | BCR  | C23-C24-C25-C26 |
| 18  | G     | 4004 | BCR  | C23-C24-C25-C30 |
| 18  | V     | 4021 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4001 | BCR  | C23-C24-C25-C30 |
| 18  | a     | 4004 | BCR  | C23-C24-C25-C26 |
| 18  | a     | 4004 | BCR  | C23-C24-C25-C30 |
| 18  | m     | 4021 | BCR  | C1-C6-C7-C8     |
| 14  | A     | 1103 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1103 | CLA  | C10-C11-C12-C13 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 14         | a            | 1103       | CLA         | C10-C11-C12-C13 |
| 21         | B            | 6002       | LMT         | C9-C10-C11-C12  |
| 21         | H            | 6002       | LMT         | C9-C10-C11-C12  |
| 21         | b            | 6002       | LMT         | C9-C10-C11-C12  |
| 18         | B            | 4010       | BCR         | C36-C18-C19-C20 |
| 18         | H            | 4010       | BCR         | C36-C18-C19-C20 |
| 18         | b            | 4010       | BCR         | C36-C18-C19-C20 |
| 18         | B            | 4005       | BCR         | C11-C12-C13-C14 |
| 18         | B            | 4010       | BCR         | C17-C18-C19-C20 |
| 18         | K            | 4001       | BCR         | C17-C18-C19-C20 |
| 18         | H            | 4005       | BCR         | C11-C12-C13-C14 |
| 18         | H            | 4010       | BCR         | C17-C18-C19-C20 |
| 18         | T            | 4001       | BCR         | C17-C18-C19-C20 |
| 18         | b            | 4010       | BCR         | C17-C18-C19-C20 |
| 18         | k            | 4001       | BCR         | C17-C18-C19-C20 |
| 14         | H            | 1225       | CLA         | C13-C15-C16-C17 |
| 16         | B            | 2002       | PQN         | C18-C20-C21-C22 |
| 16         | H            | 2002       | PQN         | C18-C20-C21-C22 |
| 16         | b            | 2002       | PQN         | C18-C20-C21-C22 |
| 14         | A            | 1125       | CLA         | C16-C17-C18-C20 |
| 14         | B            | 1228       | CLA         | C6-C7-C8-C9     |
| 14         | G            | 1125       | CLA         | C16-C17-C18-C20 |
| 14         | H            | 1228       | CLA         | C6-C7-C8-C9     |
| 14         | a            | 1125       | CLA         | C16-C17-C18-C20 |
| 14         | b            | 1228       | CLA         | C6-C7-C8-C9     |
| 14         | a            | 1103       | CLA         | CBD-CGD-O2D-CED |
| 19         | A            | 5001       | LHG         | C7-C8-C9-C10    |
| 19         | G            | 5001       | LHG         | C7-C8-C9-C10    |
| 19         | a            | 5001       | LHG         | C7-C8-C9-C10    |
| 14         | B            | 1023       | CLA         | C10-C11-C12-C13 |
| 14         | B            | 1225       | CLA         | C13-C15-C16-C17 |
| 14         | H            | 1023       | CLA         | C10-C11-C12-C13 |
| 14         | b            | 1023       | CLA         | C10-C11-C12-C13 |
| 14         | b            | 1225       | CLA         | C13-C15-C16-C17 |
| 19         | L            | 5102       | LHG         | O6-C4-C5-C6     |
| 19         | U            | 5102       | LHG         | O6-C4-C5-C6     |
| 19         | l            | 5102       | LHG         | O6-C4-C5-C6     |
| 13         | A            | 1011       | CL0         | C12-C13-C15-C16 |
| 13         | G            | 1011       | CL0         | C12-C13-C15-C16 |
| 13         | a            | 1011       | CL0         | C12-C13-C15-C16 |
| 14         | A            | 1103       | CLA         | C11-C12-C13-C15 |
| 14         | A            | 1125       | CLA         | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1126 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1127 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 1131 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1132 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 1133 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1021 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1201 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1201 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1201 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1203 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1215 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1226 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1234 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1239 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 1103 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1125 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1126 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1127 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1131 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1132 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1133 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1021 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1201 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1201 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1201 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1203 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1215 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1226 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1234 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1239 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 1103 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1125 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1126 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1127 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1131 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1132 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1133 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1021 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1201 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1201 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1201 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1203 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1215 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1226 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1234 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1239 | CLA  | C11-C10-C8-C7   |
| 21  | L     | 6002 | LMT  | C9-C10-C11-C12  |
| 21  | U     | 6002 | LMT  | C9-C10-C11-C12  |
| 21  | l     | 6002 | LMT  | C9-C10-C11-C12  |
| 18  | A     | 4004 | BCR  | C19-C20-C21-C22 |
| 18  | I     | 4018 | BCR  | C19-C20-C21-C22 |
| 18  | M     | 4021 | BCR  | C9-C10-C11-C12  |
| 18  | G     | 4004 | BCR  | C19-C20-C21-C22 |
| 18  | R     | 4018 | BCR  | C19-C20-C21-C22 |
| 18  | V     | 4021 | BCR  | C9-C10-C11-C12  |
| 18  | a     | 4004 | BCR  | C19-C20-C21-C22 |
| 18  | i     | 4018 | BCR  | C19-C20-C21-C22 |
| 18  | m     | 4021 | BCR  | C9-C10-C11-C12  |
| 15  | B     | 1207 | F6C  | C16-C17-C18-C20 |
| 15  | H     | 1207 | F6C  | C16-C17-C18-C20 |
| 15  | b     | 1207 | F6C  | C16-C17-C18-C20 |
| 13  | A     | 1011 | CL0  | C8-C10-C11-C12  |
| 13  | G     | 1011 | CL0  | C8-C10-C11-C12  |
| 13  | a     | 1011 | CL0  | C8-C10-C11-C12  |
| 18  | B     | 4017 | BCR  | C20-C21-C22-C37 |
| 18  | I     | 4020 | BCR  | C11-C10-C9-C34  |
| 18  | R     | 4020 | BCR  | C11-C10-C9-C34  |
| 18  | i     | 4020 | BCR  | C11-C10-C9-C34  |
| 14  | A     | 1131 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1131 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1131 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 1239 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1133 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 1239 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1133 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1023 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1023 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1023 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1133 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 1205 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1210 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 1229 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1205 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1210 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1229 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1205 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1210 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1229 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1239 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1104 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1110 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1112 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1120 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1123 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1201 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1202 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1211 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1227 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1104 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1110 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1112 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1120 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1123 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1201 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1202 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1211 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1227 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1104 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1110 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1112 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1120 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1123 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1201 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1202 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1211 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1227 | CLA  | CAD-CBD-CGD-O2D |
| 15  | B     | 1238 | F6C  | C2B-C3B-CAB-CBB |
| 15  | B     | 1238 | F6C  | CAD-CBD-CGD-O2D |
| 15  | H     | 1238 | F6C  | C2B-C3B-CAB-CBB |
| 15  | H     | 1238 | F6C  | CAD-CBD-CGD-O2D |
| 15  | b     | 1238 | F6C  | C2B-C3B-CAB-CBB |
| 15  | b     | 1238 | F6C  | CAD-CBD-CGD-O2D |
| 14  | A     | 1013 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1202 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1013 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1202 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1013 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1202 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1228 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1228 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1228 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1222 | CLA  | C16-C17-C18-C19 |
| 14  | L     | 1501 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1222 | CLA  | C16-C17-C18-C19 |
| 14  | U     | 1501 | CLA  | C16-C17-C18-C19 |
| 14  | l     | 1501 | CLA  | C16-C17-C18-C19 |
| 20  | A     | 5003 | LMG  | C7-C8-C9-O8     |
| 20  | G     | 5003 | LMG  | C7-C8-C9-O8     |
| 20  | a     | 5003 | LMG  | C7-C8-C9-O8     |
| 20  | I     | 5006 | LMG  | C4-C5-C6-O5     |
| 20  | R     | 5006 | LMG  | C4-C5-C6-O5     |
| 20  | i     | 5006 | LMG  | C4-C5-C6-O5     |
| 14  | B     | 1220 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1220 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1220 | CLA  | C10-C11-C12-C13 |
| 15  | B     | 1237 | F6C  | C15-C16-C17-C18 |
| 15  | H     | 1237 | F6C  | C15-C16-C17-C18 |
| 15  | b     | 1237 | F6C  | C15-C16-C17-C18 |
| 15  | B     | 1219 | F6C  | C4B-C3B-CAB-CBB |
| 15  | H     | 1219 | F6C  | C4B-C3B-CAB-CBB |
| 15  | b     | 1219 | F6C  | C4B-C3B-CAB-CBB |
| 14  | A     | 1102 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1102 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1102 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1136 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1222 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 1101 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1106 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1106 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1111 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1113 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1113 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1115 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1115 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1117 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1117 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1128 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1129 | CLA  | CHA-CBD-CGD-O1D |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 14         | A            | 1129       | CLA         | CHA-CBD-CGD-O2D |
| 14         | A            | 1137       | CLA         | CHA-CBD-CGD-O1D |
| 14         | A            | 1137       | CLA         | CHA-CBD-CGD-O2D |
| 14         | A            | 1141       | CLA         | CHA-CBD-CGD-O1D |
| 14         | A            | 1141       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1022       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1022       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1205       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1210       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1210       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1211       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1212       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1212       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1218       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1218       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1221       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1221       | CLA         | CHA-CBD-CGD-O2D |
| 14         | B            | 1222       | CLA         | CHA-CBD-CGD-O1D |
| 14         | B            | 1222       | CLA         | CHA-CBD-CGD-O2D |
| 14         | K            | 1401       | CLA         | CHA-CBD-CGD-O1D |
| 14         | K            | 1401       | CLA         | CHA-CBD-CGD-O2D |
| 14         | L            | 1501       | CLA         | CHA-CBD-CGD-O1D |
| 14         | L            | 1501       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1101       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1106       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1106       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1111       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1113       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1113       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1115       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1115       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1117       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1117       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1128       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1129       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1129       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1137       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1137       | CLA         | CHA-CBD-CGD-O2D |
| 14         | G            | 1141       | CLA         | CHA-CBD-CGD-O1D |
| 14         | G            | 1141       | CLA         | CHA-CBD-CGD-O2D |
| 14         | H            | 1022       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1022       | CLA         | CHA-CBD-CGD-O2D |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atoms</b>    |
|------------|--------------|------------|-------------|-----------------|
| 14         | H            | 1205       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1210       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1210       | CLA         | CHA-CBD-CGD-O2D |
| 14         | H            | 1211       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1212       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1212       | CLA         | CHA-CBD-CGD-O2D |
| 14         | H            | 1218       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1218       | CLA         | CHA-CBD-CGD-O2D |
| 14         | H            | 1221       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1221       | CLA         | CHA-CBD-CGD-O2D |
| 14         | H            | 1222       | CLA         | CHA-CBD-CGD-O1D |
| 14         | H            | 1222       | CLA         | CHA-CBD-CGD-O2D |
| 14         | T            | 1401       | CLA         | CHA-CBD-CGD-O1D |
| 14         | T            | 1401       | CLA         | CHA-CBD-CGD-O2D |
| 14         | U            | 1501       | CLA         | CHA-CBD-CGD-O1D |
| 14         | U            | 1501       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1101       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1106       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1106       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1111       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1113       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1113       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1115       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1115       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1117       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1117       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1128       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1129       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1129       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1137       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1137       | CLA         | CHA-CBD-CGD-O2D |
| 14         | a            | 1141       | CLA         | CHA-CBD-CGD-O1D |
| 14         | a            | 1141       | CLA         | CHA-CBD-CGD-O2D |
| 14         | b            | 1022       | CLA         | CHA-CBD-CGD-O1D |
| 14         | b            | 1022       | CLA         | CHA-CBD-CGD-O2D |
| 14         | b            | 1205       | CLA         | CHA-CBD-CGD-O1D |
| 14         | b            | 1210       | CLA         | CHA-CBD-CGD-O1D |
| 14         | b            | 1210       | CLA         | CHA-CBD-CGD-O2D |
| 14         | b            | 1211       | CLA         | CHA-CBD-CGD-O1D |
| 14         | b            | 1212       | CLA         | CHA-CBD-CGD-O1D |
| 14         | b            | 1212       | CLA         | CHA-CBD-CGD-O2D |
| 14         | b            | 1218       | CLA         | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1218 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1221 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1221 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1222 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1222 | CLA  | CHA-CBD-CGD-O2D |
| 14  | k     | 1401 | CLA  | CHA-CBD-CGD-O1D |
| 14  | k     | 1401 | CLA  | CHA-CBD-CGD-O2D |
| 14  | l     | 1501 | CLA  | CHA-CBD-CGD-O1D |
| 14  | l     | 1501 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1239 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1239 | CLA  | C15-C16-C17-C18 |
| 14  | b     | 1239 | CLA  | C15-C16-C17-C18 |
| 21  | a     | 6002 | LMT  | C5'-C4'-O1B-C1B |
| 14  | A     | 1136 | CLA  | C5-C6-C7-C8     |
| 20  | A     | 5003 | LMG  | O7-C8-C9-O8     |
| 20  | G     | 5003 | LMG  | O7-C8-C9-O8     |
| 20  | a     | 5003 | LMG  | O7-C8-C9-O8     |
| 21  | A     | 6002 | LMT  | C5'-C4'-O1B-C1B |
| 21  | G     | 6002 | LMT  | C5'-C4'-O1B-C1B |
| 14  | a     | 1136 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1225 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1225 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1225 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1117 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1119 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1117 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1119 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1117 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1119 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1113 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 5002 | LHG  | C9-C10-C11-C12  |
| 19  | G     | 5002 | LHG  | C9-C10-C11-C12  |
| 13  | A     | 1011 | CL0  | C11-C10-C8-C9   |
| 13  | A     | 1011 | CL0  | C14-C13-C15-C16 |
| 13  | G     | 1011 | CL0  | C11-C10-C8-C9   |
| 13  | G     | 1011 | CL0  | C14-C13-C15-C16 |
| 13  | a     | 1011 | CL0  | C11-C10-C8-C9   |
| 13  | a     | 1011 | CL0  | C14-C13-C15-C16 |
| 14  | A     | 1103 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 1127 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1128 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1021 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1223 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1103 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1127 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1128 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1021 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1223 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1103 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1127 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1128 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1021 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1223 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1113 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 5002 | LHG  | C9-C10-C11-C12  |
| 14  | a     | 1113 | CLA  | O1D-CGD-O2D-CED |
| 21  | m     | 6000 | LMT  | C4'-C5'-C6'-O6' |
| 18  | b     | 4005 | BCR  | C11-C12-C13-C14 |
| 14  | A     | 1103 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1206 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1226 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1239 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1103 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1206 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1226 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1239 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1103 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1206 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1226 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1239 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1133 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1133 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1133 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1203 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1203 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1203 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1122 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1137 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1240 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1122 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1133 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1137 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1122 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1137 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1240 | CLA  | C2-C1-O2A-CGA   |
| 19  | A     | 5001 | LHG  | C24-C25-C26-C27 |
| 19  | G     | 5001 | LHG  | C24-C25-C26-C27 |
| 21  | M     | 6000 | LMT  | C4'-C5'-C6'-O6' |
| 14  | A     | 1103 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 1103 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1103 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 5001 | LHG  | C24-C25-C26-C27 |
| 14  | A     | 1123 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1221 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1123 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1221 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1123 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1221 | CLA  | C4-C3-C5-C6     |
| 21  | V     | 6000 | LMT  | C4'-C5'-C6'-O6' |
| 14  | B     | 1236 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1236 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1236 | CLA  | C2-C3-C5-C6     |
| 18  | I     | 4018 | BCR  | C14-C15-C16-C17 |
| 18  | R     | 4018 | BCR  | C14-C15-C16-C17 |
| 18  | i     | 4018 | BCR  | C14-C15-C16-C17 |
| 19  | L     | 5102 | LHG  | C3-O3-P-O5      |
| 19  | U     | 5102 | LHG  | C3-O3-P-O5      |
| 19  | l     | 5102 | LHG  | C3-O3-P-O5      |
| 14  | A     | 1125 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 1125 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1125 | CLA  | C16-C17-C18-C19 |
| 15  | B     | 1238 | F6C  | C13-C15-C16-C17 |
| 15  | H     | 1238 | F6C  | C13-C15-C16-C17 |
| 15  | b     | 1238 | F6C  | C13-C15-C16-C17 |
| 14  | B     | 1228 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1102 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1228 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1228 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1118 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 1118 | CLA  | CBD-CGD-O2D-CED |
| 15  | B     | 1219 | F6C  | C6-C7-C8-C10    |
| 15  | H     | 1219 | F6C  | C6-C7-C8-C10    |
| 15  | b     | 1219 | F6C  | C6-C7-C8-C10    |
| 14  | A     | 1111 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1129 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1141 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1022 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 1223 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1111 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1129 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1141 | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 1022 | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 1223 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1111 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1129 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1141 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 1022 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 1223 | CLA  | CAD-CBD-CGD-O1D |
| 15  | B     | 1219 | F6C  | CAD-CBD-CGD-O1D |
| 15  | H     | 1219 | F6C  | CAD-CBD-CGD-O1D |
| 15  | b     | 1219 | F6C  | CAD-CBD-CGD-O1D |
| 20  | I     | 5006 | LMG  | C30-C31-C32-C33 |
| 14  | A     | 1013 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1013 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1013 | CLA  | O1A-CGA-O2A-C1  |
| 20  | R     | 5006 | LMG  | C30-C31-C32-C33 |
| 20  | i     | 5006 | LMG  | C30-C31-C32-C33 |
| 14  | B     | 1210 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 1118 | CLA  | CBD-CGD-O2D-CED |
| 21  | B     | 6004 | LMT  | C3'-C4'-O1B-C1B |
| 21  | H     | 6004 | LMT  | C3'-C4'-O1B-C1B |
| 21  | b     | 6004 | LMT  | C3'-C4'-O1B-C1B |
| 14  | A     | 1102 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1102 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1210 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1206 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 1231 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1206 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1231 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 1206 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1231 | CLA  | C16-C17-C18-C20 |
| 13  | A     | 1011 | CL0  | C11-C10-C8-C7   |
| 13  | G     | 1011 | CL0  | C11-C10-C8-C7   |
| 13  | a     | 1011 | CL0  | C11-C10-C8-C7   |
| 14  | A     | 1104 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 1115 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 1117 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1119 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 1127 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 1128 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1203 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1204 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1205 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1220 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1221 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1240 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 1104 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 1115 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1117 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1127 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 1128 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1203 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1204 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1205 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1220 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1221 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1240 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 1104 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 1115 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1117 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1127 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 1128 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1203 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1204 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1205 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1220 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1221 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1240 | CLA  | C11-C10-C8-C7   |
| 19  | L     | 5102 | LHG  | O6-C4-C5-O7     |
| 19  | U     | 5102 | LHG  | O6-C4-C5-O7     |
| 19  | l     | 5102 | LHG  | O6-C4-C5-O7     |
| 14  | B     | 1023 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1023 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1102 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1102 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1102 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1023 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1210 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1214 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1214 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1214 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 1127 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1127 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1127 | CLA  | CAA-CBA-CGA-O2A |
| 15  | B     | 1207 | F6C  | C1B-C2B-CMB-OMB |
| 15  | B     | 1230 | F6C  | C1B-C2B-CMB-OMB |
| 15  | H     | 1207 | F6C  | C1B-C2B-CMB-OMB |
| 15  | H     | 1230 | F6C  | C1B-C2B-CMB-OMB |
| 15  | b     | 1207 | F6C  | C1B-C2B-CMB-OMB |
| 15  | b     | 1230 | F6C  | C1B-C2B-CMB-OMB |
| 21  | B     | 6001 | LMT  | C5-C6-C7-C8     |
| 21  | H     | 6001 | LMT  | C5-C6-C7-C8     |
| 21  | b     | 6001 | LMT  | C5-C6-C7-C8     |
| 14  | G     | 1118 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 1210 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1210 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1210 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1119 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1119 | CLA  | C2-C3-C5-C6     |
| 14  | L     | 1501 | CLA  | C13-C15-C16-C17 |
| 14  | U     | 1501 | CLA  | C13-C15-C16-C17 |
| 14  | l     | 1501 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1125 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 1127 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 1132 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1136 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1215 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1221 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1226 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 1125 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1127 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1132 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1136 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1215 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1221 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1226 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 1125 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1127 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1132 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 1136 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1215 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1221 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1226 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1118 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1118 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1125 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1125 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1125 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1116 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1116 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1116 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 4006 | BCR  | C18-C19-C20-C21 |
| 18  | I     | 4020 | BCR  | C18-C19-C20-C21 |
| 18  | M     | 4021 | BCR  | C18-C19-C20-C21 |
| 18  | H     | 4006 | BCR  | C18-C19-C20-C21 |
| 18  | R     | 4020 | BCR  | C18-C19-C20-C21 |
| 18  | V     | 4021 | BCR  | C18-C19-C20-C21 |
| 18  | b     | 4006 | BCR  | C18-C19-C20-C21 |
| 18  | i     | 4020 | BCR  | C18-C19-C20-C21 |
| 18  | m     | 4021 | BCR  | C18-C19-C20-C21 |
| 18  | B     | 4004 | BCR  | C9-C10-C11-C12  |
| 18  | B     | 4006 | BCR  | C13-C14-C15-C16 |
| 18  | H     | 4004 | BCR  | C9-C10-C11-C12  |
| 18  | H     | 4006 | BCR  | C13-C14-C15-C16 |
| 18  | a     | 4001 | BCR  | C19-C20-C21-C22 |
| 18  | b     | 4006 | BCR  | C13-C14-C15-C16 |
| 18  | a     | 4003 | BCR  | C36-C18-C19-C20 |
| 14  | A     | 1136 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 1136 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1136 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 1132 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1216 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1132 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1216 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1132 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1216 | CLA  | C10-C11-C12-C13 |
| 18  | H     | 4017 | BCR  | C20-C21-C22-C37 |
| 18  | b     | 4017 | BCR  | C20-C21-C22-C37 |
| 16  | a     | 2001 | PQN  | C13-C15-C16-C17 |
| 14  | B     | 1021 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1021 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1021 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1228 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 1228 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1228 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1231 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1231 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1231 | CLA  | C16-C17-C18-C19 |
| 16  | A     | 2001 | PQN  | C13-C15-C16-C17 |
| 16  | G     | 2001 | PQN  | C13-C15-C16-C17 |
| 14  | A     | 1136 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1136 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1136 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1203 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1203 | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 1240 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1203 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1127 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 1127 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1127 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1214 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 1214 | CLA  | C3-C5-C6-C7     |
| 19  | L     | 5102 | LHG  | C15-C16-C17-C18 |
| 19  | U     | 5102 | LHG  | C15-C16-C17-C18 |
| 19  | l     | 5102 | LHG  | C15-C16-C17-C18 |
| 14  | A     | 1125 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1125 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 4001 | BCR  | C19-C20-C21-C22 |
| 18  | G     | 4001 | BCR  | C19-C20-C21-C22 |
| 14  | b     | 1214 | CLA  | C3-C5-C6-C7     |
| 18  | I     | 4020 | BCR  | C5-C6-C7-C8     |
| 18  | R     | 4020 | BCR  | C5-C6-C7-C8     |
| 18  | i     | 4020 | BCR  | C5-C6-C7-C8     |
| 15  | B     | 1237 | F6C  | C3A-C2A-CAA-CBA |
| 15  | H     | 1237 | F6C  | C3A-C2A-CAA-CBA |
| 15  | b     | 1237 | F6C  | C3A-C2A-CAA-CBA |
| 14  | G     | 1125 | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 6002 | LMT  | O5'-C1'-O1'-C1  |
| 21  | G     | 6002 | LMT  | O5'-C1'-O1'-C1  |
| 21  | a     | 6002 | LMT  | O5'-C1'-O1'-C1  |
| 14  | B     | 1222 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1222 | CLA  | C8-C10-C11-C12  |
| 21  | A     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 21  | G     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 21  | a     | 6003 | LMT  | C2'-C1'-O1'-C1  |
| 14  | H     | 1222 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | L     | 5102 | LHG  | C4-O6-P-O3      |
| 19  | U     | 5102 | LHG  | C4-O6-P-O3      |
| 19  | l     | 5102 | LHG  | C4-O6-P-O3      |
| 21  | B     | 6004 | LMT  | C2-C3-C4-C5     |
| 21  | H     | 6004 | LMT  | C2-C3-C4-C5     |
| 21  | b     | 6004 | LMT  | C2-C3-C4-C5     |
| 14  | A     | 1104 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1104 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1104 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 1228 | CLA  | C2-C3-C5-C6     |
| 14  | L     | 1502 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1228 | CLA  | C2-C3-C5-C6     |
| 14  | U     | 1502 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1228 | CLA  | C2-C3-C5-C6     |
| 14  | l     | 1502 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 1122 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 1115 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 1125 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1204 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1206 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1115 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1125 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1204 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1206 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1115 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1125 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1204 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1206 | CLA  | C11-C12-C13-C14 |
| 15  | H     | 1238 | F6C  | C14-C13-C15-C16 |
| 15  | b     | 1238 | F6C  | C14-C13-C15-C16 |
| 14  | B     | 1239 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1239 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1239 | CLA  | C5-C6-C7-C8     |
| 18  | b     | 4004 | BCR  | C9-C10-C11-C12  |
| 14  | B     | 1203 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 1203 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 1203 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 1127 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 1127 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 1127 | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 1503 | CLA  | C13-C15-C16-C17 |
| 14  | U     | 1503 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | l     | 1503 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1122 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1122 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 4003 | BCR  | C36-C18-C19-C20 |
| 18  | G     | 4003 | BCR  | C36-C18-C19-C20 |
| 14  | B     | 1022 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1022 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1022 | CLA  | C6-C7-C8-C9     |
| 15  | B     | 1237 | F6C  | C2-C3-C5-C6     |
| 15  | H     | 1237 | F6C  | C2-C3-C5-C6     |
| 15  | b     | 1237 | F6C  | C2-C3-C5-C6     |
| 14  | B     | 1214 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1214 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1214 | CLA  | C11-C12-C13-C15 |
| 21  | A     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 21  | G     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 15  | B     | 1230 | F6C  | C2B-C3B-CAB-CBB |
| 15  | H     | 1230 | F6C  | C2B-C3B-CAB-CBB |
| 15  | b     | 1230 | F6C  | C2B-C3B-CAB-CBB |
| 14  | B     | 1204 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 1204 | CLA  | O1A-CGA-O2A-C1  |
| 15  | B     | 1219 | F6C  | C2A-CAA-CBA-CGA |
| 15  | H     | 1219 | F6C  | C2A-CAA-CBA-CGA |
| 15  | b     | 1219 | F6C  | C2A-CAA-CBA-CGA |
| 21  | a     | 6001 | LMT  | O5B-C5B-C6B-O6B |
| 14  | H     | 1204 | CLA  | O1A-CGA-O2A-C1  |
| 15  | B     | 1207 | F6C  | CBA-CGA-O2A-C1  |
| 15  | H     | 1207 | F6C  | CBA-CGA-O2A-C1  |
| 15  | b     | 1207 | F6C  | CBA-CGA-O2A-C1  |
| 21  | I     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | R     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 21  | i     | 6001 | LMT  | O5'-C1'-O1'-C1  |
| 18  | A     | 4002 | BCR  | C19-C20-C21-C22 |
| 18  | B     | 4014 | BCR  | C15-C16-C17-C18 |
| 18  | I     | 4020 | BCR  | C9-C10-C11-C12  |
| 18  | G     | 4002 | BCR  | C19-C20-C21-C22 |
| 18  | H     | 4014 | BCR  | C15-C16-C17-C18 |
| 18  | R     | 4020 | BCR  | C9-C10-C11-C12  |
| 18  | a     | 4002 | BCR  | C19-C20-C21-C22 |
| 18  | b     | 4014 | BCR  | C15-C16-C17-C18 |
| 18  | i     | 4020 | BCR  | C9-C10-C11-C12  |
| 13  | A     | 1011 | CL0  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | G     | 1011 | CL0  | O1A-CGA-O2A-C1  |
| 13  | a     | 1011 | CL0  | O1A-CGA-O2A-C1  |
| 14  | A     | 1103 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 1103 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 1103 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1103 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1103 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1103 | CLA  | C16-C17-C18-C20 |
| 15  | B     | 1230 | F6C  | C4B-C3B-CAB-CBB |
| 15  | H     | 1230 | F6C  | C4B-C3B-CAB-CBB |
| 15  | b     | 1230 | F6C  | C4B-C3B-CAB-CBB |
| 14  | L     | 1503 | CLA  | C5-C6-C7-C8     |
| 14  | U     | 1503 | CLA  | C5-C6-C7-C8     |
| 19  | G     | 5002 | LHG  | C10-C11-C12-C13 |
| 14  | A     | 1138 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1138 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1138 | CLA  | C2-C3-C5-C6     |
| 19  | A     | 5002 | LHG  | C10-C11-C12-C13 |
| 14  | b     | 1216 | CLA  | C13-C15-C16-C17 |
| 14  | l     | 1503 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 5002 | LHG  | C10-C11-C12-C13 |
| 14  | B     | 1221 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 1221 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 1216 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 1216 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1104 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1104 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 1104 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 1136 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1136 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1136 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 1204 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 1204 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 1204 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 1126 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1206 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1218 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1222 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1126 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1206 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1218 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1222 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1126 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1206 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1218 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1222 | CLA  | C3A-C2A-CAA-CBA |
| 13  | A     | 1011 | CL0  | CAA-CBA-CGA-O2A |
| 13  | G     | 1011 | CL0  | CAA-CBA-CGA-O2A |
| 13  | a     | 1011 | CL0  | CAA-CBA-CGA-O2A |
| 21  | B     | 6003 | LMT  | C2-C1-O1'-C1'   |
| 21  | H     | 6003 | LMT  | C2-C1-O1'-C1'   |
| 21  | b     | 6003 | LMT  | C2-C1-O1'-C1'   |
| 14  | B     | 1205 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1210 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 1225 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1205 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1210 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1225 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1205 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1210 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1225 | CLA  | C14-C13-C15-C16 |
| 15  | B     | 1238 | F6C  | C14-C13-C15-C16 |
| 16  | B     | 2002 | PQN  | C19-C18-C20-C21 |
| 16  | H     | 2002 | PQN  | C19-C18-C20-C21 |
| 16  | b     | 2002 | PQN  | C19-C18-C20-C21 |
| 14  | H     | 1206 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 1101 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 4004 | BCR  | C16-C17-C18-C36 |
| 18  | A     | 4006 | BCR  | C16-C17-C18-C36 |
| 18  | B     | 4006 | BCR  | C11-C10-C9-C34  |
| 18  | B     | 4010 | BCR  | C16-C17-C18-C36 |
| 18  | G     | 4004 | BCR  | C16-C17-C18-C36 |
| 18  | G     | 4006 | BCR  | C16-C17-C18-C36 |
| 18  | H     | 4006 | BCR  | C11-C10-C9-C34  |
| 18  | H     | 4010 | BCR  | C16-C17-C18-C36 |
| 18  | a     | 4004 | BCR  | C16-C17-C18-C36 |
| 18  | a     | 4006 | BCR  | C16-C17-C18-C36 |
| 18  | b     | 4006 | BCR  | C11-C10-C9-C34  |
| 18  | b     | 4010 | BCR  | C16-C17-C18-C36 |
| 14  | A     | 1101 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1101 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1140 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1140 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1140 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 1022 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1206 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 1022 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1022 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1206 | CLA  | C16-C17-C18-C20 |
| 21  | L     | 6101 | LMT  | O5'-C1'-O1'-C1  |
| 21  | U     | 6101 | LMT  | O5'-C1'-O1'-C1  |
| 21  | l     | 6101 | LMT  | O5'-C1'-O1'-C1  |
| 14  | a     | 1126 | CLA  | C10-C11-C12-C13 |
| 21  | A     | 6001 | LMT  | C2-C3-C4-C5     |
| 21  | G     | 6001 | LMT  | C2-C3-C4-C5     |
| 21  | a     | 6001 | LMT  | C2-C3-C4-C5     |
| 14  | A     | 1126 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1126 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1138 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1138 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1138 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1012 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1127 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1133 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1227 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1231 | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 1502 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1012 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1127 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1133 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1227 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1231 | CLA  | C1A-C2A-CAA-CBA |
| 14  | U     | 1502 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1012 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1127 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1133 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1227 | CLA  | C1A-C2A-CAA-CBA |
| 14  | l     | 1502 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1103 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1223 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 1240 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 1103 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1223 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 1240 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 1103 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 1223 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1240 | CLA  | C6-C7-C8-C10    |
| 21  | G     | 6003 | LMT  | C4'-C5'-C6'-O6' |
| 14  | L     | 1501 | CLA  | C2A-CAA-CBA-CGA |
| 14  | U     | 1501 | CLA  | C2A-CAA-CBA-CGA |
| 14  | l     | 1501 | CLA  | C2A-CAA-CBA-CGA |
| 21  | A     | 6003 | LMT  | C4'-C5'-C6'-O6' |
| 14  | B     | 1211 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1211 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 1211 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 6003 | LMT  | O5B-C1B-O1B-C4' |
| 21  | H     | 6003 | LMT  | O5B-C1B-O1B-C4' |
| 21  | A     | 6001 | LMT  | O5B-C1B-O1B-C4' |
| 21  | G     | 6001 | LMT  | O5B-C1B-O1B-C4' |
| 21  | b     | 6003 | LMT  | O5B-C1B-O1B-C4' |
| 21  | a     | 6003 | LMT  | C4'-C5'-C6'-O6' |
| 21  | a     | 6001 | LMT  | O5B-C1B-O1B-C4' |
| 14  | H     | 1217 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1128 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 1128 | CLA  | CBD-CGD-O2D-CED |
| 20  | A     | 5003 | LMG  | C42-C43-C44-C45 |
| 20  | G     | 5003 | LMG  | C42-C43-C44-C45 |
| 20  | a     | 5003 | LMG  | C42-C43-C44-C45 |
| 18  | A     | 4004 | BCR  | C16-C17-C18-C19 |
| 18  | A     | 4006 | BCR  | C16-C17-C18-C19 |
| 18  | B     | 4006 | BCR  | C11-C10-C9-C8   |
| 18  | G     | 4004 | BCR  | C16-C17-C18-C19 |
| 18  | G     | 4006 | BCR  | C16-C17-C18-C19 |
| 18  | H     | 4006 | BCR  | C11-C10-C9-C8   |
| 18  | a     | 4004 | BCR  | C16-C17-C18-C19 |
| 18  | a     | 4006 | BCR  | C16-C17-C18-C19 |
| 18  | b     | 4006 | BCR  | C11-C10-C9-C8   |
| 18  | V     | 4021 | BCR  | C14-C15-C16-C17 |
| 18  | L     | 4022 | BCR  | C19-C20-C21-C22 |
| 18  | U     | 4022 | BCR  | C19-C20-C21-C22 |
| 18  | i     | 4018 | BCR  | C9-C10-C11-C12  |
| 18  | l     | 4022 | BCR  | C19-C20-C21-C22 |
| 14  | B     | 1217 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1101 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1115 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1115 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 1115 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 1128 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1137 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 1137 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 1101 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1101 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1217 | CLA  | O1D-CGD-O2D-CED |
| 13  | A     | 1011 | CL0  | C2-C1-O2A-CGA   |
| 13  | G     | 1011 | CL0  | C2-C1-O2A-CGA   |
| 13  | a     | 1011 | CL0  | C2-C1-O2A-CGA   |
| 14  | H     | 1221 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 1104 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1123 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1104 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1123 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1104 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1123 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1137 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 1229 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1231 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1229 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1231 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1229 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1231 | CLA  | C14-C13-C15-C16 |
| 16  | B     | 2002 | PQN  | C16-C17-C18-C19 |
| 16  | H     | 2002 | PQN  | C16-C17-C18-C19 |
| 16  | b     | 2002 | PQN  | C16-C17-C18-C19 |
| 21  | H     | 6003 | LMT  | C3-C4-C5-C6     |
| 21  | B     | 6003 | LMT  | C3-C4-C5-C6     |
| 21  | b     | 6003 | LMT  | C3-C4-C5-C6     |
| 21  | G     | 6001 | LMT  | C2B-C1B-O1B-C4' |
| 14  | A     | 1130 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 1130 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1130 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 4006 | BCR  | C1-C6-C7-C8     |
| 18  | A     | 4006 | BCR  | C5-C6-C7-C8     |
| 18  | B     | 4004 | BCR  | C1-C6-C7-C8     |
| 18  | I     | 4020 | BCR  | C1-C6-C7-C8     |
| 18  | G     | 4006 | BCR  | C1-C6-C7-C8     |
| 18  | G     | 4006 | BCR  | C5-C6-C7-C8     |
| 18  | H     | 4004 | BCR  | C1-C6-C7-C8     |
| 18  | R     | 4020 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4006 | BCR  | C1-C6-C7-C8     |
| 18  | a     | 4006 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | b     | 4004 | BCR  | C1-C6-C7-C8     |
| 18  | i     | 4020 | BCR  | C1-C6-C7-C8     |
| 19  | G     | 5002 | LHG  | C24-C25-C26-C27 |
| 14  | A     | 1110 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1110 | CLA  | CAA-CBA-CGA-O2A |
| 19  | A     | 5002 | LHG  | C24-C25-C26-C27 |
| 21  | A     | 6001 | LMT  | C2B-C1B-O1B-C4' |
| 21  | a     | 6001 | LMT  | C2B-C1B-O1B-C4' |
| 18  | I     | 4018 | BCR  | C9-C10-C11-C12  |
| 18  | R     | 4018 | BCR  | C9-C10-C11-C12  |
| 19  | a     | 5002 | LHG  | C24-C25-C26-C27 |
| 14  | A     | 1127 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1127 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1127 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 4002 | BCR  | C7-C8-C9-C10    |
| 18  | A     | 4003 | BCR  | C17-C18-C19-C20 |
| 18  | G     | 4002 | BCR  | C7-C8-C9-C10    |
| 18  | G     | 4003 | BCR  | C17-C18-C19-C20 |
| 18  | a     | 4002 | BCR  | C7-C8-C9-C10    |
| 18  | a     | 4003 | BCR  | C17-C18-C19-C20 |
| 14  | B     | 1210 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1210 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1210 | CLA  | C2-C3-C5-C6     |
| 15  | B     | 1207 | F6C  | C2A-CAA-CBA-CGA |
| 15  | H     | 1207 | F6C  | C2A-CAA-CBA-CGA |
| 15  | b     | 1207 | F6C  | C2A-CAA-CBA-CGA |
| 14  | A     | 1141 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1110 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1141 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1141 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1128 | CLA  | O1D-CGD-O2D-CED |
| 19  | G     | 5002 | LHG  | C32-C33-C34-C35 |
| 14  | A     | 1104 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 1104 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1128 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 1115 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 1115 | CLA  | C10-C11-C12-C13 |
| 19  | A     | 5002 | LHG  | C32-C33-C34-C35 |
| 19  | a     | 5002 | LHG  | C32-C33-C34-C35 |
| 14  | G     | 1115 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 1128 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 1104 | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1207 | F6C  | C16-C17-C18-C19 |
| 15  | b     | 1207 | F6C  | C16-C17-C18-C19 |
| 14  | L     | 1502 | CLA  | C4-C3-C5-C6     |
| 14  | U     | 1502 | CLA  | C4-C3-C5-C6     |
| 14  | l     | 1502 | CLA  | C4-C3-C5-C6     |
| 15  | B     | 1238 | F6C  | C4-C3-C5-C6     |
| 15  | H     | 1238 | F6C  | C4-C3-C5-C6     |
| 15  | b     | 1238 | F6C  | C4-C3-C5-C6     |
| 14  | B     | 1221 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1221 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1221 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 1221 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 1221 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 1221 | CLA  | C6-C7-C8-C10    |
| 16  | B     | 2002 | PQN  | C17-C18-C20-C21 |
| 16  | H     | 2002 | PQN  | C17-C18-C20-C21 |
| 16  | b     | 2002 | PQN  | C17-C18-C20-C21 |
| 21  | L     | 6002 | LMT  | C1-C2-C3-C4     |
| 21  | U     | 6002 | LMT  | C1-C2-C3-C4     |
| 20  | B     | 5002 | LMG  | C34-C35-C36-C37 |
| 20  | b     | 5002 | LMG  | C34-C35-C36-C37 |
| 18  | B     | 4010 | BCR  | C19-C20-C21-C22 |
| 18  | H     | 4010 | BCR  | C19-C20-C21-C22 |
| 18  | b     | 4010 | BCR  | C19-C20-C21-C22 |
| 21  | I     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 21  | R     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 21  | i     | 6001 | LMT  | C2'-C1'-O1'-C1  |
| 14  | A     | 1141 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1141 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1141 | CLA  | CAA-CBA-CGA-O1A |
| 20  | H     | 5002 | LMG  | C34-C35-C36-C37 |
| 21  | l     | 6002 | LMT  | C1-C2-C3-C4     |
| 14  | B     | 1215 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1215 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1215 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 1103 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 1103 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 1103 | CLA  | C16-C17-C18-C19 |
| 15  | H     | 1207 | F6C  | C16-C17-C18-C19 |
| 21  | b     | 6002 | LMT  | C4'-C5'-C6'-O6' |
| 13  | A     | 1011 | CL0  | CBA-CGA-O2A-C1  |
| 13  | G     | 1011 | CL0  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | a     | 1011 | CL0  | CBA-CGA-O2A-C1  |
| 14  | A     | 1124 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1124 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 6002 | LMT  | C4'-C5'-C6'-O6' |
| 21  | H     | 6002 | LMT  | C4'-C5'-C6'-O6' |
| 19  | U     | 5101 | LHG  | O7-C7-C8-C9     |
| 14  | A     | 1125 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1201 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 1240 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 1240 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 1125 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1201 | CLA  | C11-C10-C8-C9   |
| 14  | H     | 1240 | CLA  | C6-C7-C8-C9     |
| 14  | H     | 1240 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 1125 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1201 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 1240 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 1240 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 1111 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 1130 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1111 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 1130 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1111 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 1130 | CLA  | C3A-C2A-CAA-CBA |
| 19  | L     | 5101 | LHG  | O7-C7-C8-C9     |
| 19  | l     | 5101 | LHG  | O7-C7-C8-C9     |
| 14  | G     | 1107 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1118 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 1135 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1210 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1212 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1217 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1226 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 1234 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1118 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 1135 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1210 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1212 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1217 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1226 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 1234 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 1118 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1135 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1210 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1212 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1217 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1226 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 1234 | CLA  | CAD-CBD-CGD-O2D |
| 18  | G     | 4005 | BCR  | C9-C10-C11-C12  |
| 14  | A     | 1103 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 1103 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 1103 | CLA  | C3-C5-C6-C7     |
| 16  | B     | 2002 | PQN  | C23-C25-C26-C27 |
| 14  | A     | 1107 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1107 | CLA  | CAA-CBA-CGA-O2A |
| 16  | H     | 2002 | PQN  | C23-C25-C26-C27 |
| 14  | a     | 1124 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1127 | CLA  | C2-C3-C5-C6     |
| 14  | L     | 1502 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1127 | CLA  | C2-C3-C5-C6     |
| 14  | U     | 1502 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1127 | CLA  | C2-C3-C5-C6     |
| 14  | l     | 1502 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 1239 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1239 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1239 | CLA  | CAA-CBA-CGA-O2A |
| 20  | H     | 5002 | LMG  | O7-C10-C11-C12  |
| 20  | b     | 5002 | LMG  | O7-C10-C11-C12  |
| 14  | L     | 1502 | CLA  | C10-C11-C12-C13 |
| 14  | l     | 1502 | CLA  | C10-C11-C12-C13 |
| 16  | b     | 2002 | PQN  | C23-C25-C26-C27 |
| 20  | B     | 5002 | LMG  | O7-C10-C11-C12  |
| 14  | a     | 1110 | CLA  | CAA-CBA-CGA-O1A |
| 14  | U     | 1502 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1013 | CLA  | O2A-C1-C2-C3    |
| 14  | L     | 1503 | CLA  | O2A-C1-C2-C3    |
| 14  | G     | 1013 | CLA  | O2A-C1-C2-C3    |
| 14  | U     | 1503 | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 1013 | CLA  | O2A-C1-C2-C3    |
| 14  | l     | 1503 | CLA  | O2A-C1-C2-C3    |
| 15  | B     | 1238 | F6C  | C4B-C3B-CAB-CBB |
| 15  | H     | 1238 | F6C  | C4B-C3B-CAB-CBB |
| 15  | b     | 1238 | F6C  | C4B-C3B-CAB-CBB |
| 14  | A     | 1013 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1013 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1013 | CLA  | C2A-CAA-CBA-CGA |
| 19  | L     | 5102 | LHG  | O8-C23-C24-C25  |
| 19  | U     | 5102 | LHG  | O8-C23-C24-C25  |
| 14  | A     | 1110 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1110 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1013 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1108 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1114 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1114 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1126 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1126 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1133 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1133 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1134 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 1139 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 1139 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1021 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1021 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1203 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1203 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1204 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1204 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1215 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1215 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1223 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1224 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1224 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 1225 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 1225 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1013 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1108 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1114 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1114 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1126 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1126 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1133 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1133 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1134 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 1139 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 1139 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1021 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 1021 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1203 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1203 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1204 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1204 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1215 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1215 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1223 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1224 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1224 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 1225 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 1225 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1013 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1108 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1114 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1114 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1126 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1126 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1133 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1133 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1134 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 1139 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 1139 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1021 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1021 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1203 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1203 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1204 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1204 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1215 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1215 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1223 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1224 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1224 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 1225 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 1225 | CLA  | CHA-CBD-CGD-O2D |
| 15  | B     | 1237 | F6C  | CHA-CBD-CGD-O1D |
| 15  | B     | 1237 | F6C  | CHA-CBD-CGD-O2D |
| 15  | H     | 1237 | F6C  | CHA-CBD-CGD-O1D |
| 15  | H     | 1237 | F6C  | CHA-CBD-CGD-O2D |
| 15  | b     | 1237 | F6C  | CHA-CBD-CGD-O1D |
| 15  | b     | 1237 | F6C  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 4005 | BCR  | C9-C10-C11-C12  |
| 14  | B     | 1233 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 1215 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1215 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 1215 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1103 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1236 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1103 | CLA  | CAA-CBA-CGA-O2A |
| 19  | l     | 5102 | LHG  | O8-C23-C24-C25  |
| 15  | B     | 1238 | F6C  | C2-C3-C5-C6     |
| 15  | H     | 1238 | F6C  | C2-C3-C5-C6     |
| 15  | b     | 1238 | F6C  | C2-C3-C5-C6     |
| 18  | B     | 4010 | BCR  | C16-C17-C18-C19 |
| 18  | H     | 4010 | BCR  | C16-C17-C18-C19 |
| 18  | b     | 4010 | BCR  | C16-C17-C18-C19 |
| 14  | H     | 1233 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1233 | CLA  | CAA-CBA-CGA-O1A |
| 15  | A     | 1121 | F6C  | CAA-CBA-CGA-O2A |
| 14  | A     | 1103 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1235 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1236 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1235 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1235 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1236 | CLA  | CAA-CBA-CGA-O2A |
| 15  | B     | 1237 | F6C  | CAA-CBA-CGA-O2A |
| 15  | H     | 1237 | F6C  | CAA-CBA-CGA-O2A |
| 15  | b     | 1237 | F6C  | CAA-CBA-CGA-O2A |
| 21  | b     | 6001 | LMT  | C9-C10-C11-C12  |
| 20  | H     | 5002 | LMG  | C21-C22-C23-C24 |
| 20  | b     | 5002 | LMG  | C21-C22-C23-C24 |
| 21  | B     | 6001 | LMT  | C9-C10-C11-C12  |
| 21  | H     | 6001 | LMT  | C9-C10-C11-C12  |
| 15  | G     | 1121 | F6C  | CAA-CBA-CGA-O2A |
| 15  | a     | 1121 | F6C  | CAA-CBA-CGA-O2A |
| 20  | B     | 5002 | LMG  | C21-C22-C23-C24 |
| 14  | B     | 1217 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1233 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1217 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1217 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1233 | CLA  | CAA-CBA-CGA-O2A |
| 19  | A     | 5001 | LHG  | O1-C1-C2-O2     |
| 19  | G     | 5001 | LHG  | O1-C1-C2-O2     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | a     | 5001 | LHG  | O1-C1-C2-O2     |
| 21  | a     | 6002 | LMT  | C3'-C4'-O1B-C1B |
| 14  | H     | 1233 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1235 | CLA  | C4-C3-C5-C6     |
| 21  | A     | 6002 | LMT  | C3'-C4'-O1B-C1B |
| 21  | G     | 6002 | LMT  | C3'-C4'-O1B-C1B |
| 14  | A     | 1132 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 1103 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 1123 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1203 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 1103 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 1123 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1203 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 1103 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 1123 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1203 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1216 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1216 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1216 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1107 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 1203 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1223 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 1203 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 1223 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 1203 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 1223 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 4005 | BCR  | C9-C10-C11-C12  |
| 18  | M     | 4021 | BCR  | C14-C15-C16-C17 |
| 18  | m     | 4021 | BCR  | C14-C15-C16-C17 |
| 14  | K     | 1401 | CLA  | CAA-CBA-CGA-O2A |
| 14  | T     | 1401 | CLA  | CAA-CBA-CGA-O2A |
| 14  | k     | 1401 | CLA  | CAA-CBA-CGA-O2A |
| 21  | H     | 6003 | LMT  | C4-C5-C6-C7     |
| 14  | G     | 1132 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 6003 | LMT  | C4-C5-C6-C7     |
| 21  | b     | 6003 | LMT  | C4-C5-C6-C7     |
| 14  | B     | 1227 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1107 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1107 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1227 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1227 | CLA  | CAA-CBA-CGA-O2A |
| 19  | L     | 5101 | LHG  | O9-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | U     | 5101 | LHG  | O9-C7-C8-C9     |
| 19  | l     | 5101 | LHG  | O9-C7-C8-C9     |
| 14  | a     | 1132 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 1235 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 1235 | CLA  | C4-C3-C5-C6     |
| 21  | a     | 6002 | LMT  | O1'-C1-C2-C3    |
| 21  | A     | 6002 | LMT  | O1'-C1-C2-C3    |
| 21  | G     | 6002 | LMT  | O1'-C1-C2-C3    |
| 20  | H     | 5002 | LMG  | O9-C10-C11-C12  |
| 20  | b     | 5002 | LMG  | O9-C10-C11-C12  |
| 14  | B     | 1203 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1203 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 1210 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 1210 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 21  | H     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 13  | A     | 1011 | CL0  | C1A-C2A-CAA-CBA |
| 13  | G     | 1011 | CL0  | C1A-C2A-CAA-CBA |
| 13  | a     | 1011 | CL0  | C1A-C2A-CAA-CBA |
| 14  | A     | 1111 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1119 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1123 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 1218 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1111 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1119 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 1123 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1218 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1111 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1119 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 1123 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1218 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 1231 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 1131 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1131 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1239 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1239 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1239 | CLA  | CAA-CBA-CGA-O1A |
| 20  | B     | 5002 | LMG  | O9-C10-C11-C12  |
| 14  | b     | 1203 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 1135 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 1135 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 1135 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | b     | 6004 | LMT  | C4'-C5'-C6'-O6' |
| 14  | B     | 1203 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 1203 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 1203 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 1131 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 1203 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1203 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1203 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1210 | CLA  | C3-C5-C6-C7     |
| 19  | A     | 5001 | LHG  | C2-C3-O3-P      |
| 19  | G     | 5001 | LHG  | C2-C3-O3-P      |
| 19  | a     | 5001 | LHG  | C2-C3-O3-P      |
| 19  | L     | 5101 | LHG  | C27-C28-C29-C30 |
| 14  | B     | 1216 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1216 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1216 | CLA  | CAA-CBA-CGA-O1A |
| 19  | U     | 5101 | LHG  | C27-C28-C29-C30 |
| 21  | A     | 6002 | LMT  | C2'-C1'-O1'-C1  |
| 21  | G     | 6002 | LMT  | C2'-C1'-O1'-C1  |
| 21  | a     | 6002 | LMT  | C2'-C1'-O1'-C1  |
| 19  | l     | 5101 | LHG  | C27-C28-C29-C30 |
| 19  | L     | 5102 | LHG  | C4-O6-P-O5      |
| 19  | U     | 5102 | LHG  | C4-O6-P-O5      |
| 19  | l     | 5102 | LHG  | C4-O6-P-O5      |
| 14  | B     | 1236 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1236 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1236 | CLA  | CAA-CBA-CGA-O1A |
| 15  | B     | 1237 | F6C  | CAA-CBA-CGA-O1A |
| 19  | G     | 5002 | LHG  | C16-C17-C18-C19 |
| 14  | H     | 1231 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 1231 | CLA  | C8-C10-C11-C12  |
| 15  | H     | 1237 | F6C  | CAA-CBA-CGA-O1A |
| 15  | b     | 1237 | F6C  | CAA-CBA-CGA-O1A |
| 19  | L     | 5102 | LHG  | O10-C23-C24-C25 |
| 19  | U     | 5102 | LHG  | O10-C23-C24-C25 |
| 19  | l     | 5102 | LHG  | O10-C23-C24-C25 |
| 19  | a     | 5002 | LHG  | C16-C17-C18-C19 |
| 14  | B     | 1231 | CLA  | C8-C10-C11-C12  |
| 14  | K     | 1401 | CLA  | CAA-CBA-CGA-O1A |
| 14  | T     | 1401 | CLA  | CAA-CBA-CGA-O1A |
| 15  | G     | 1121 | F6C  | CAA-CBA-CGA-O1A |
| 14  | G     | 1138 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1138 | CLA  | C6-C7-C8-C9     |
| 20  | H     | 5002 | LMG  | C4-C5-C6-O5     |
| 18  | A     | 4004 | BCR  | C10-C11-C12-C13 |
| 18  | L     | 4019 | BCR  | C10-C11-C12-C13 |
| 18  | G     | 4004 | BCR  | C10-C11-C12-C13 |
| 18  | a     | 4004 | BCR  | C10-C11-C12-C13 |
| 18  | l     | 4019 | BCR  | C10-C11-C12-C13 |
| 14  | G     | 1013 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 5002 | LHG  | C16-C17-C18-C19 |
| 20  | B     | 5002 | LMG  | C4-C5-C6-O5     |
| 14  | B     | 1217 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1217 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1217 | CLA  | CAA-CBA-CGA-O1A |
| 14  | k     | 1401 | CLA  | CAA-CBA-CGA-O1A |
| 15  | A     | 1121 | F6C  | CAA-CBA-CGA-O1A |
| 15  | a     | 1121 | F6C  | CAA-CBA-CGA-O1A |
| 14  | A     | 1013 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 1013 | CLA  | C8-C10-C11-C12  |
| 20  | b     | 5002 | LMG  | C4-C5-C6-O5     |
| 14  | A     | 1138 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 1133 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1134 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1135 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 1215 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 1228 | CLA  | CAD-CBD-CGD-O1D |
| 14  | L     | 1502 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1133 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1134 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 1135 | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 1215 | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 1228 | CLA  | CAD-CBD-CGD-O1D |
| 14  | U     | 1502 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1133 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1134 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 1135 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 1215 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 1228 | CLA  | CAD-CBD-CGD-O1D |
| 14  | l     | 1502 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 1117 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 1136 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 1117 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 1136 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 1117 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 1136 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 1102 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1102 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1102 | CLA  | CAA-CBA-CGA-O2A |
| 20  | I     | 5006 | LMG  | O8-C28-C29-C30  |
| 20  | R     | 5006 | LMG  | O8-C28-C29-C30  |
| 20  | i     | 5006 | LMG  | O8-C28-C29-C30  |
| 14  | B     | 1227 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1227 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1227 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 1203 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 1220 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1220 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1123 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1231 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 1231 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 1231 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 1235 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1203 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1235 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1203 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1235 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1103 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 1103 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 1103 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 1123 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1210 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 1228 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 1229 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 1234 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 1239 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 1123 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1210 | CLA  | C11-C12-C13-C15 |
| 14  | H     | 1228 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 1229 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 1234 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 1239 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 1123 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1210 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 1228 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 1229 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 1234 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 1239 | CLA  | C11-C12-C13-C15 |
| 15  | B     | 1237 | F6C  | C6-C7-C8-C10    |
| 15  | H     | 1237 | F6C  | C6-C7-C8-C10    |
| 15  | b     | 1237 | F6C  | C6-C7-C8-C10    |
| 14  | G     | 1134 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1123 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1125 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1137 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1123 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1125 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1137 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1125 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1137 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1220 | CLA  | CAA-CBA-CGA-O2A |
| 19  | L     | 5101 | LHG  | O8-C23-C24-C25  |
| 19  | U     | 5101 | LHG  | O8-C23-C24-C25  |
| 18  | L     | 4022 | BCR  | C17-C18-C19-C20 |
| 18  | U     | 4022 | BCR  | C17-C18-C19-C20 |
| 18  | l     | 4022 | BCR  | C17-C18-C19-C20 |
| 14  | A     | 1137 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1137 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1137 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1134 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1134 | CLA  | CAA-CBA-CGA-O2A |
| 18  | K     | 4001 | BCR  | C15-C16-C17-C18 |
| 18  | T     | 4001 | BCR  | C15-C16-C17-C18 |
| 18  | k     | 4001 | BCR  | C15-C16-C17-C18 |
| 14  | B     | 1226 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1226 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 1123 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1123 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1123 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1125 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1125 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1139 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1139 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1212 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1139 | CLA  | CAA-CBA-CGA-O1A |

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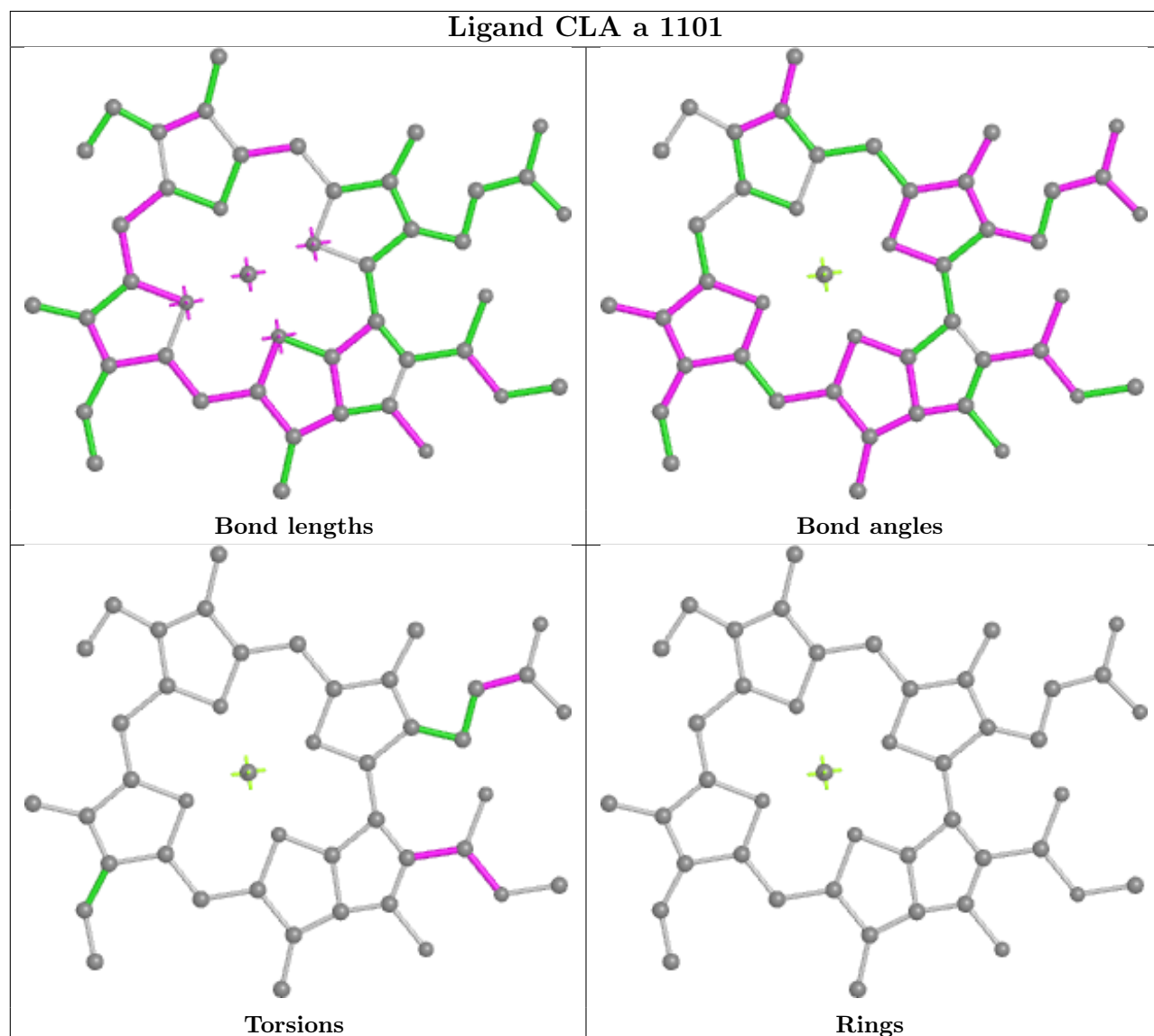
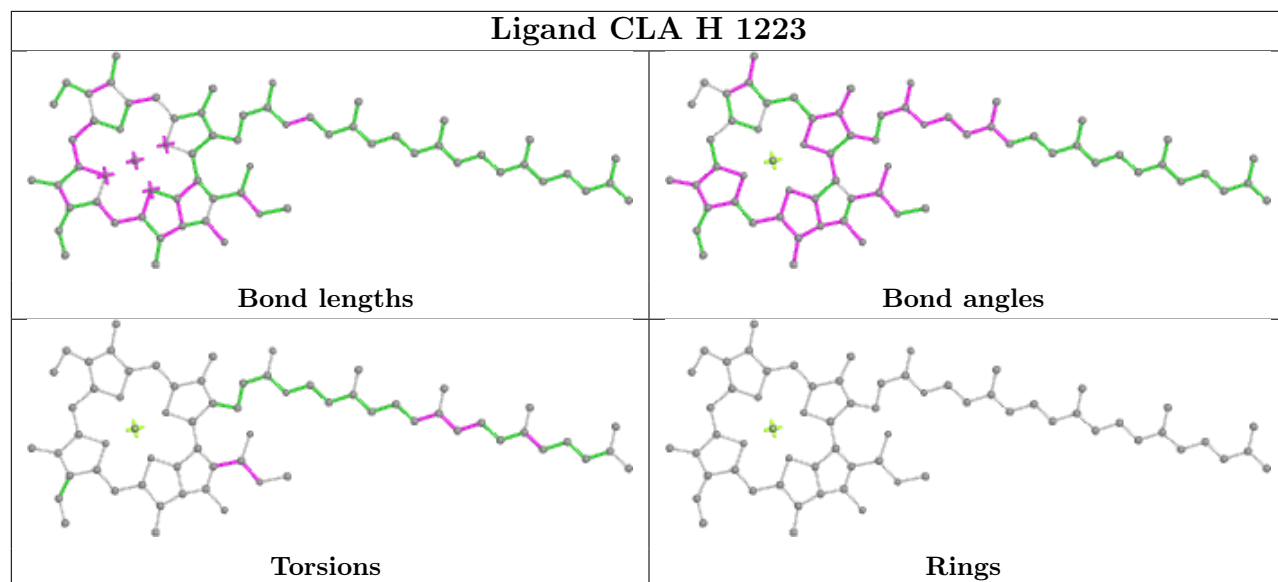
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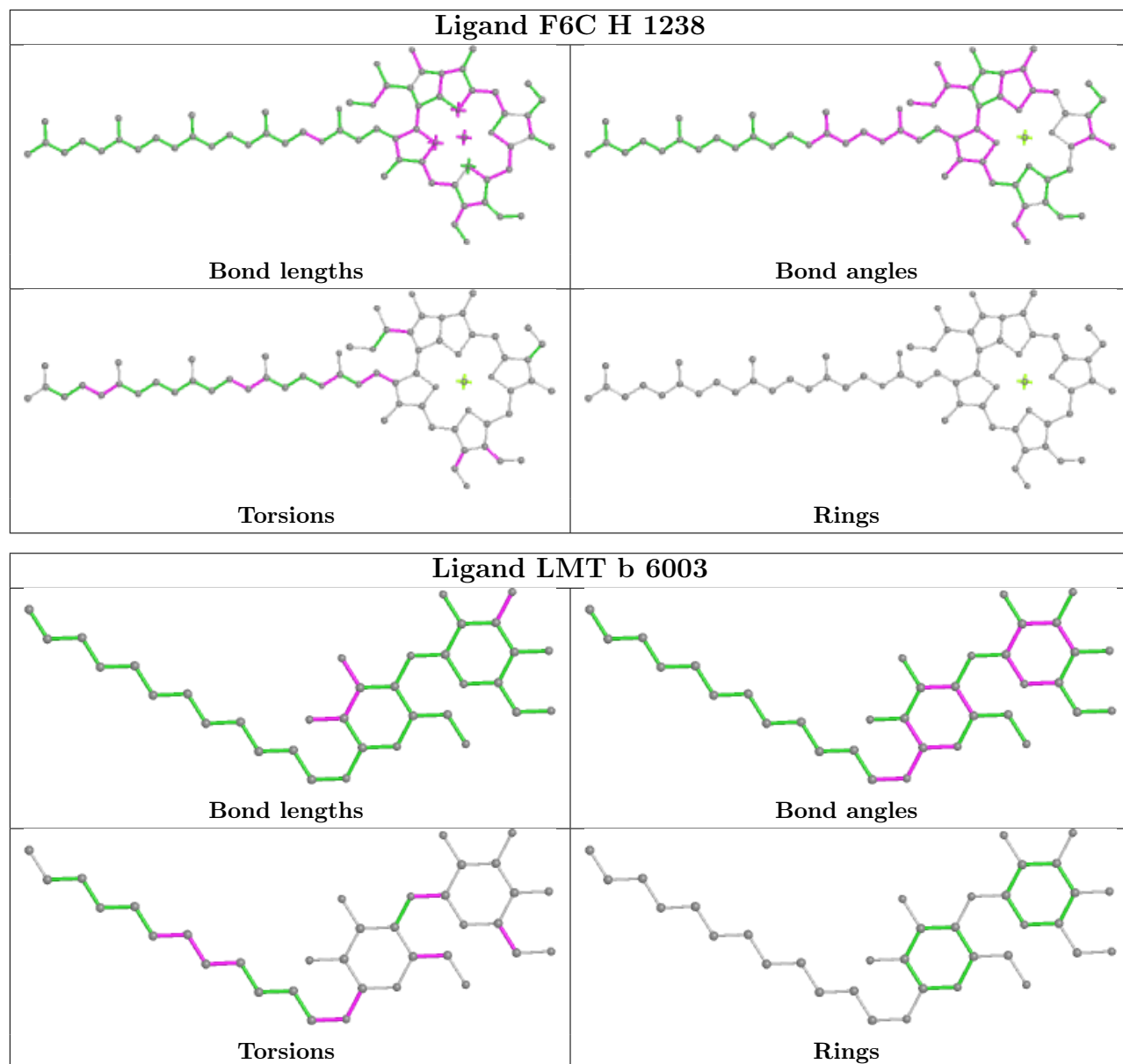
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 1139 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1212 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1139 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1139 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1212 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 1225 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 1225 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 1103 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 1220 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1103 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1125 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 1220 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1103 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 1220 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 1124 | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 1502 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 1124 | CLA  | CAA-CBA-CGA-O2A |
| 14  | U     | 1502 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 1124 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 1226 | CLA  | CAA-CBA-CGA-O2A |
| 14  | l     | 1502 | CLA  | CAA-CBA-CGA-O2A |
| 19  | l     | 5101 | LHG  | O8-C23-C24-C25  |
| 14  | A     | 1134 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 1134 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 1134 | CLA  | CAA-CBA-CGA-O1A |

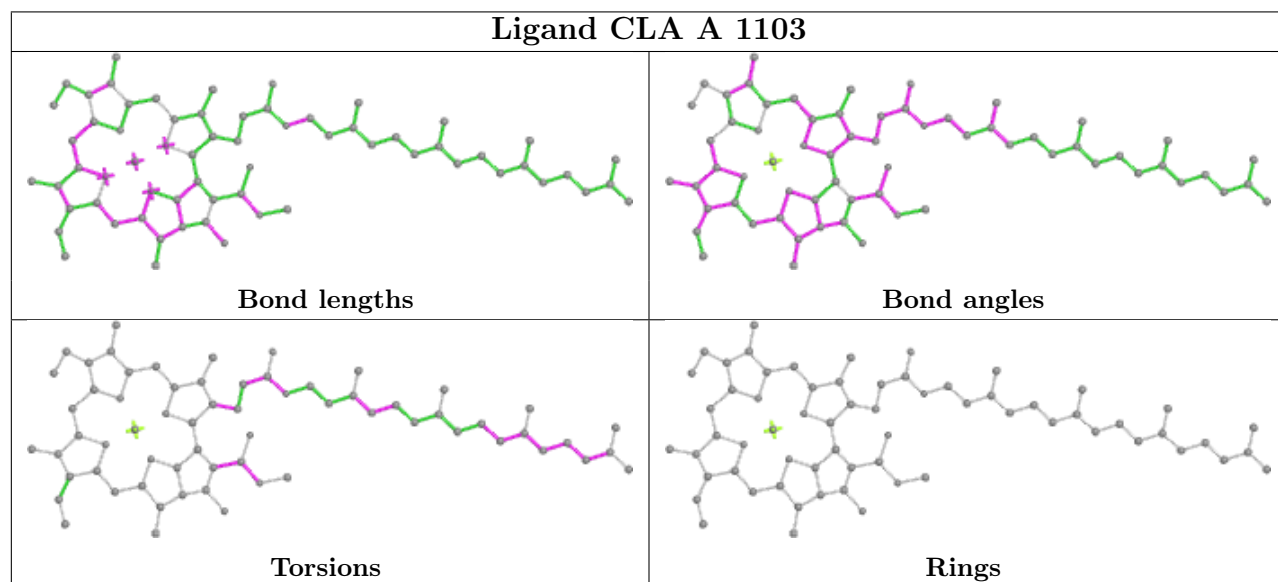
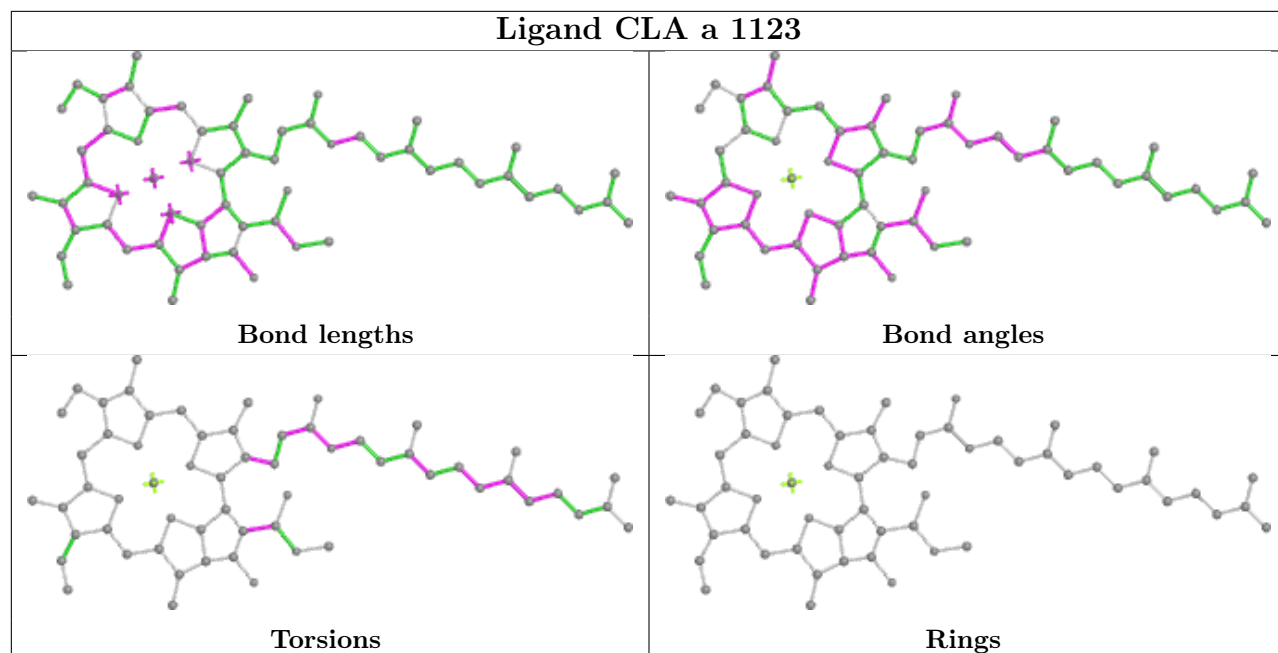
There are no ring outliers.

No monomer is involved in short contacts.

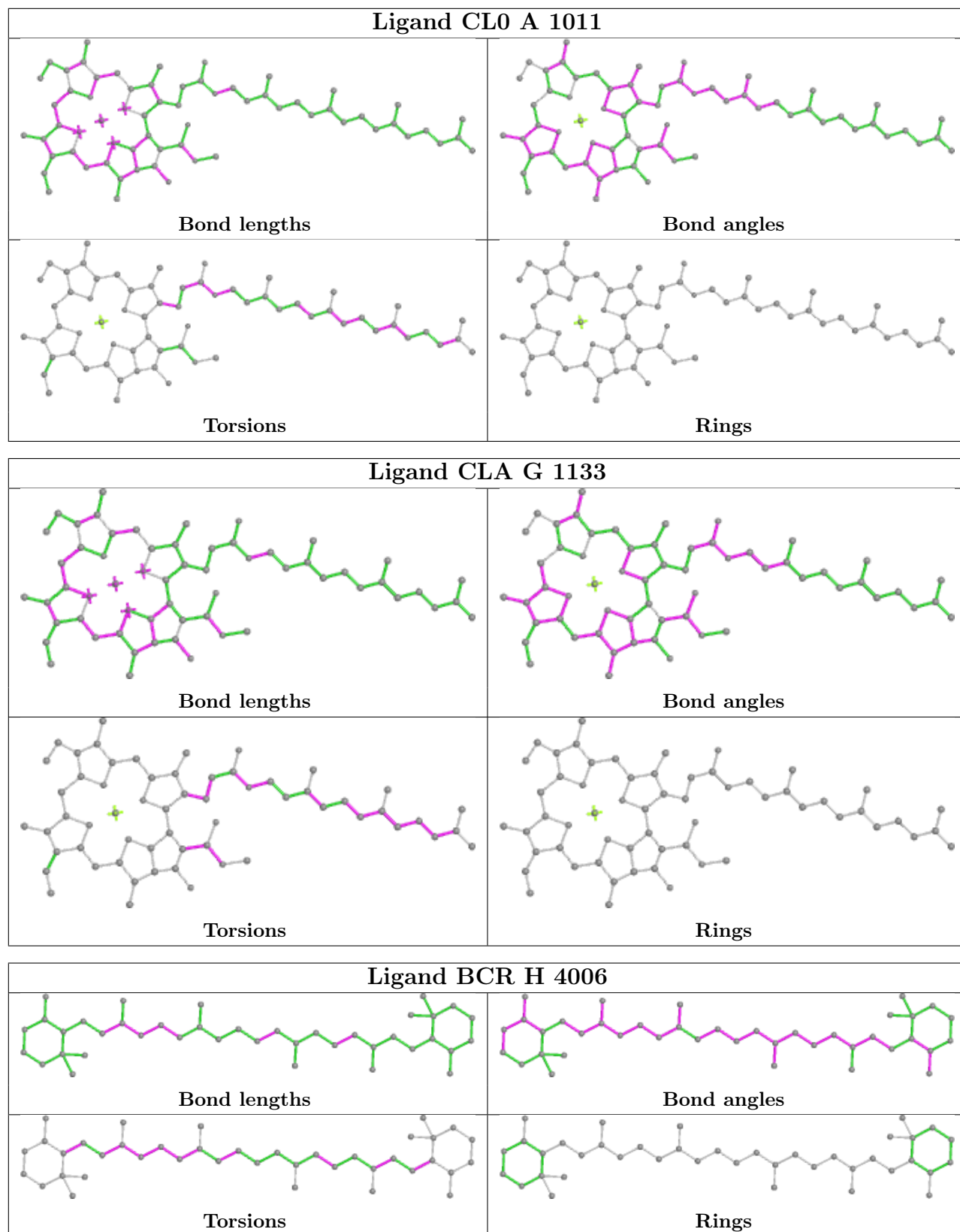
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

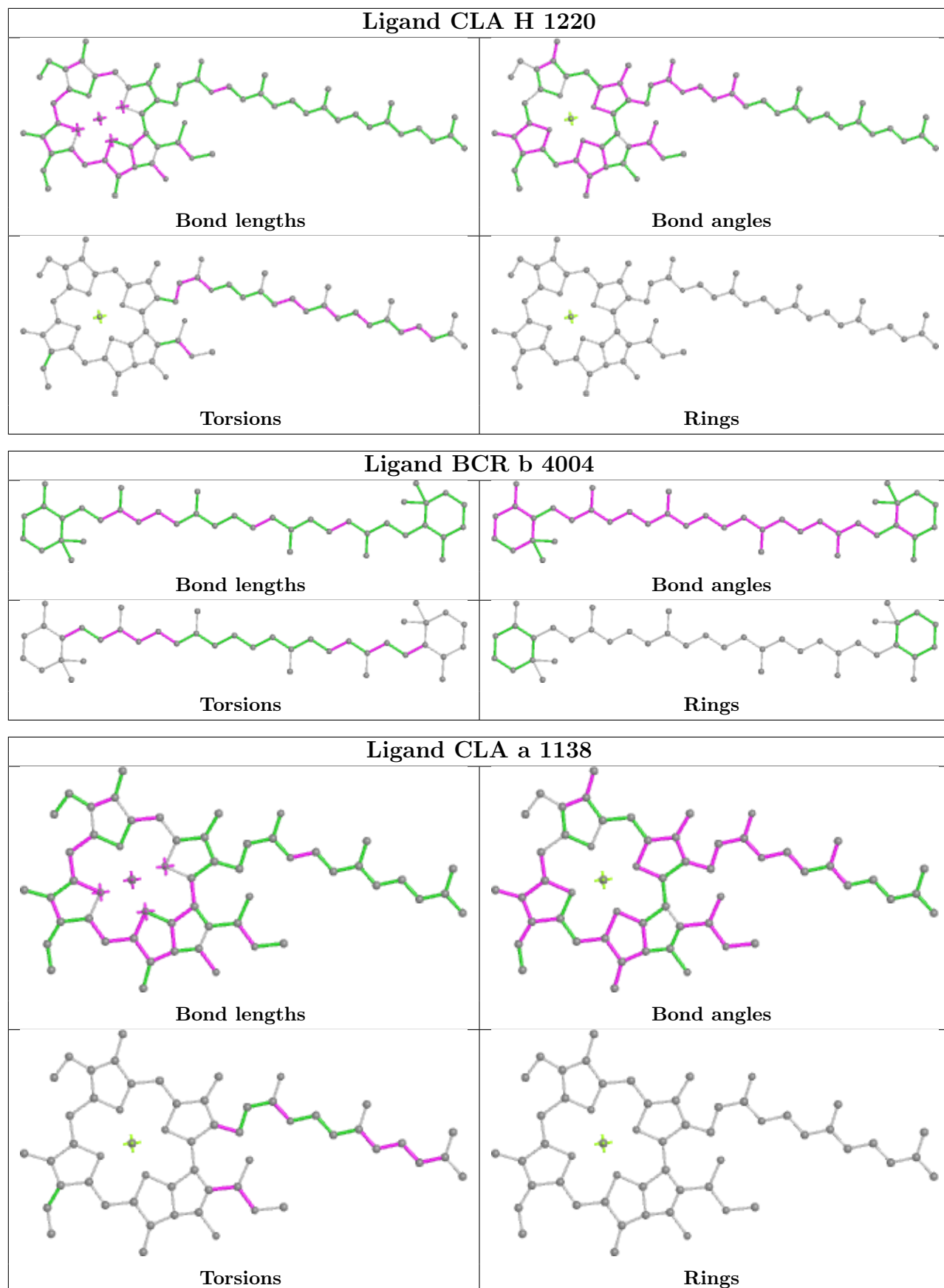


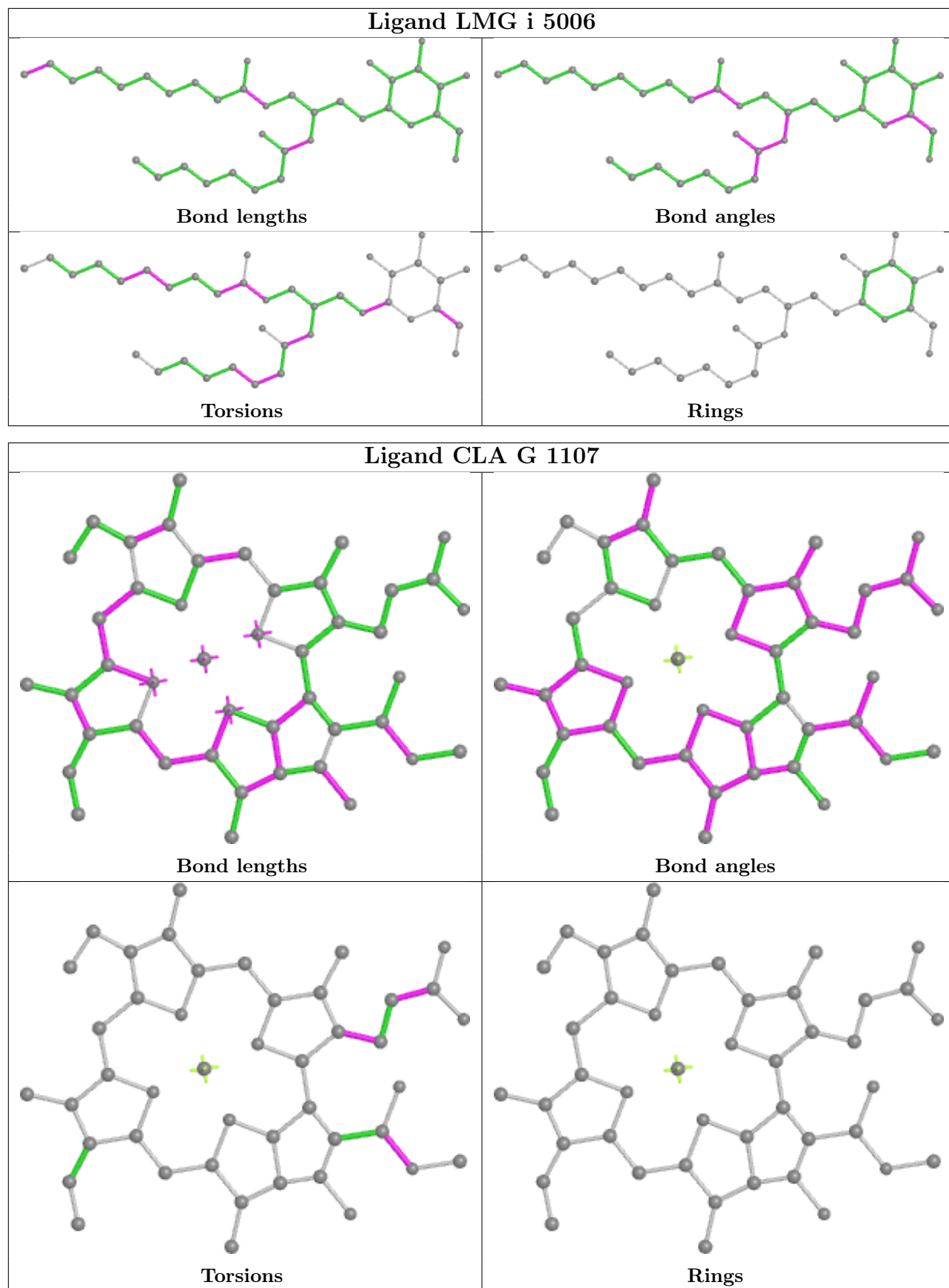


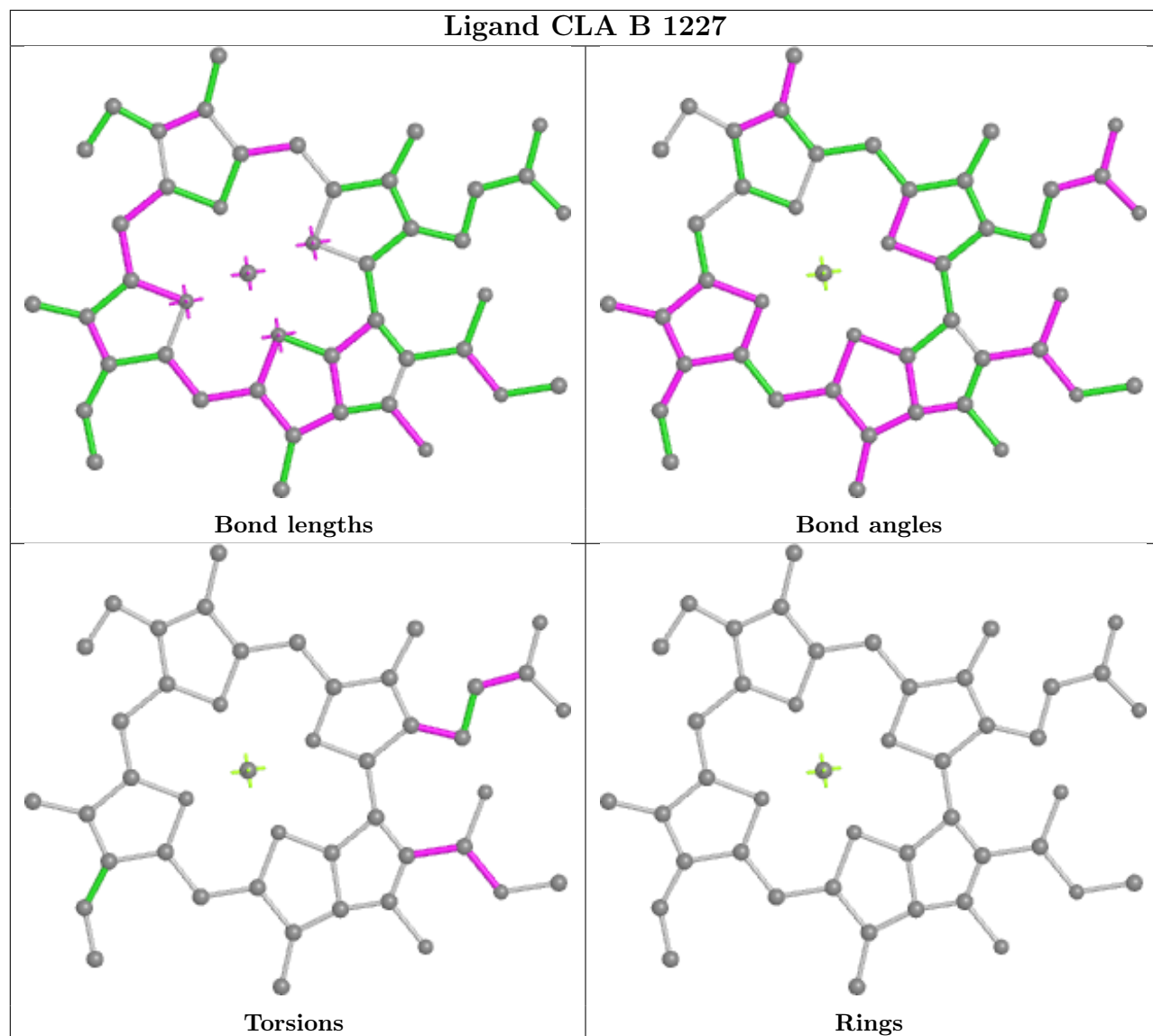


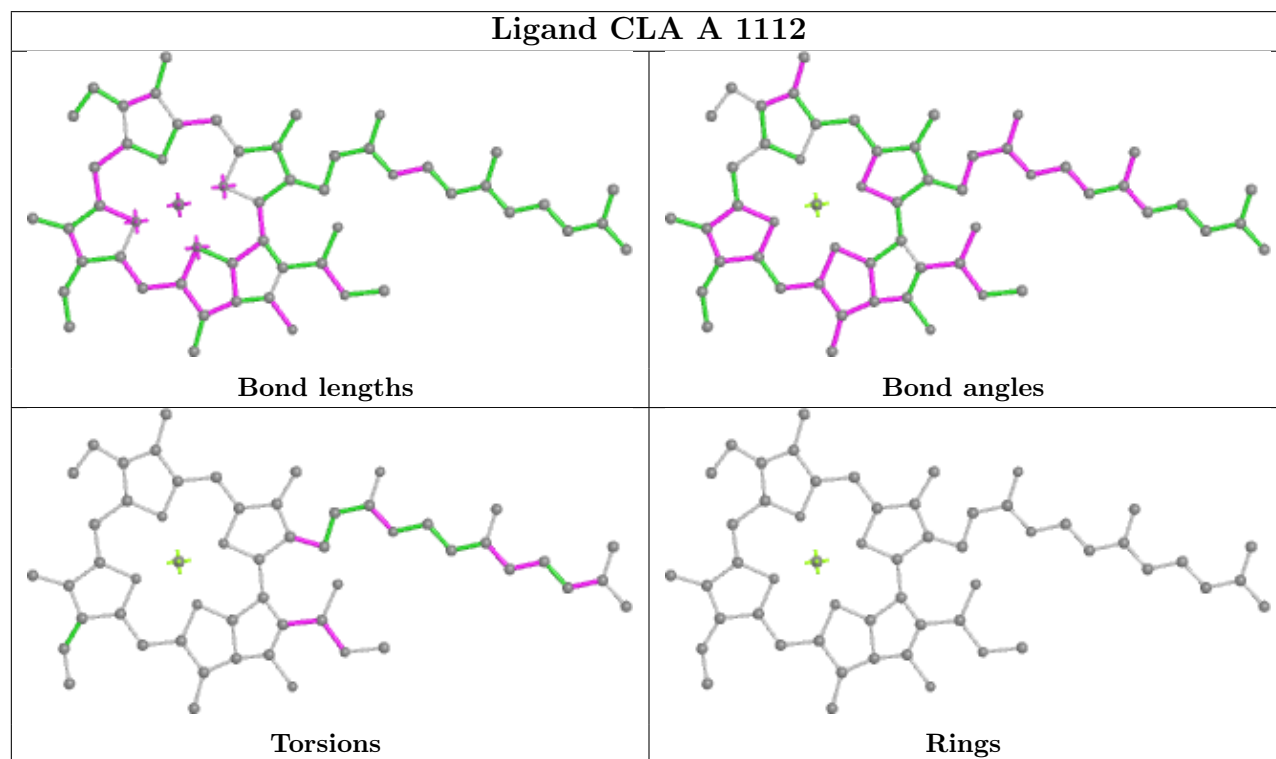
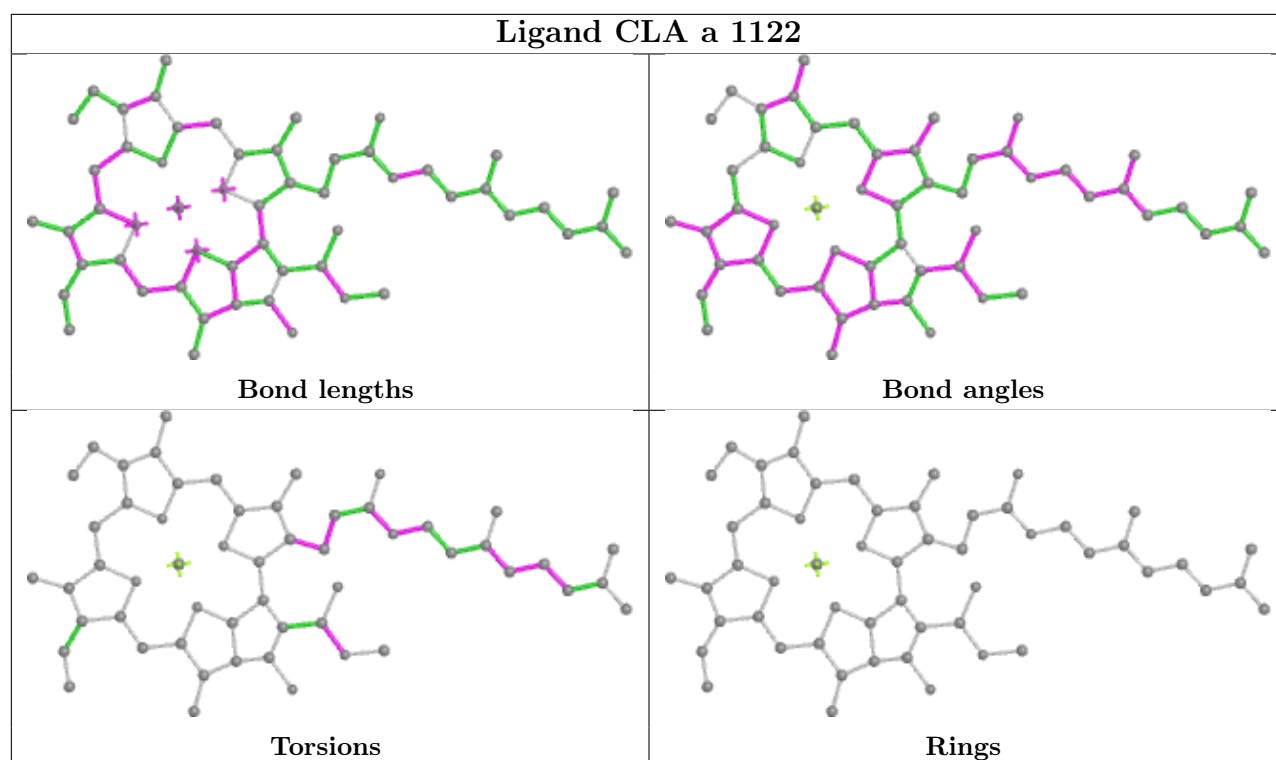


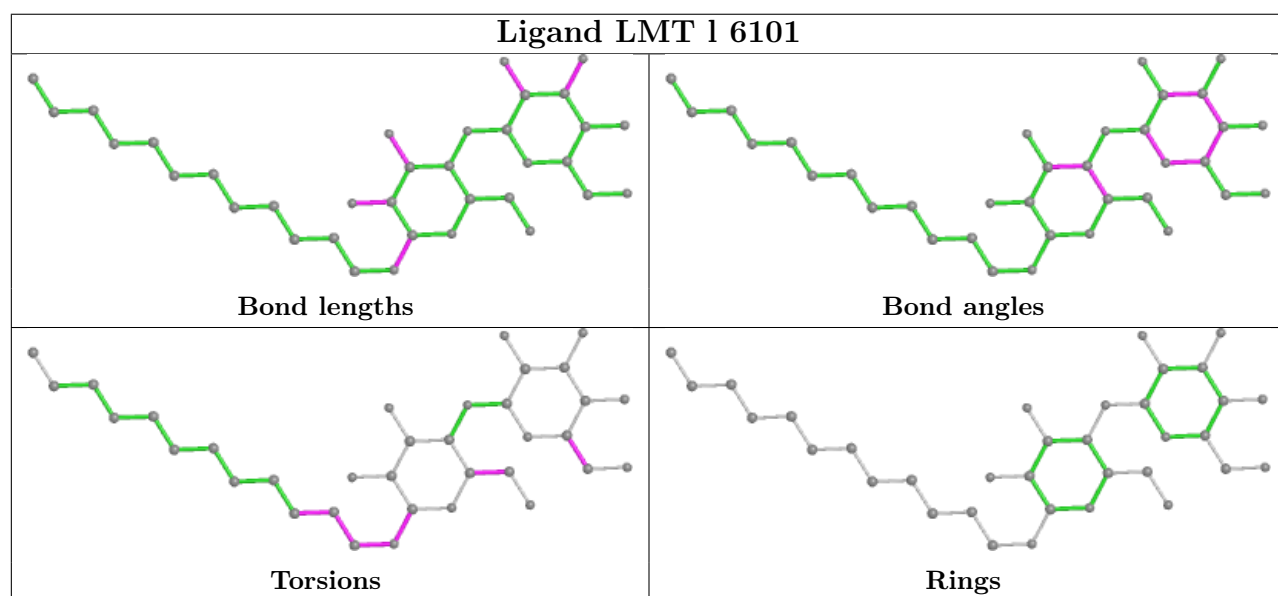
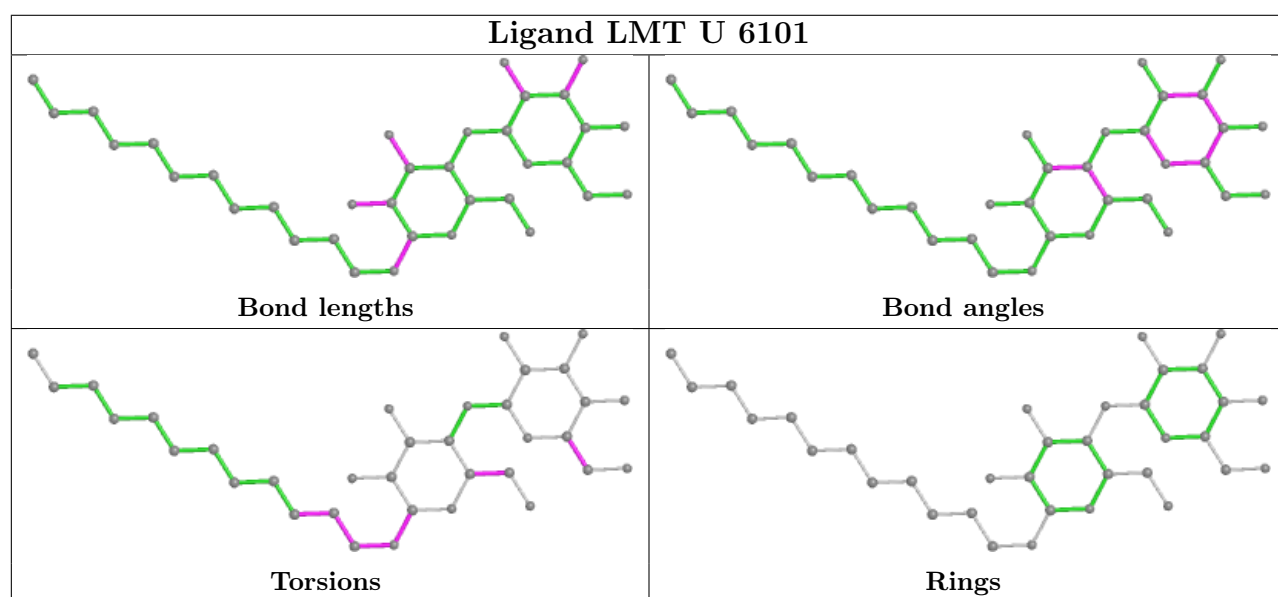
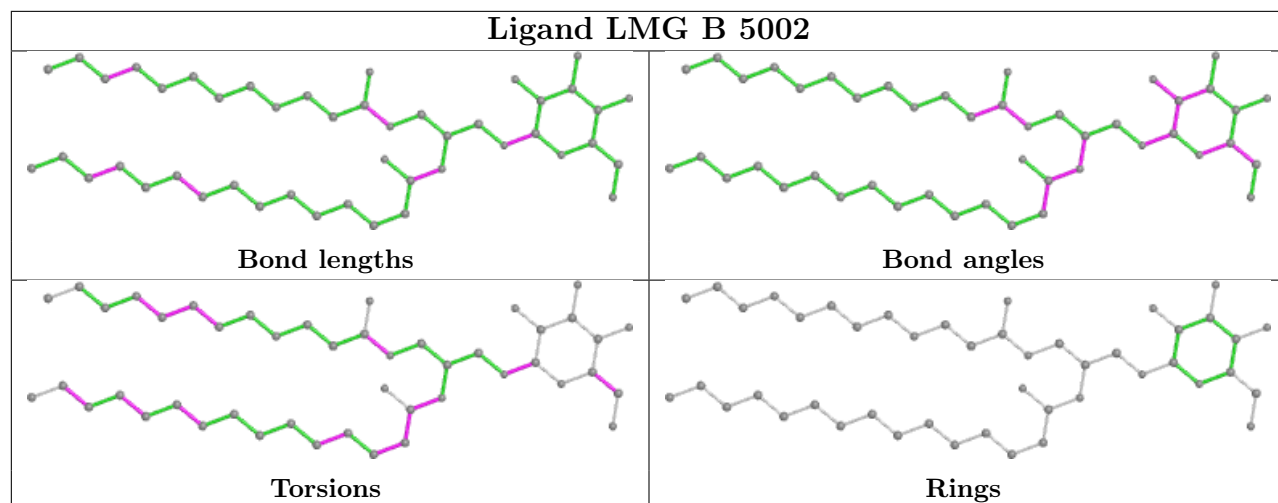


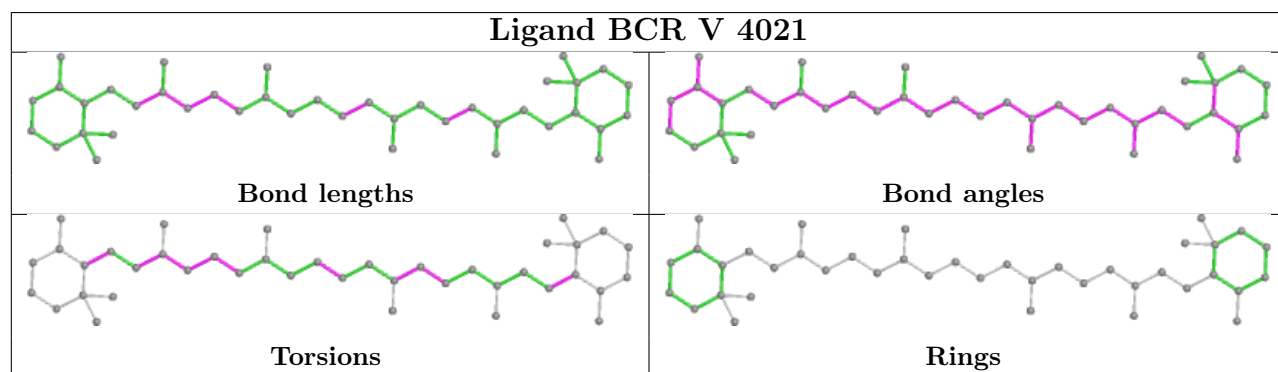
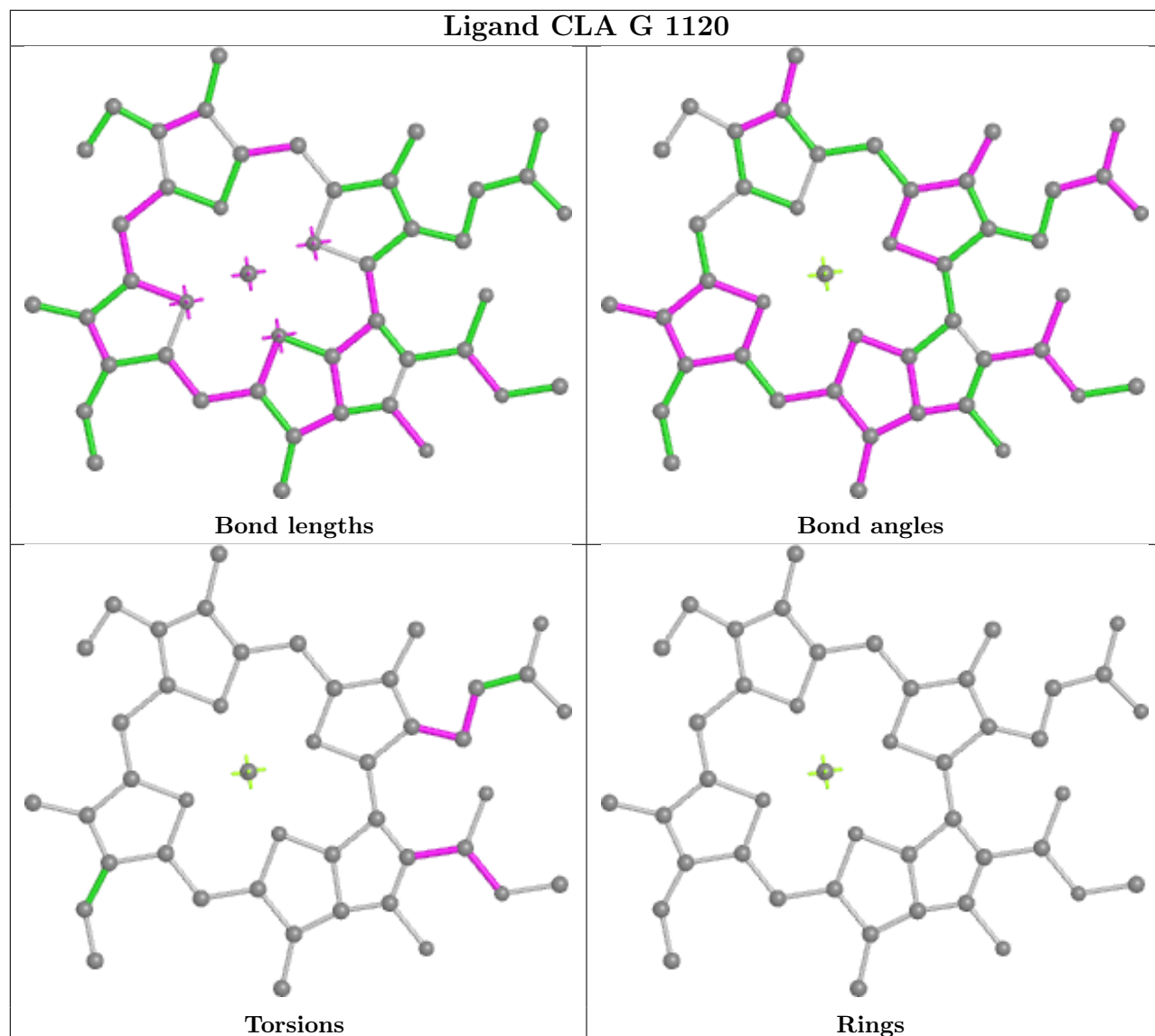


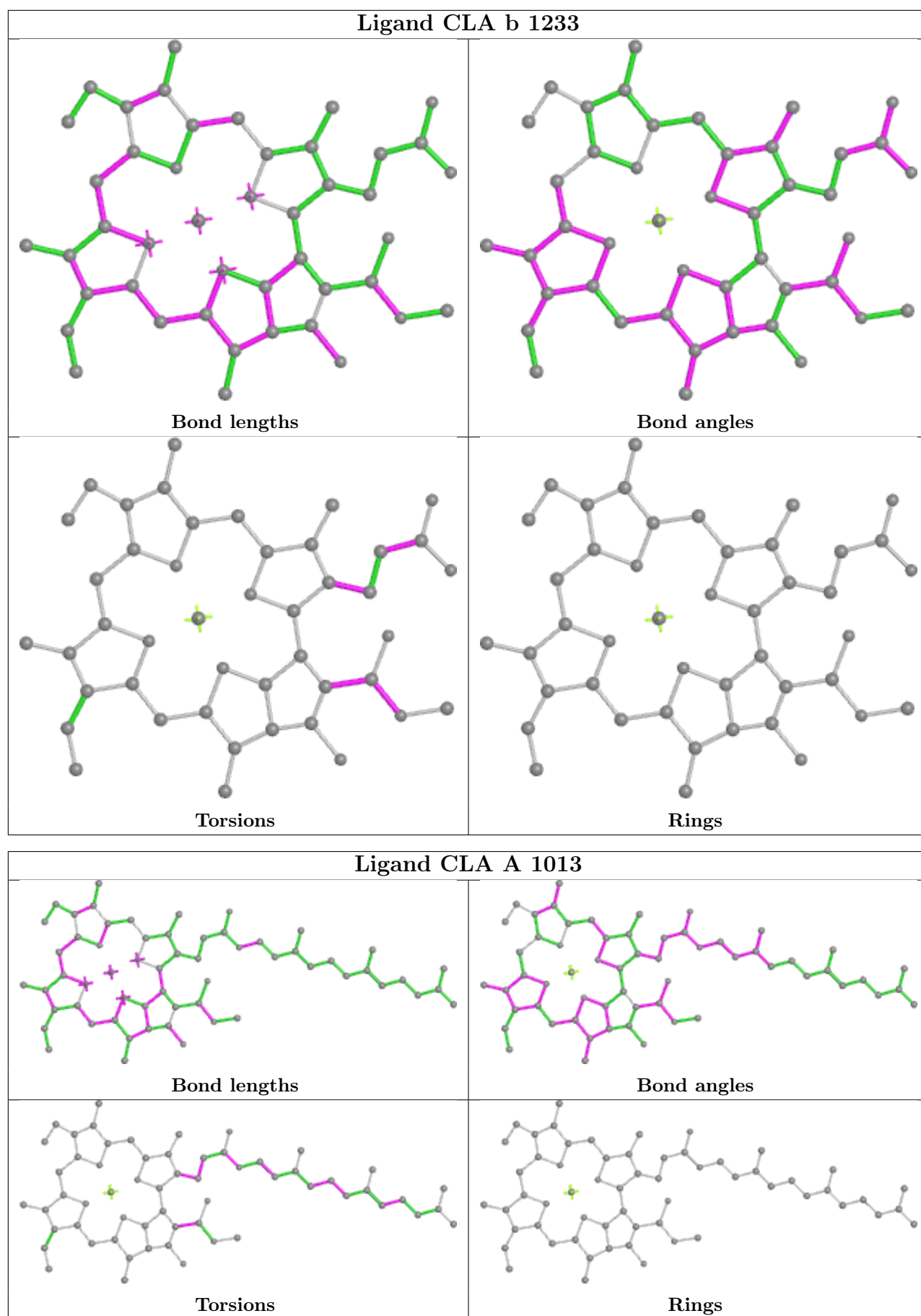




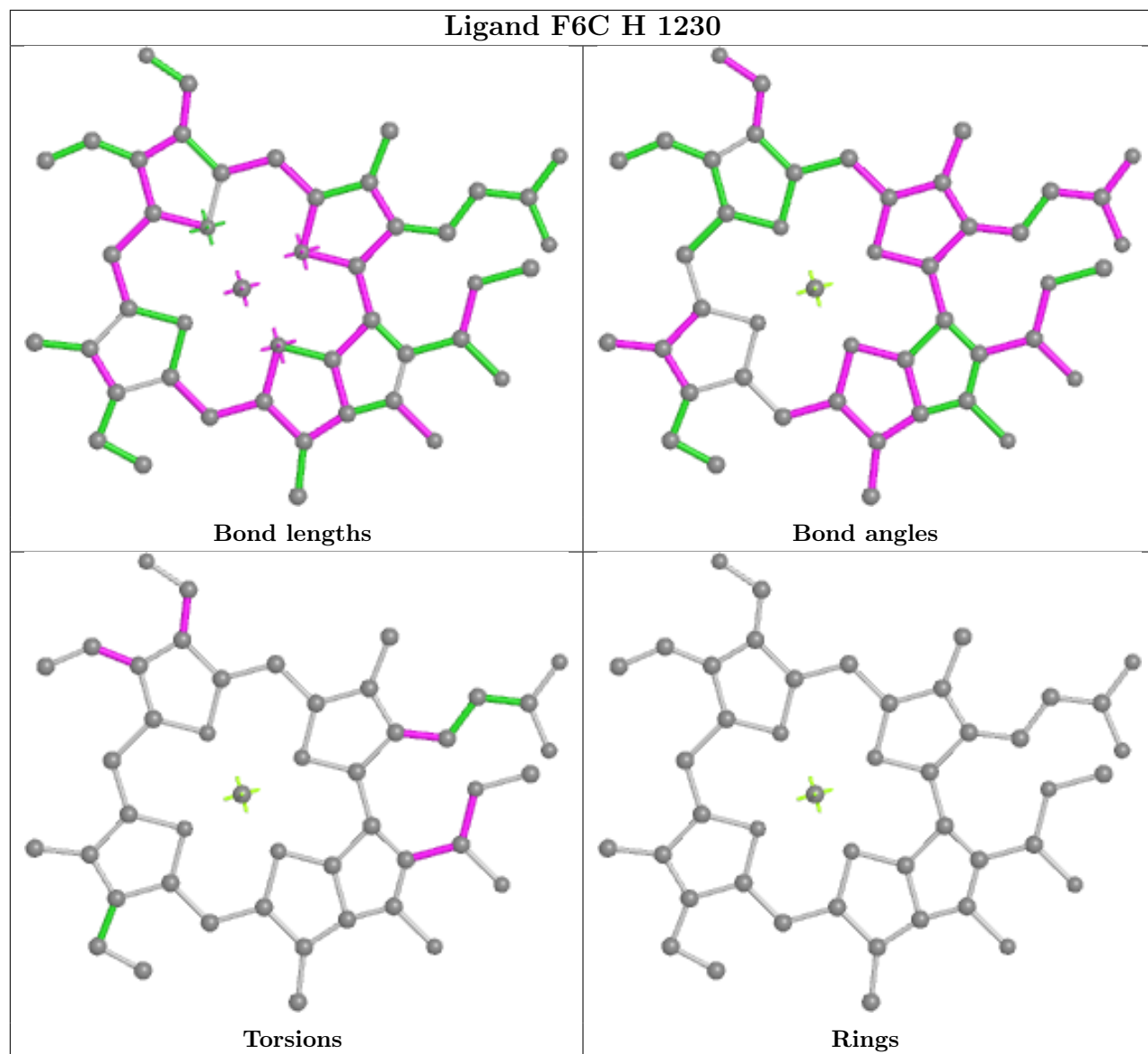


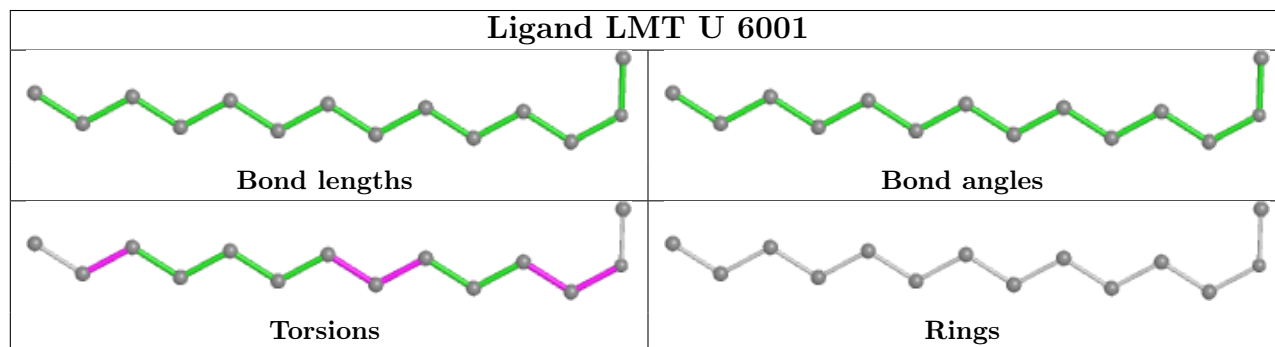
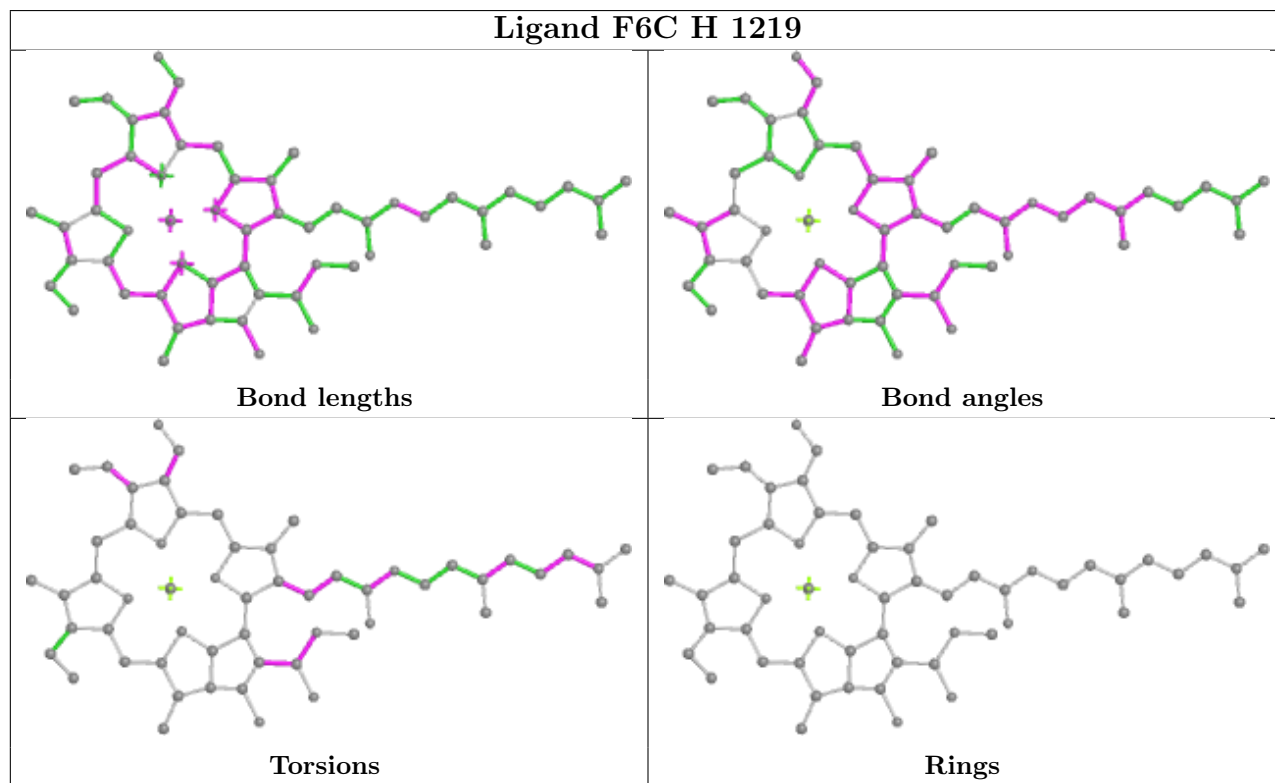
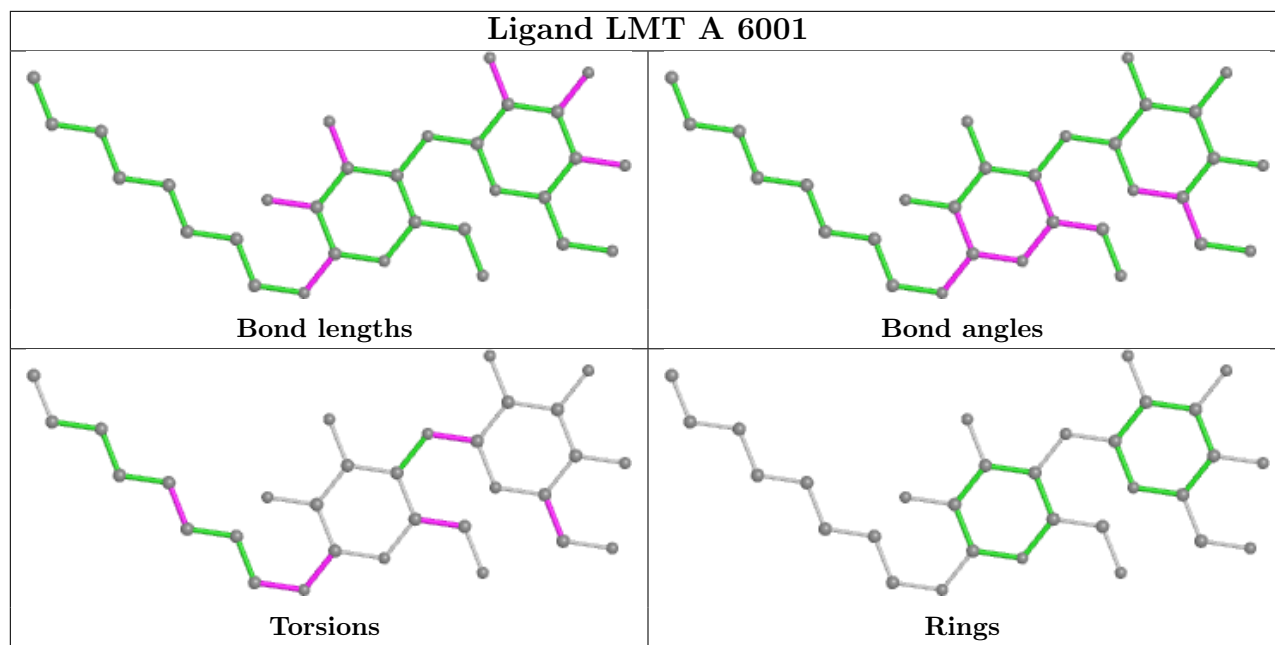


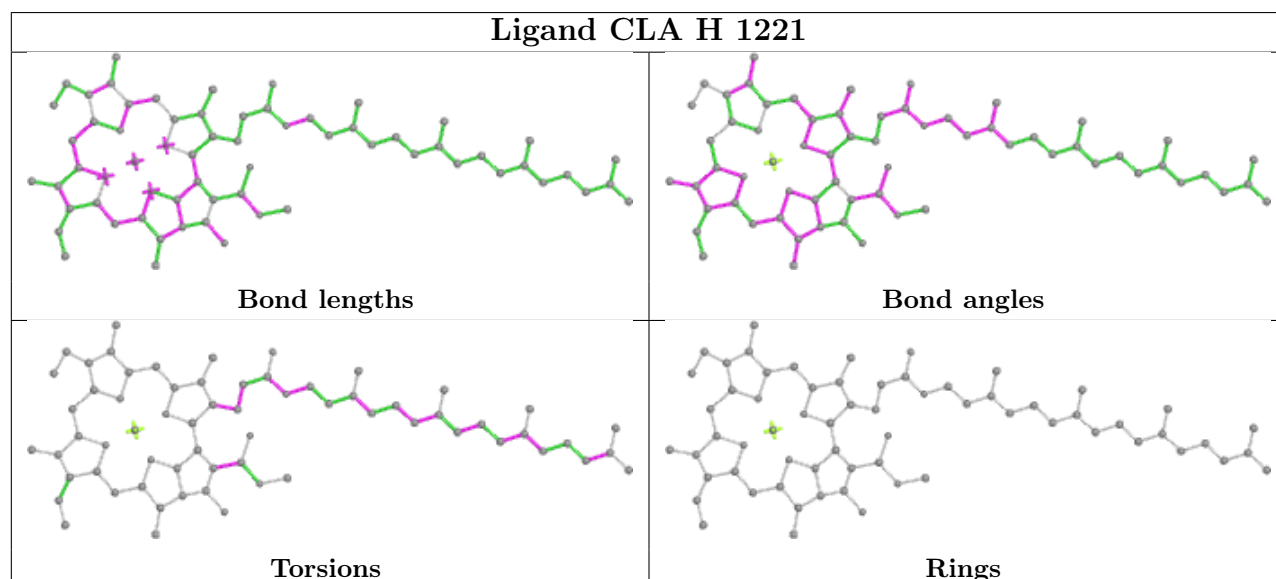
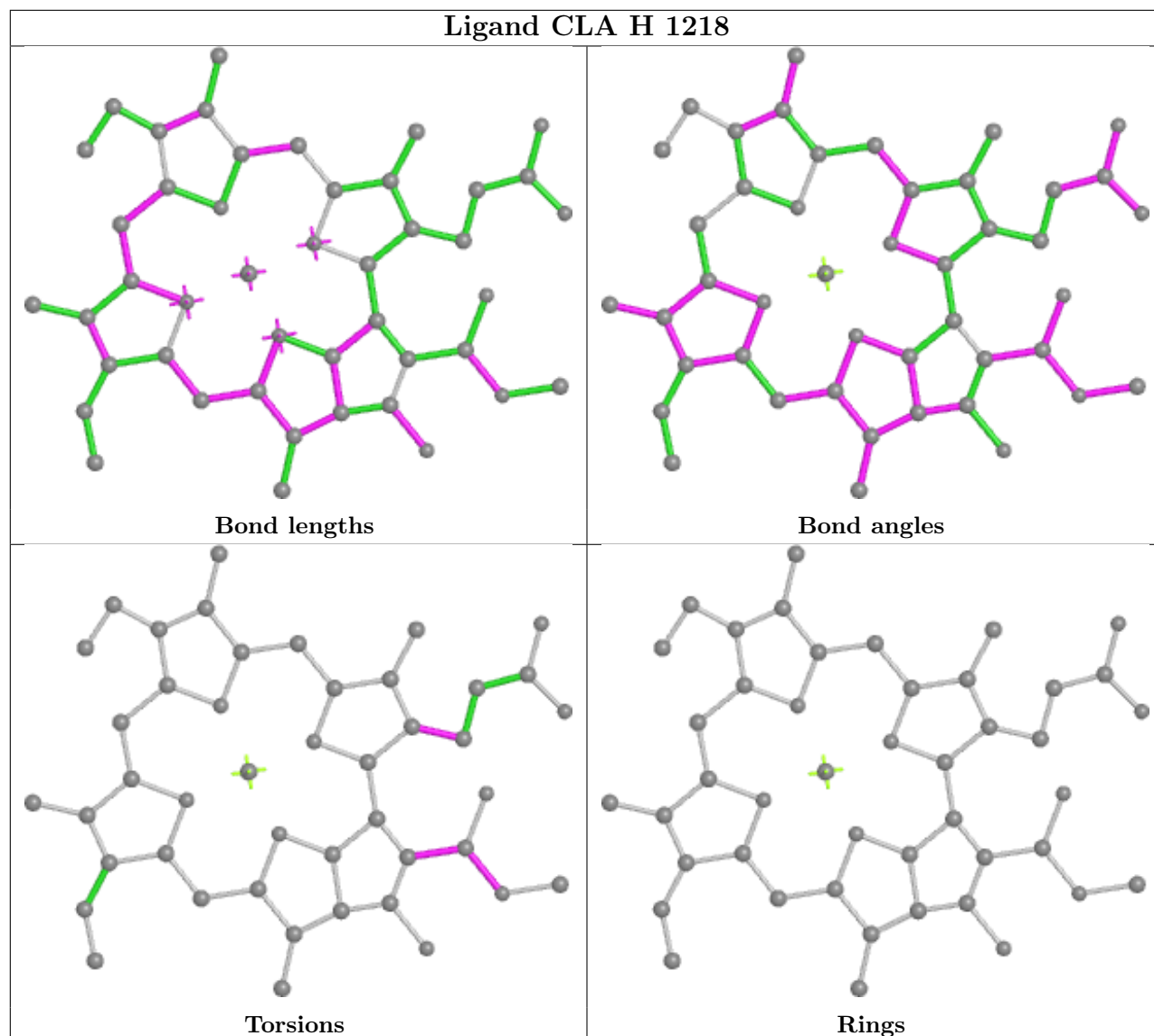


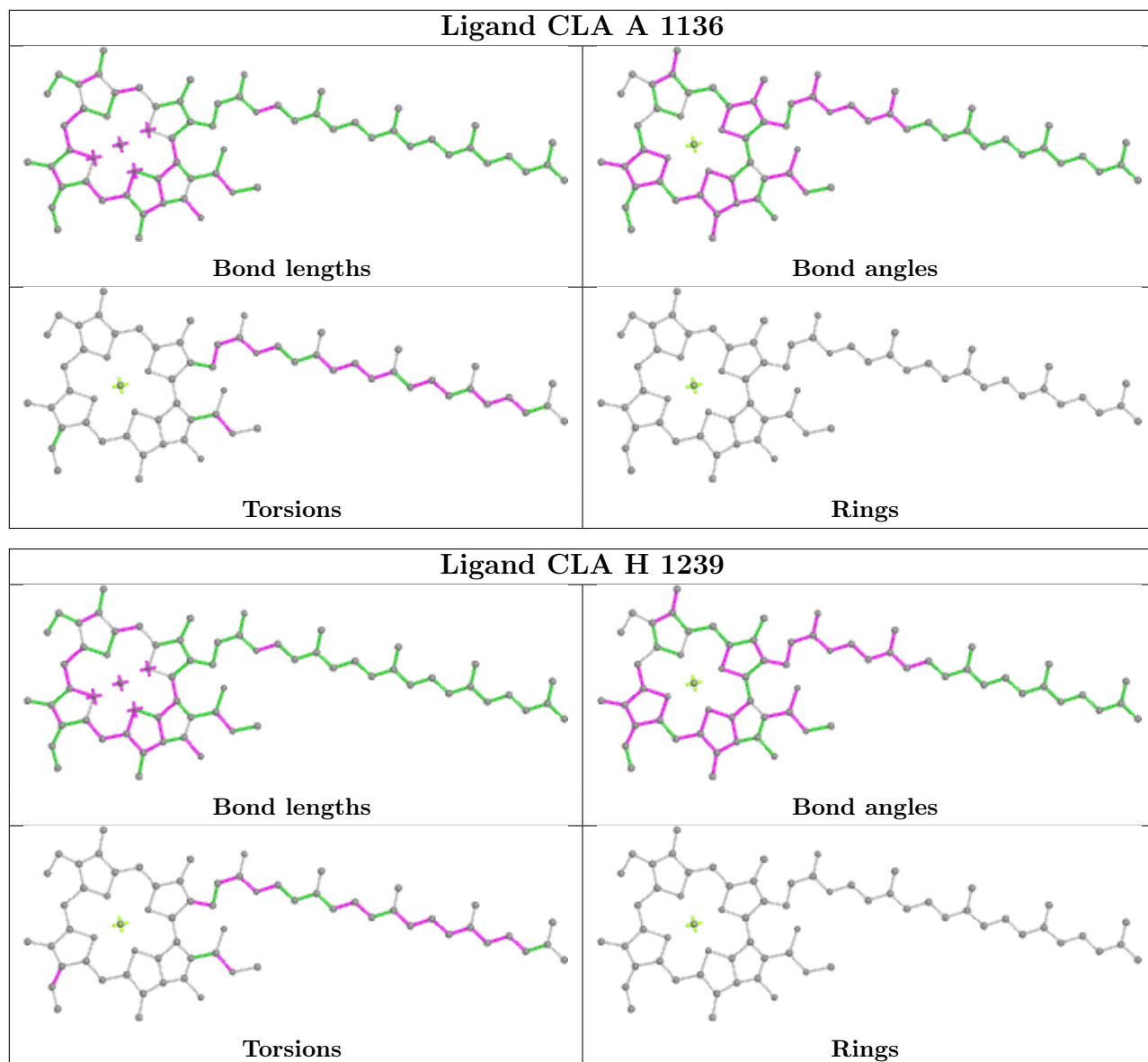


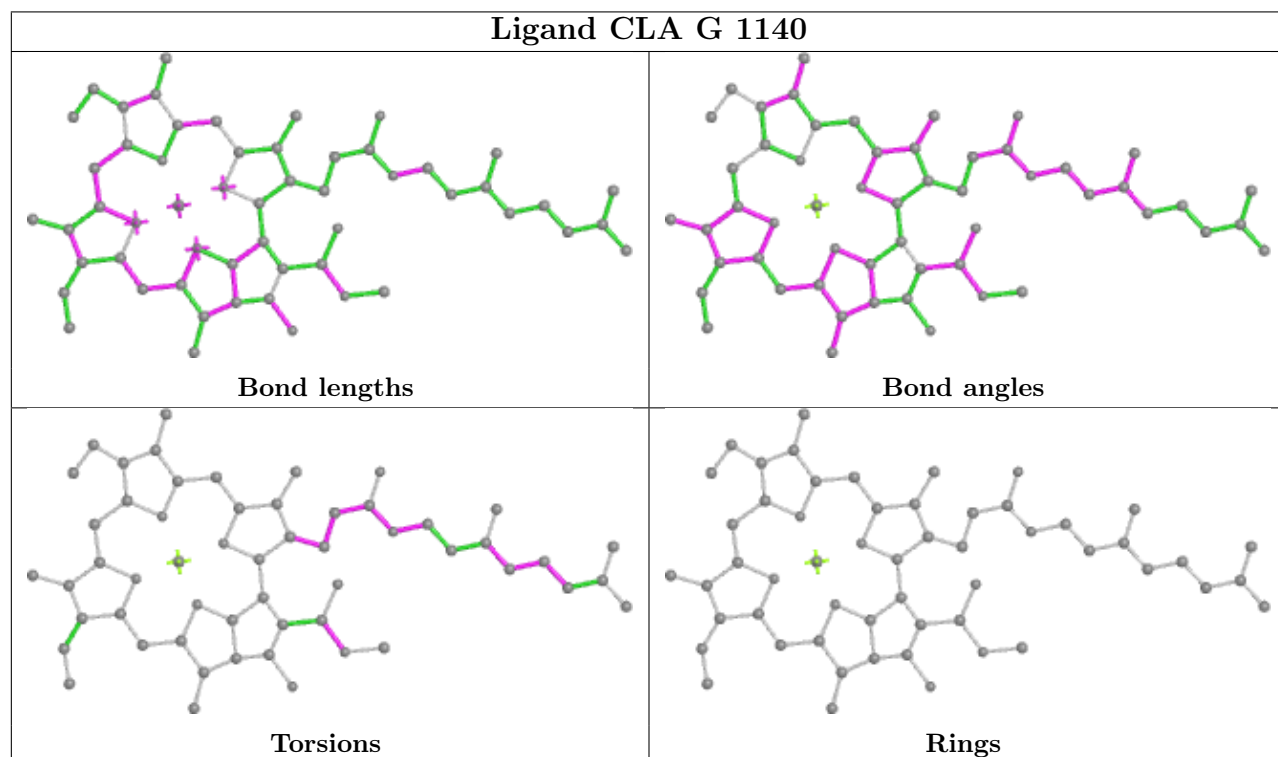
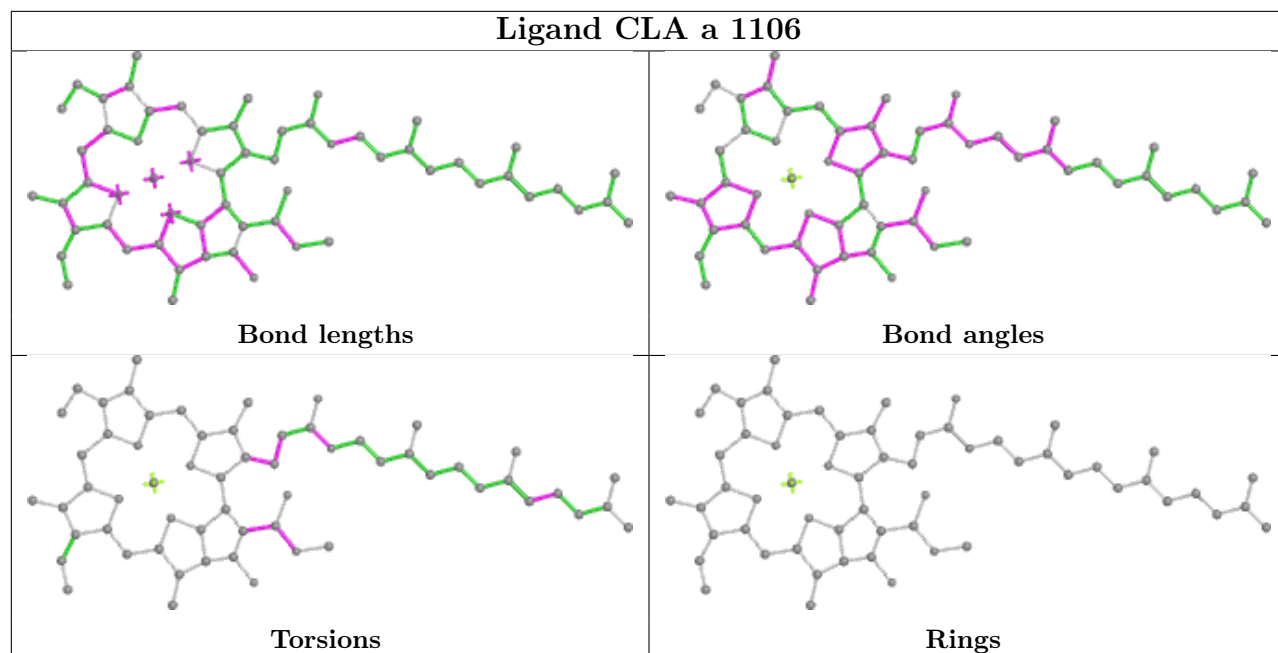


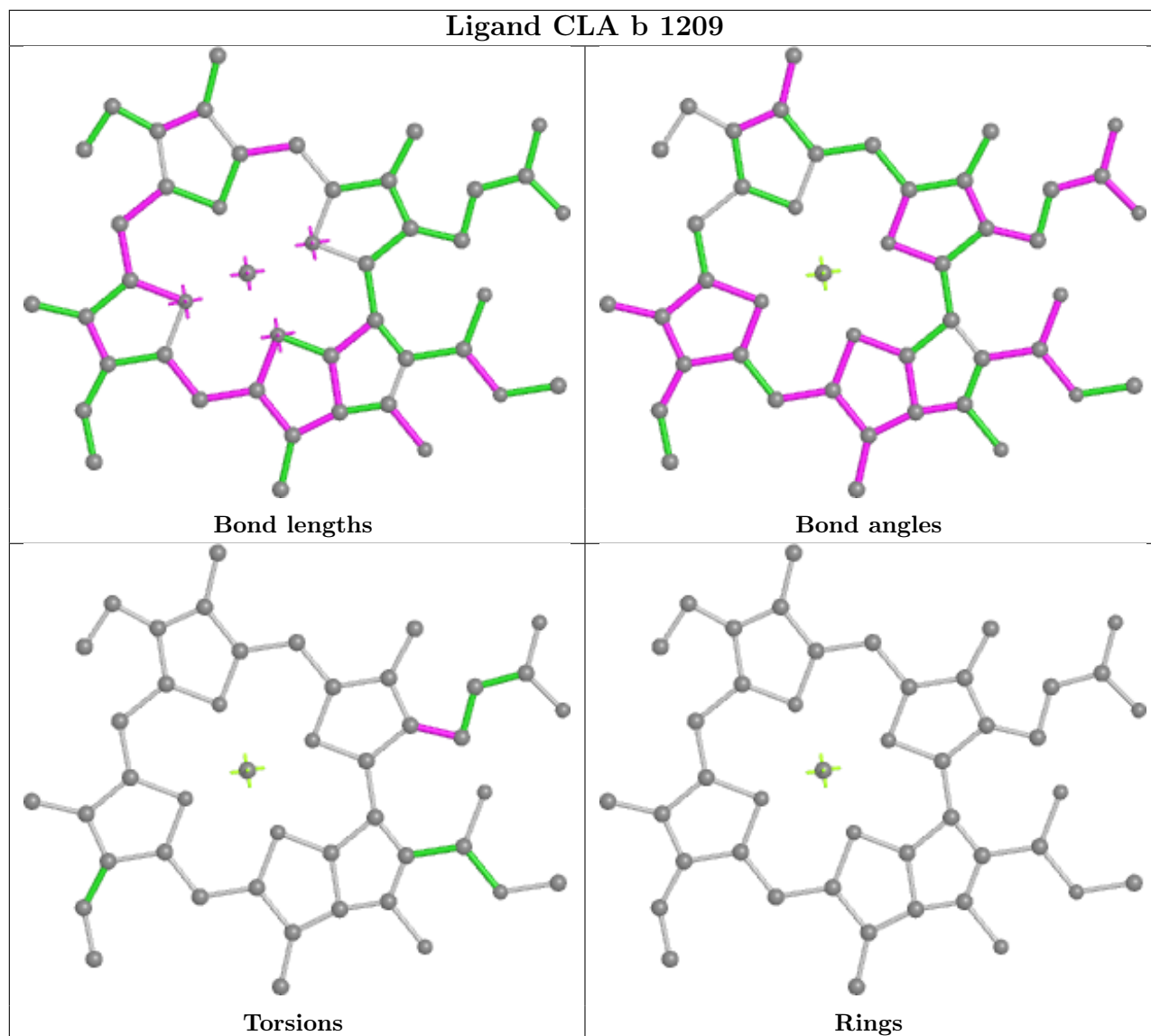


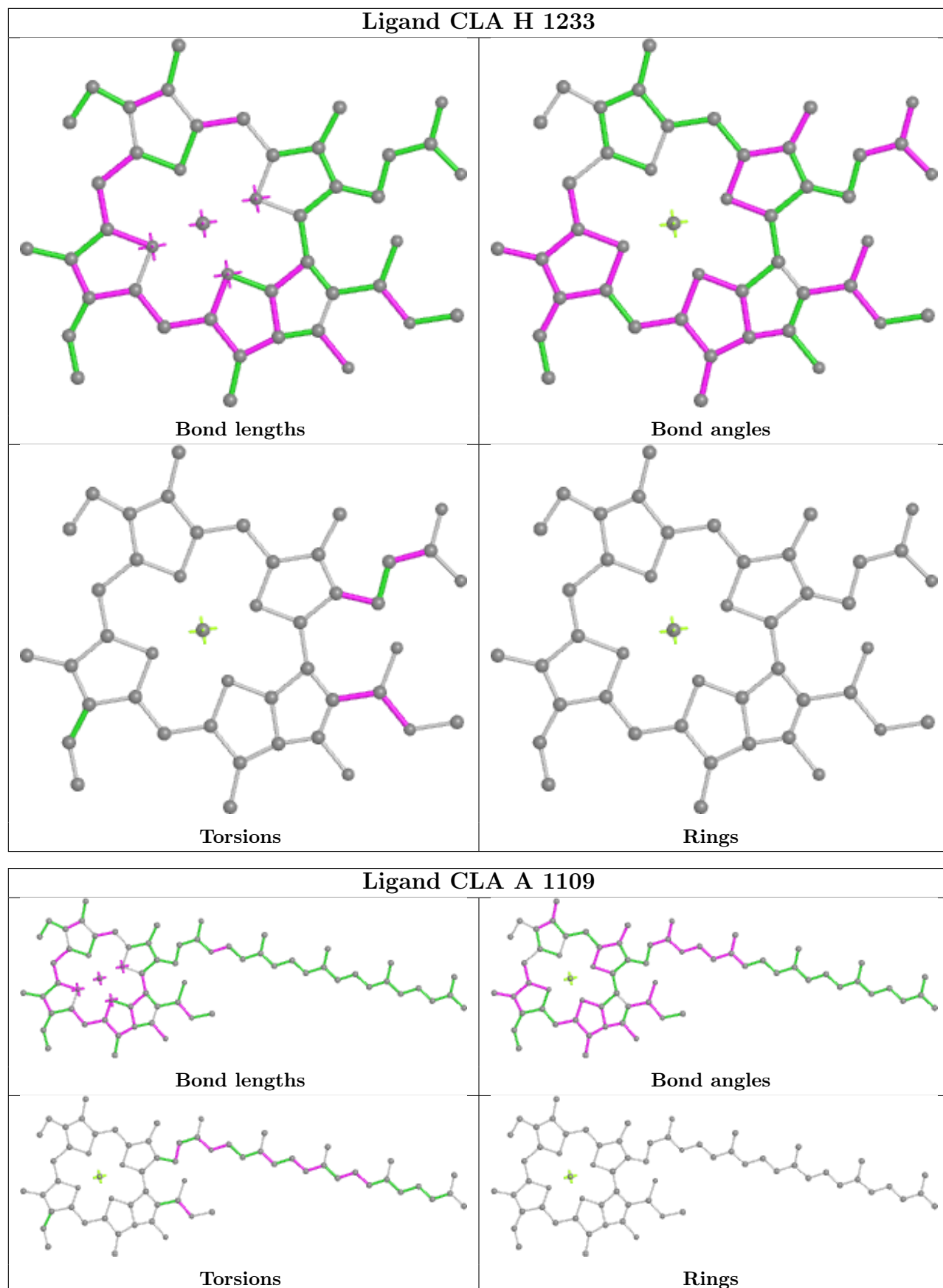


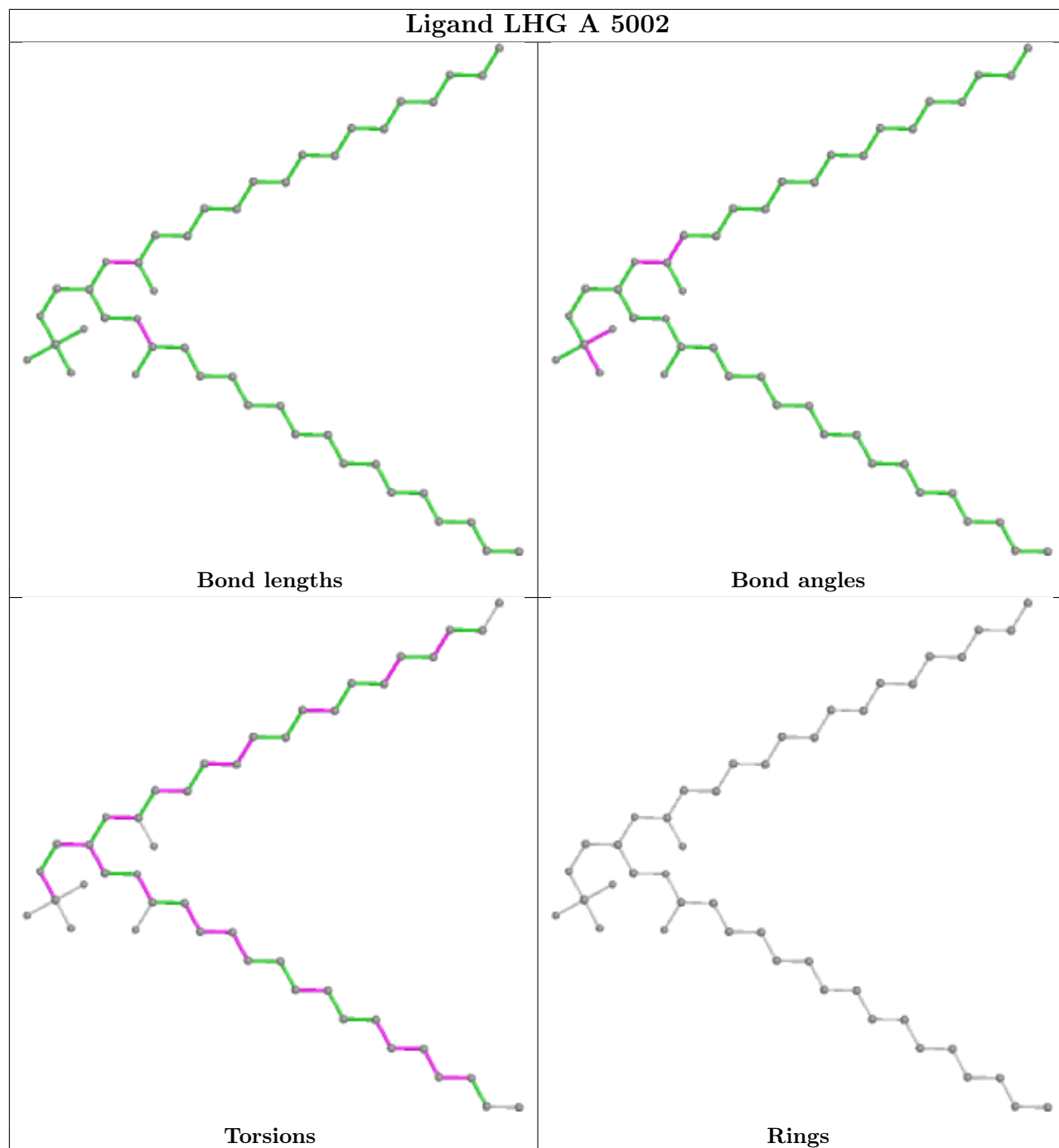




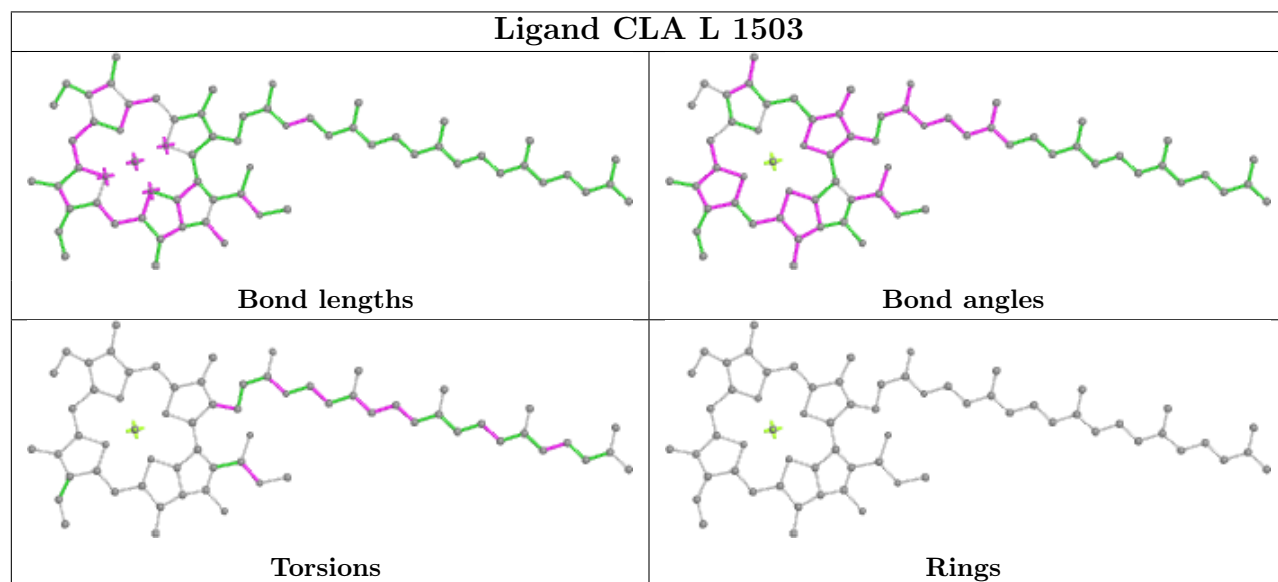
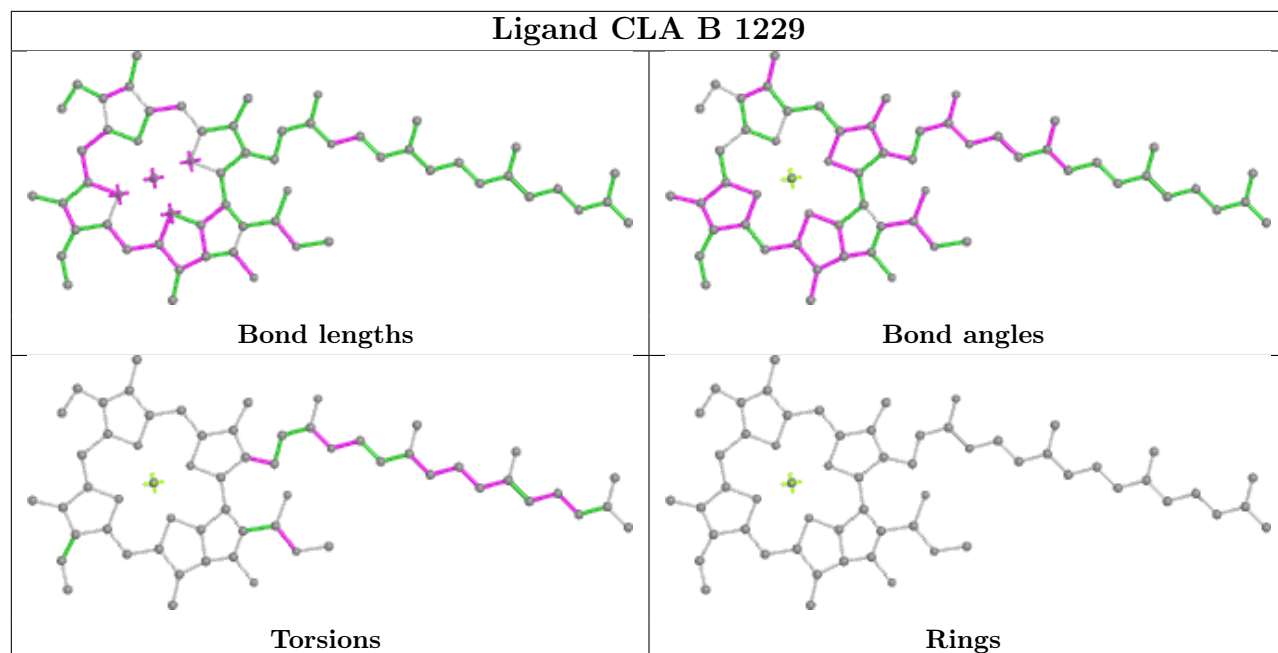


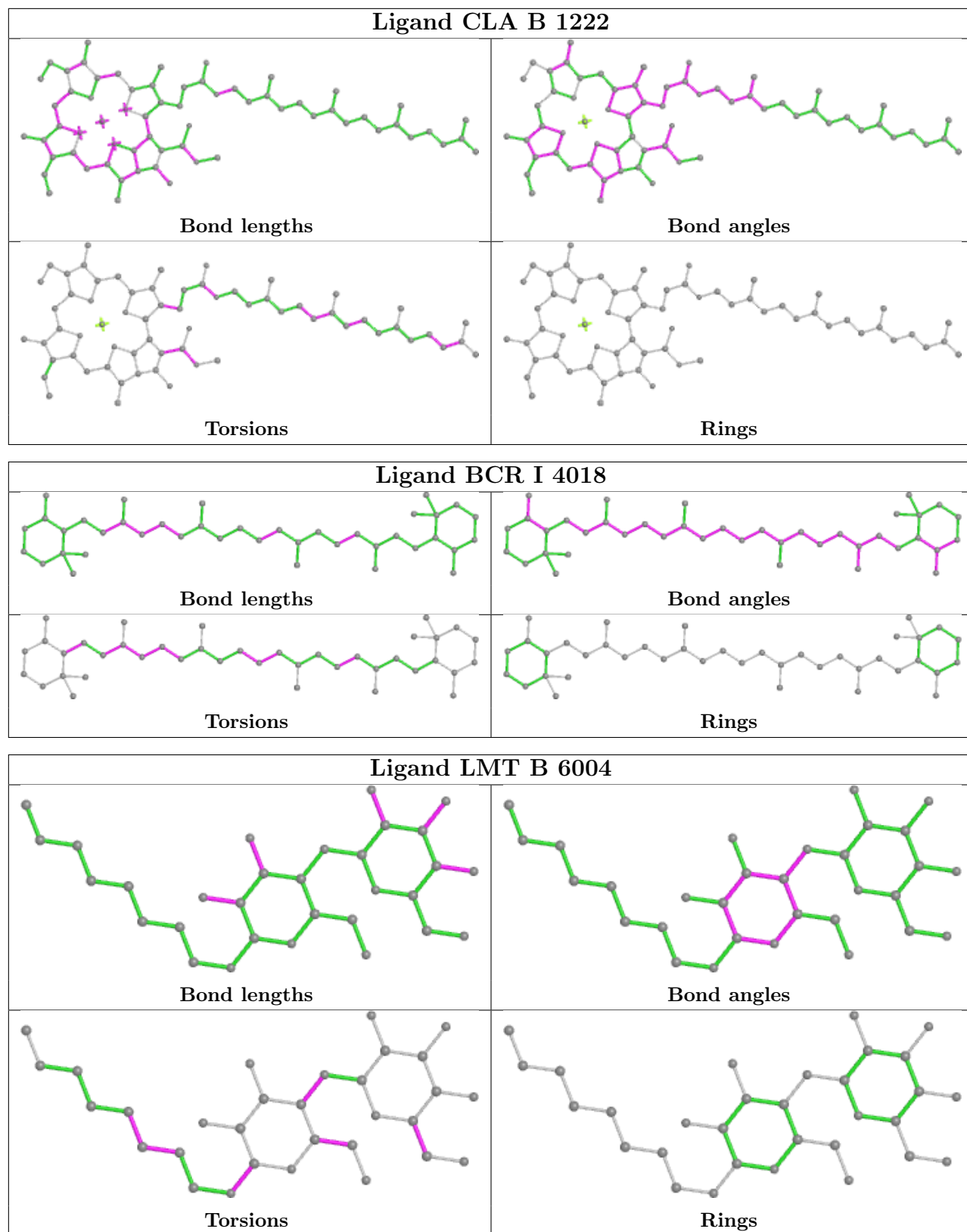


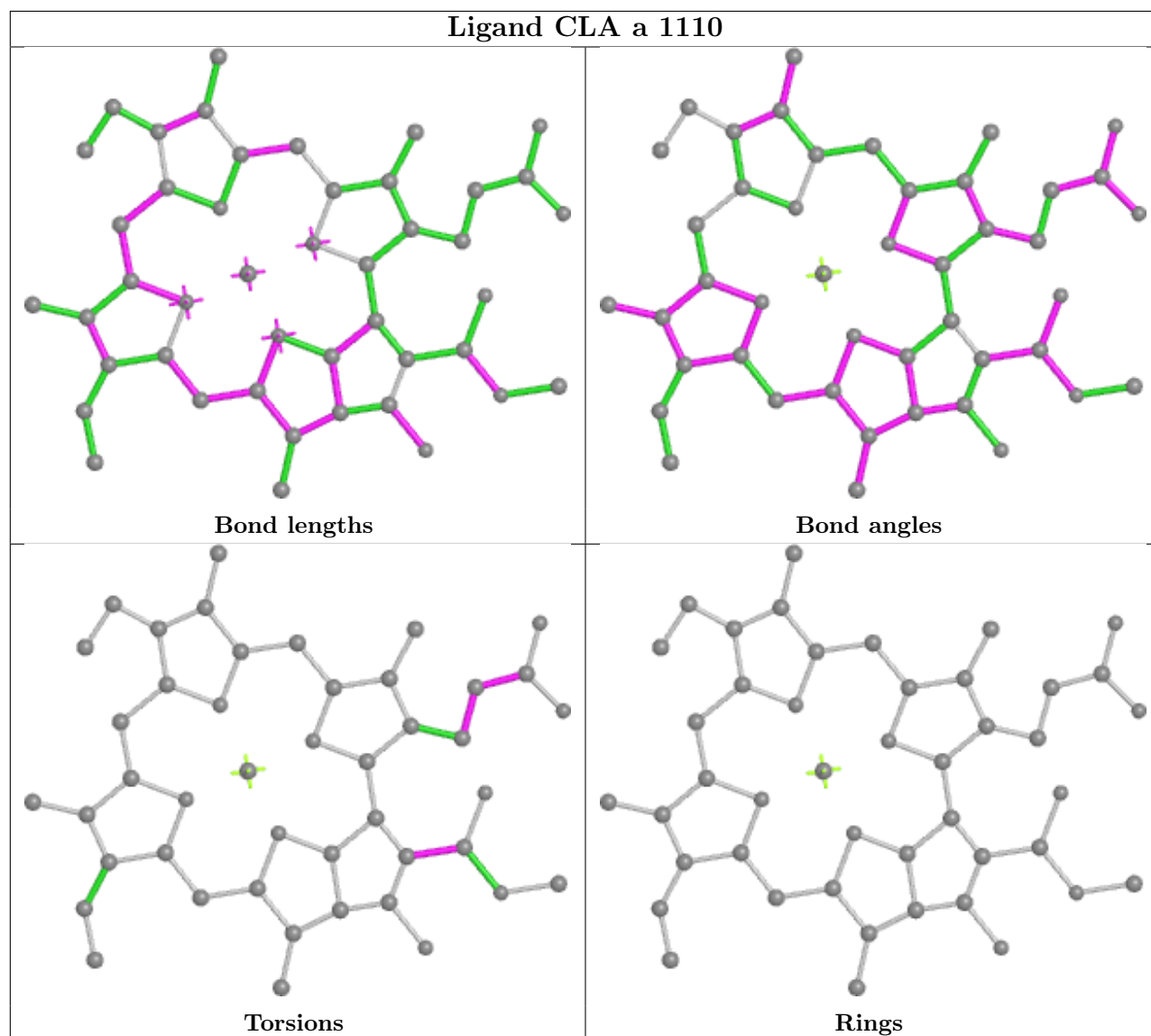
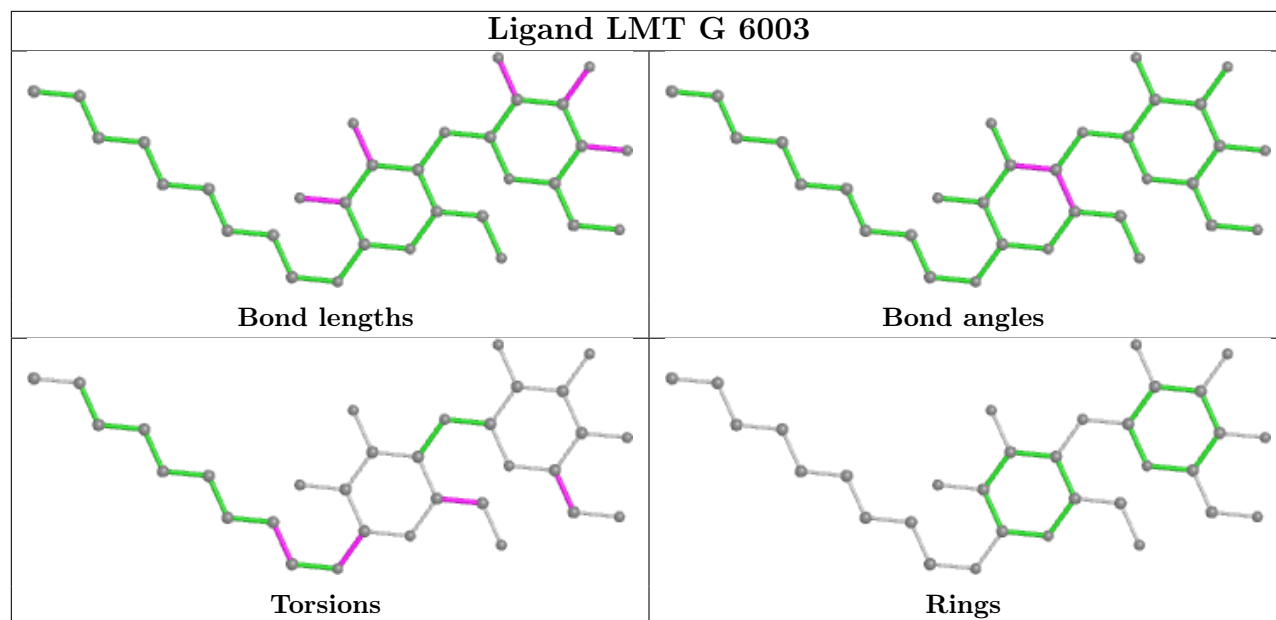


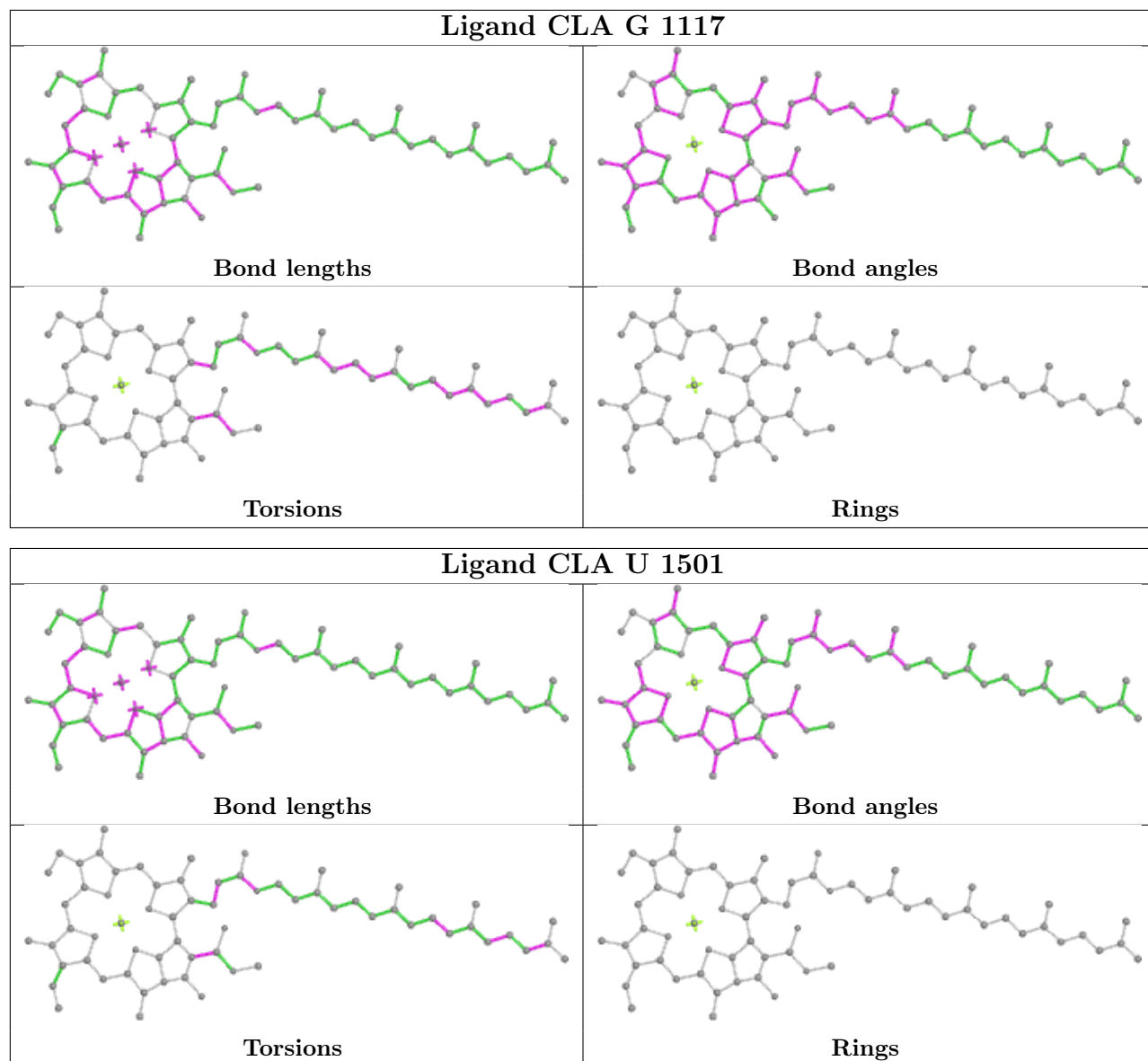


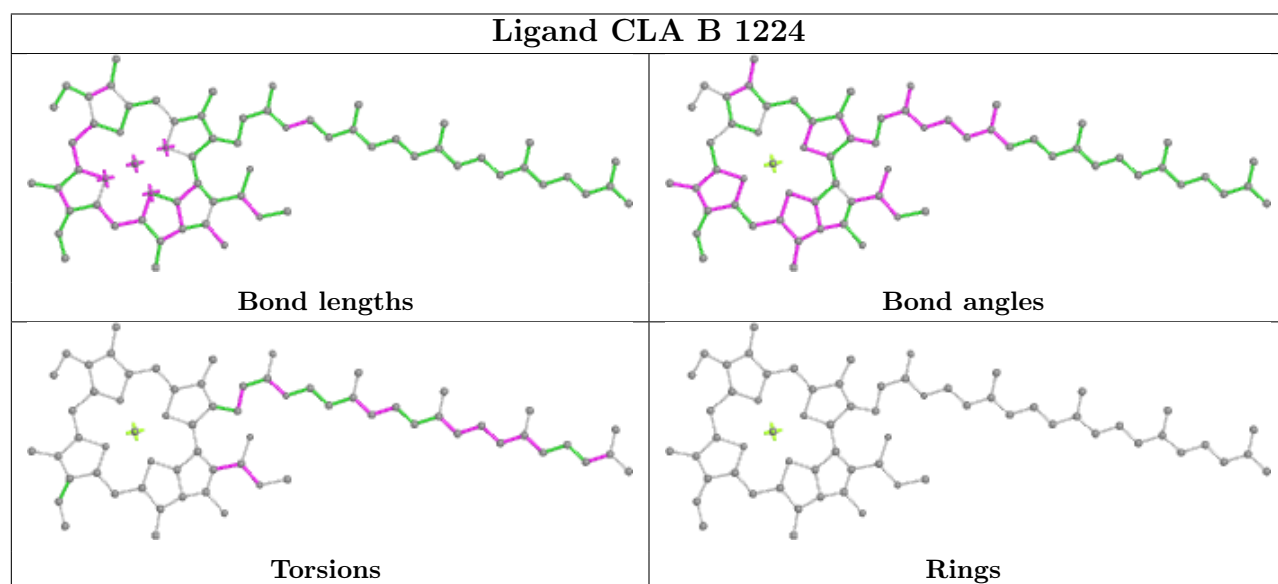
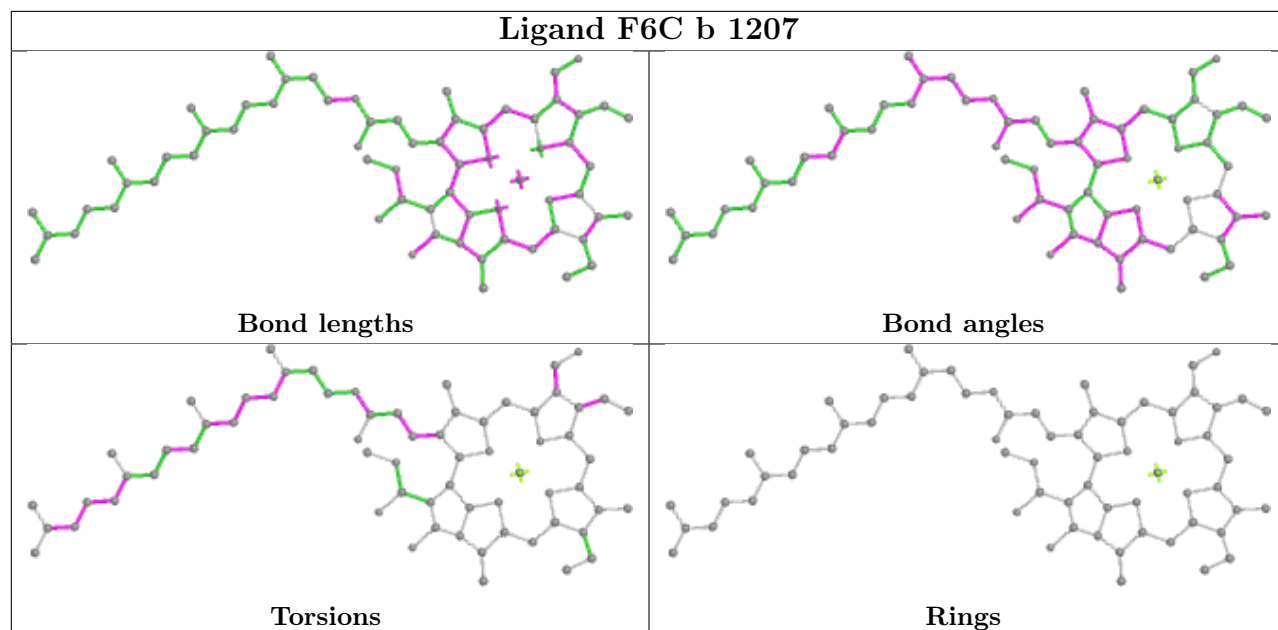


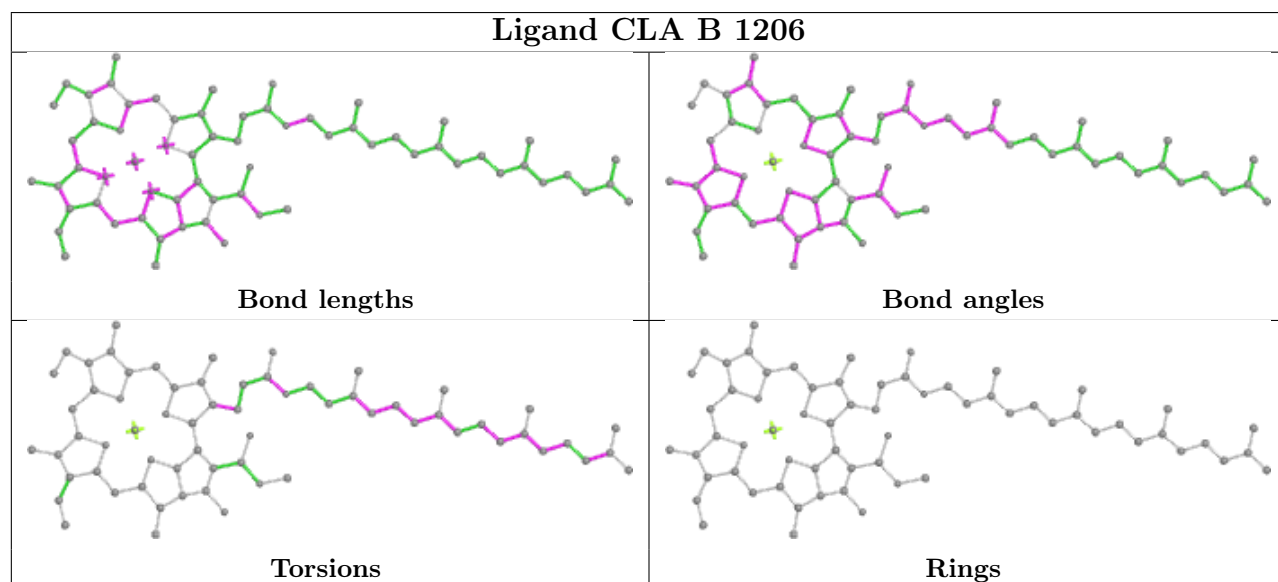
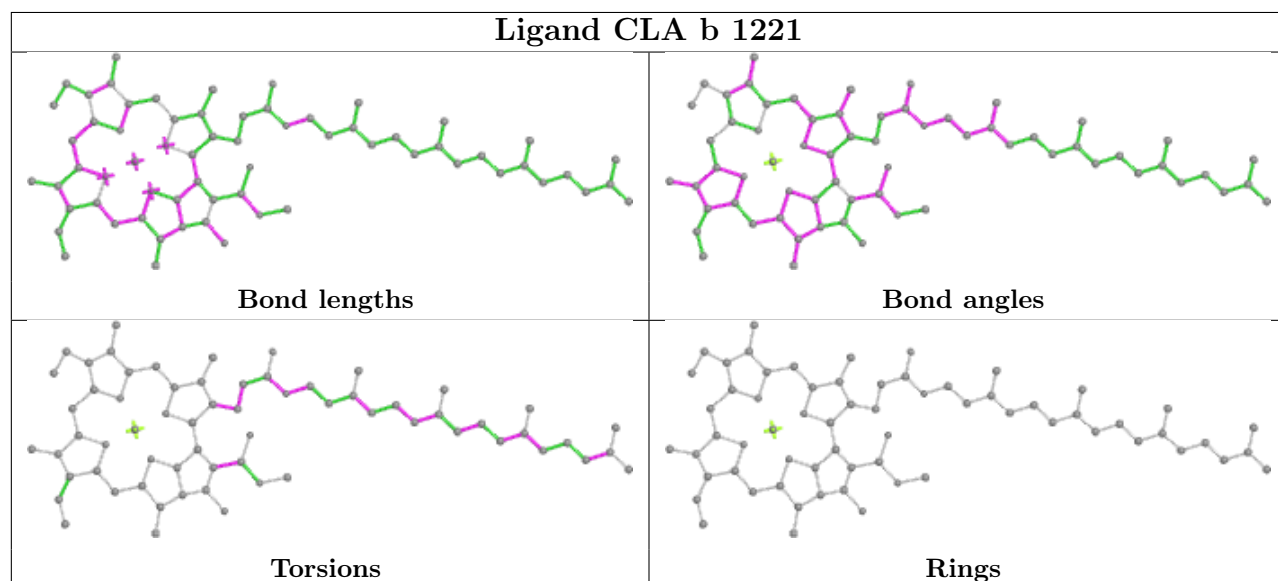
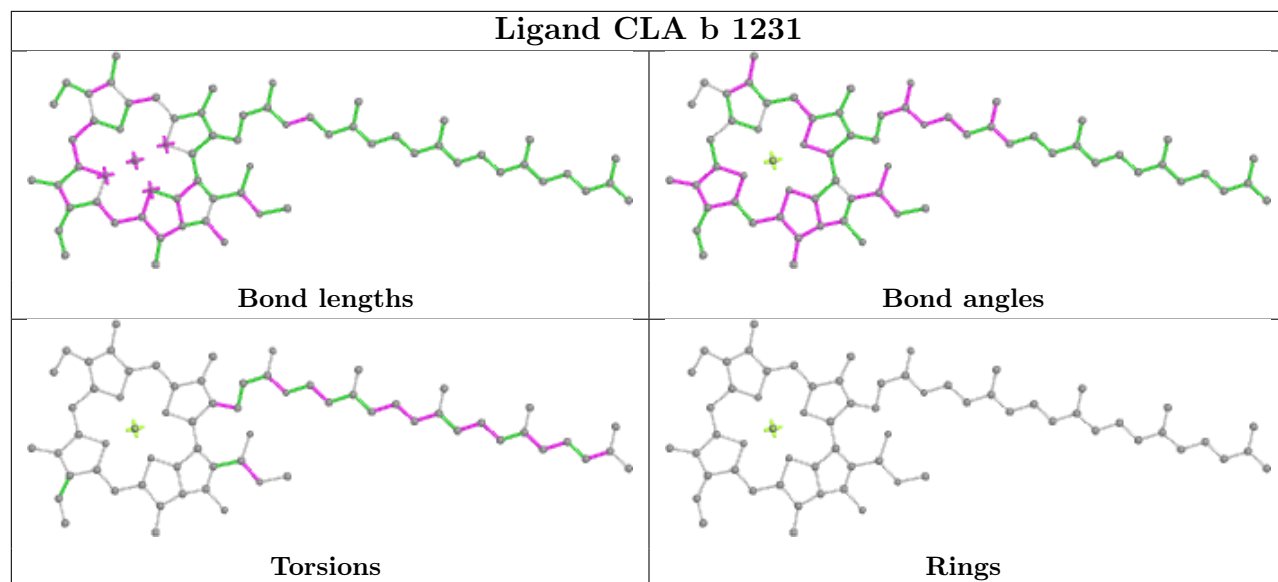


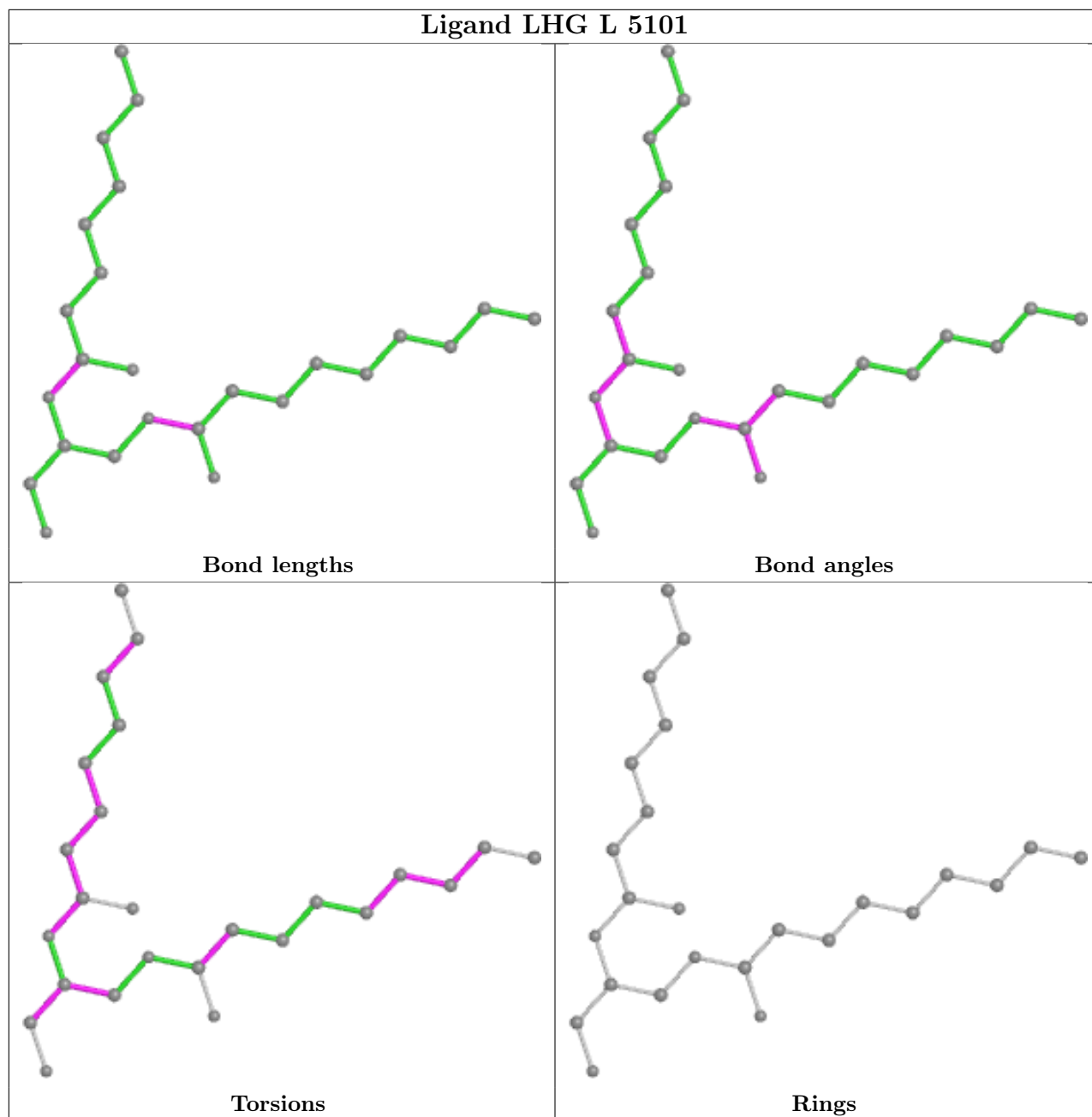
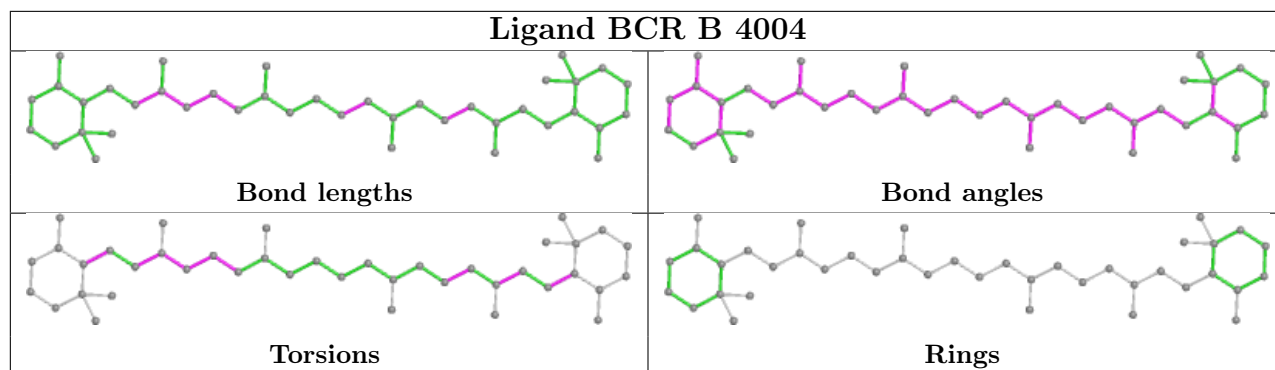


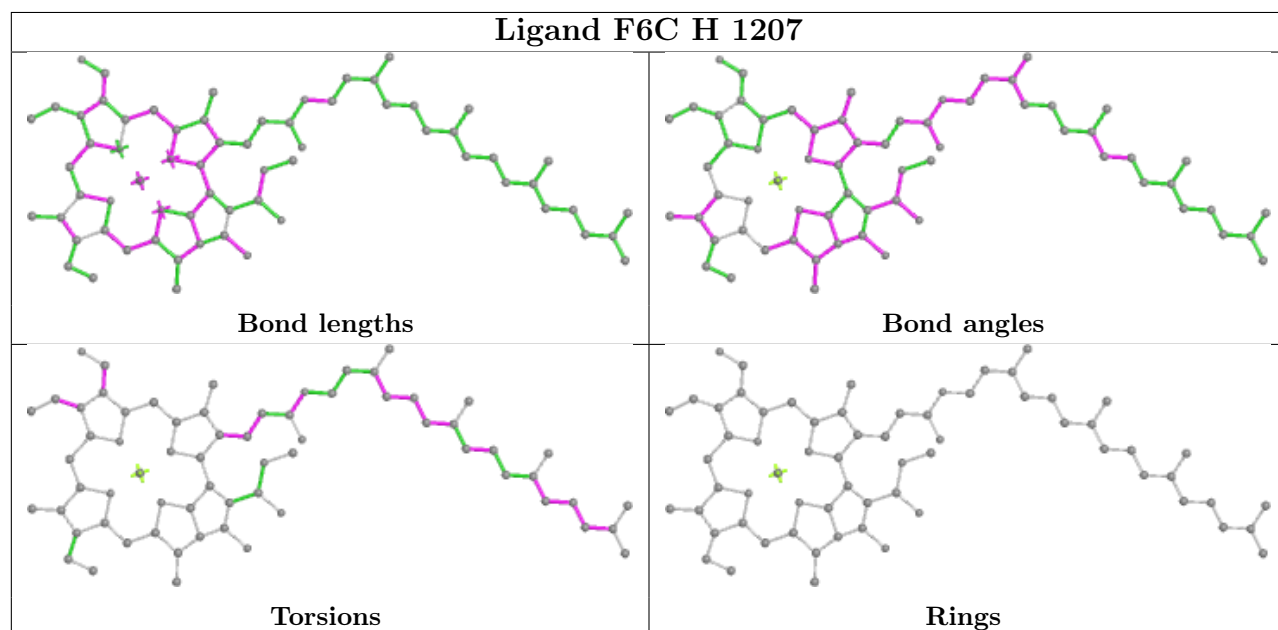
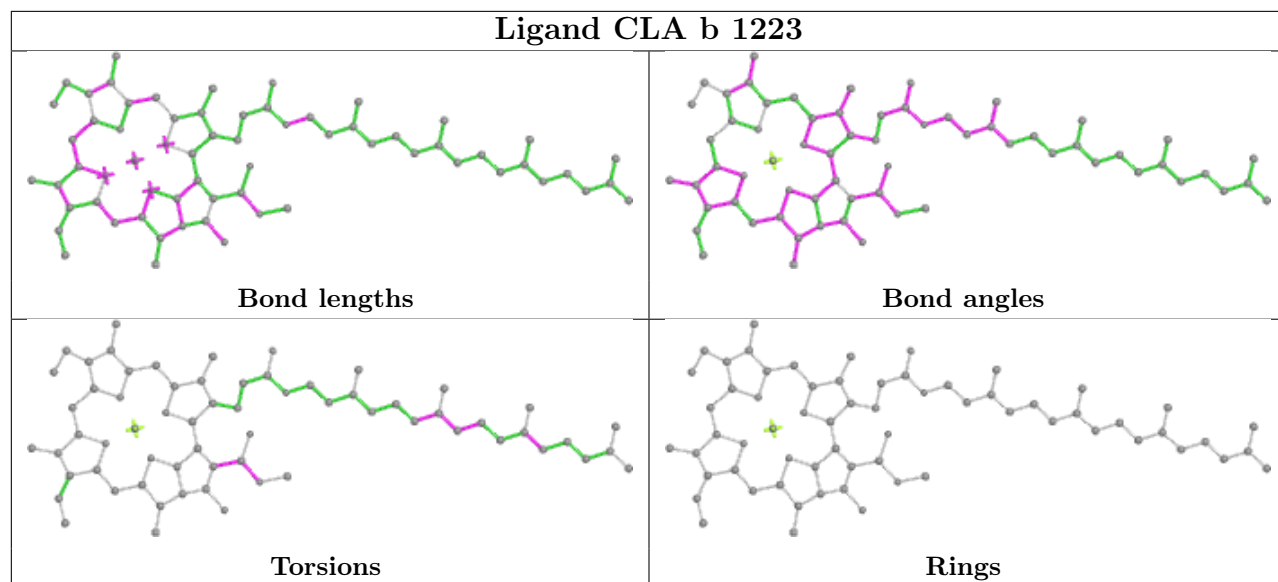




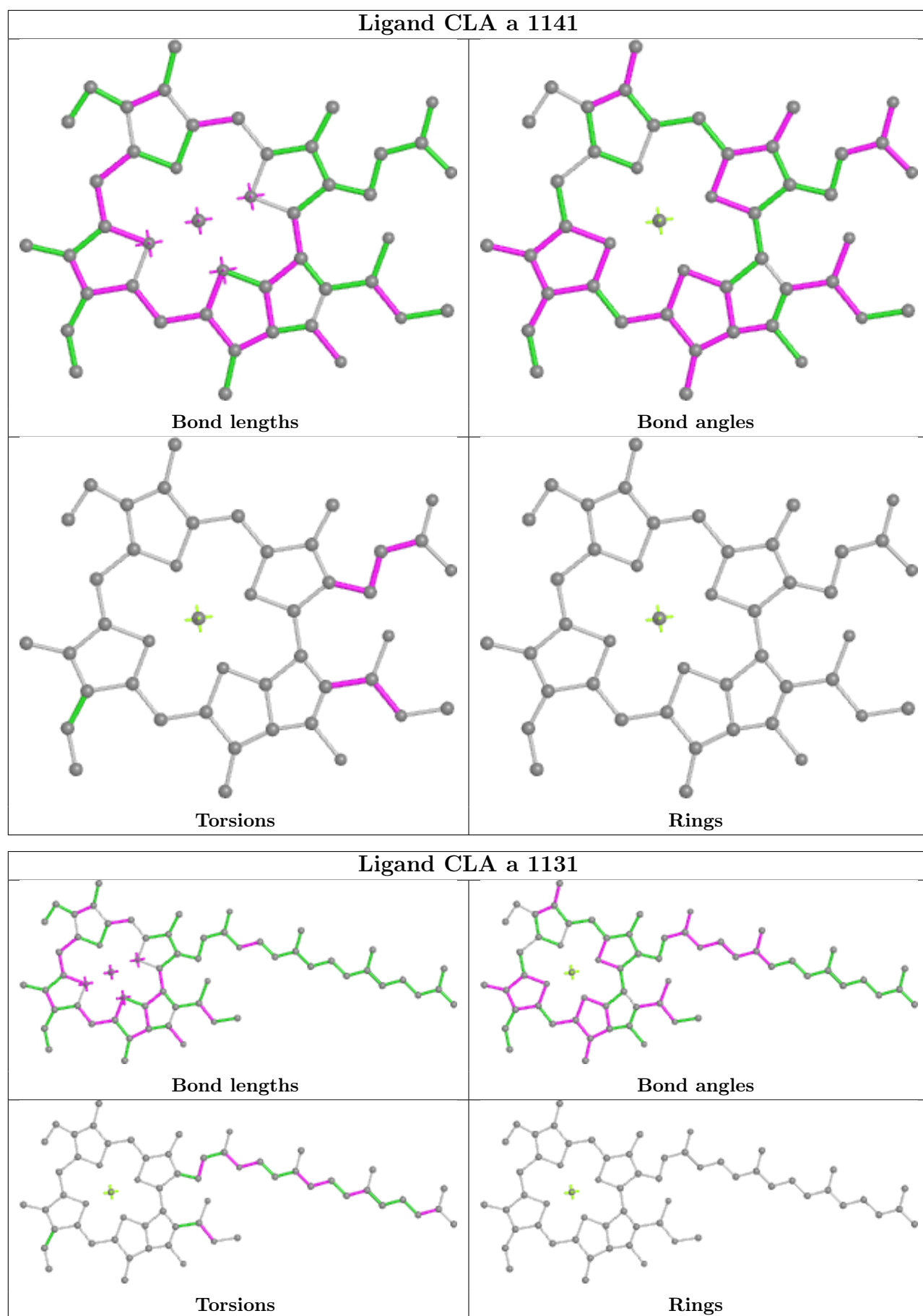


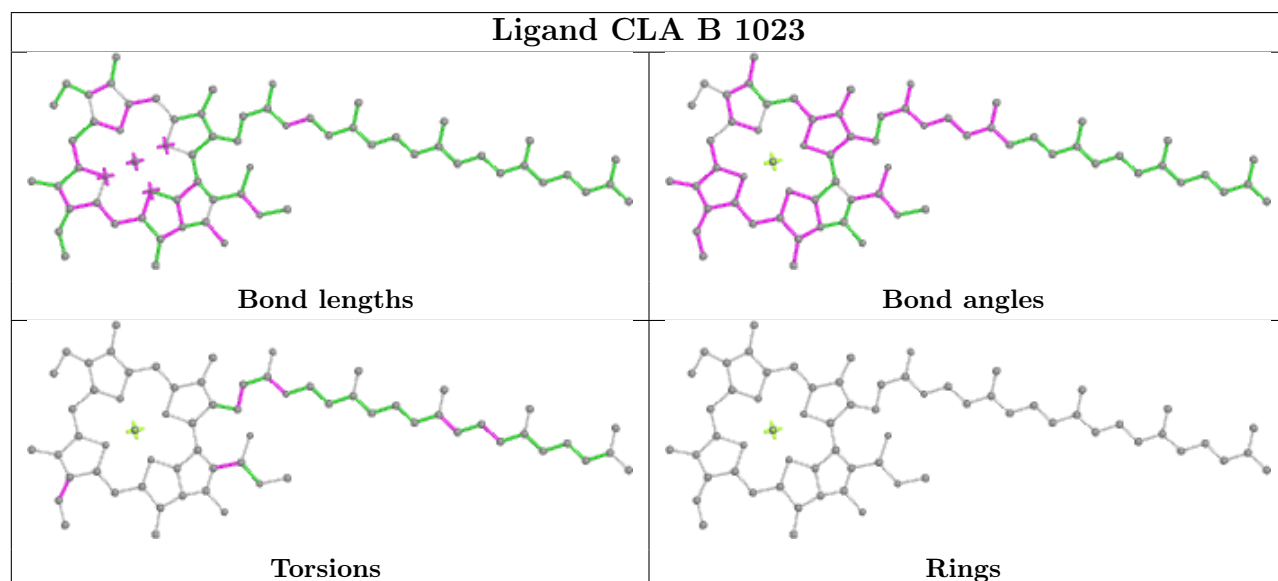
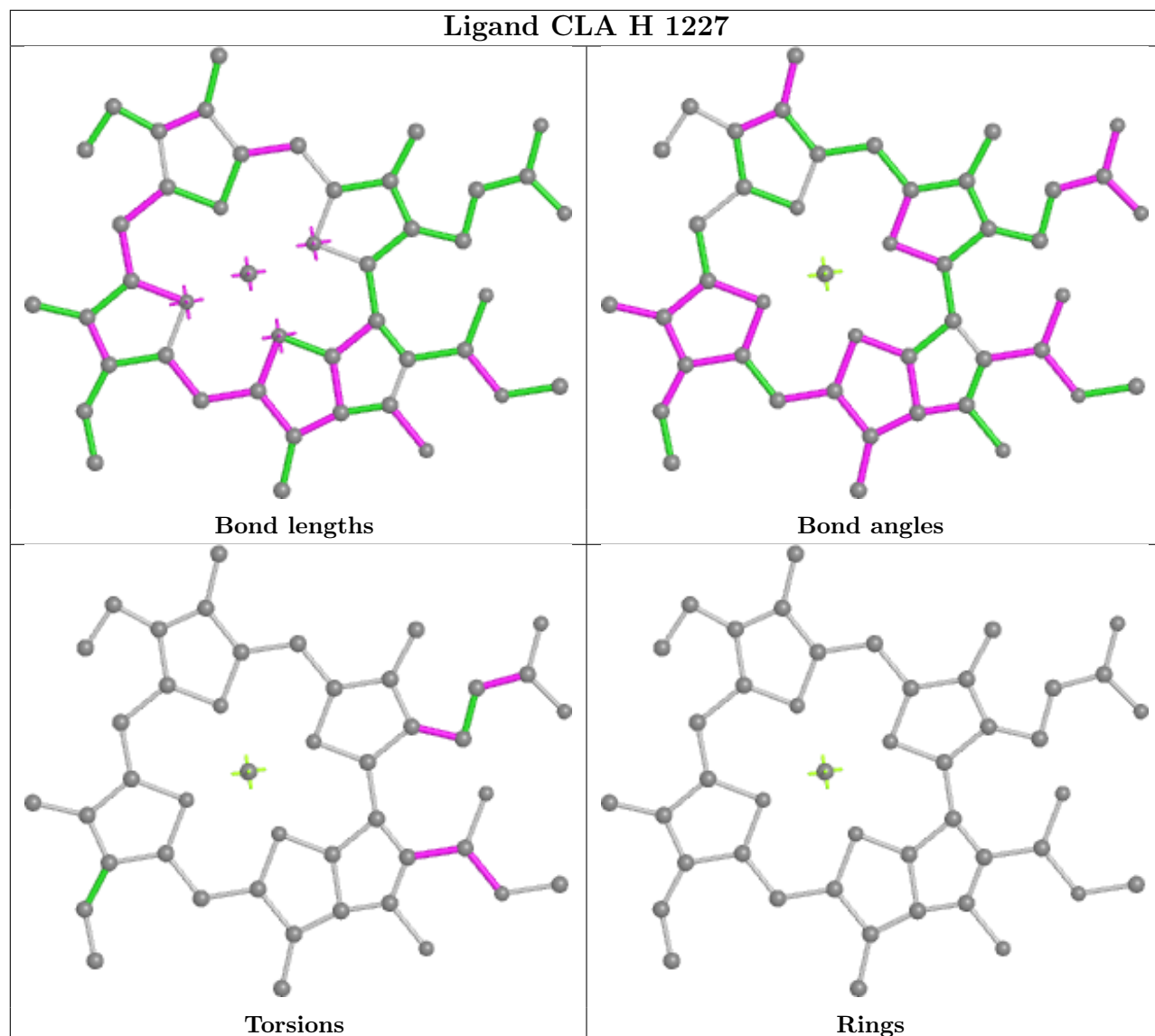


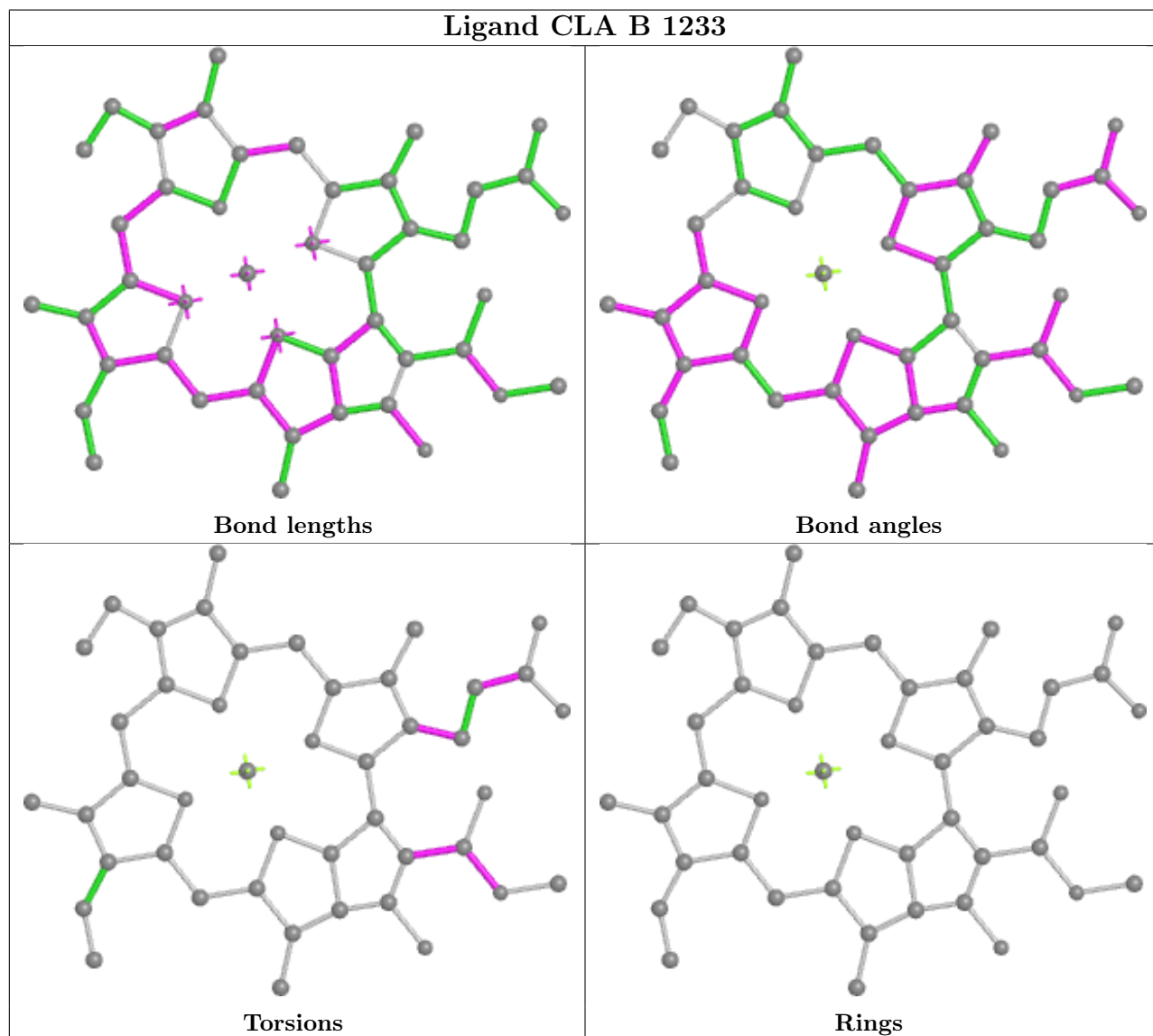
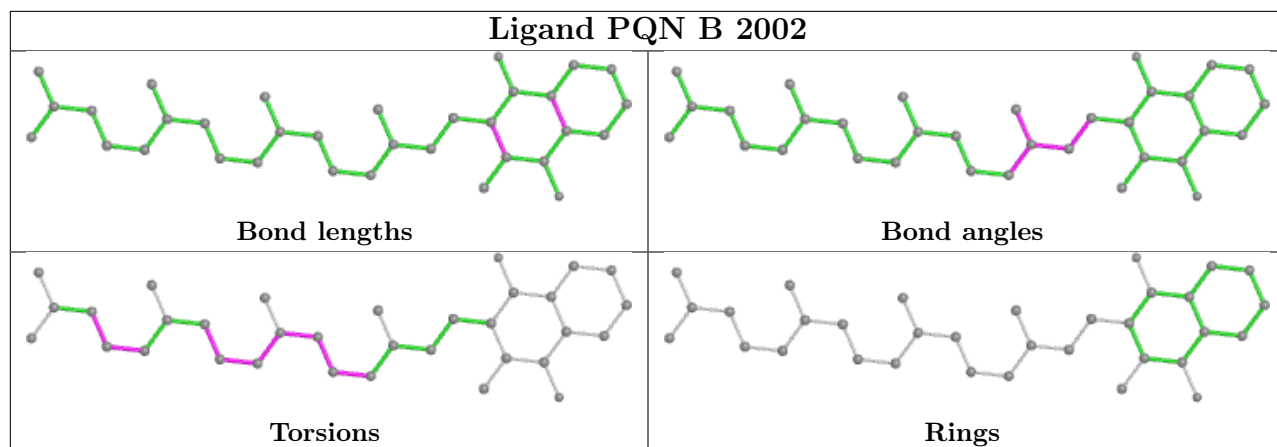


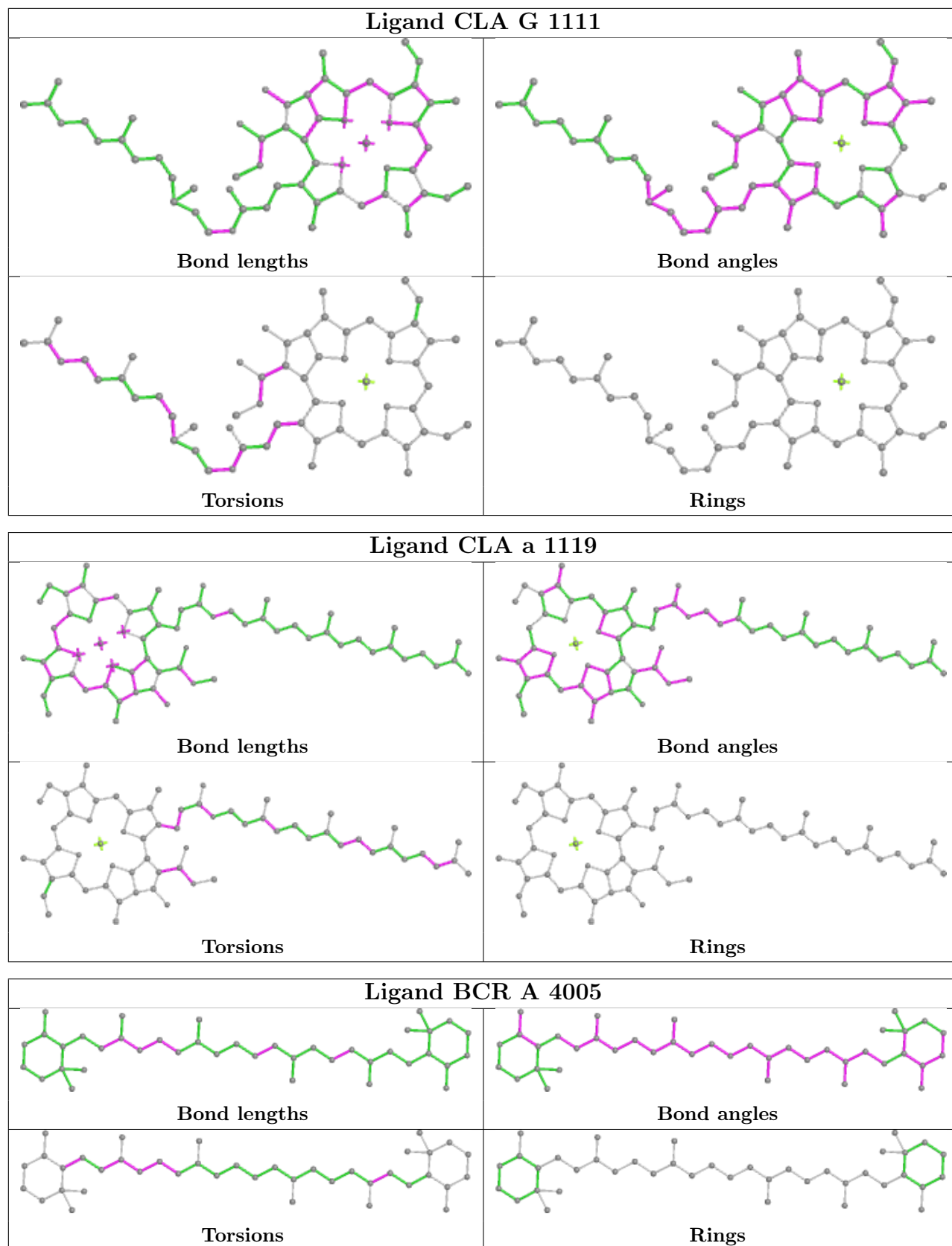


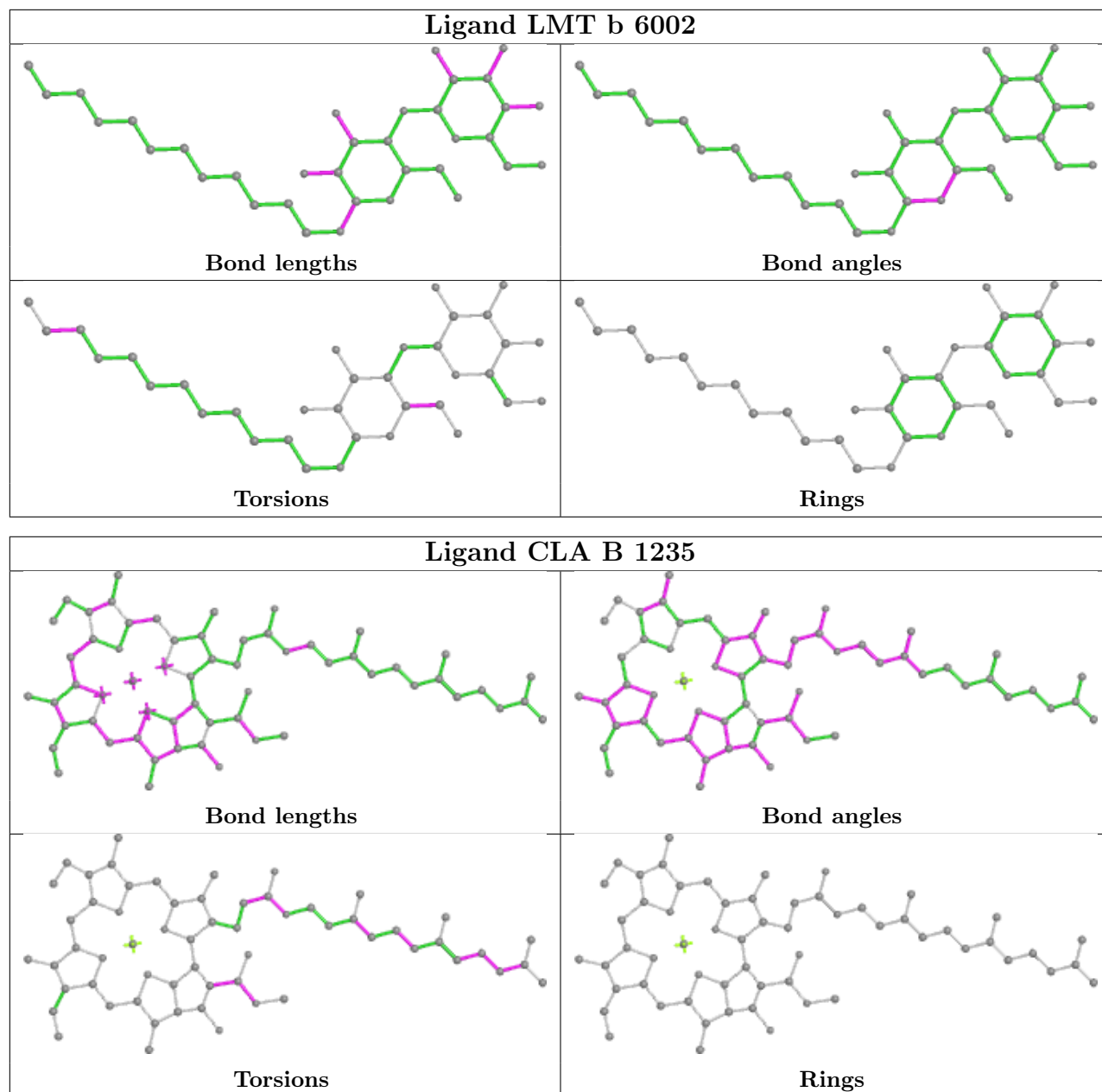


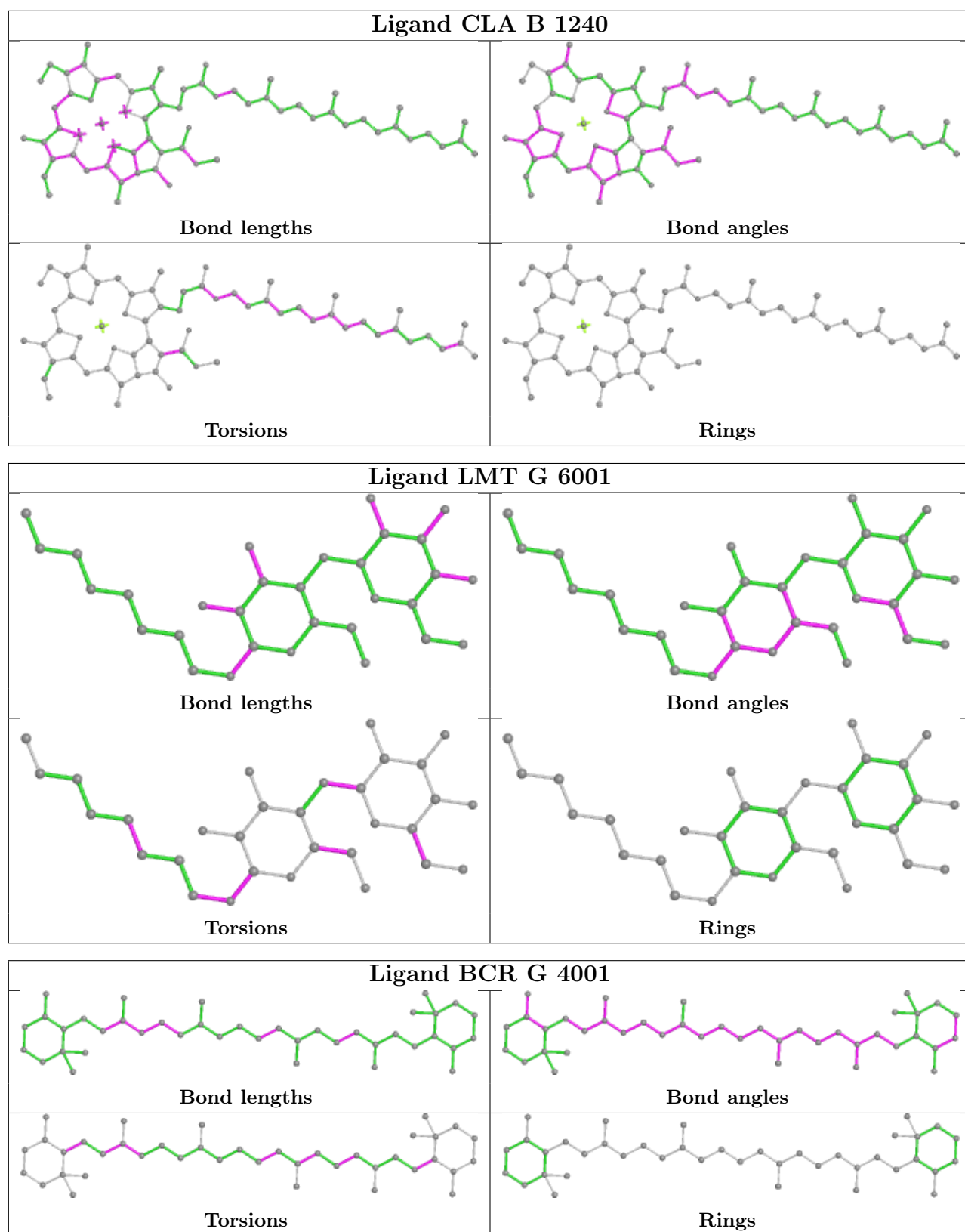


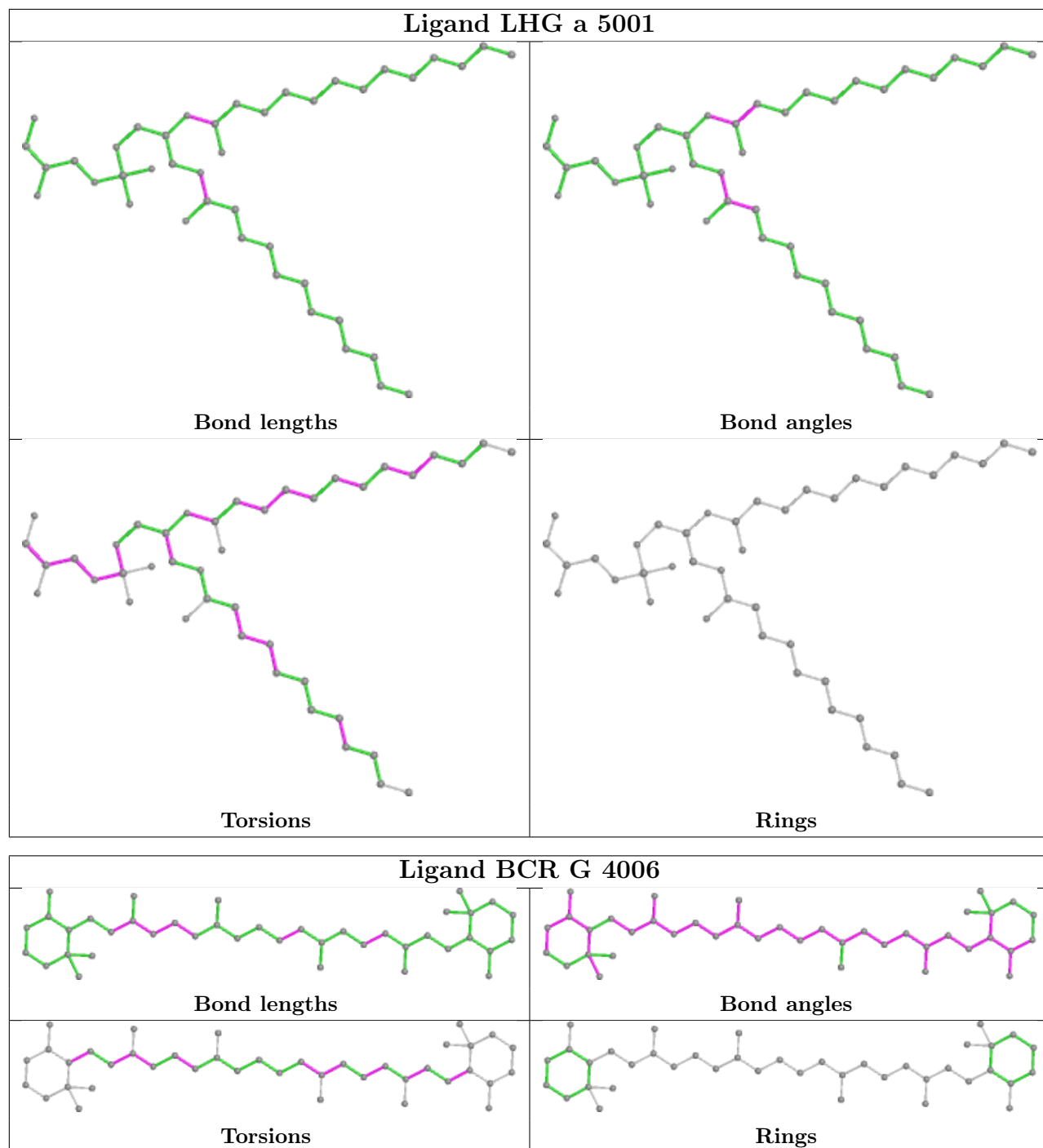


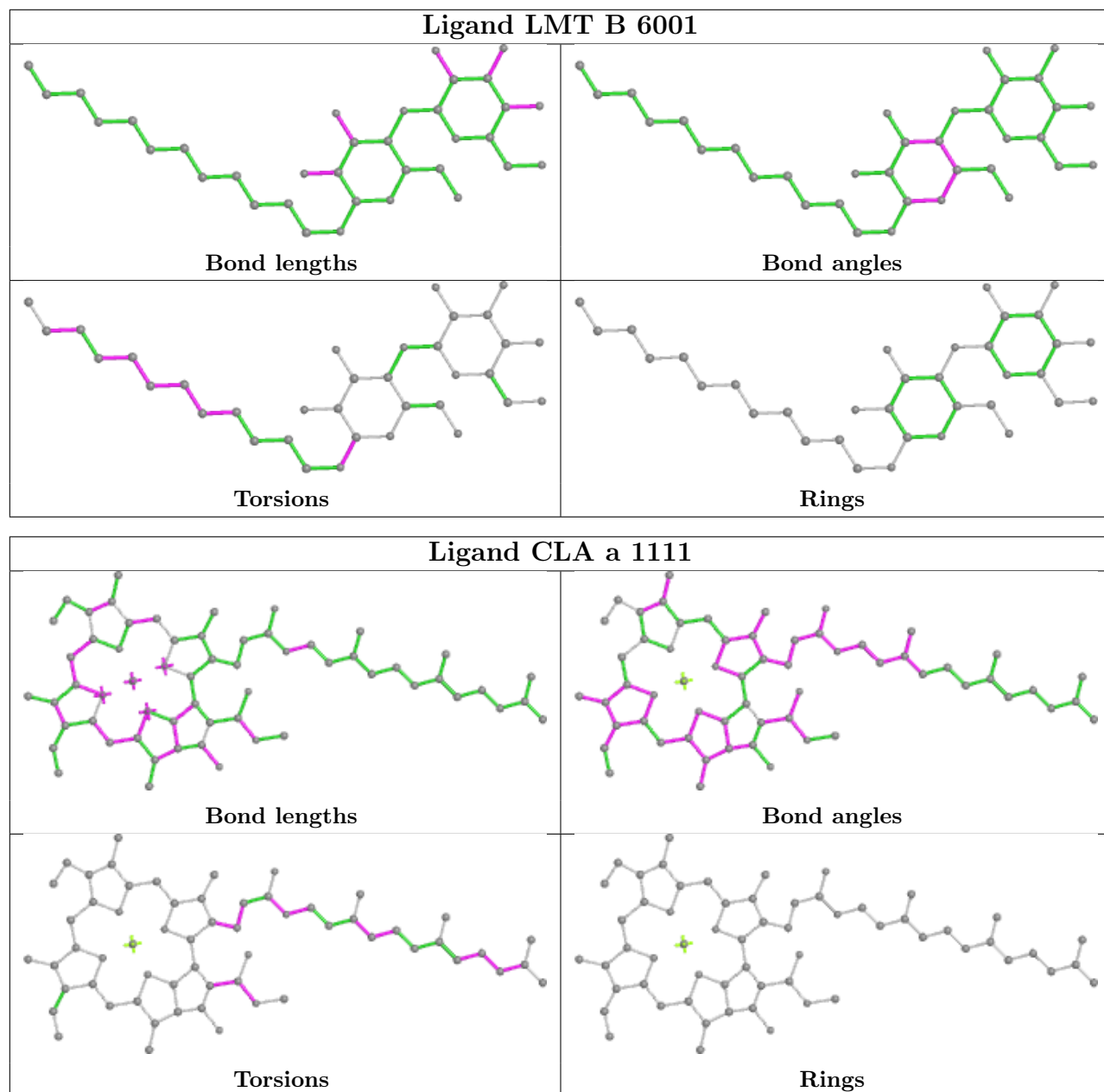




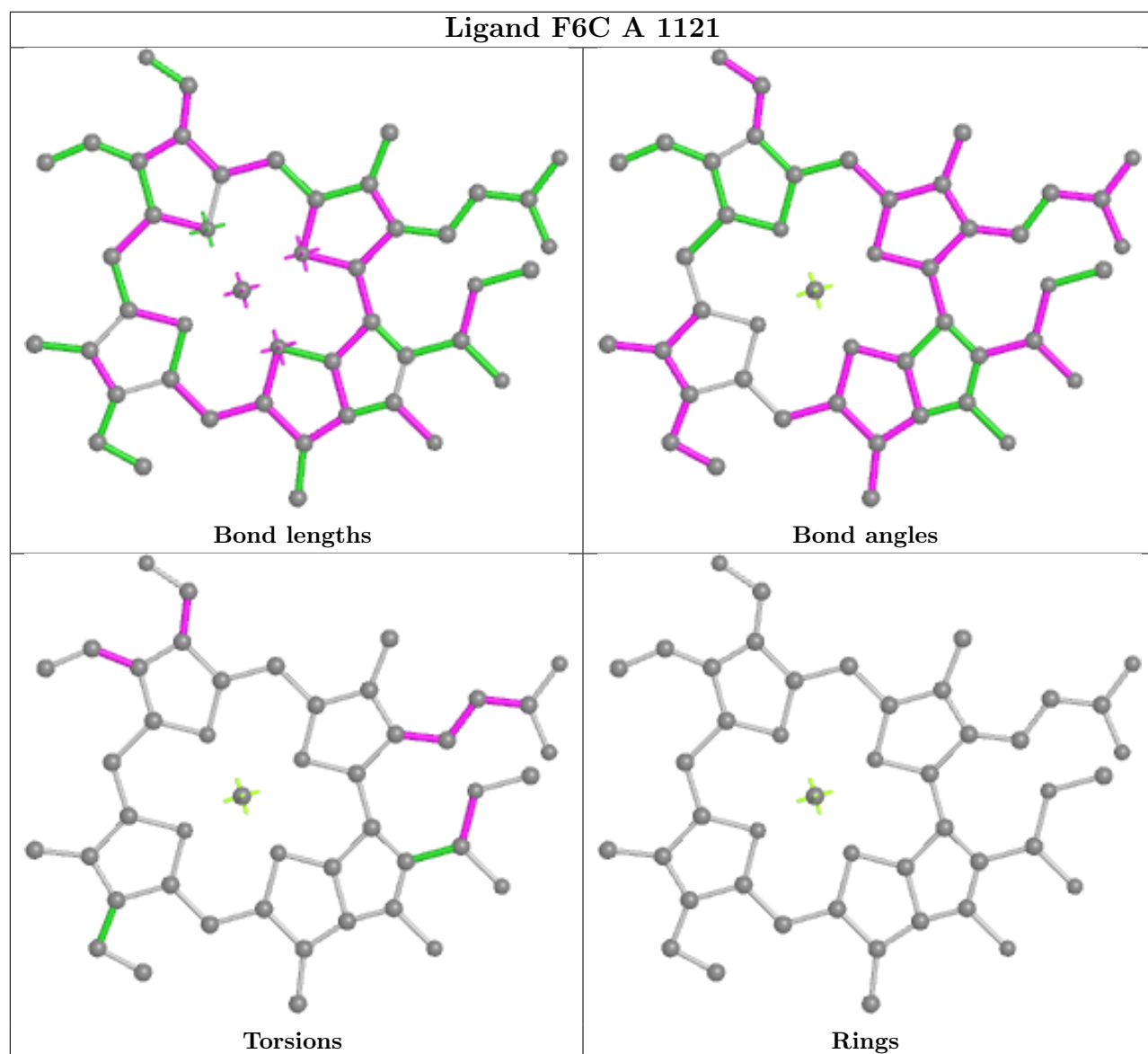
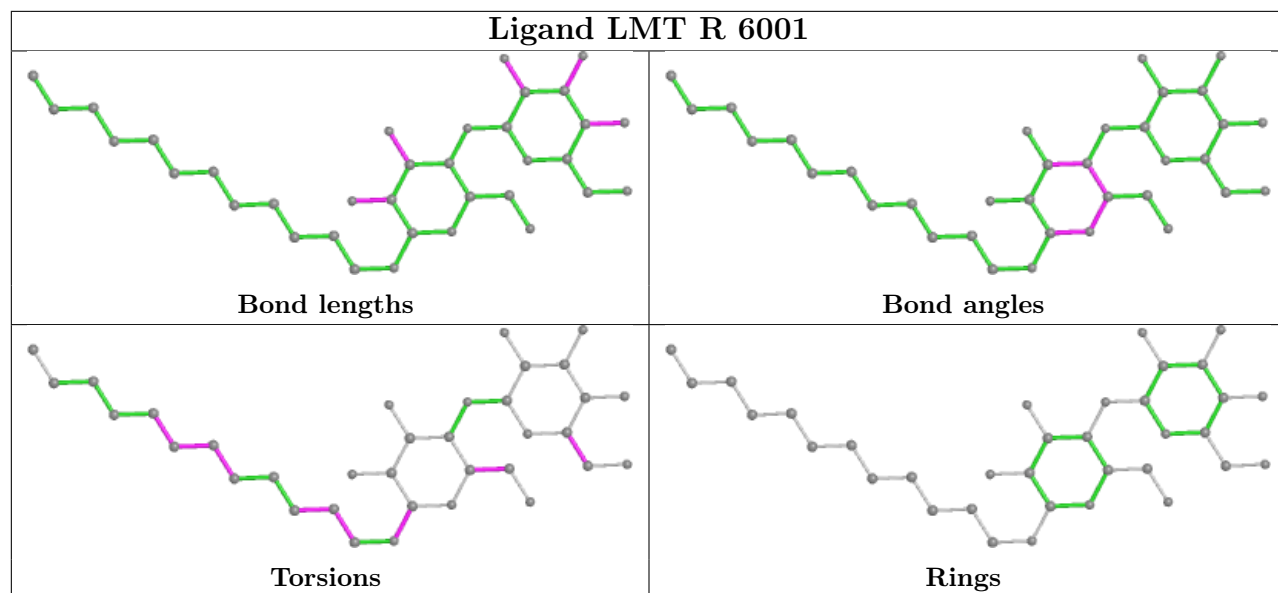


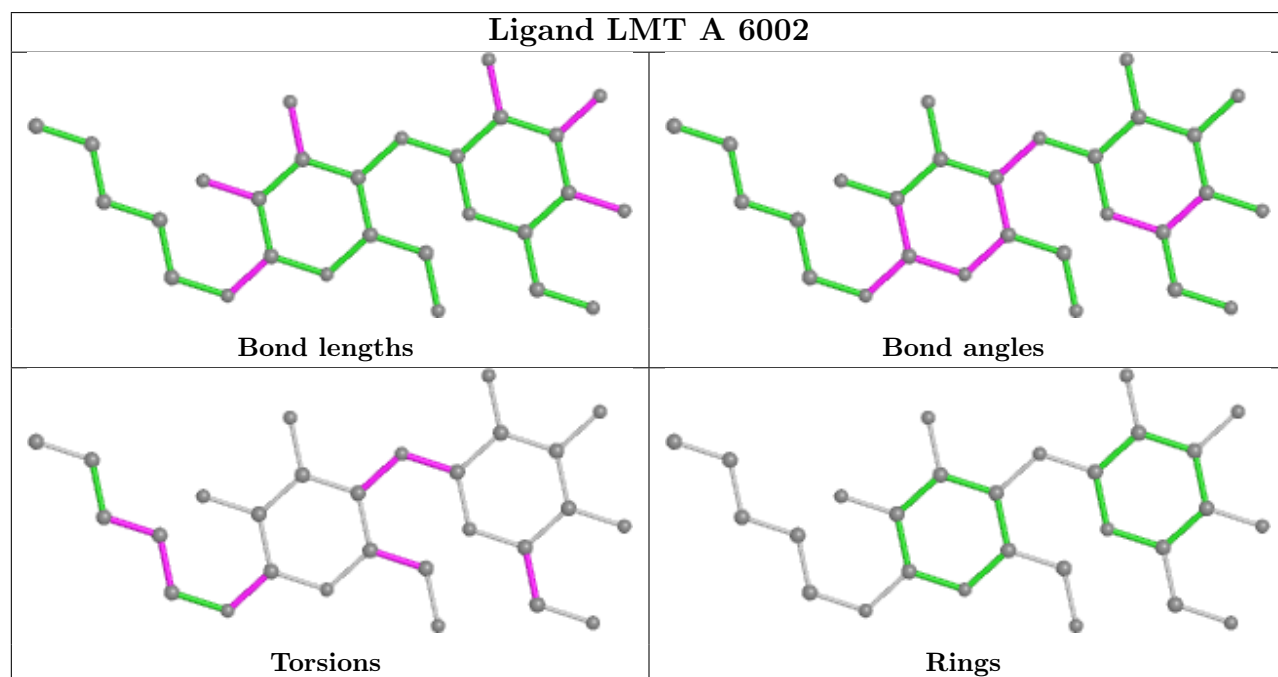
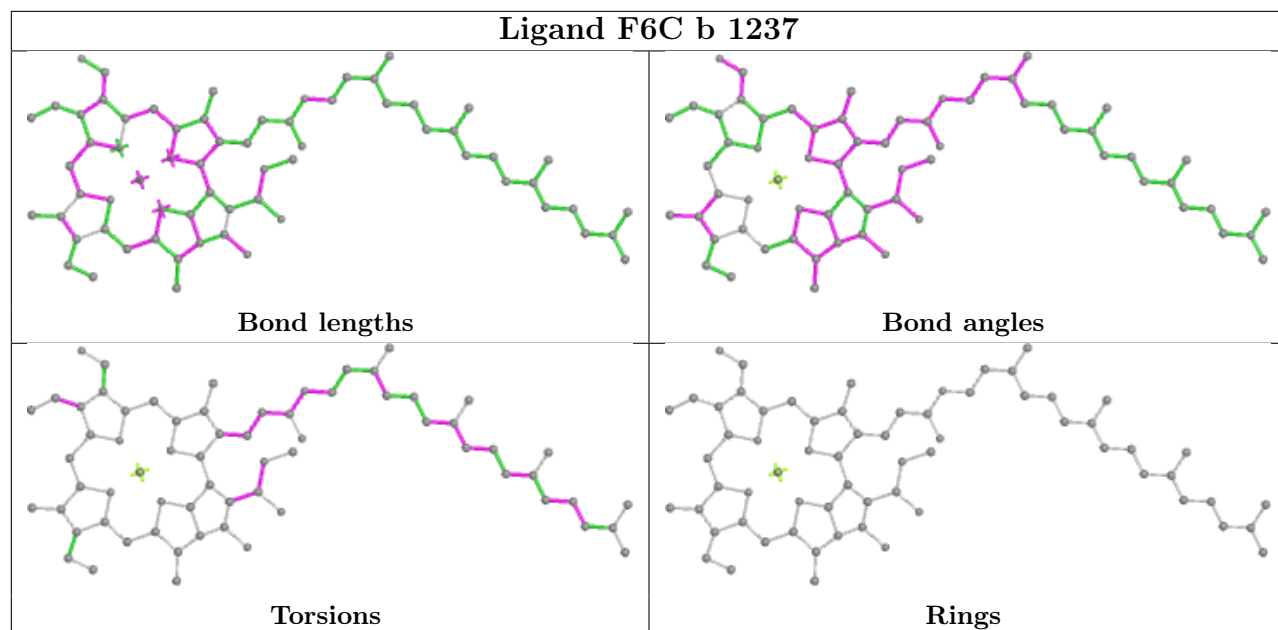


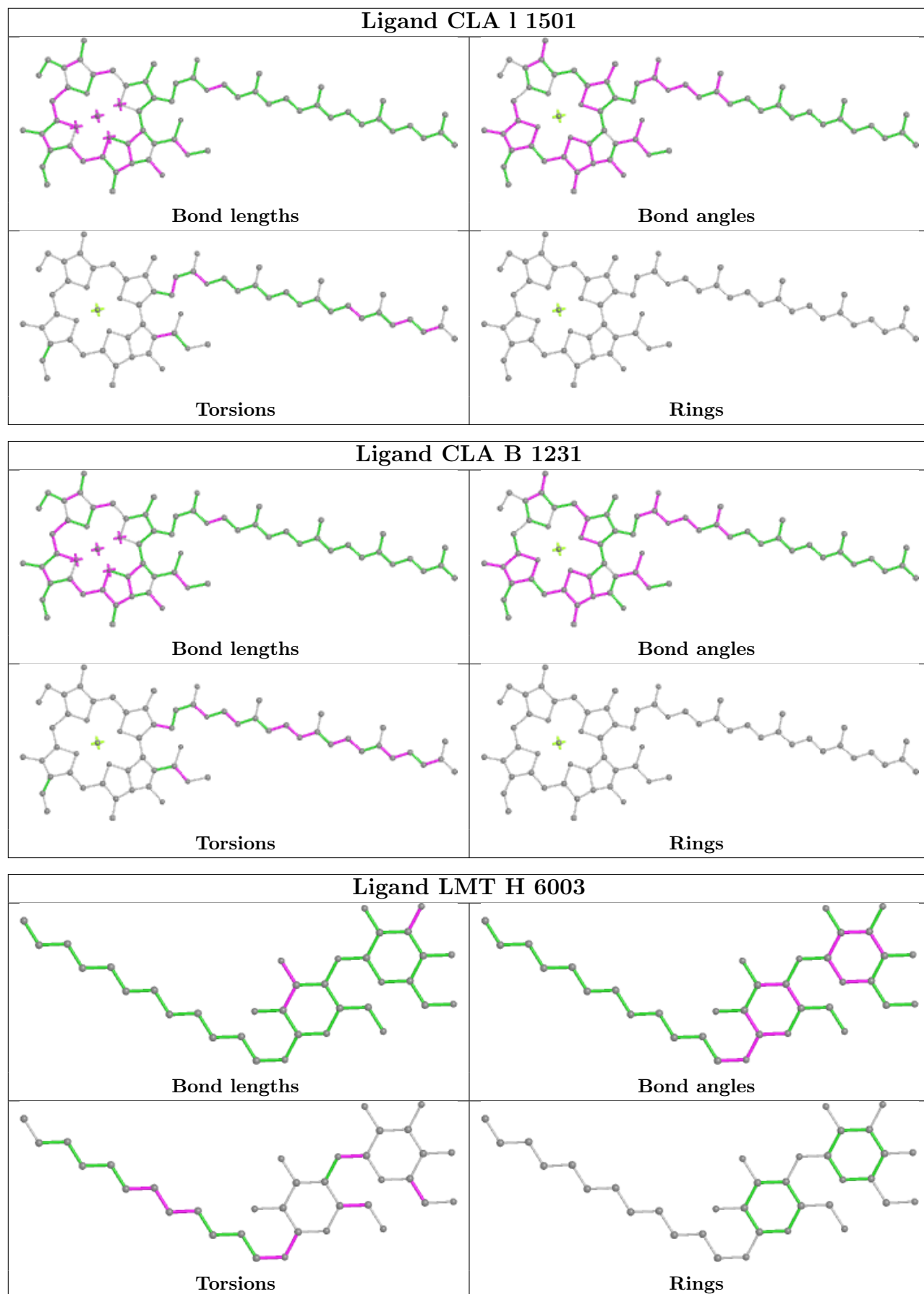


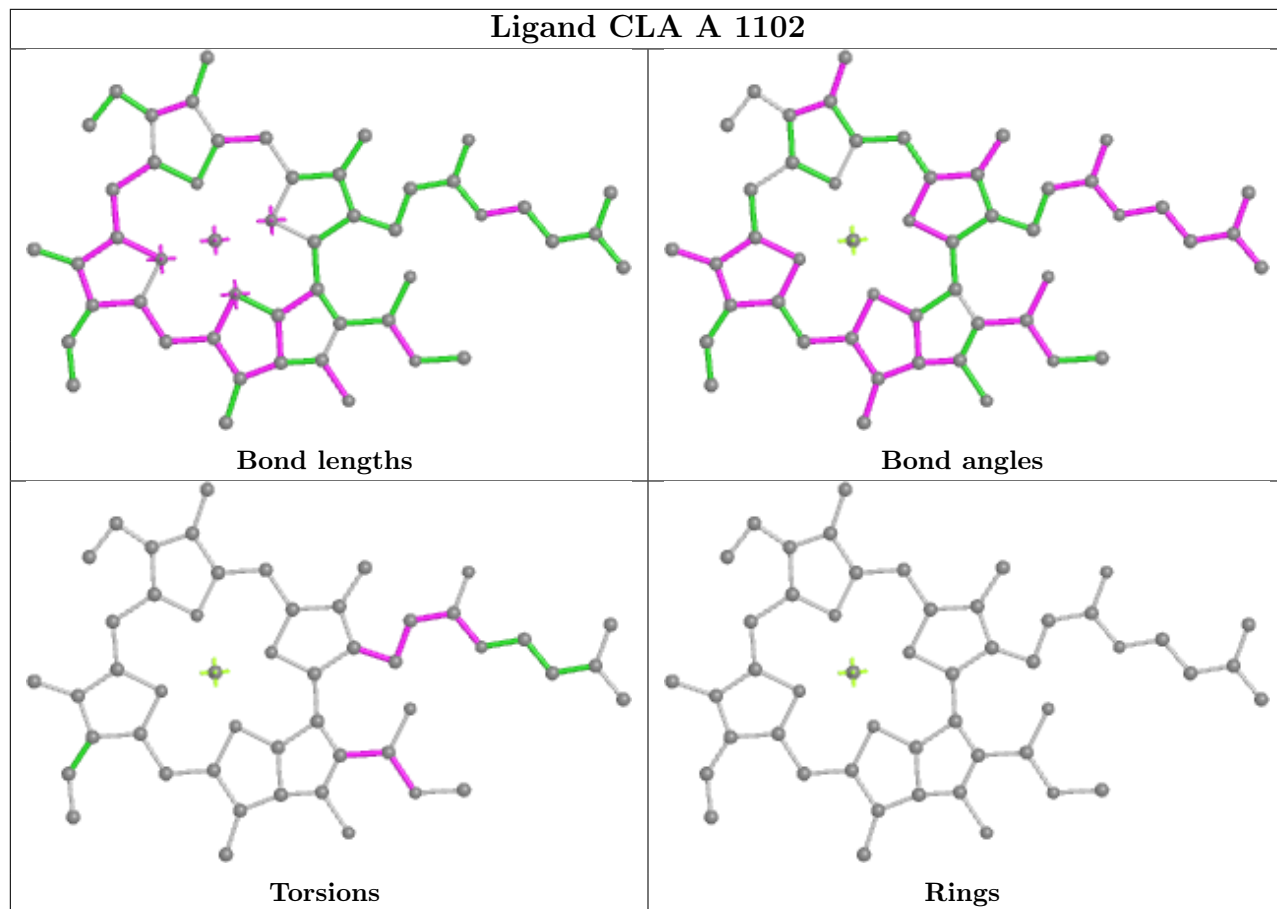
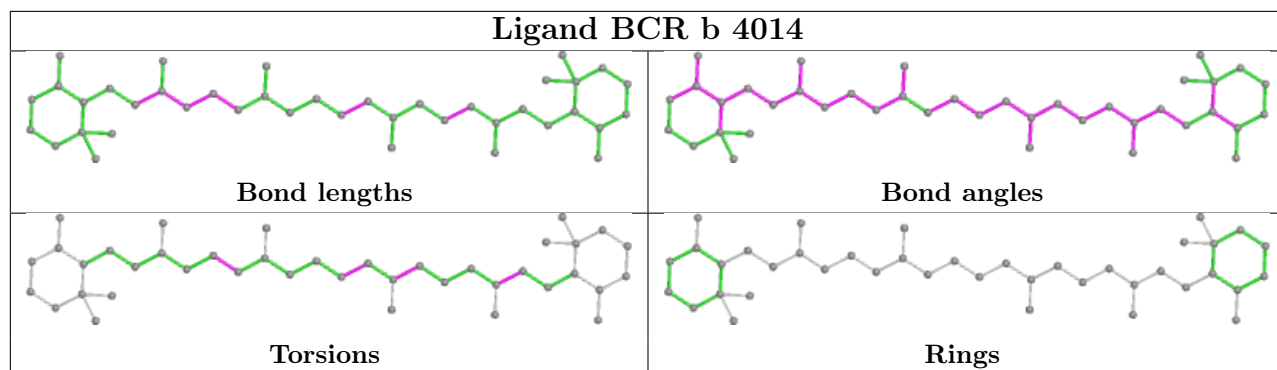


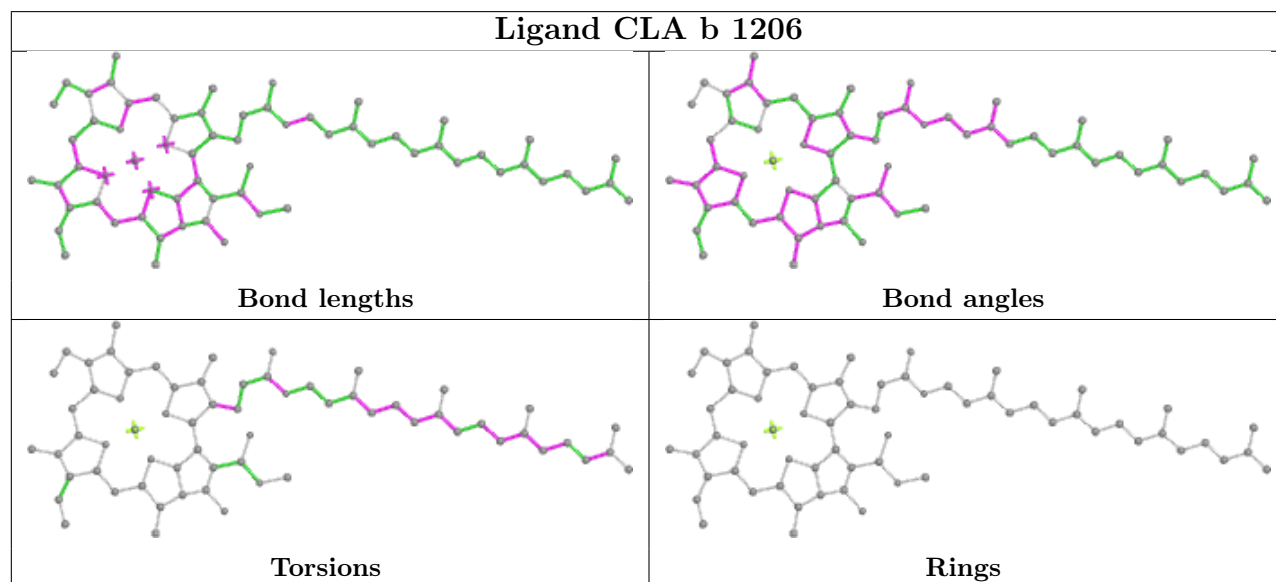
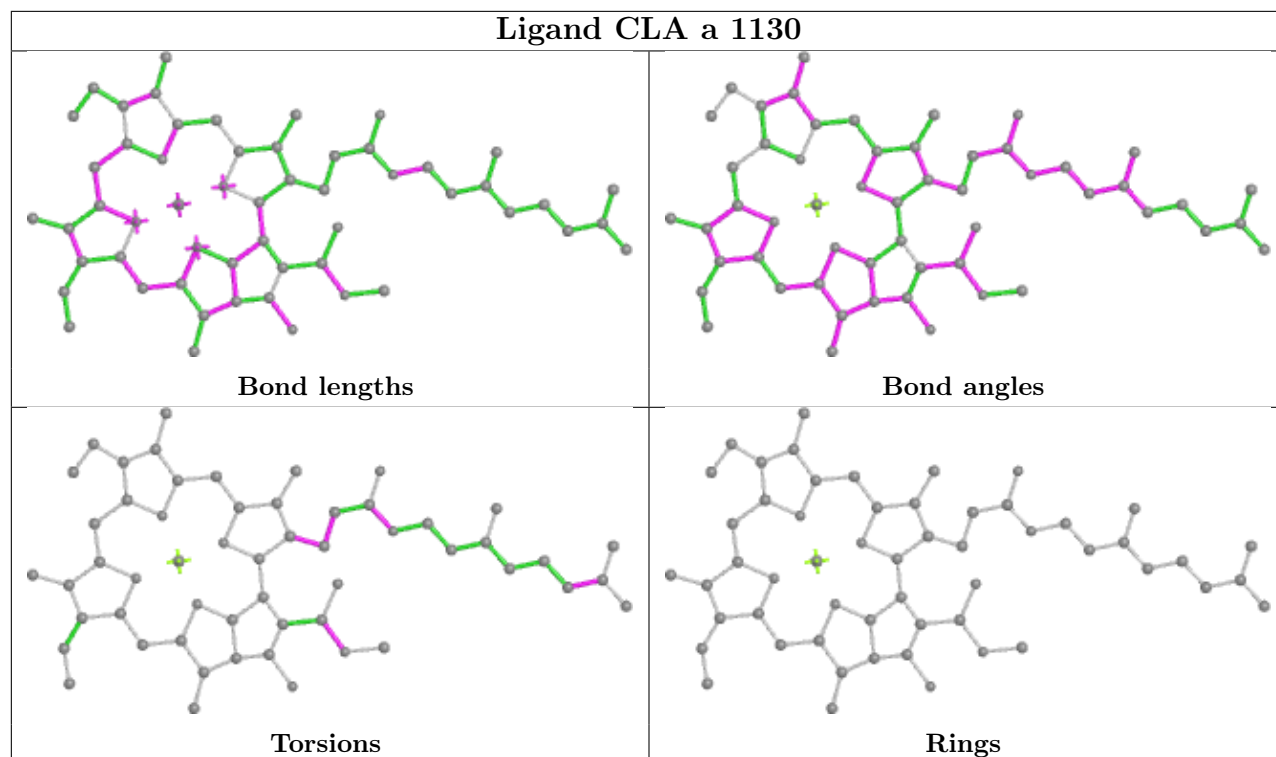


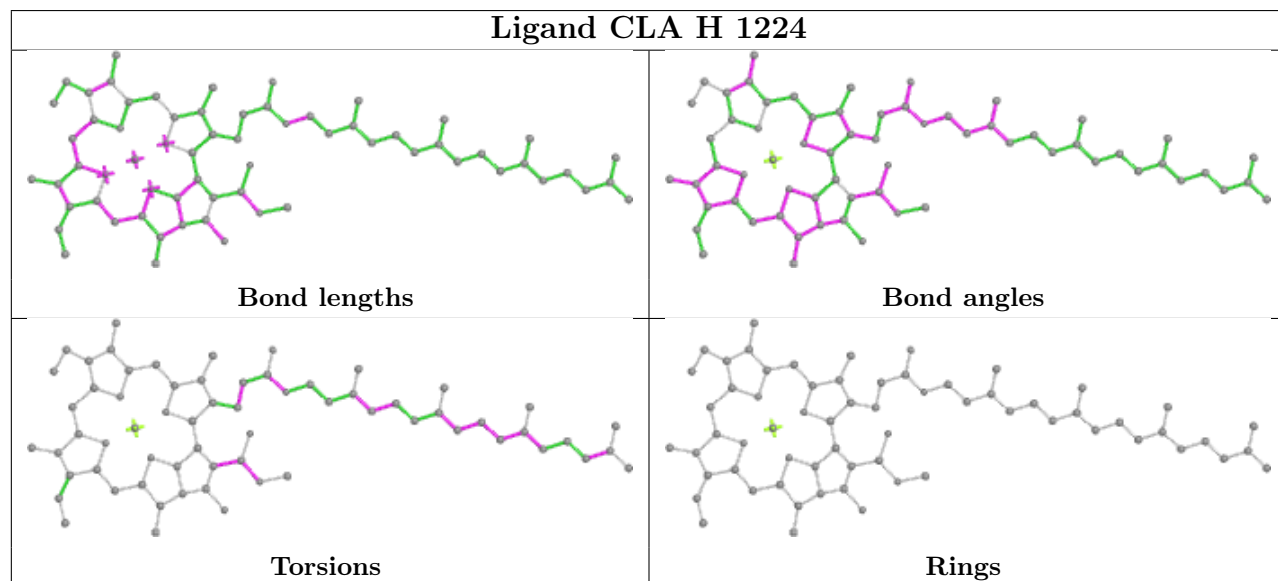
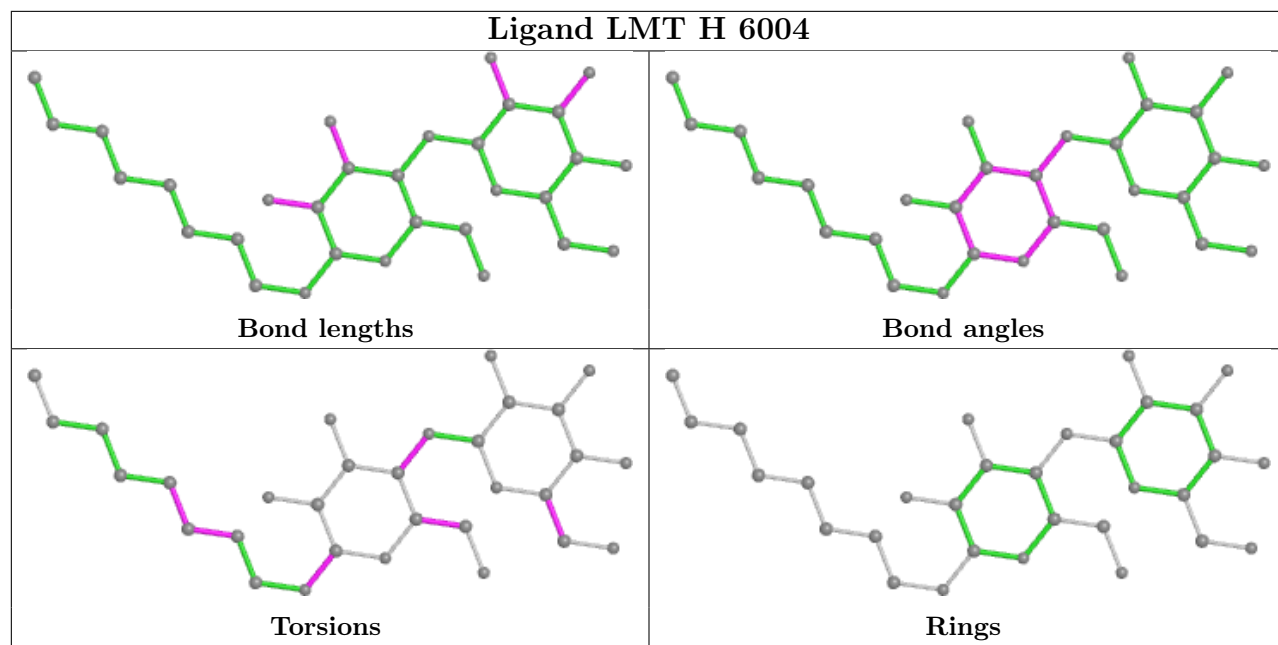


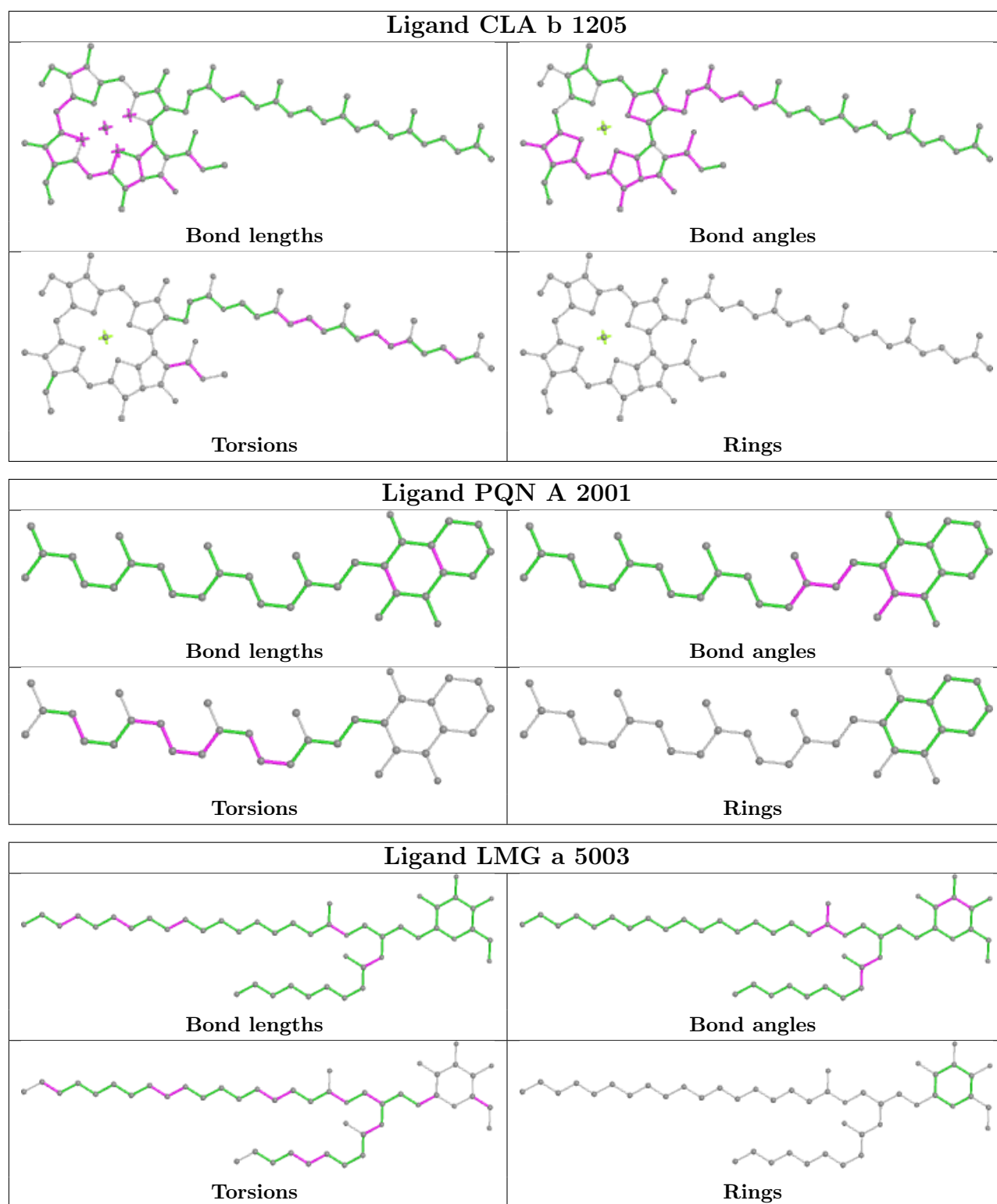


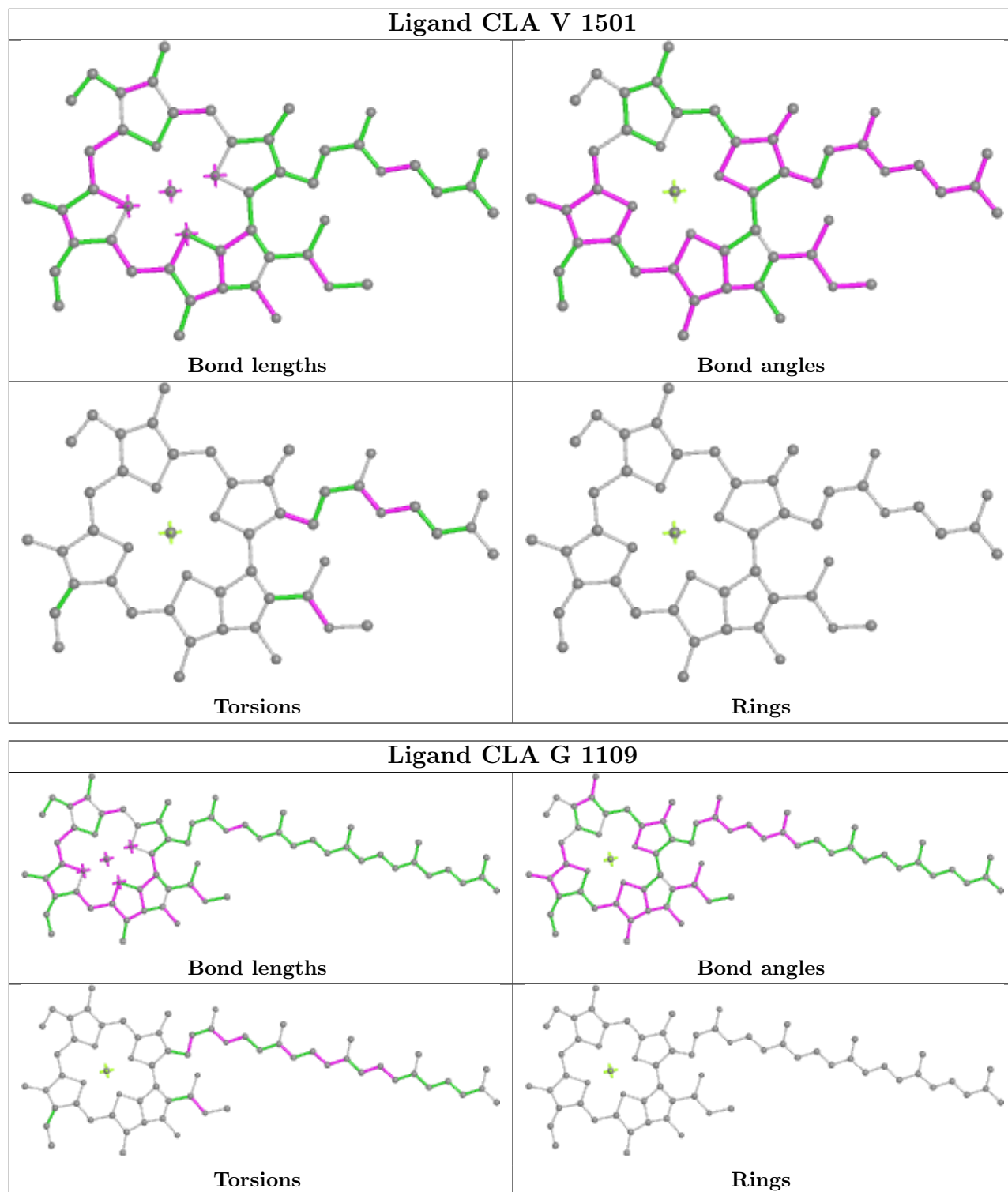




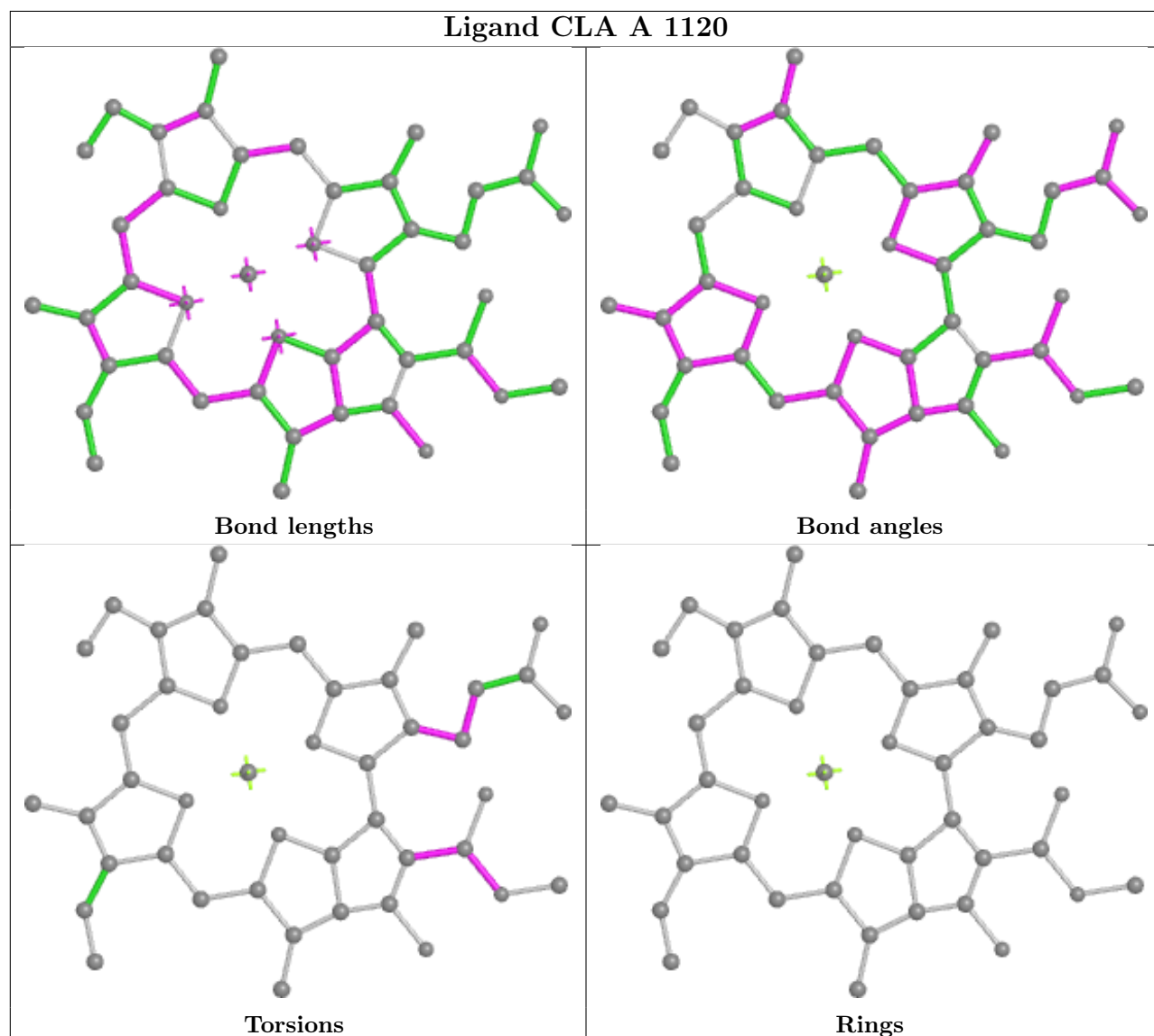
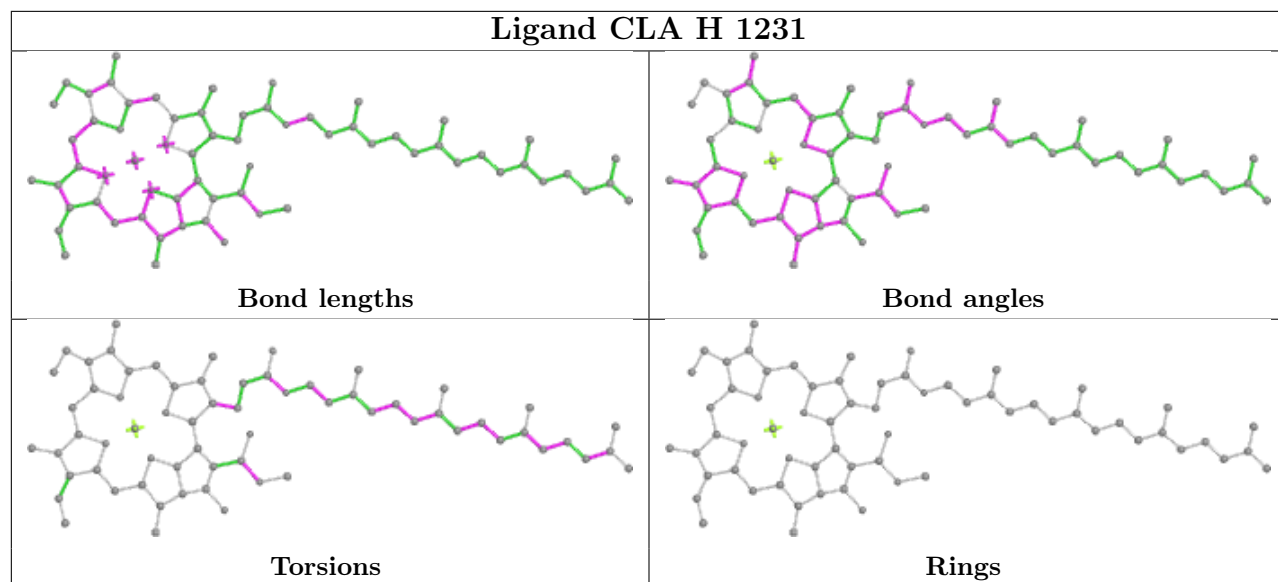


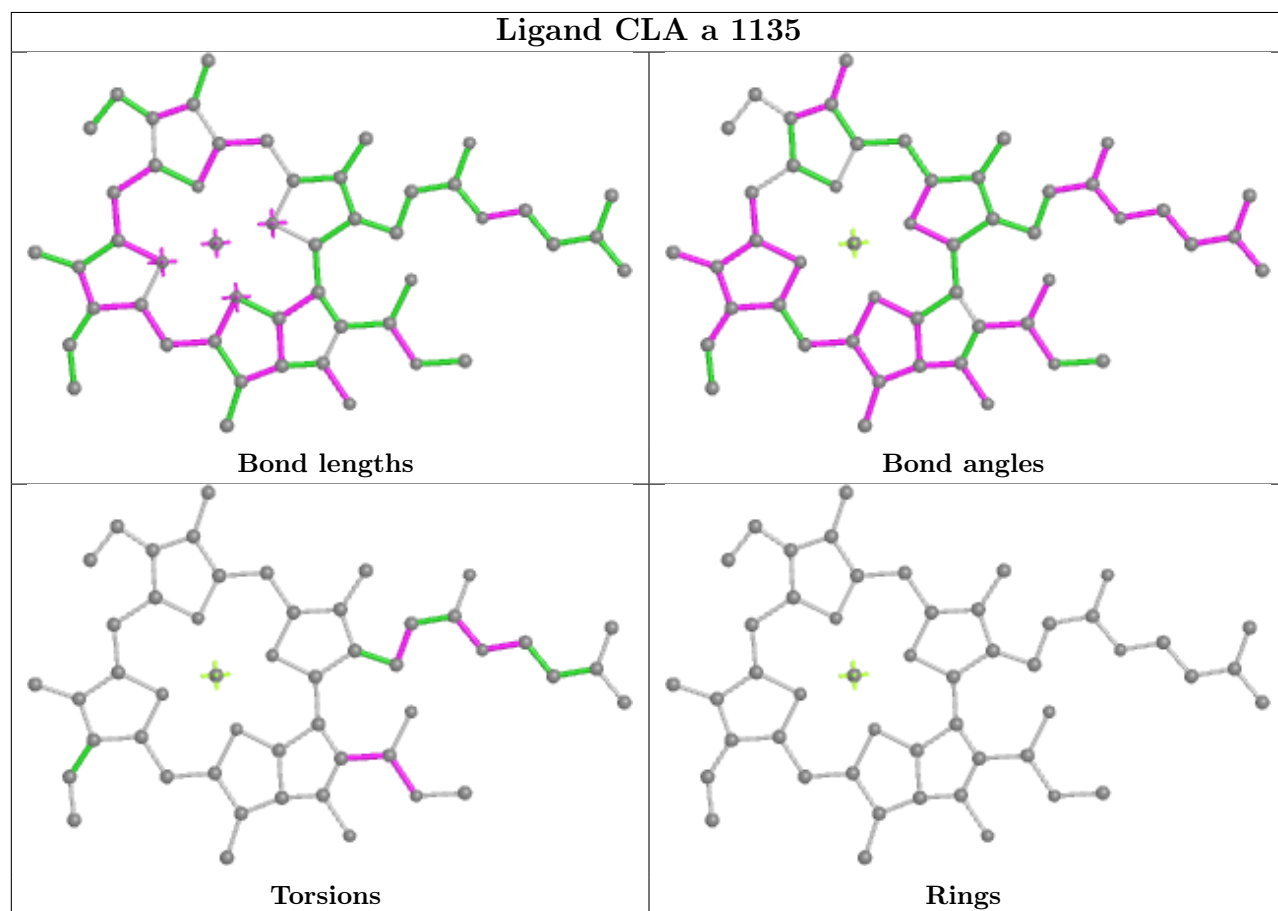
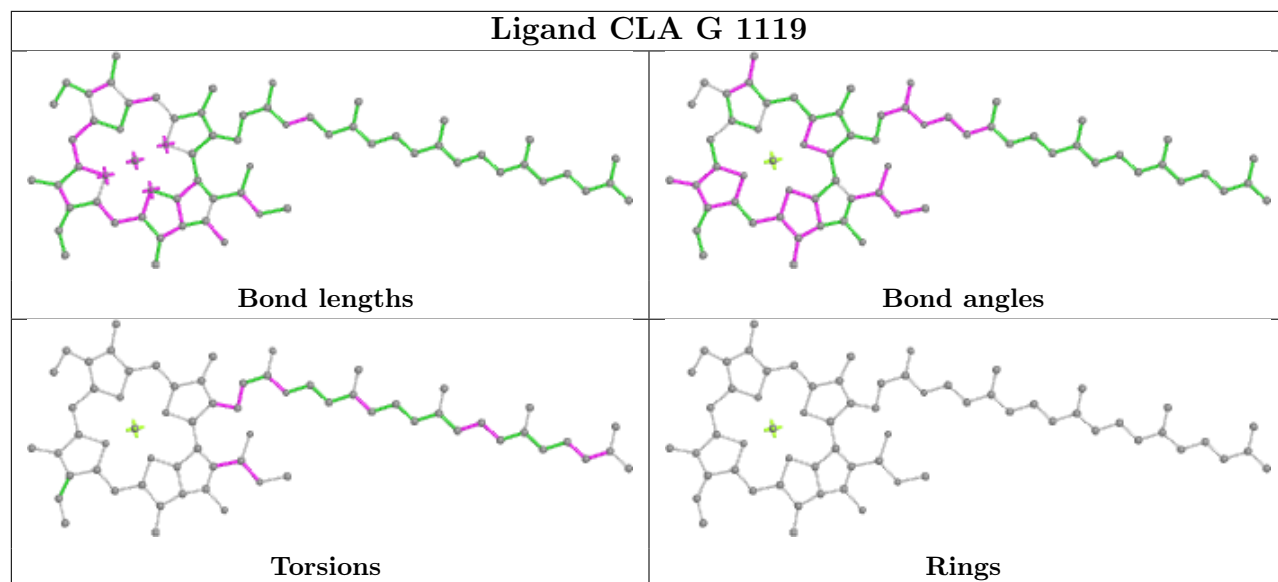


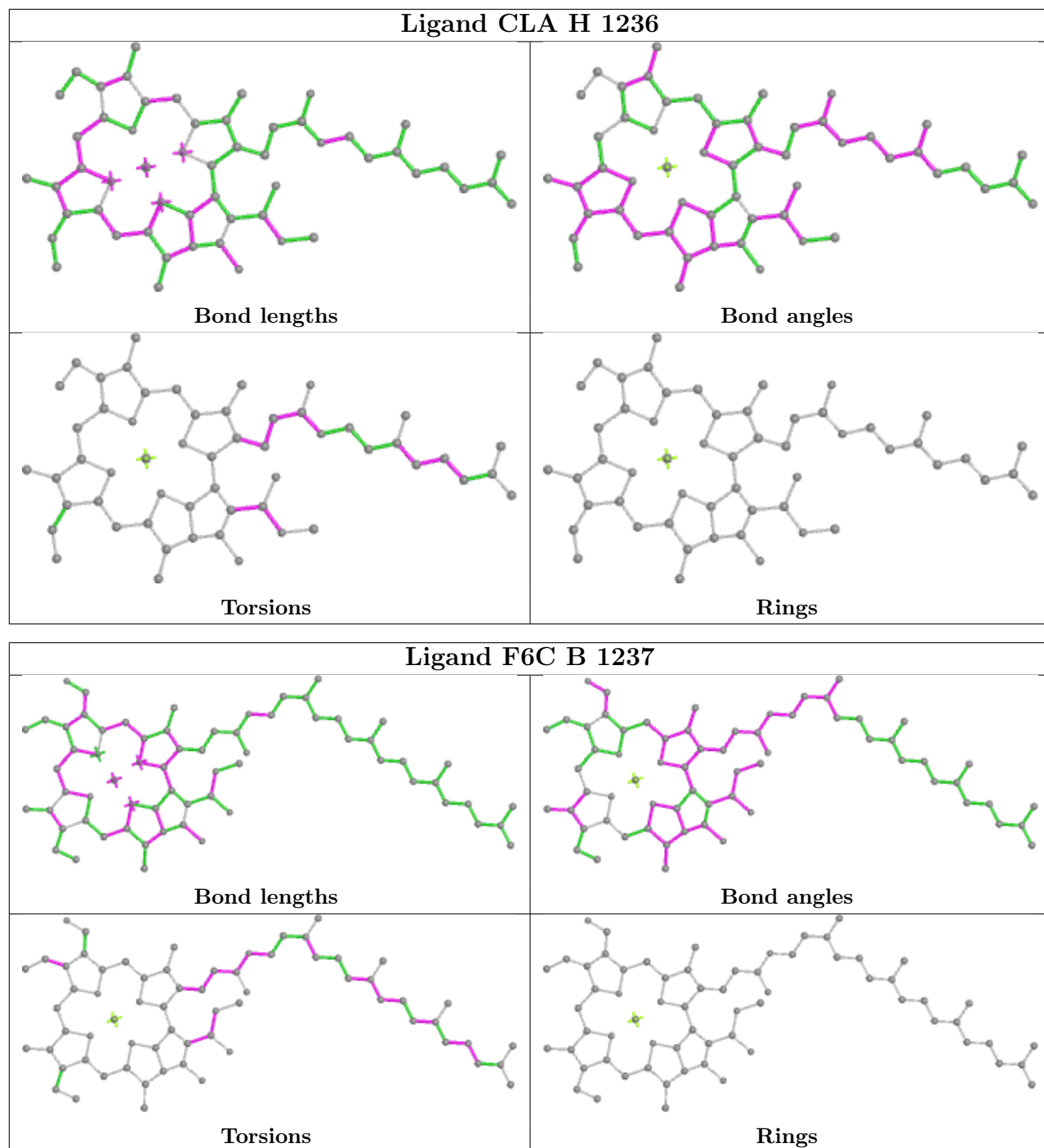


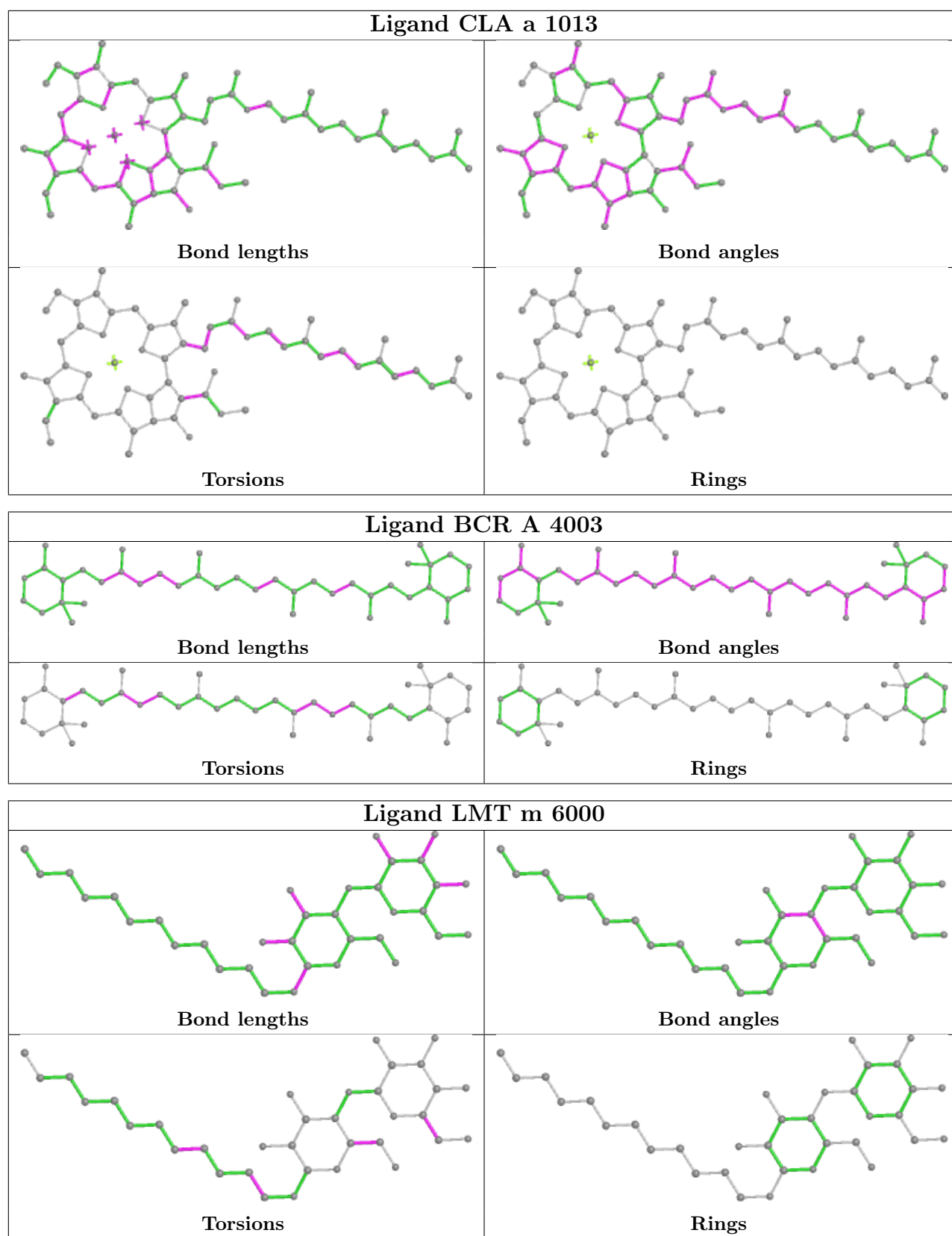


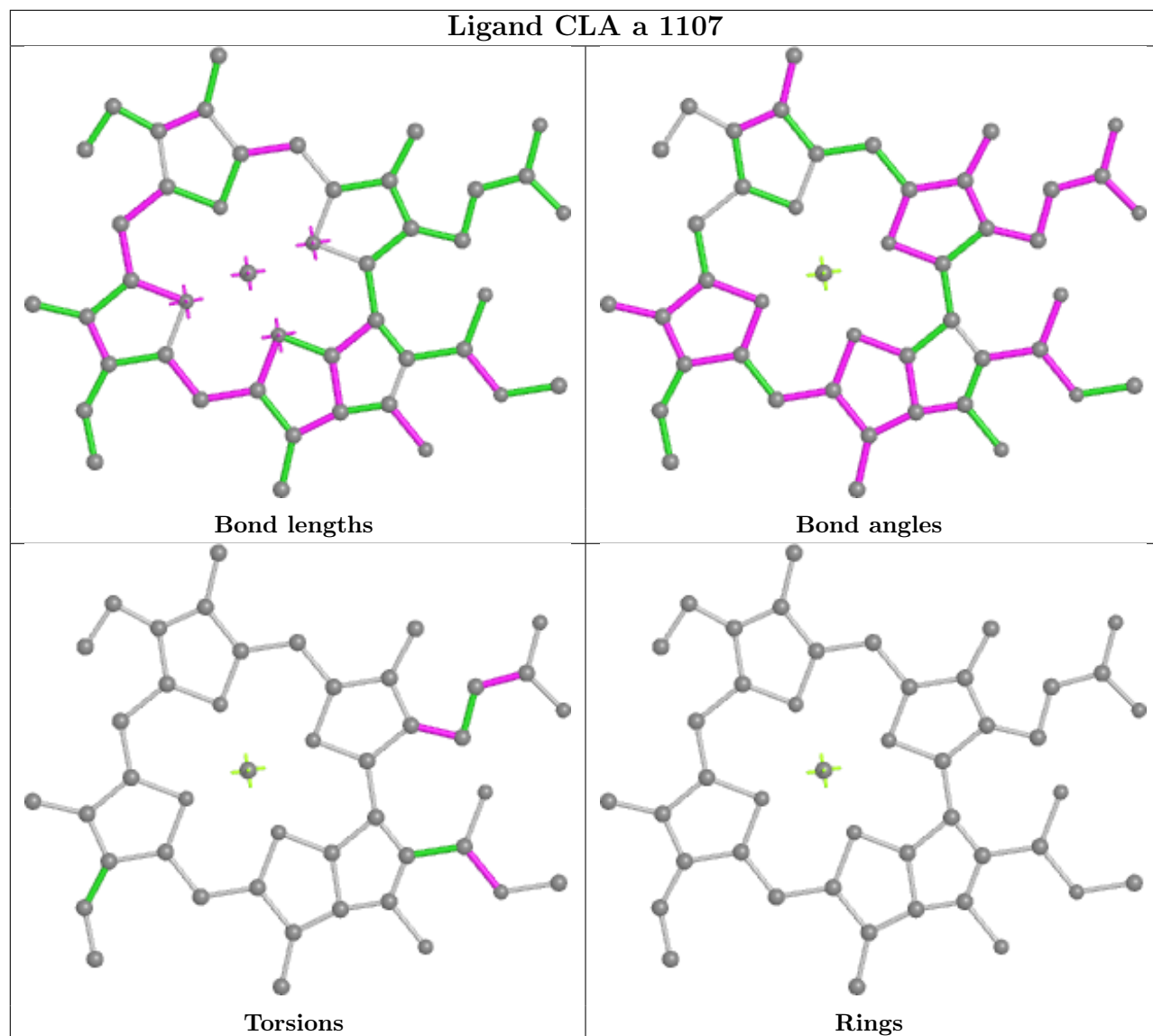


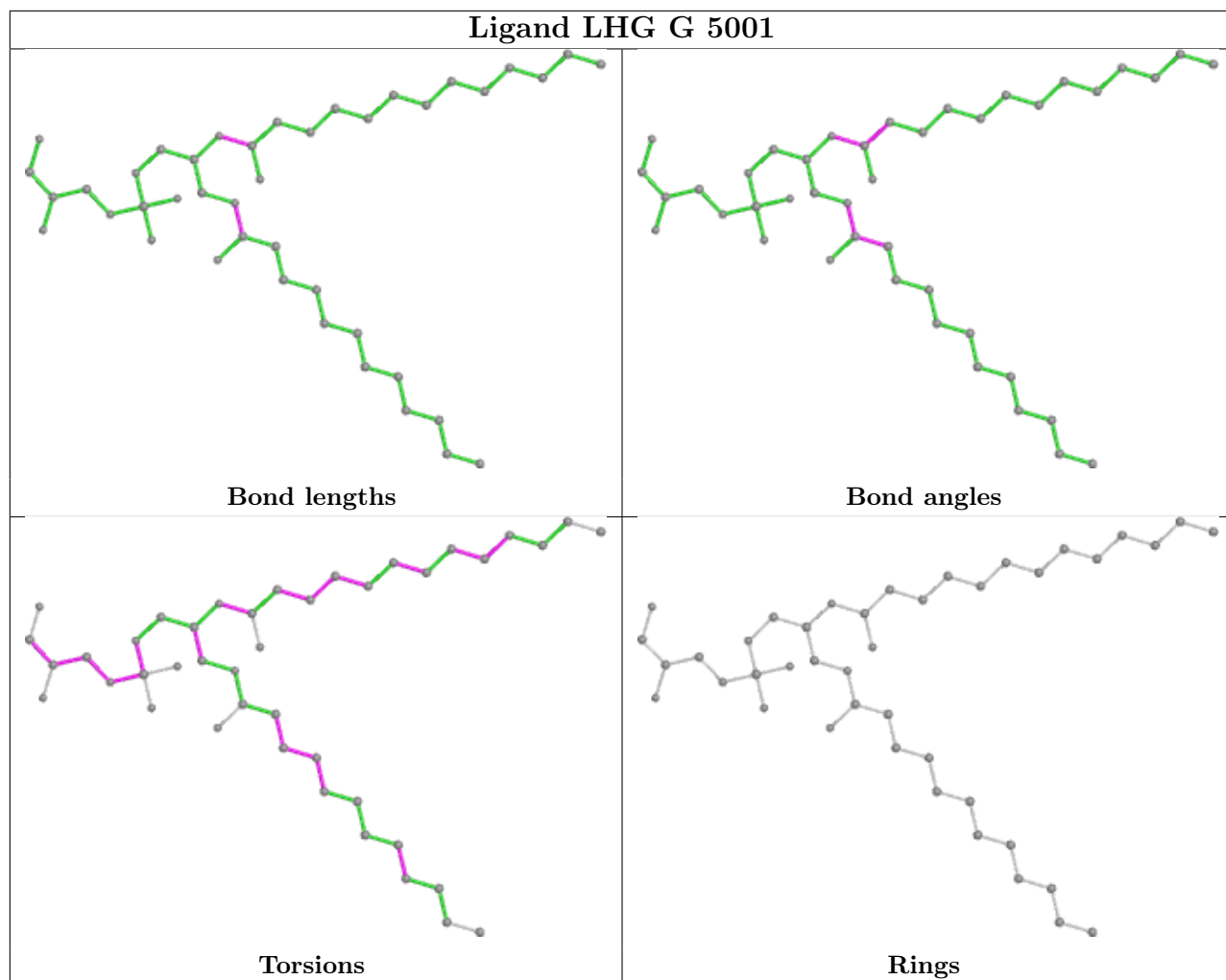


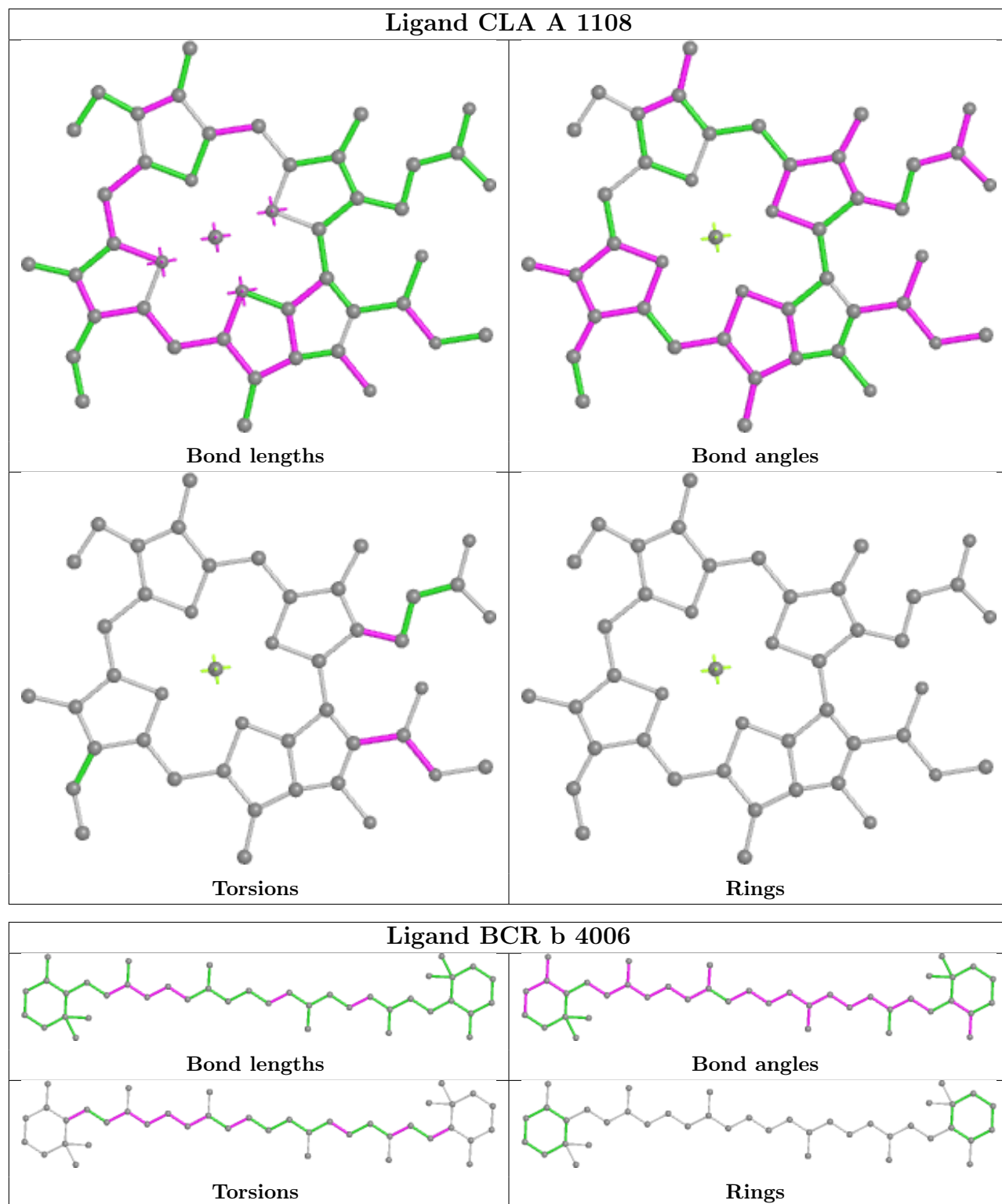


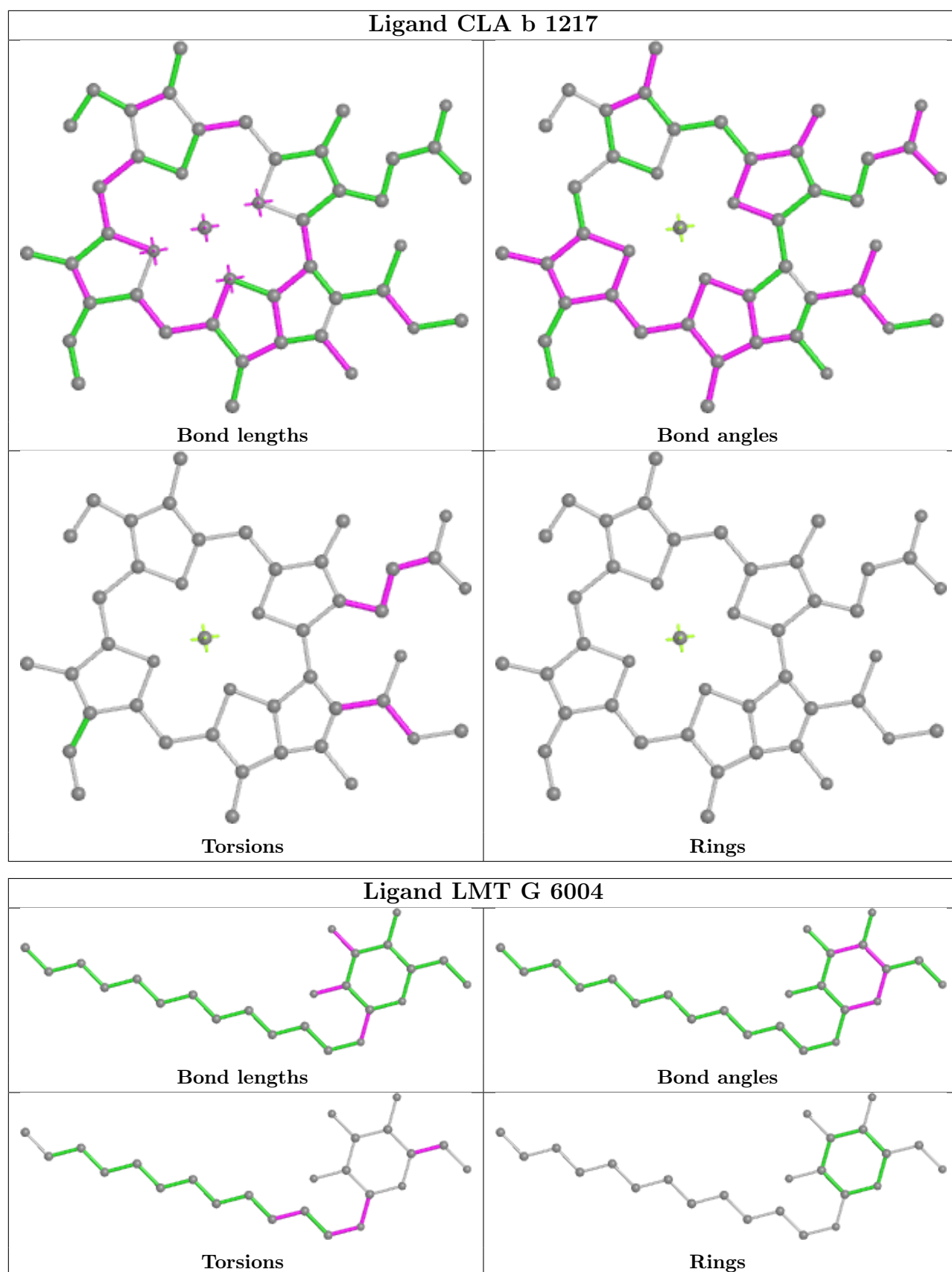




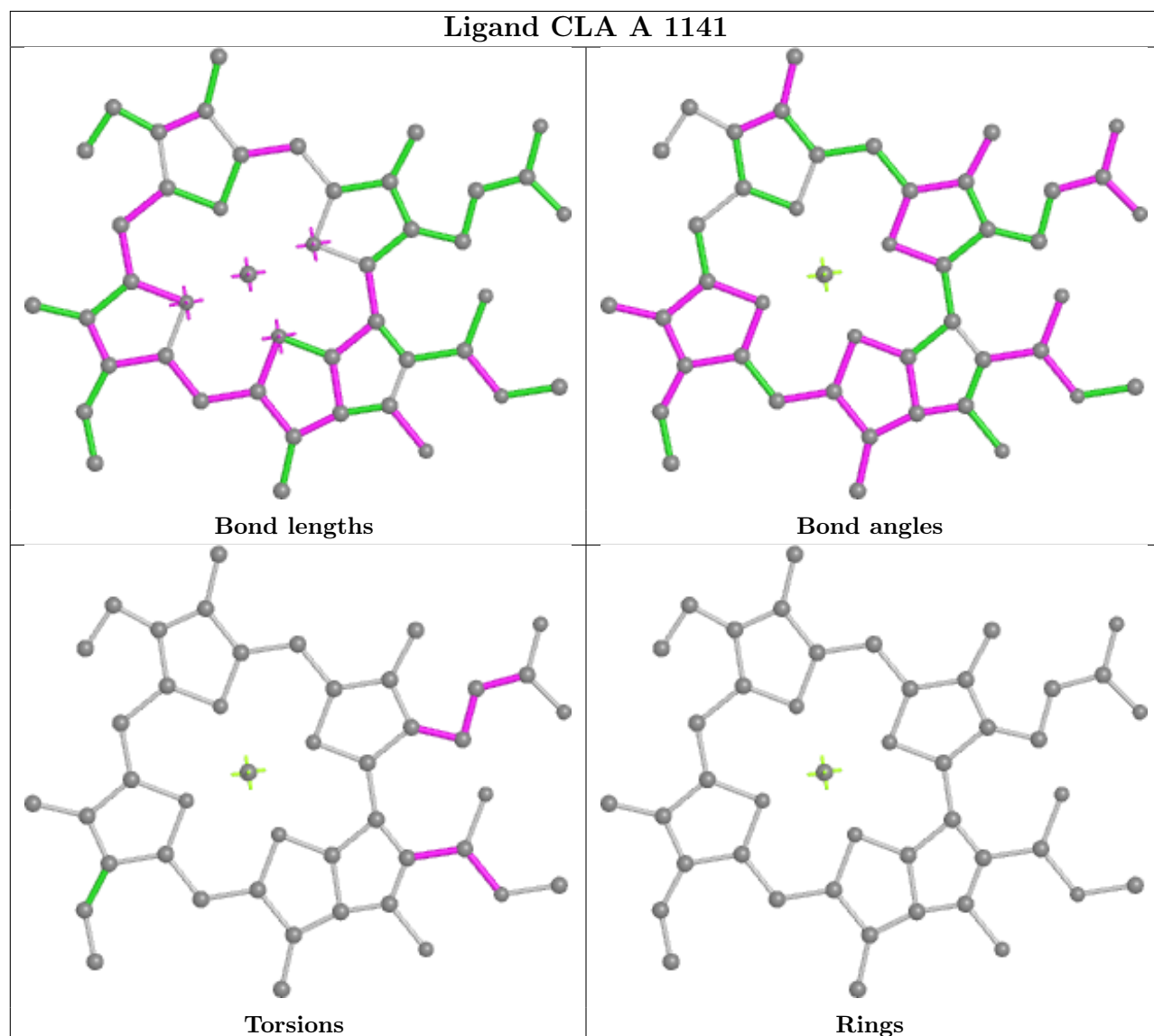
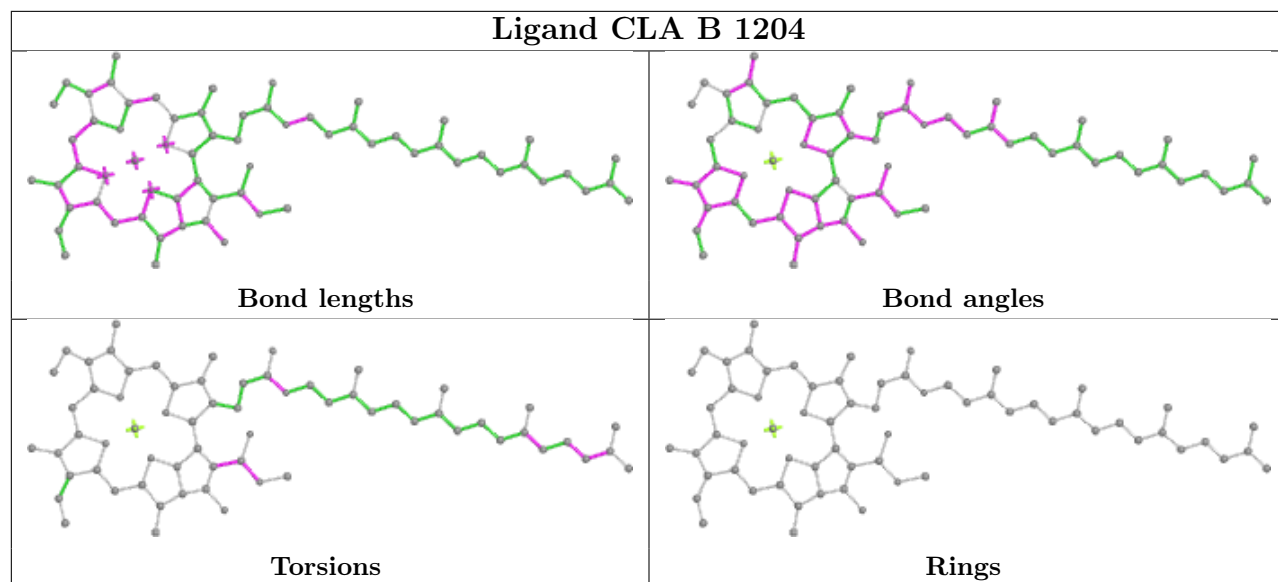


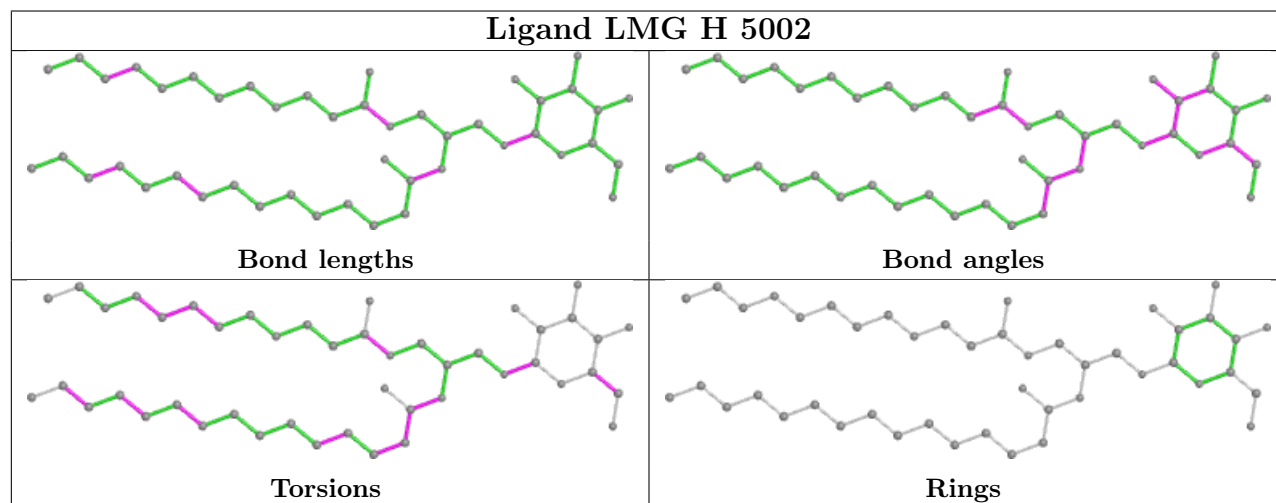
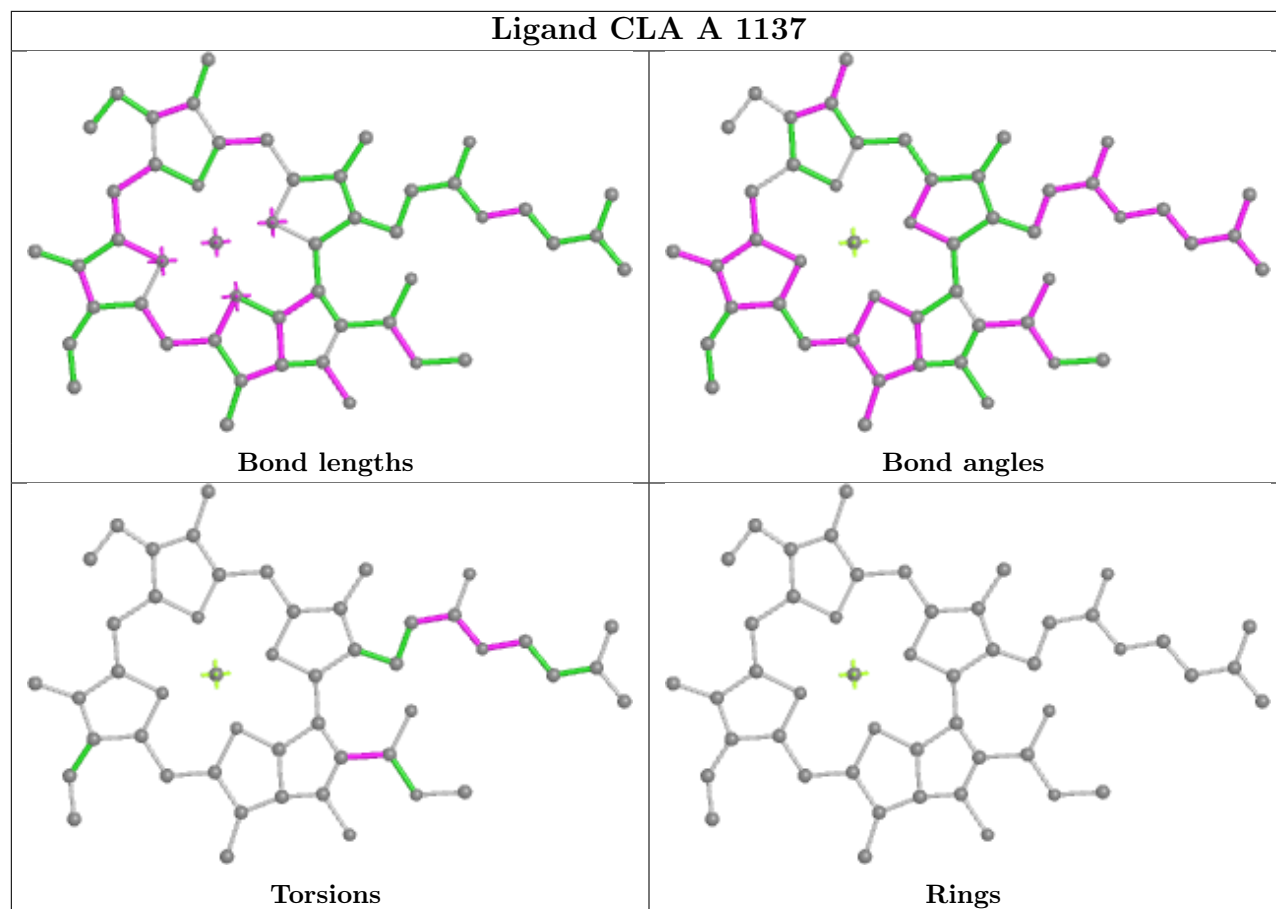


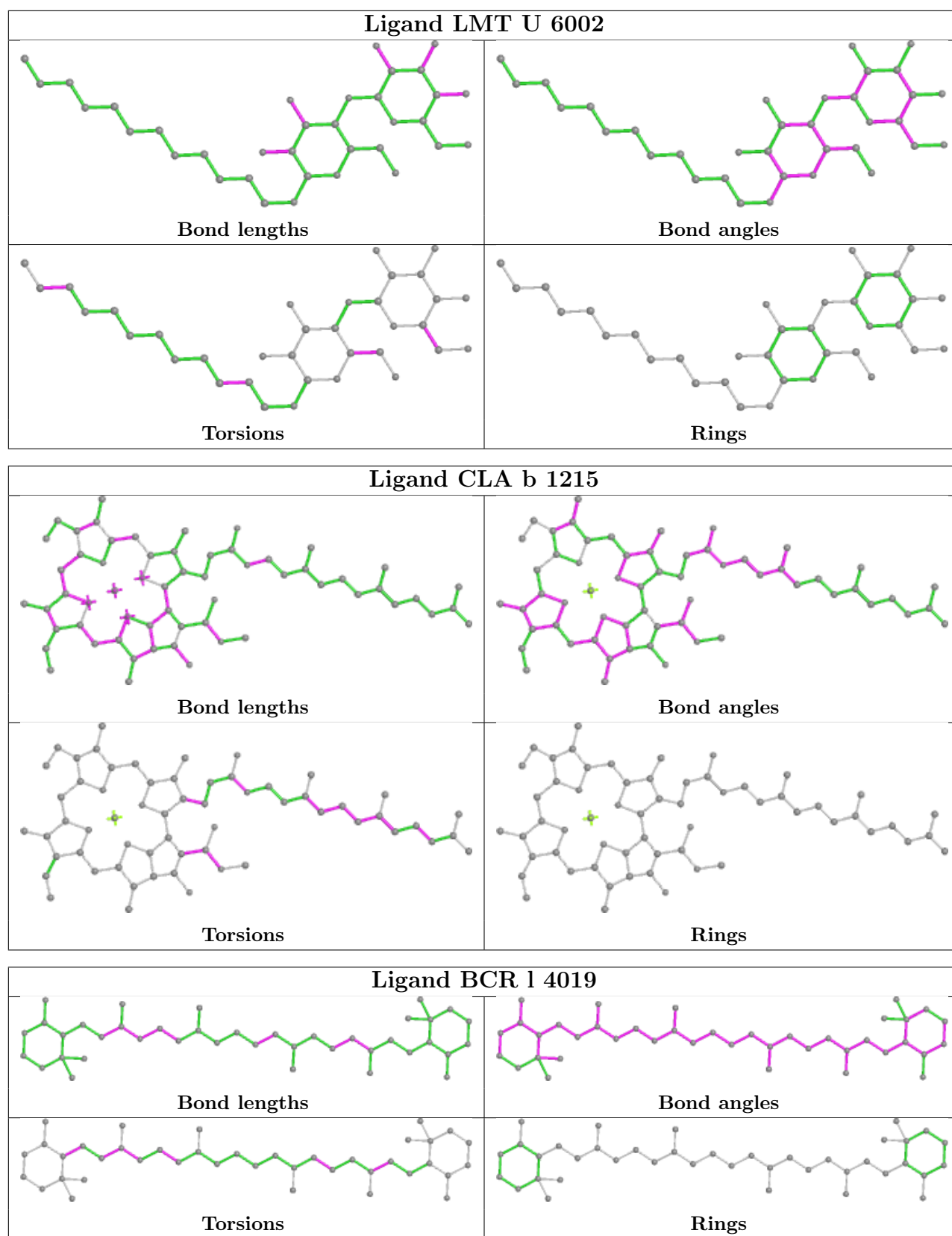


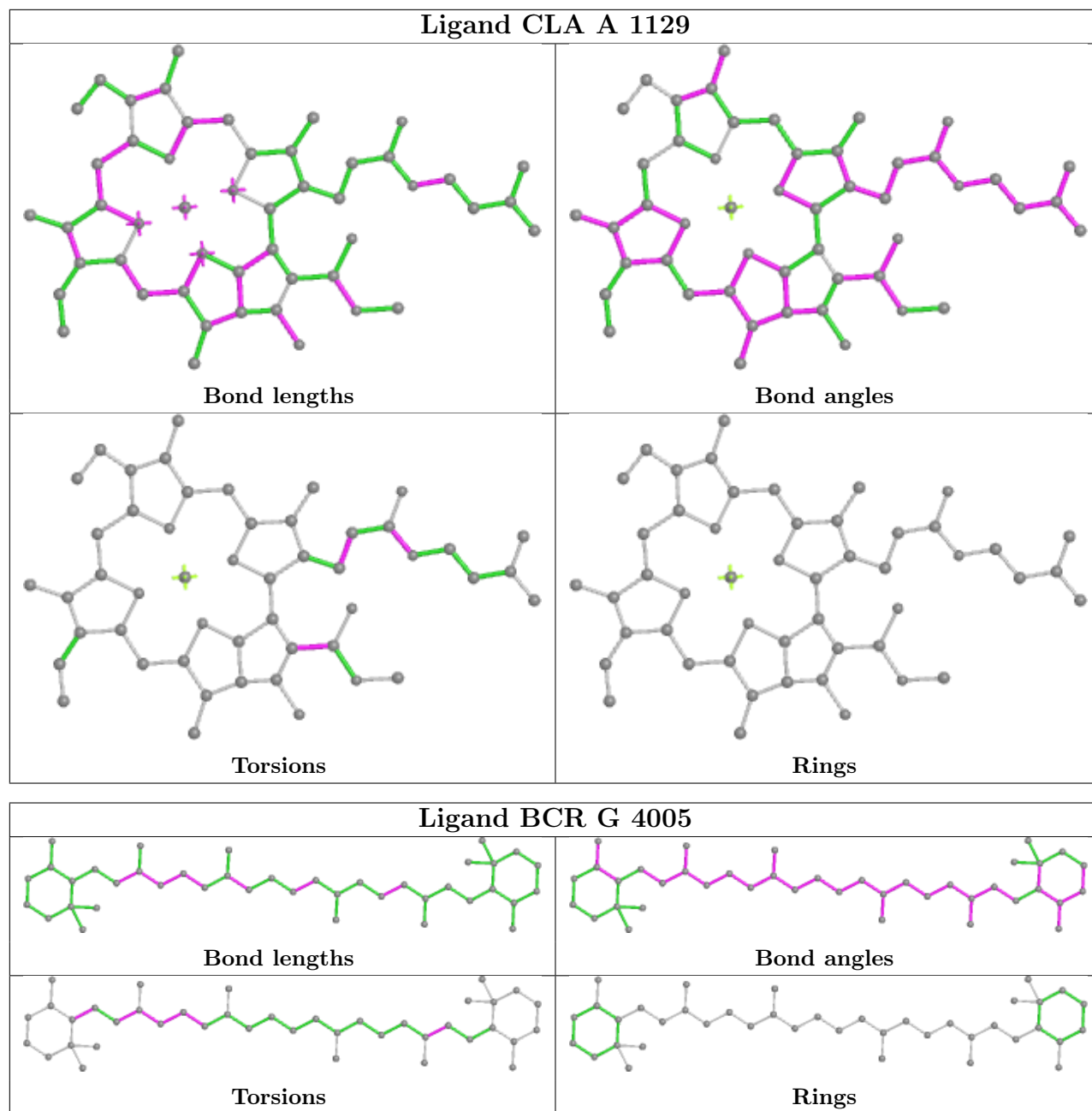


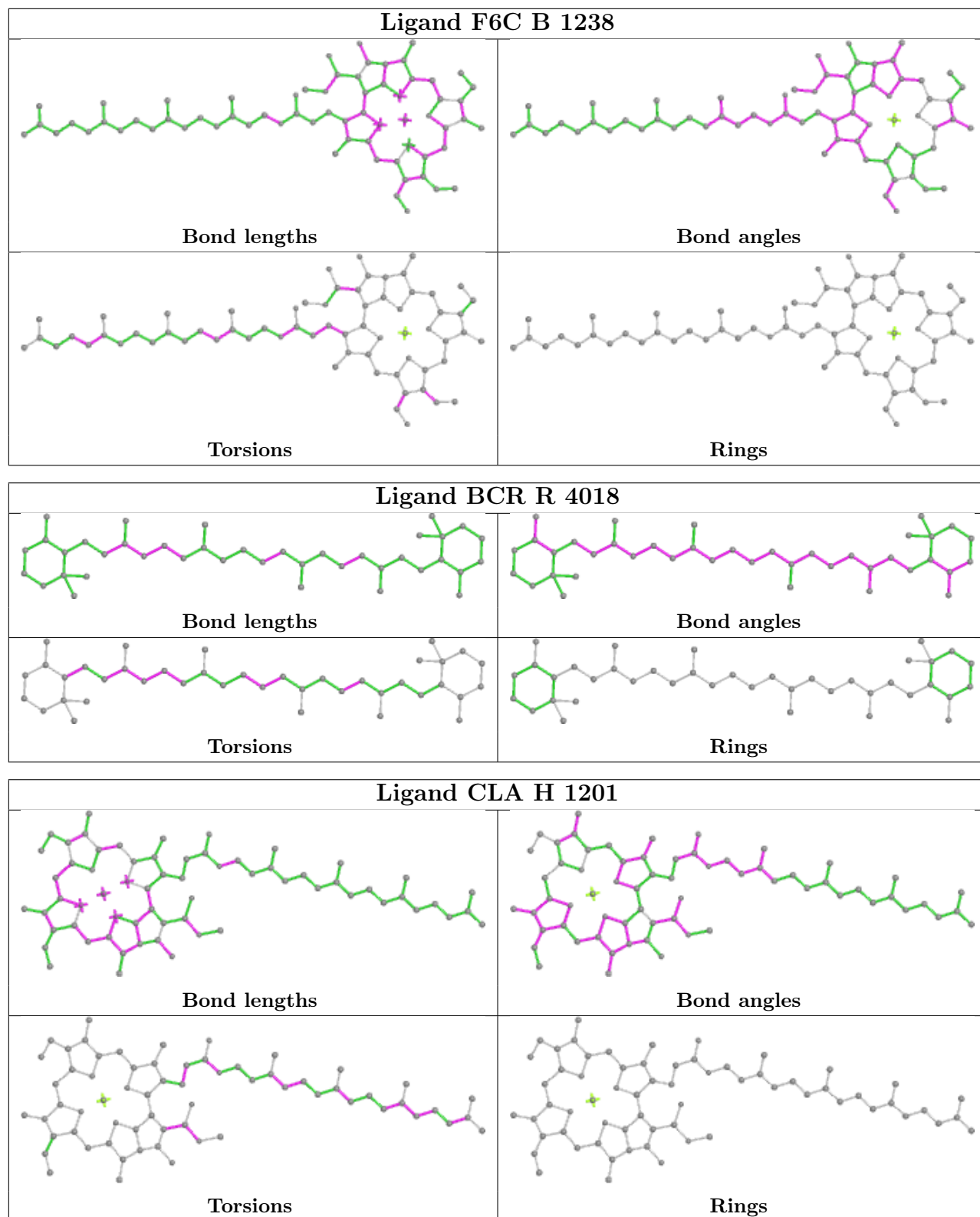


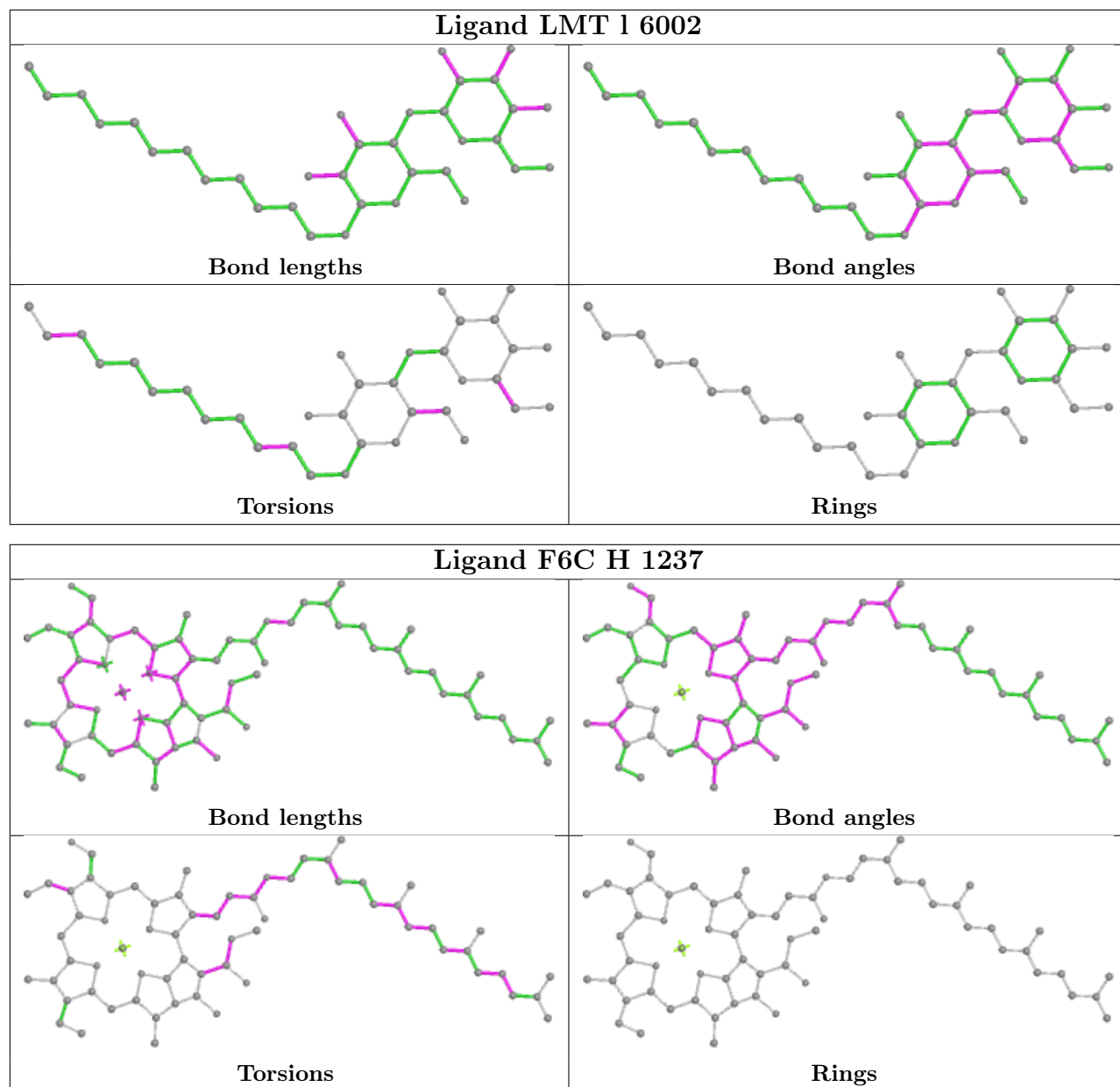


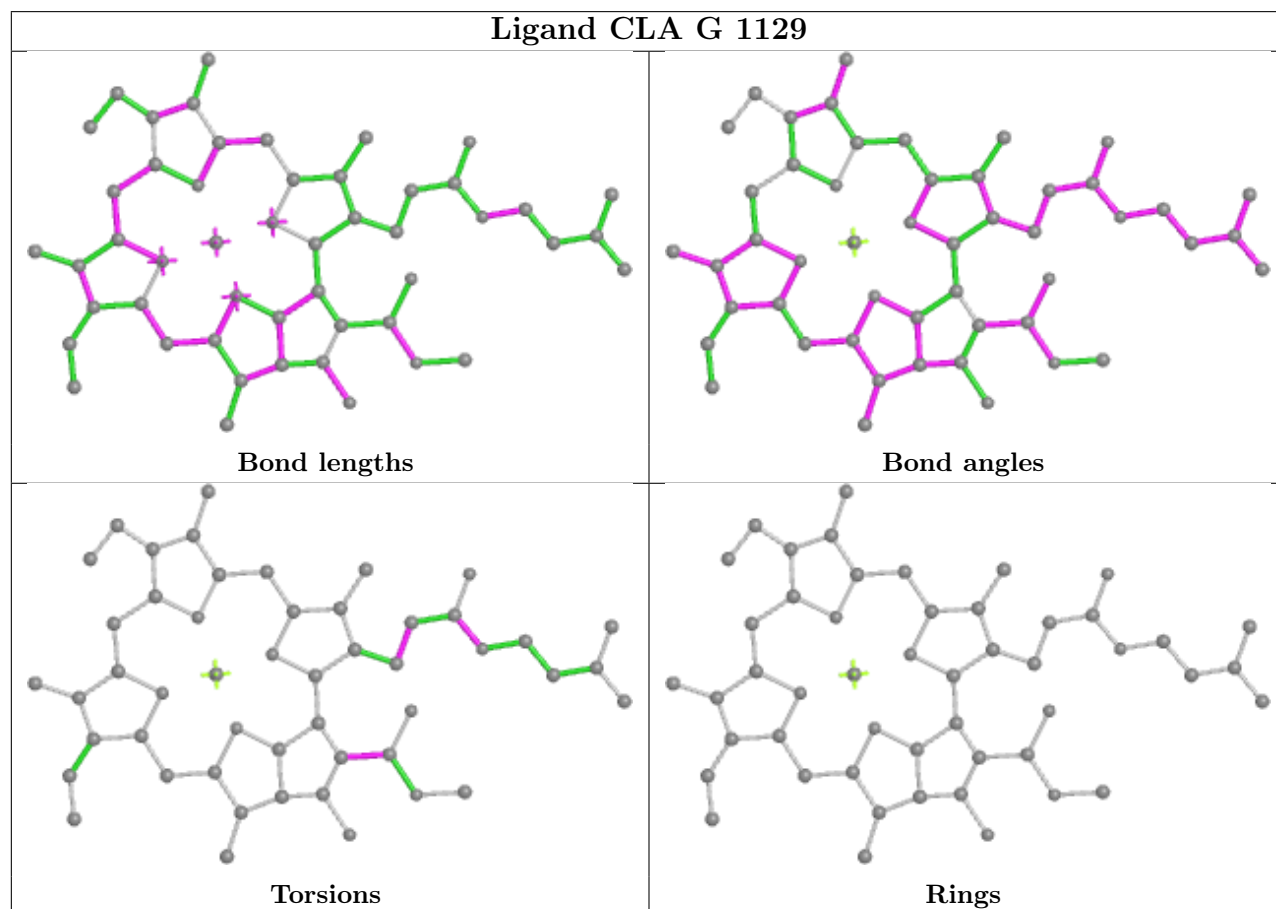
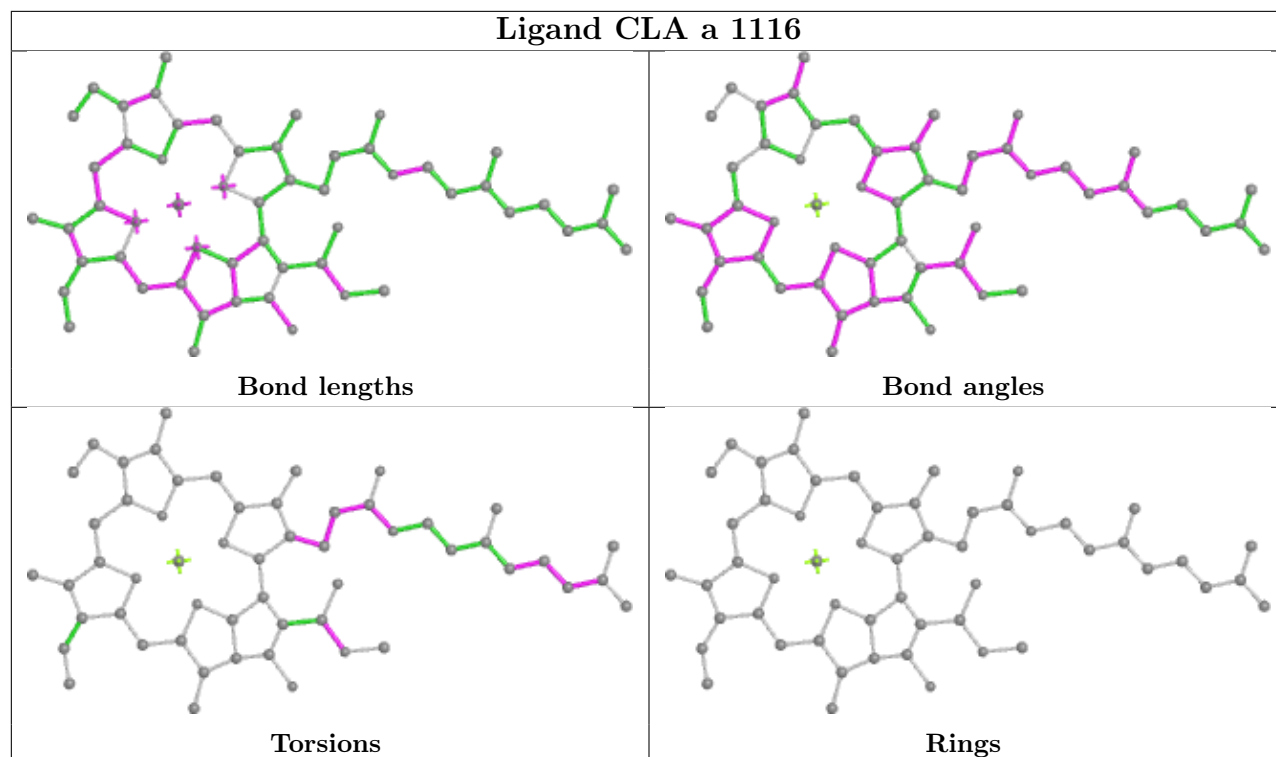


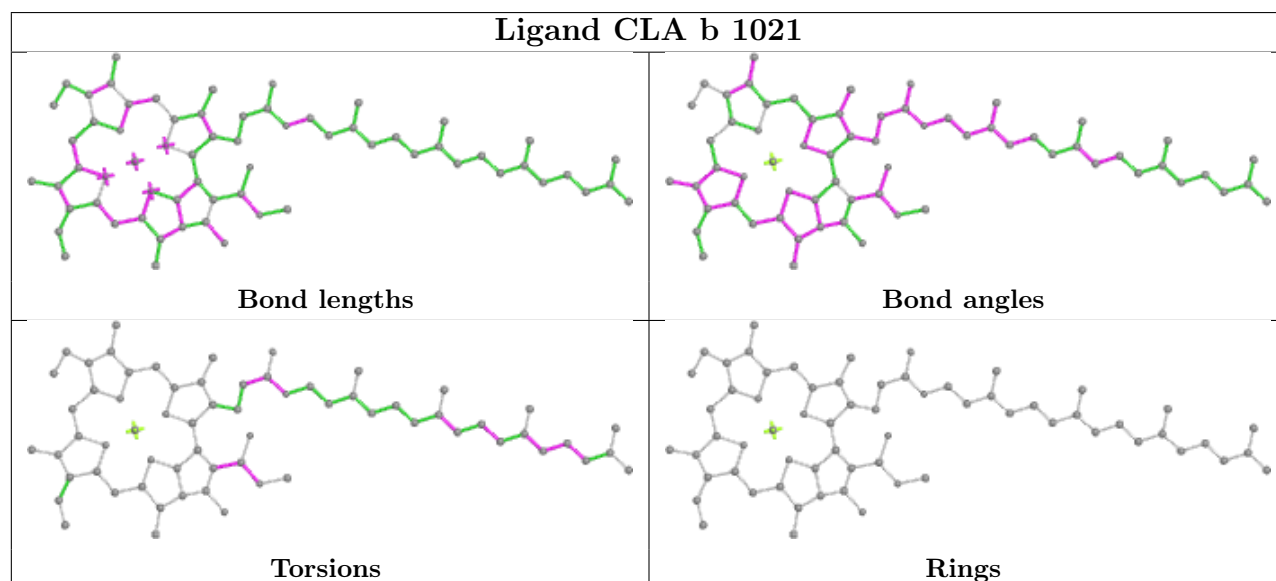
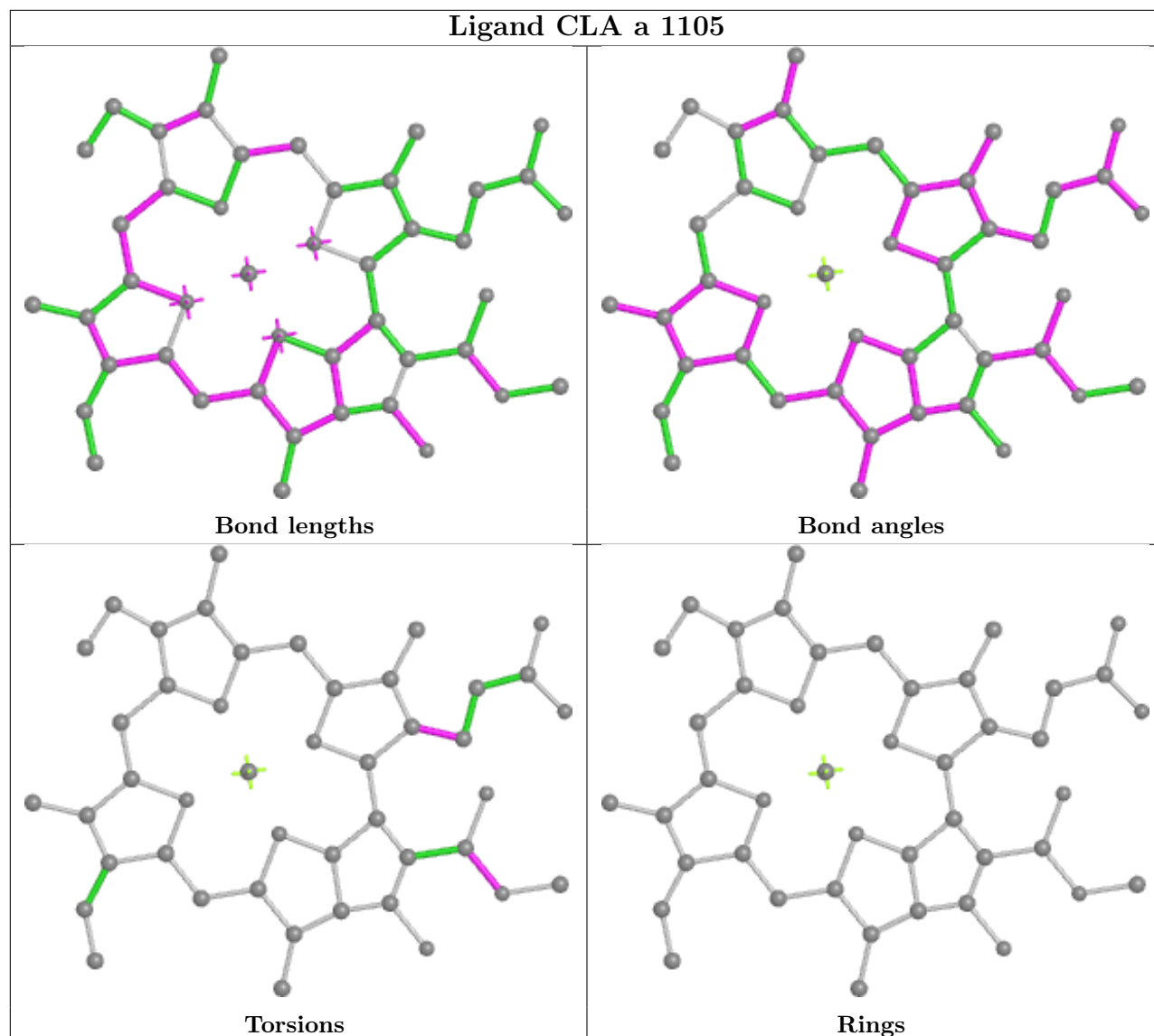




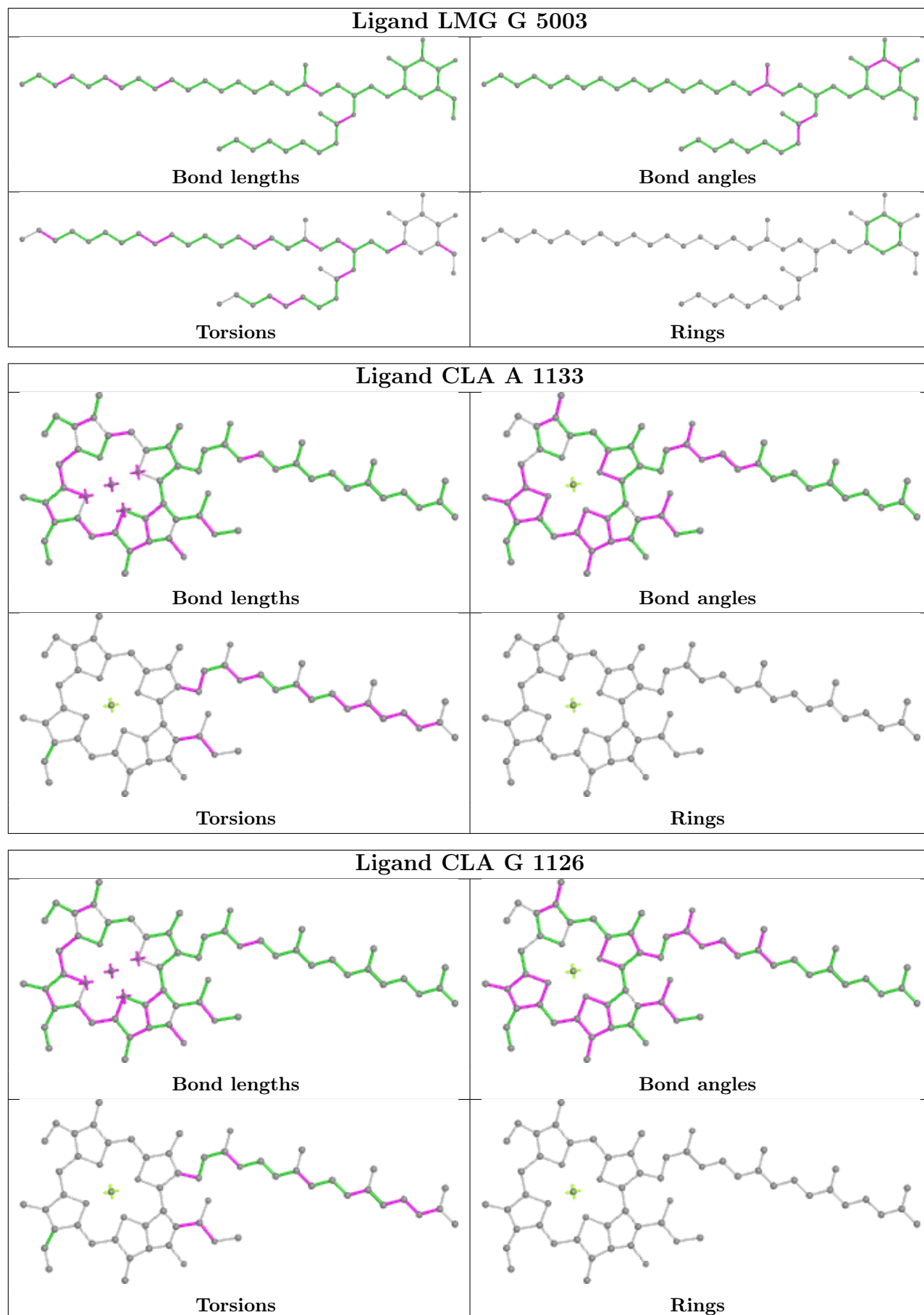


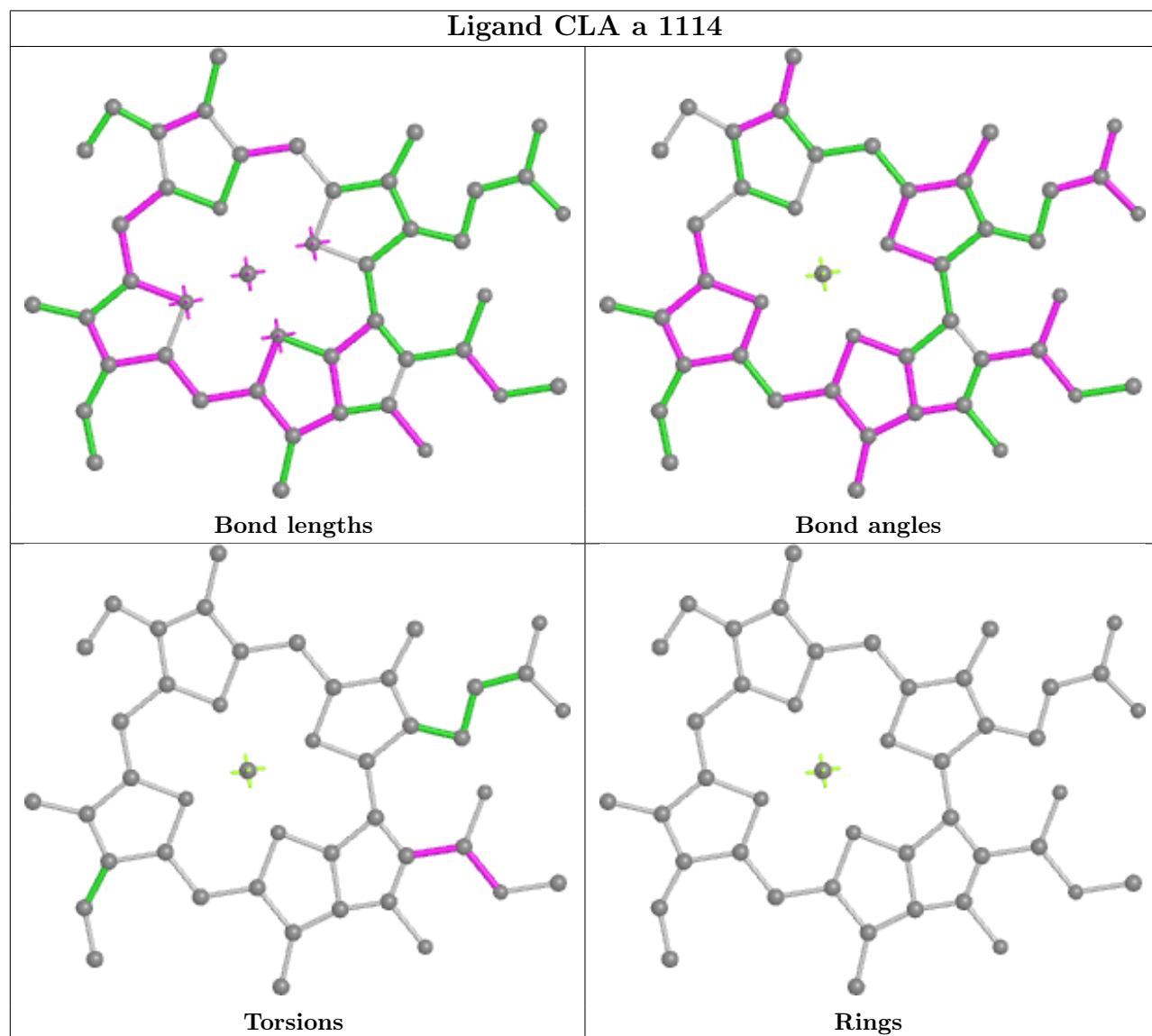
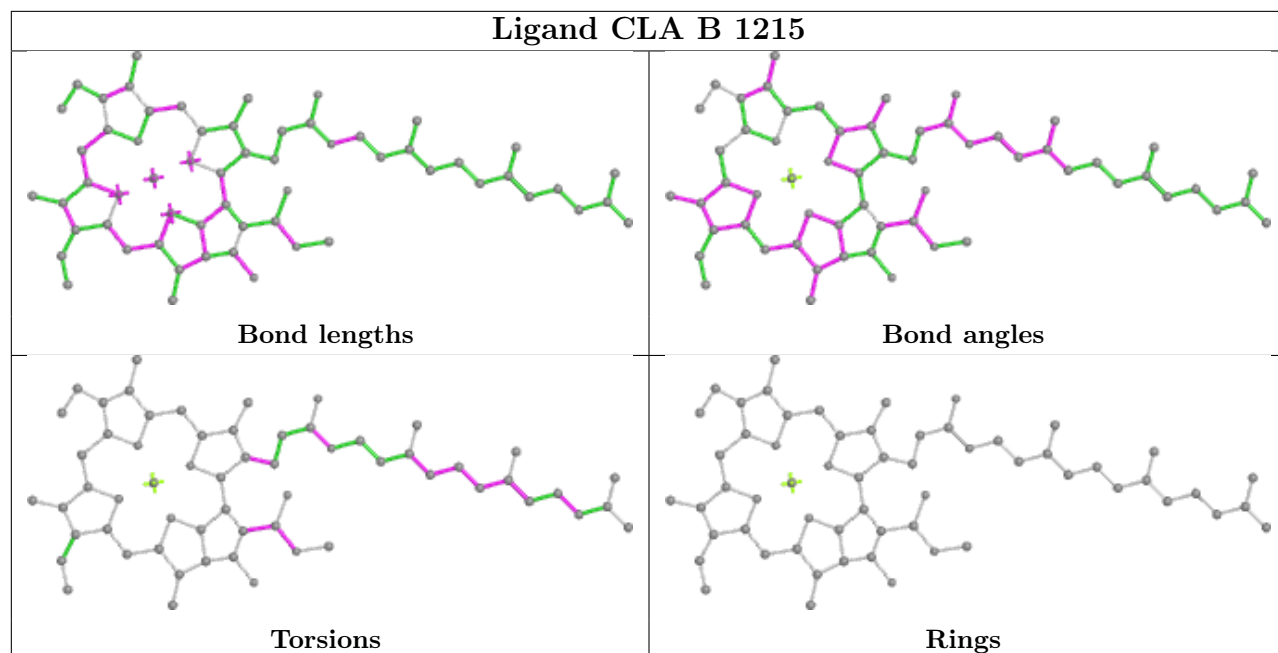


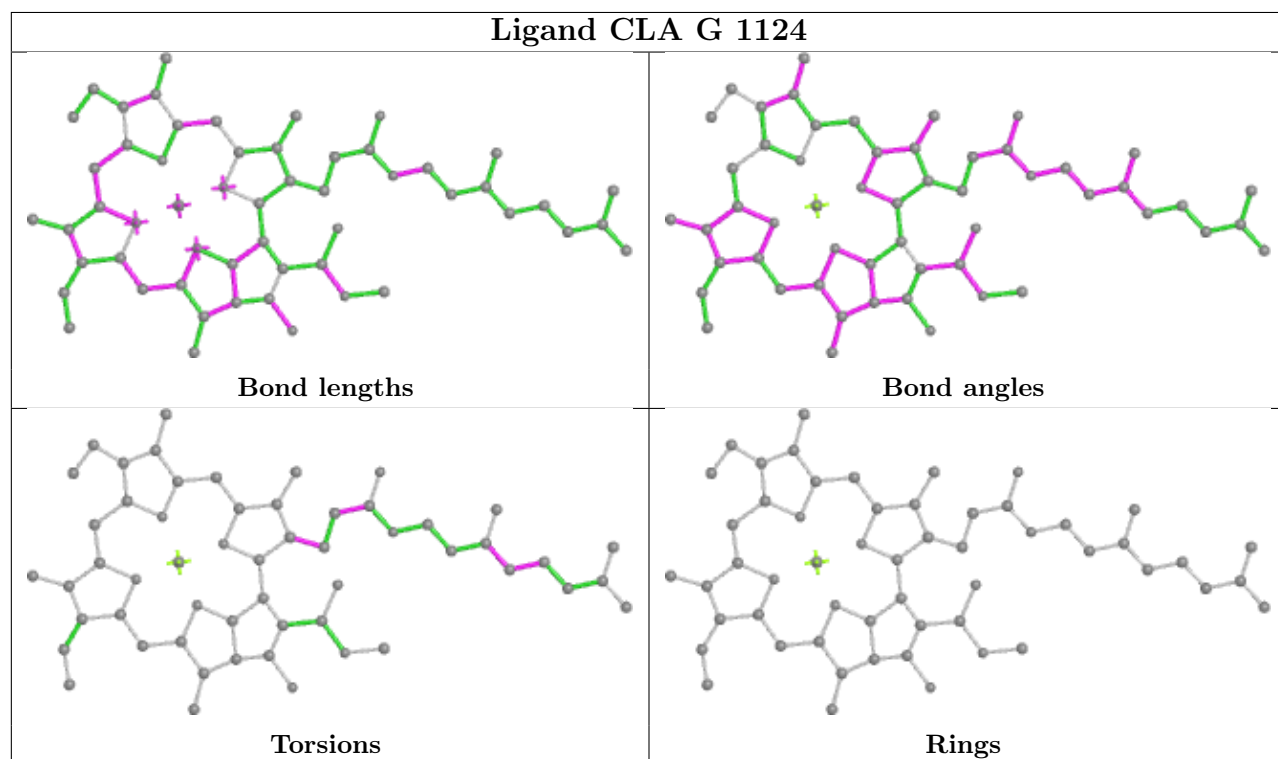
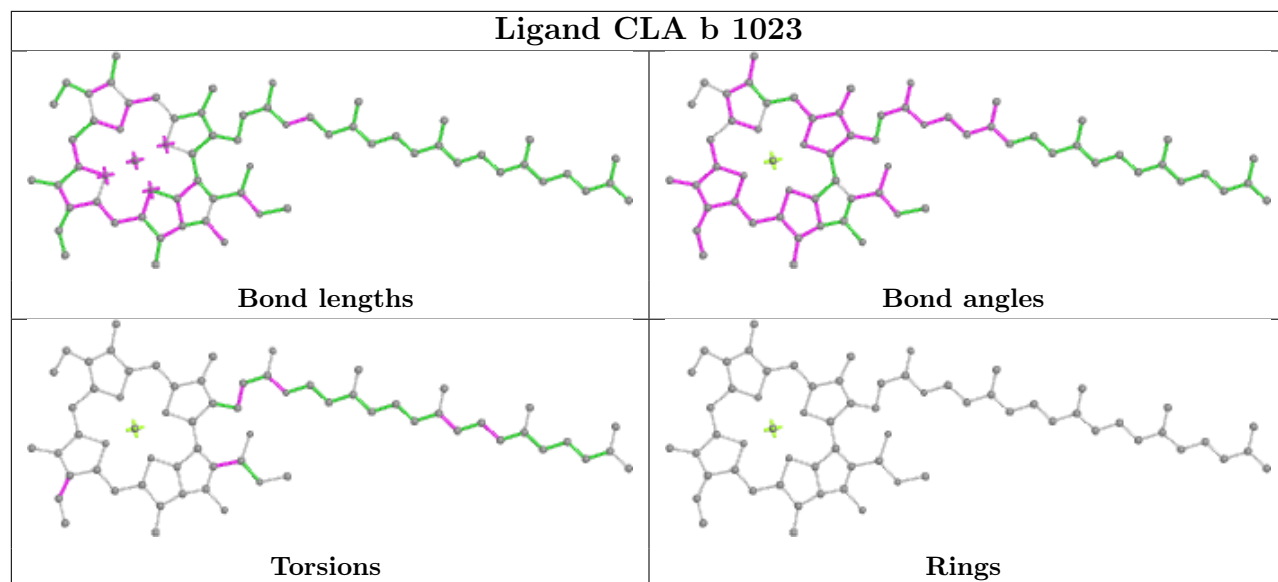


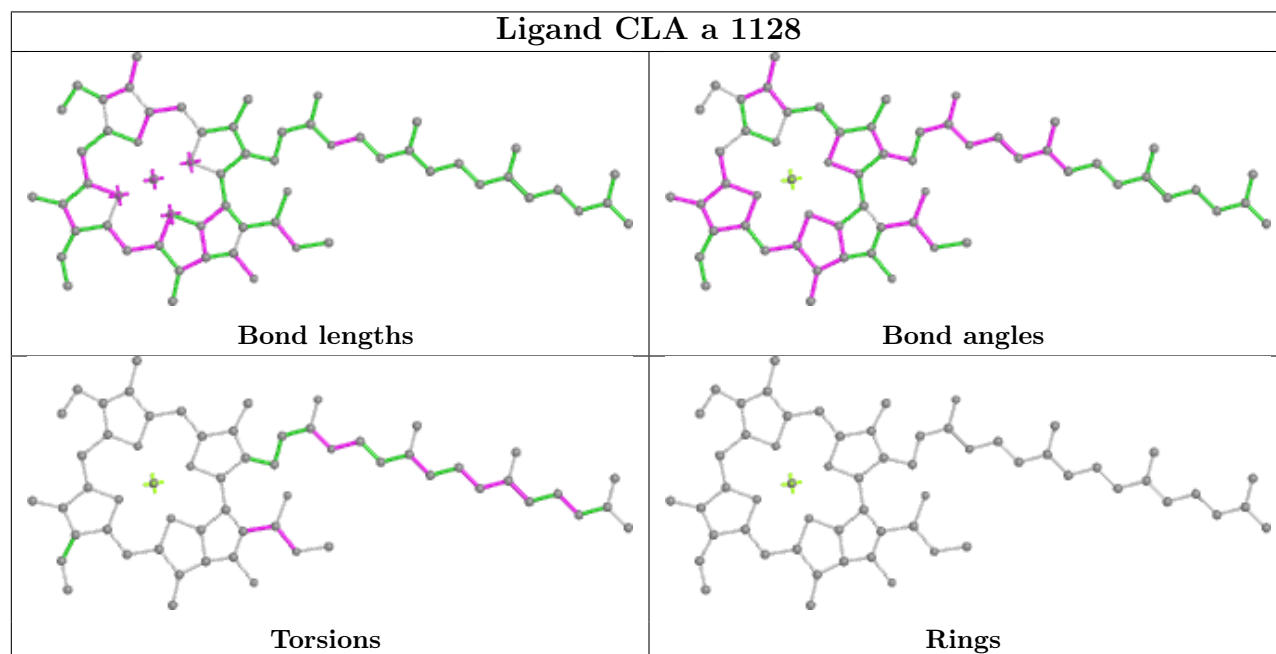
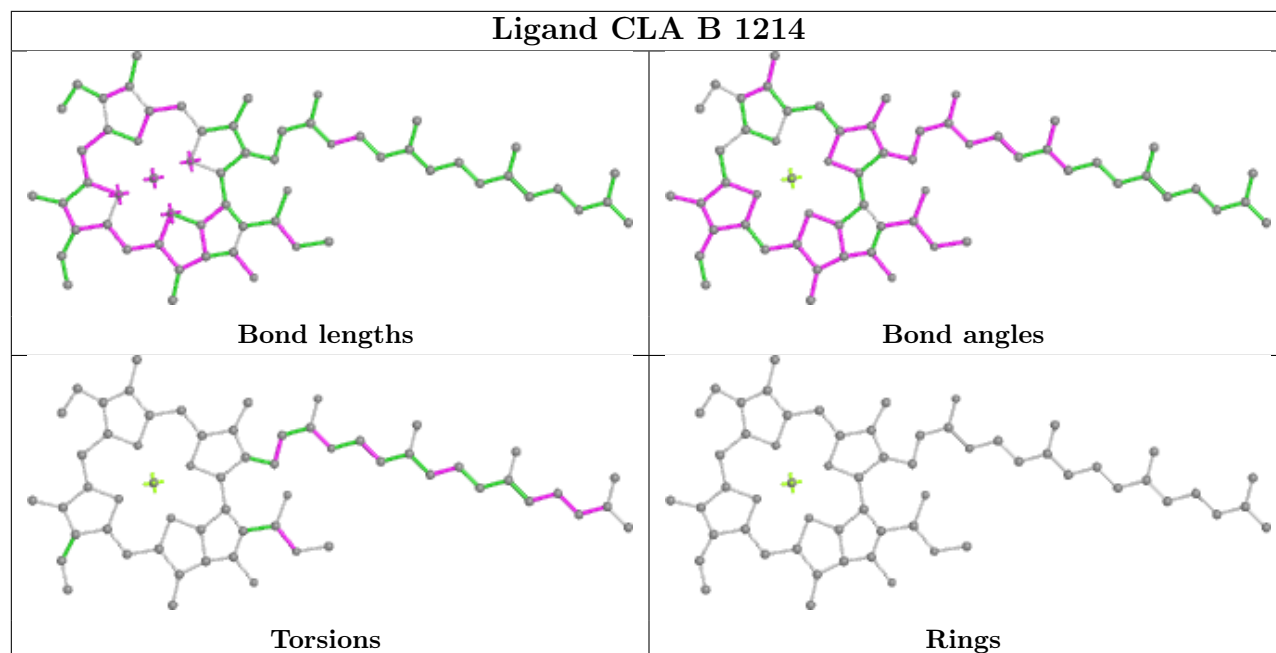


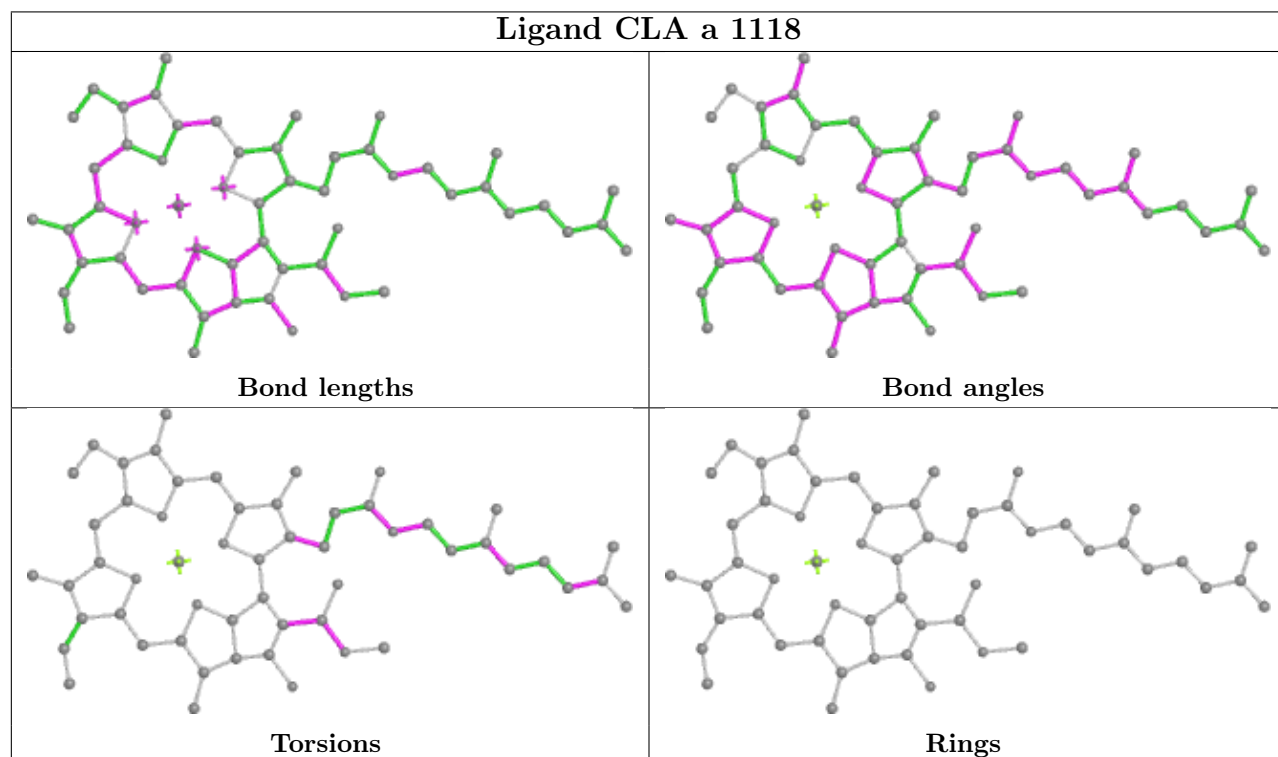
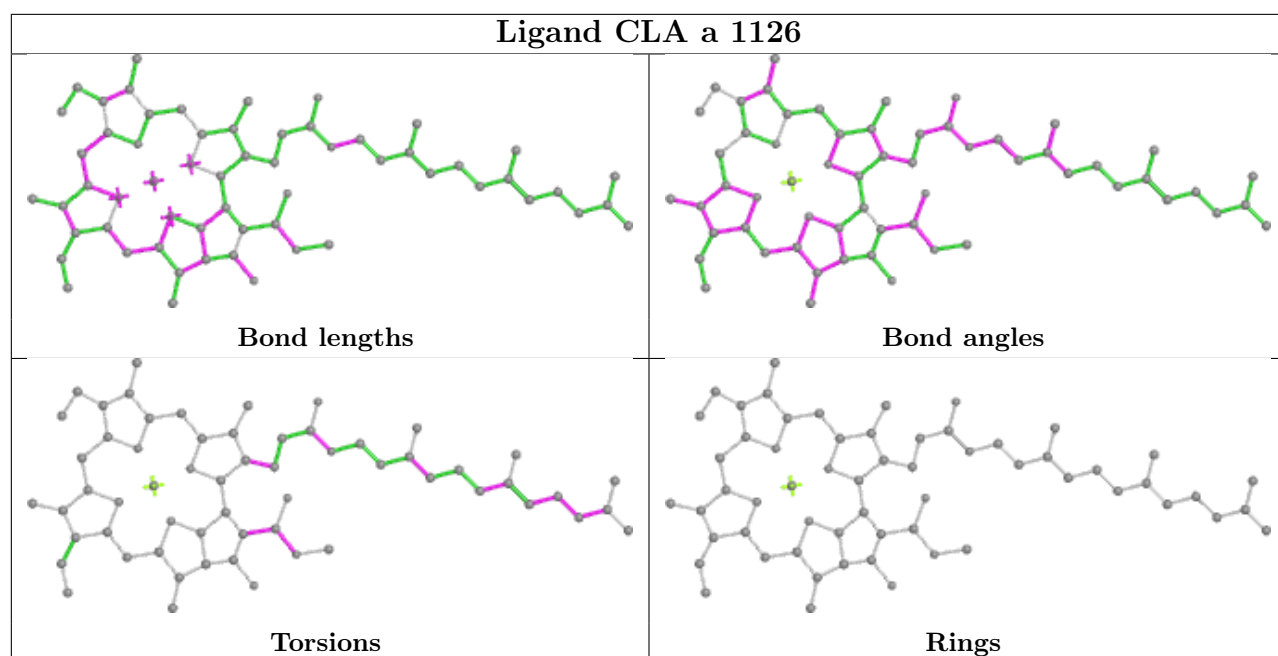


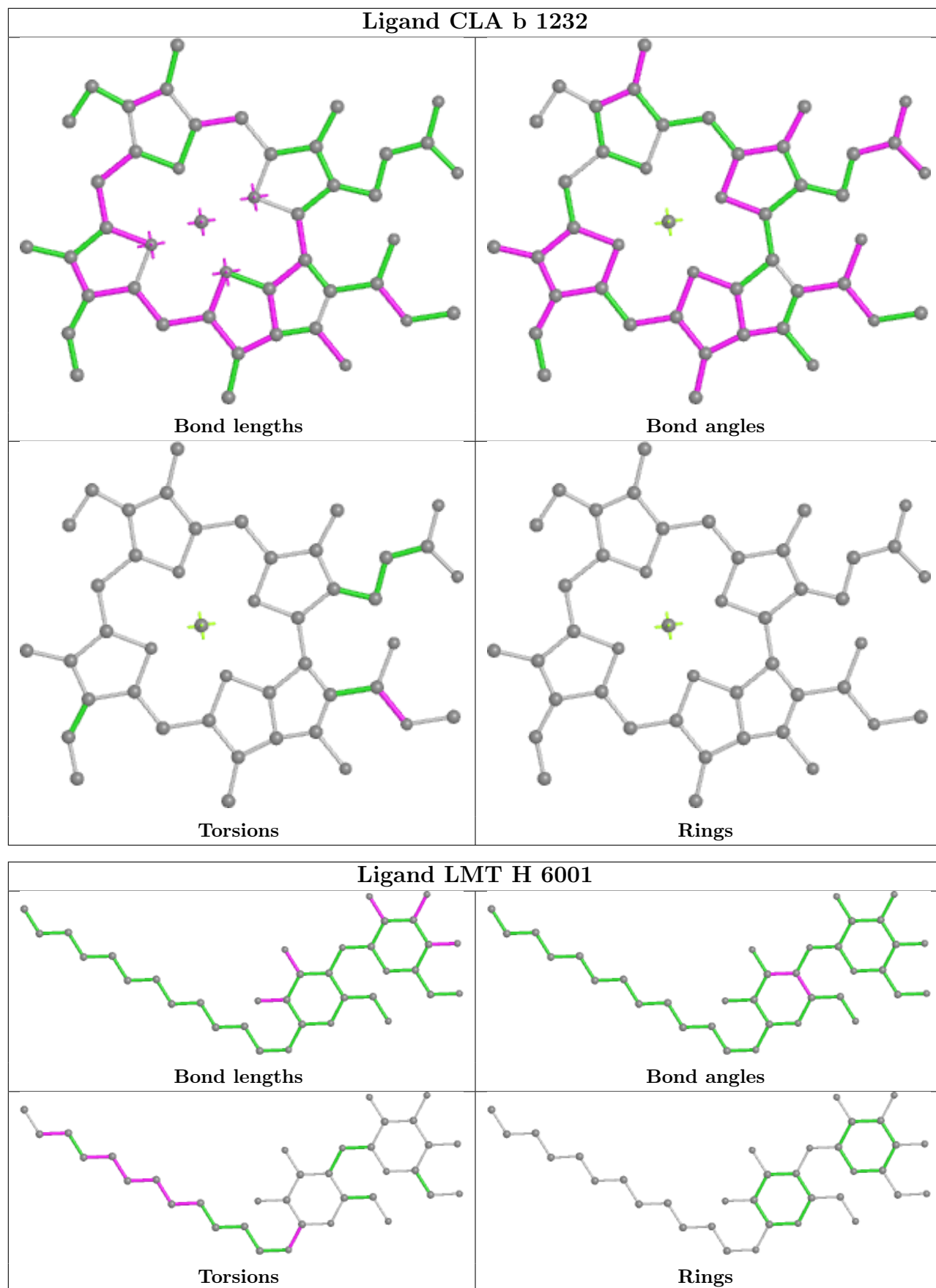


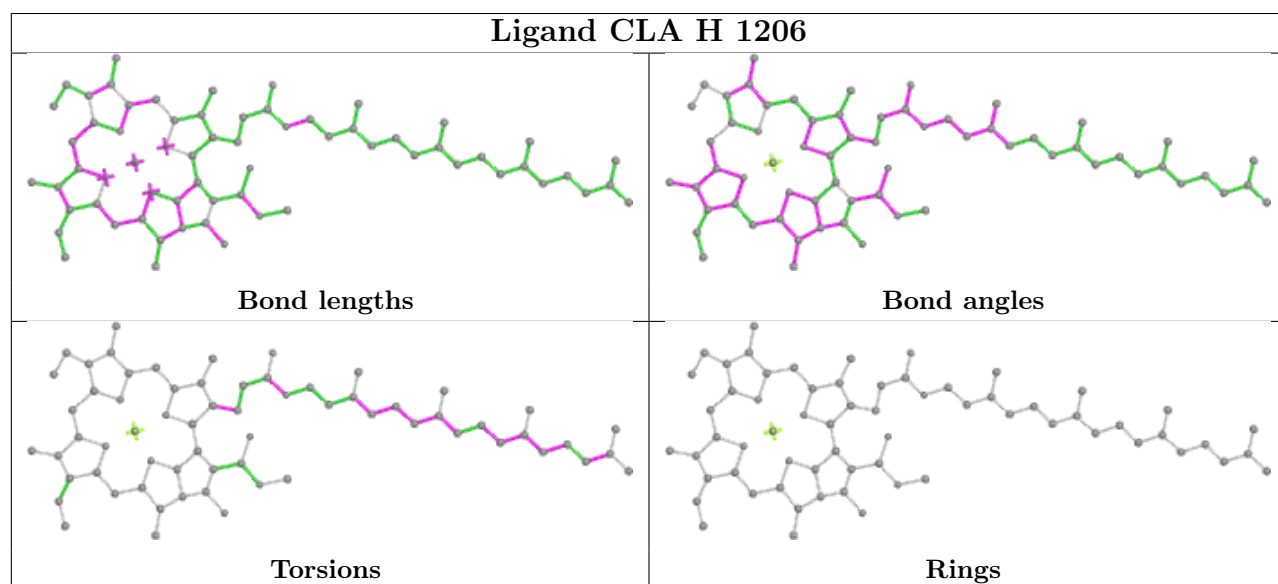
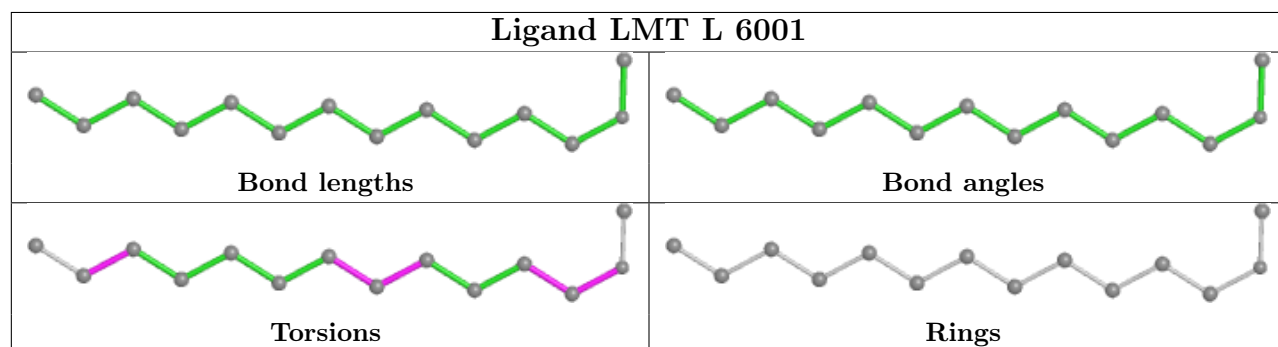
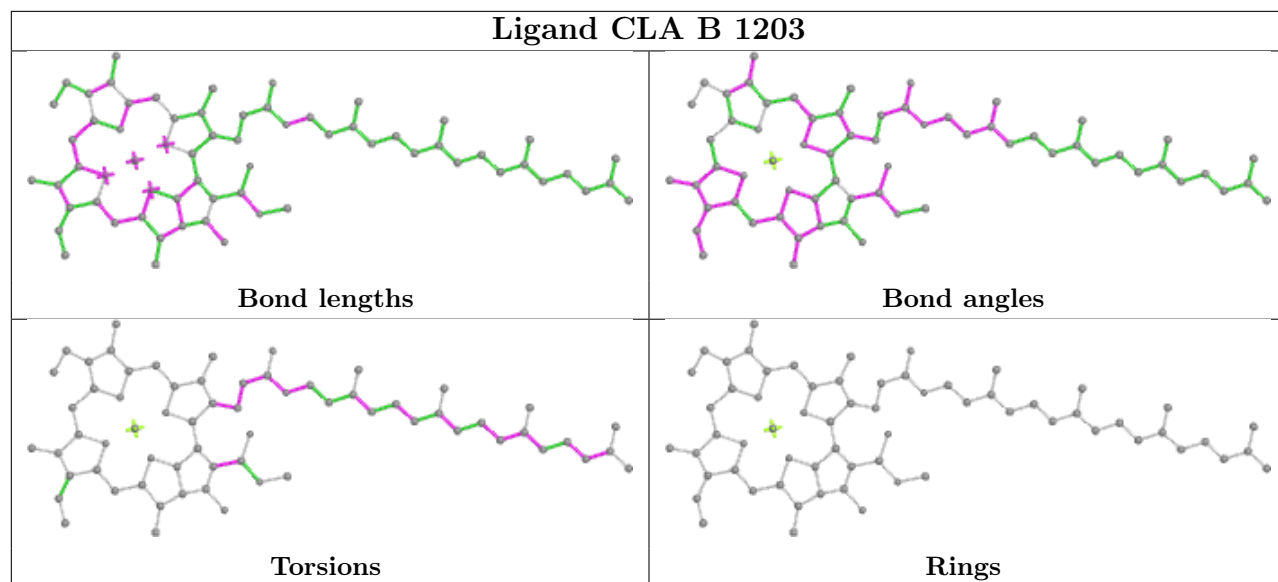


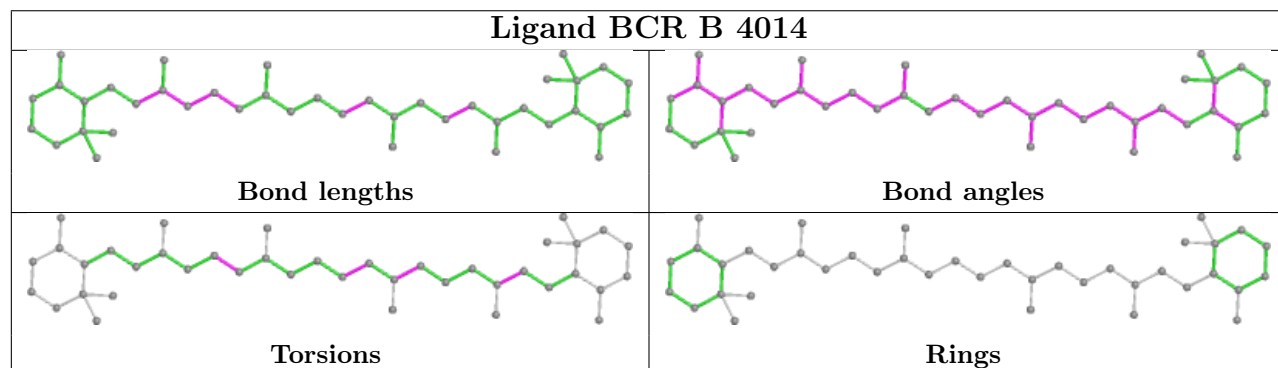
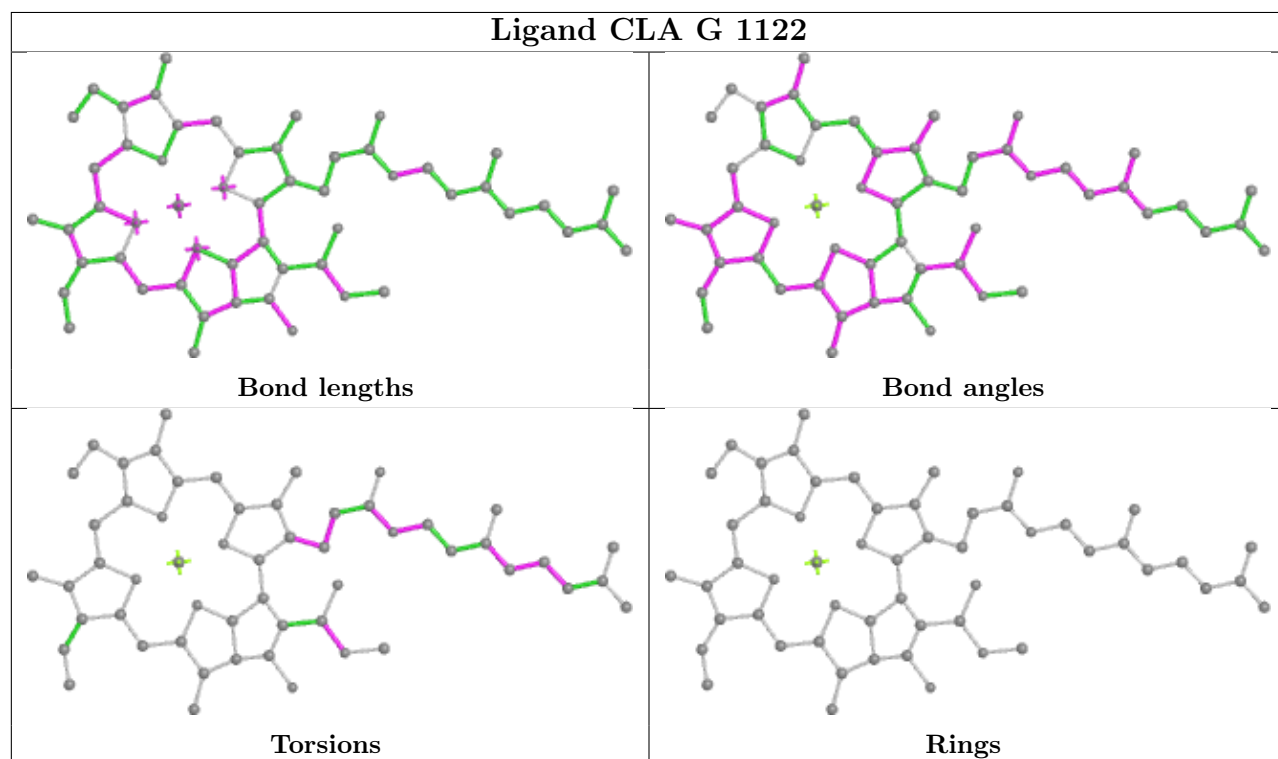
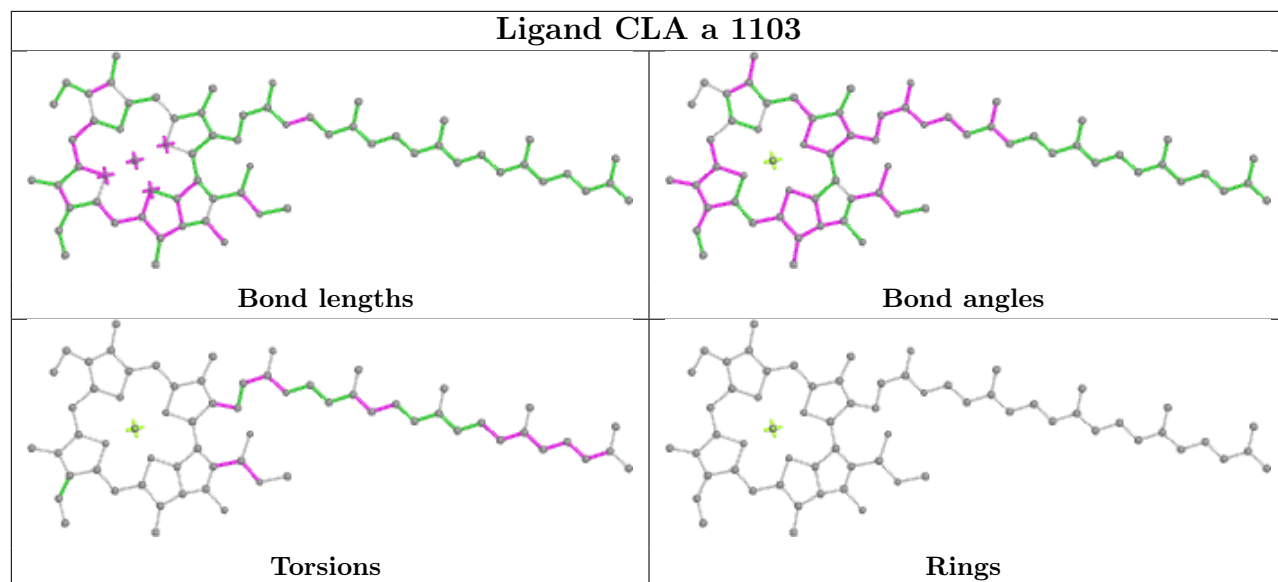




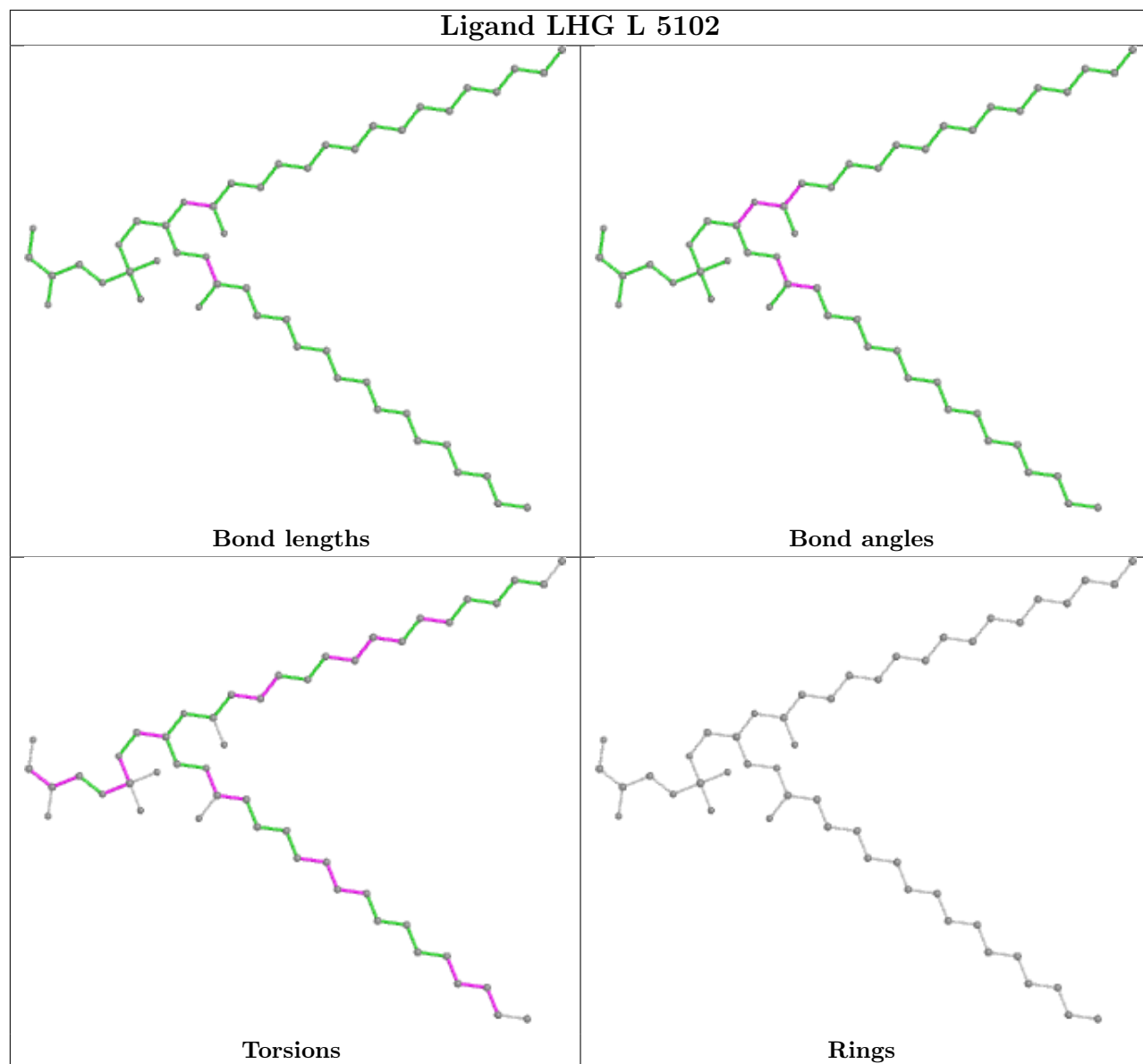


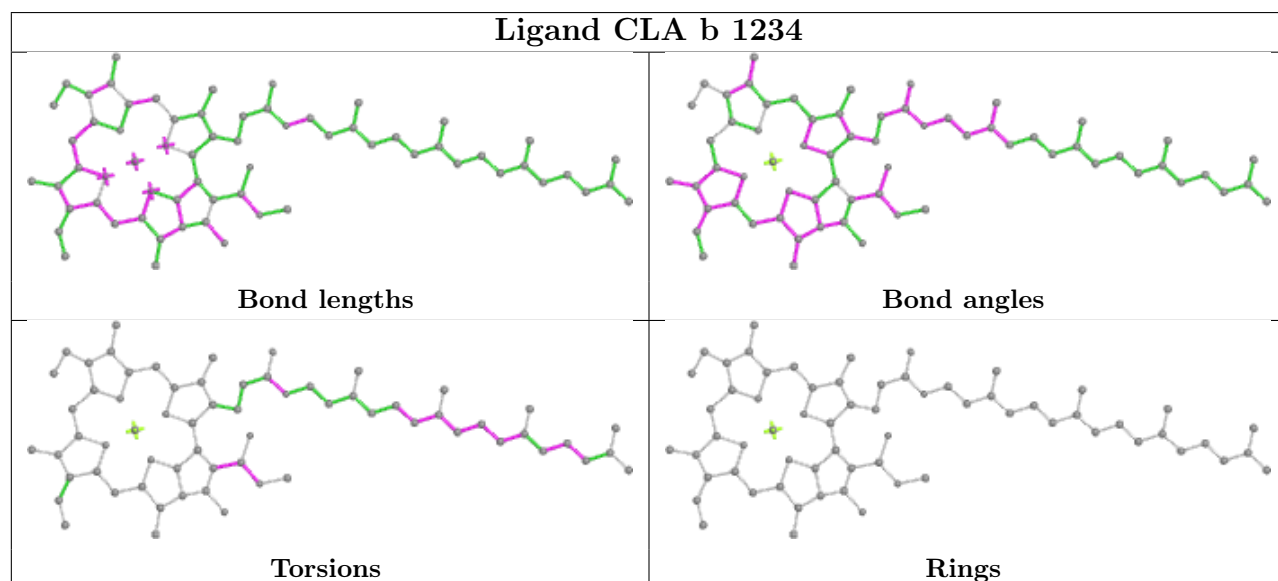
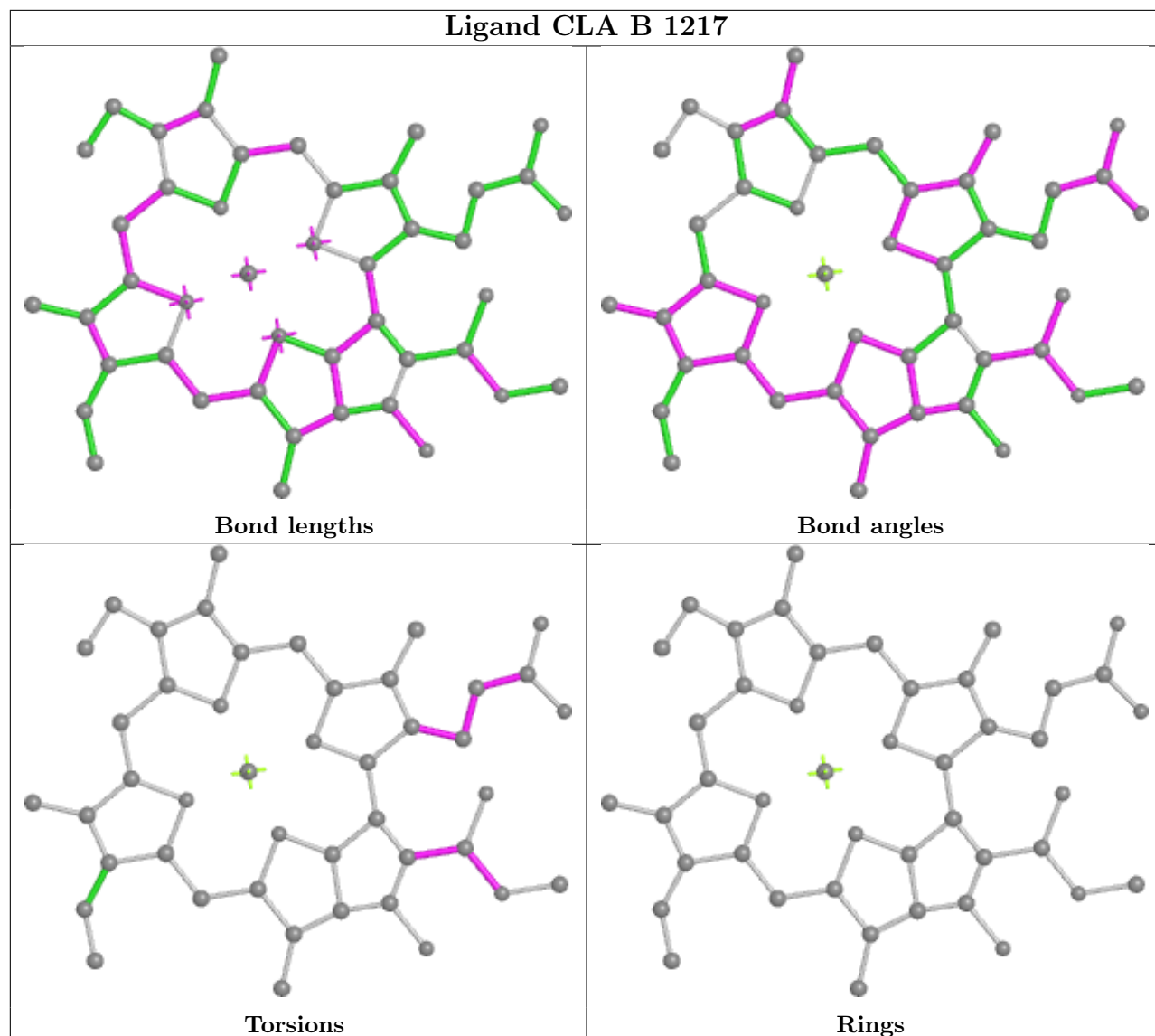


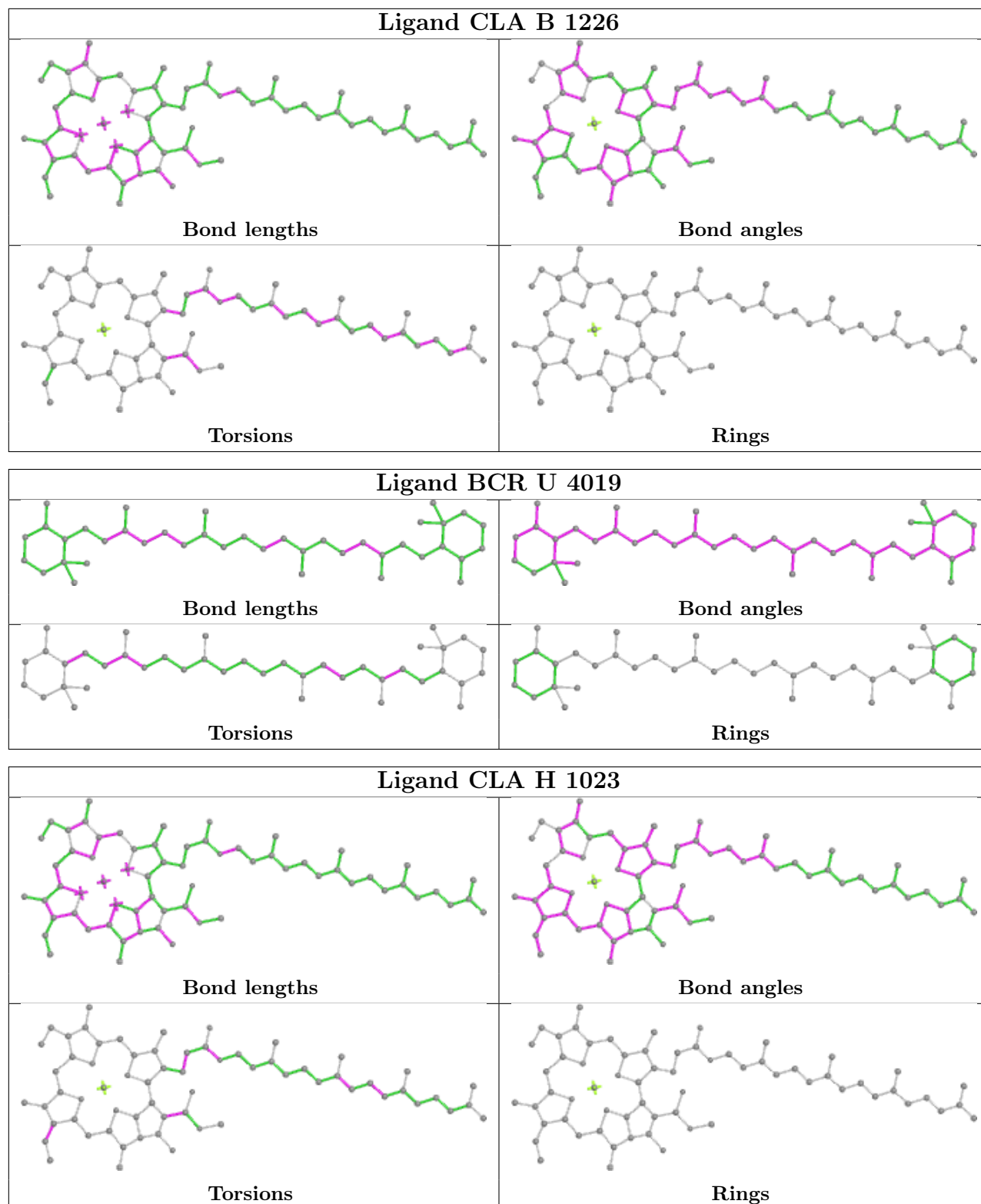


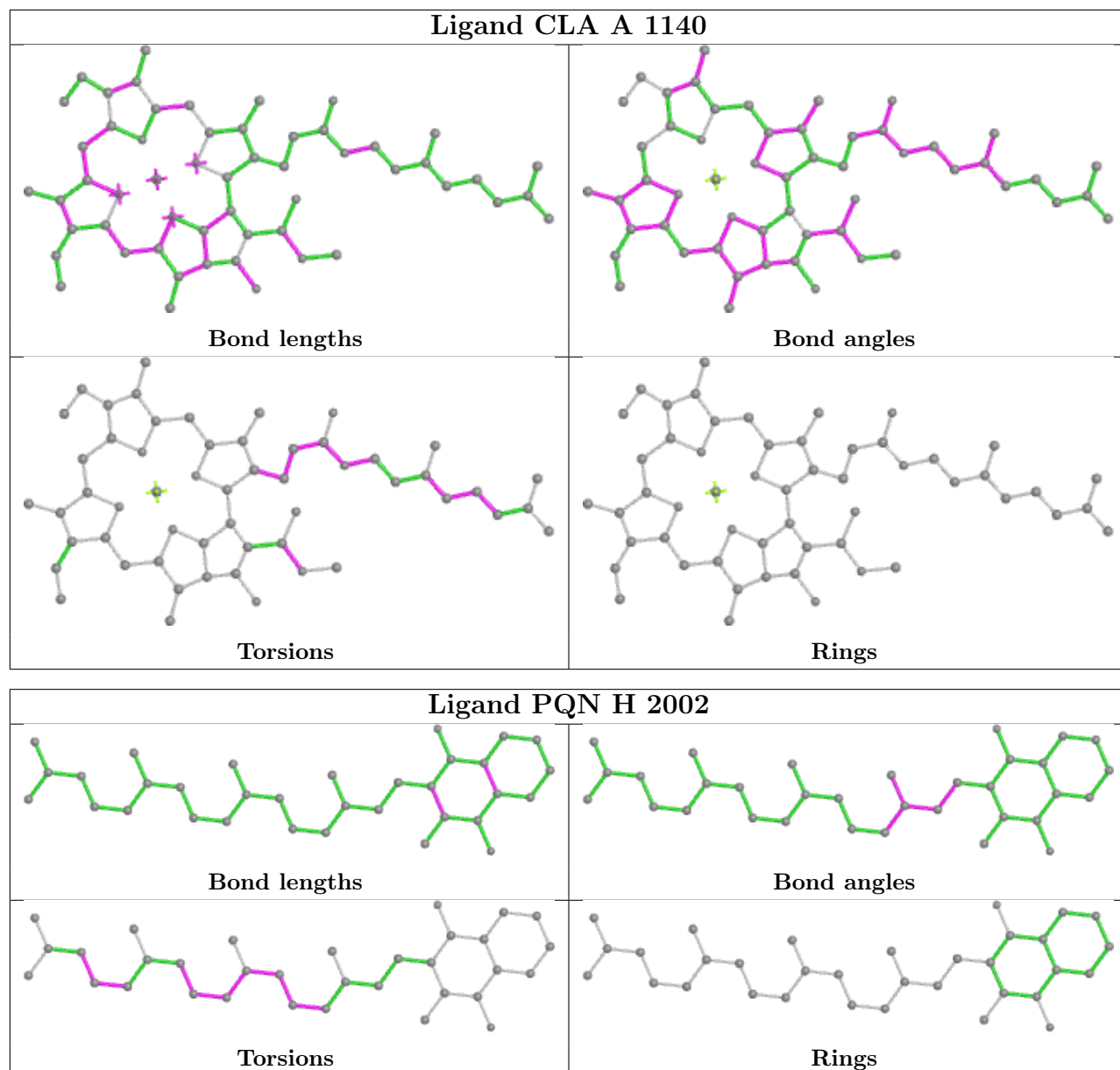


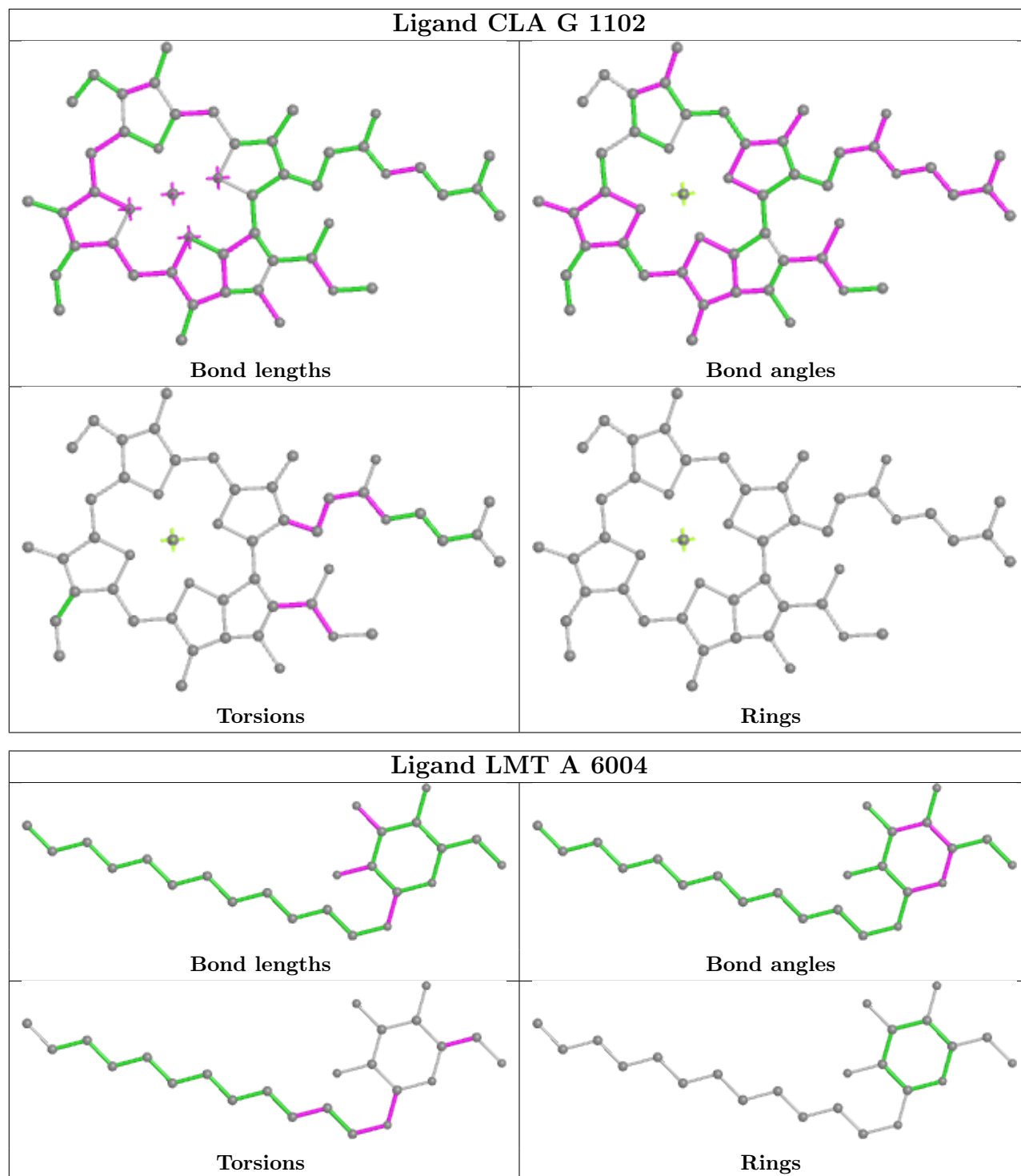


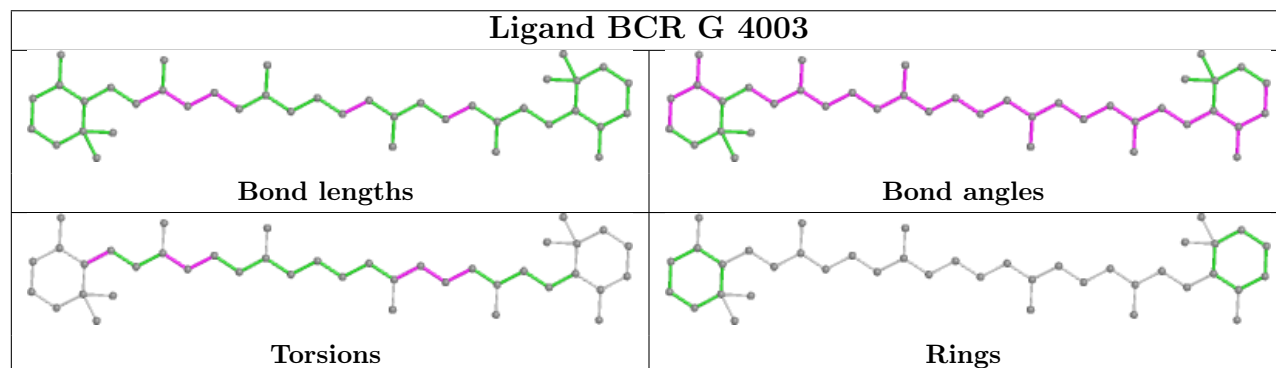
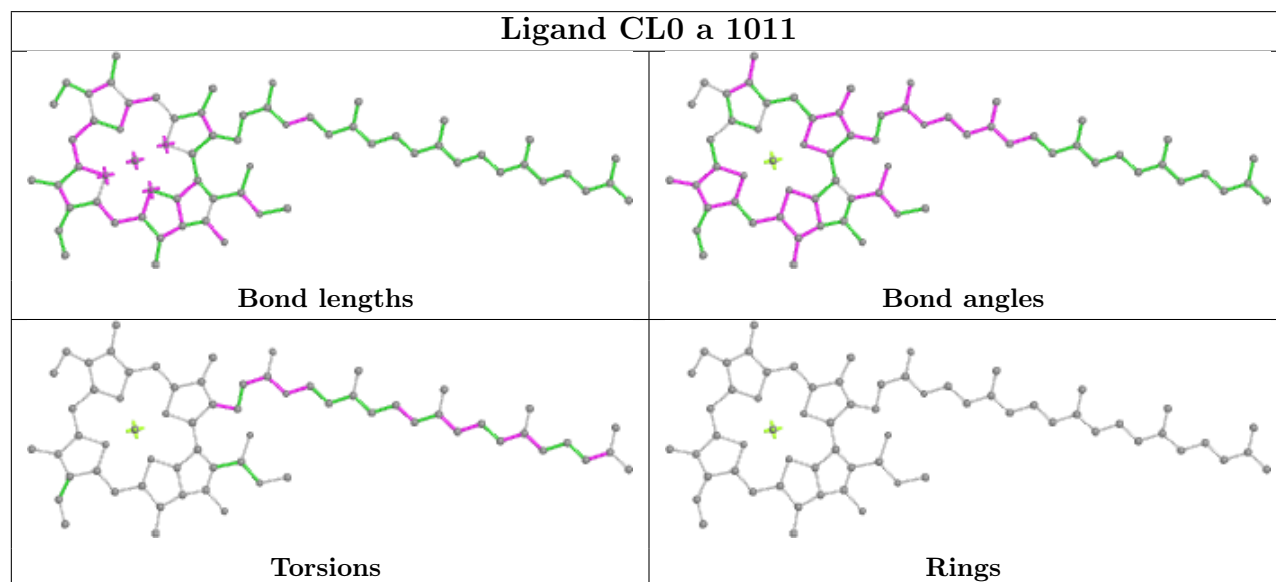
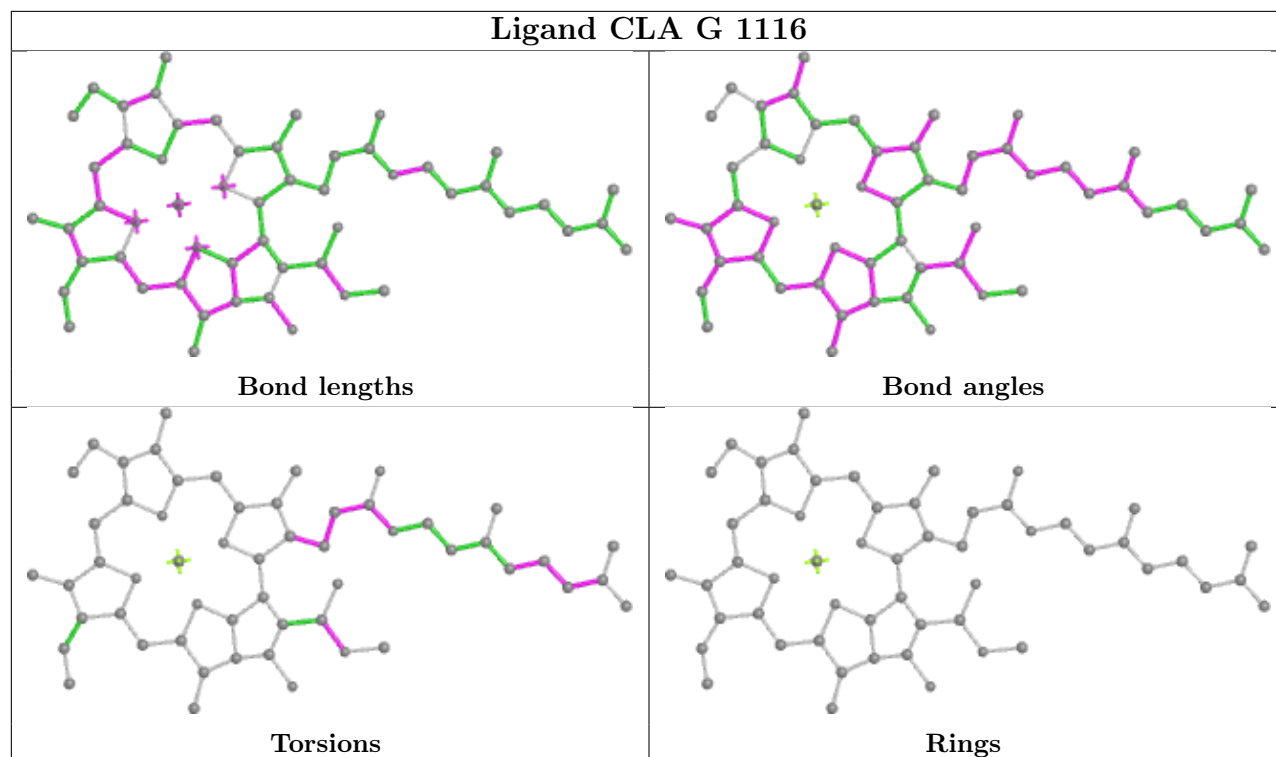


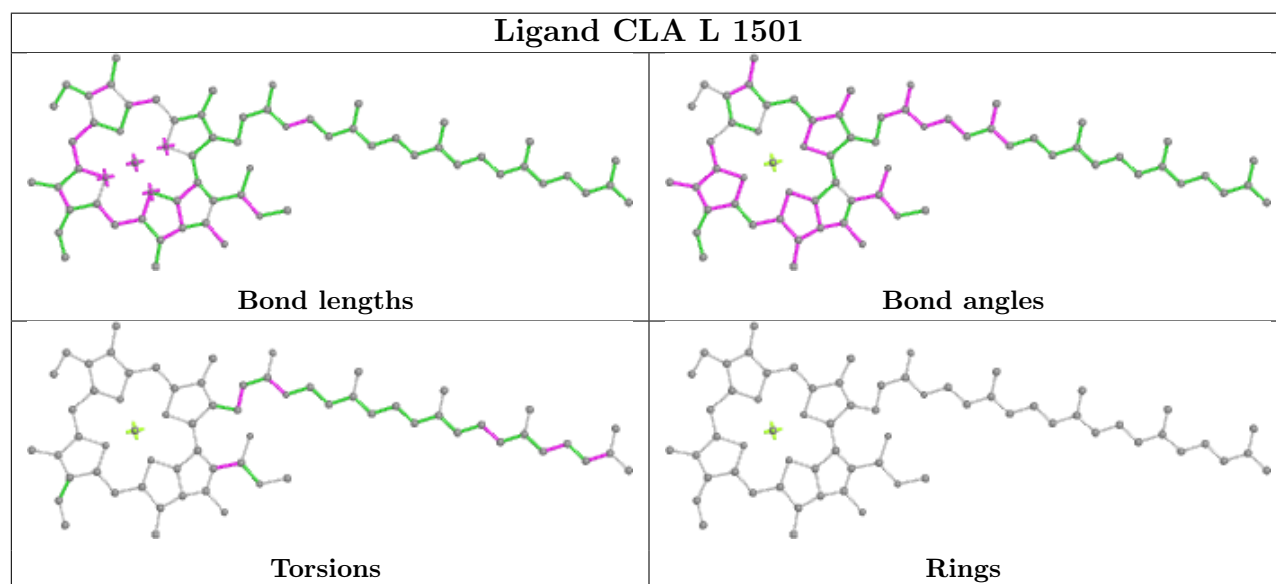
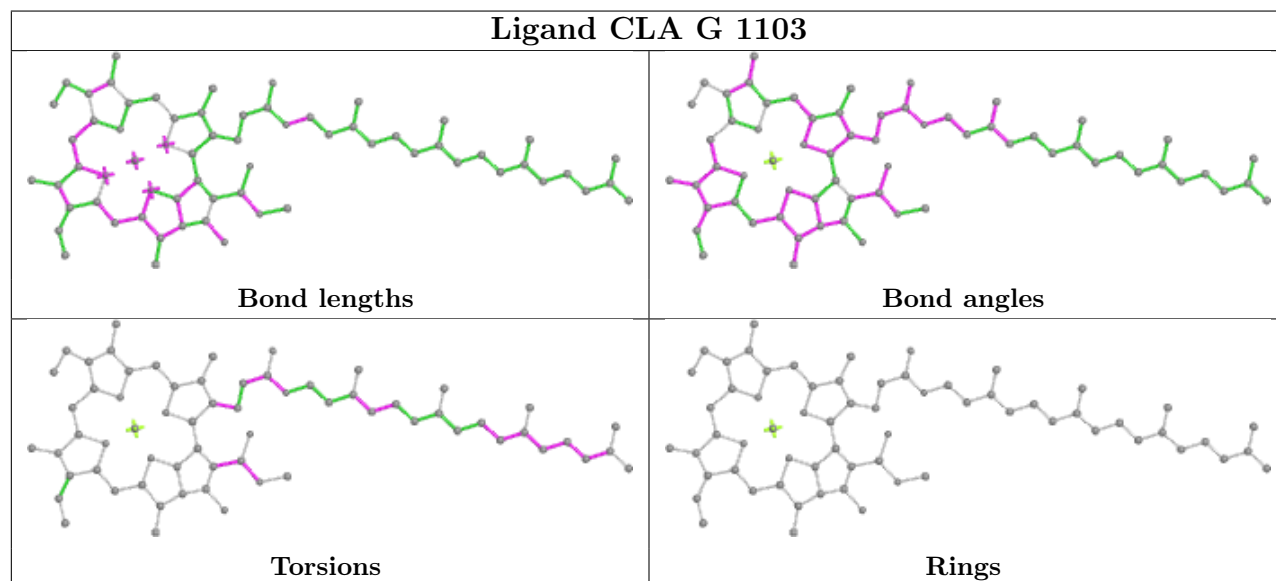
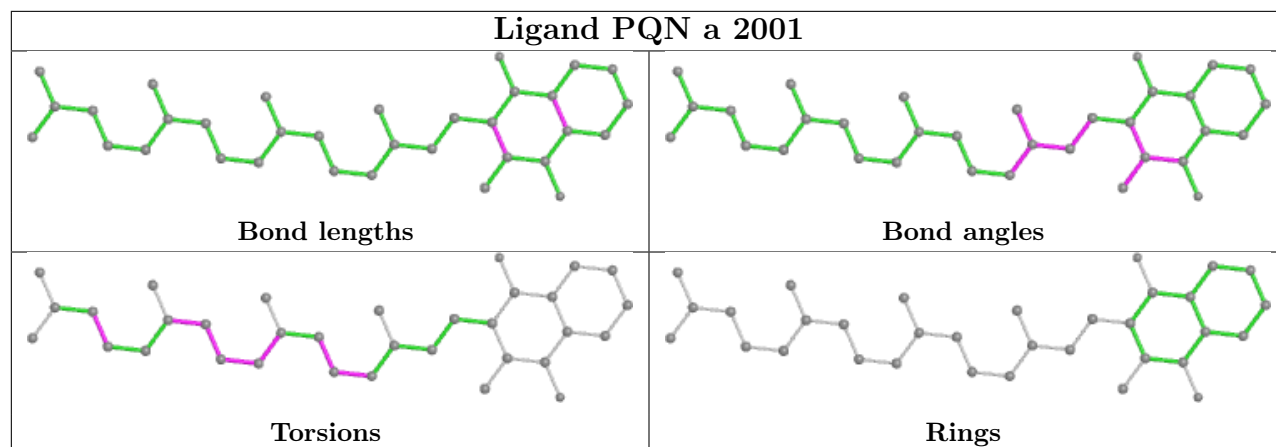


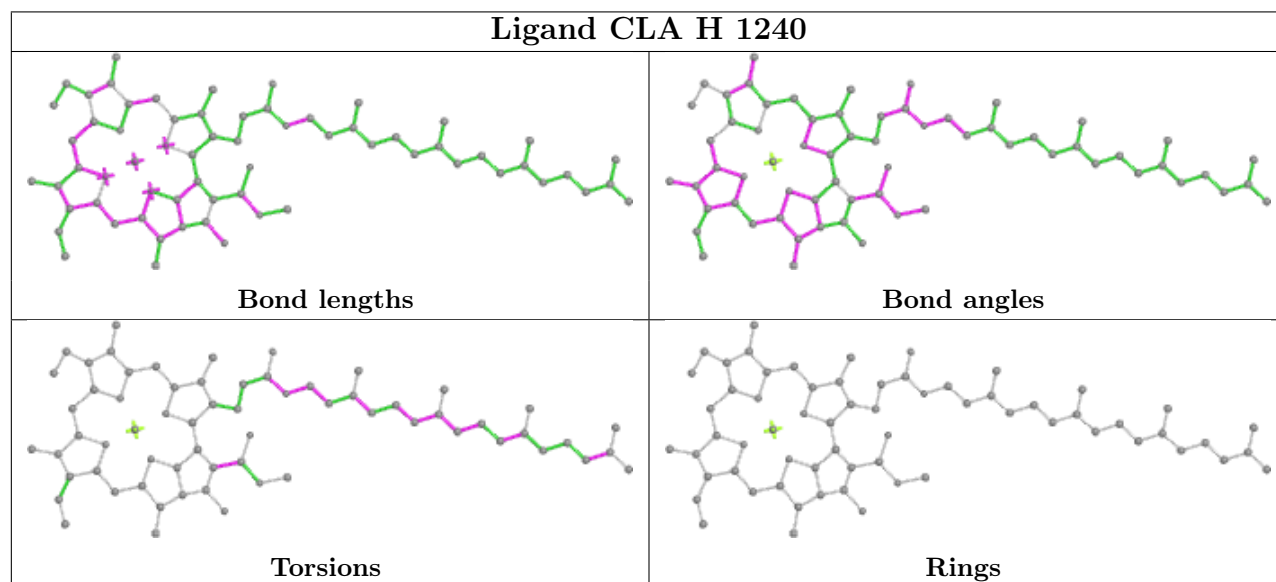
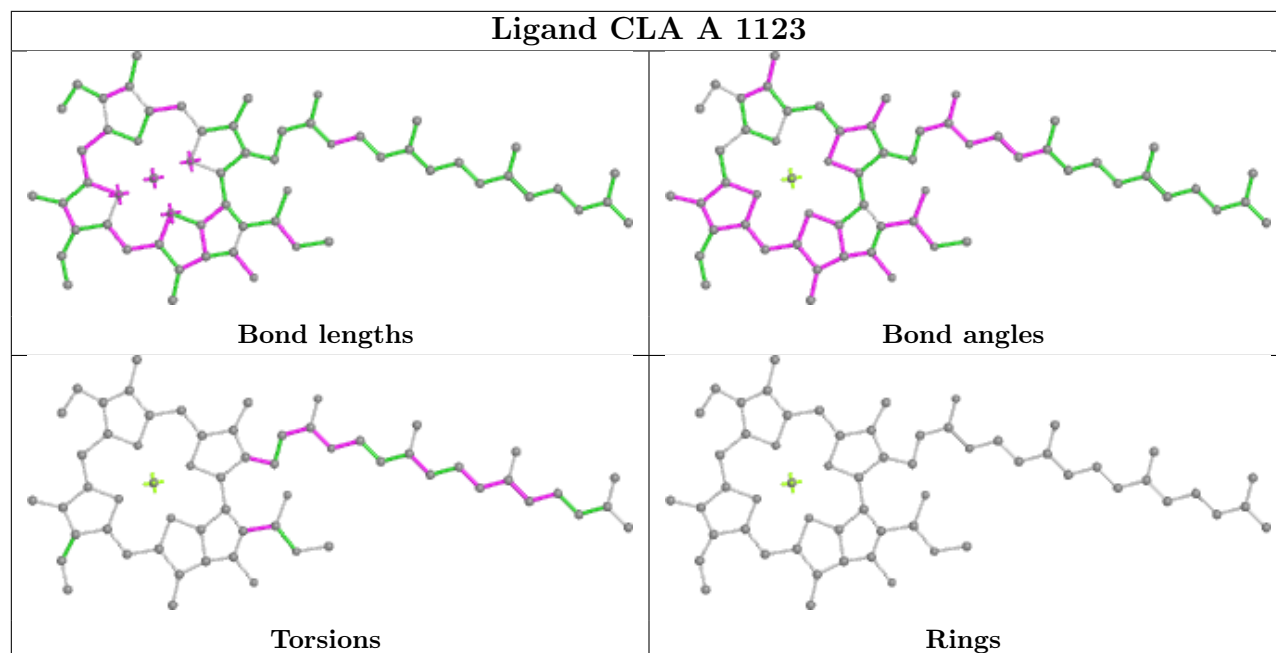




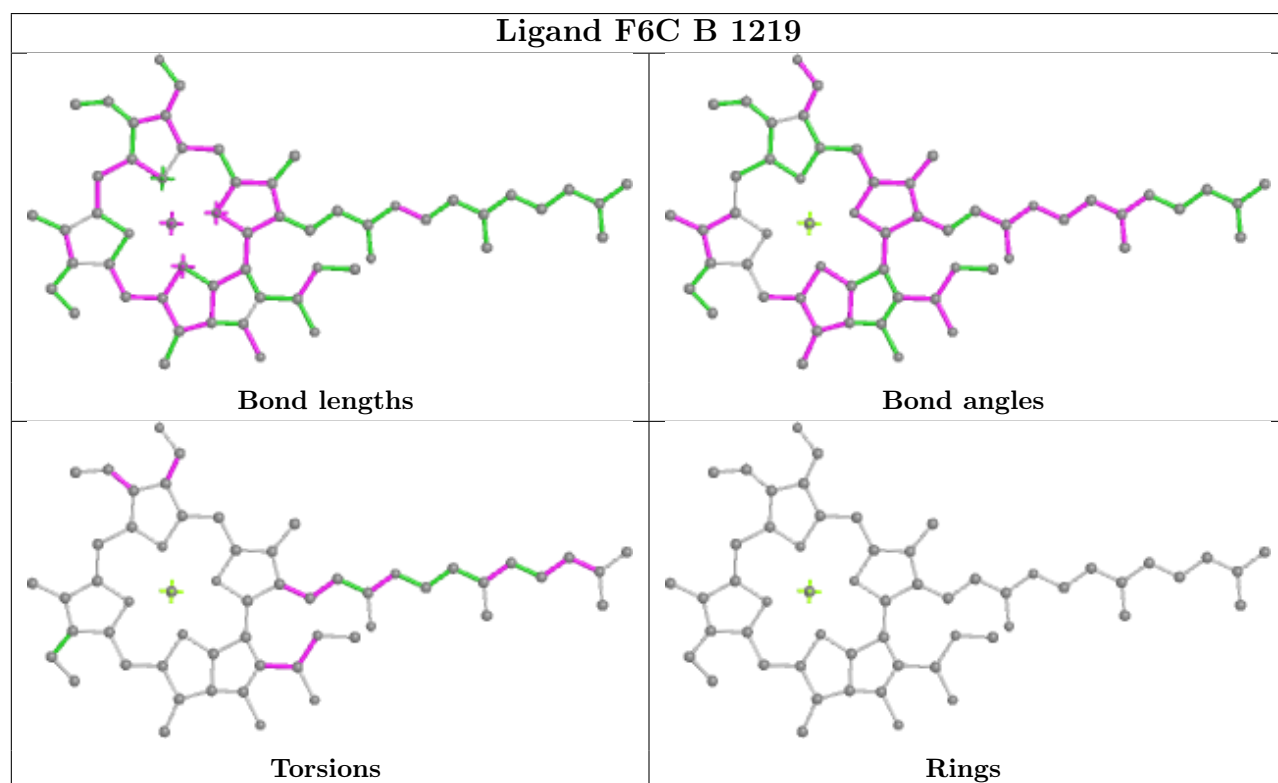
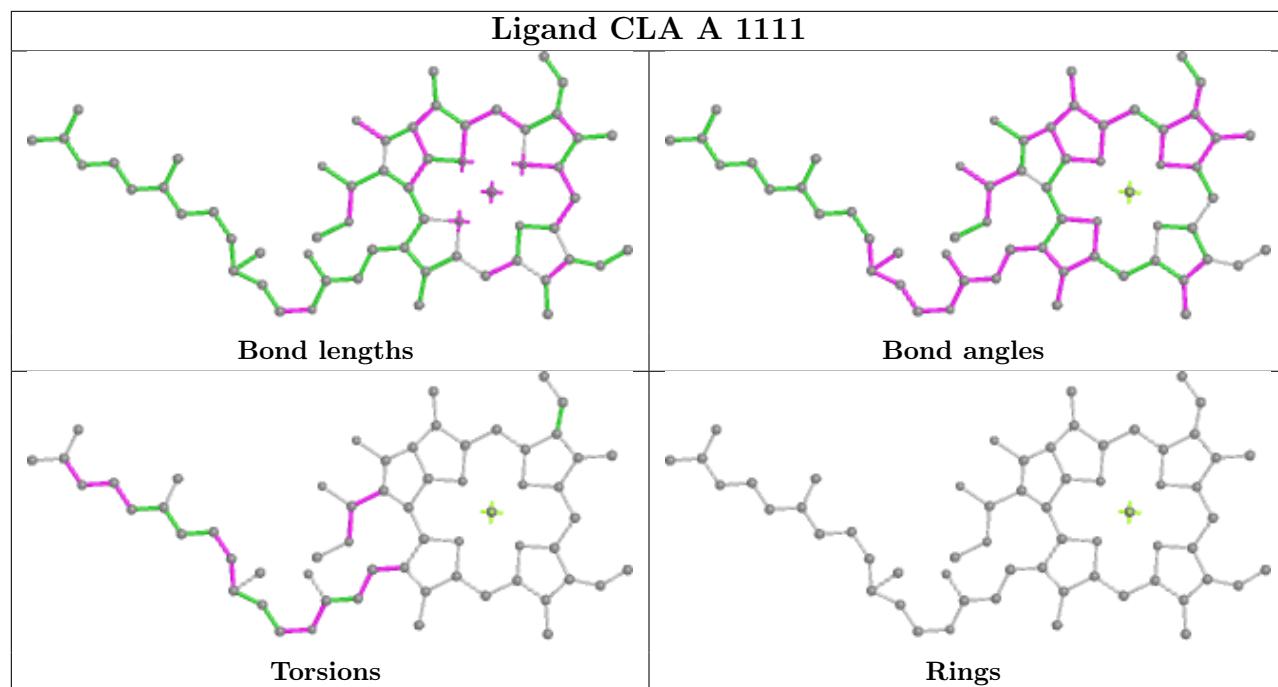


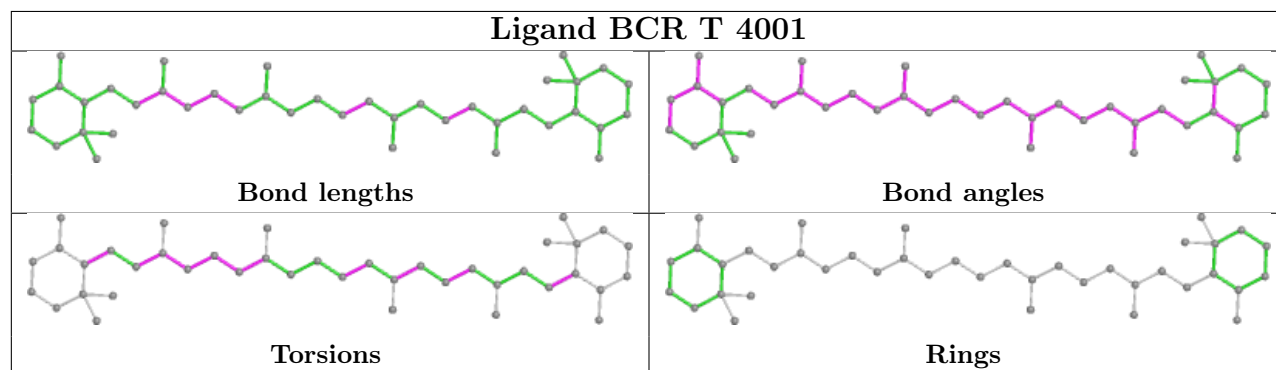
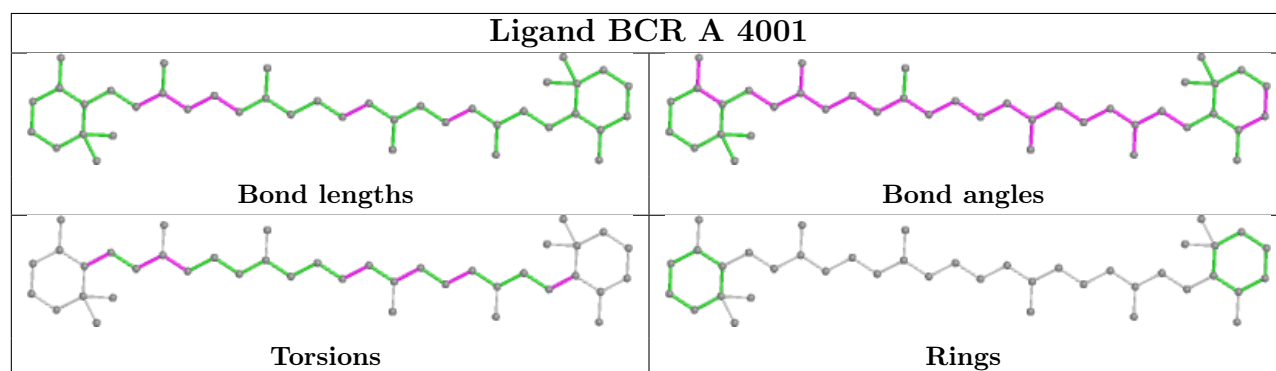
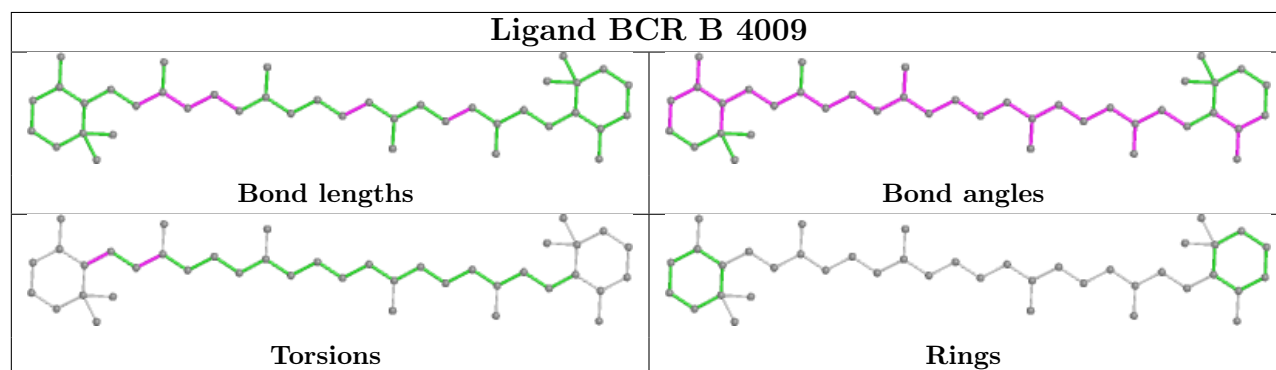
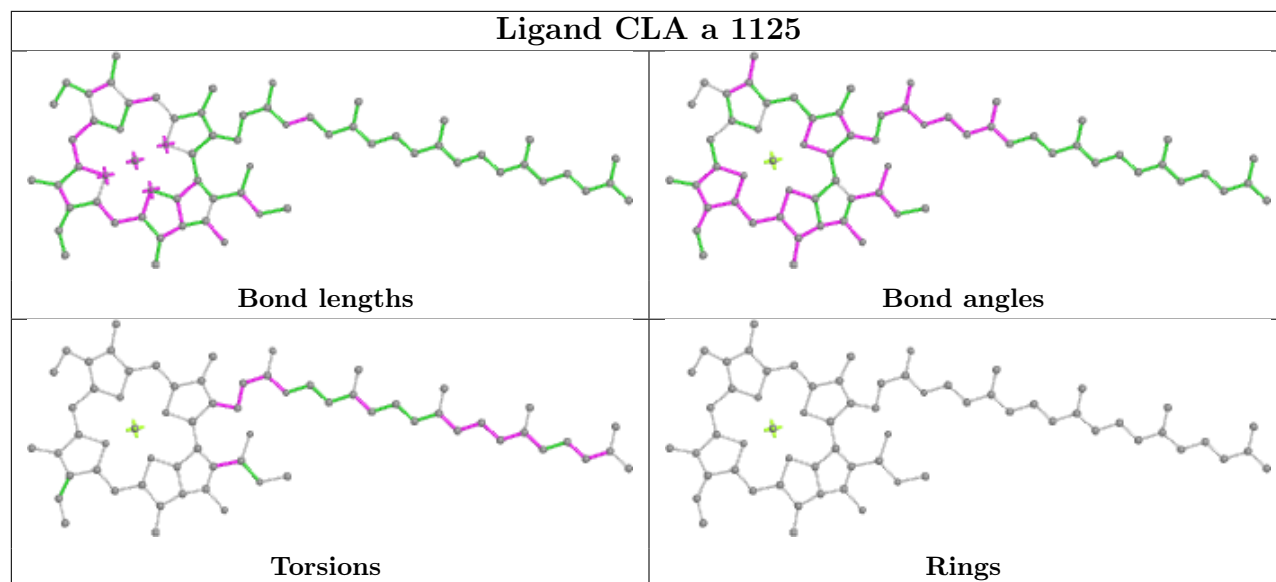


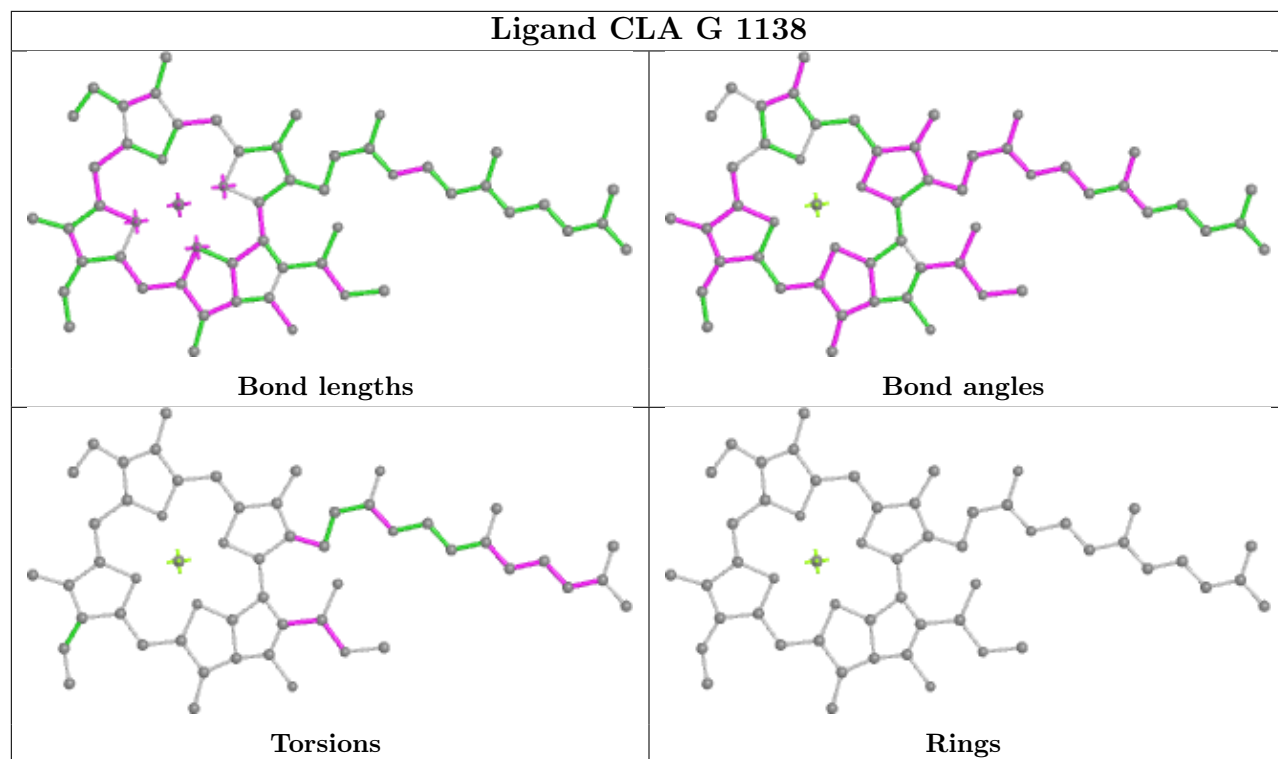


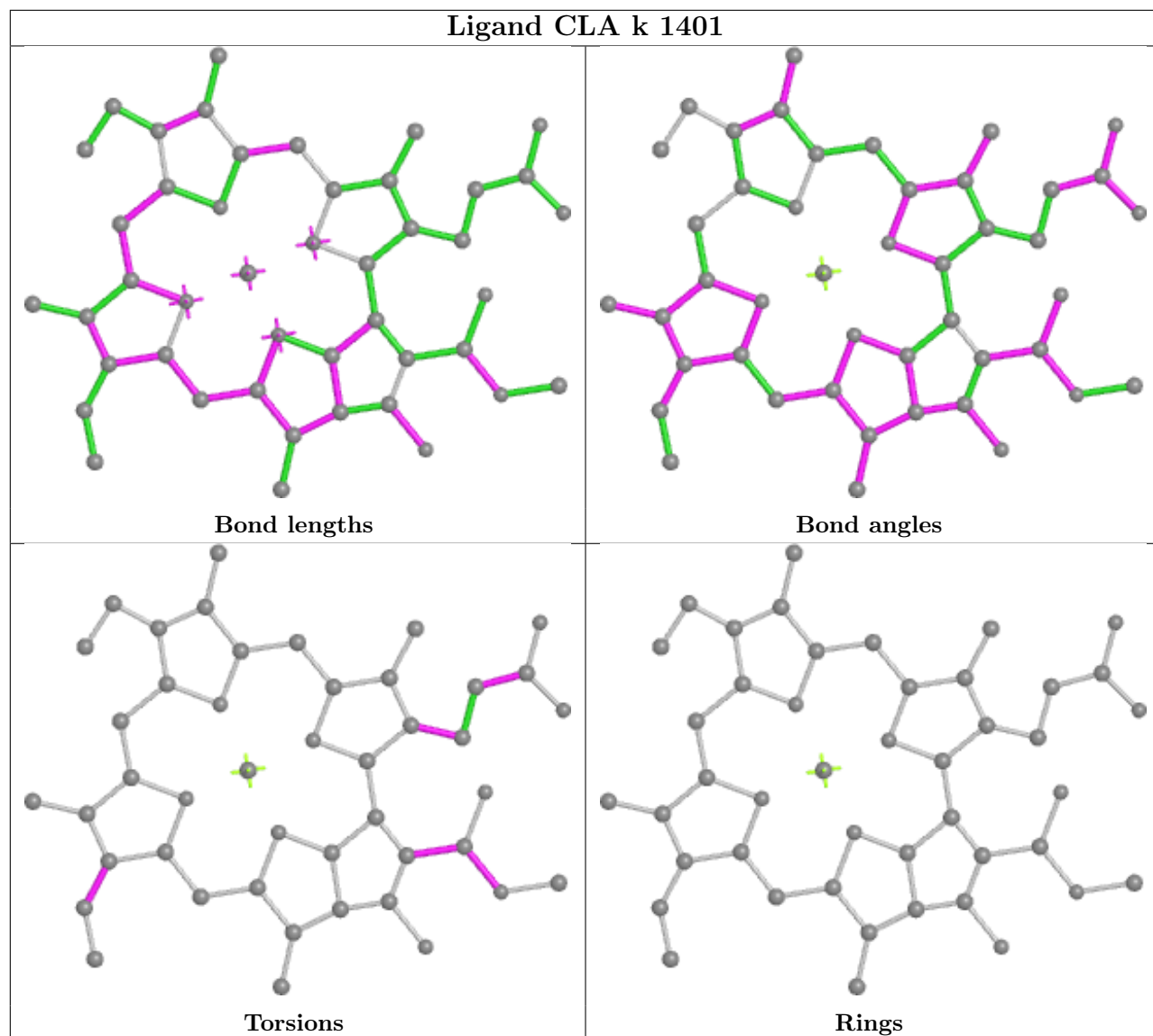


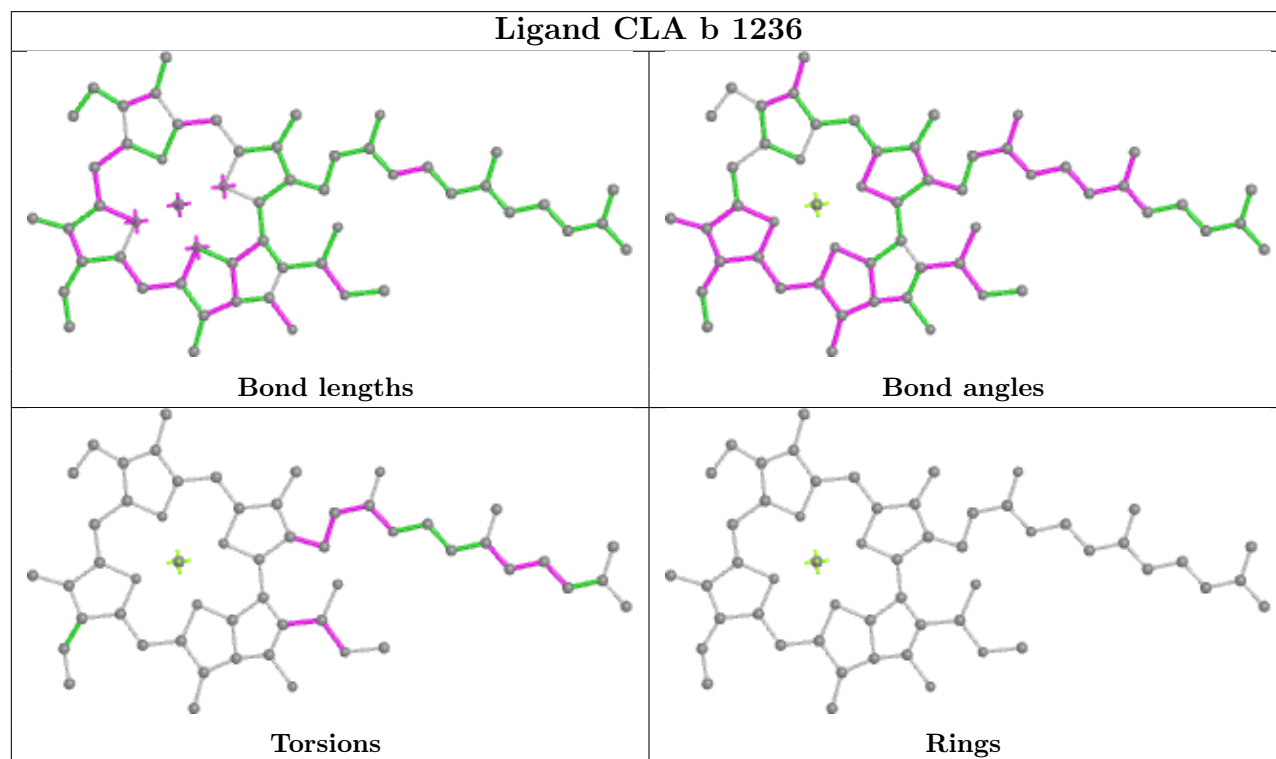
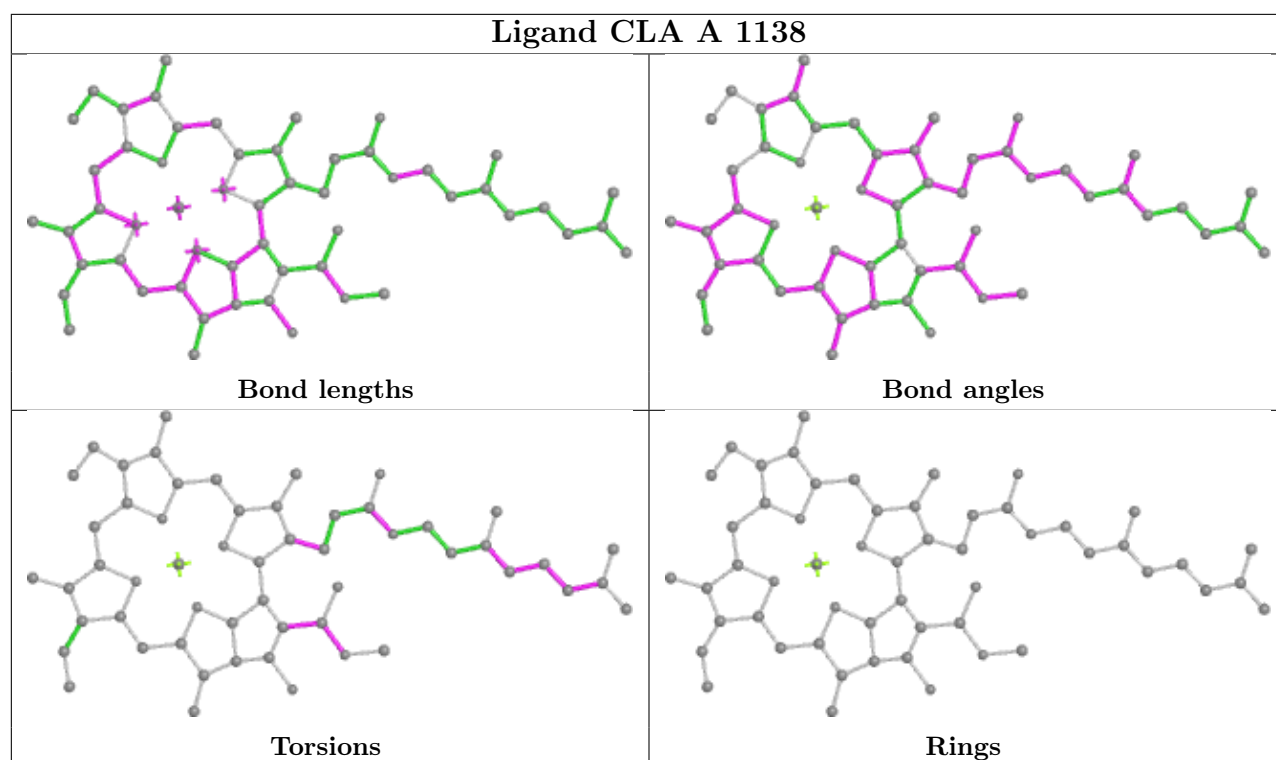


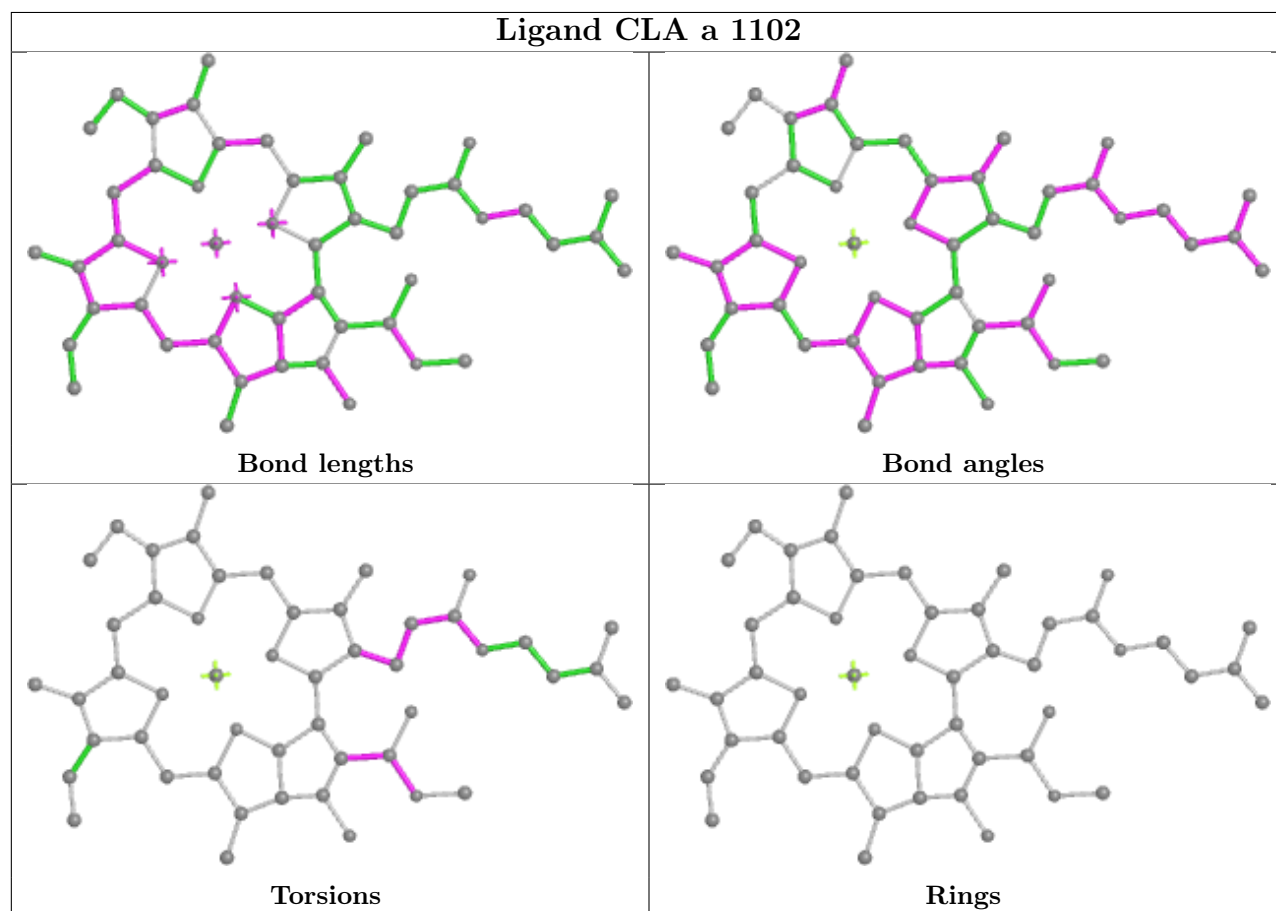
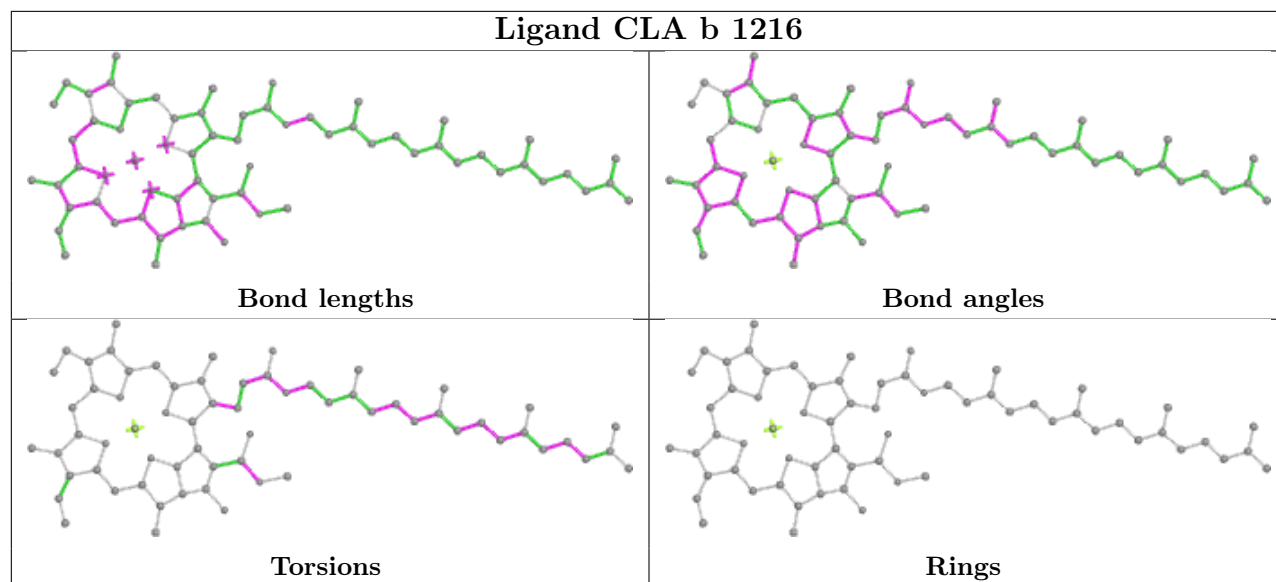


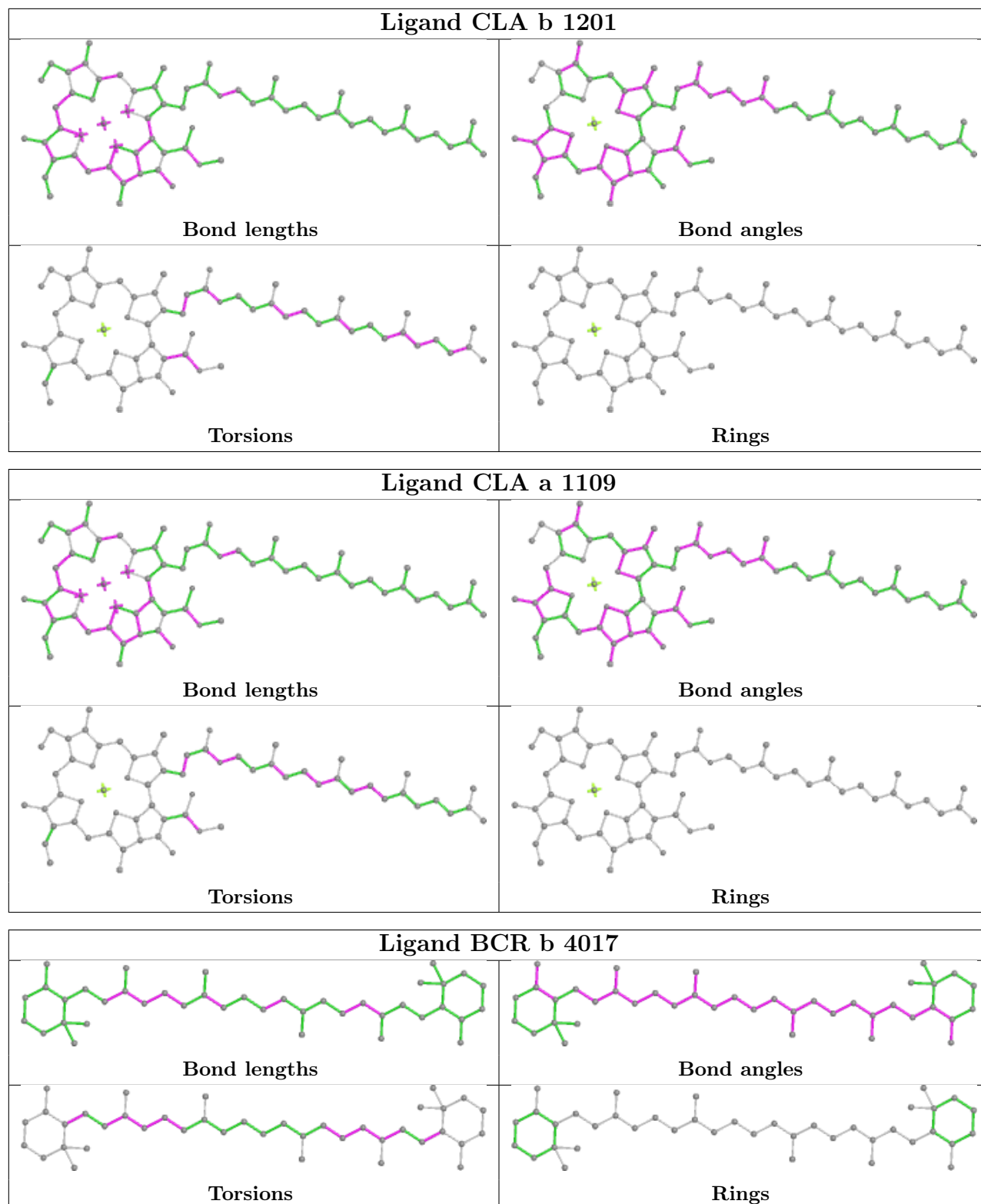


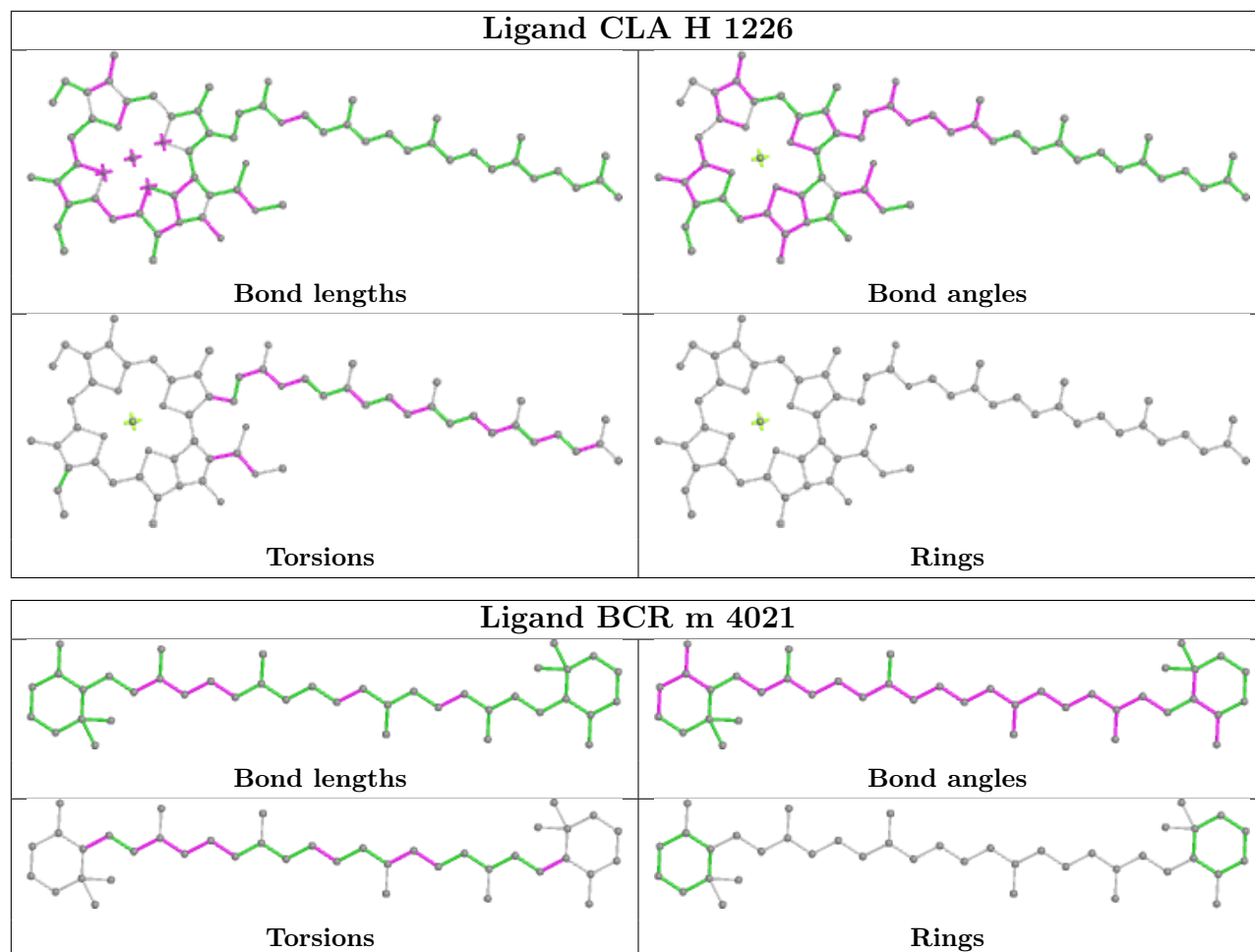




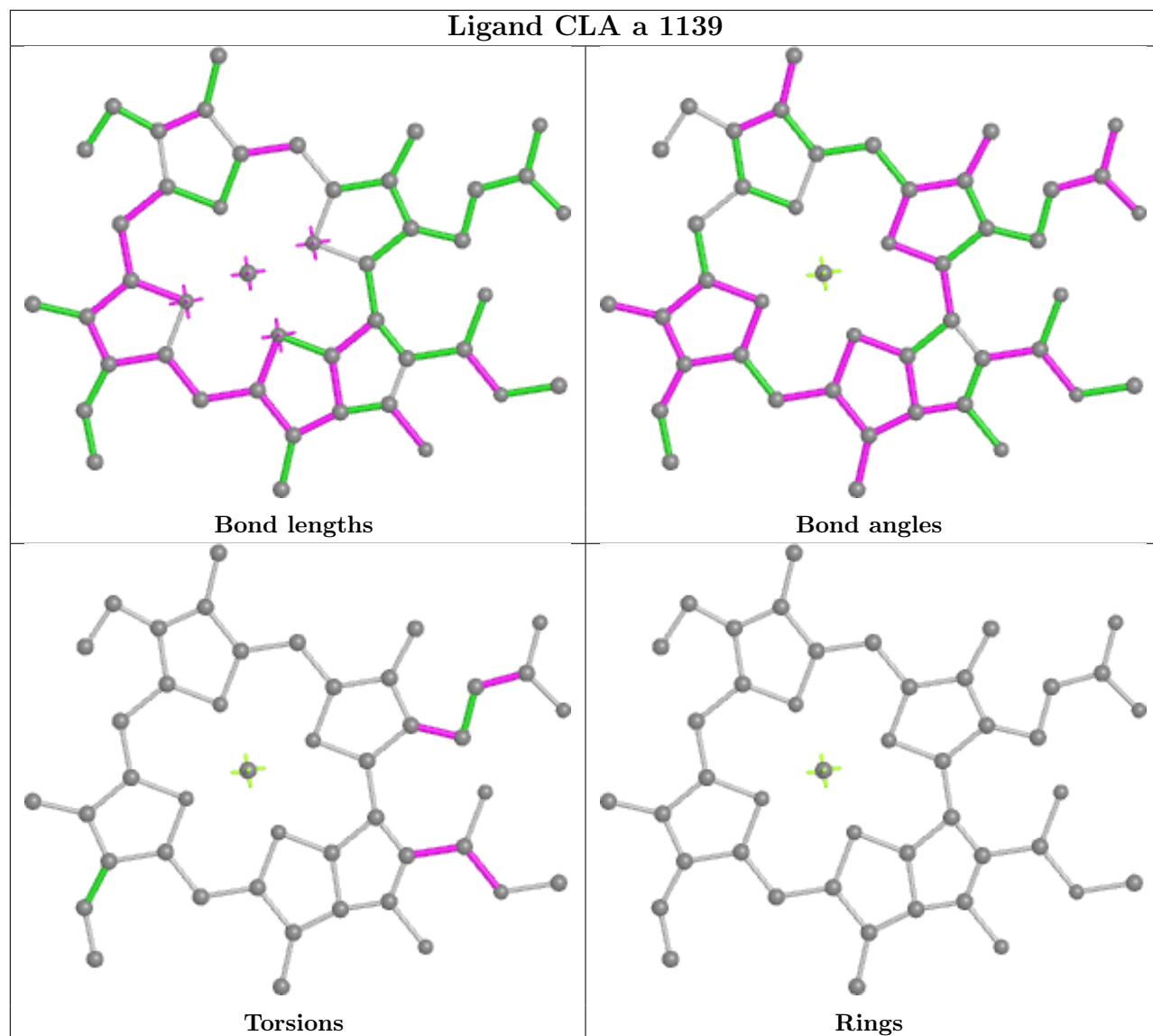


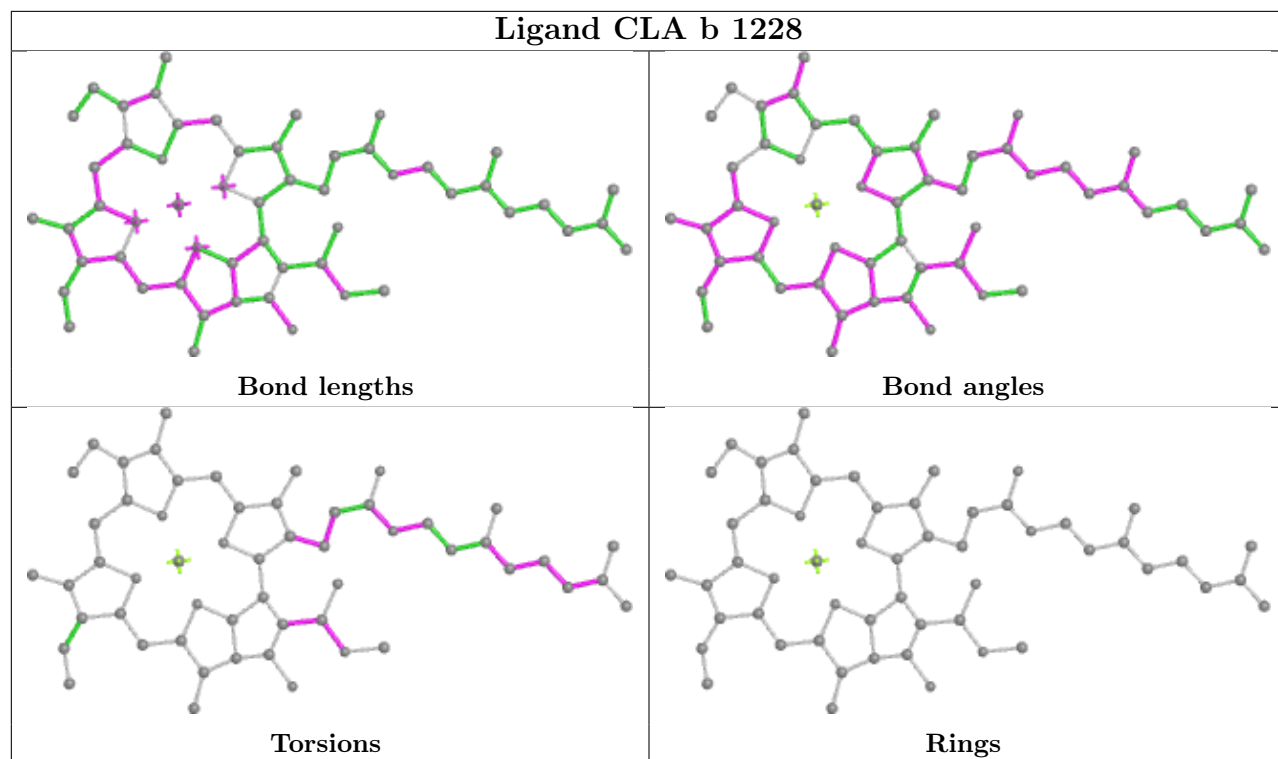


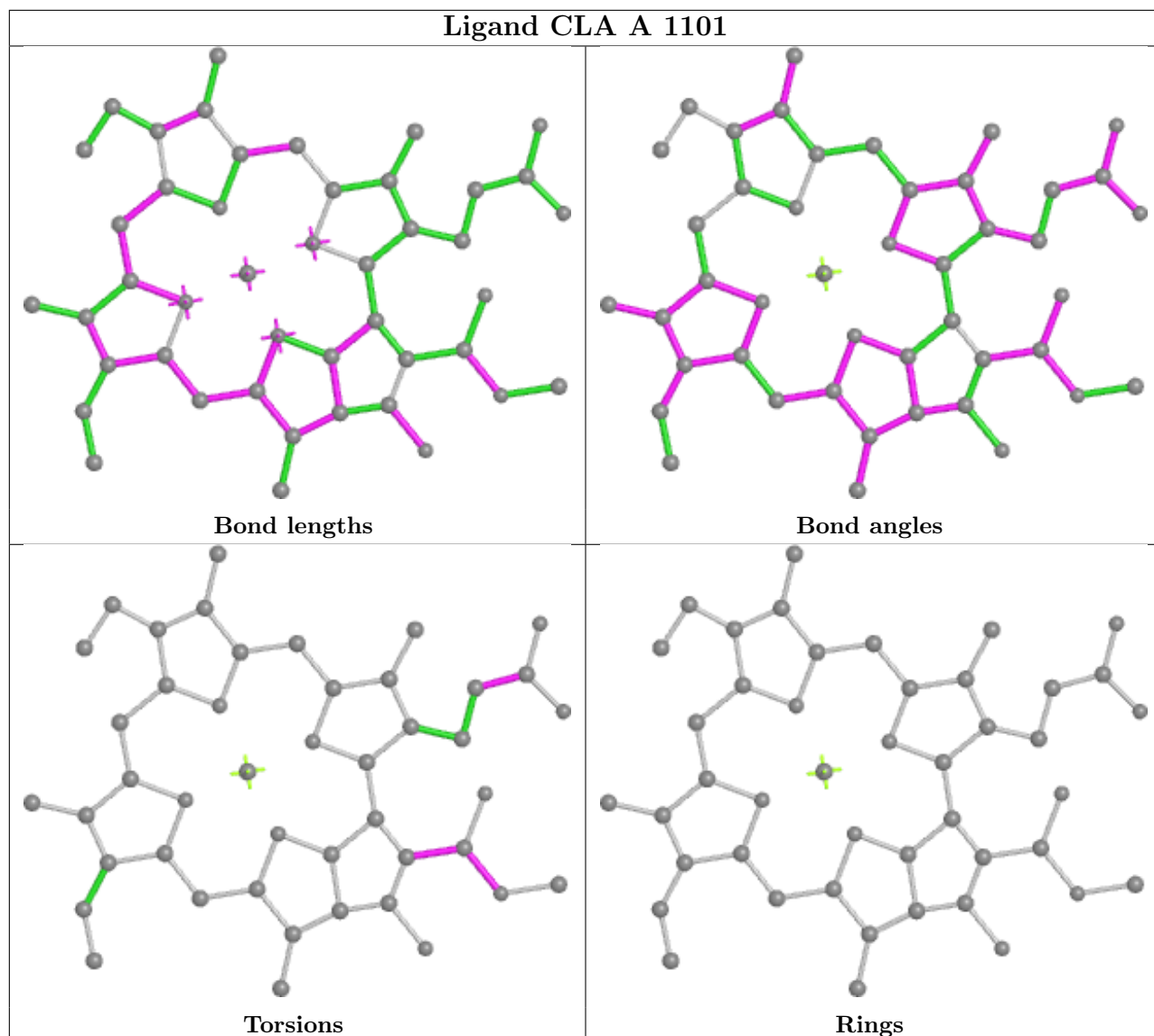


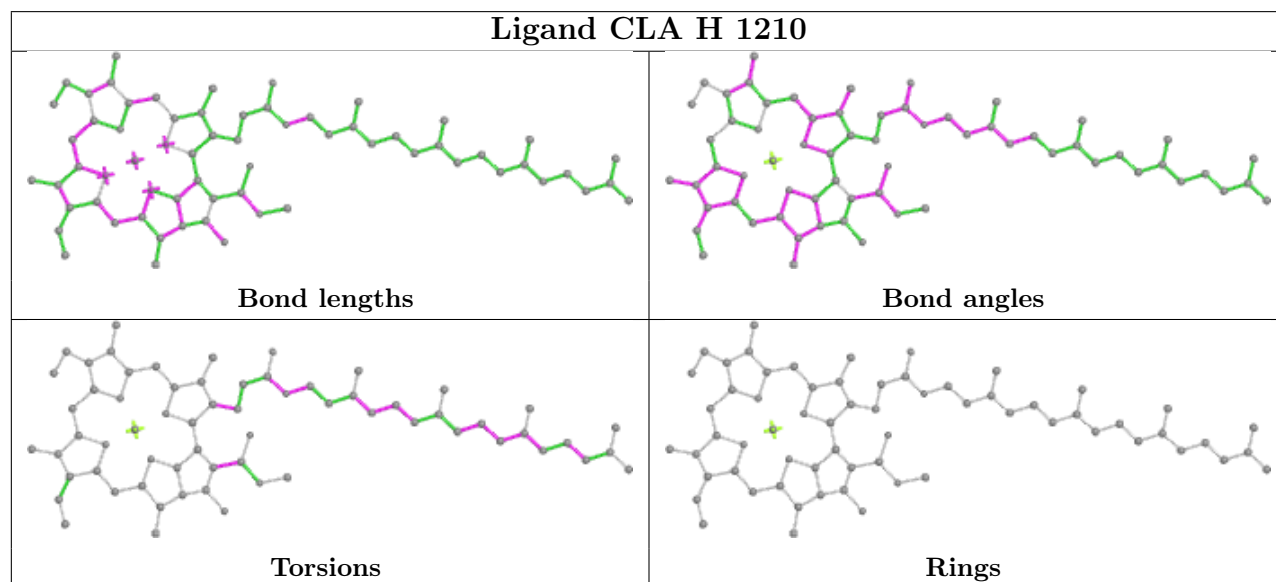
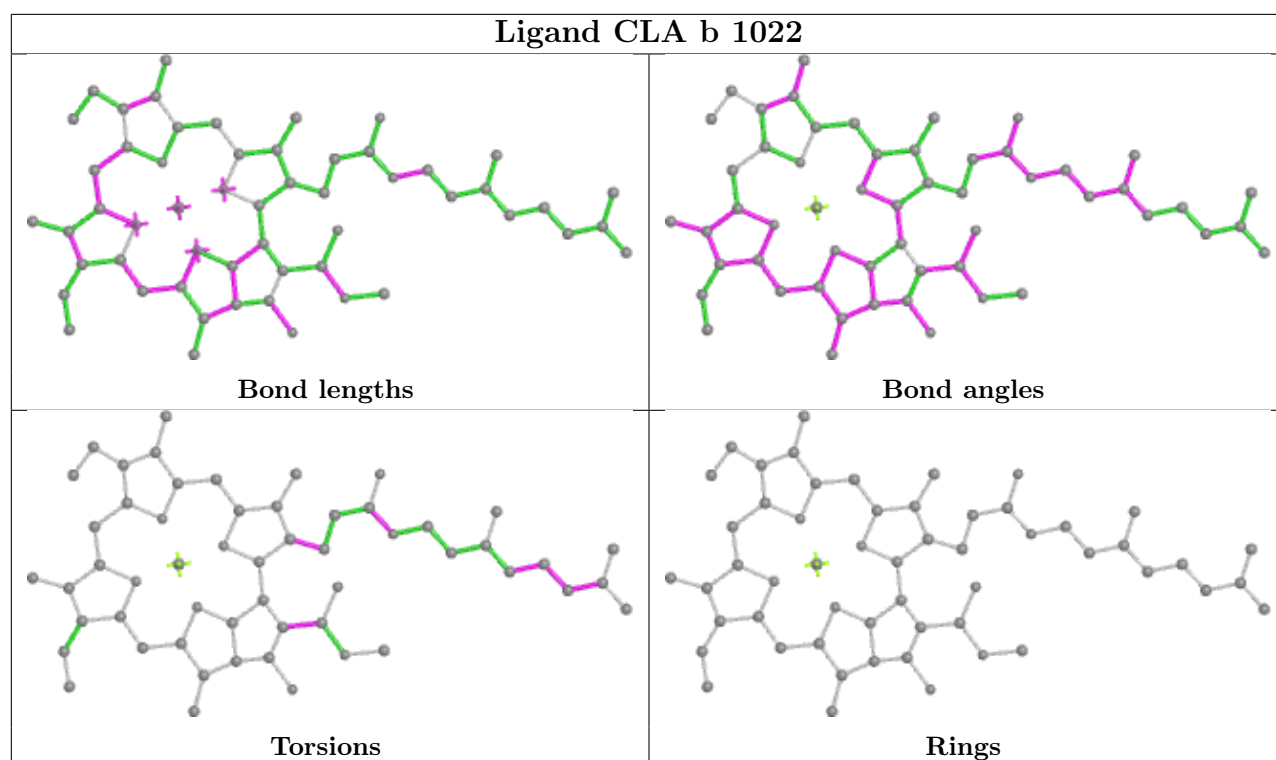


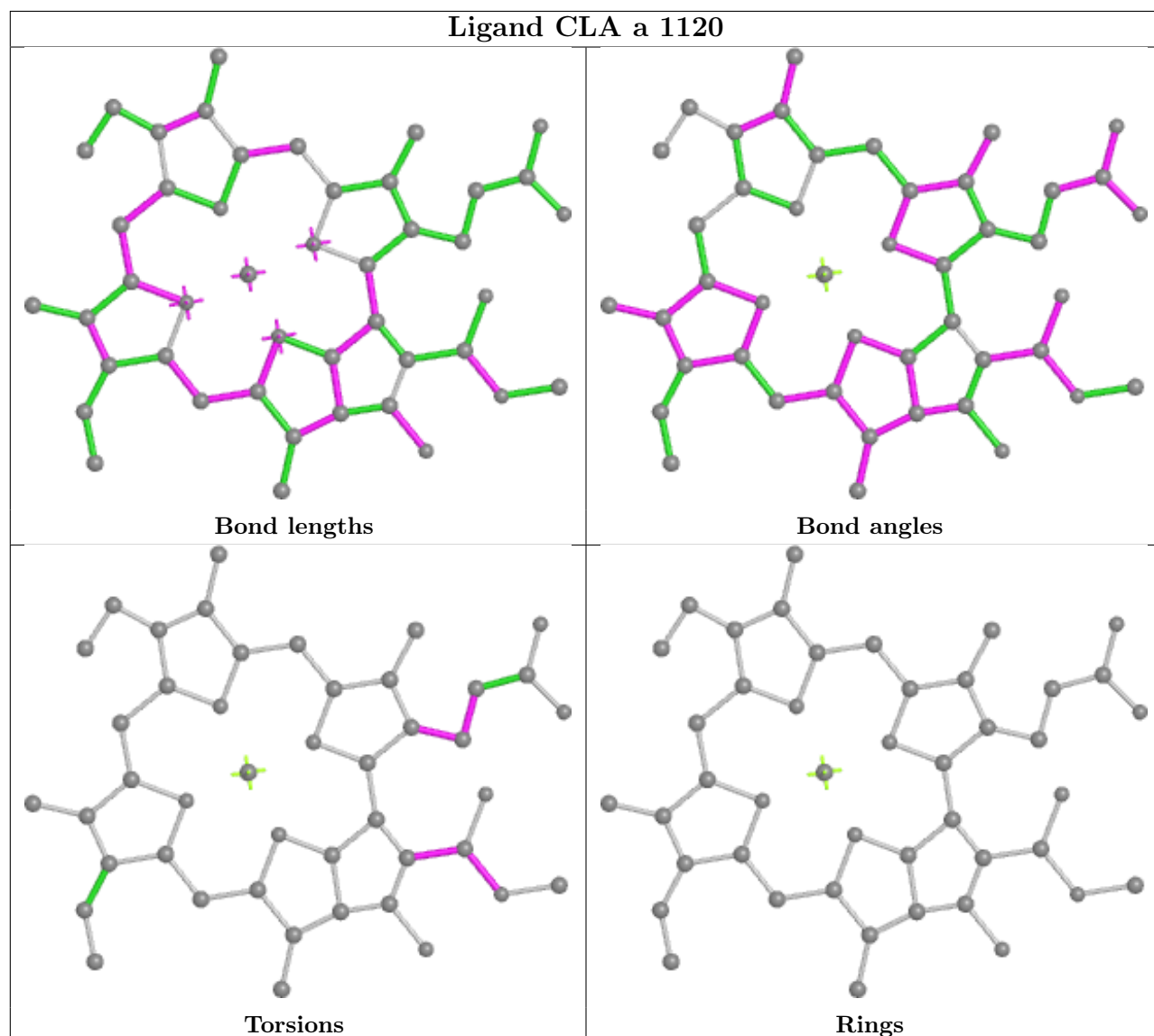
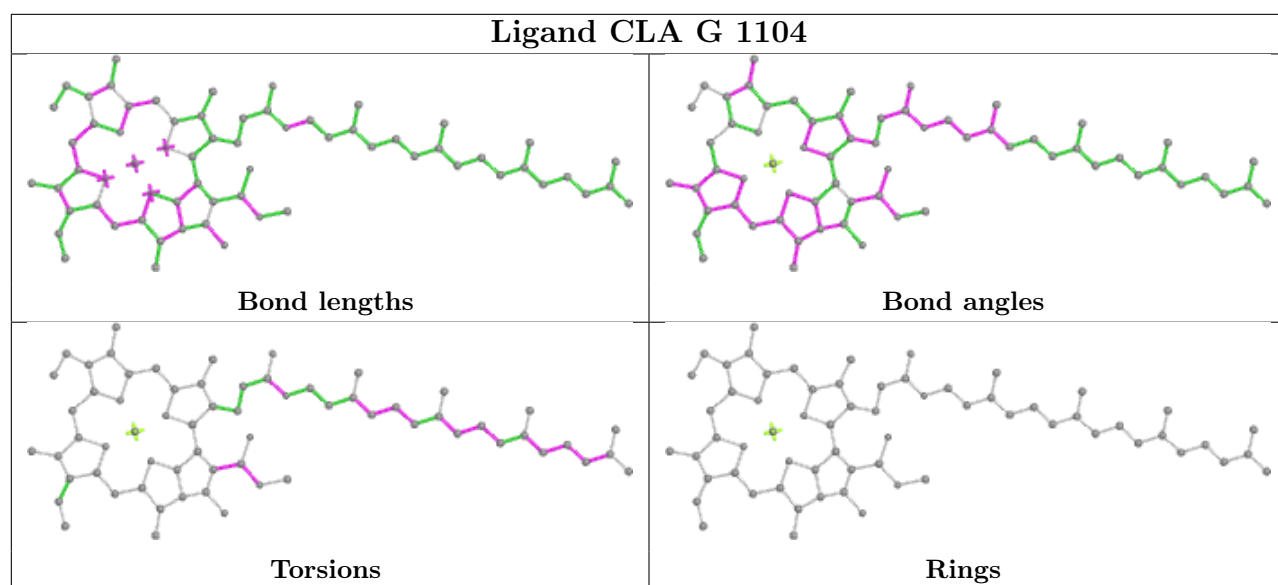


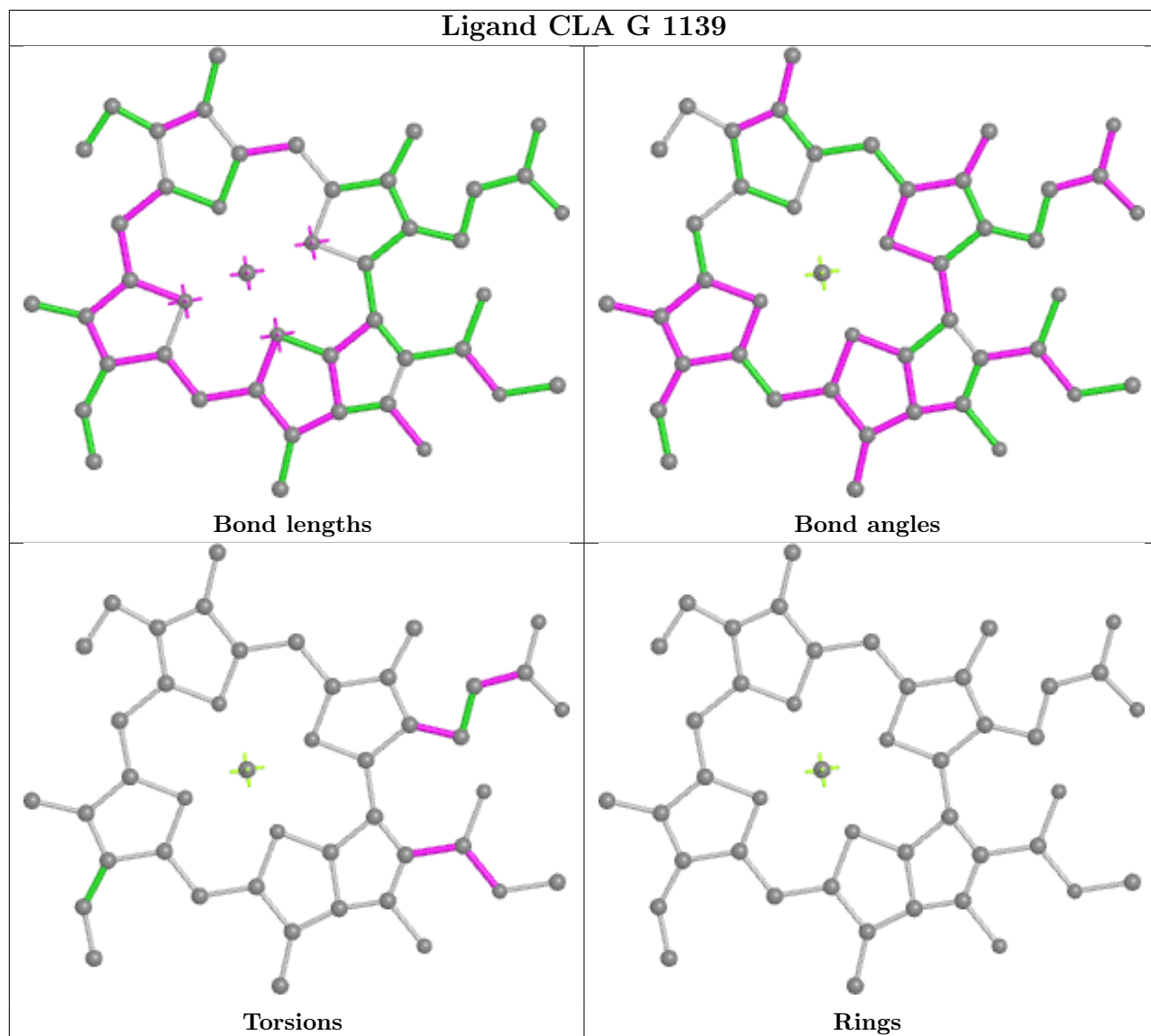
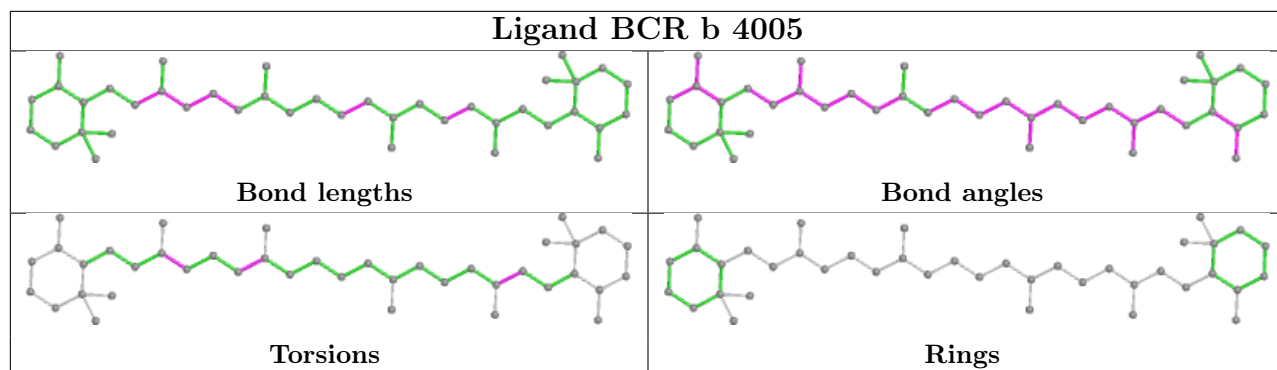


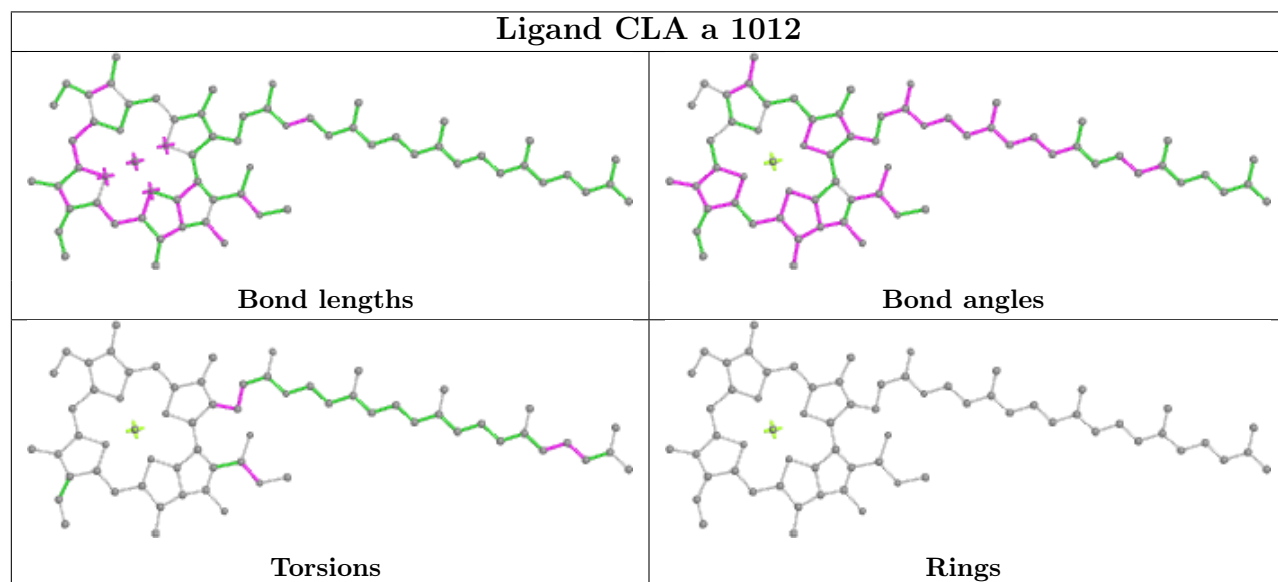
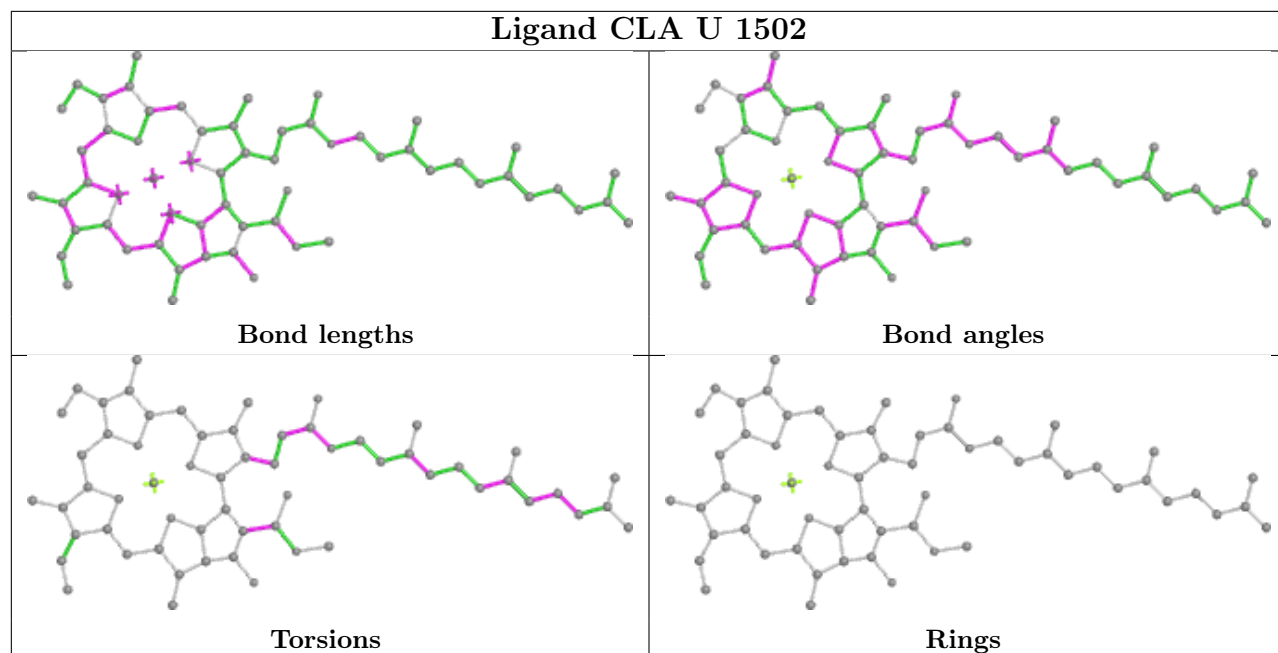


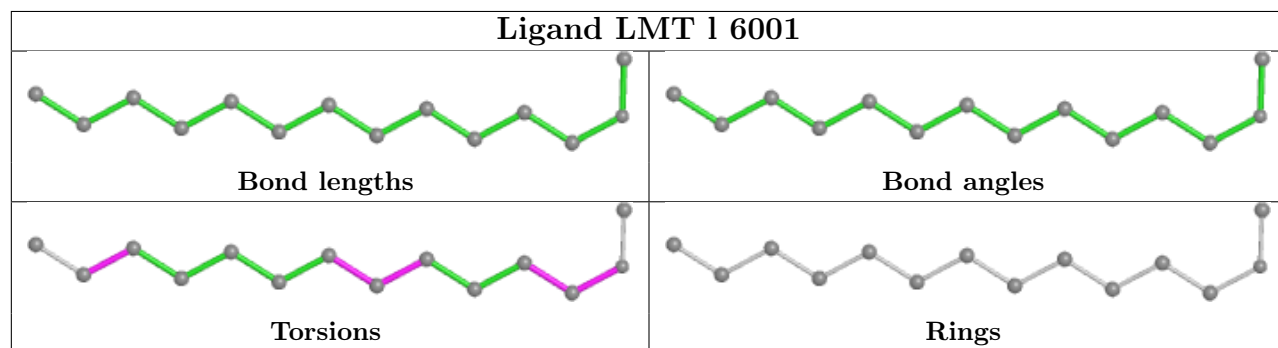
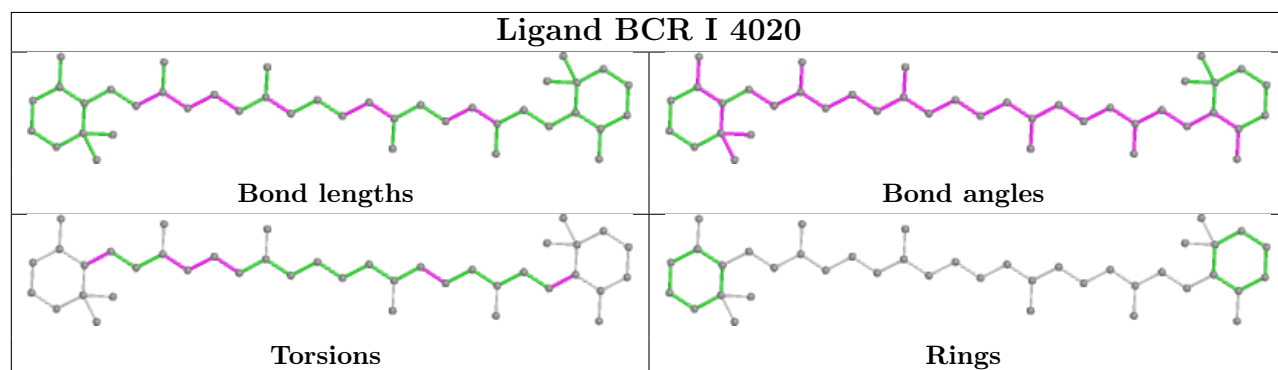
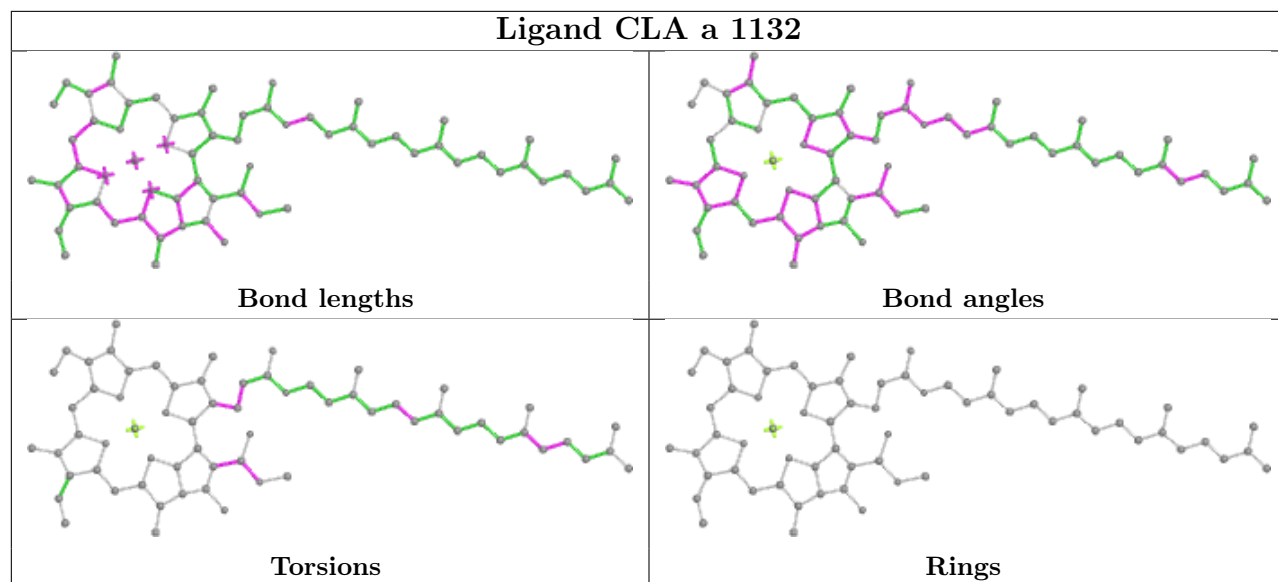




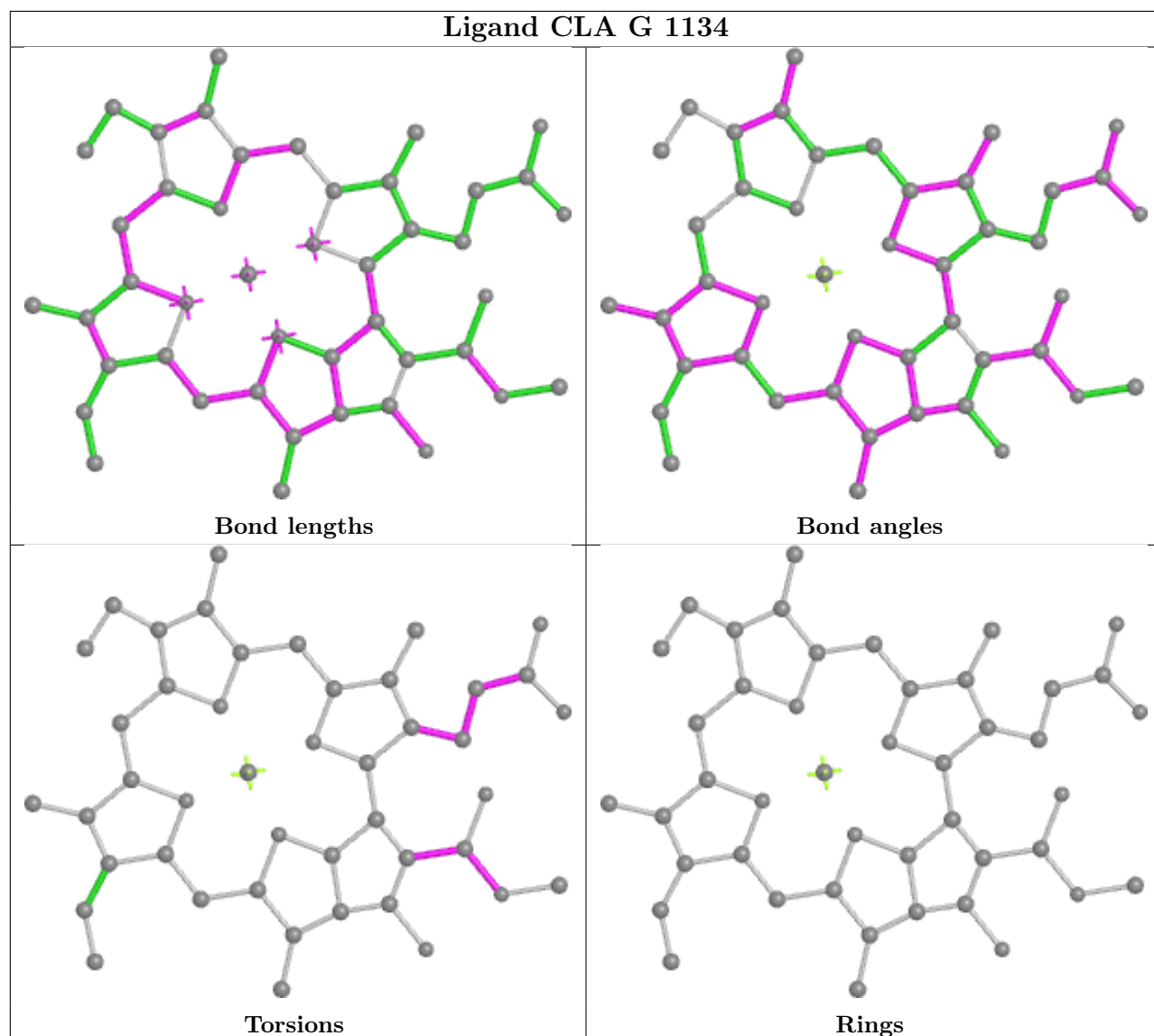
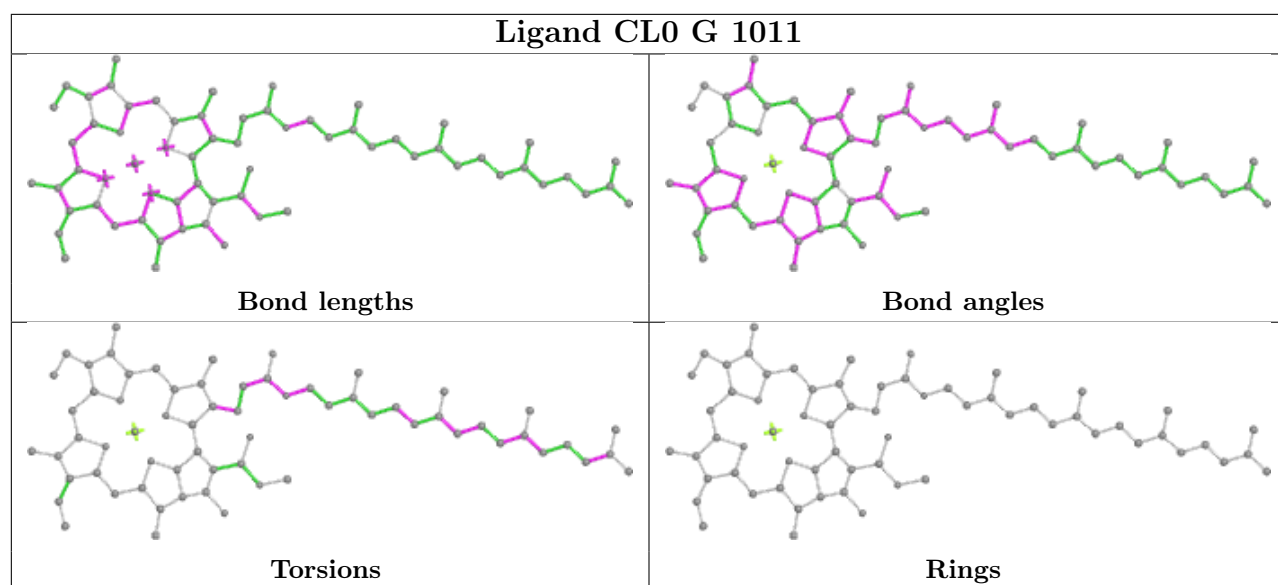


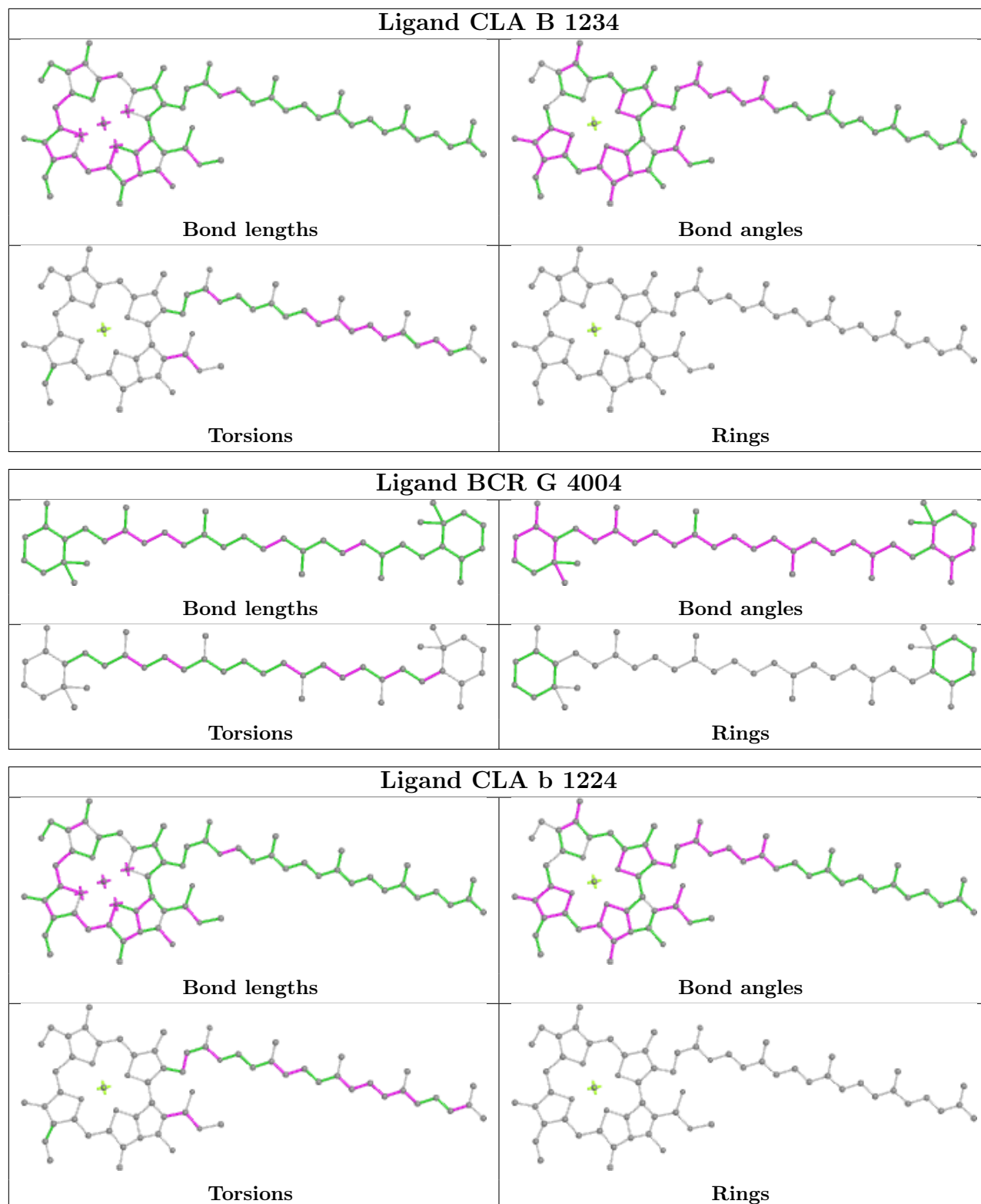


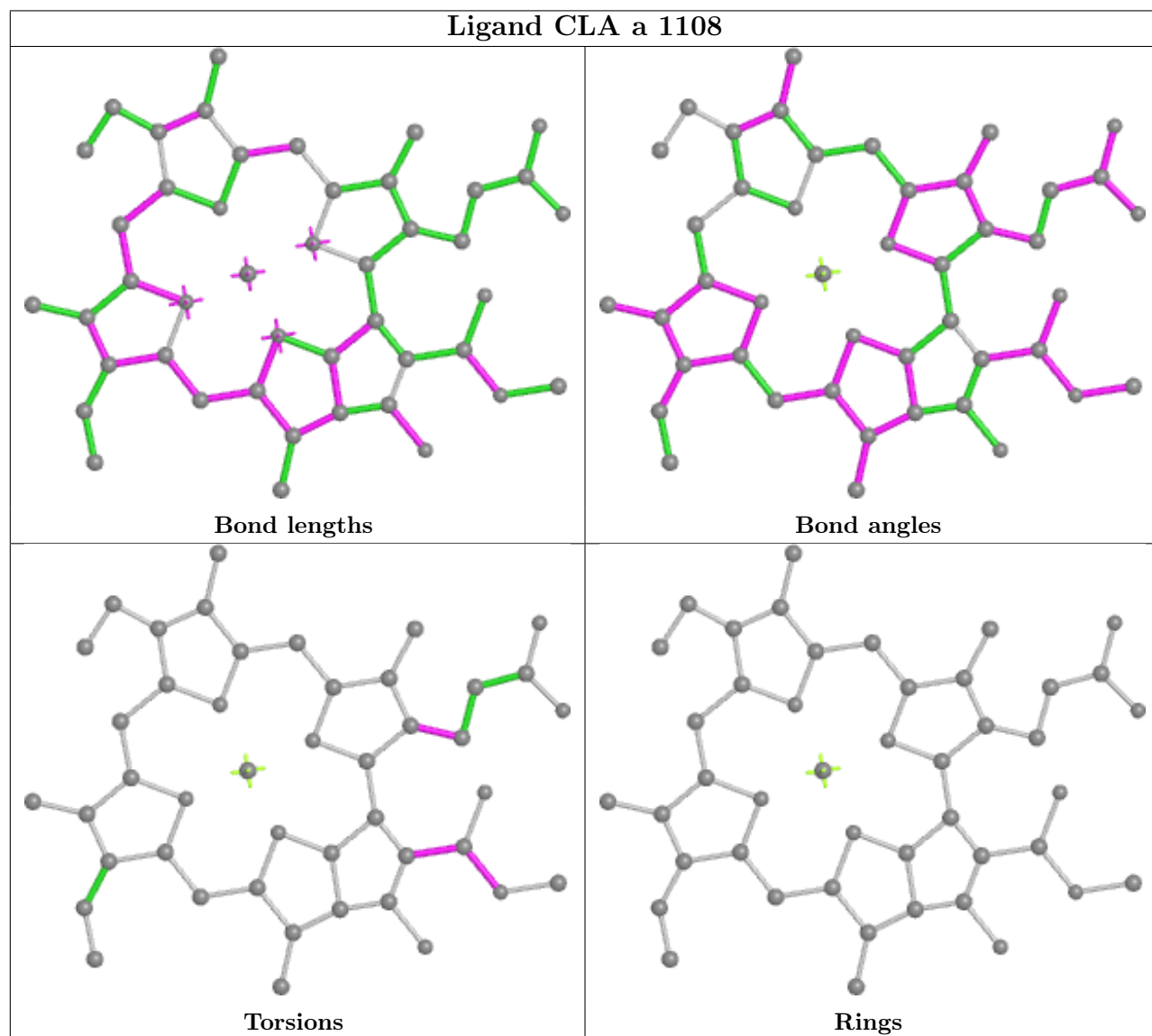
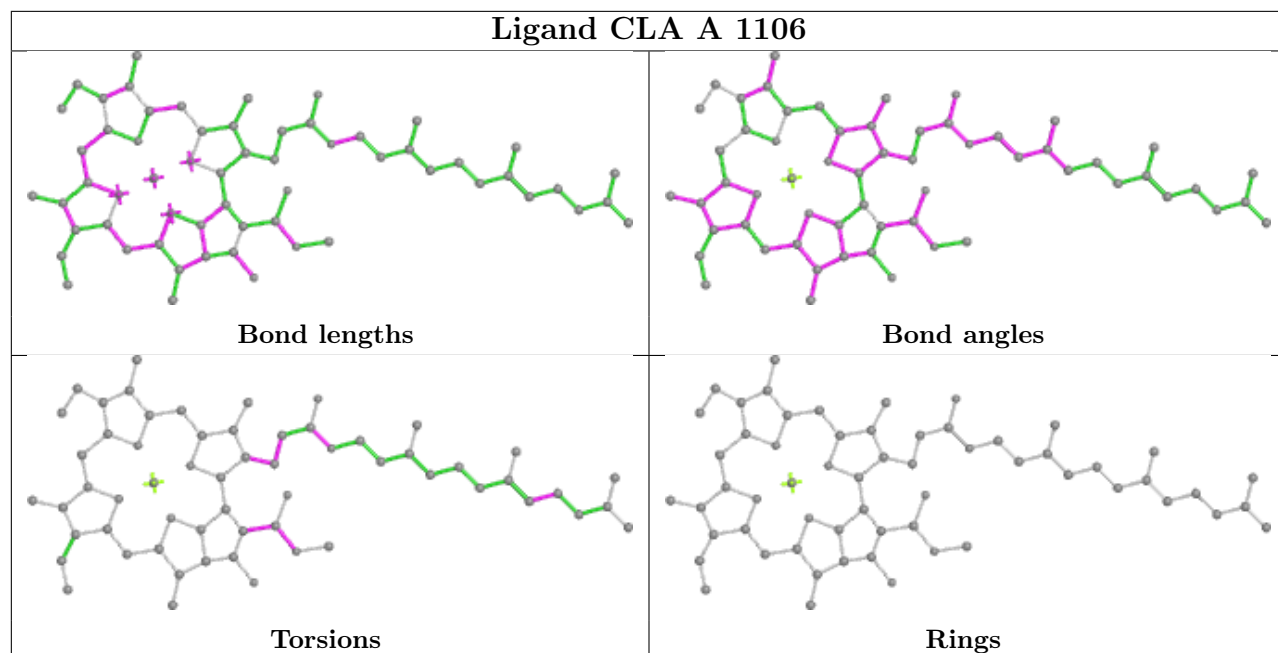


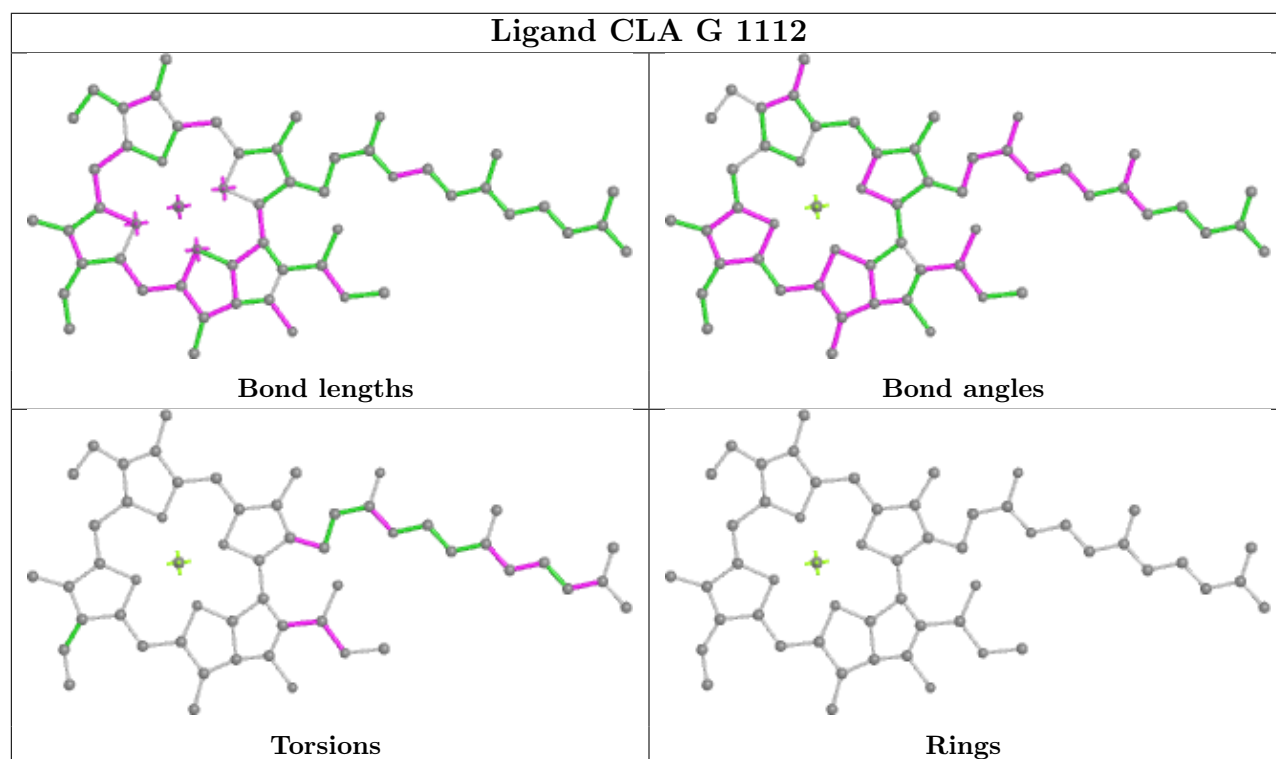
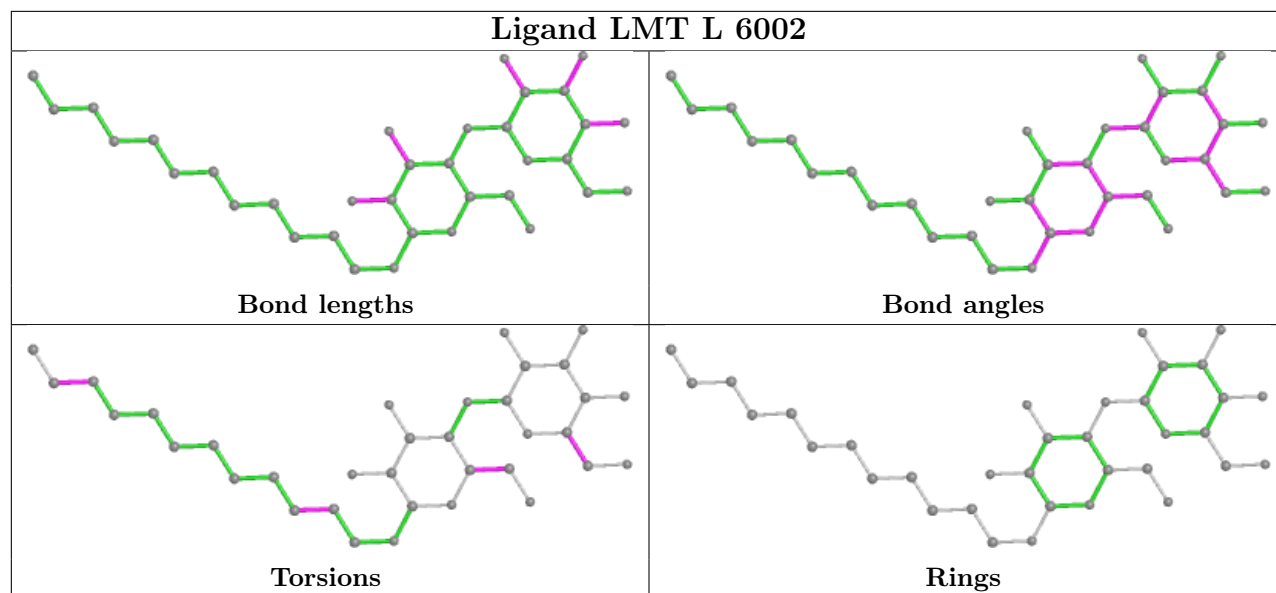


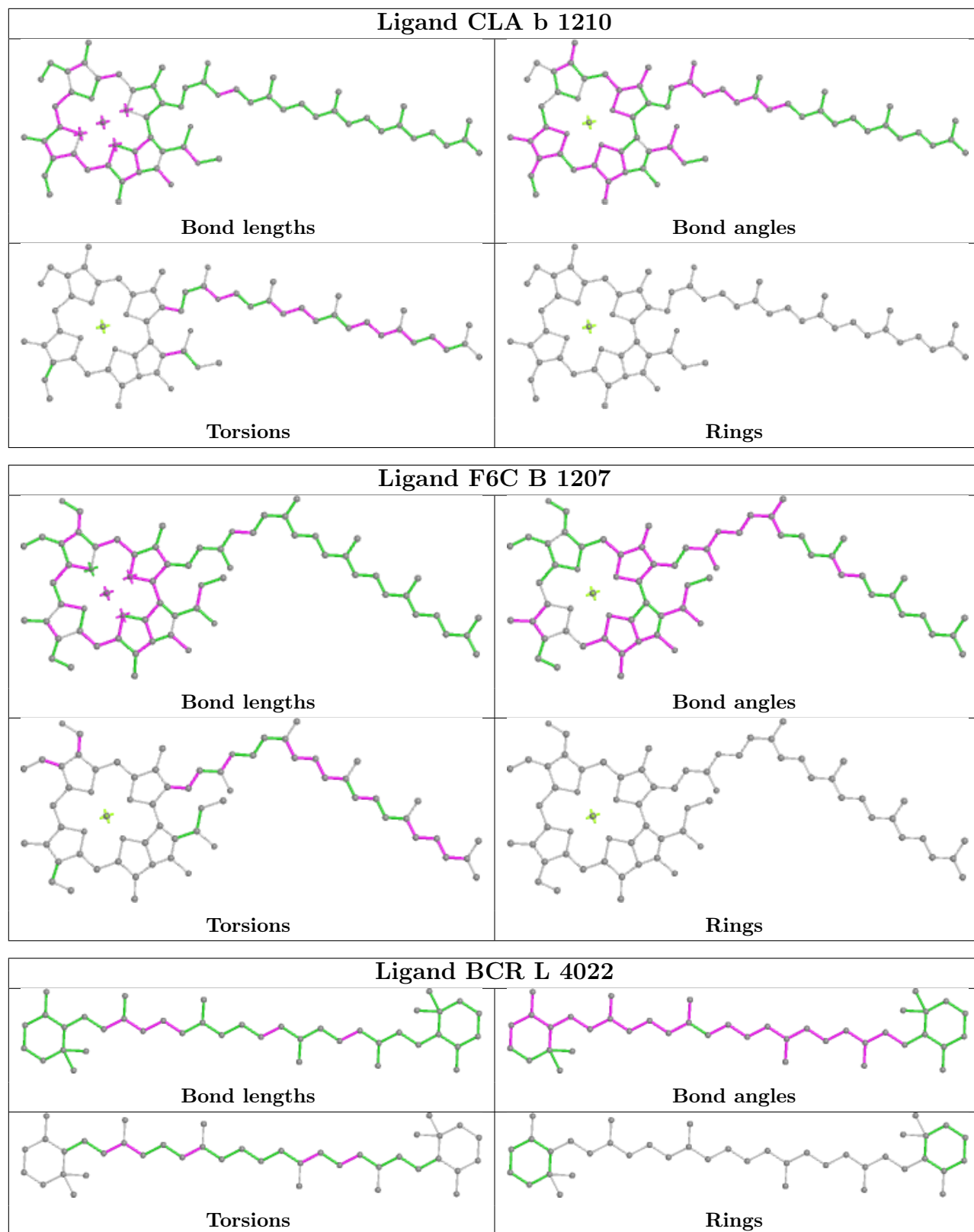


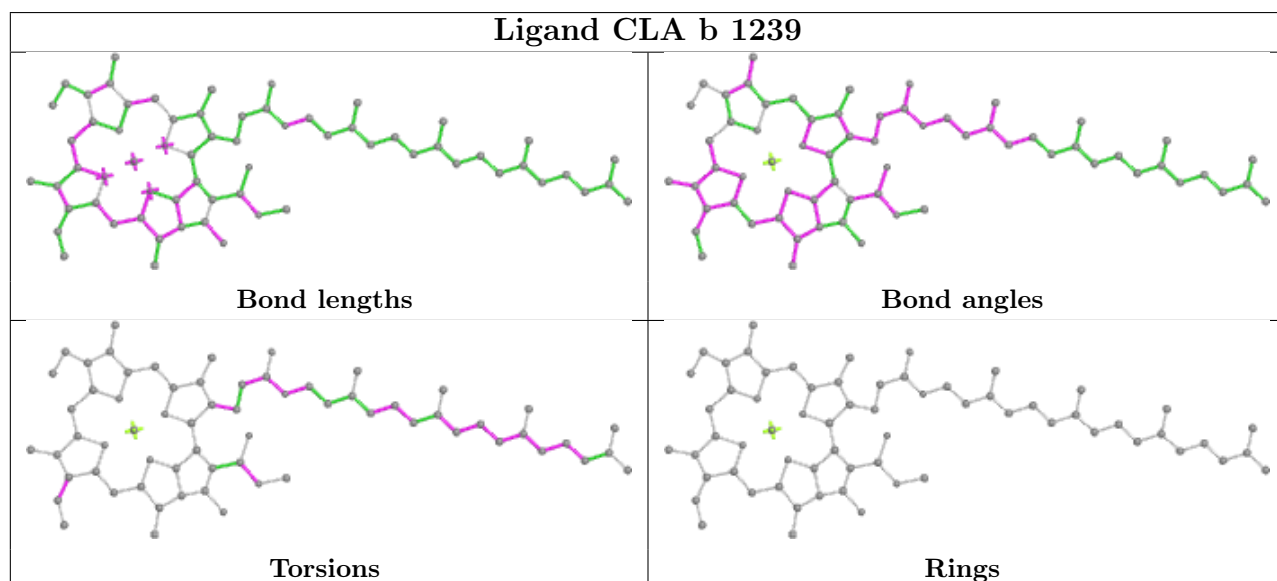
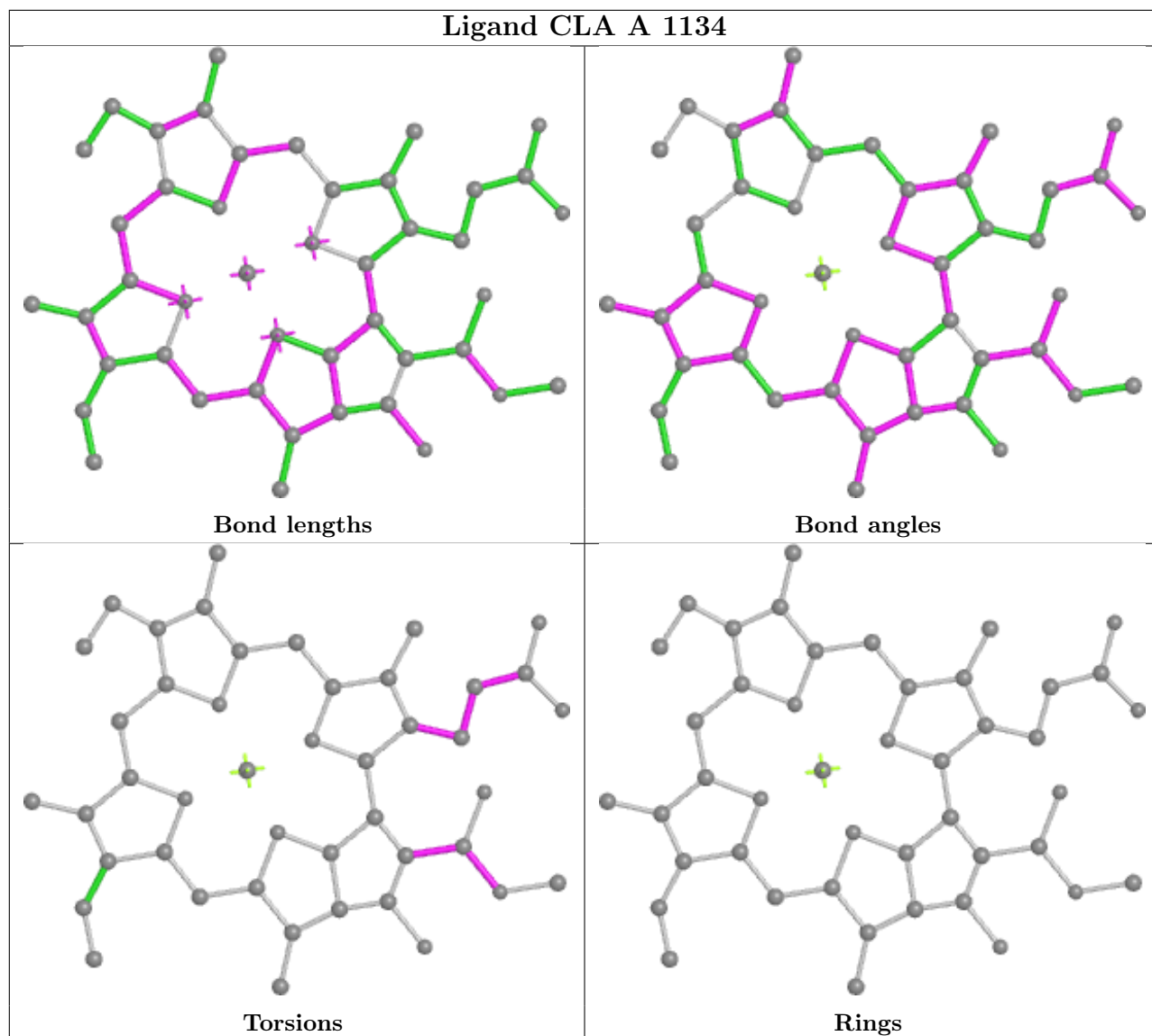


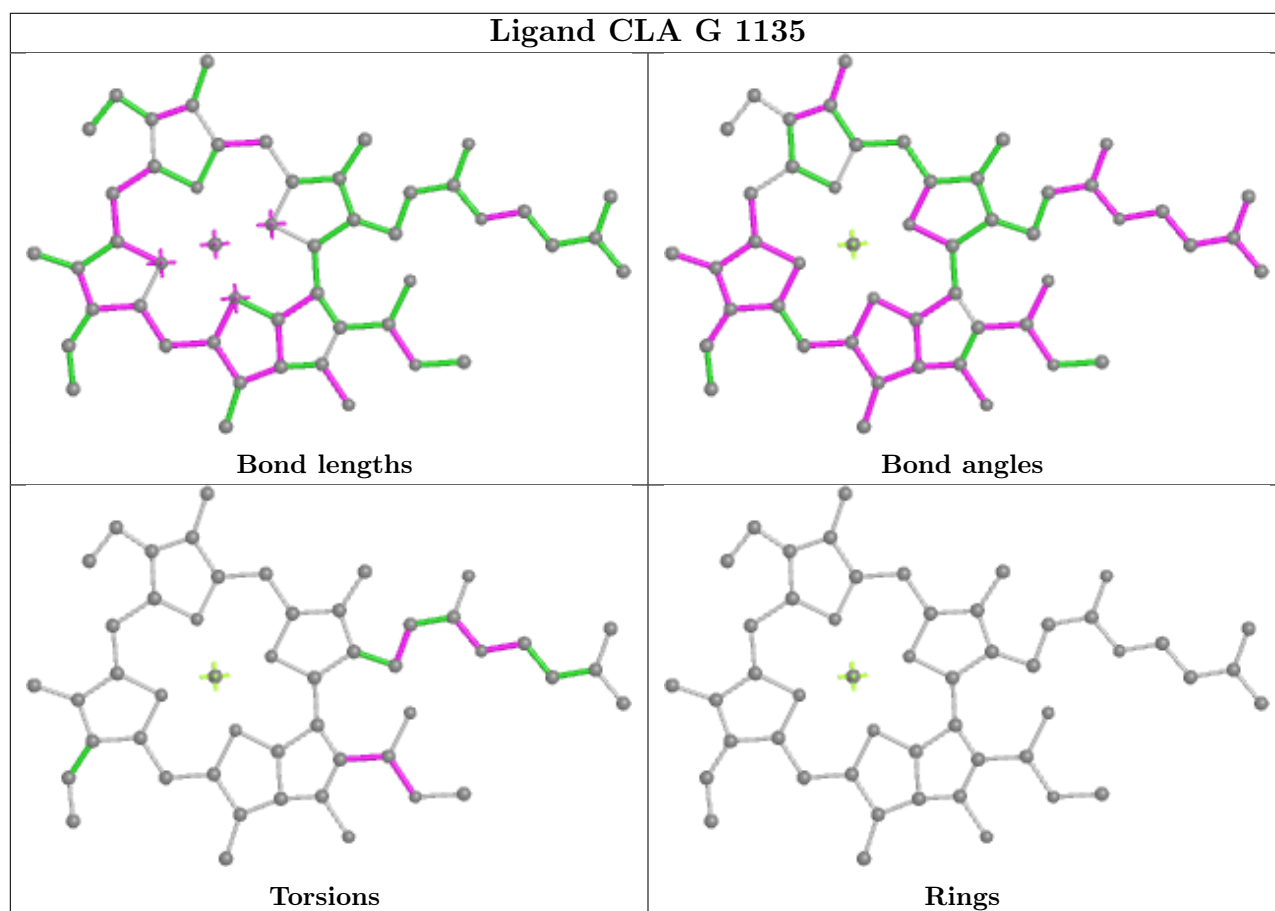
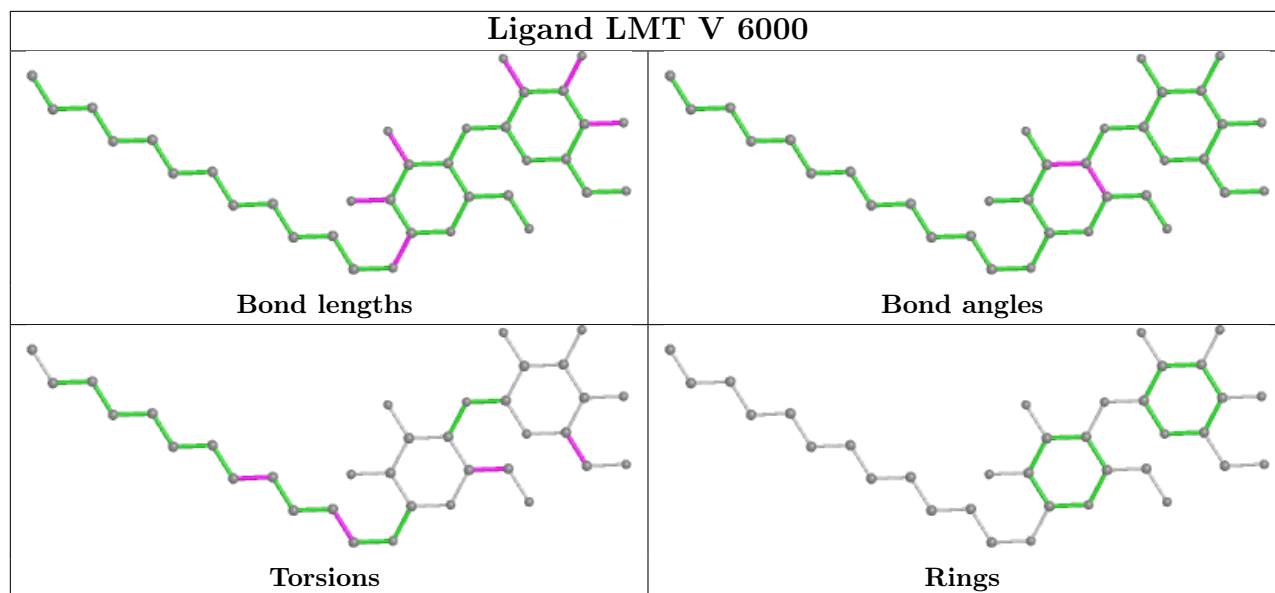


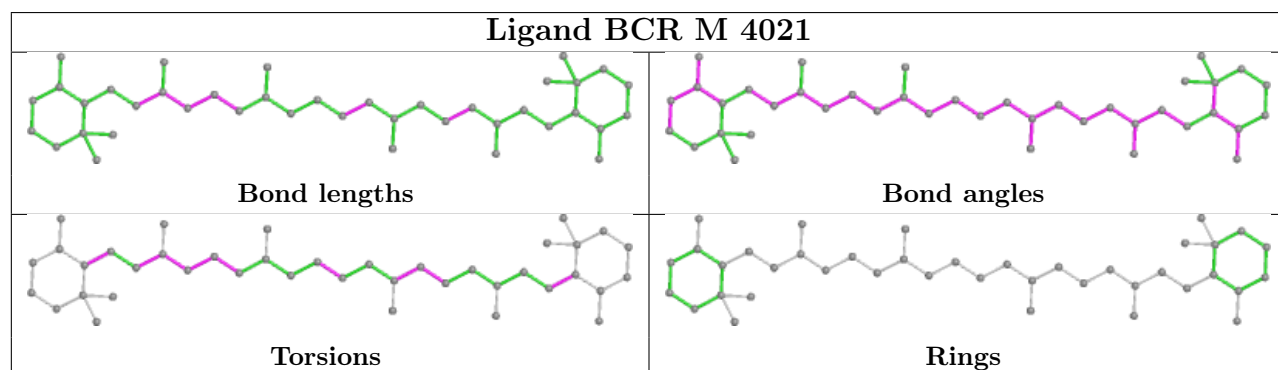
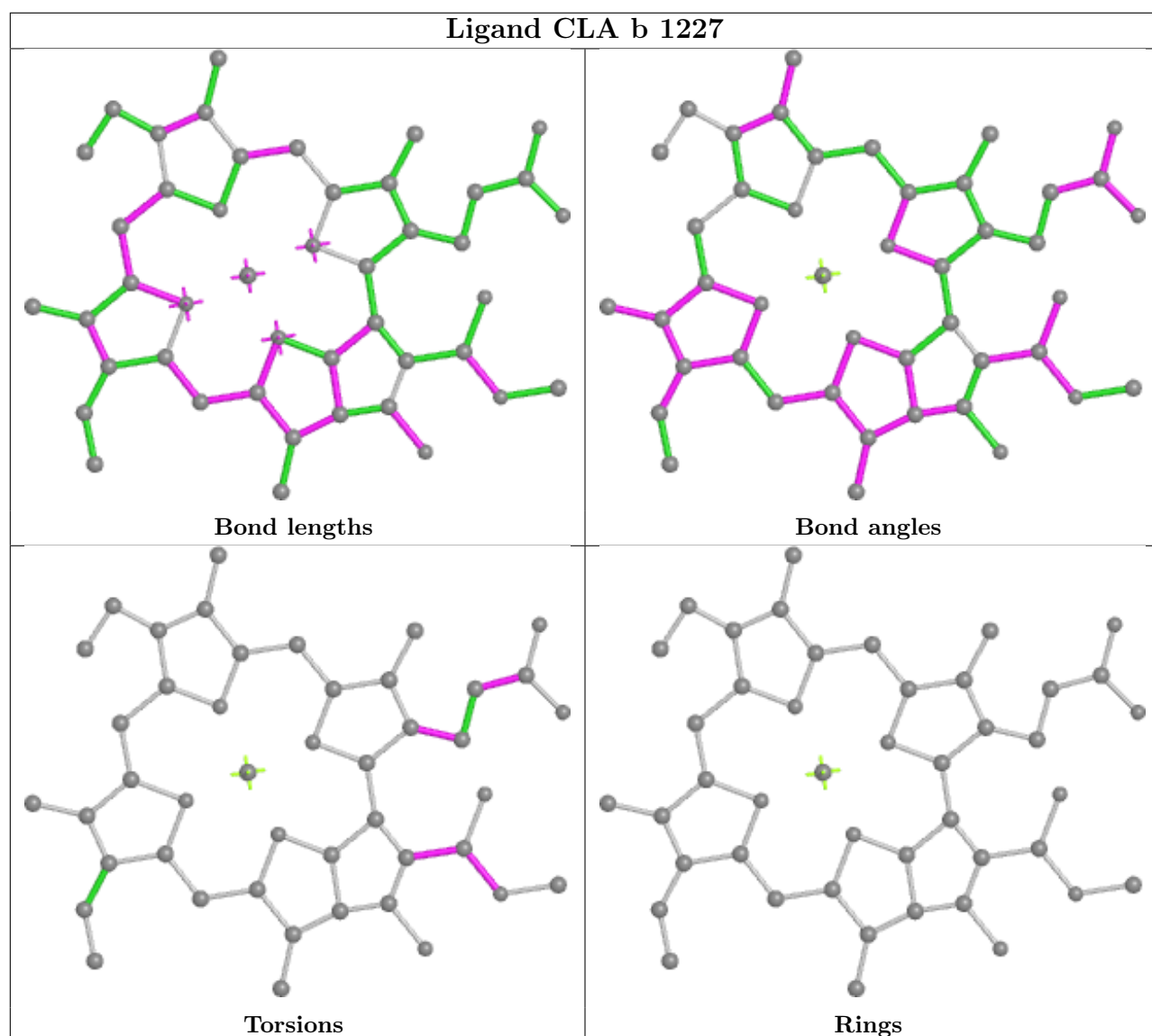




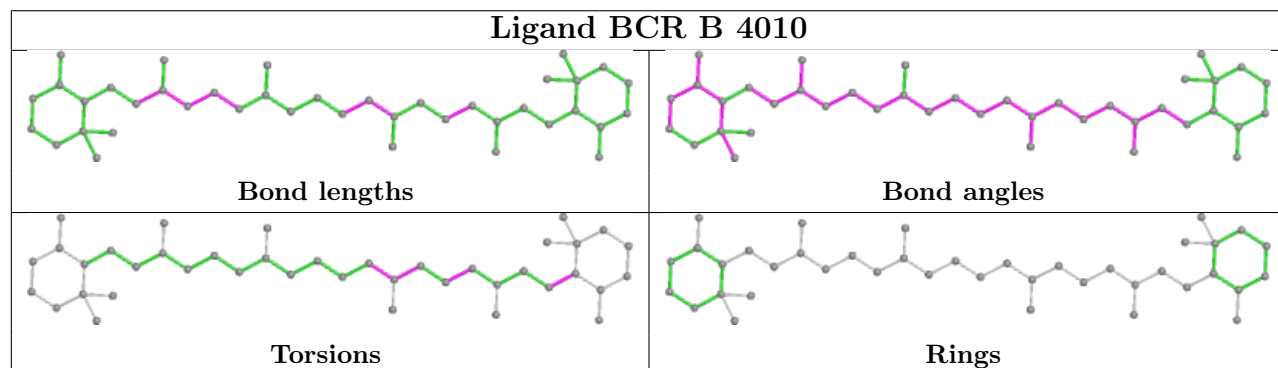
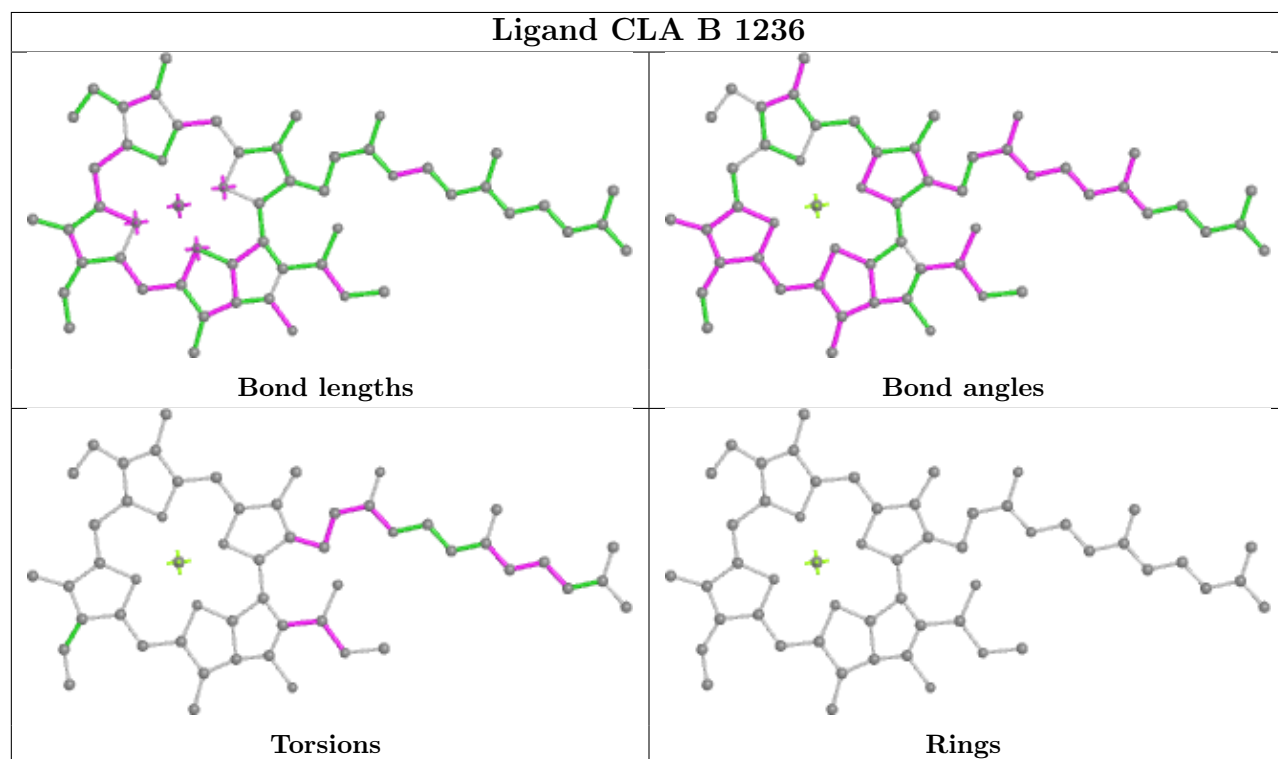
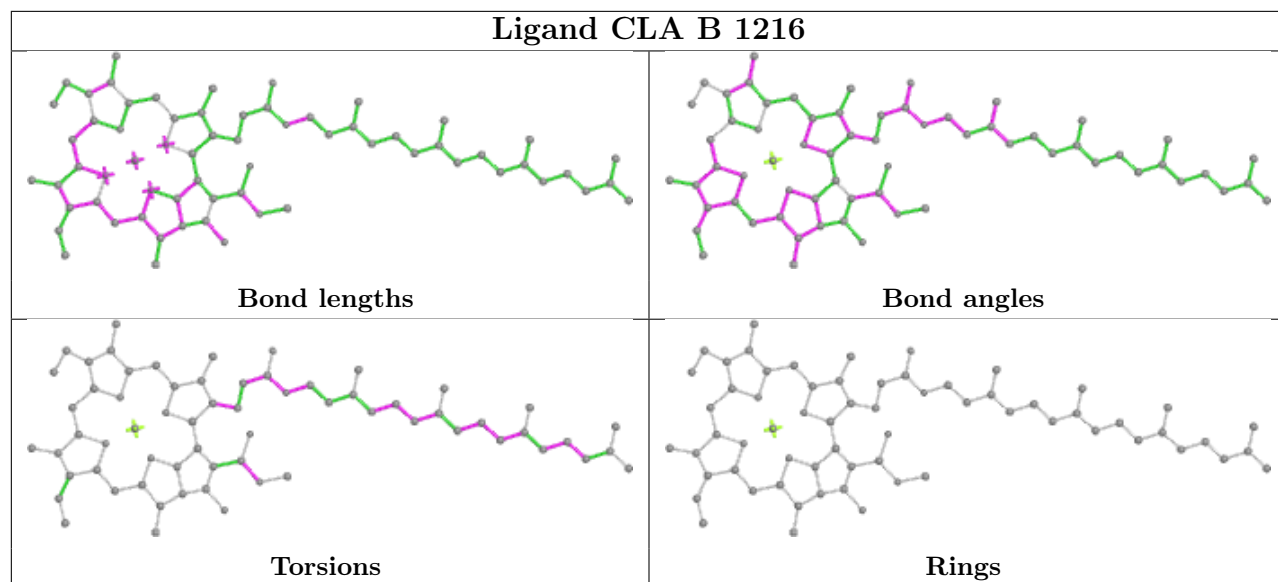


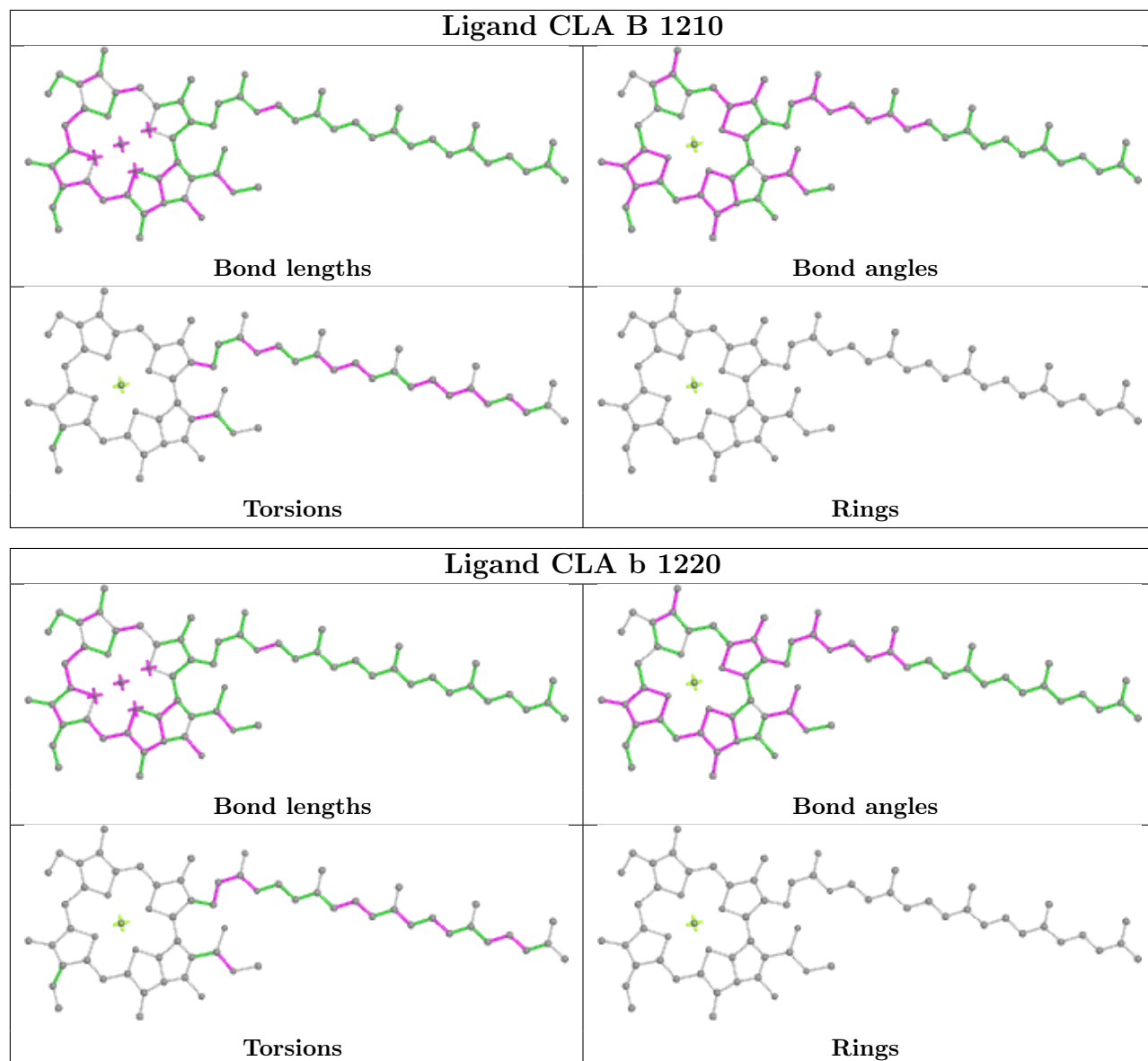


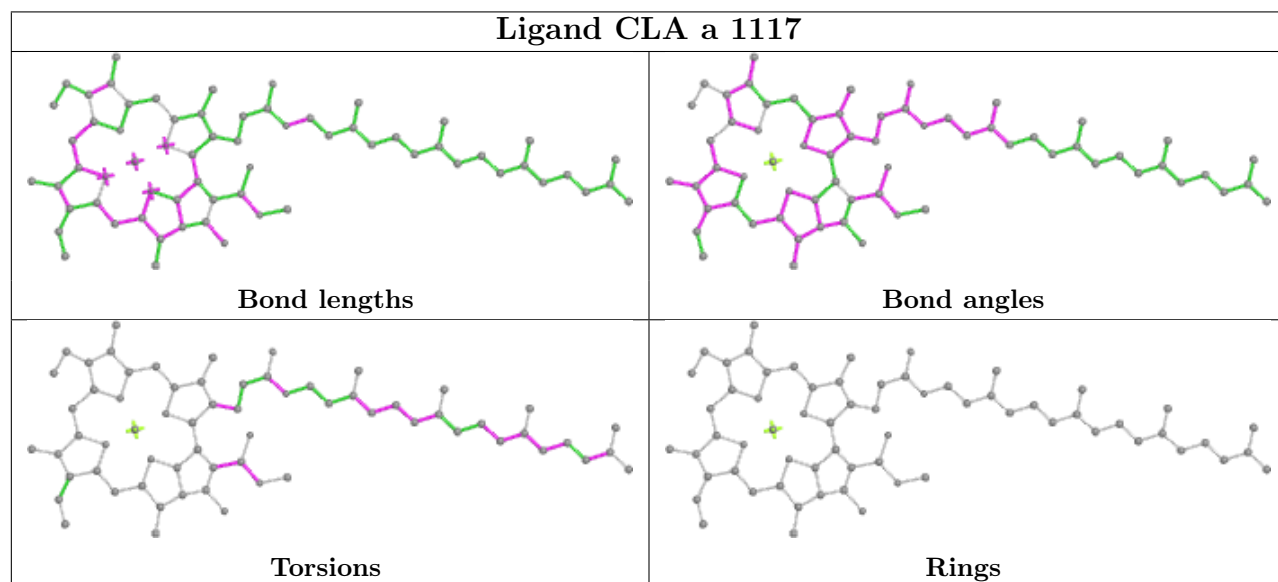
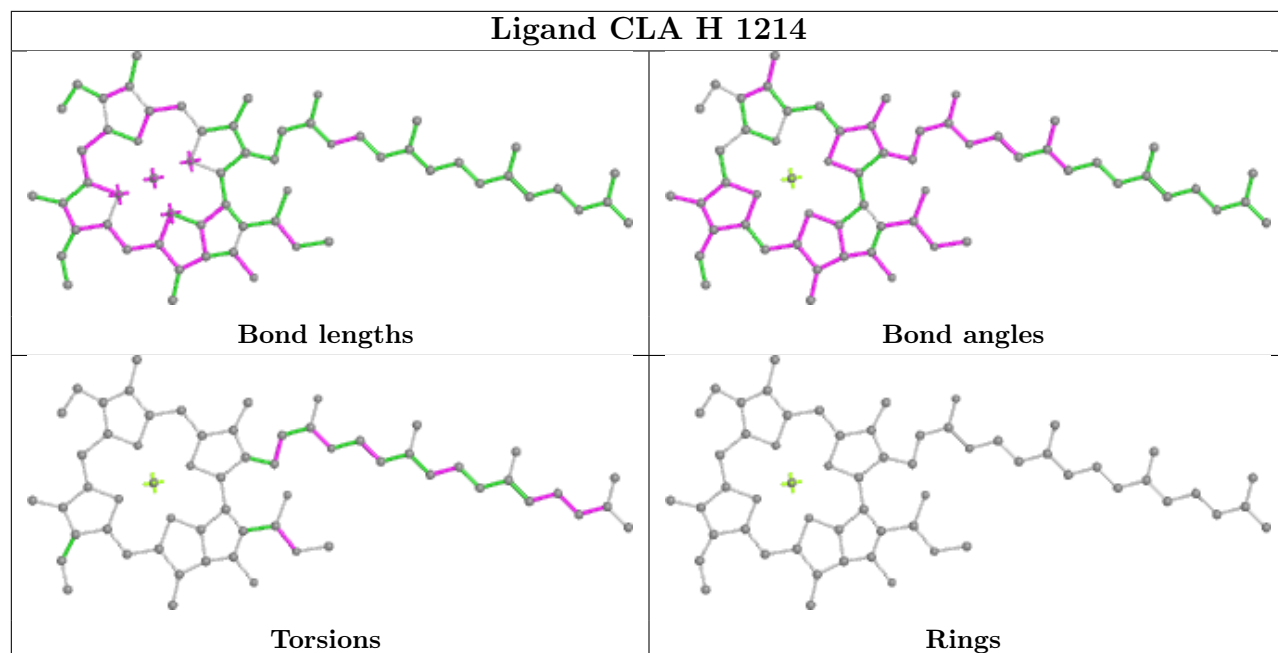


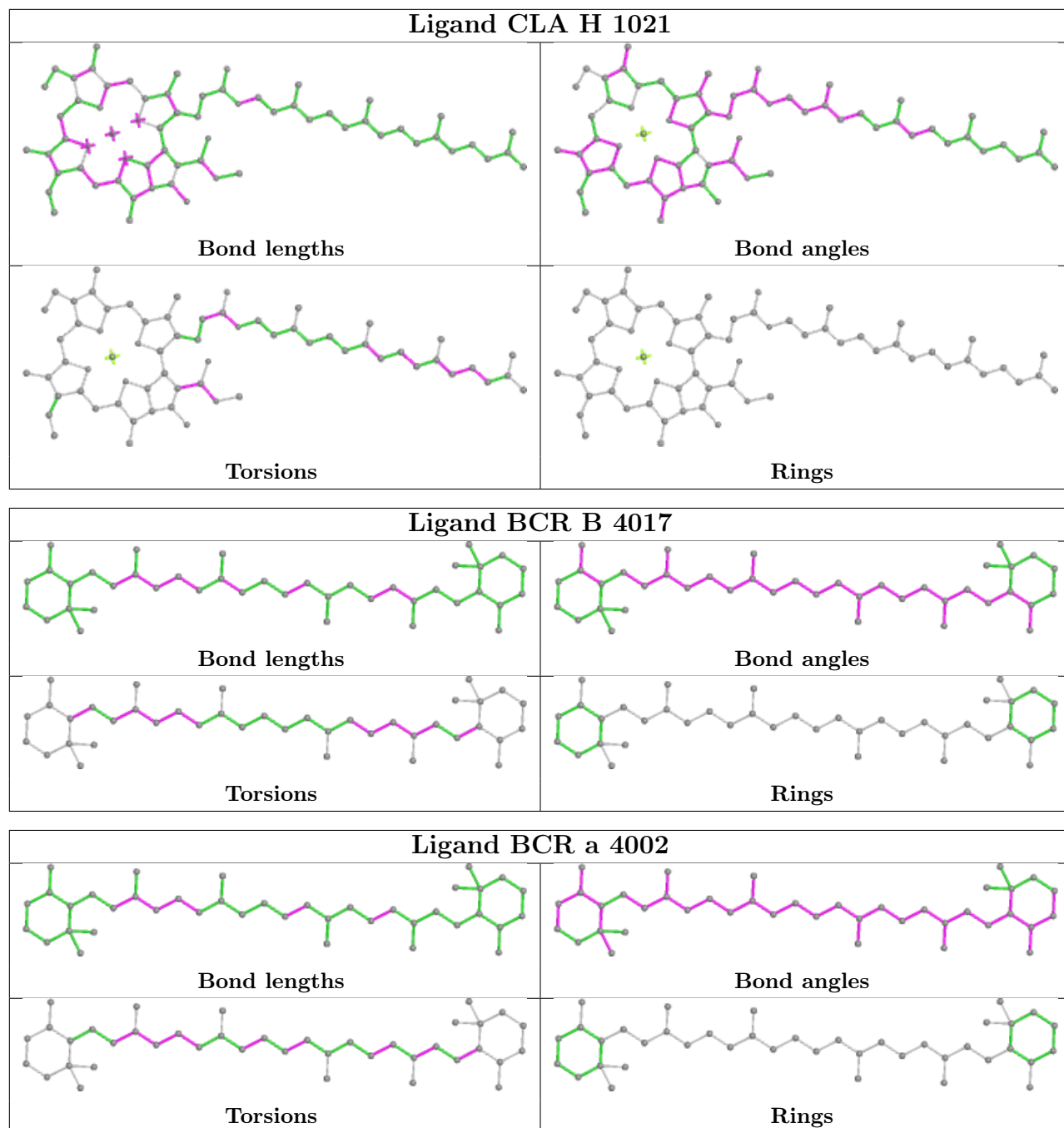


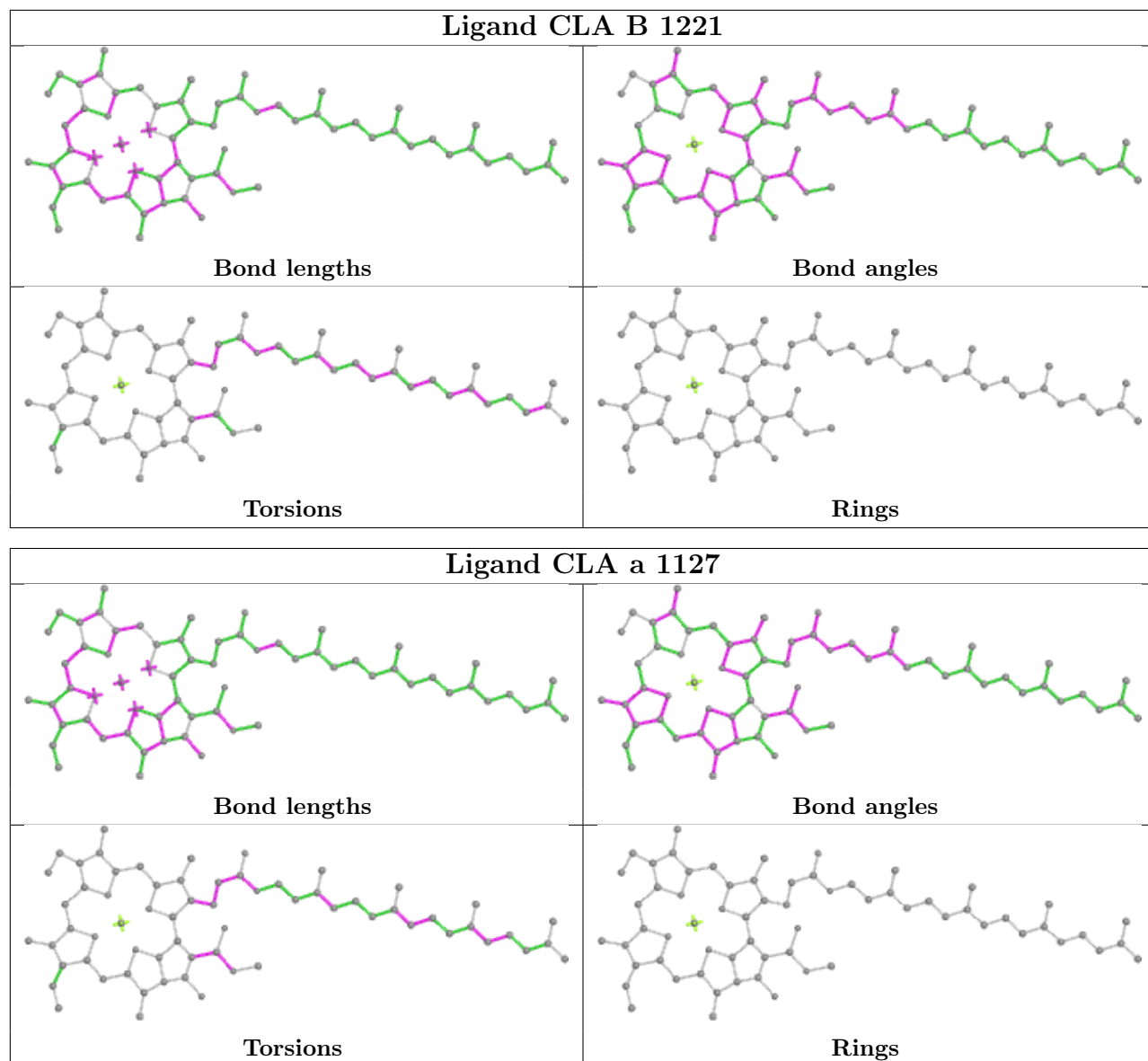


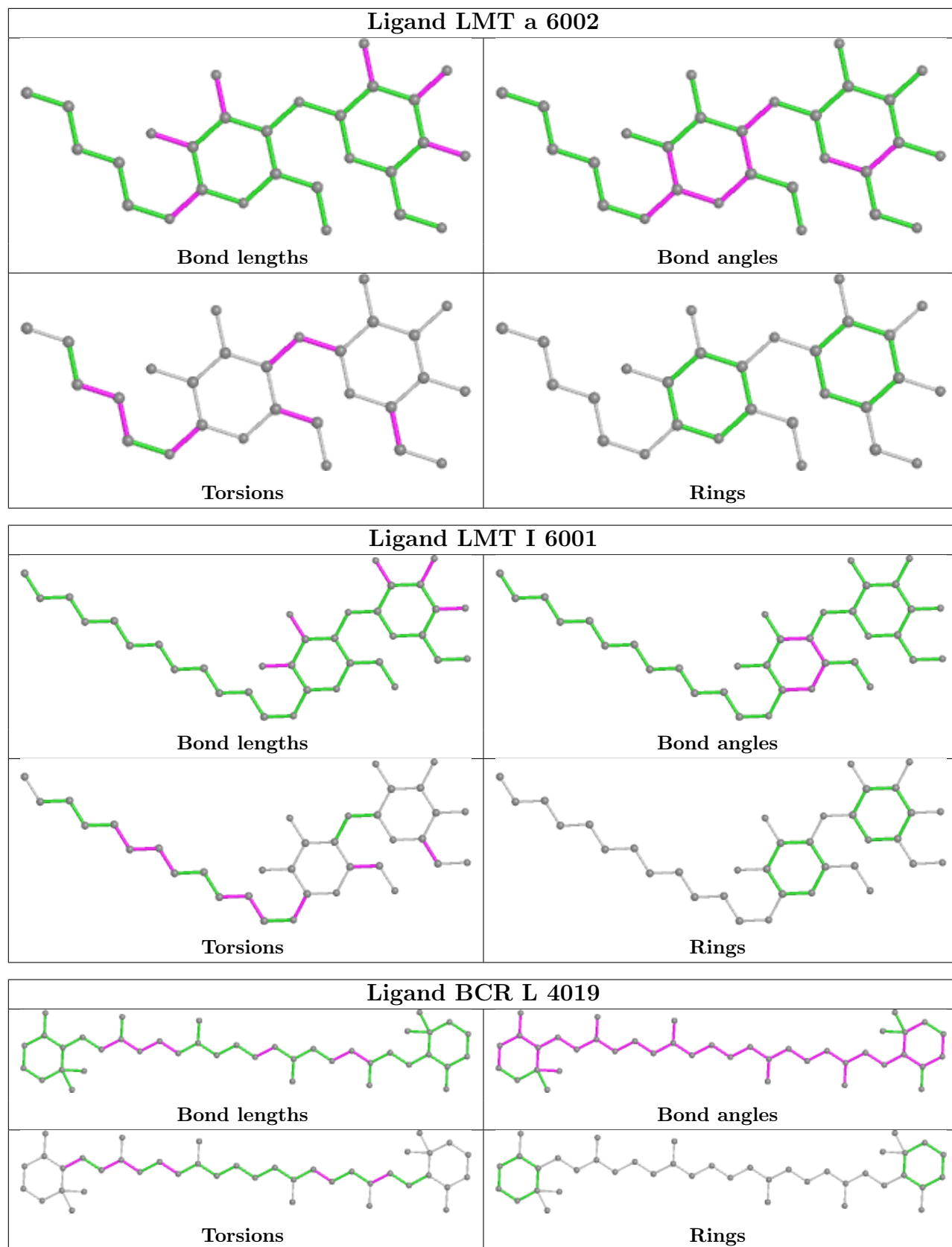


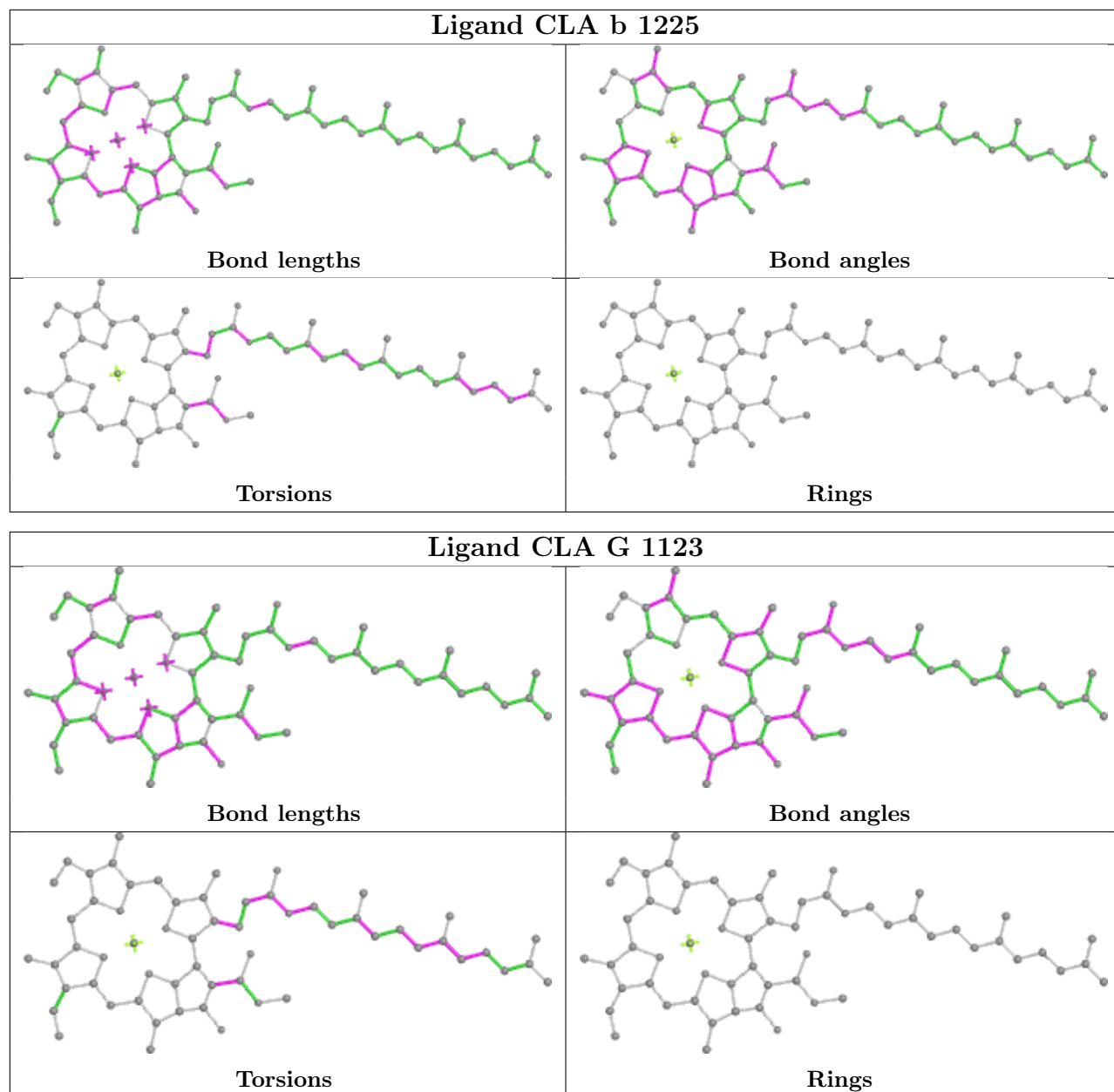


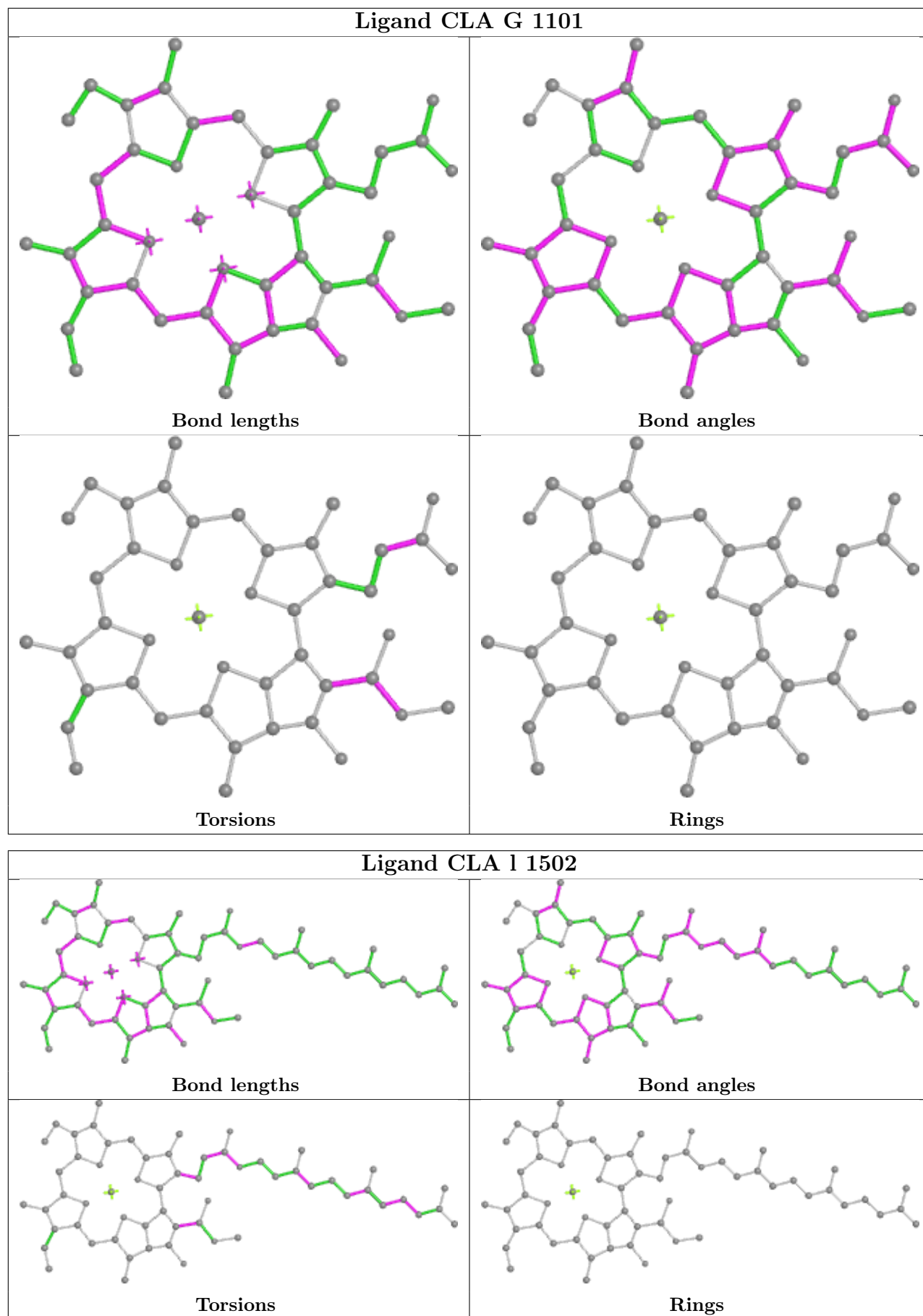




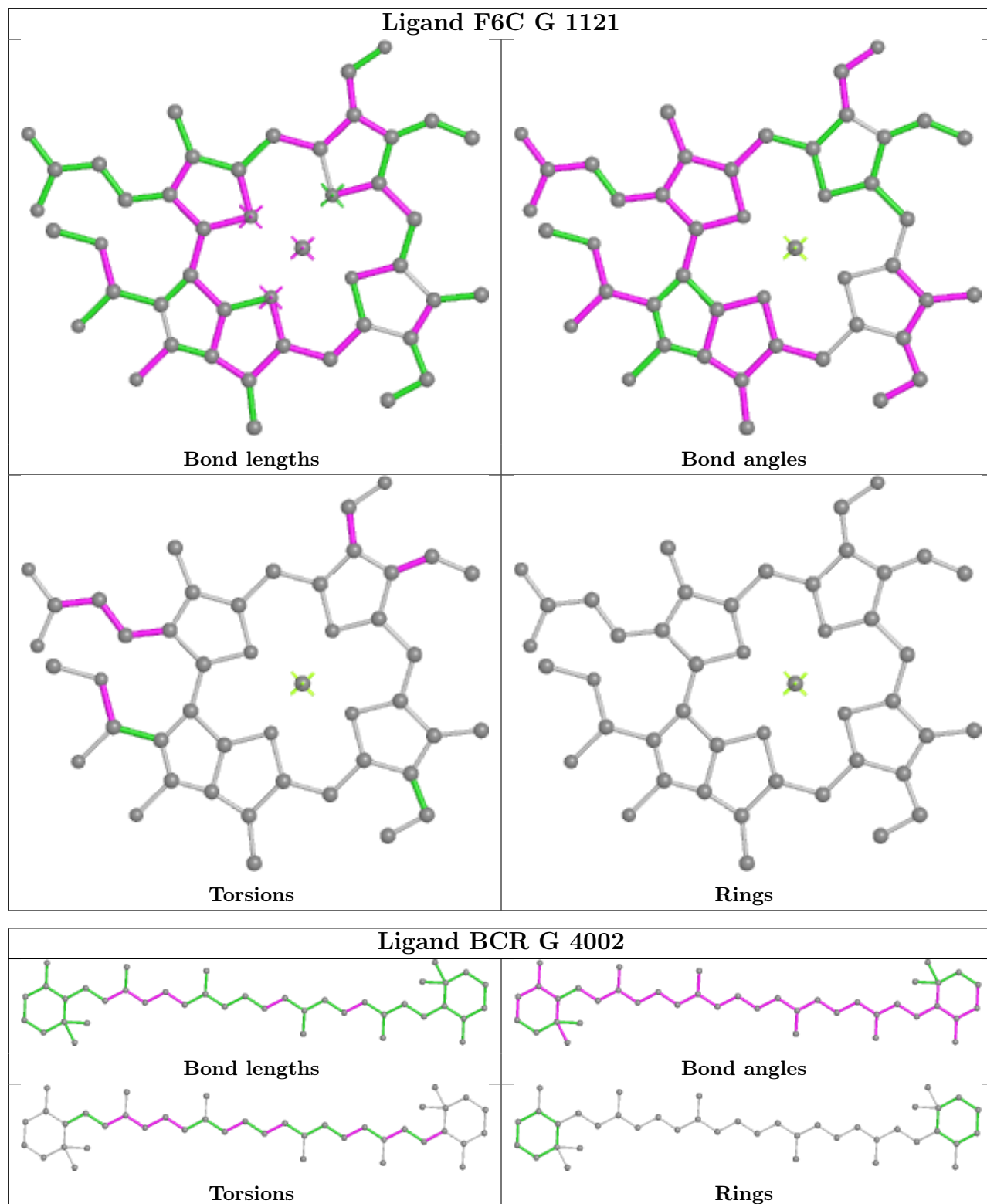


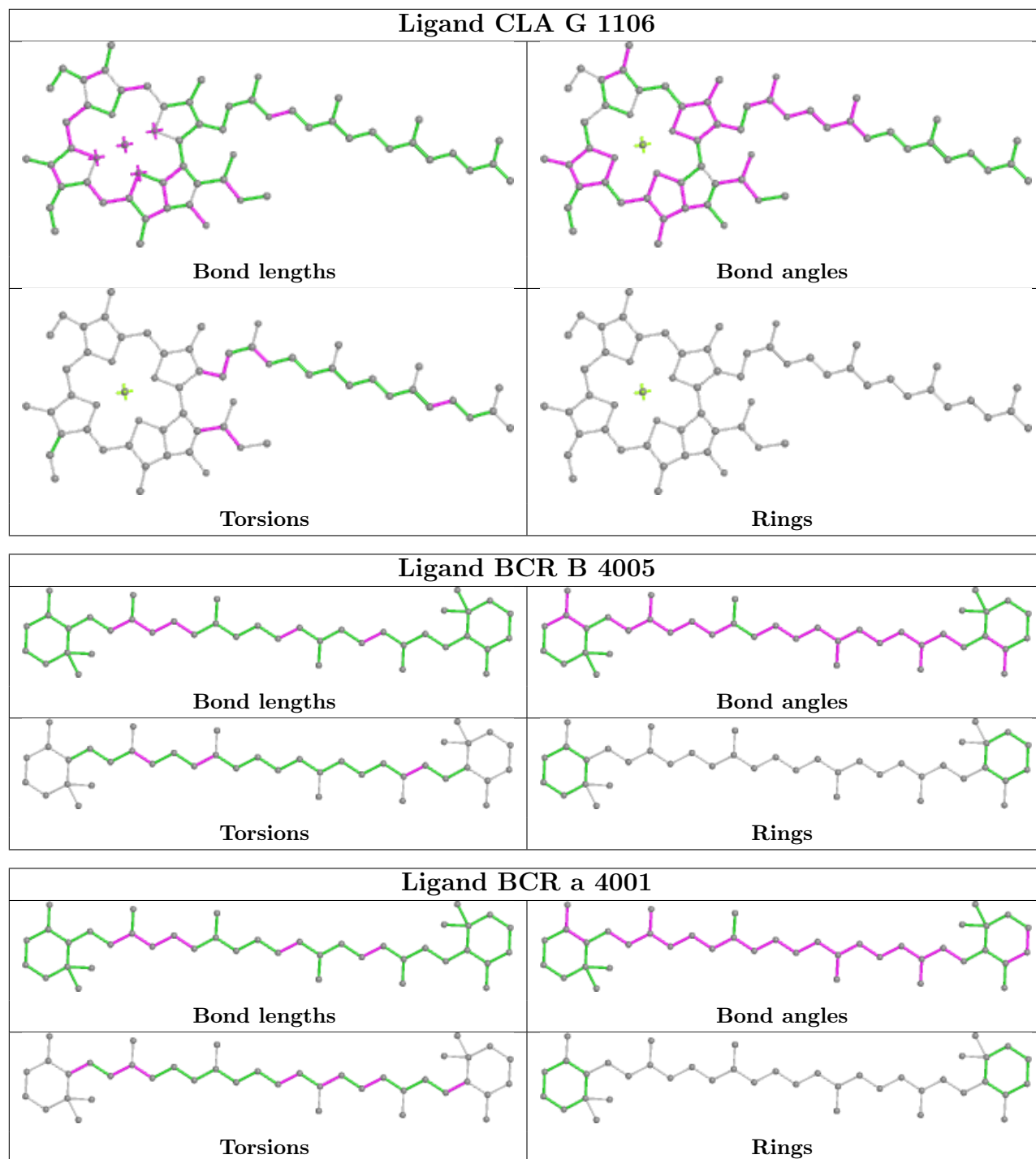


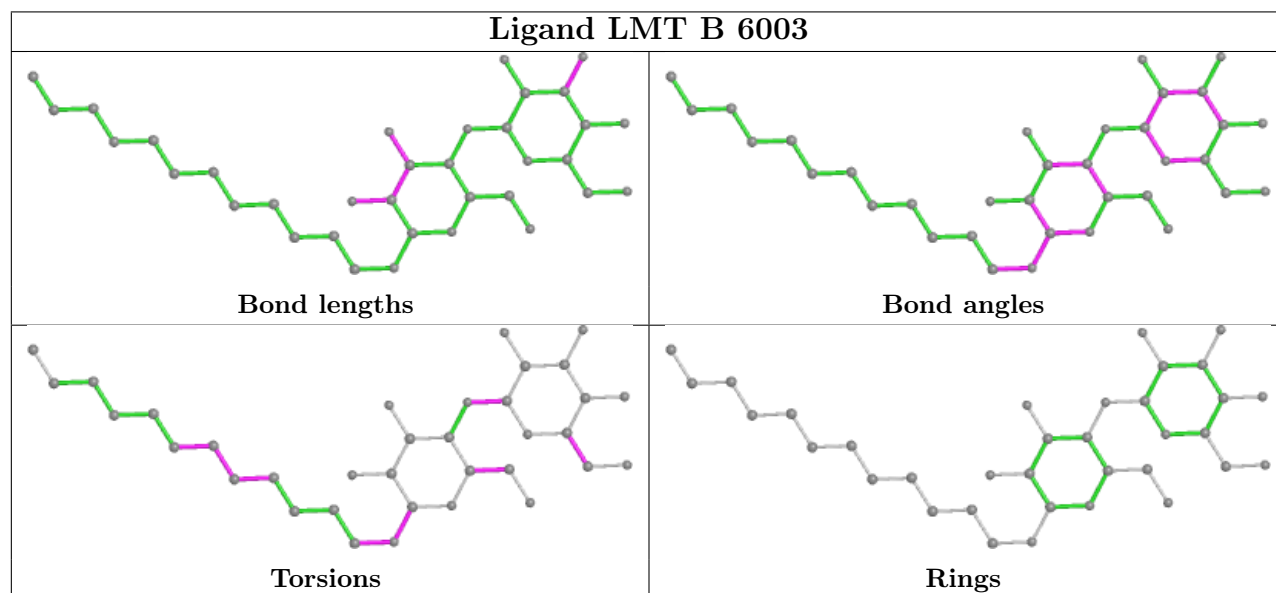
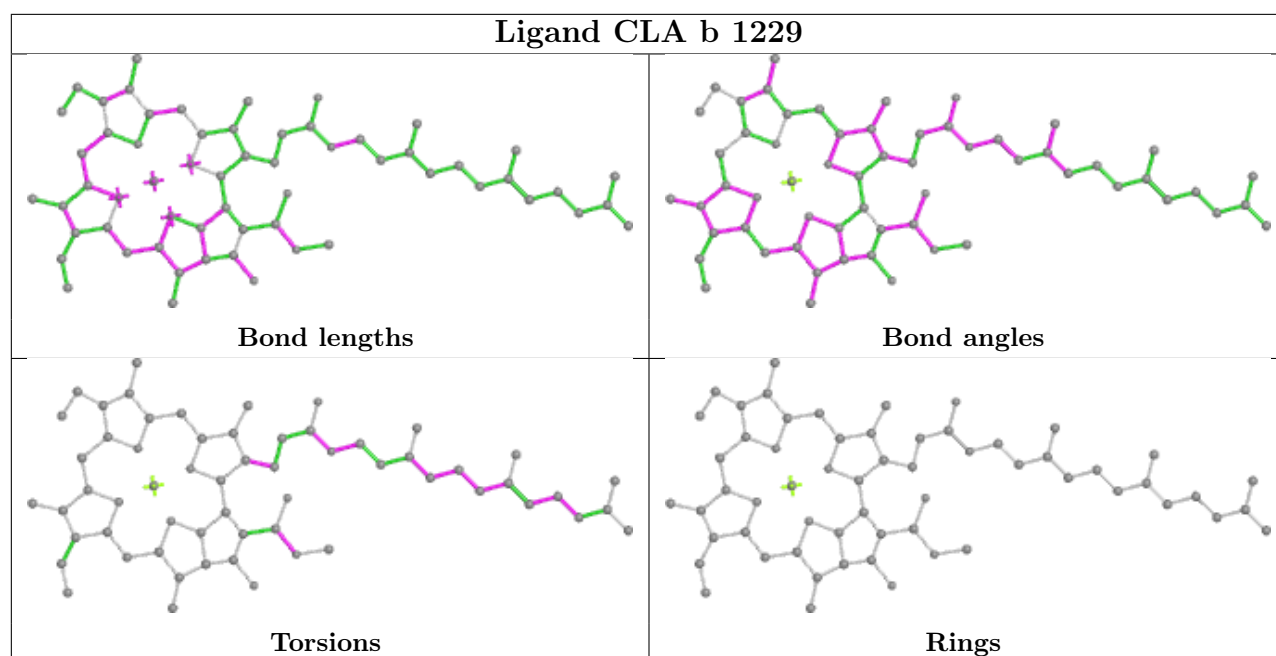


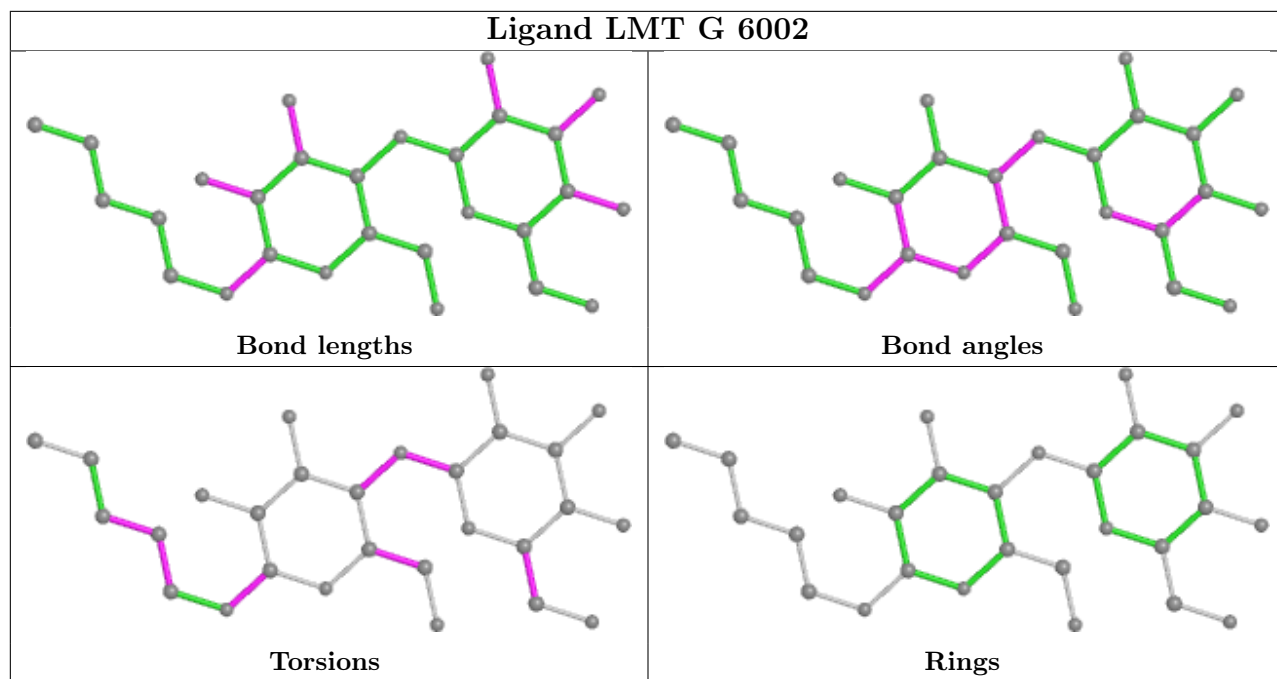


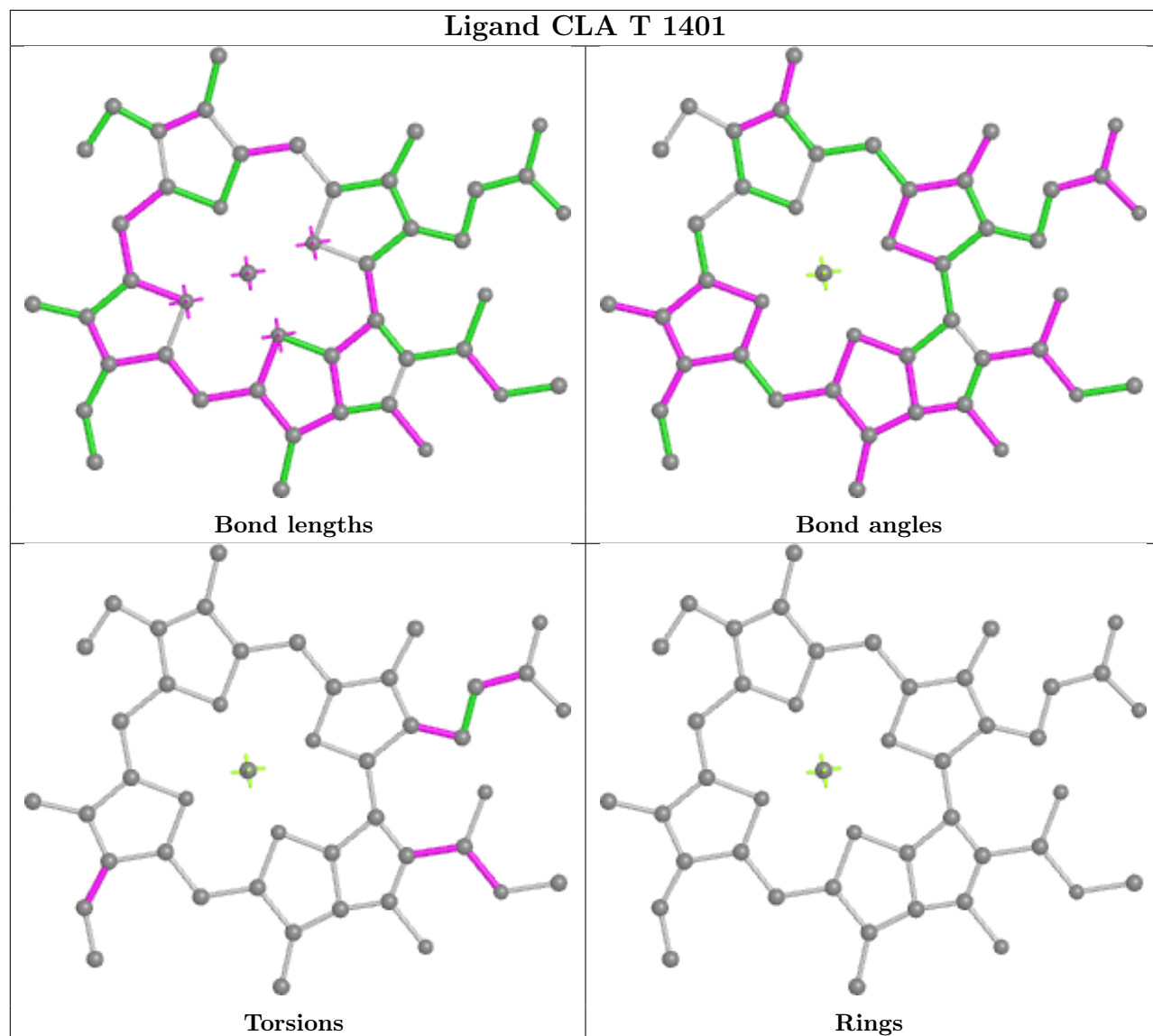


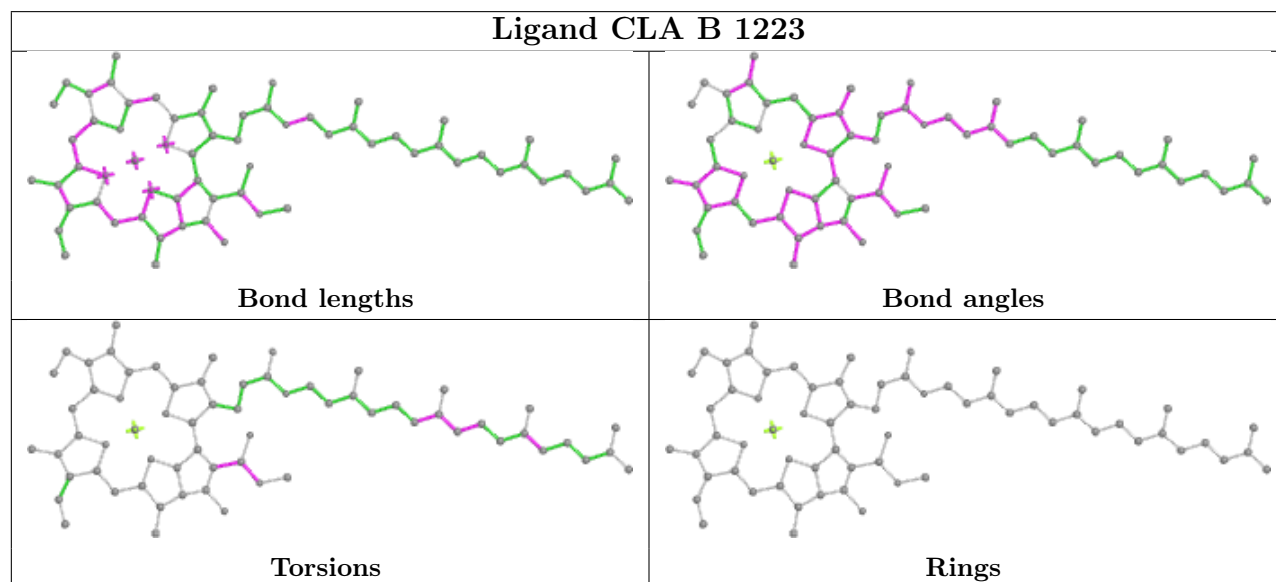
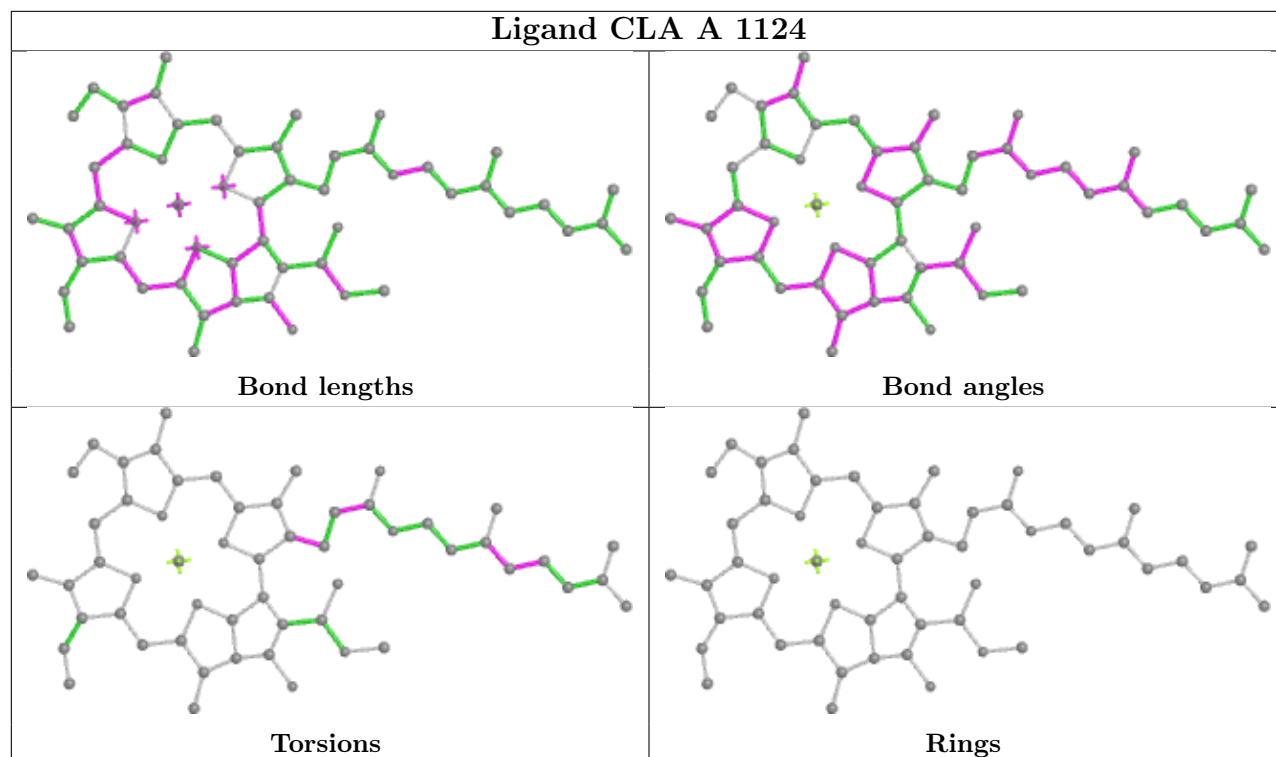


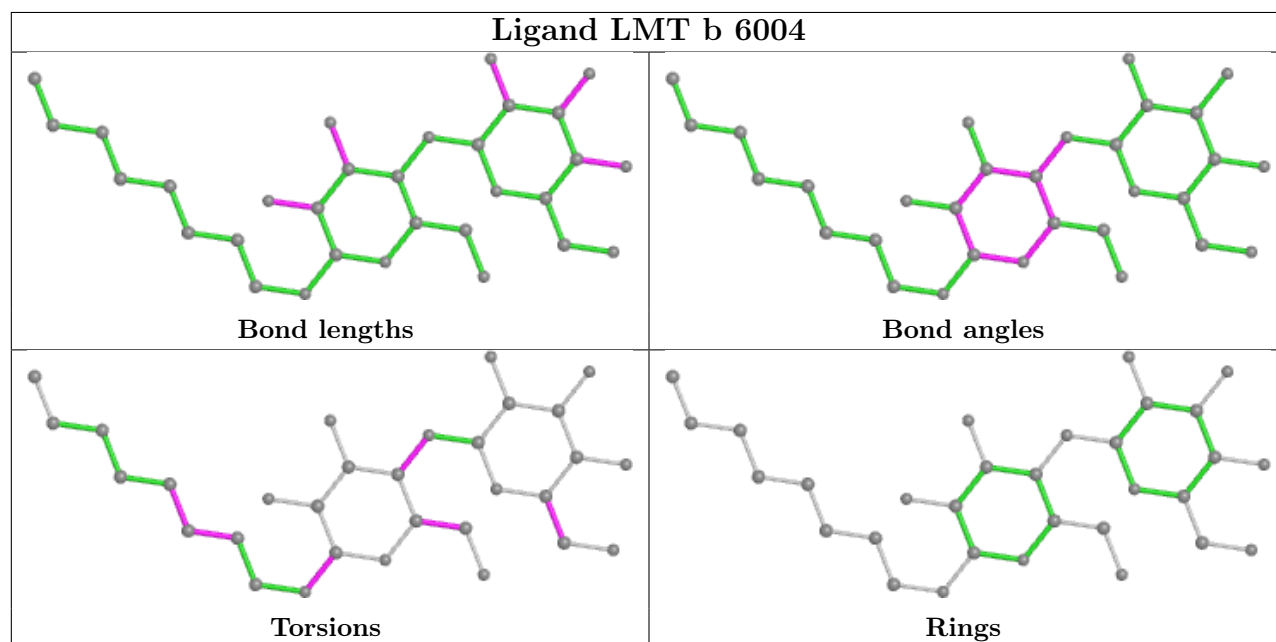
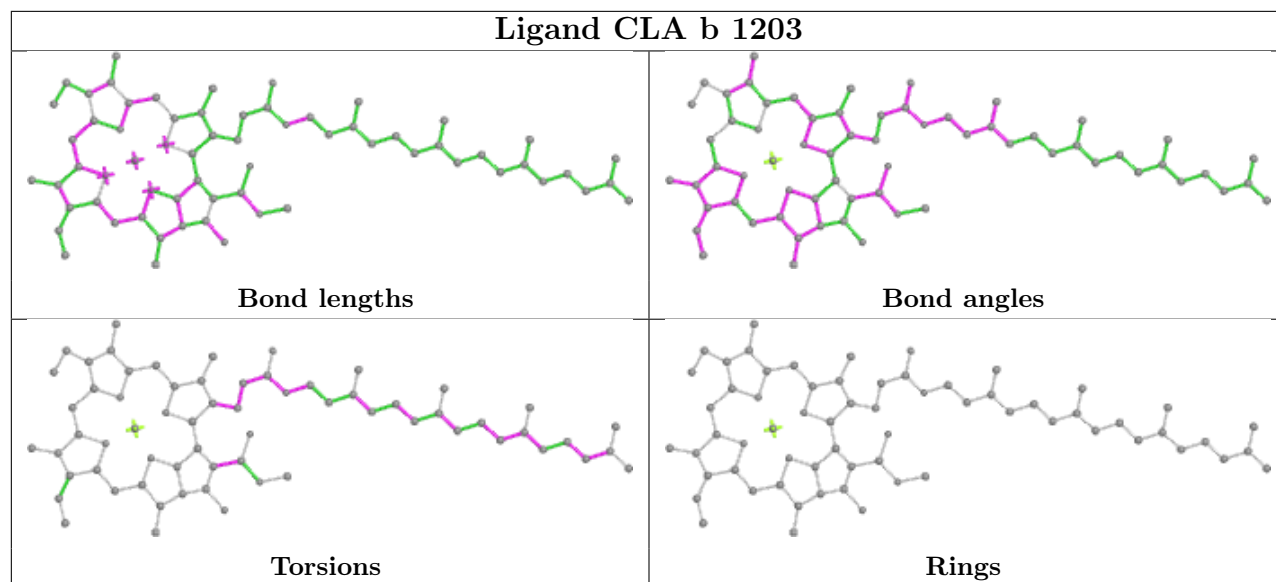


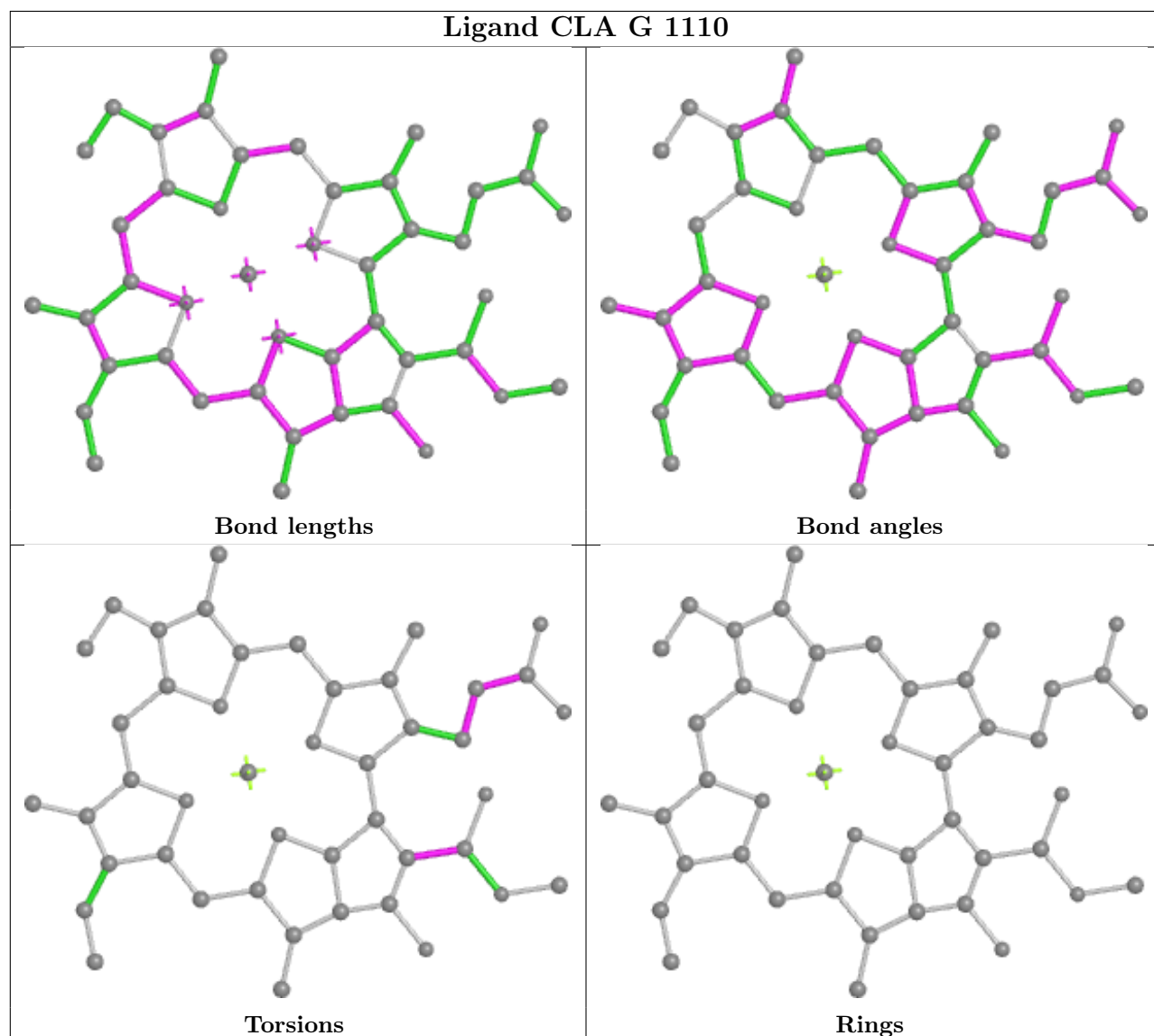
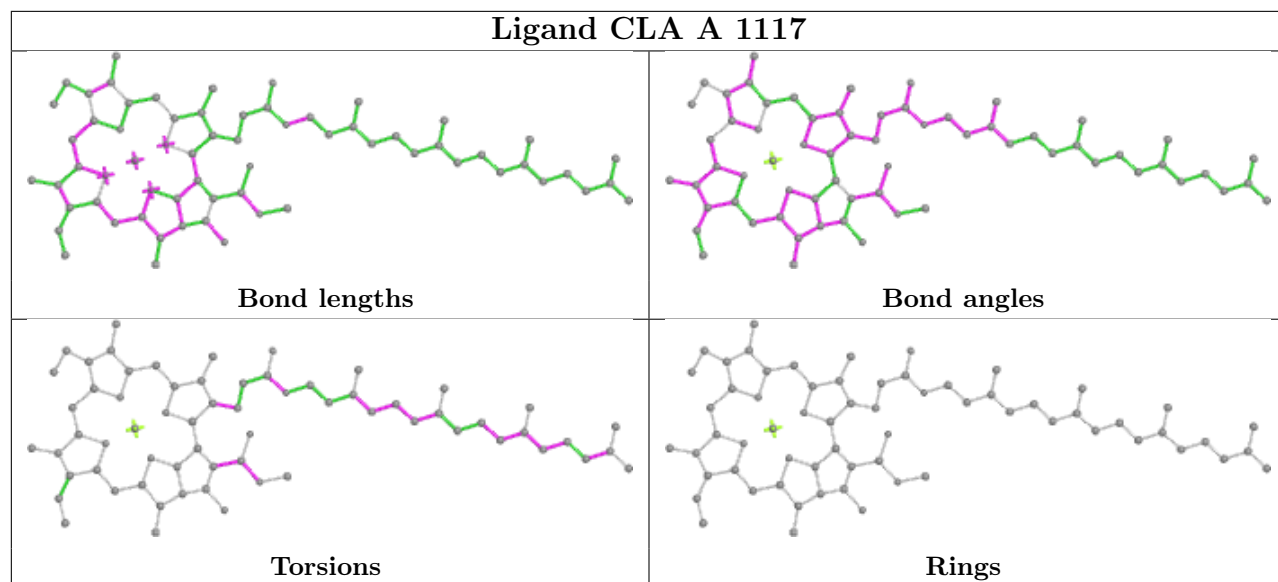




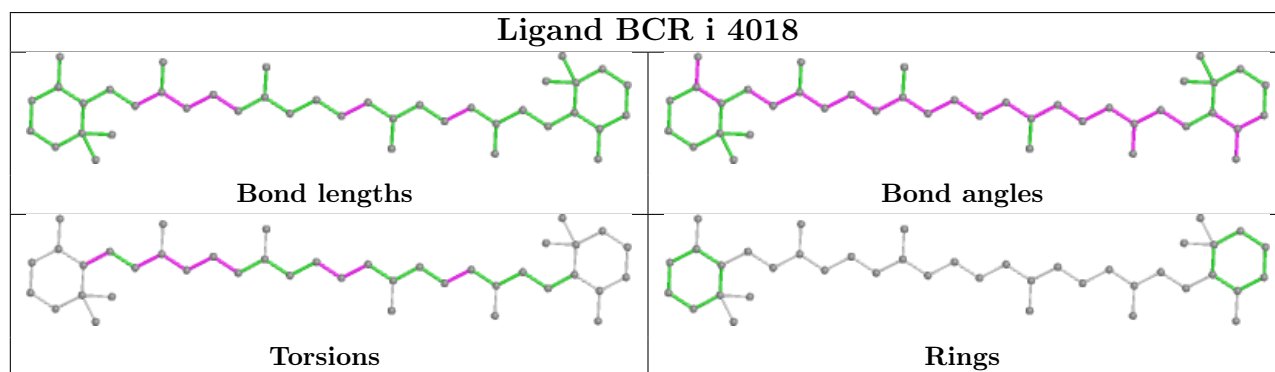
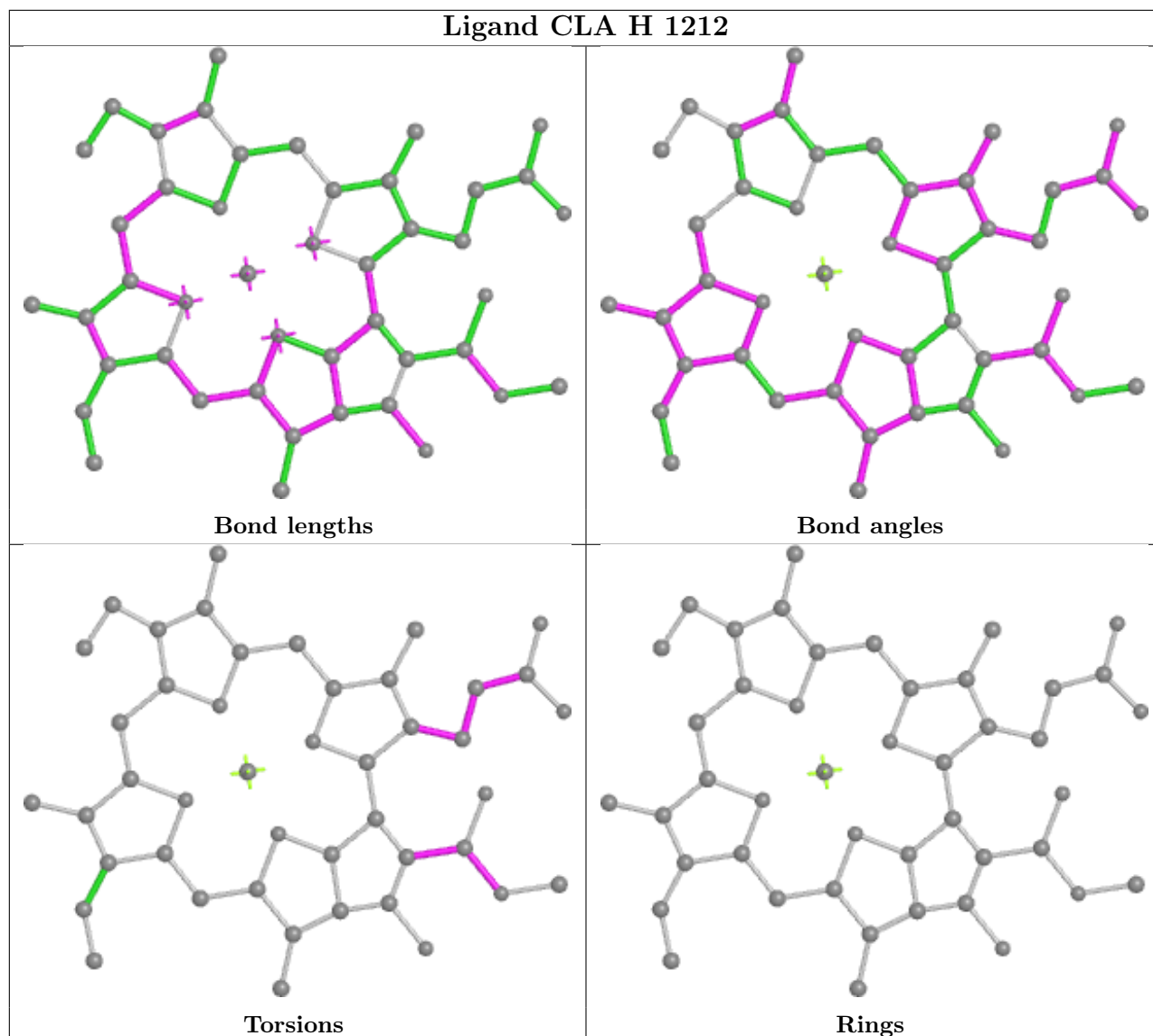


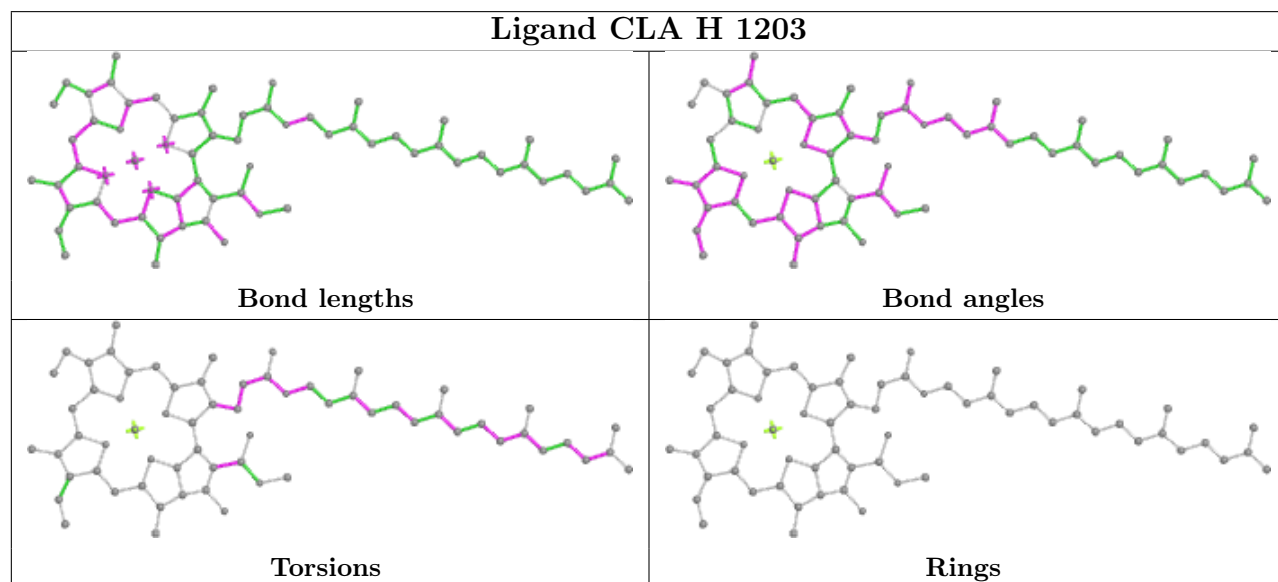
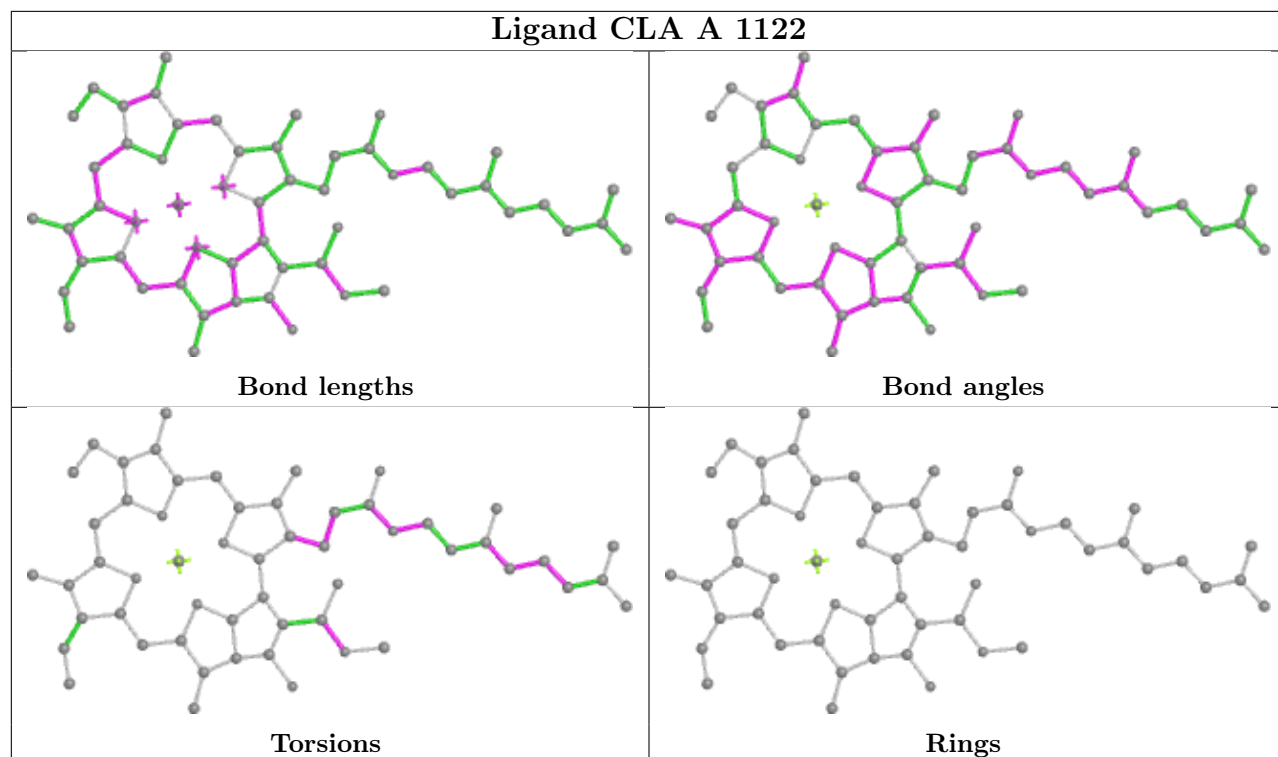


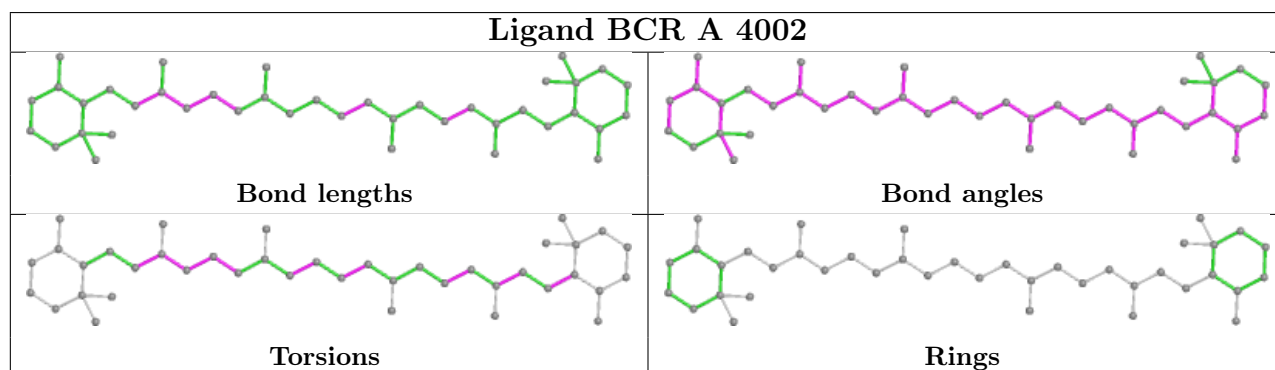
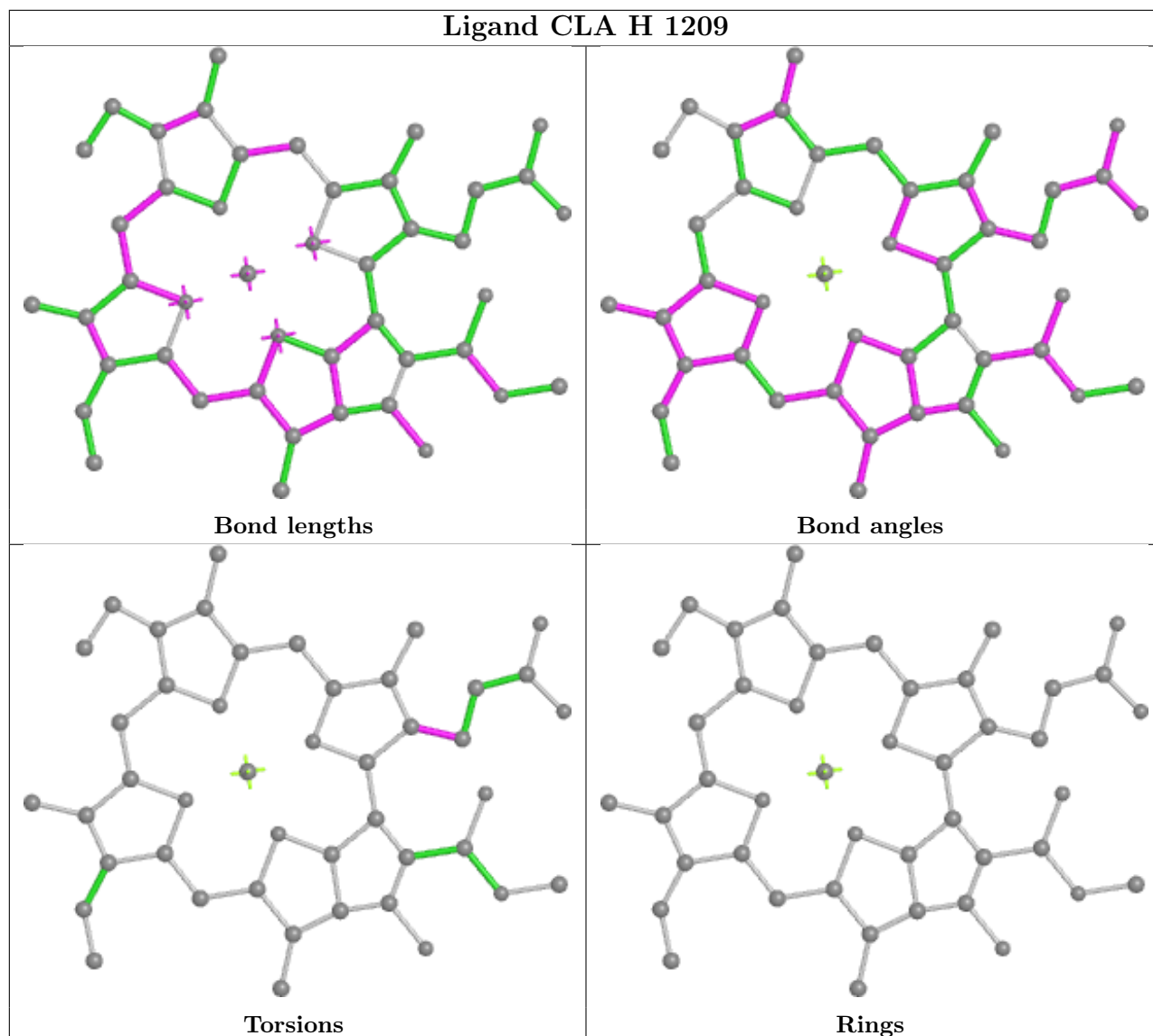


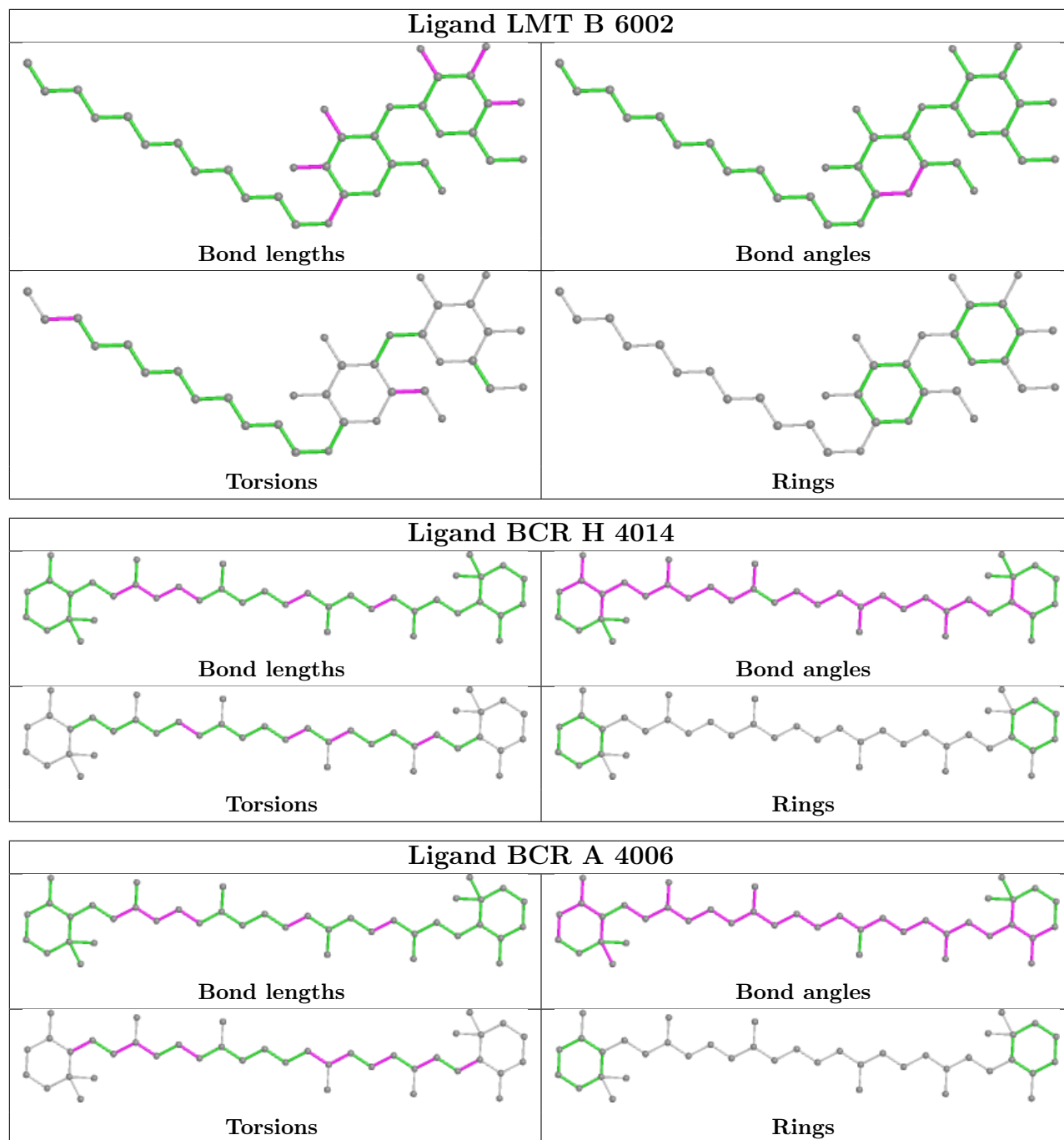


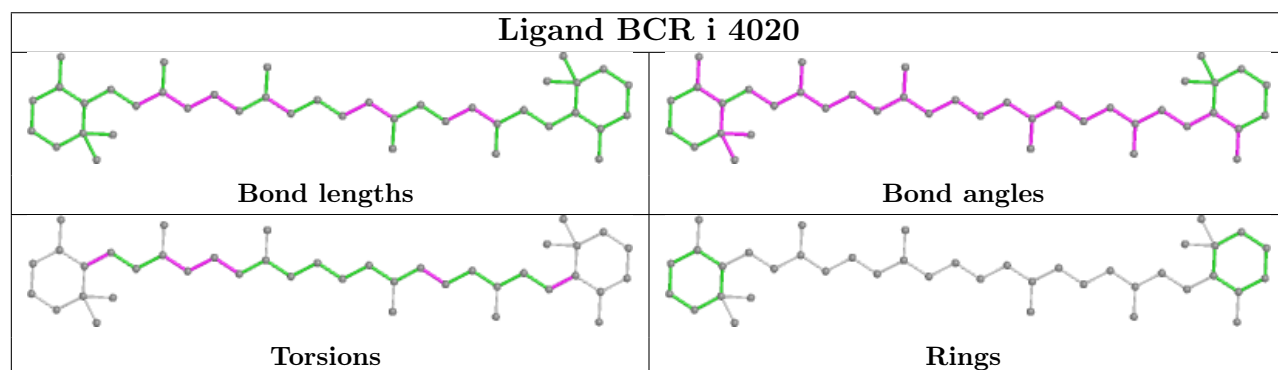
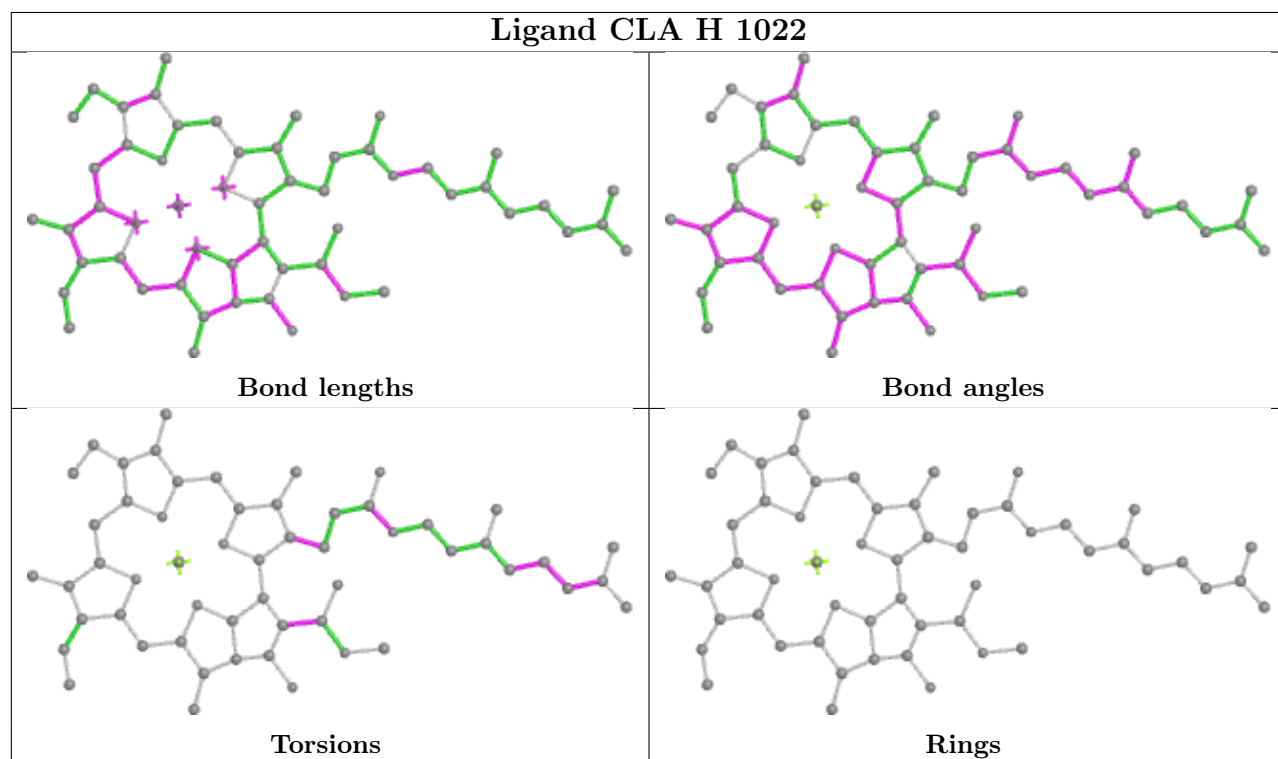
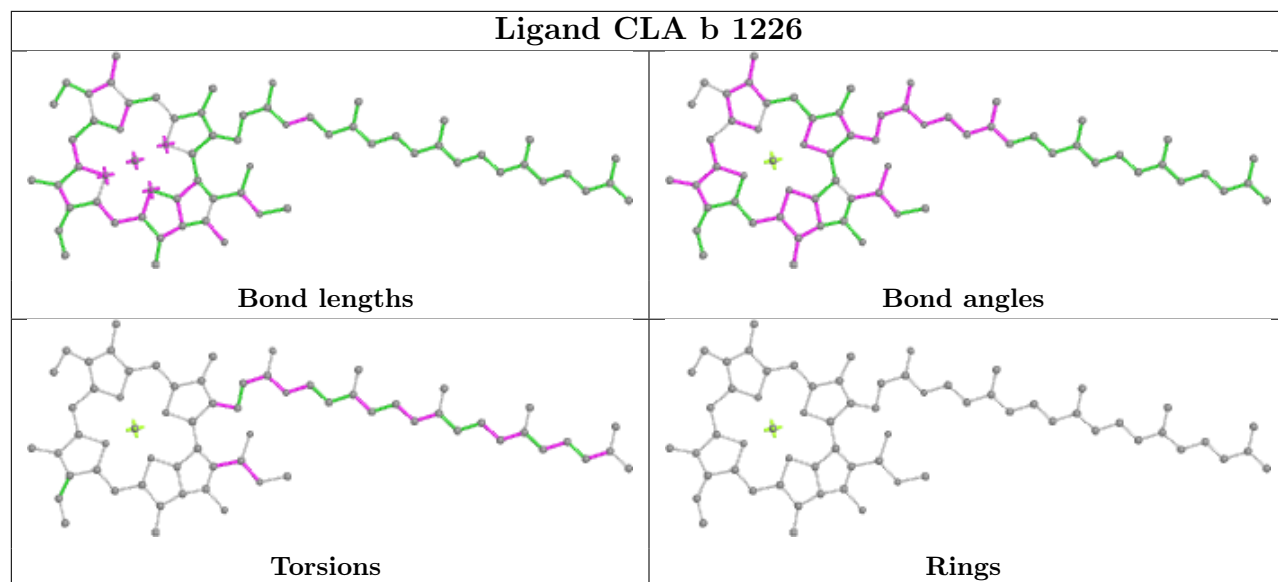


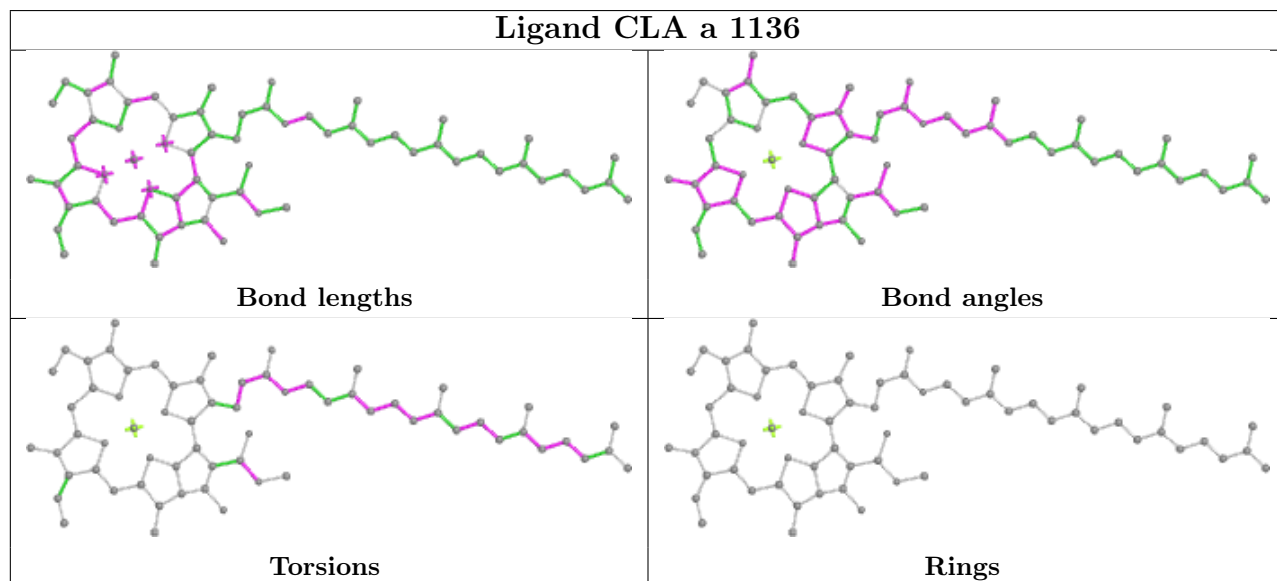
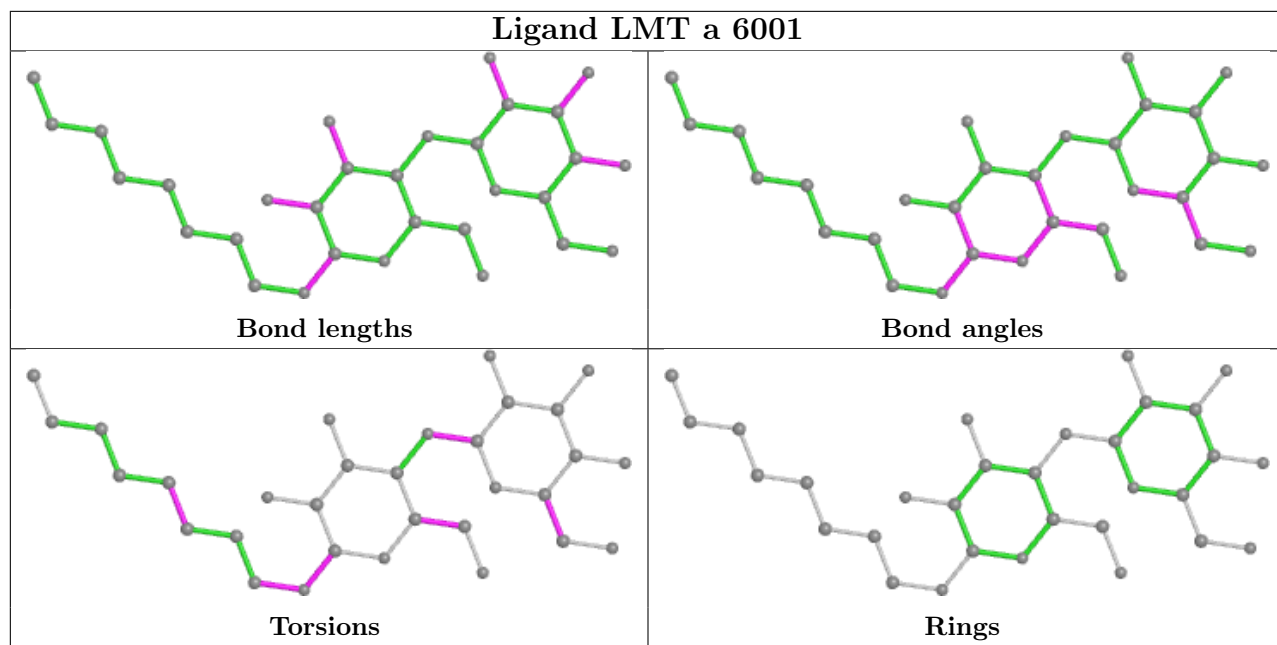


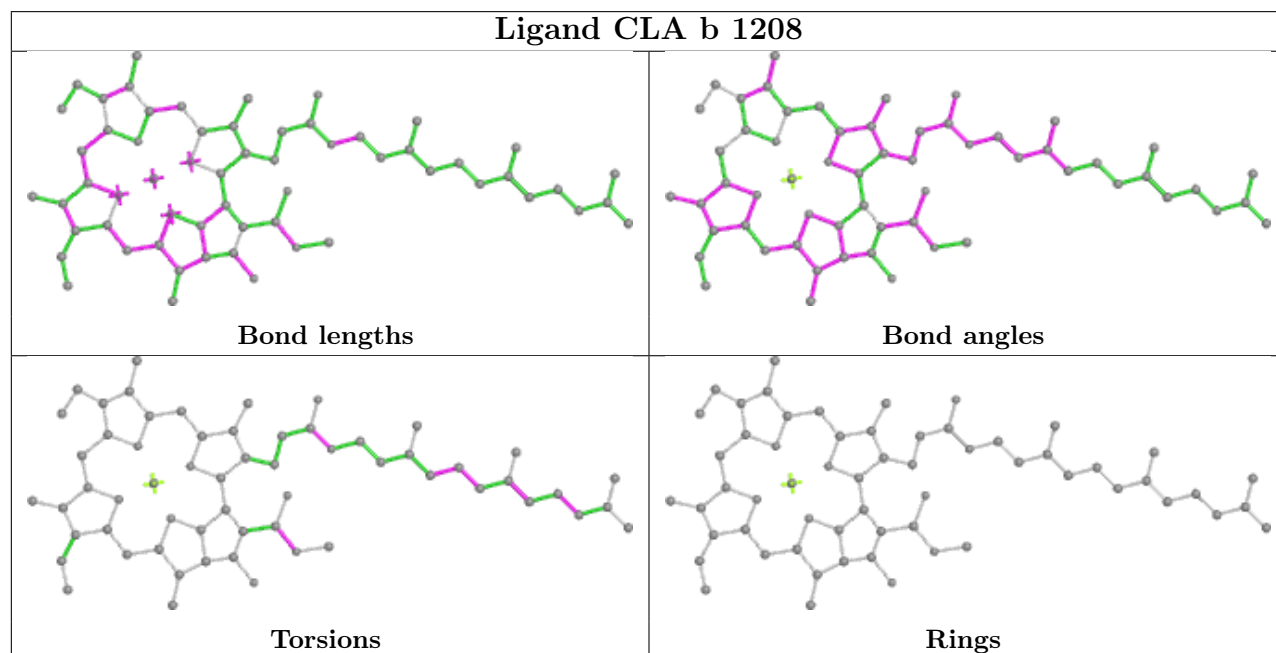
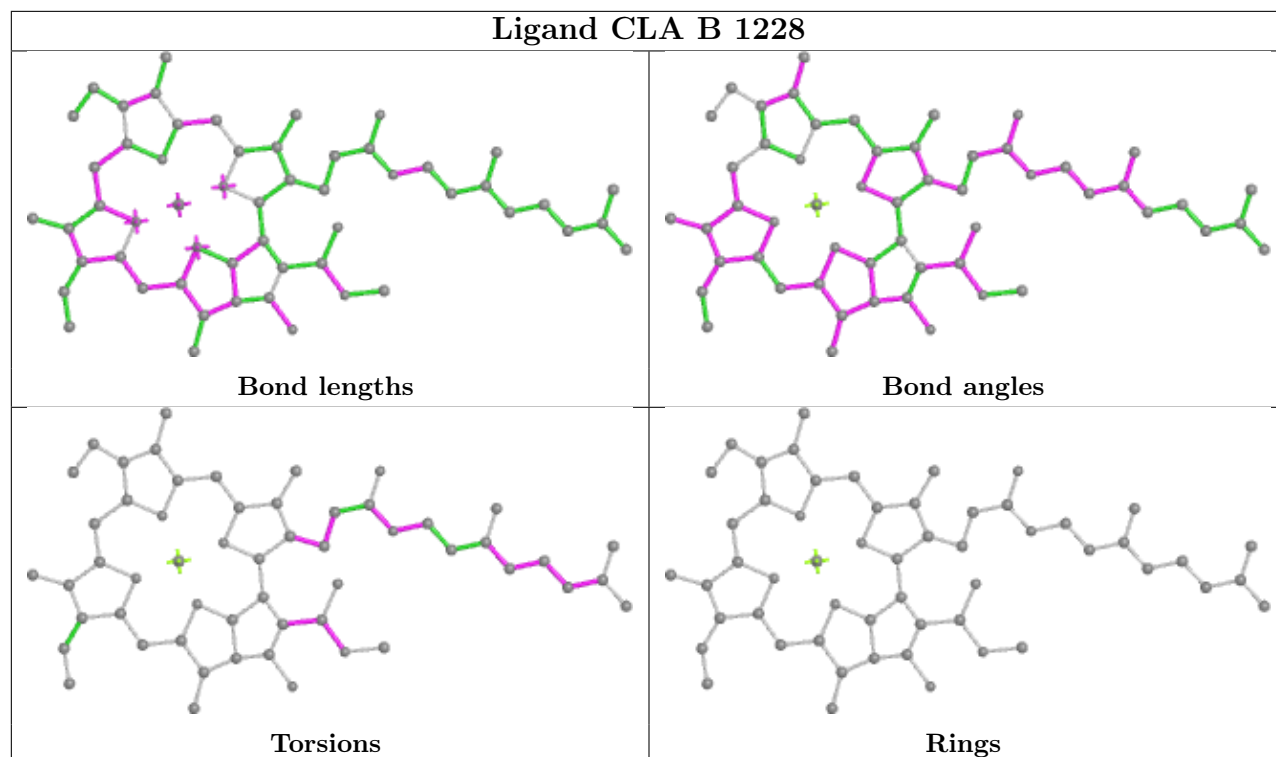


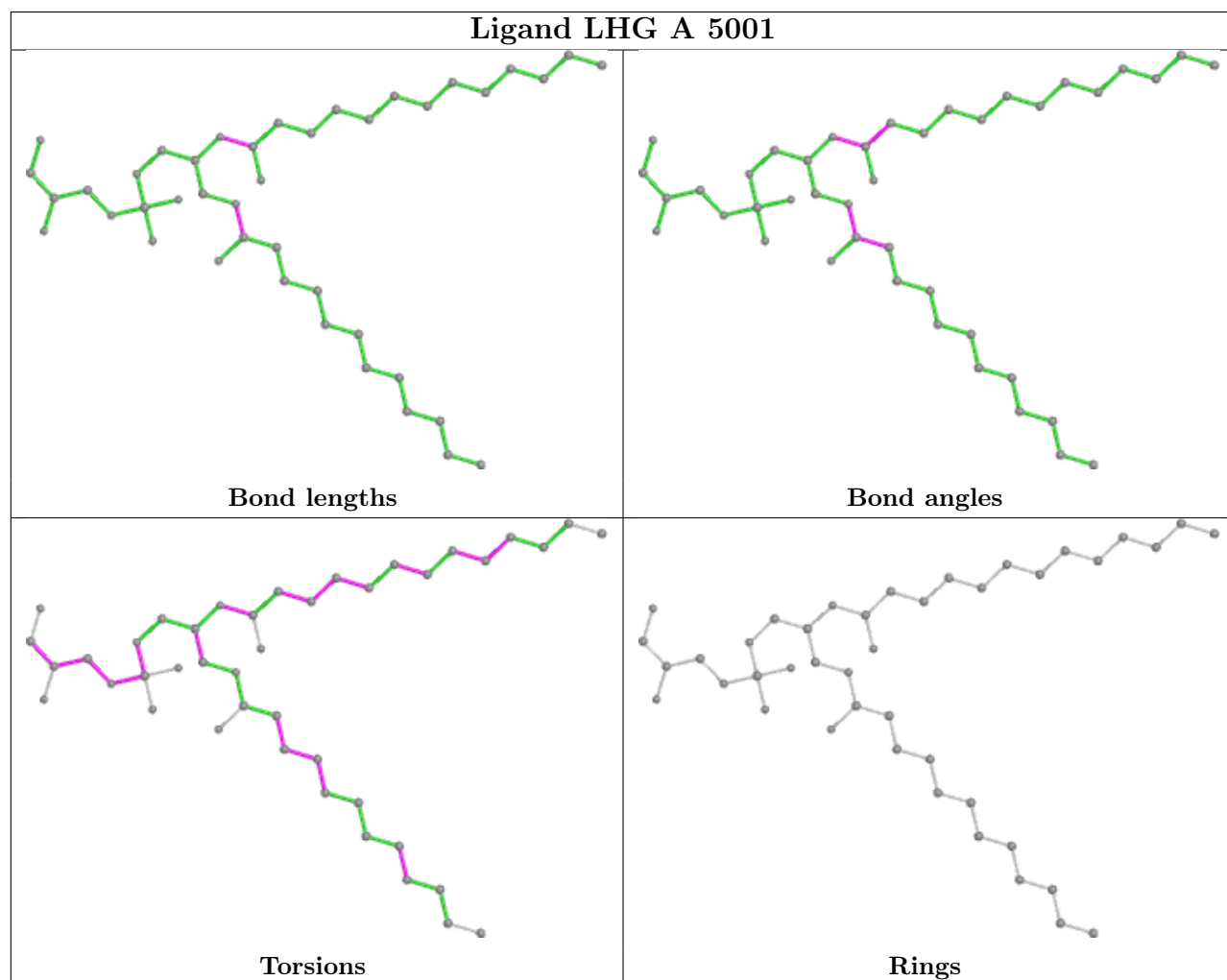
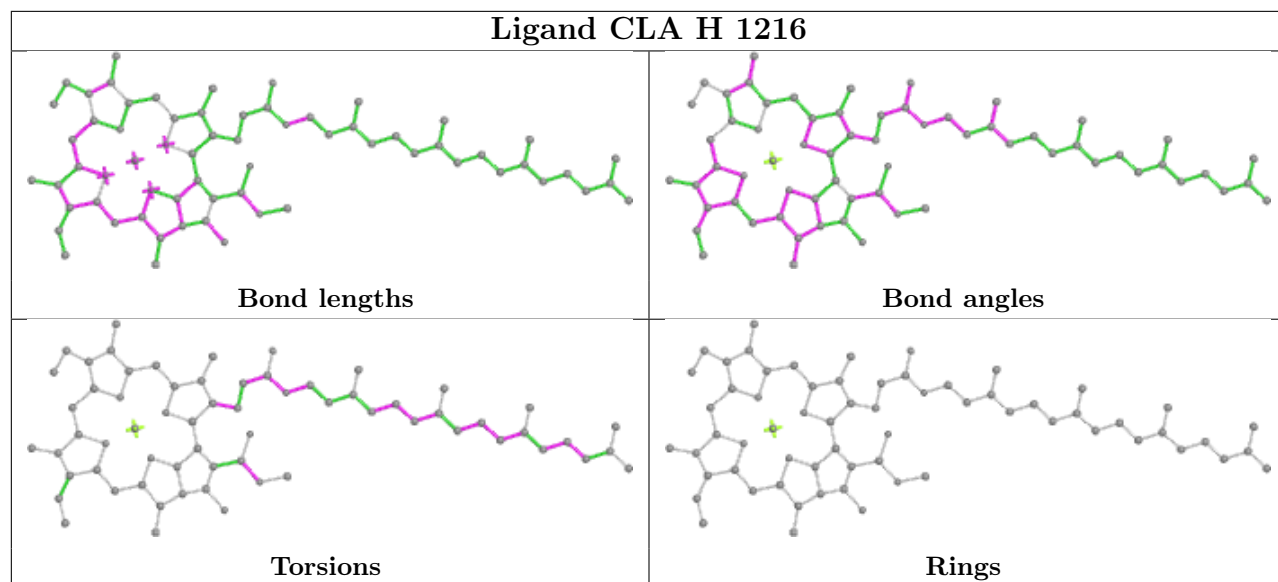




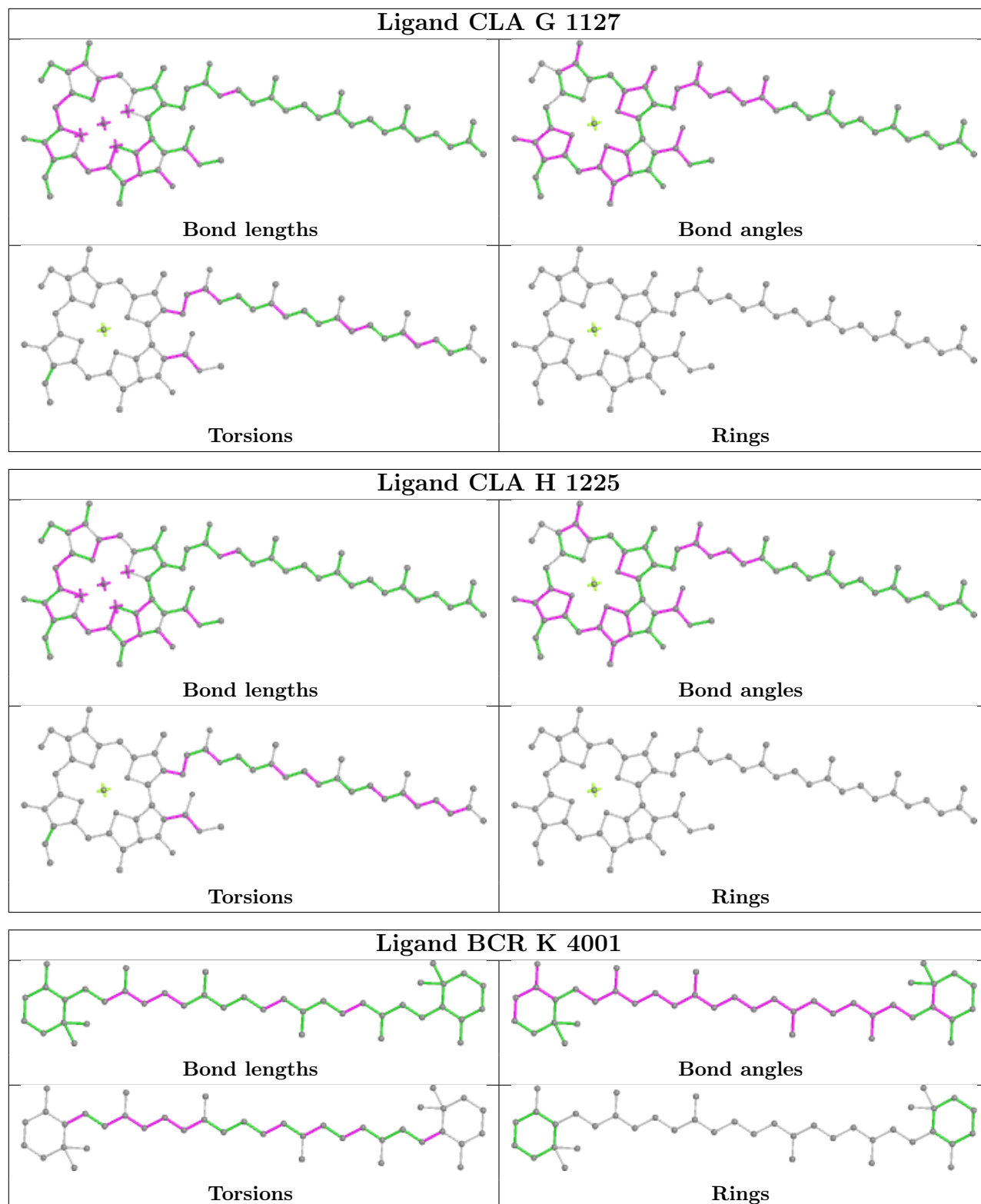


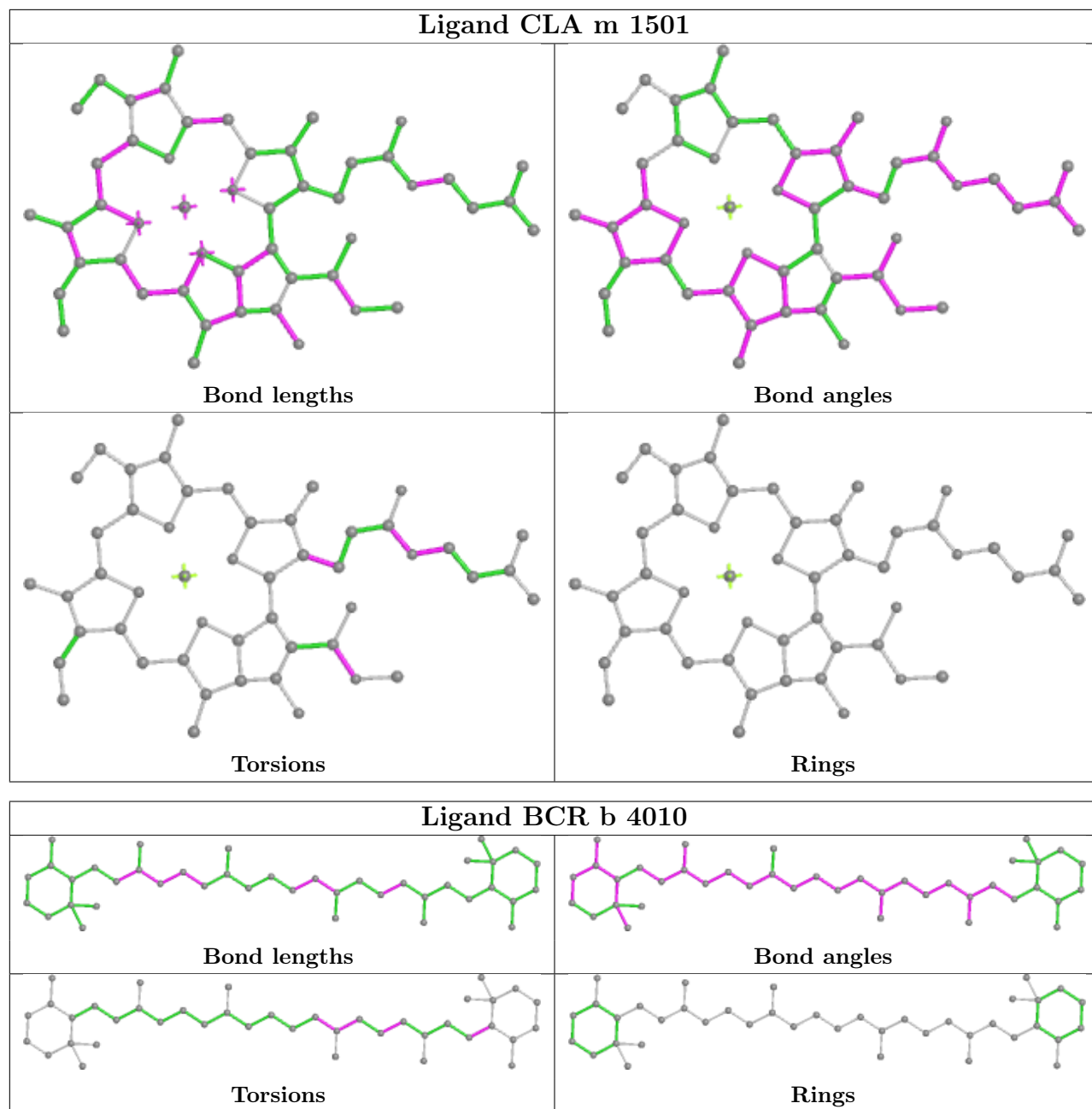


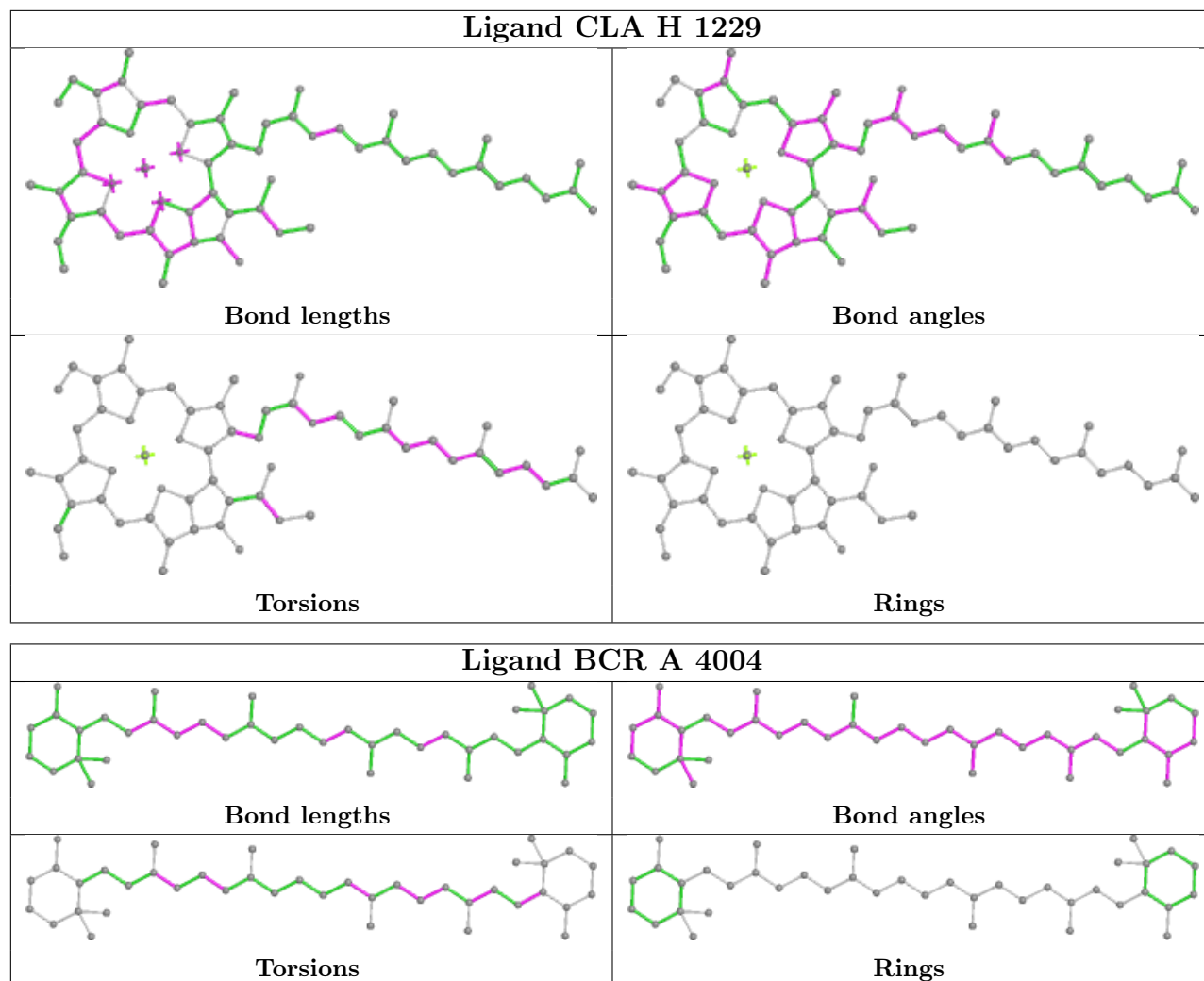


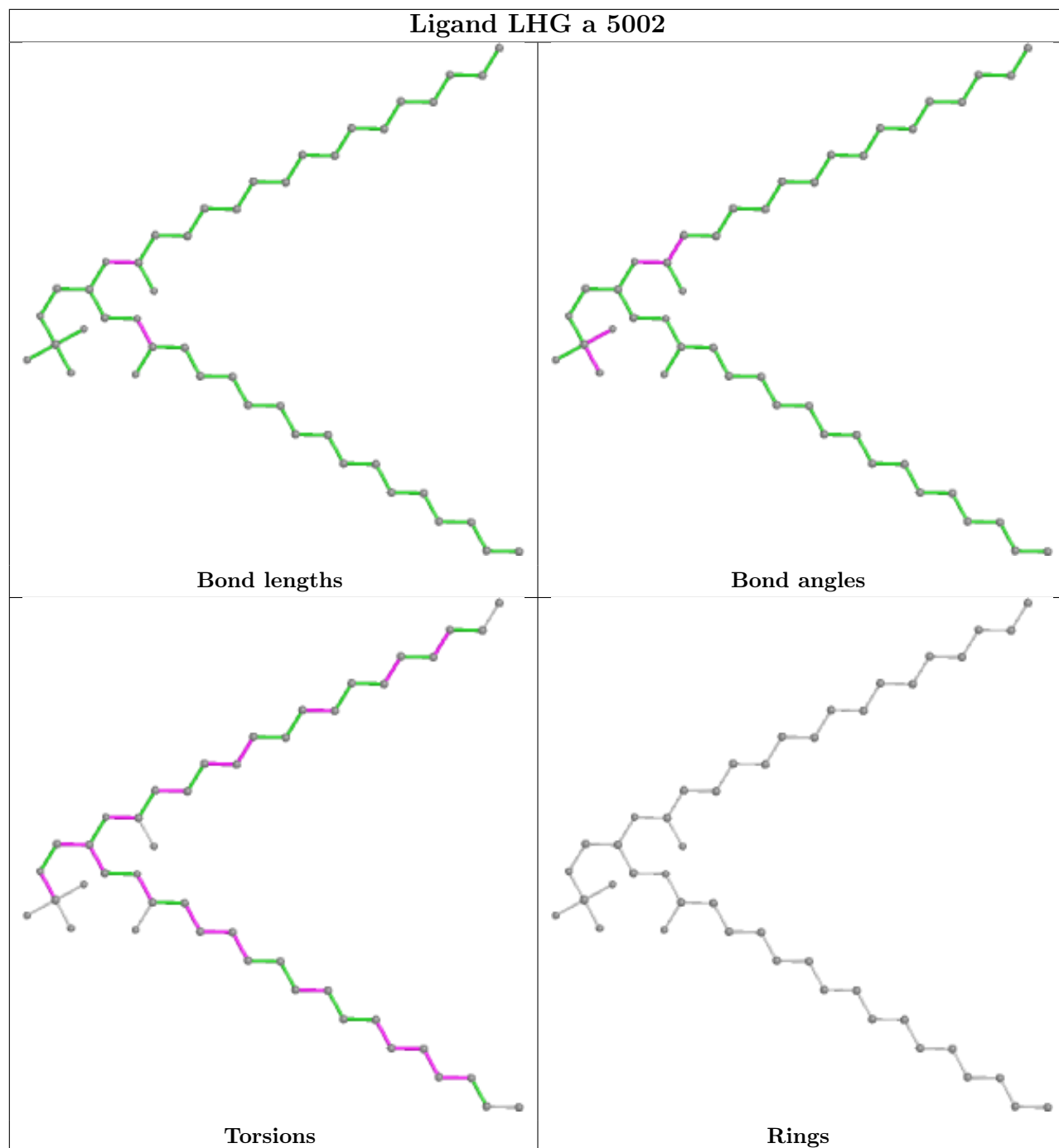


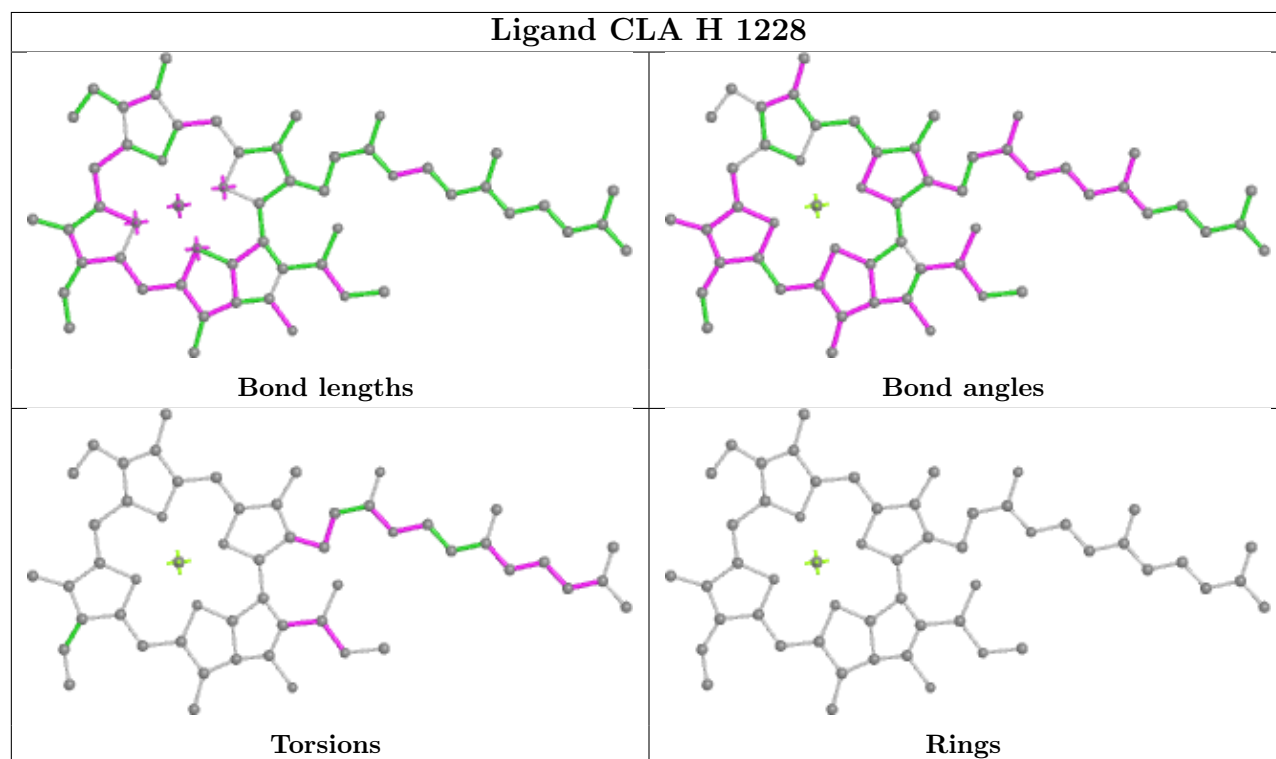
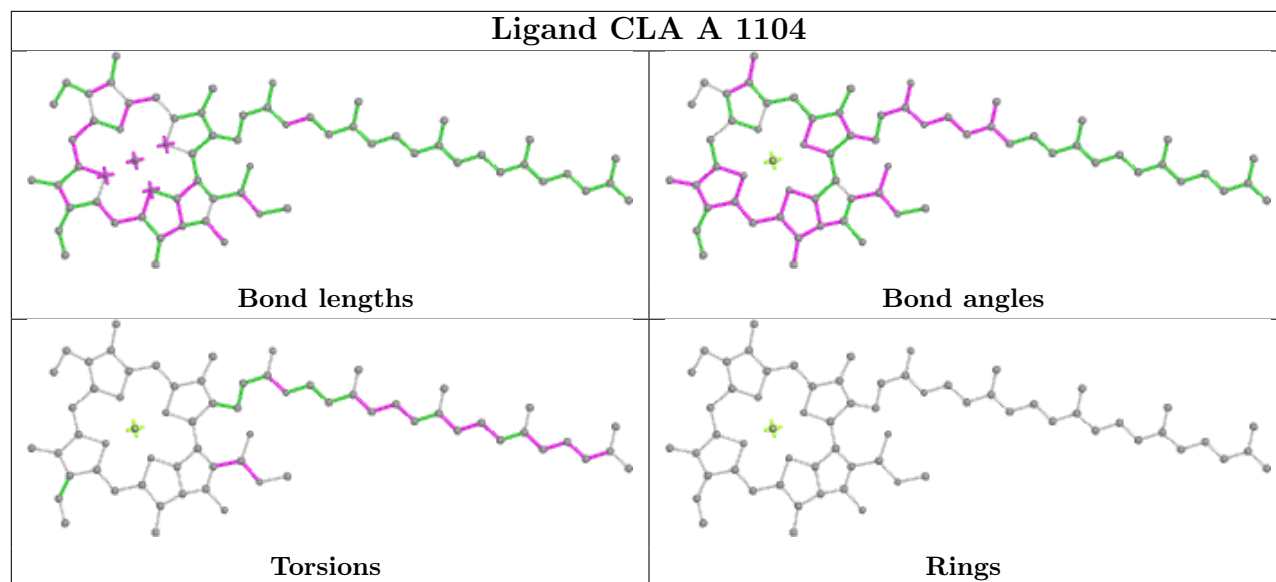


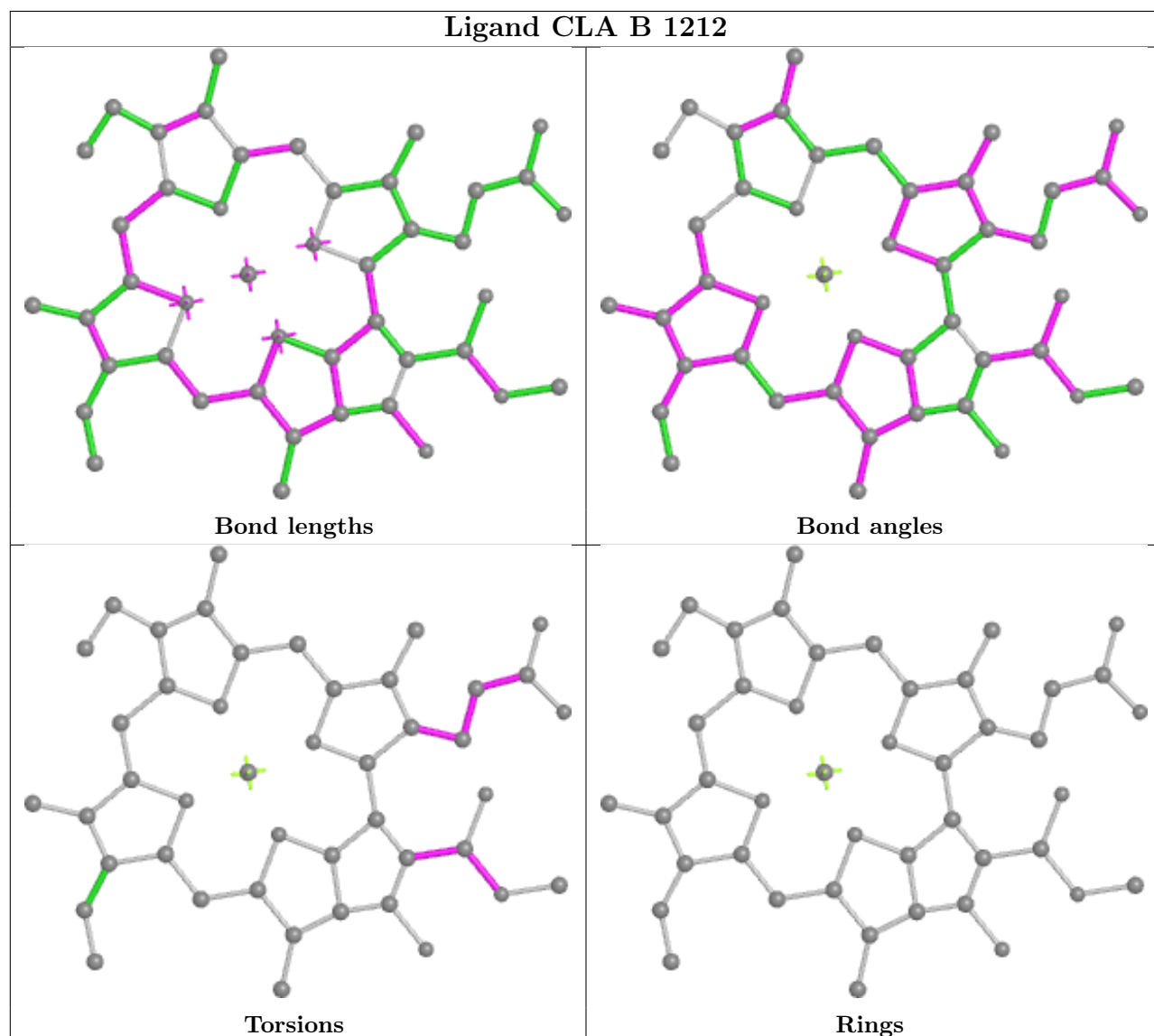
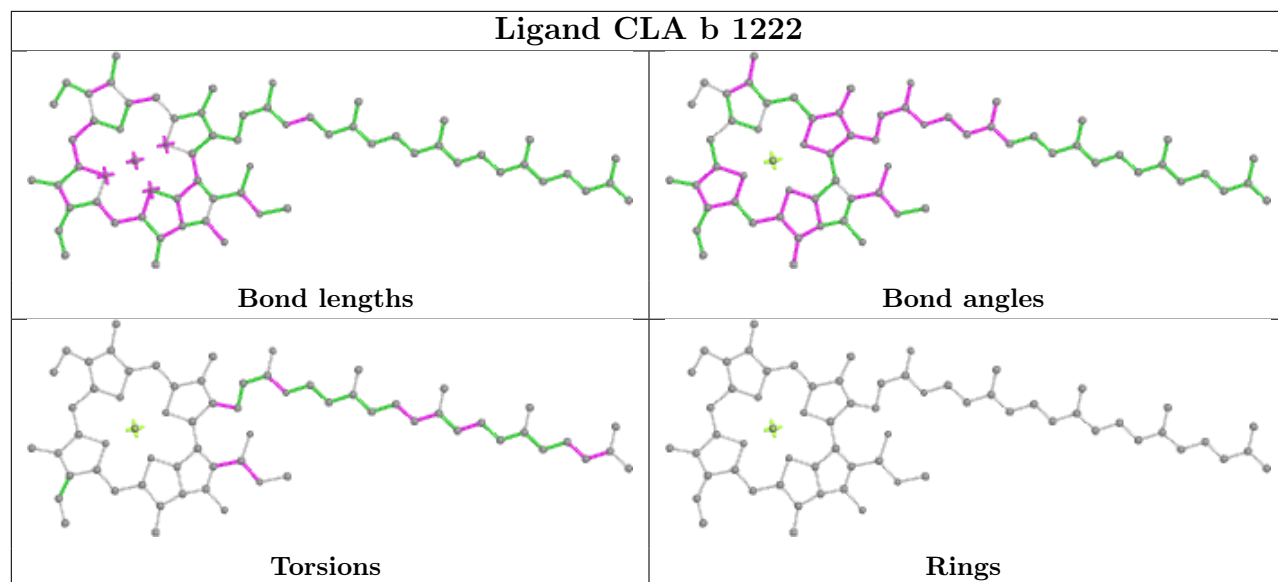


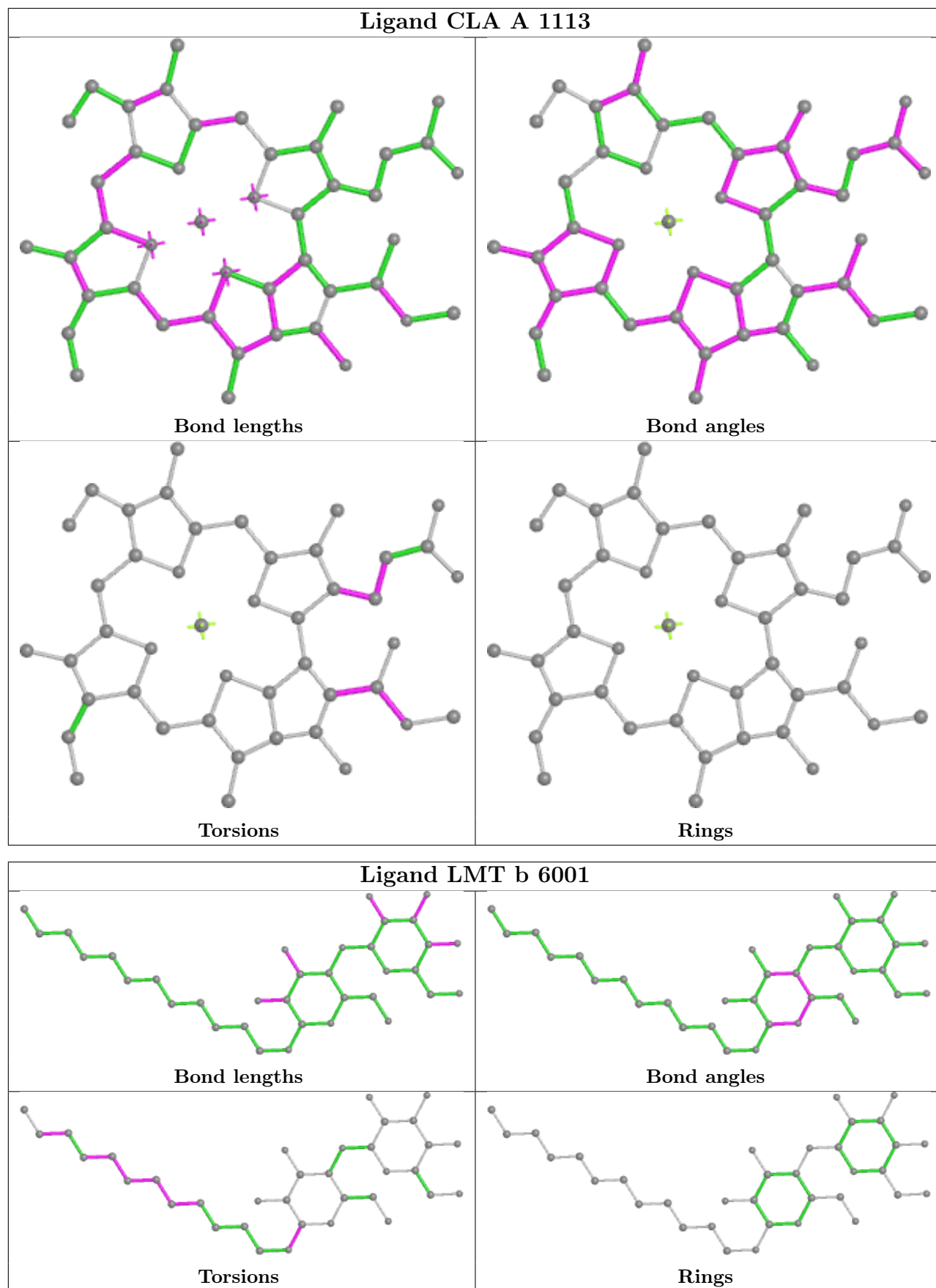


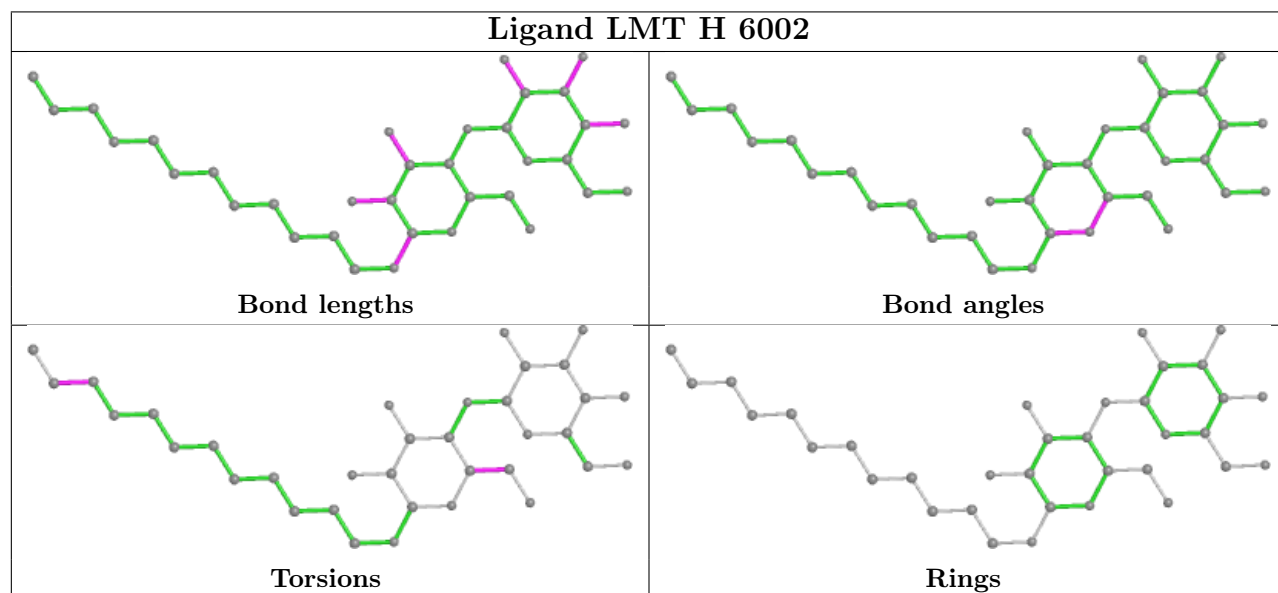
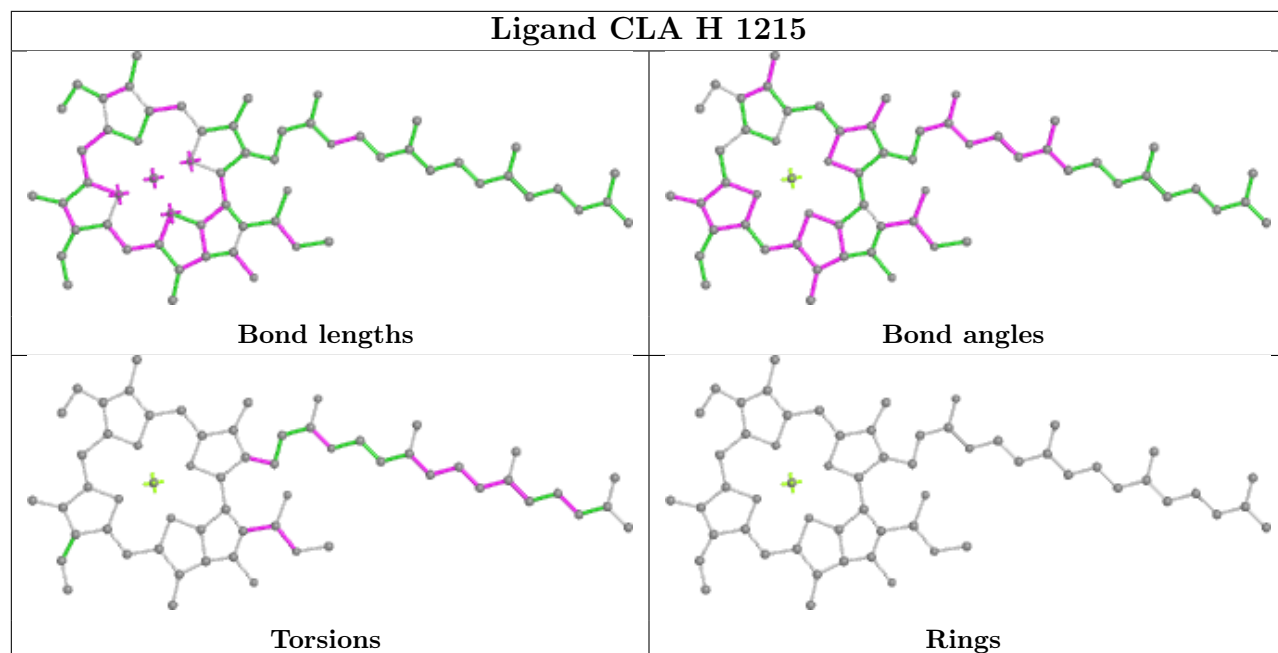




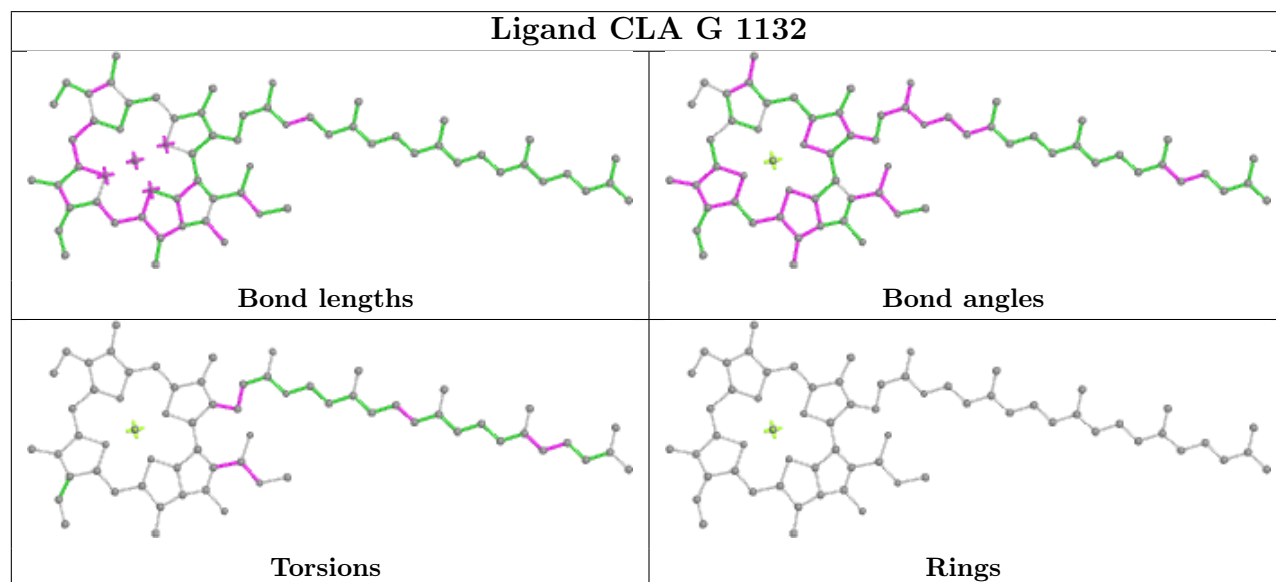
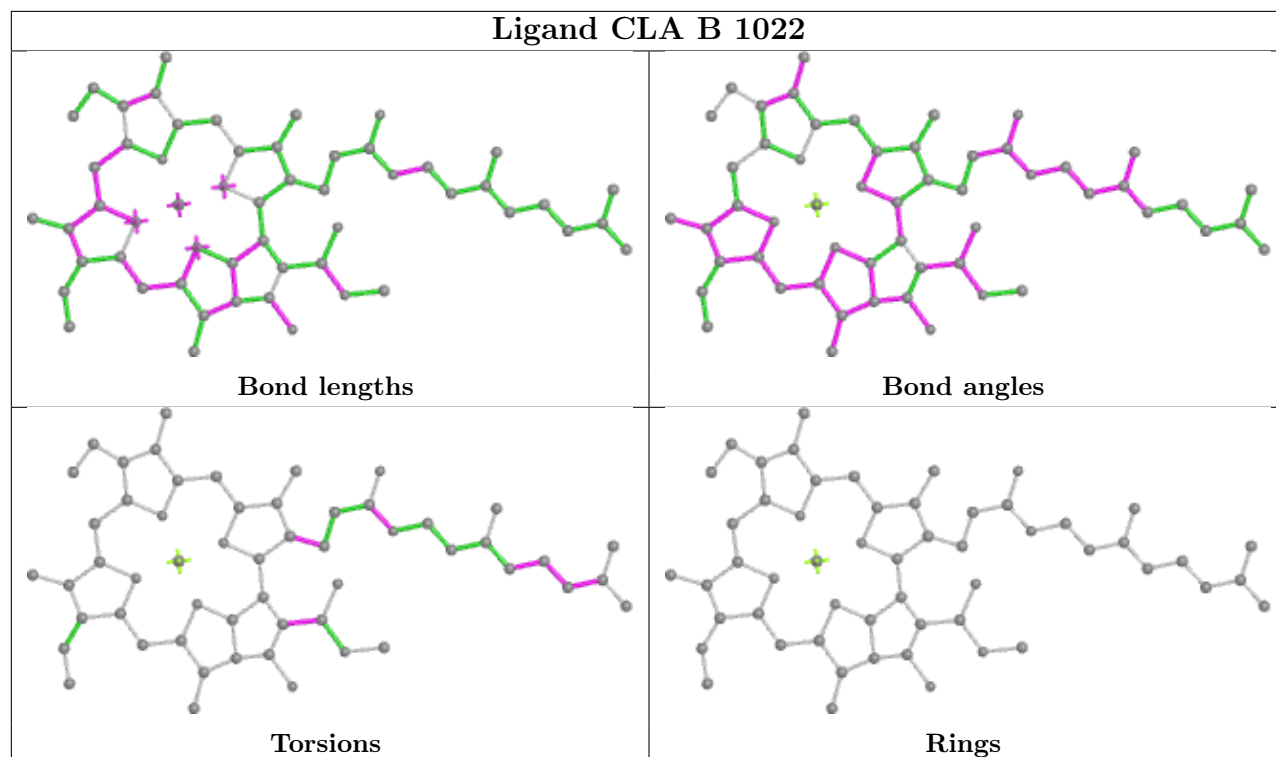


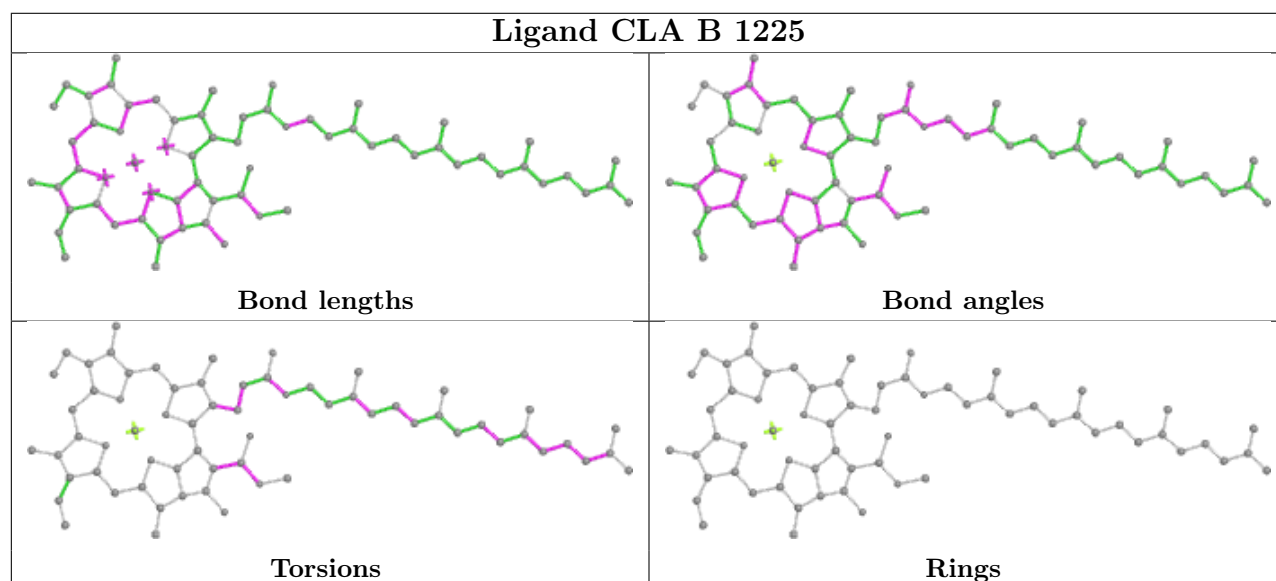
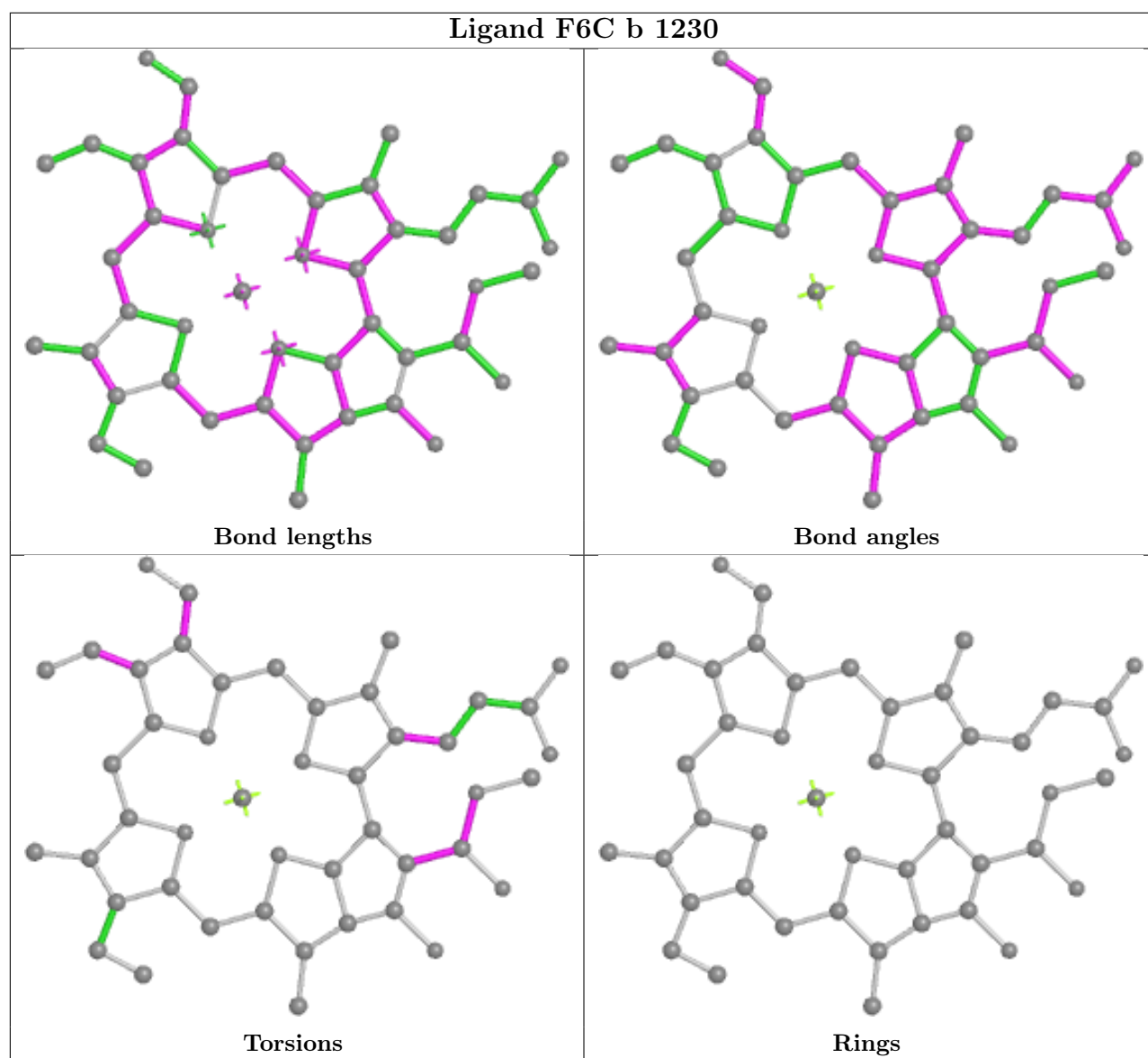


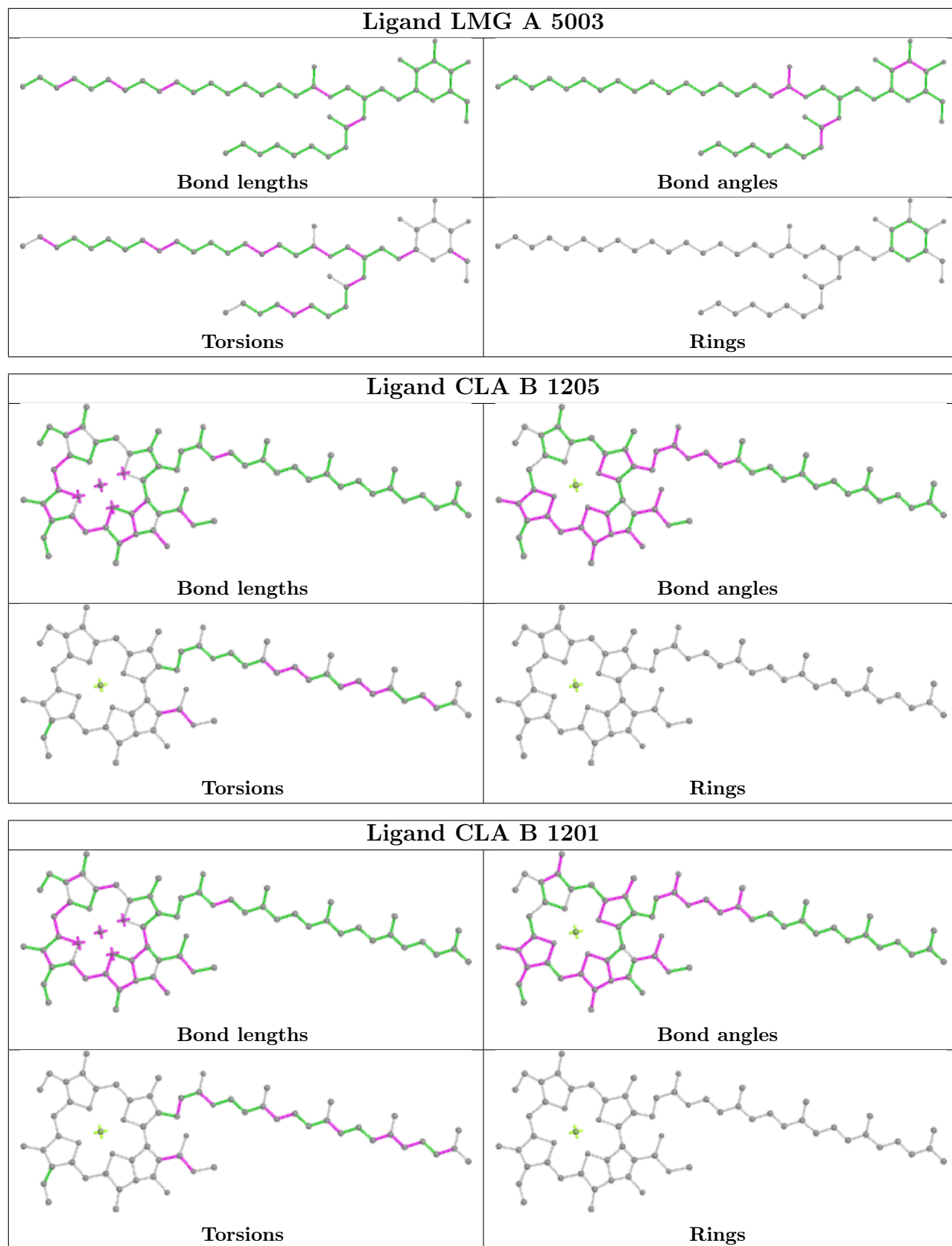


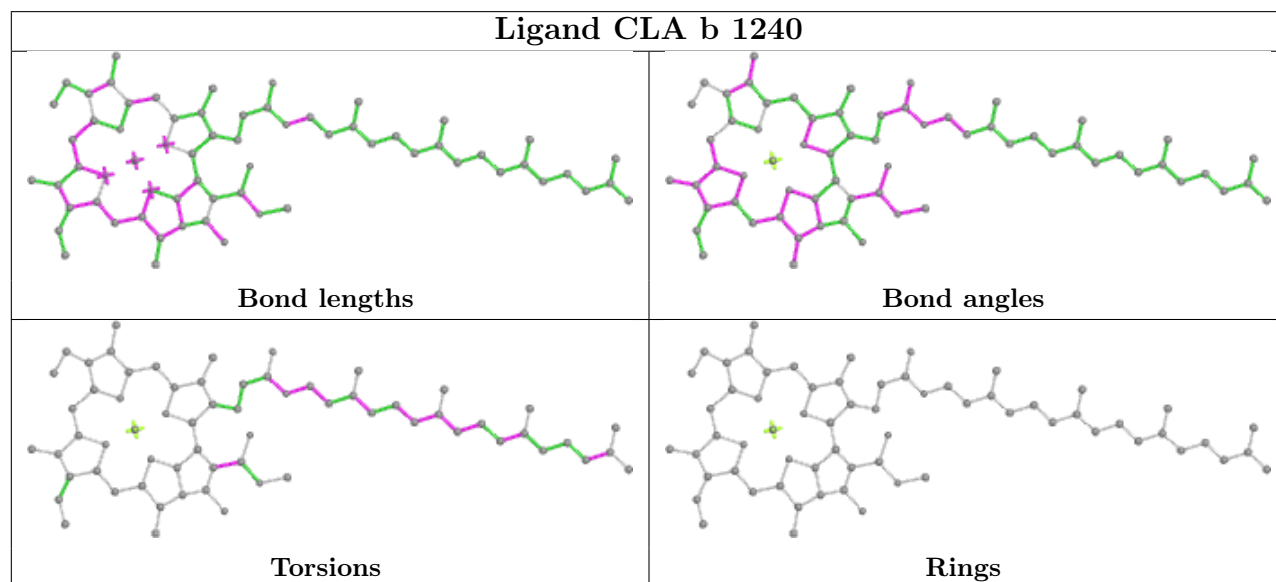
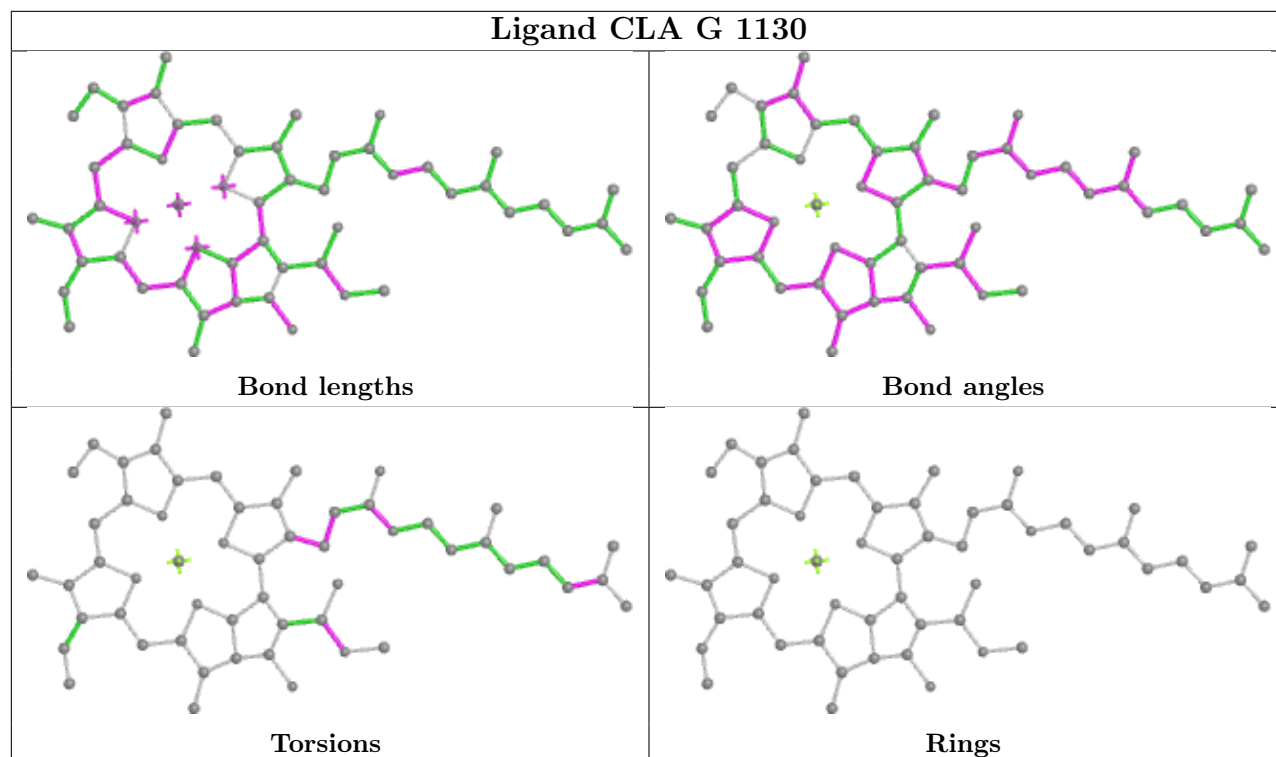


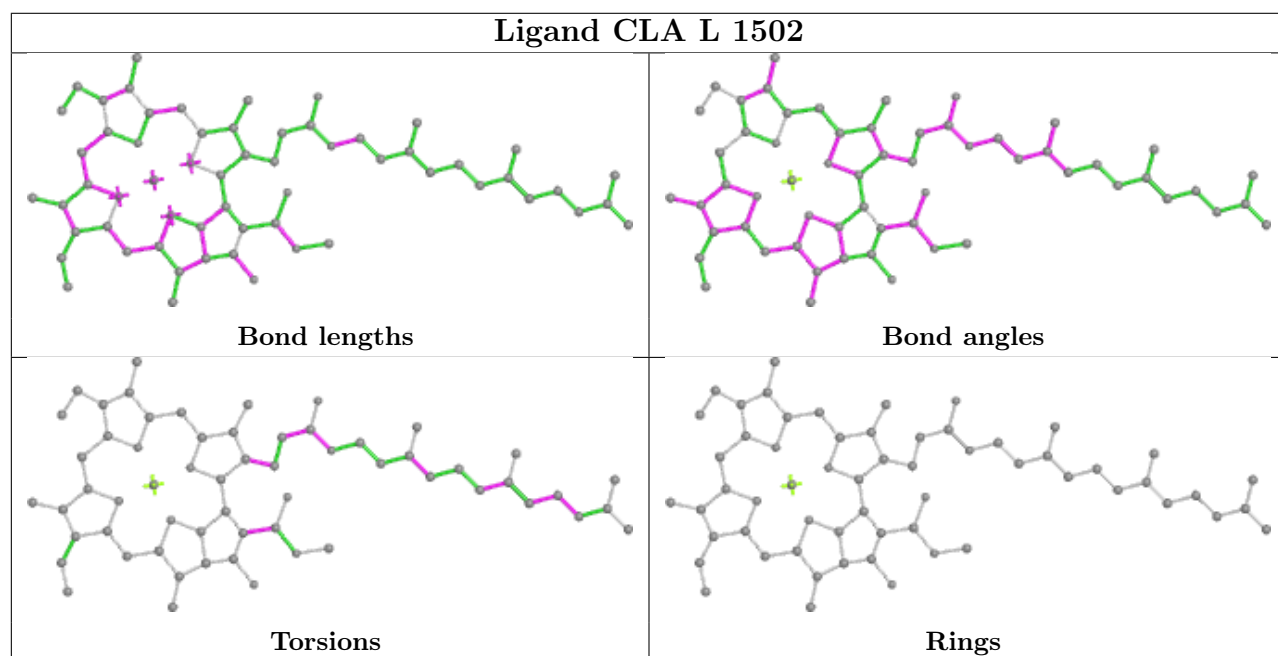
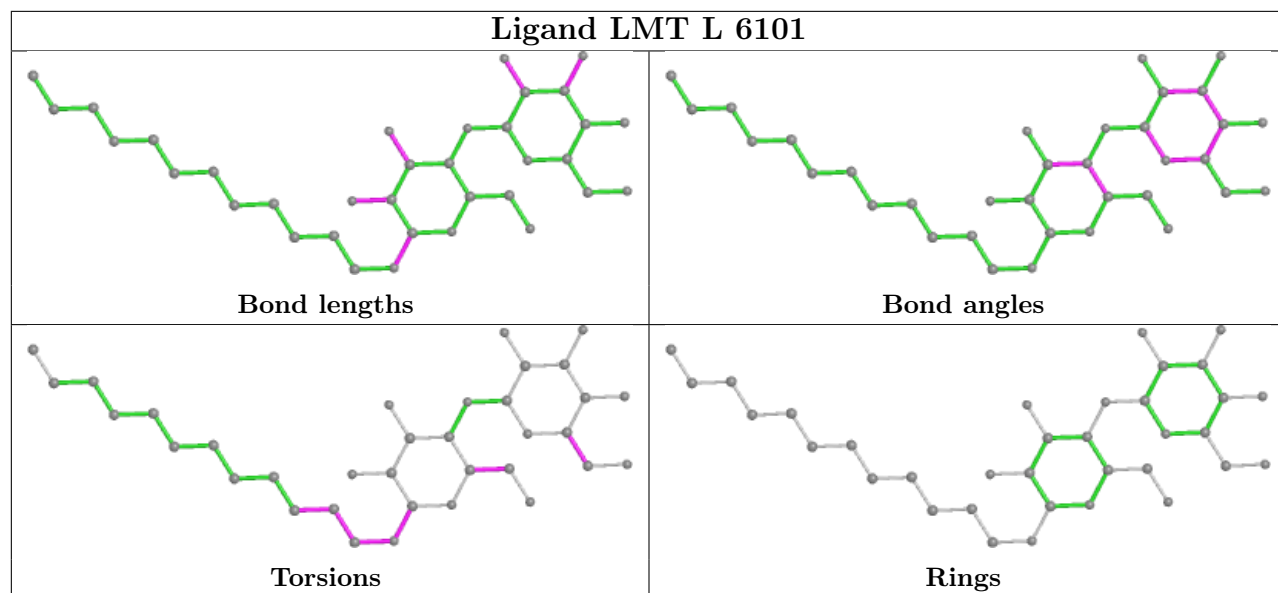


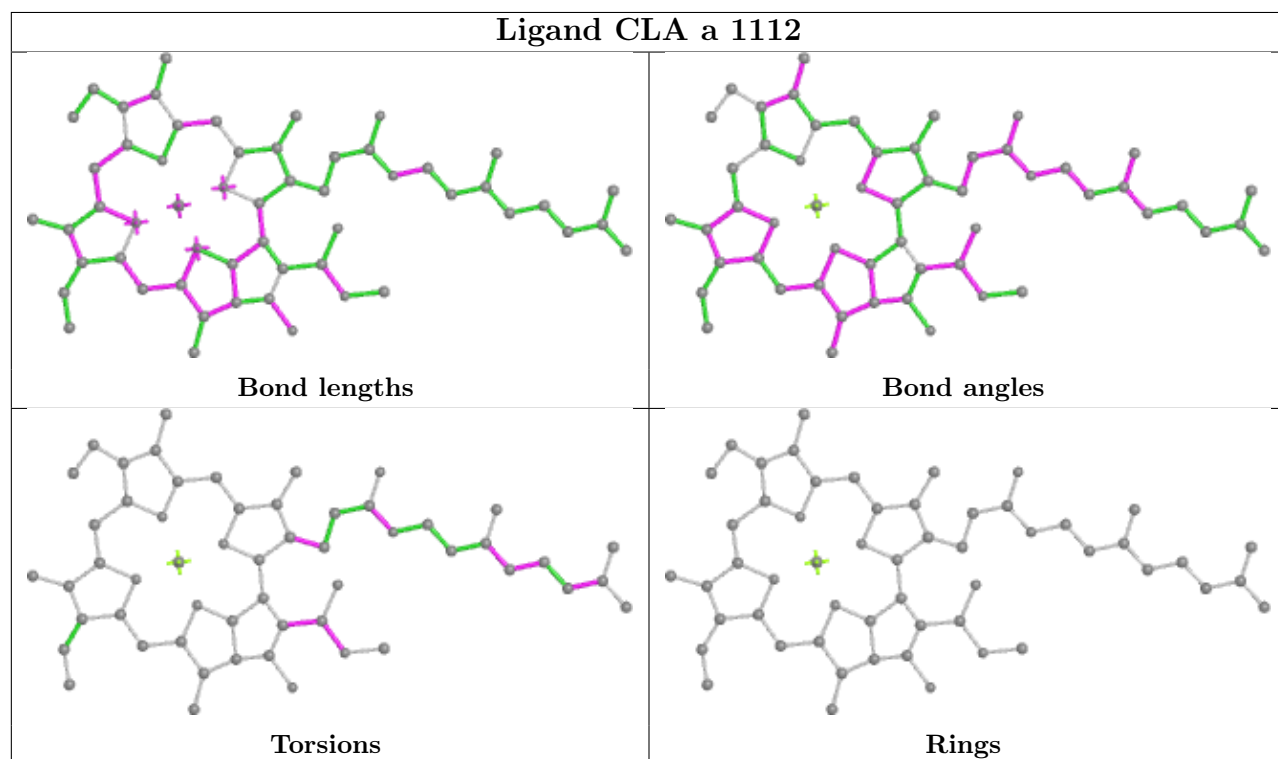
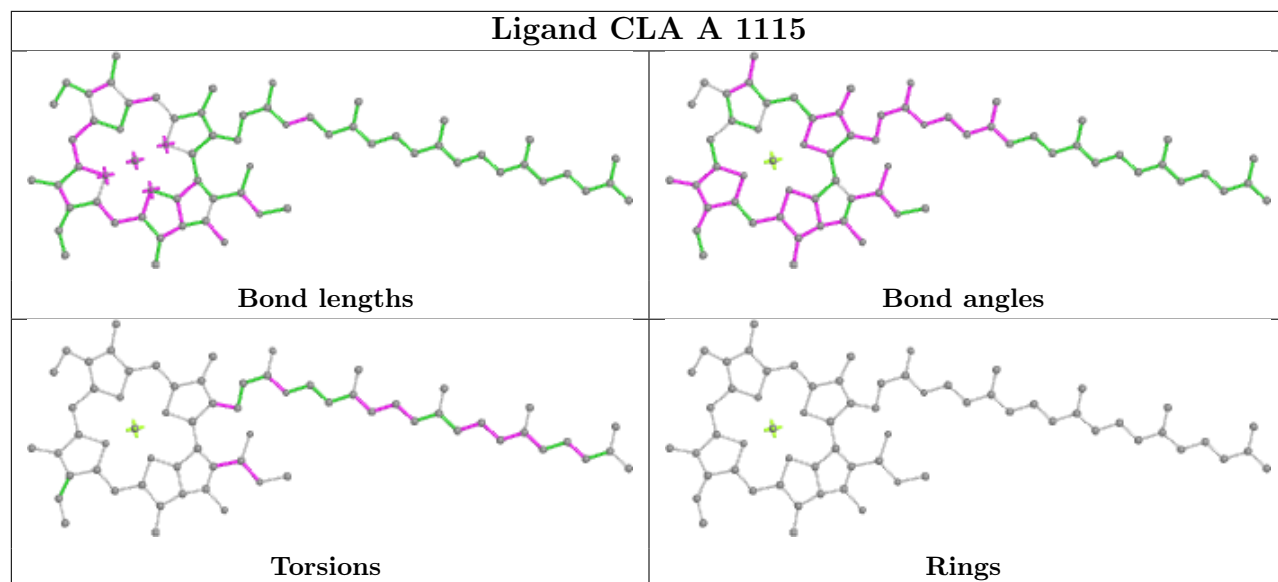


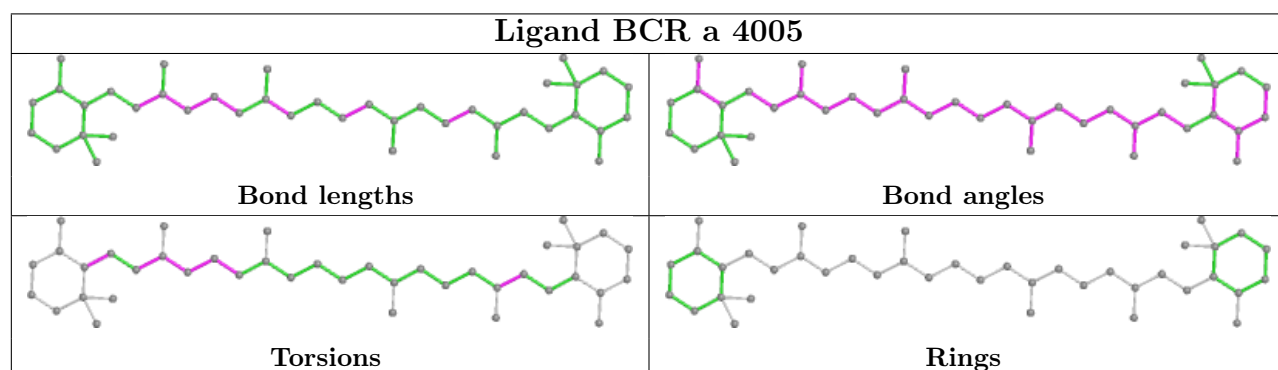
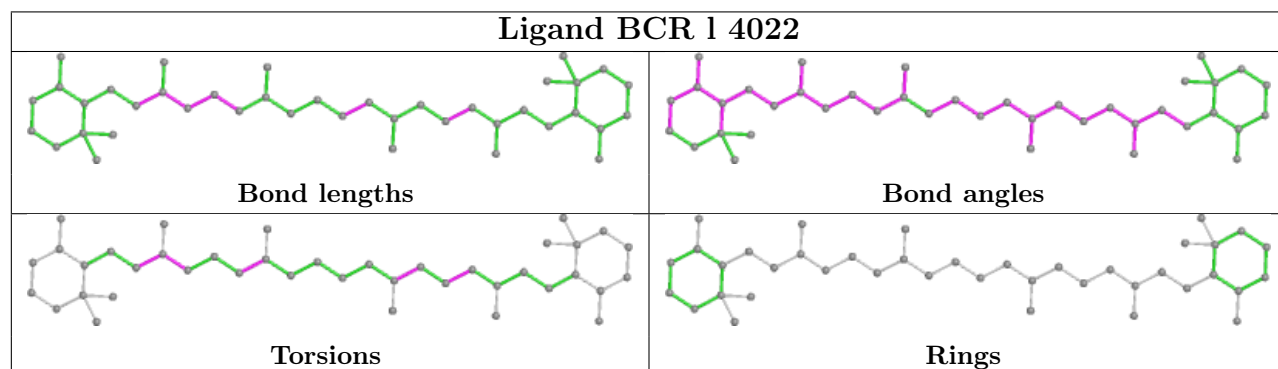
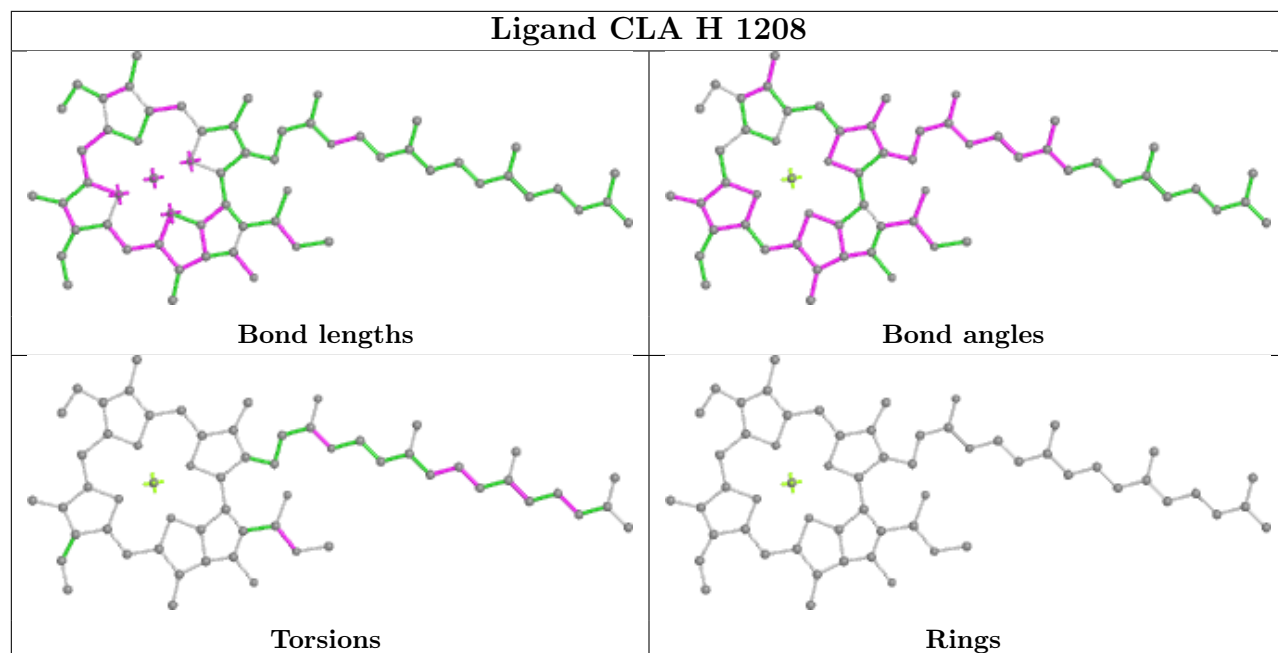


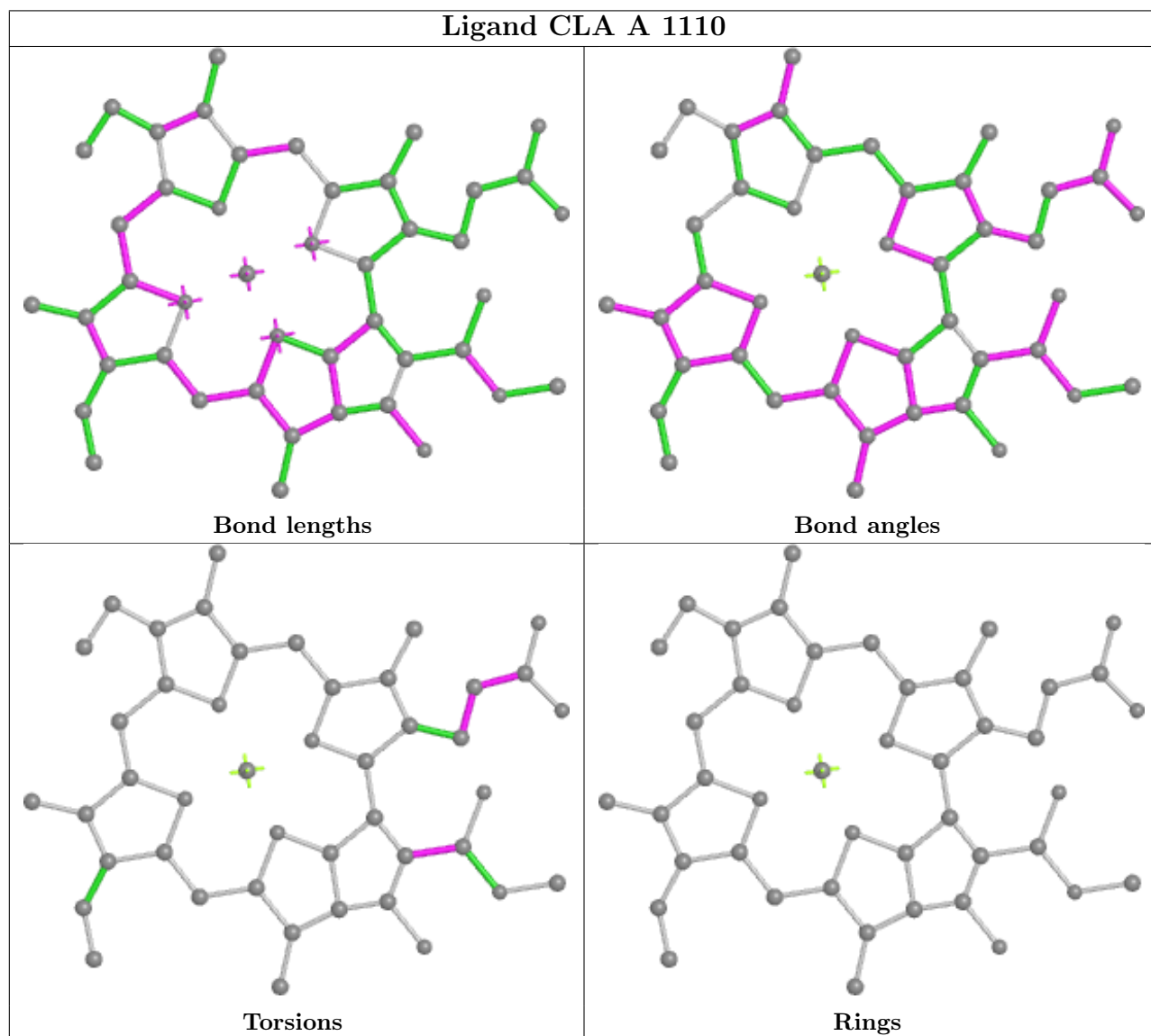
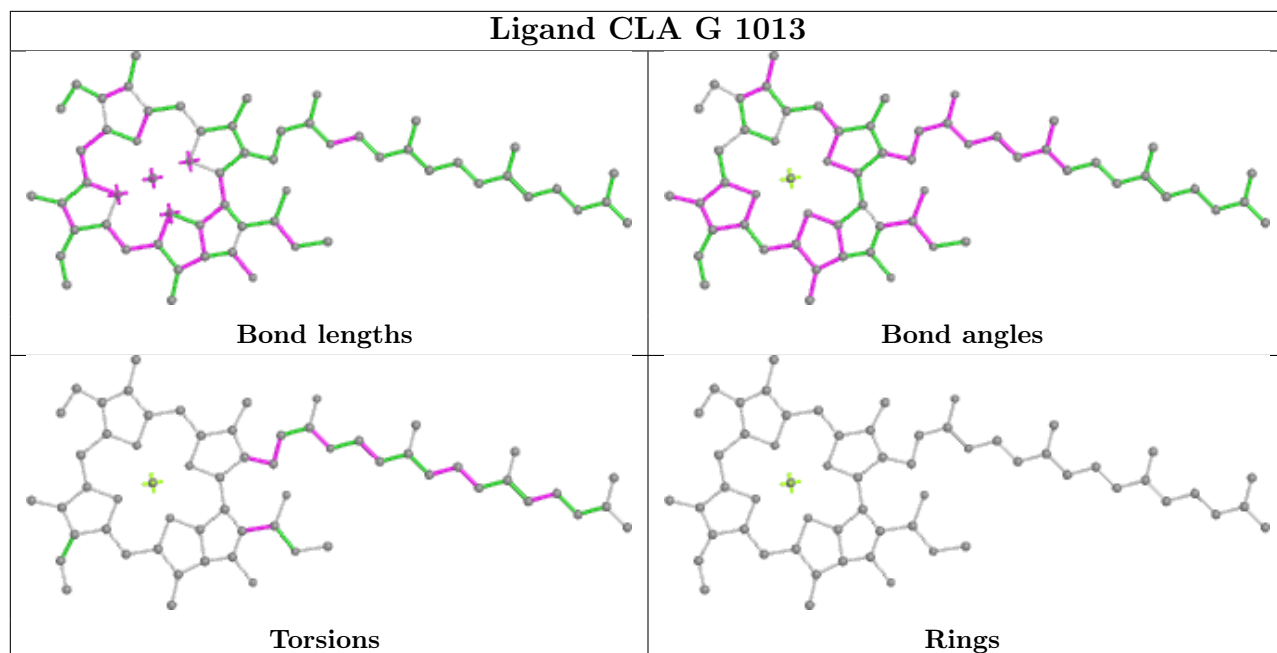




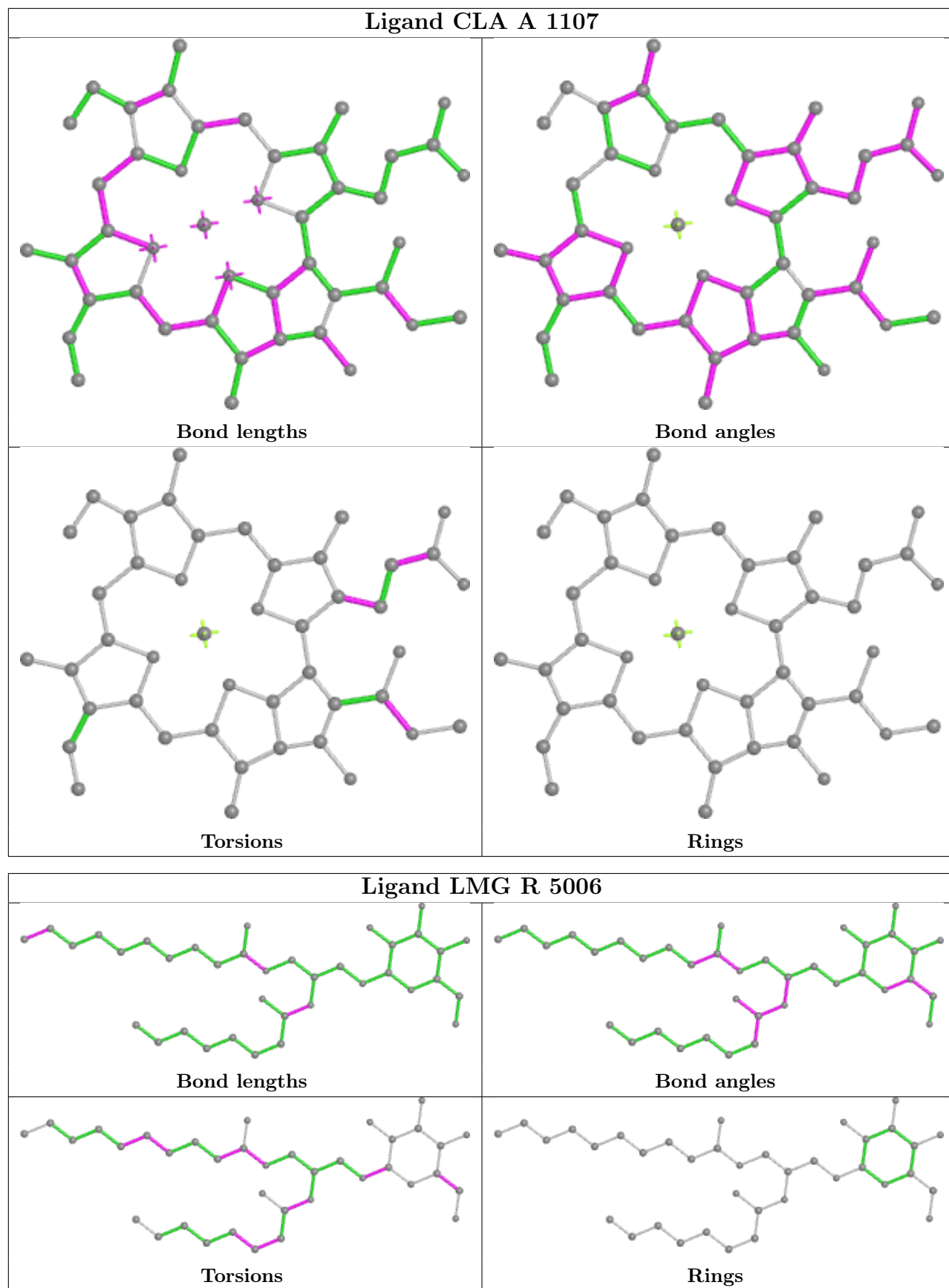


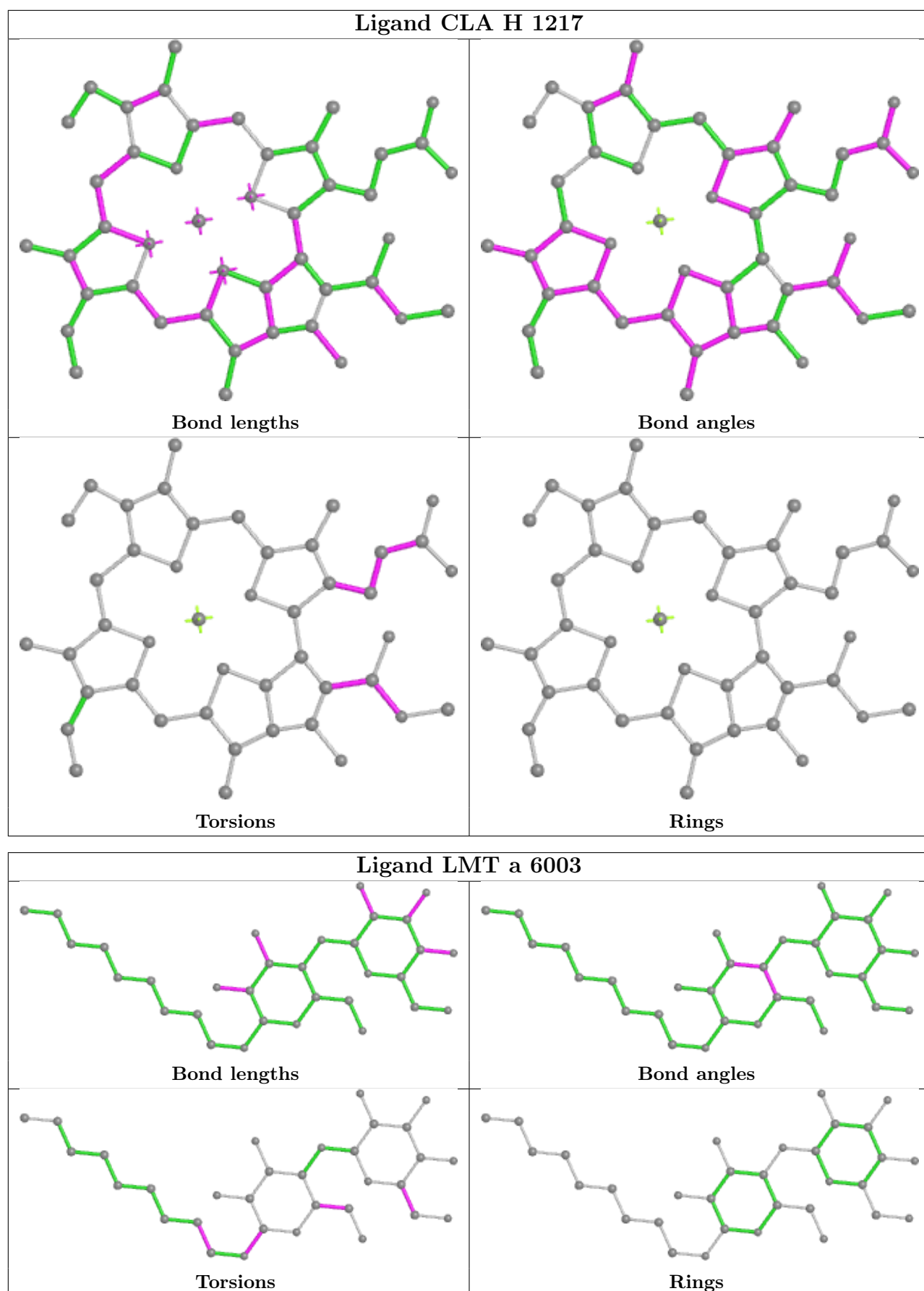


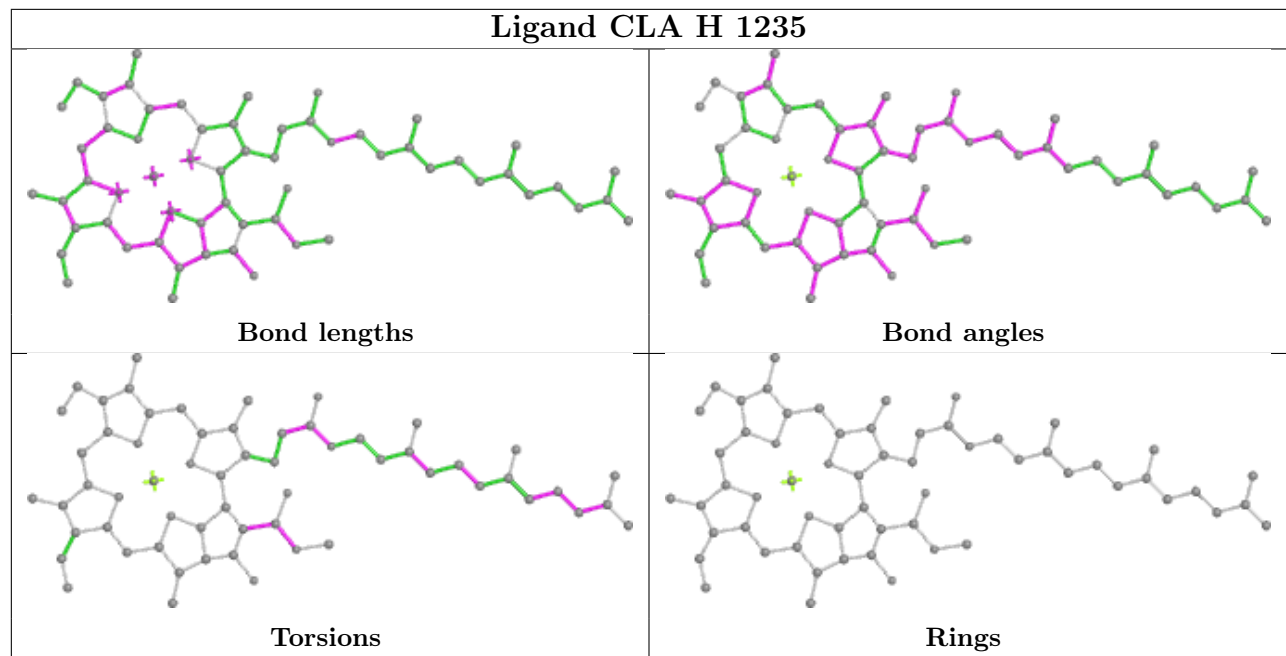


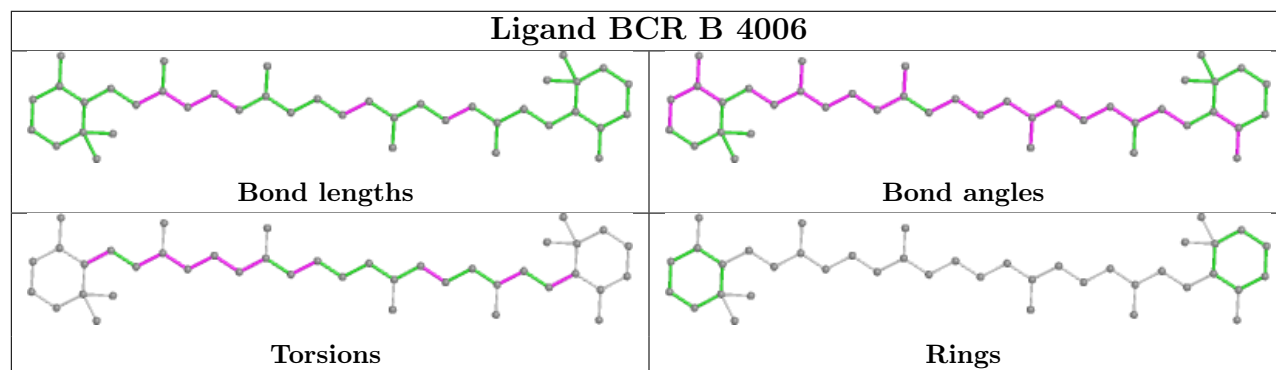
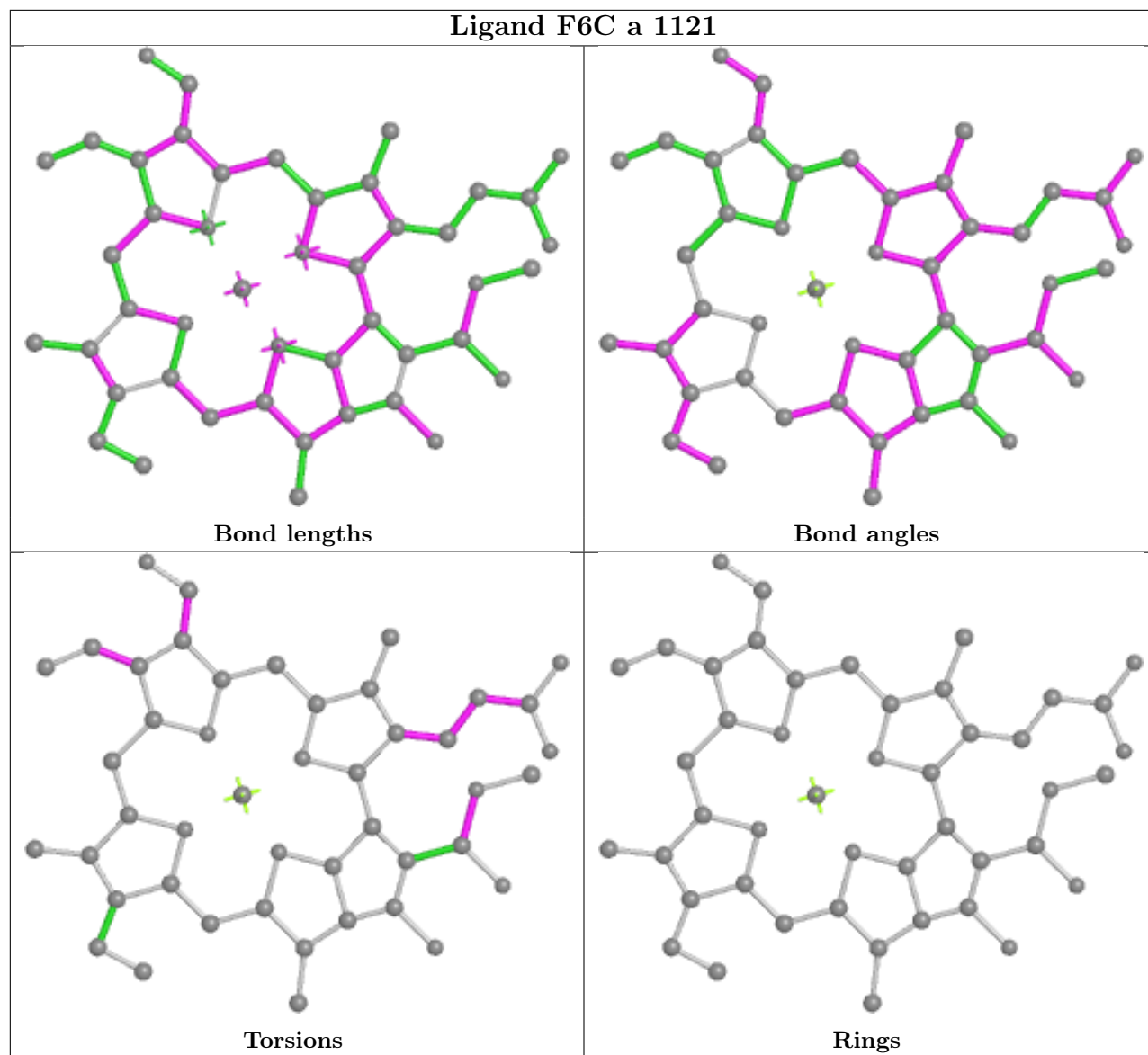


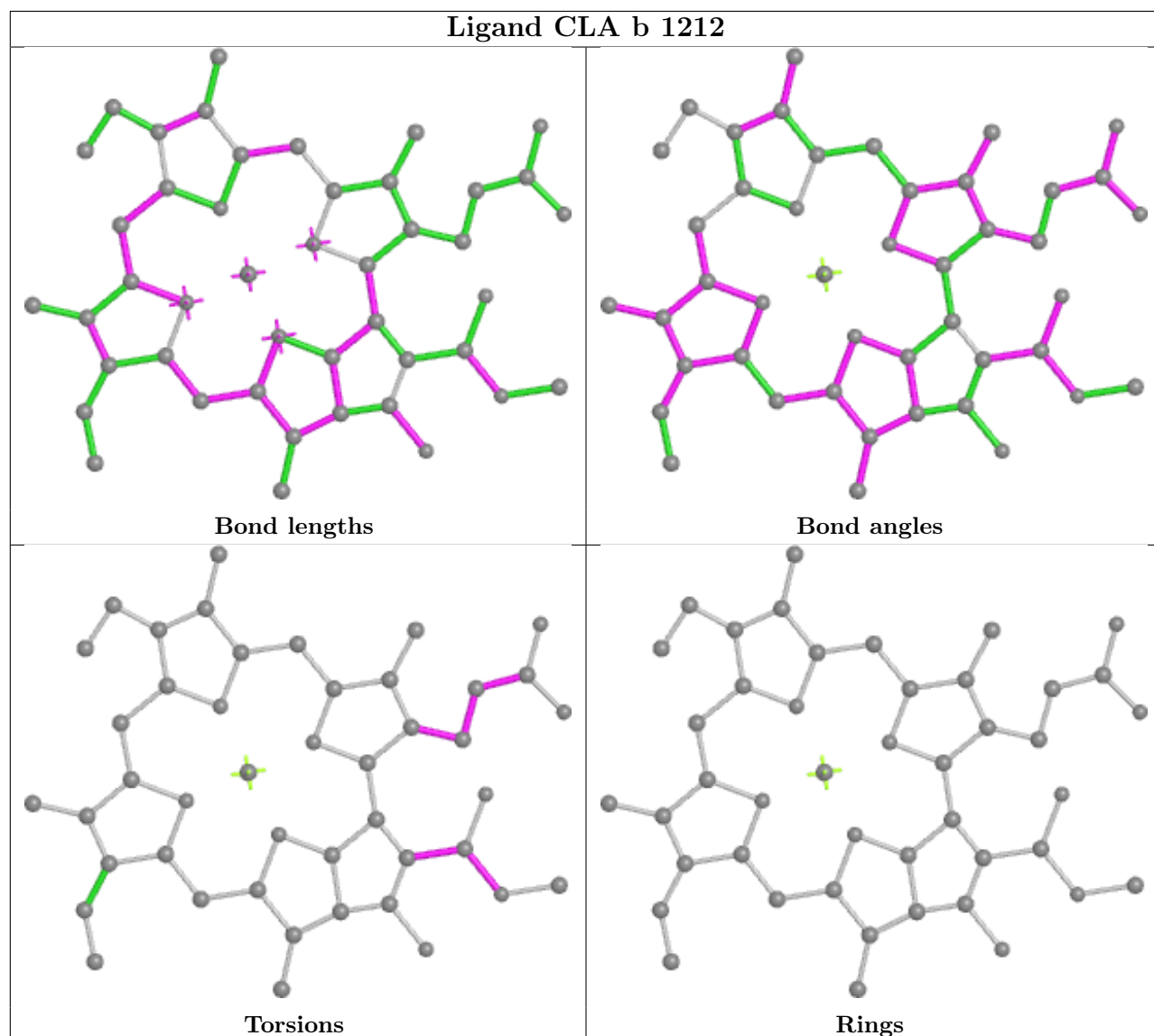
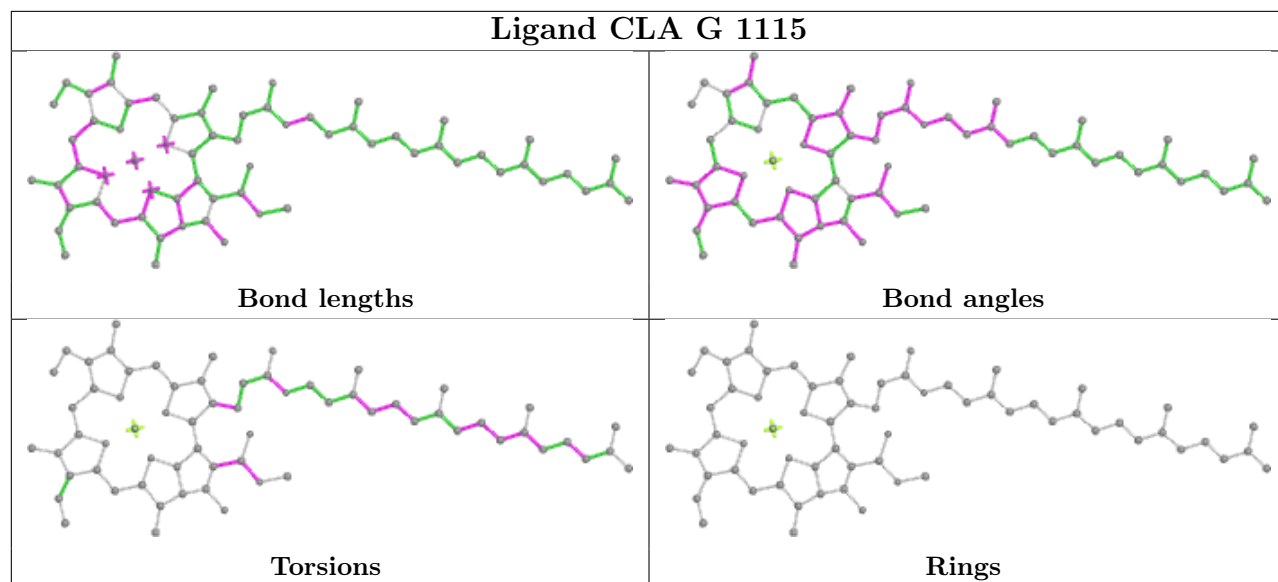


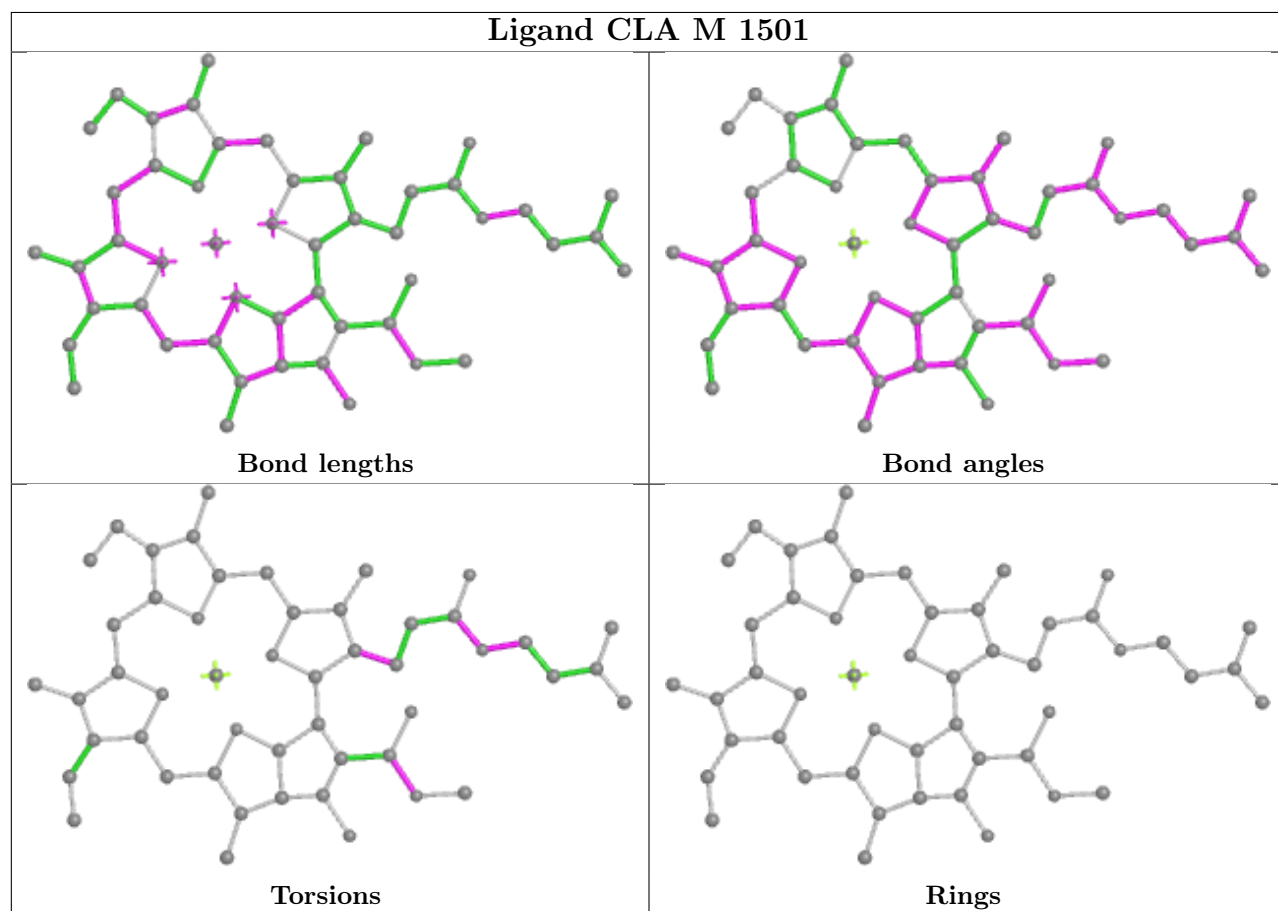
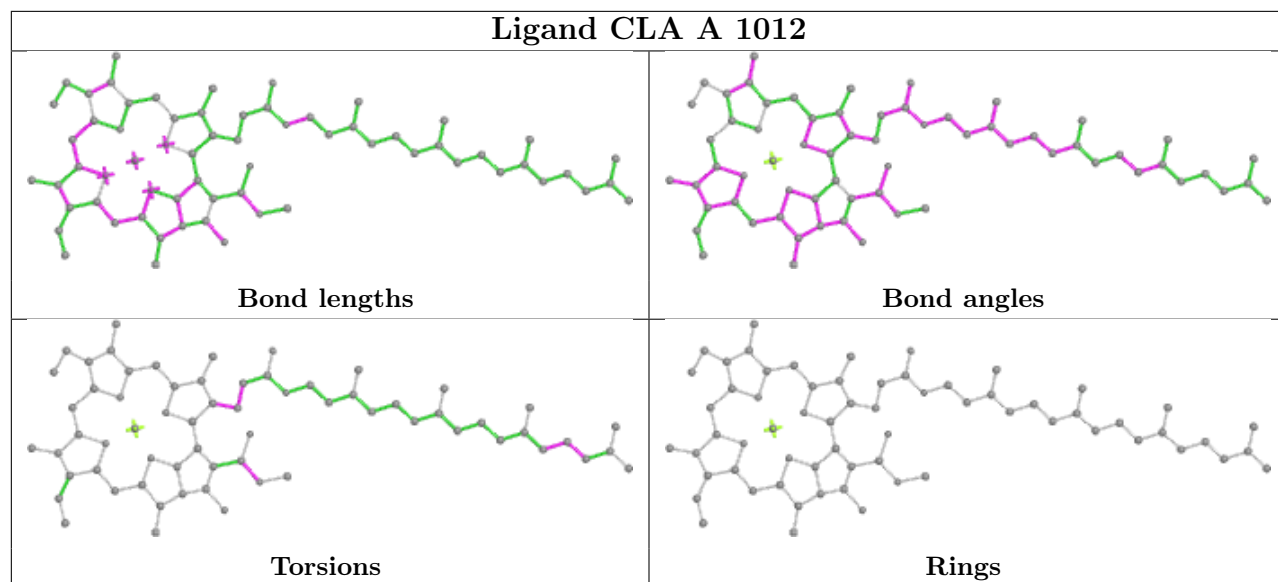


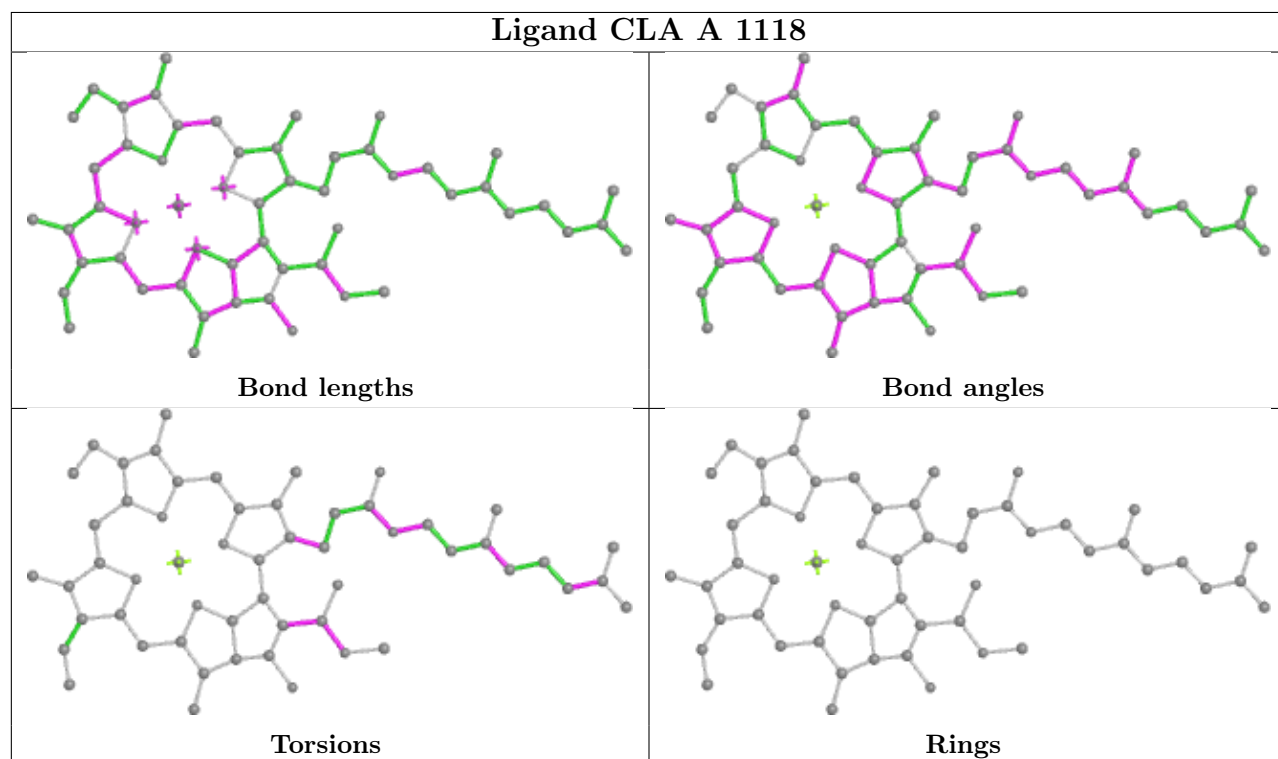
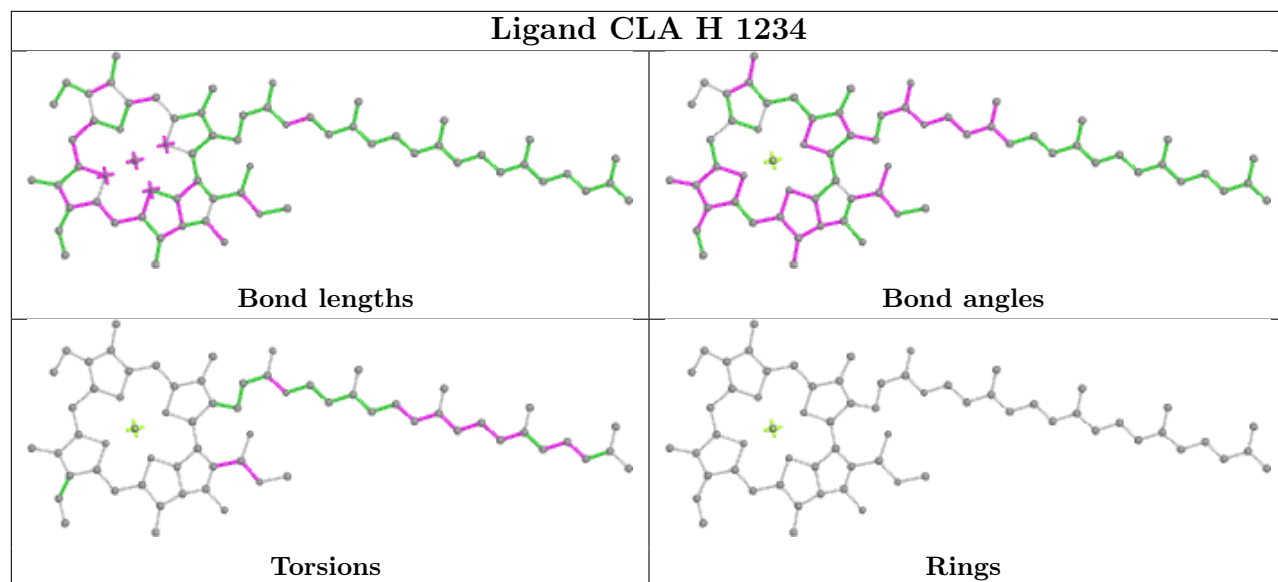


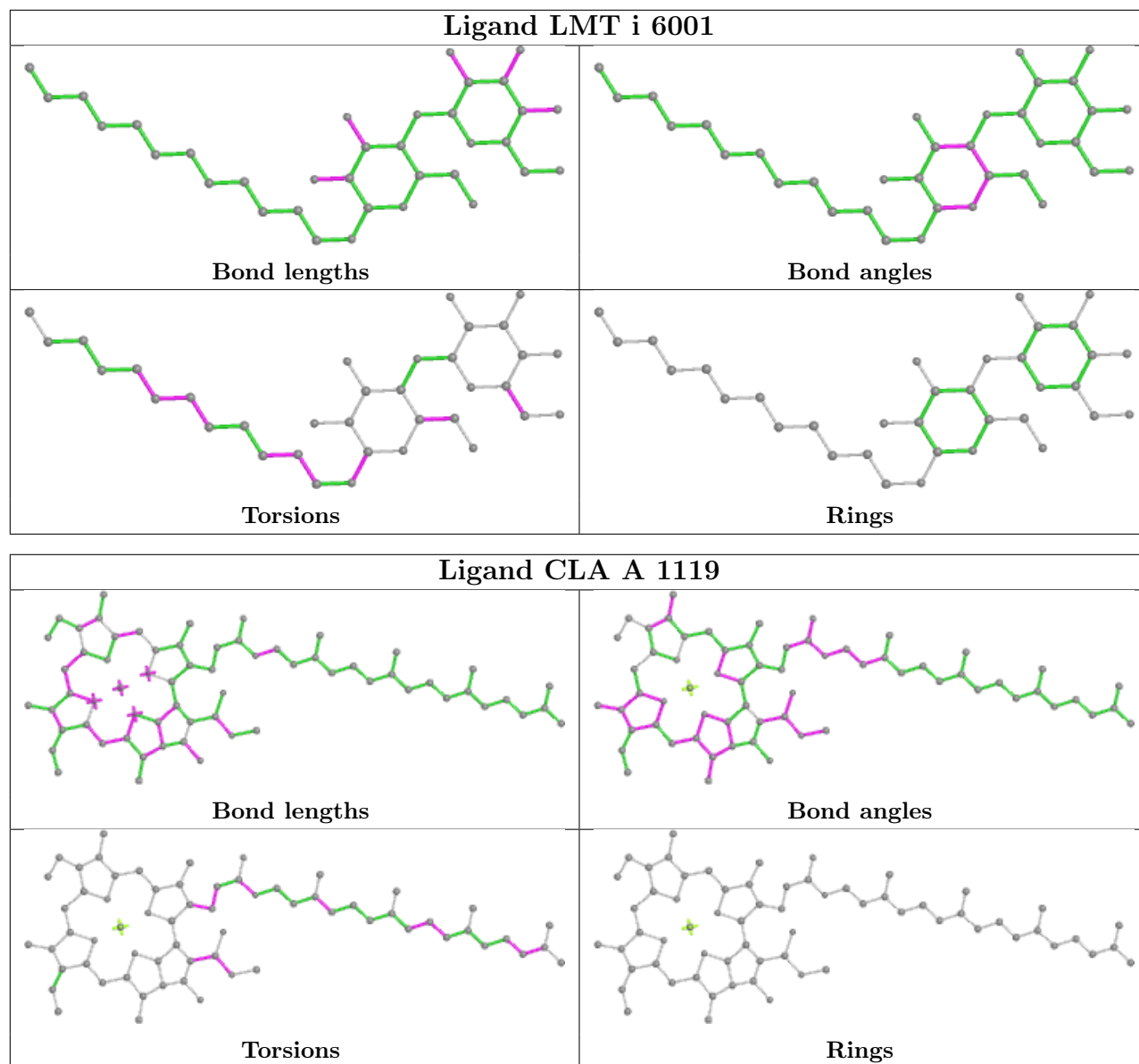




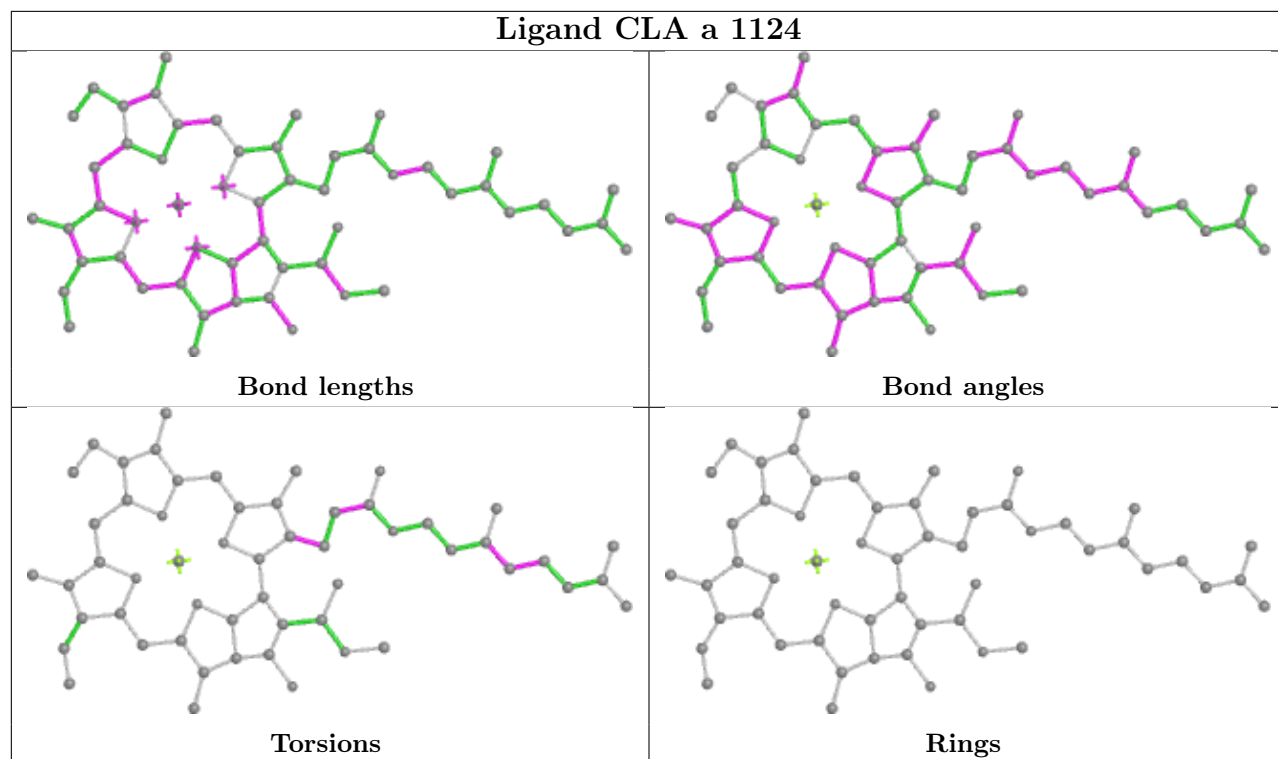


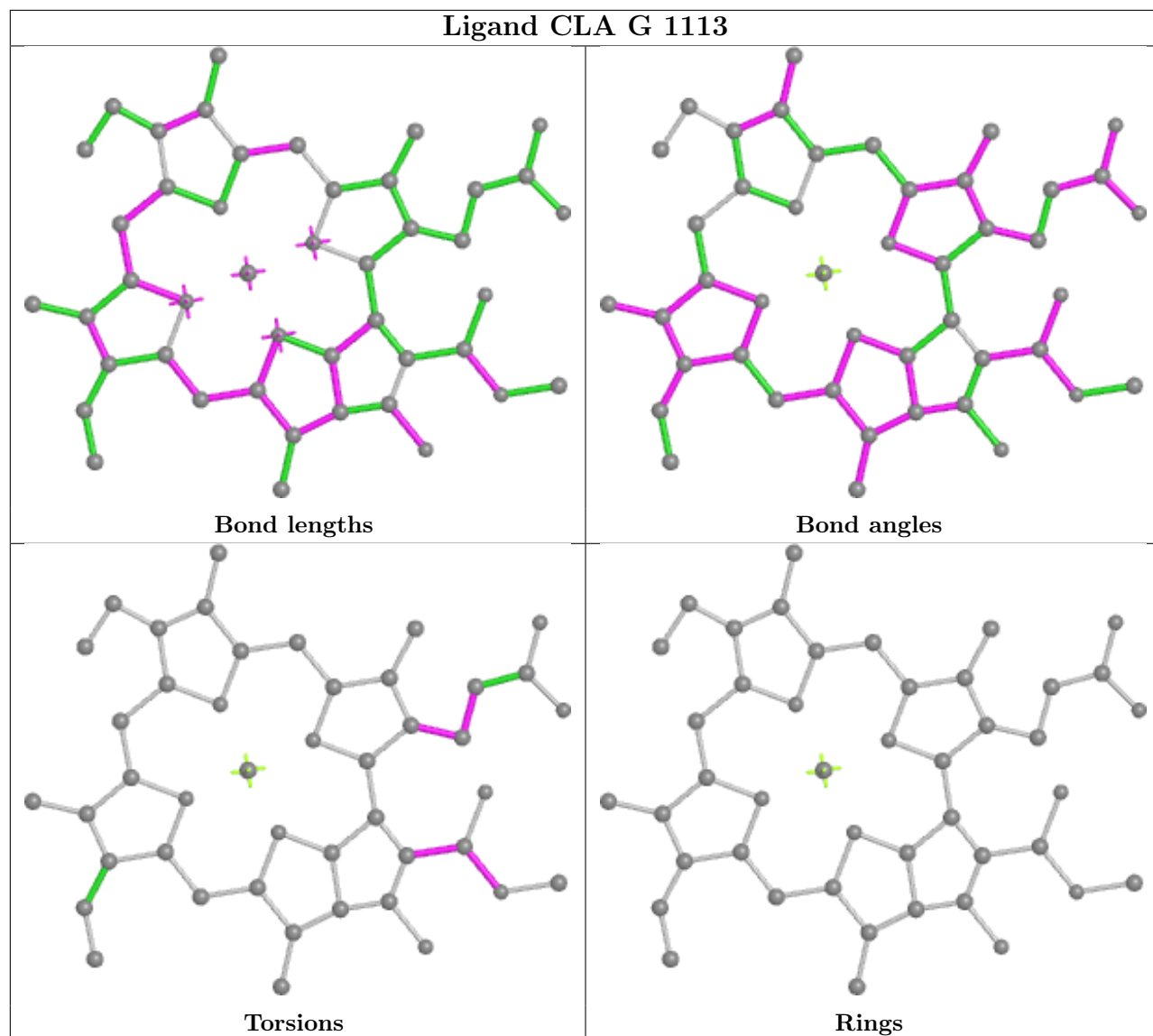


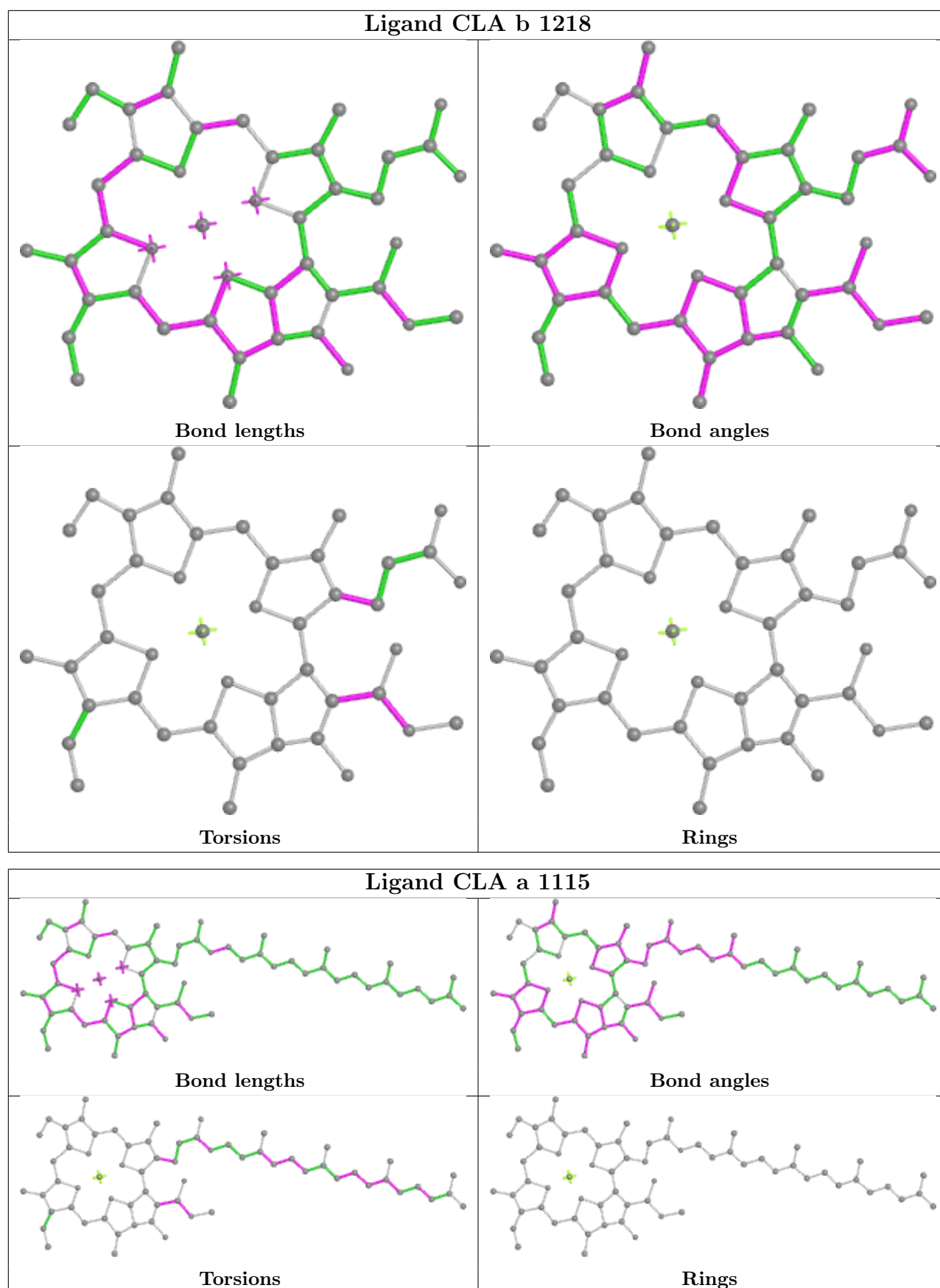


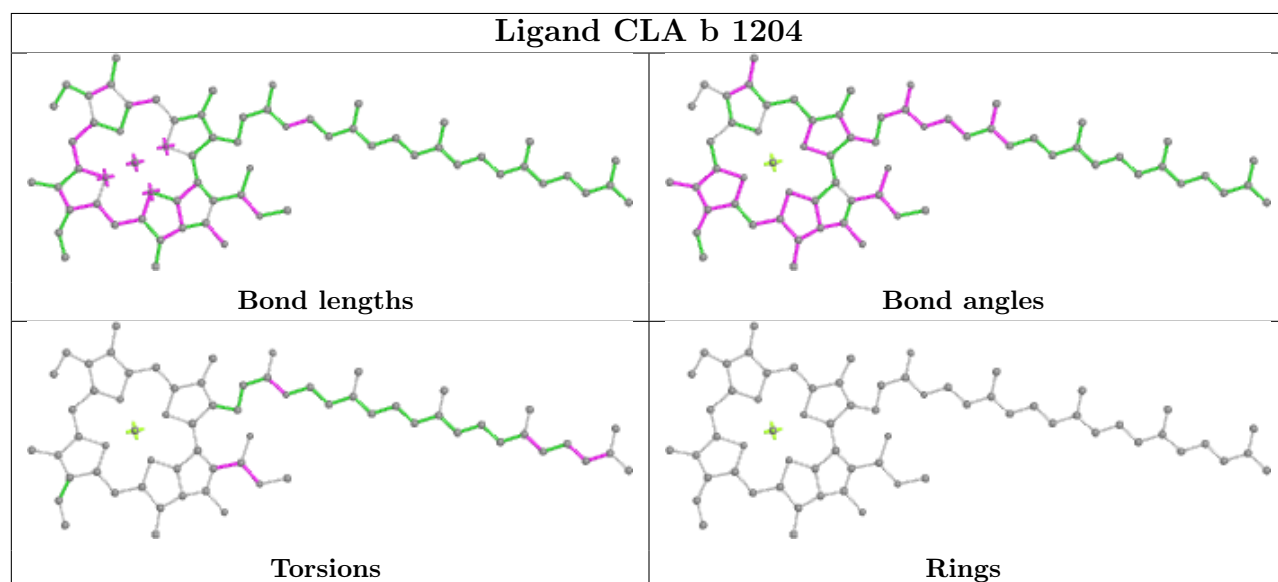
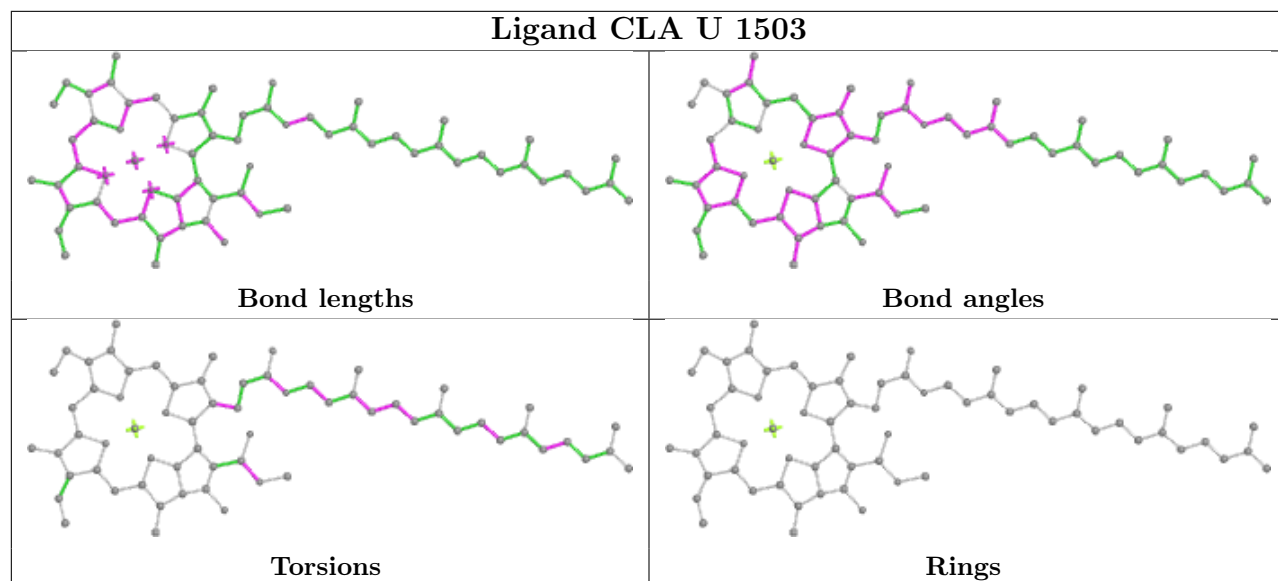
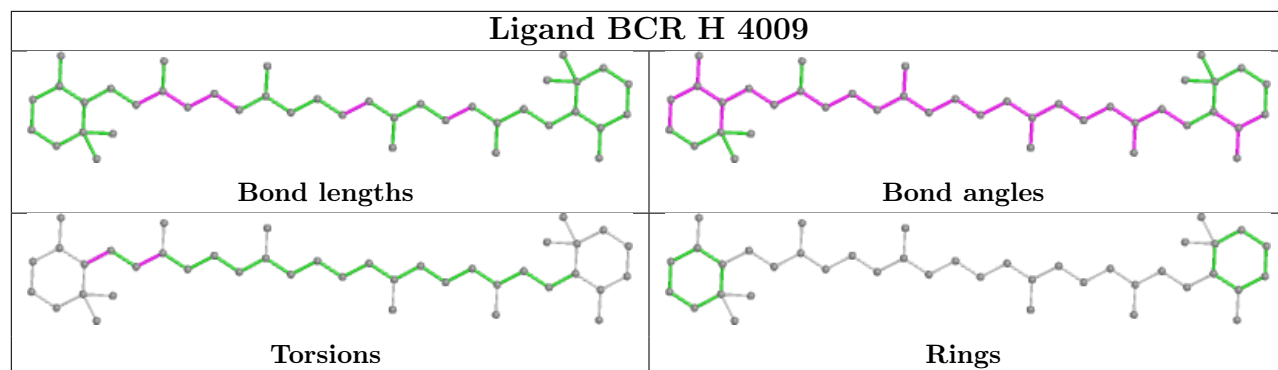


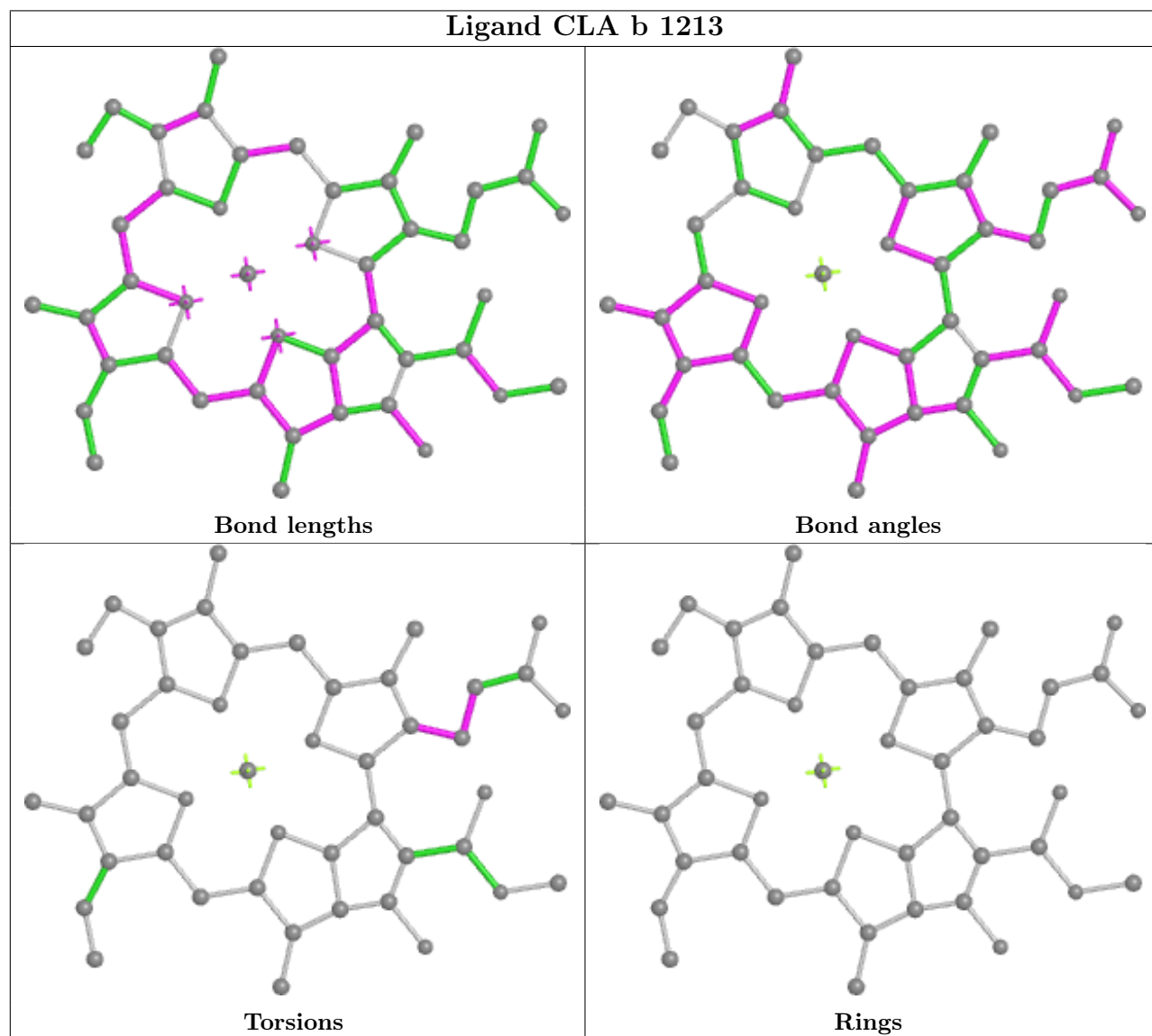
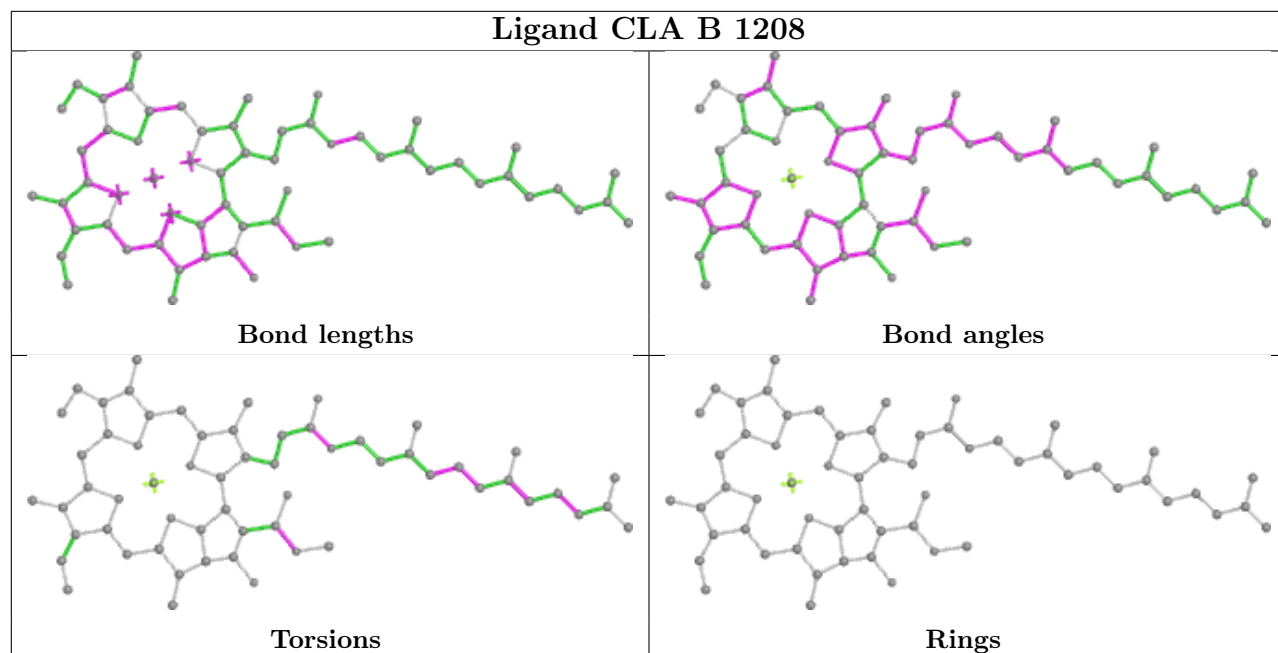


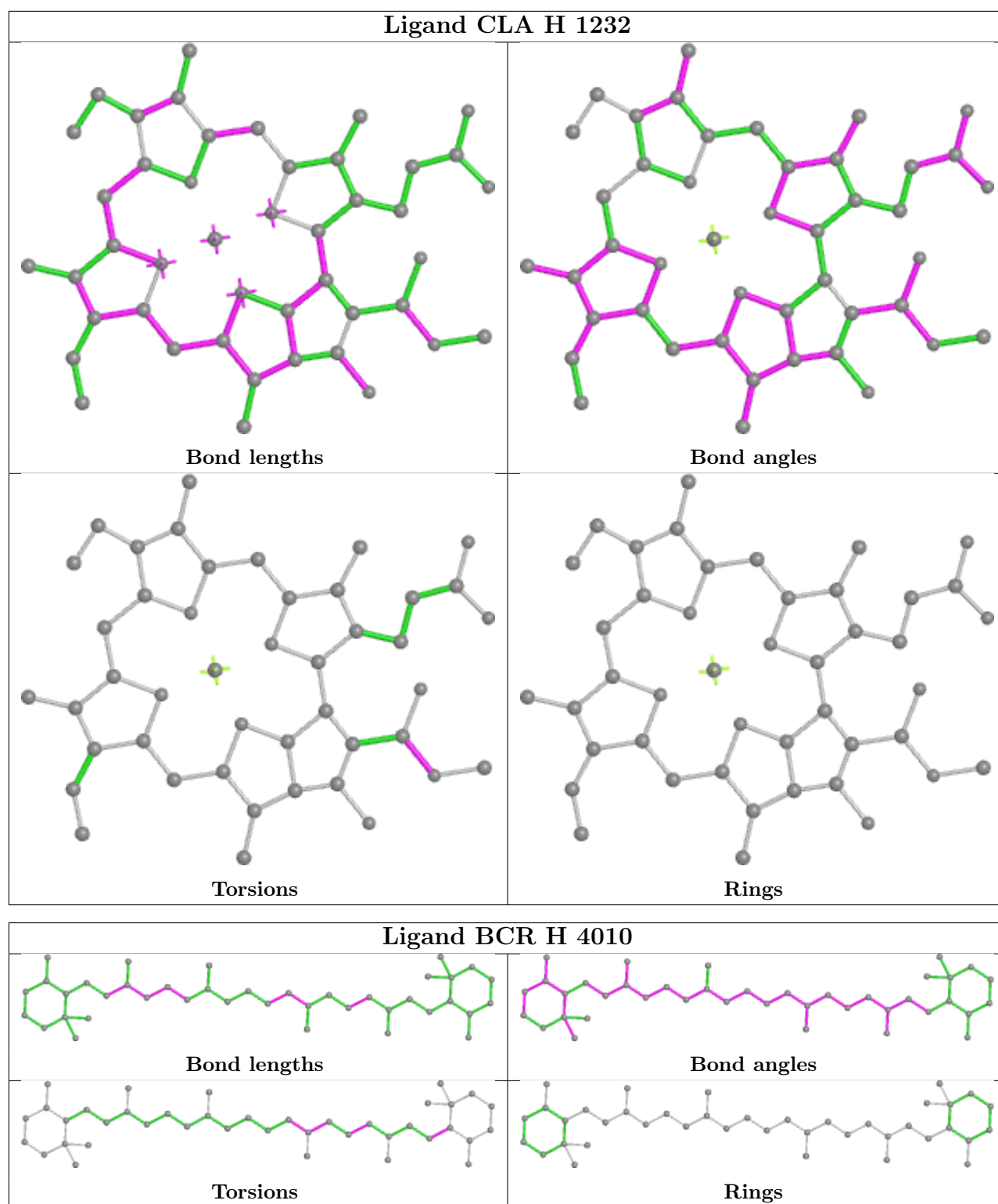


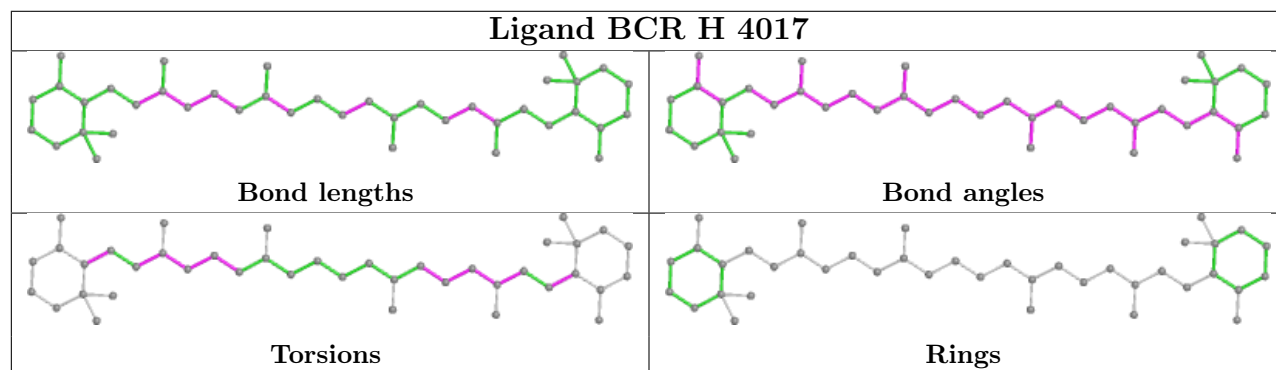
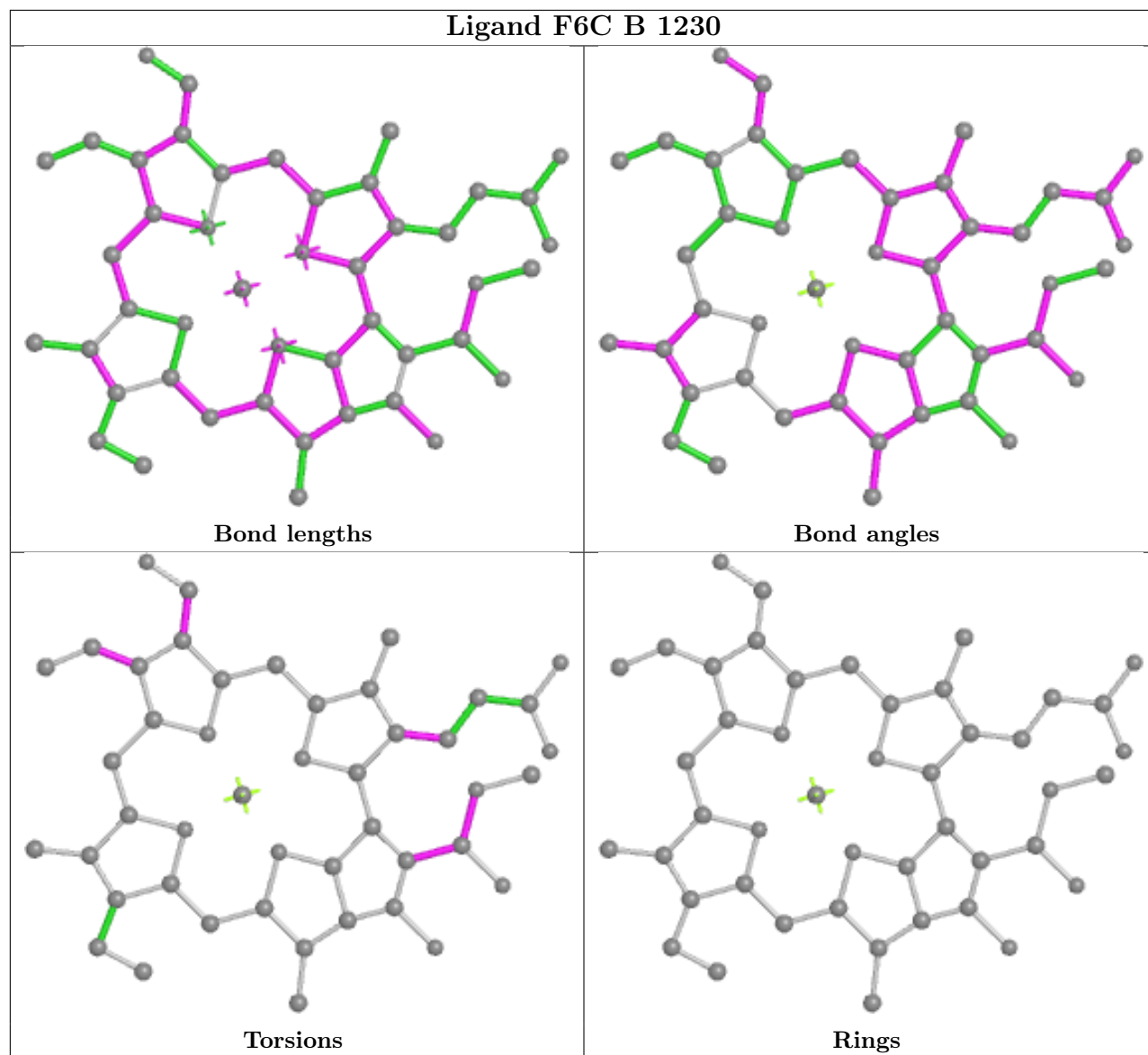


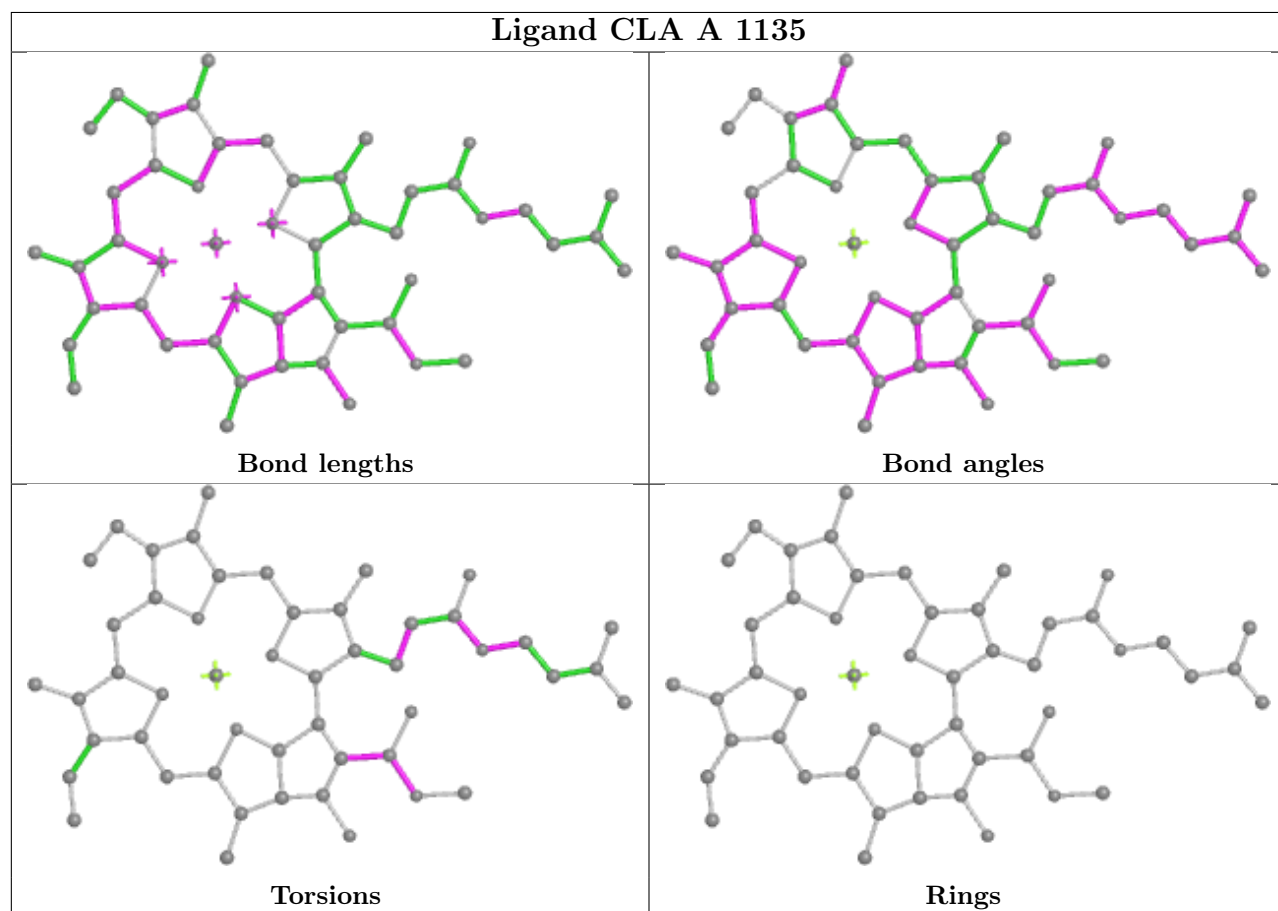
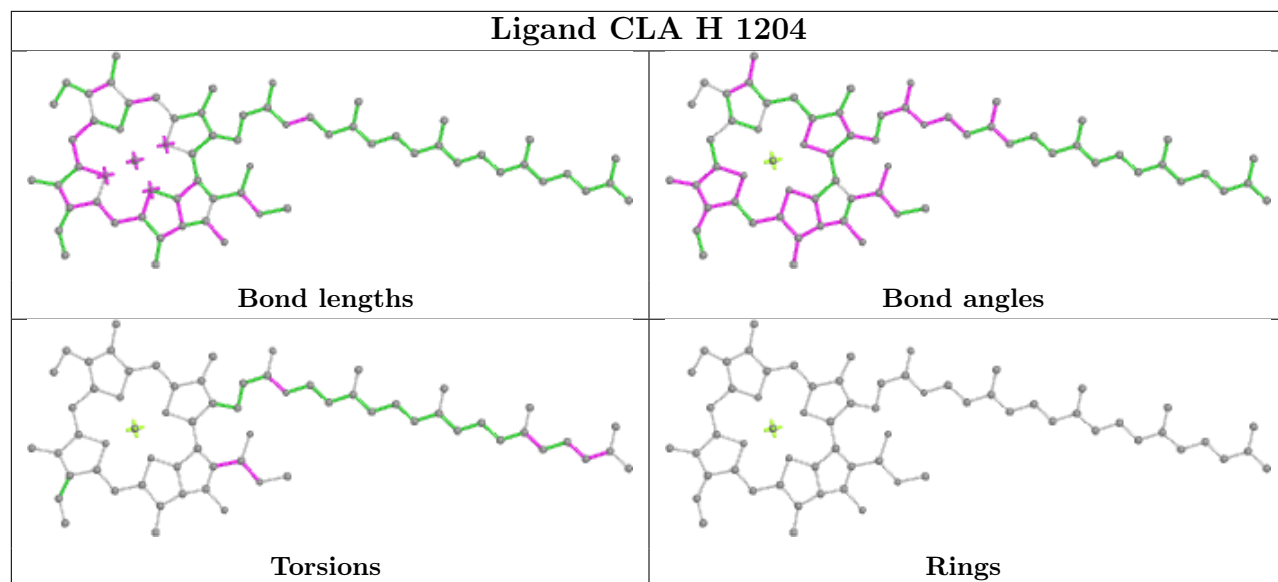




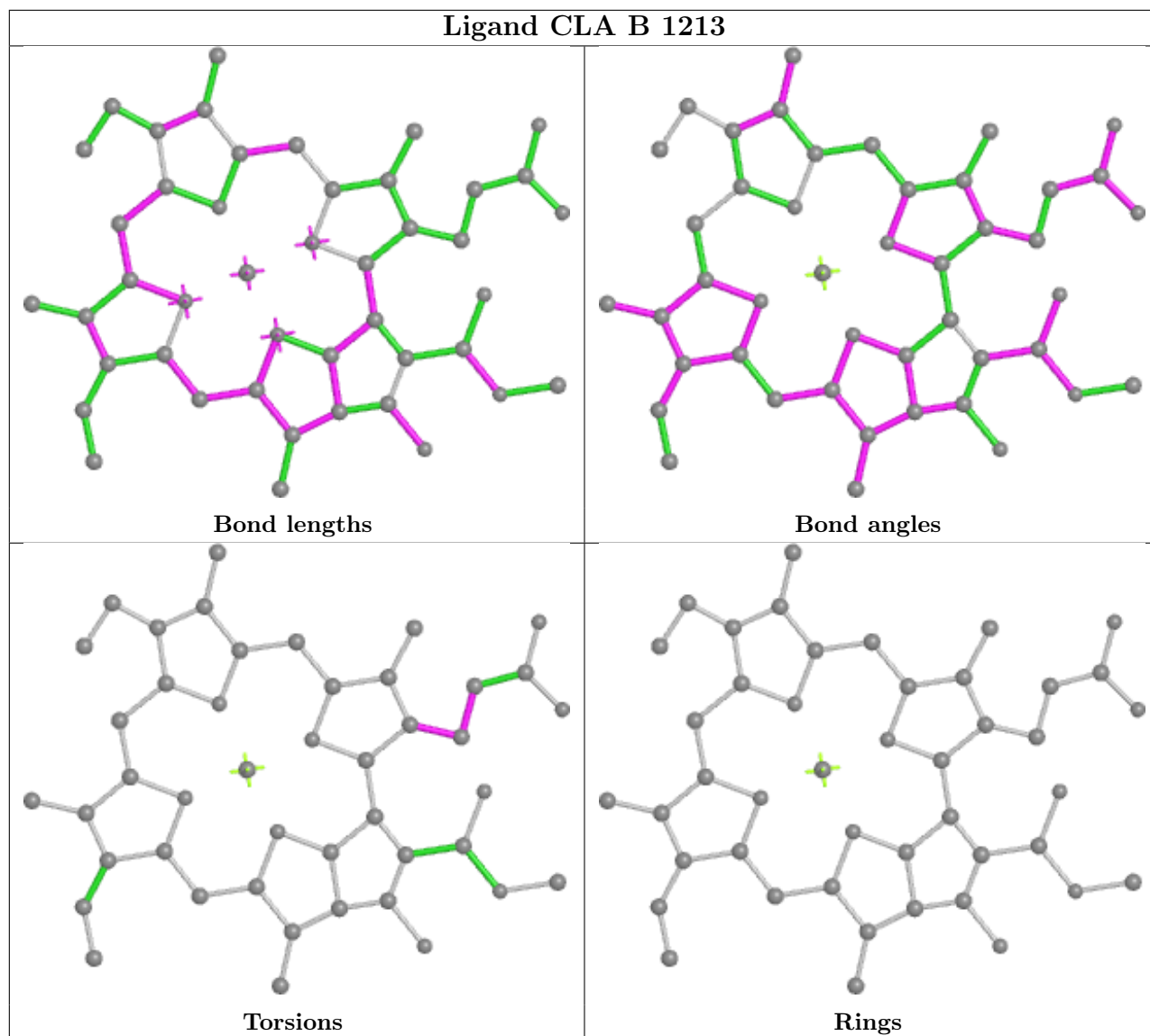
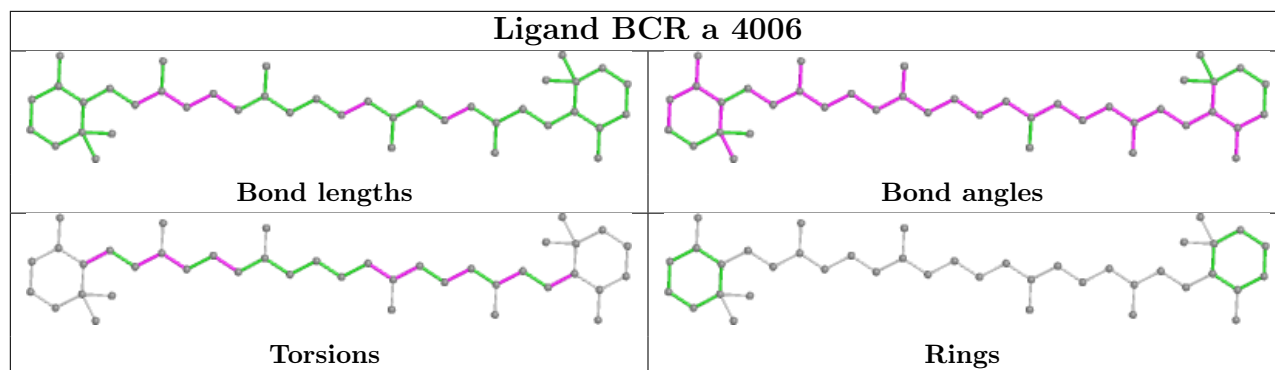


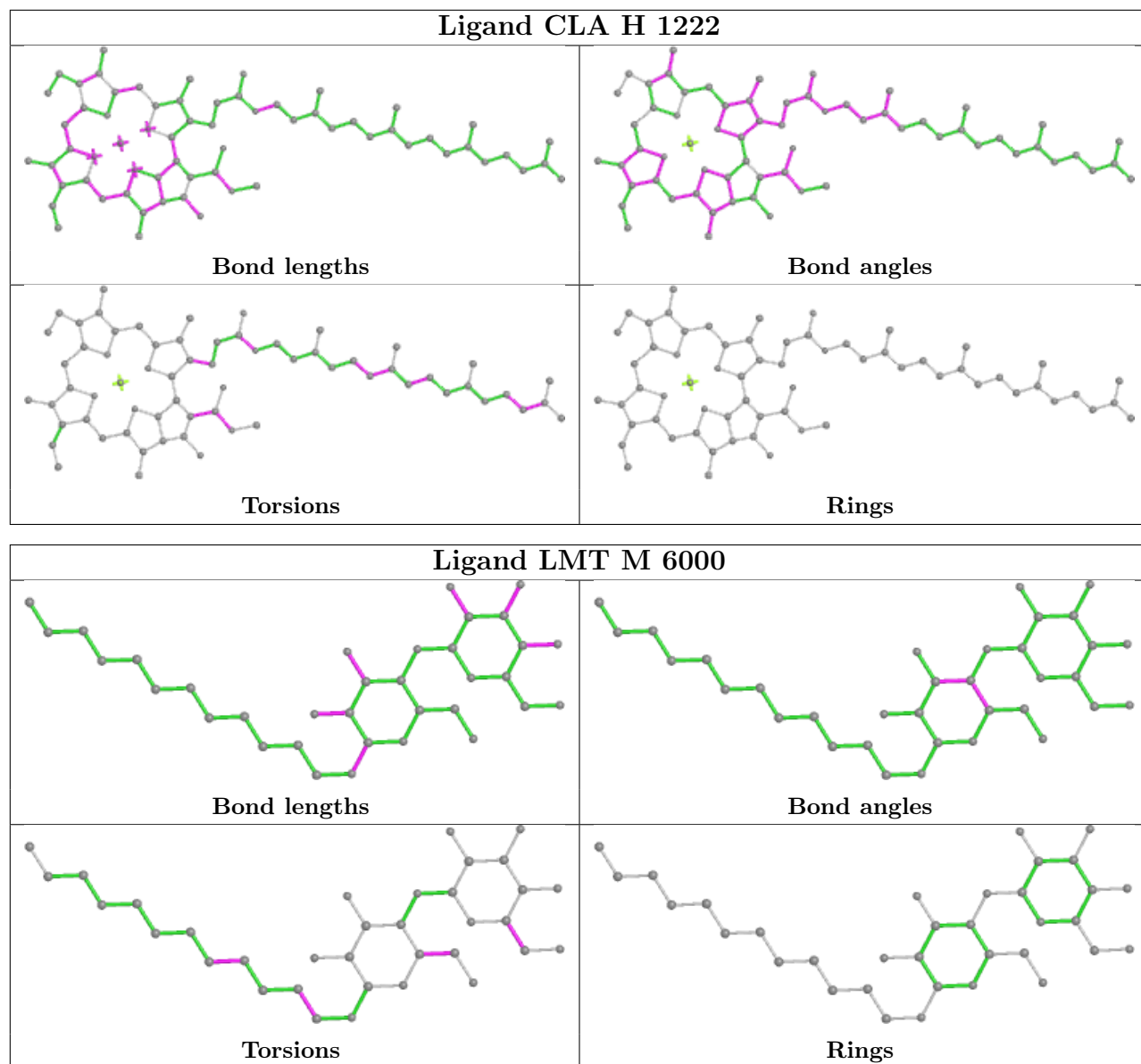


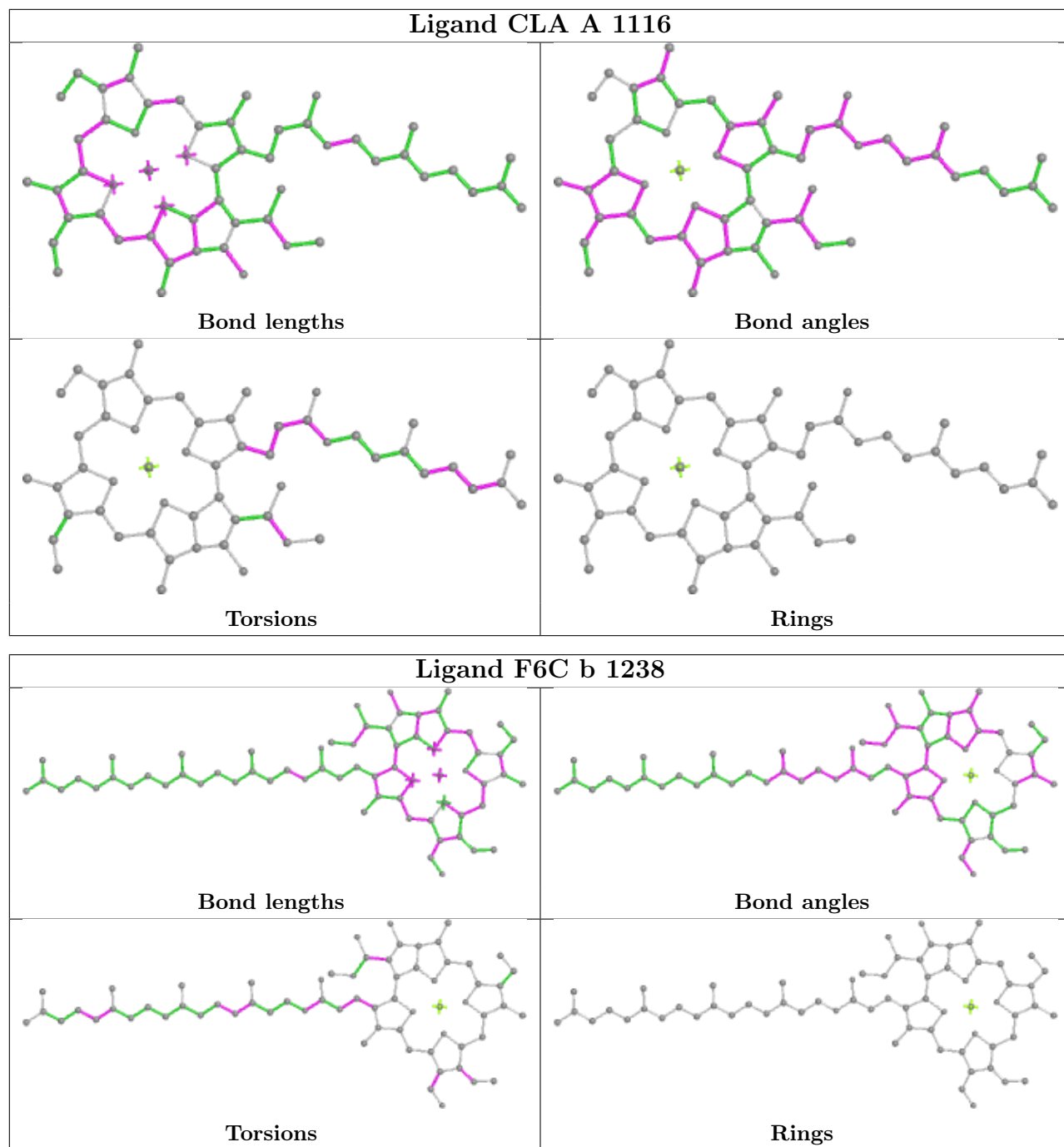


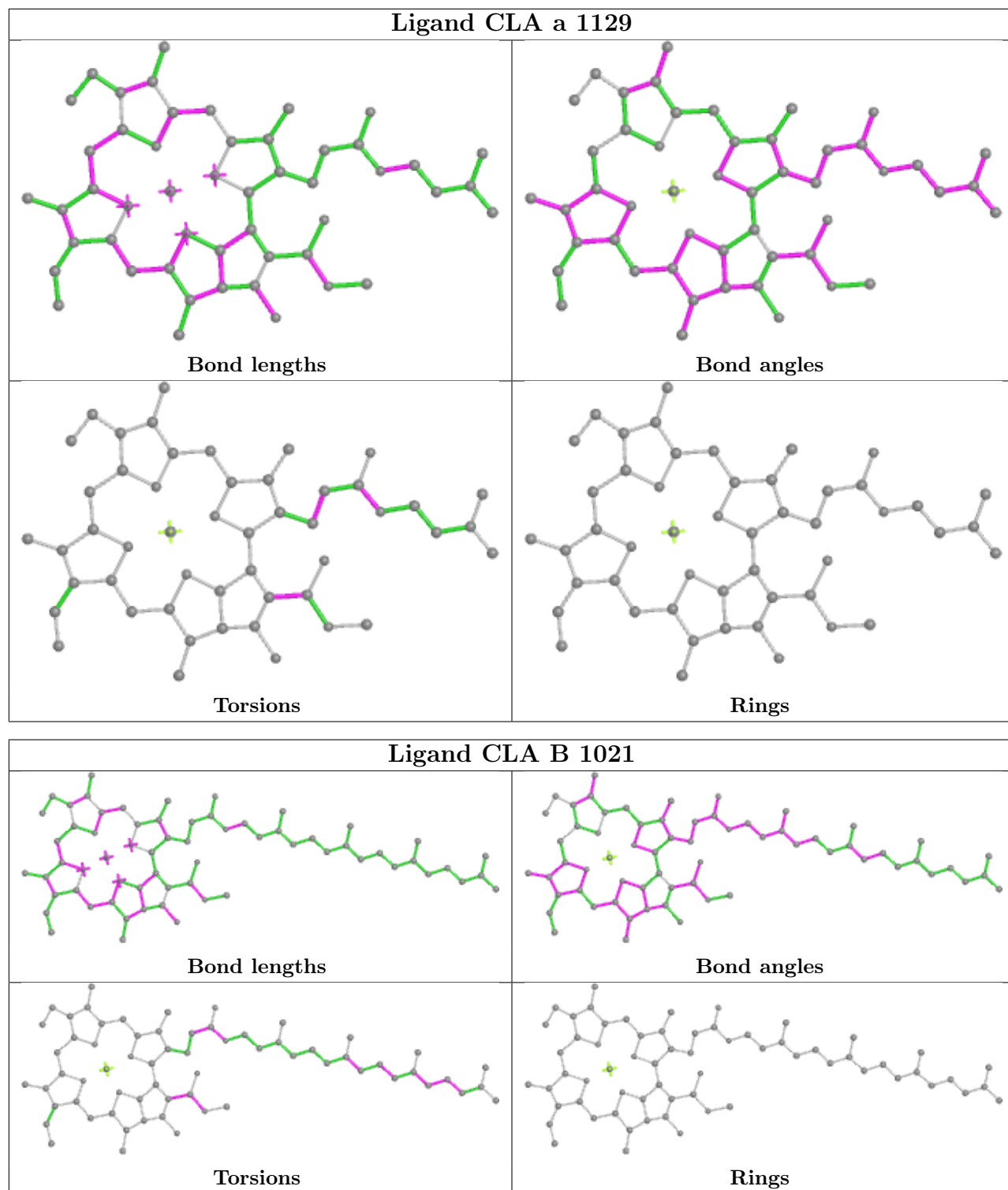


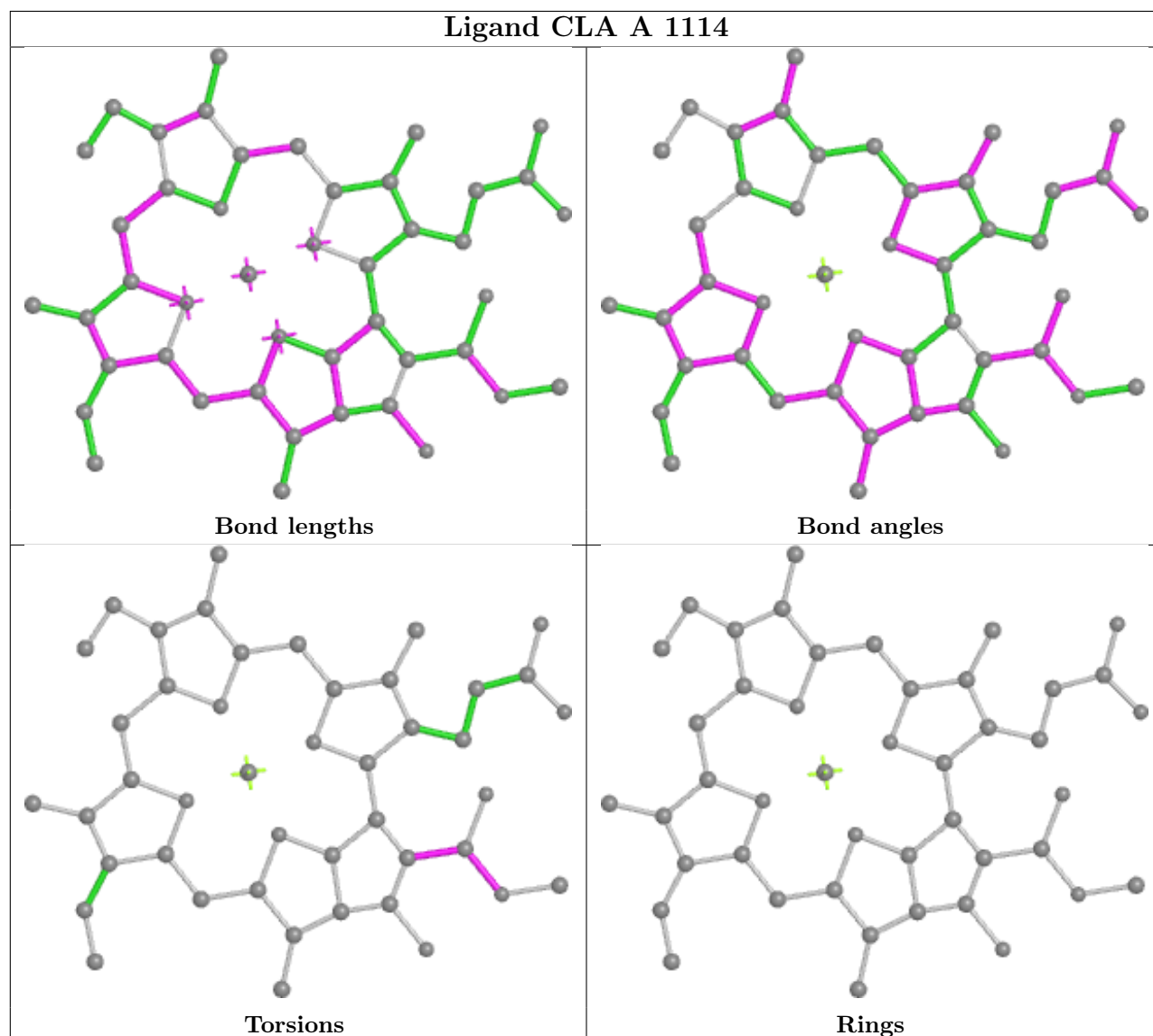
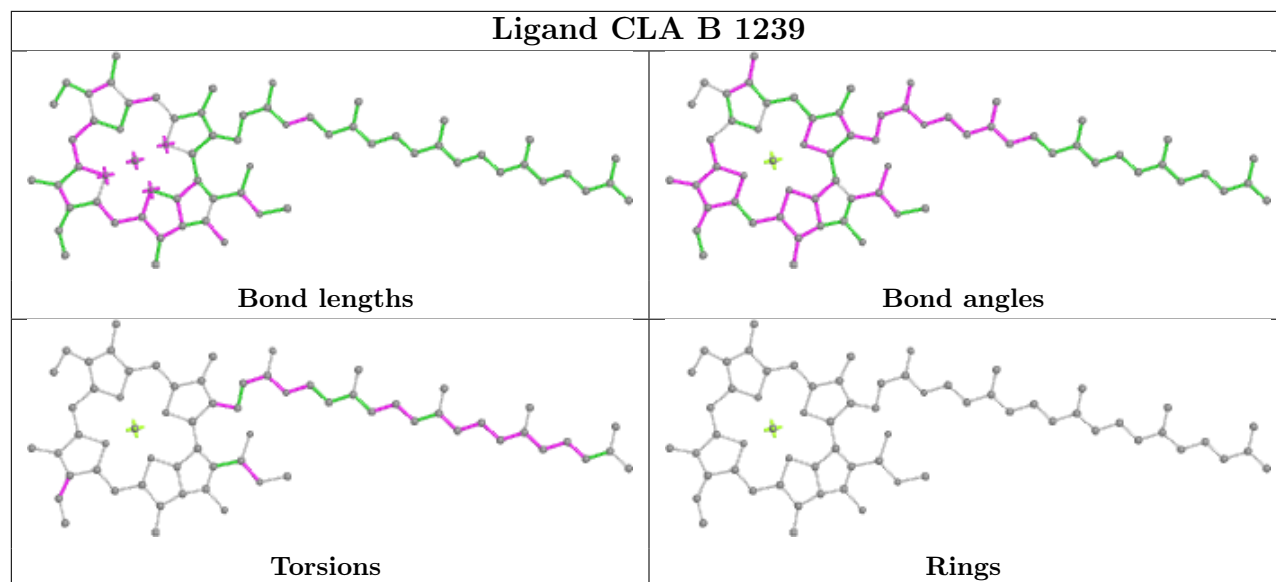


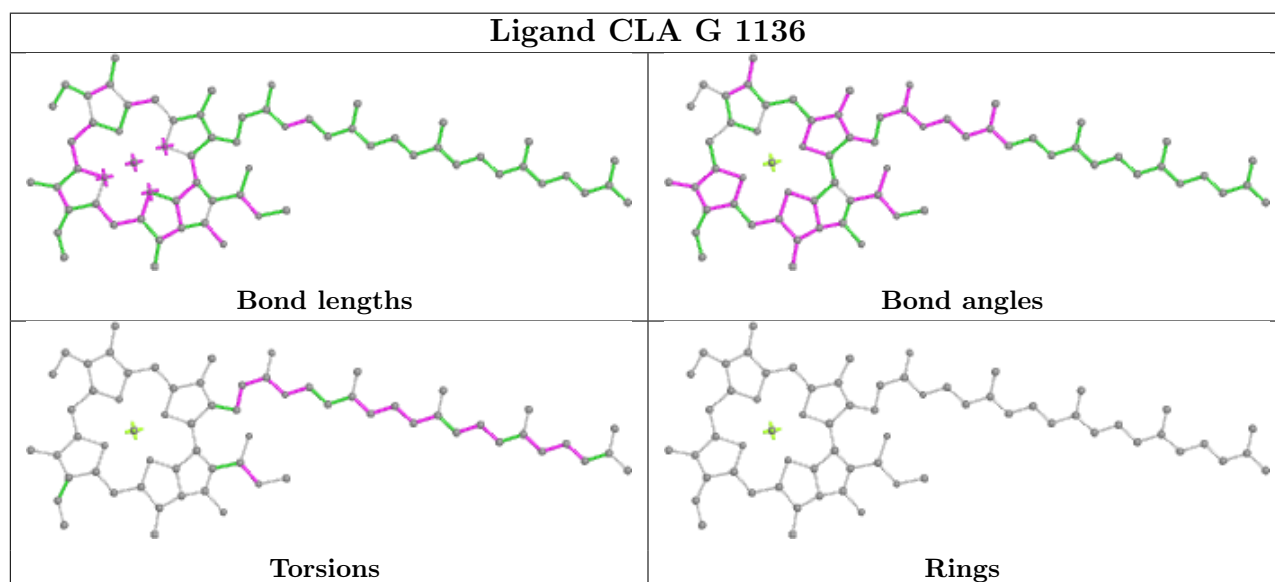
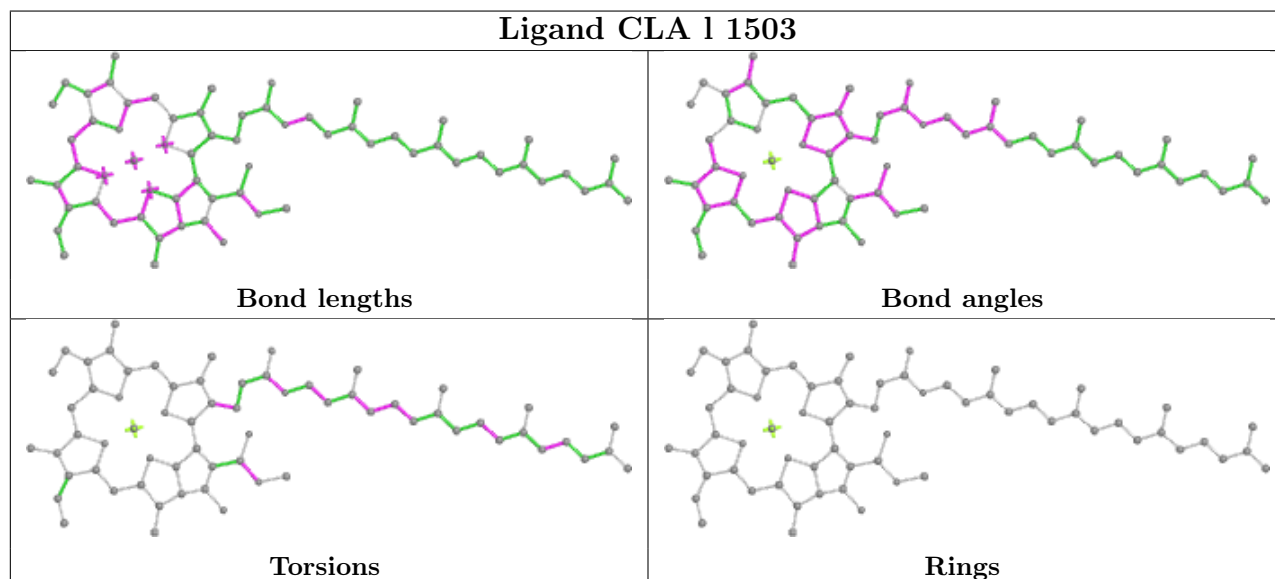
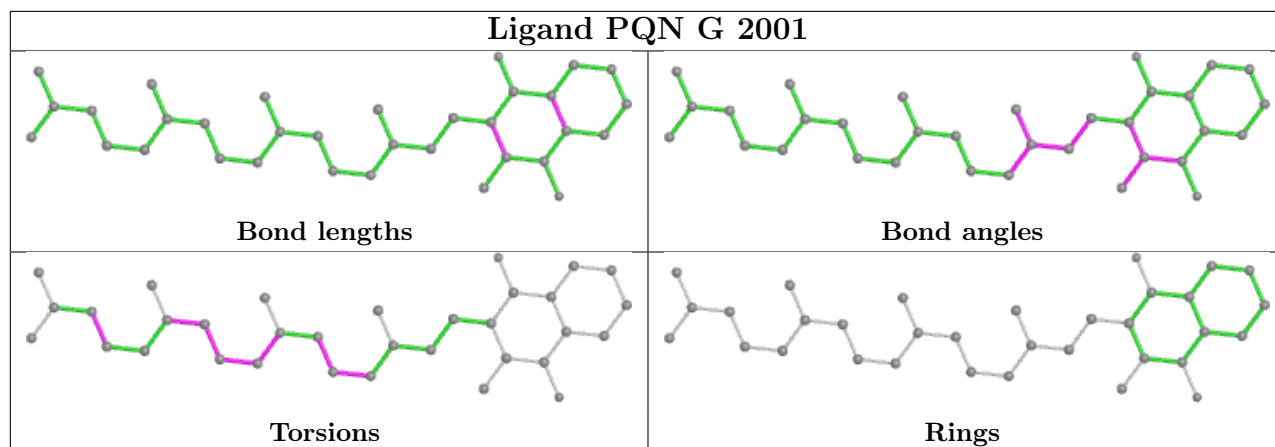


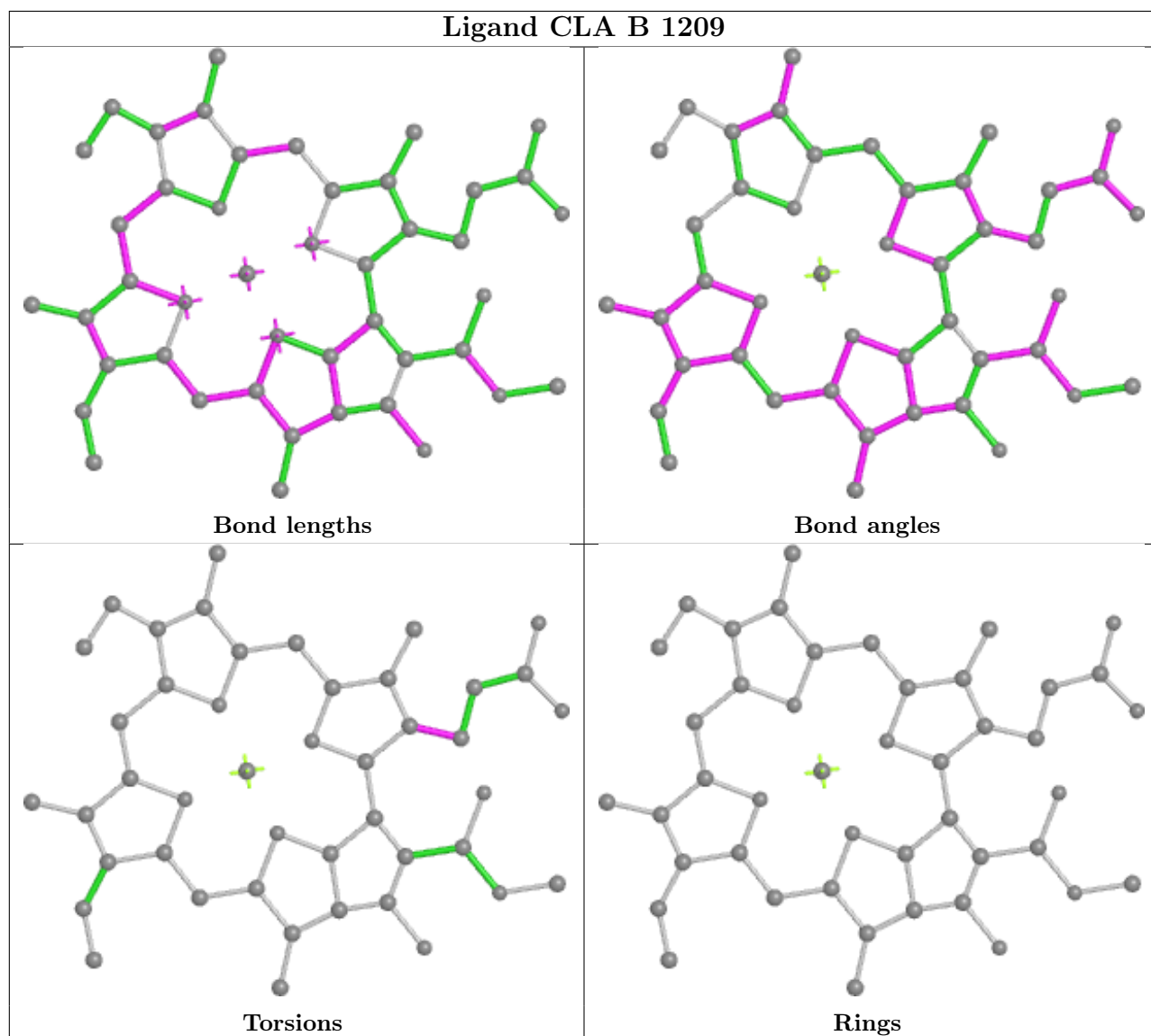
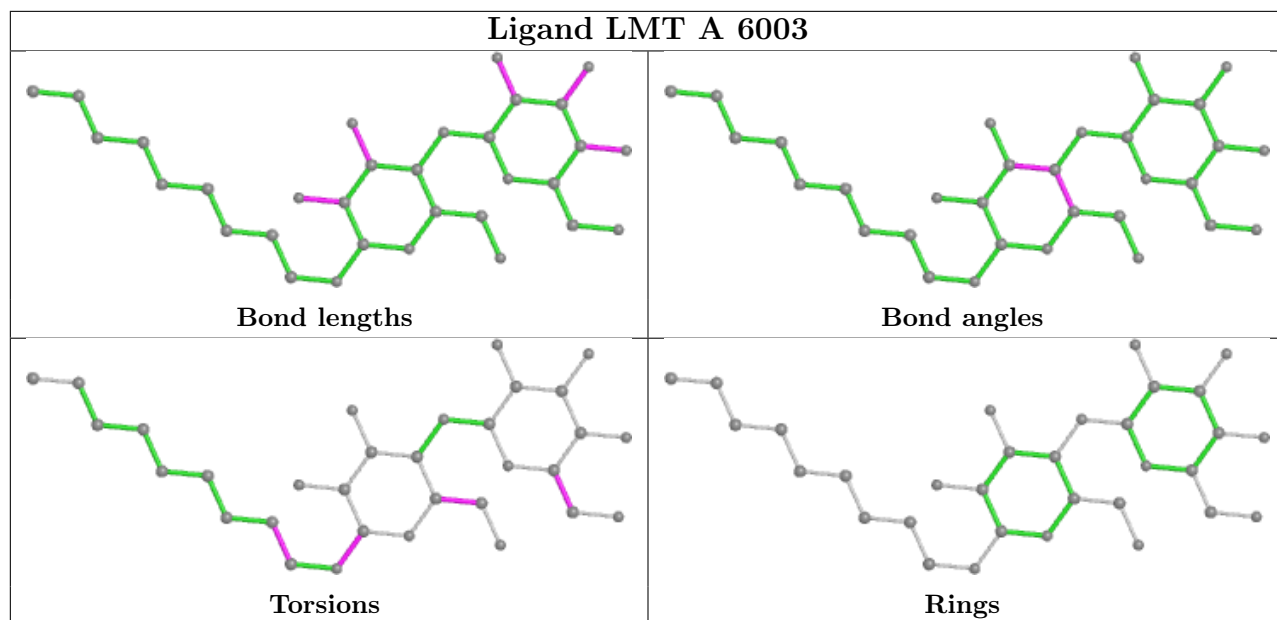


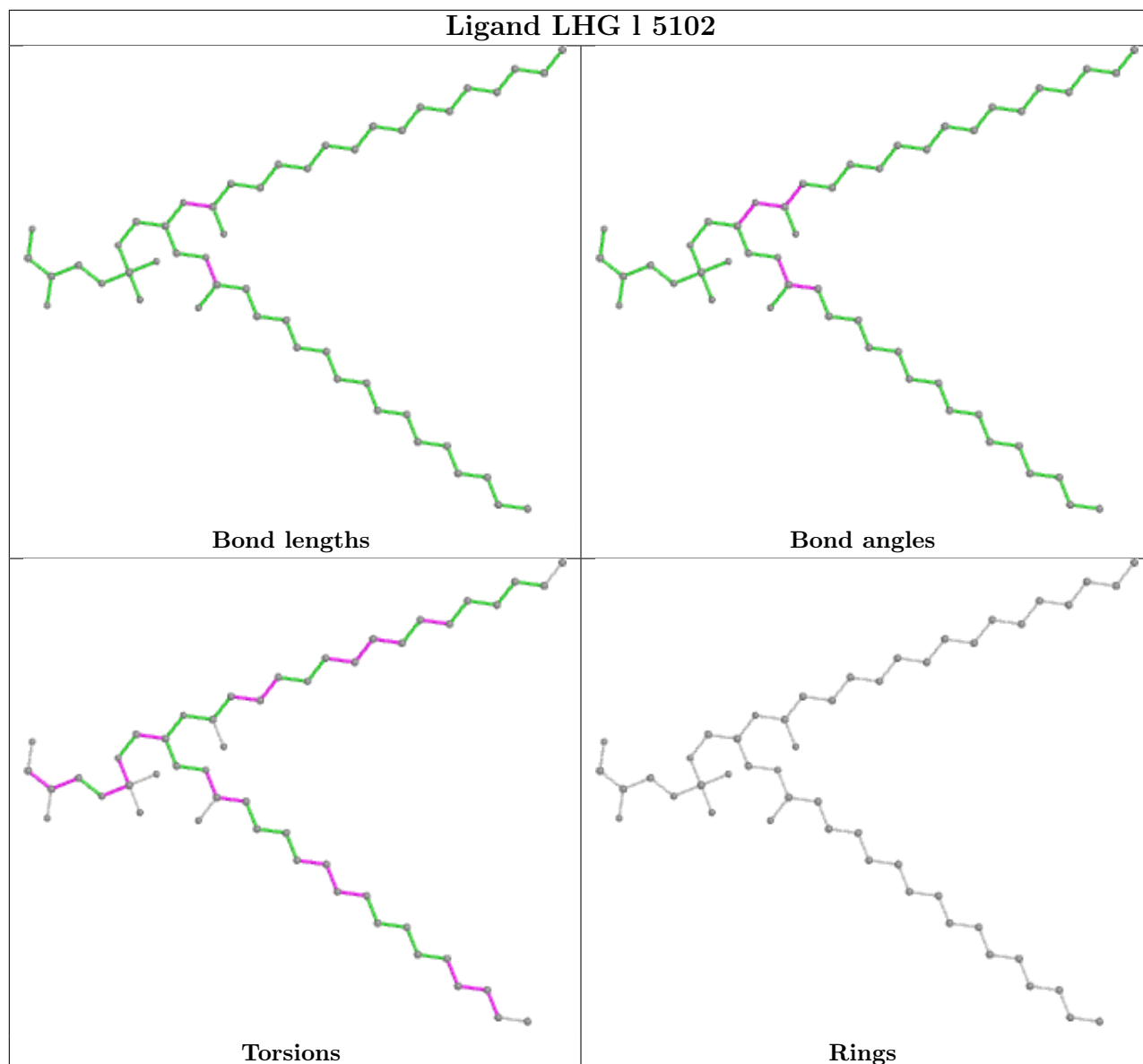
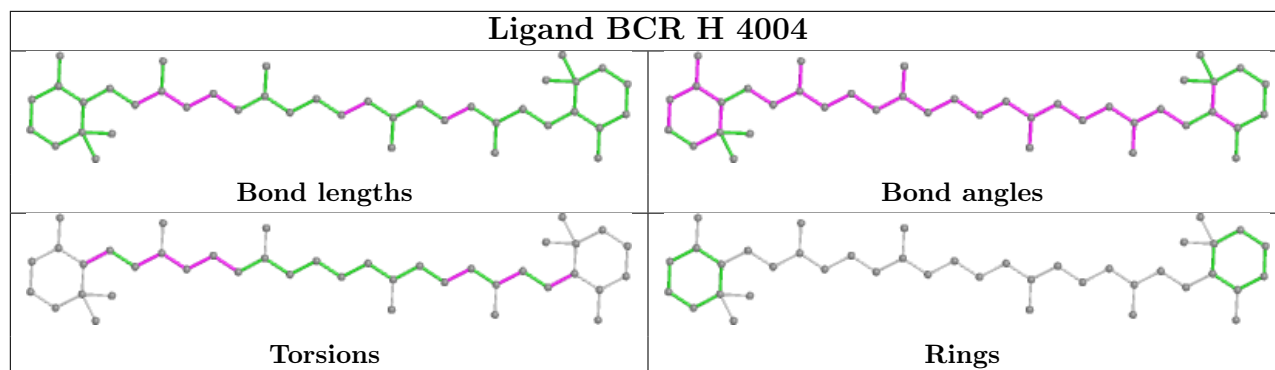




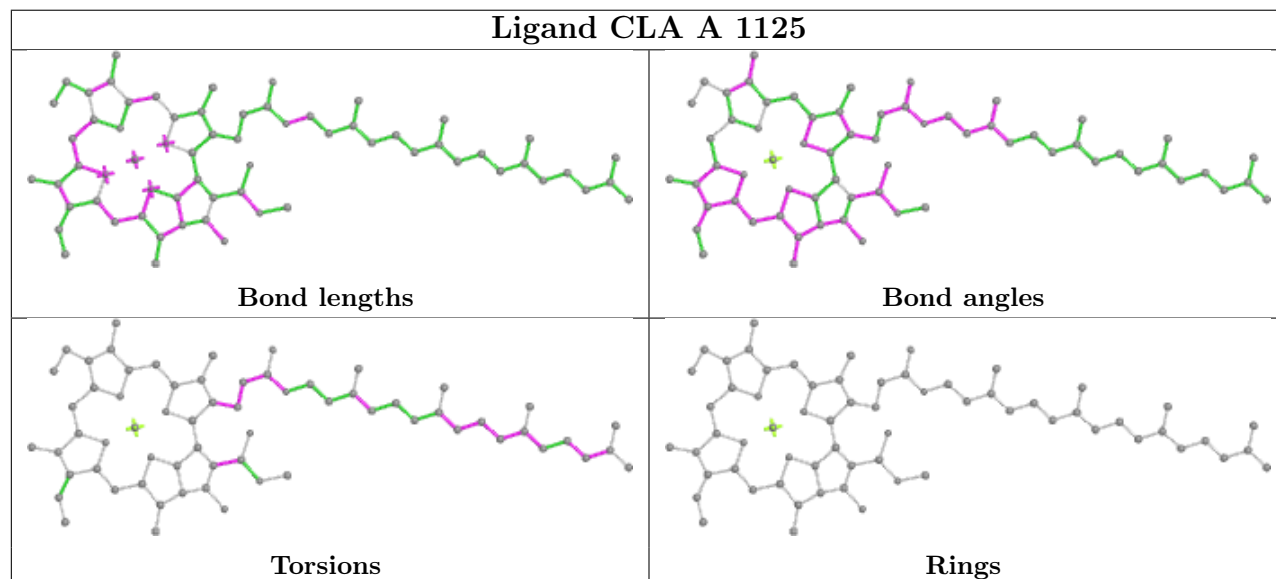
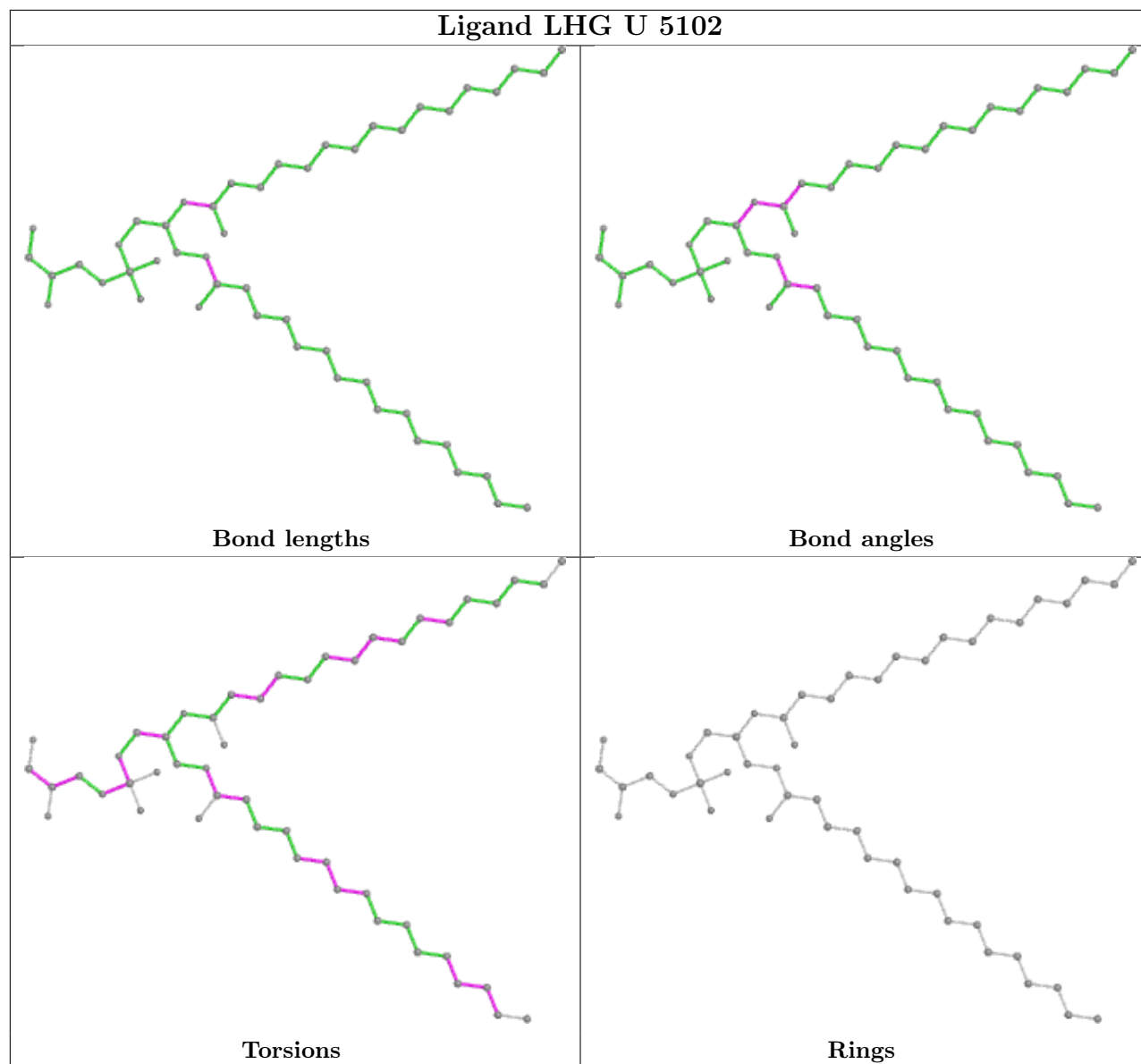


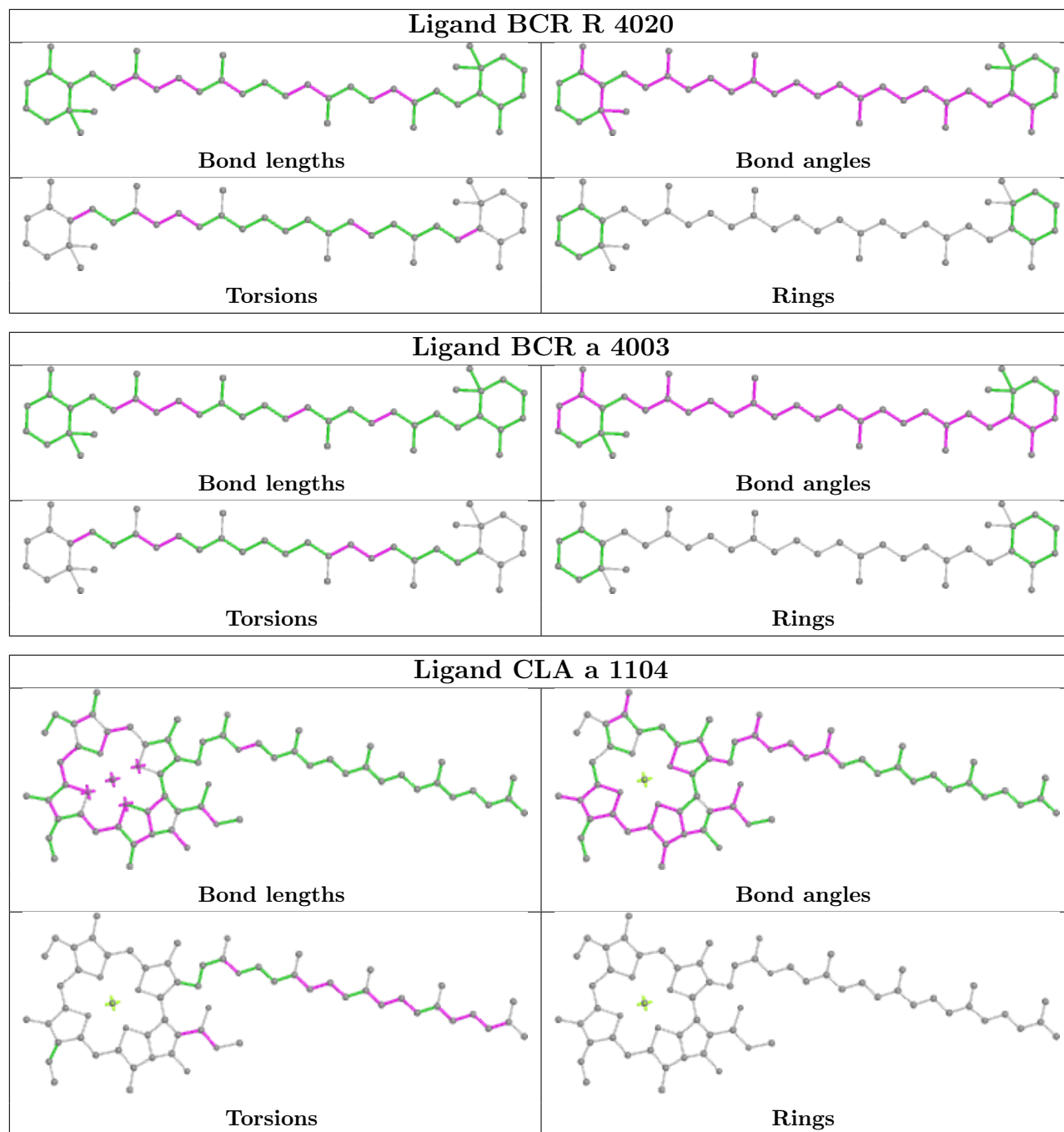


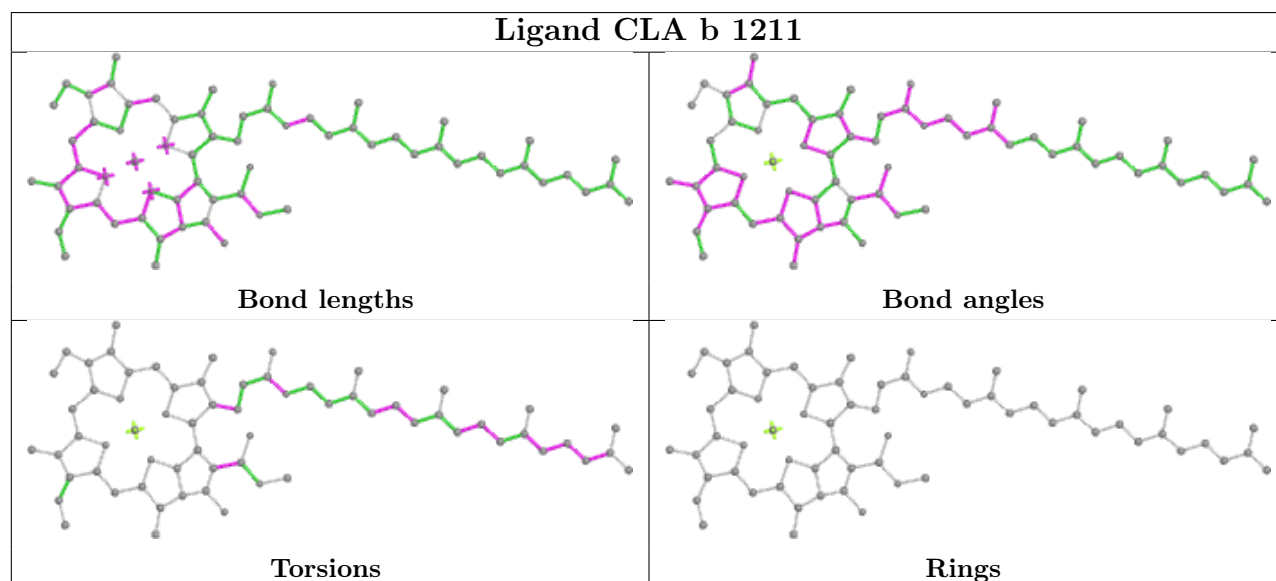
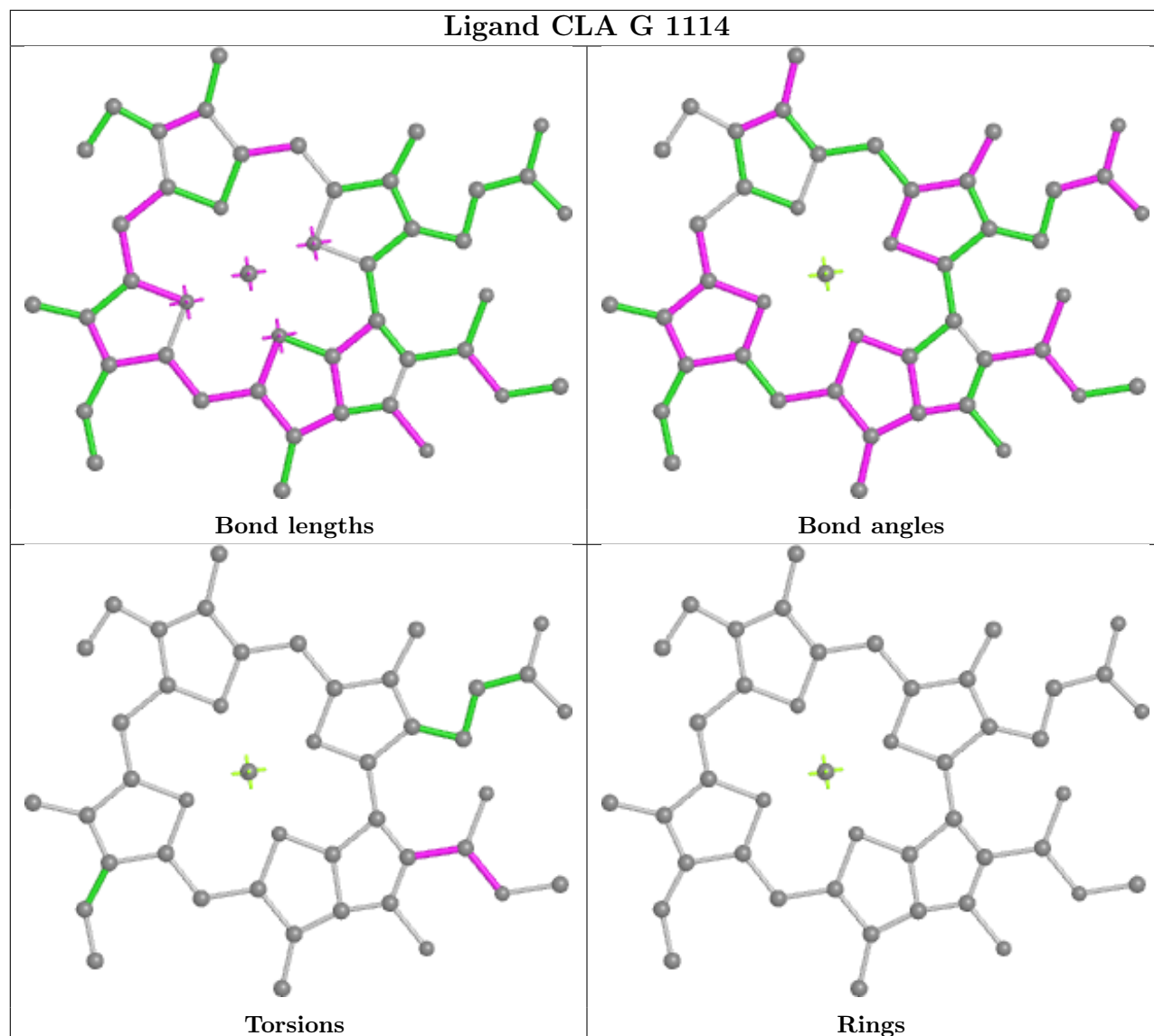


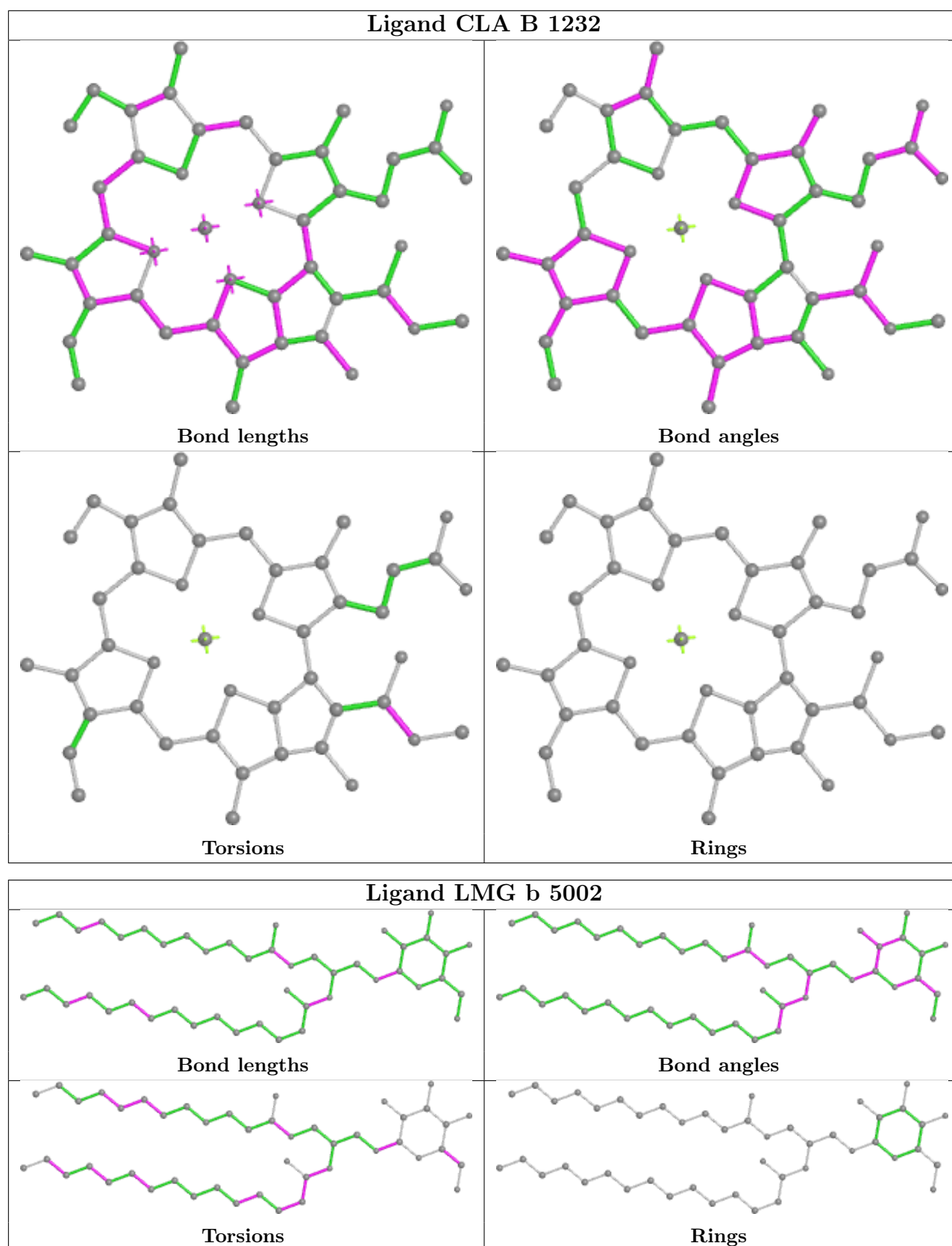


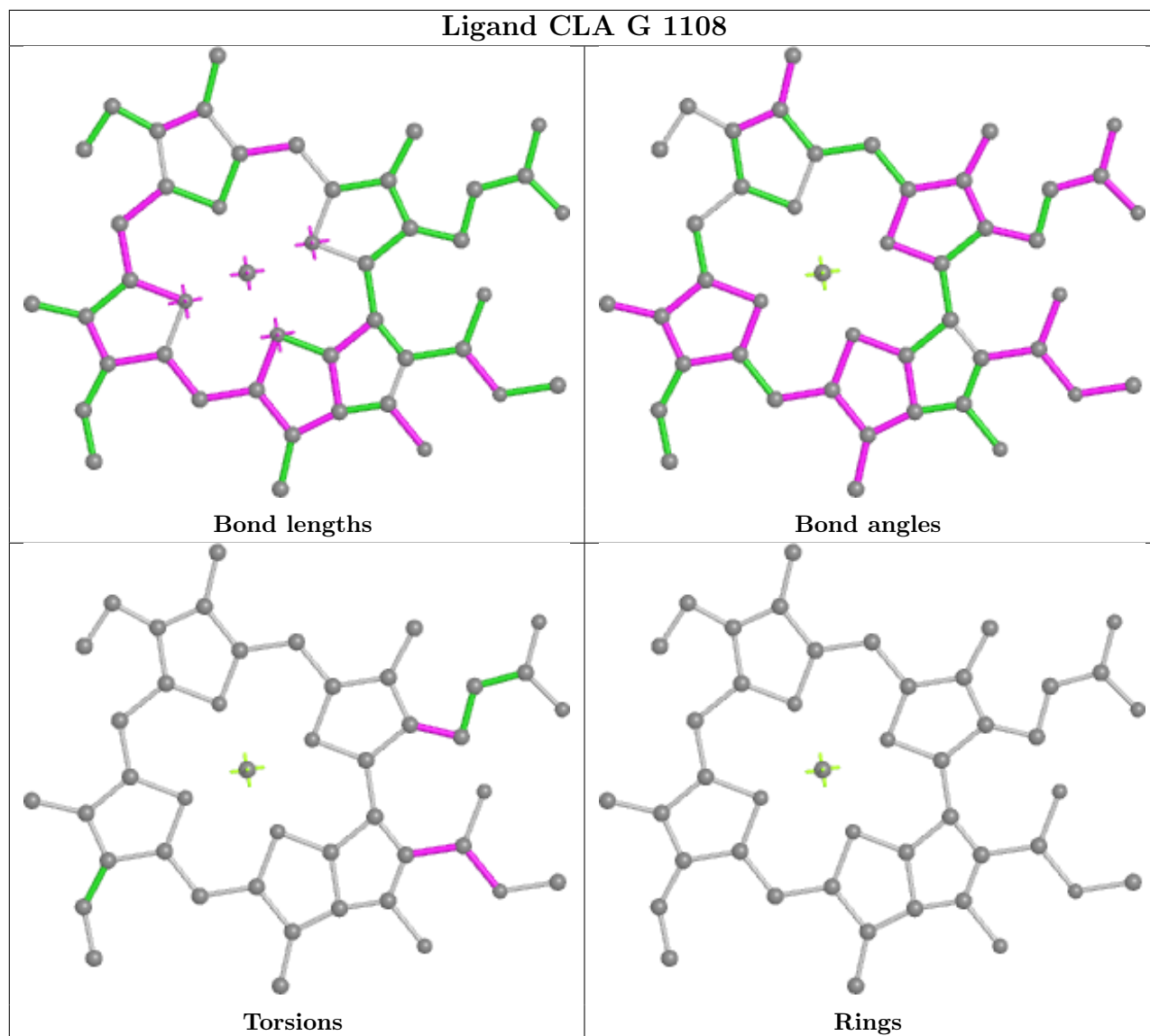
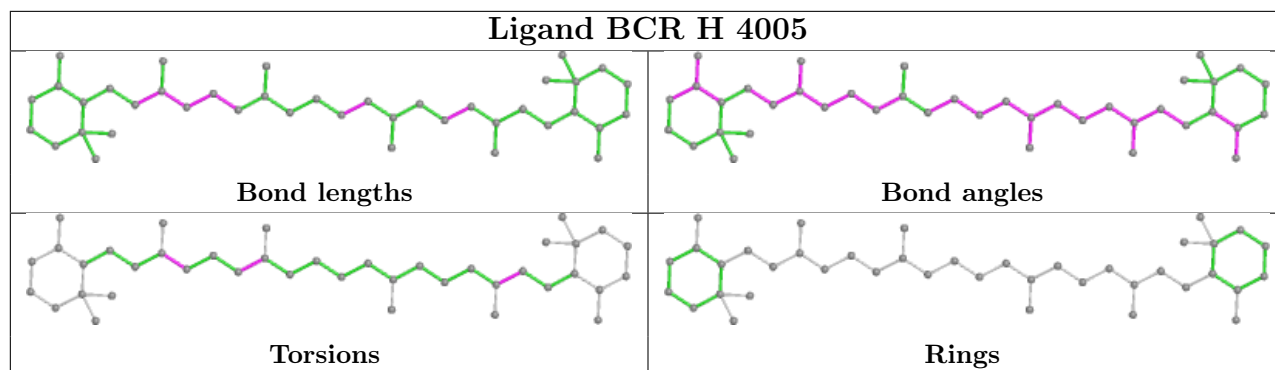


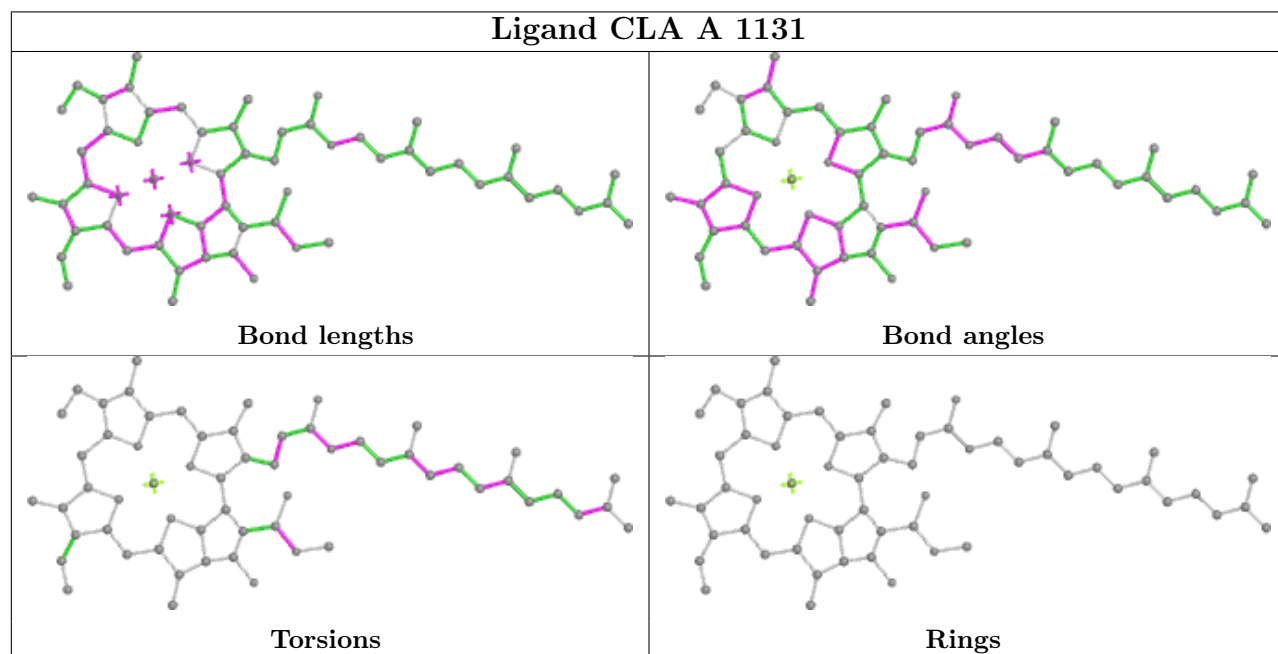
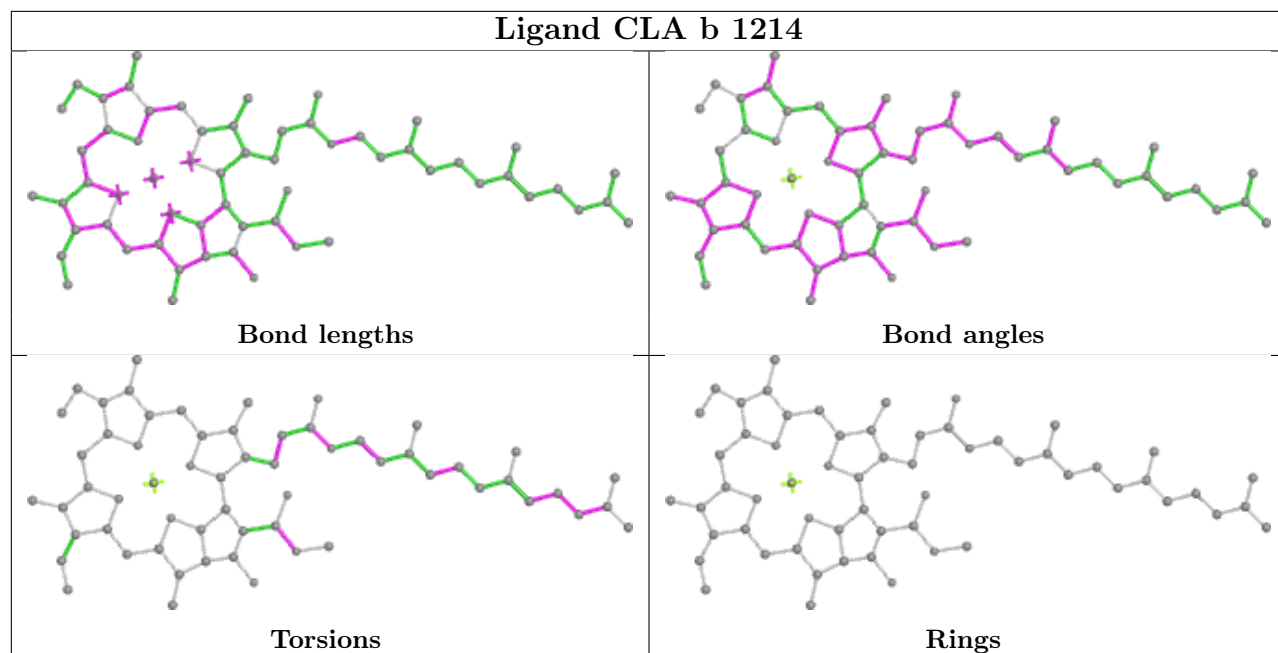


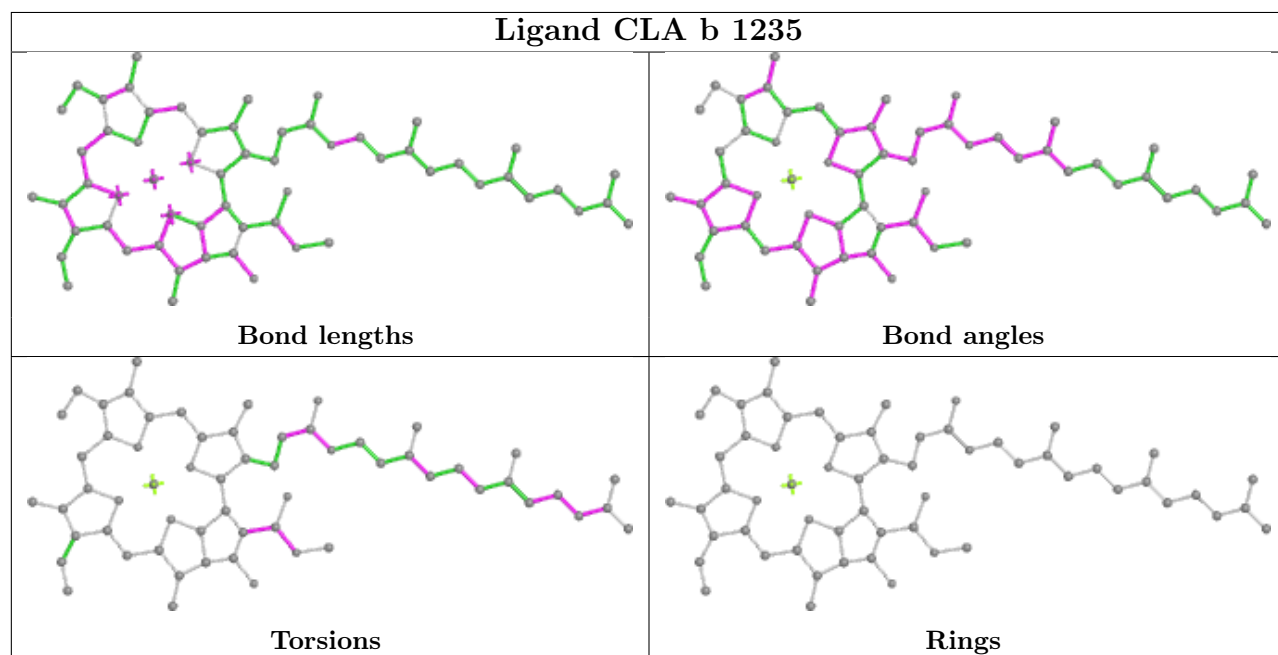
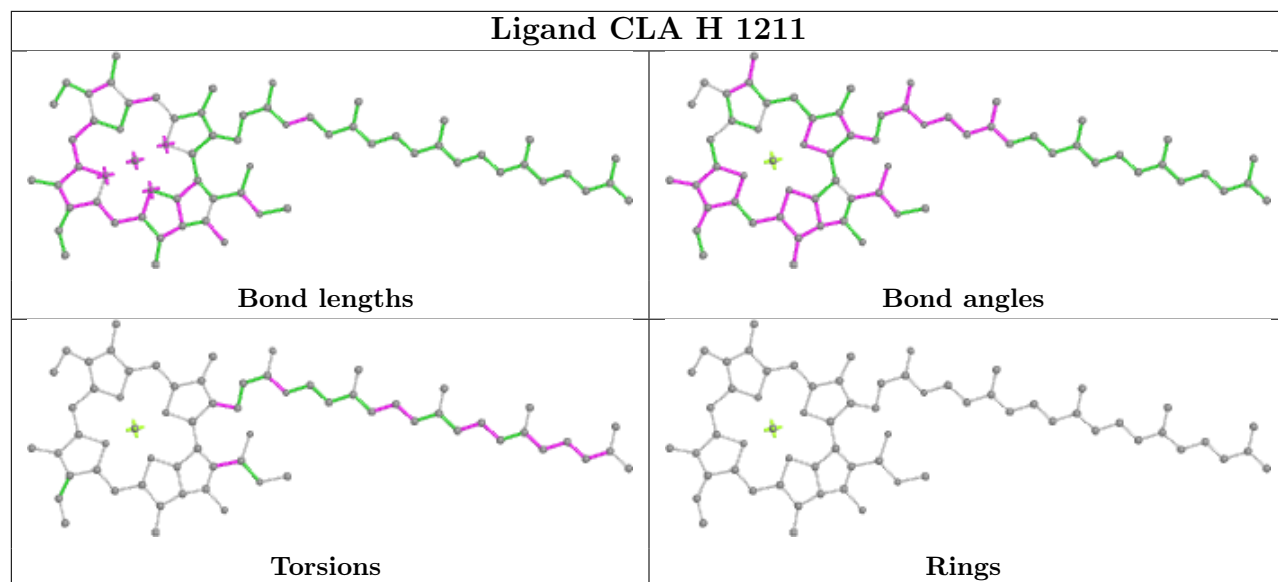


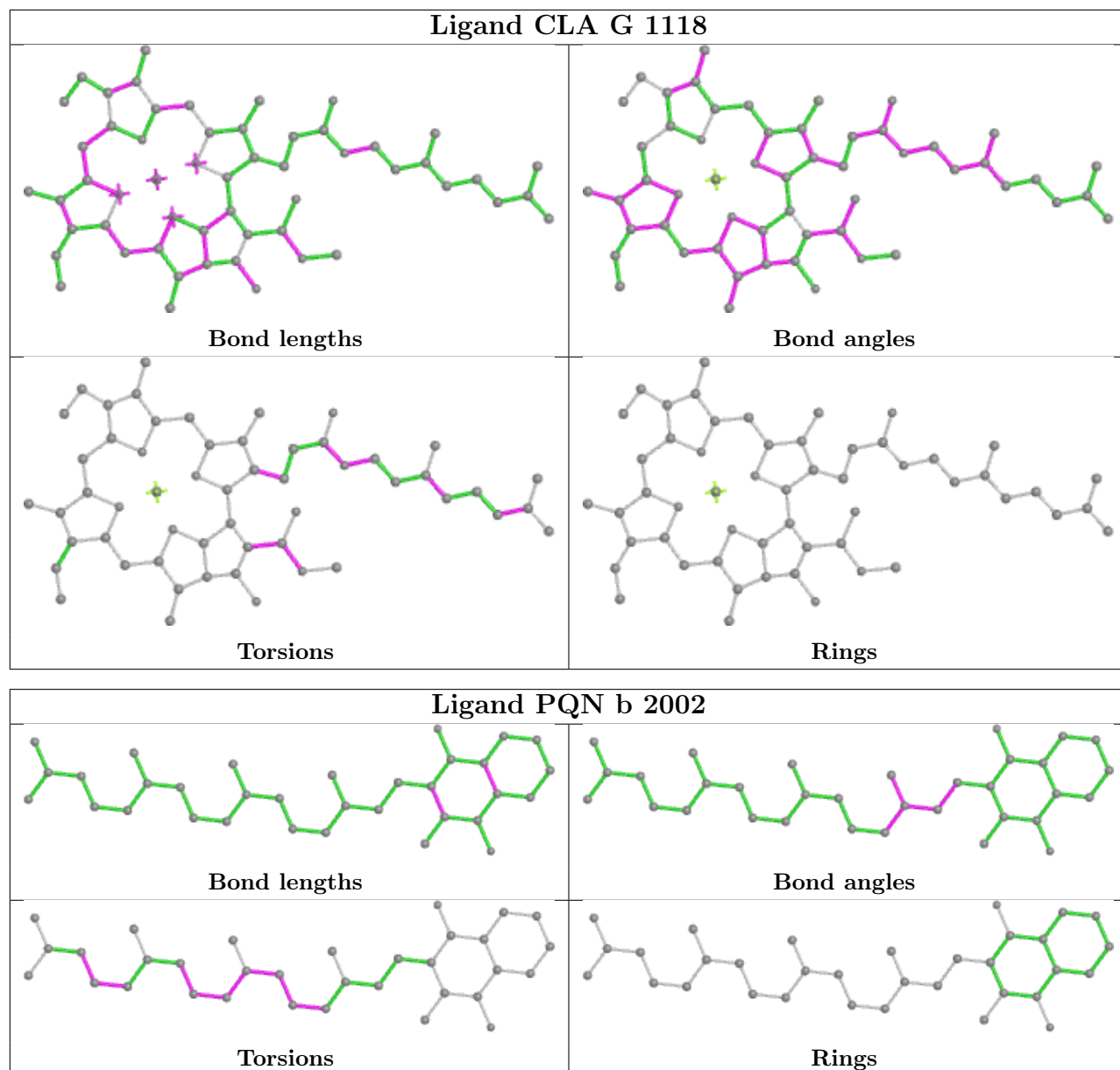




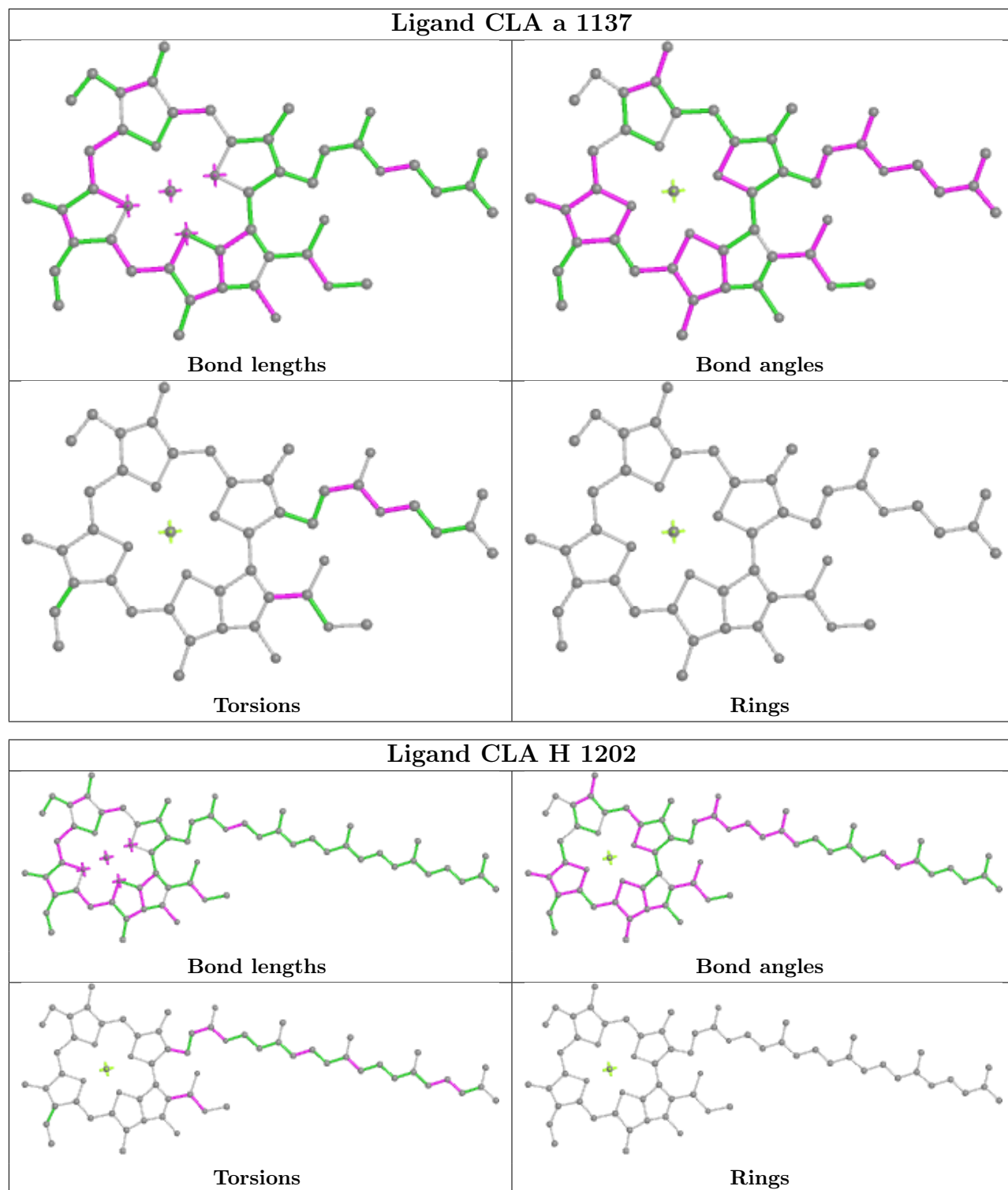


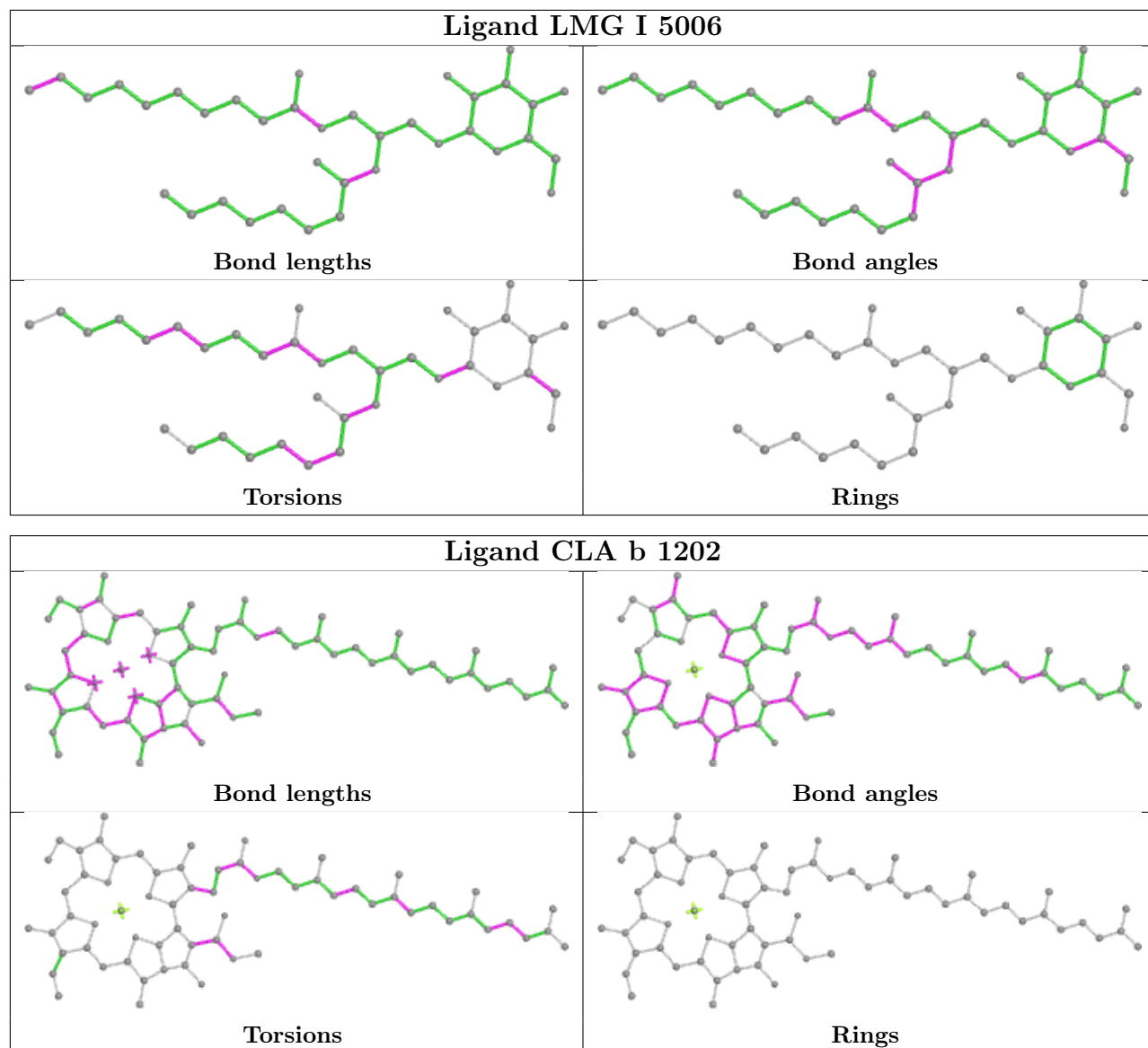


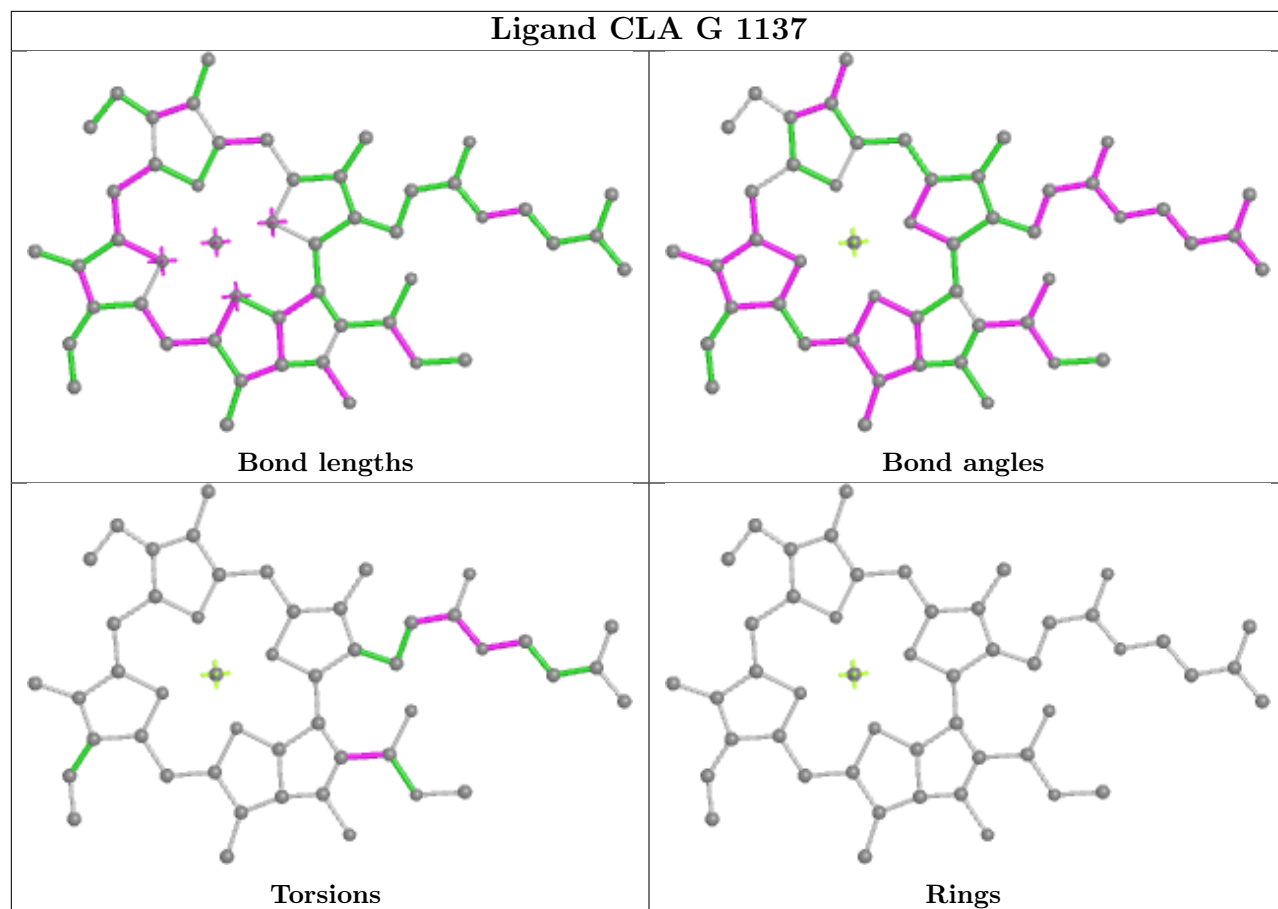


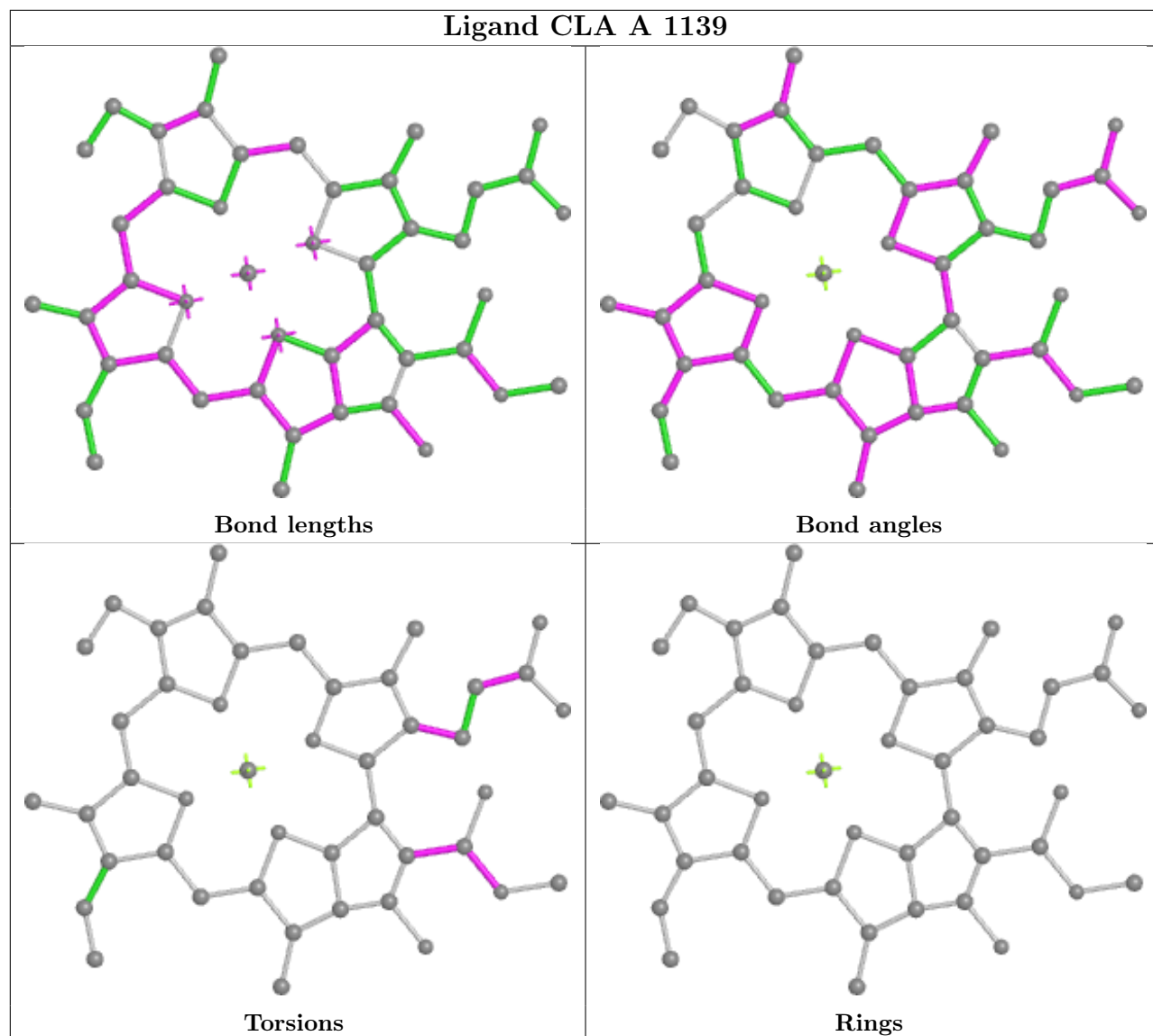


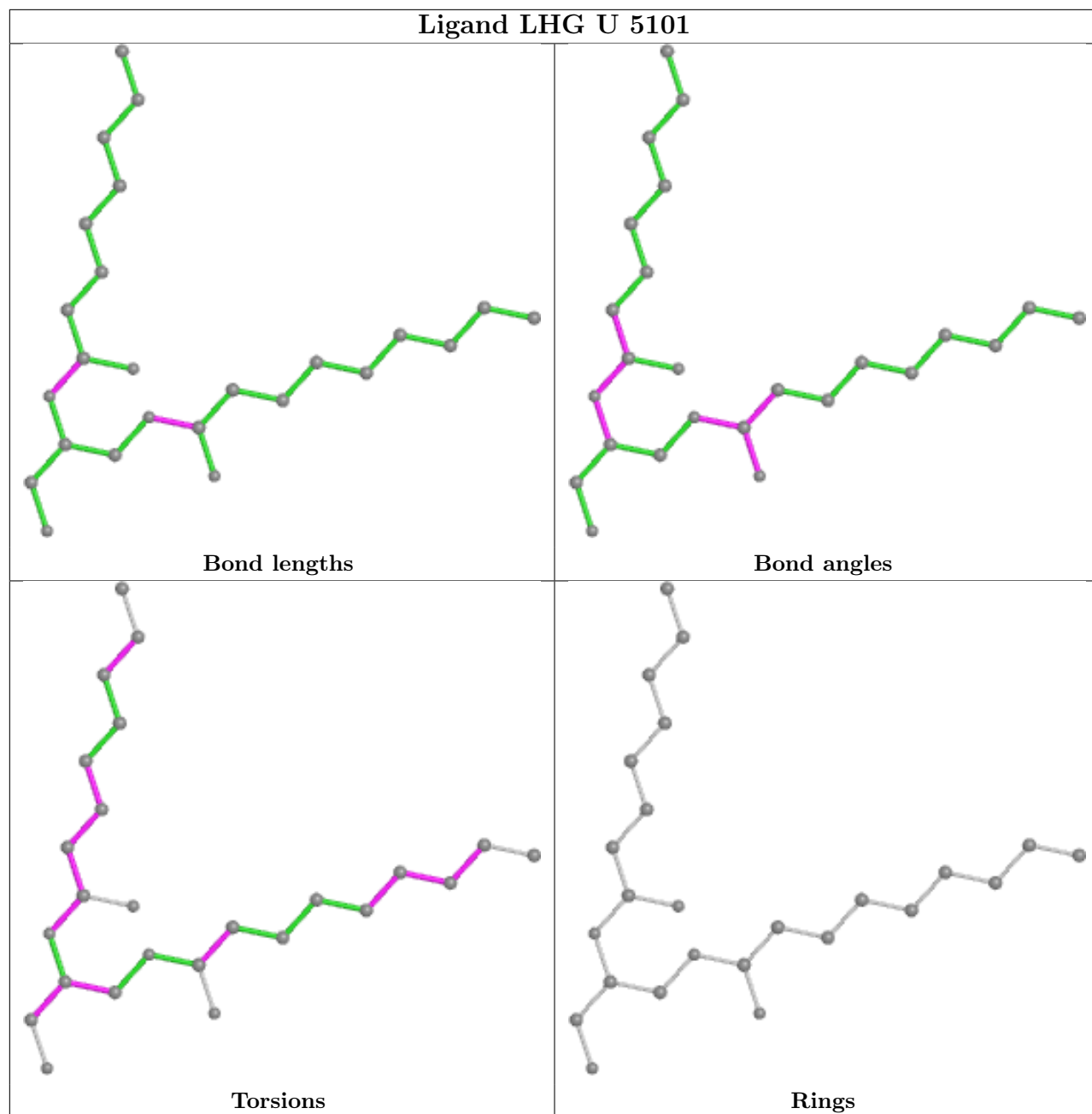


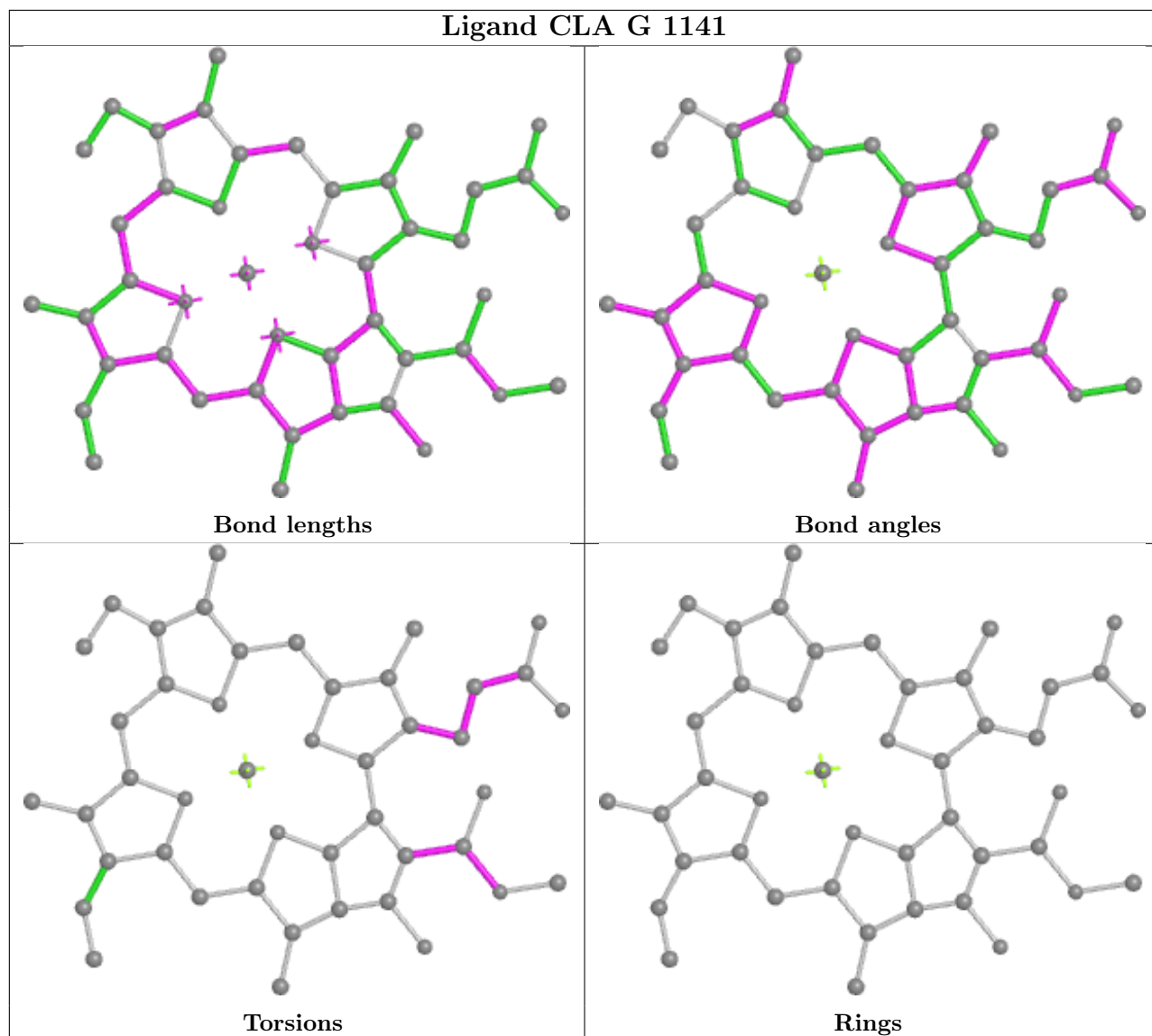


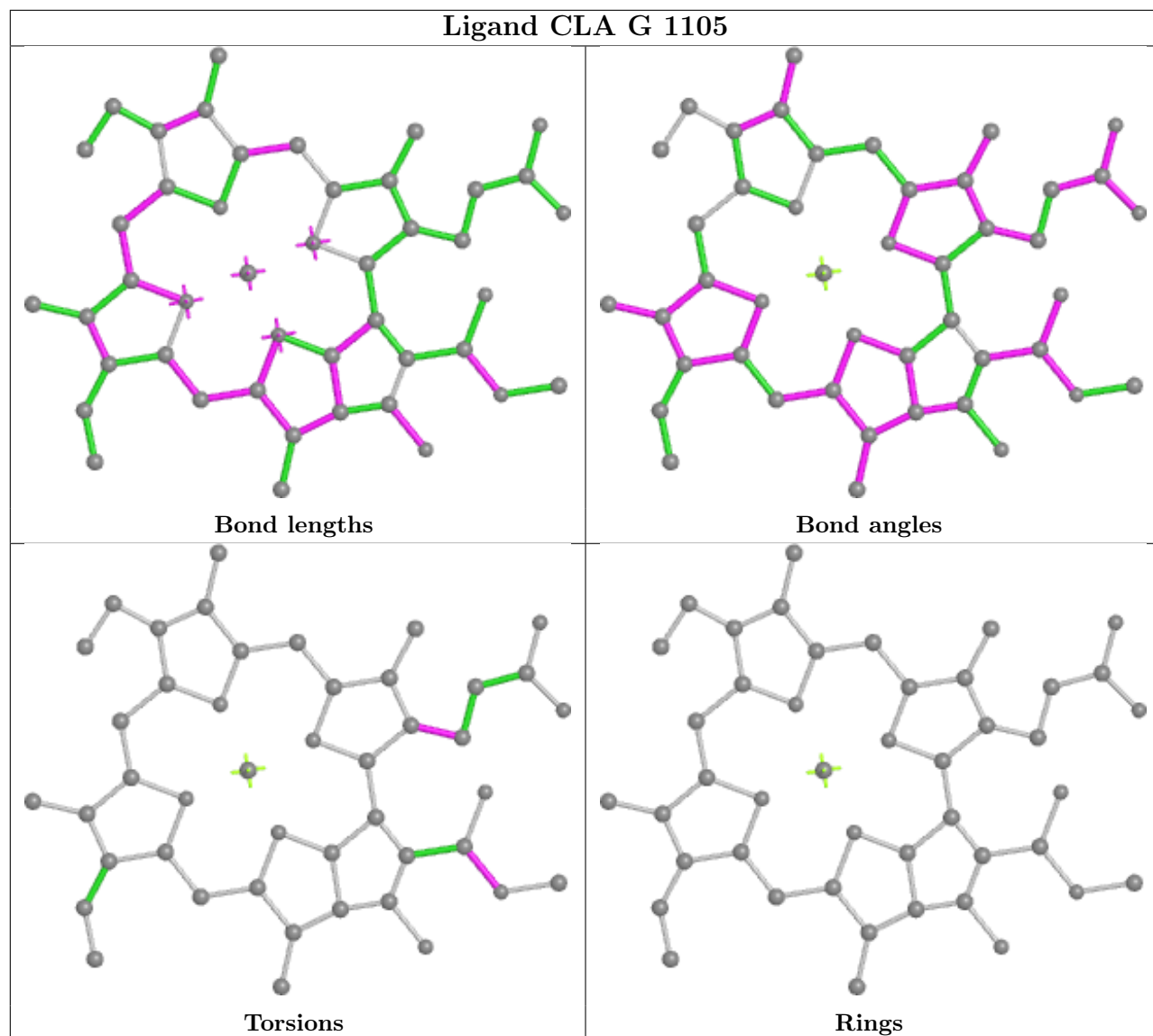


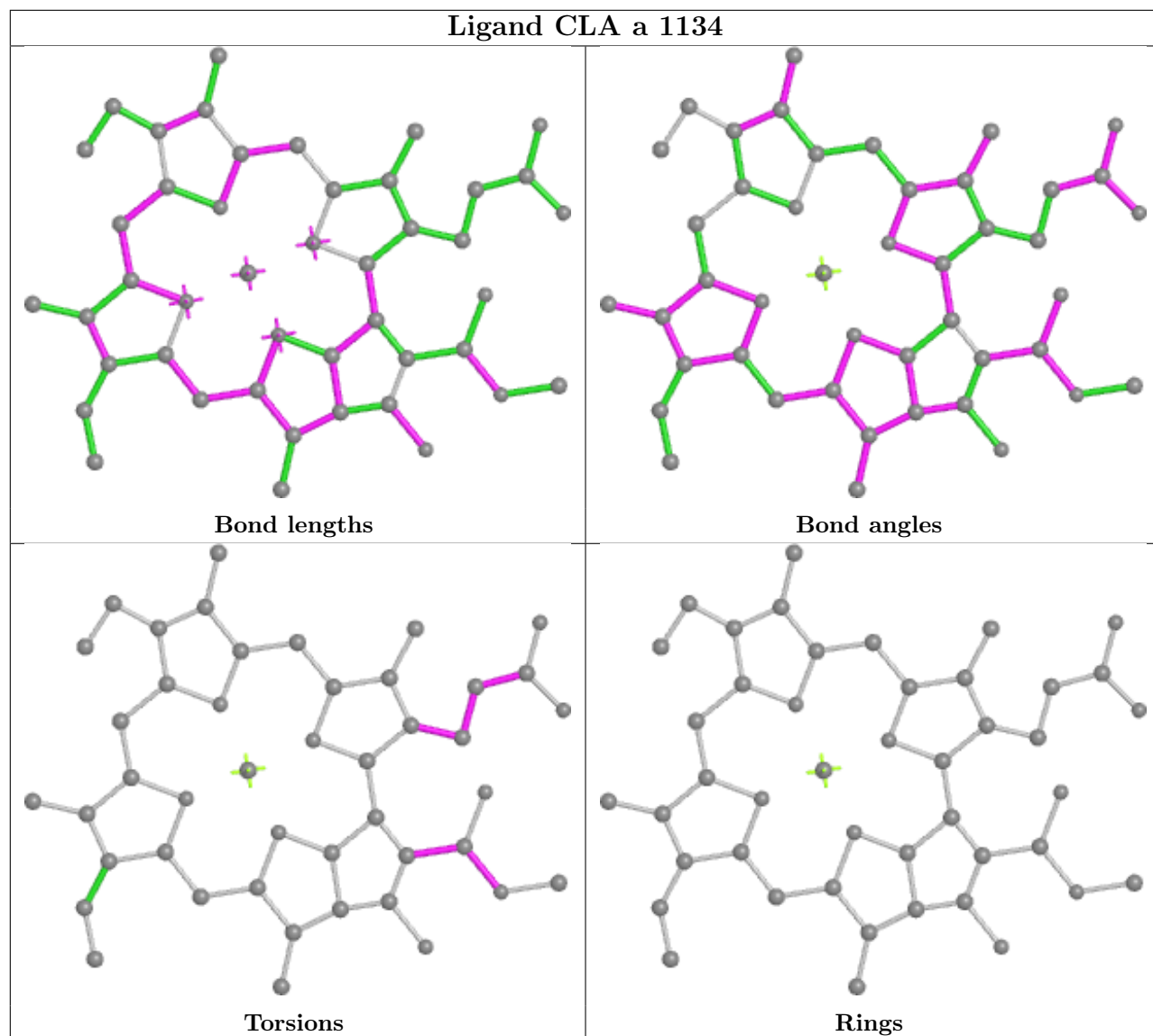




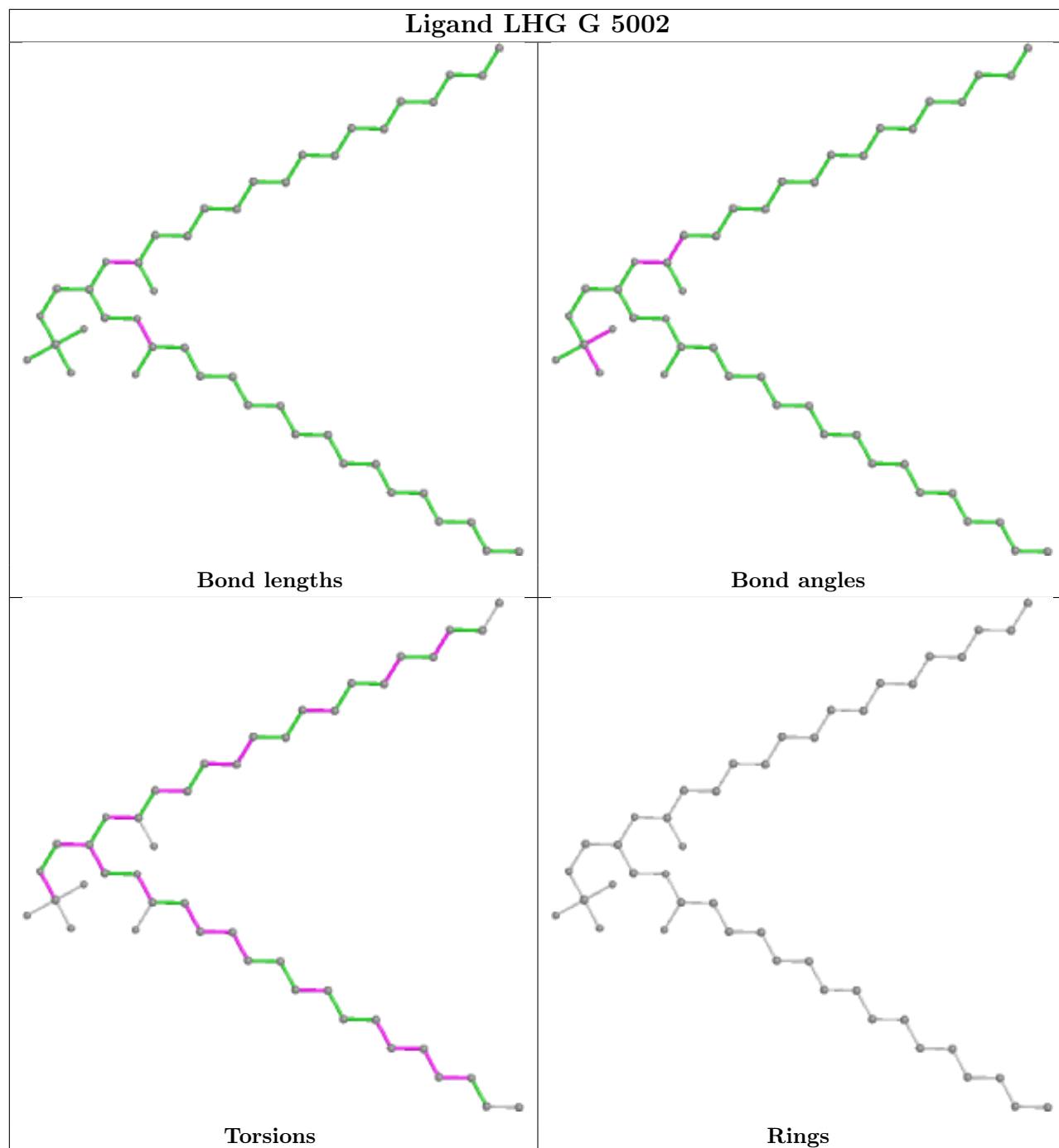


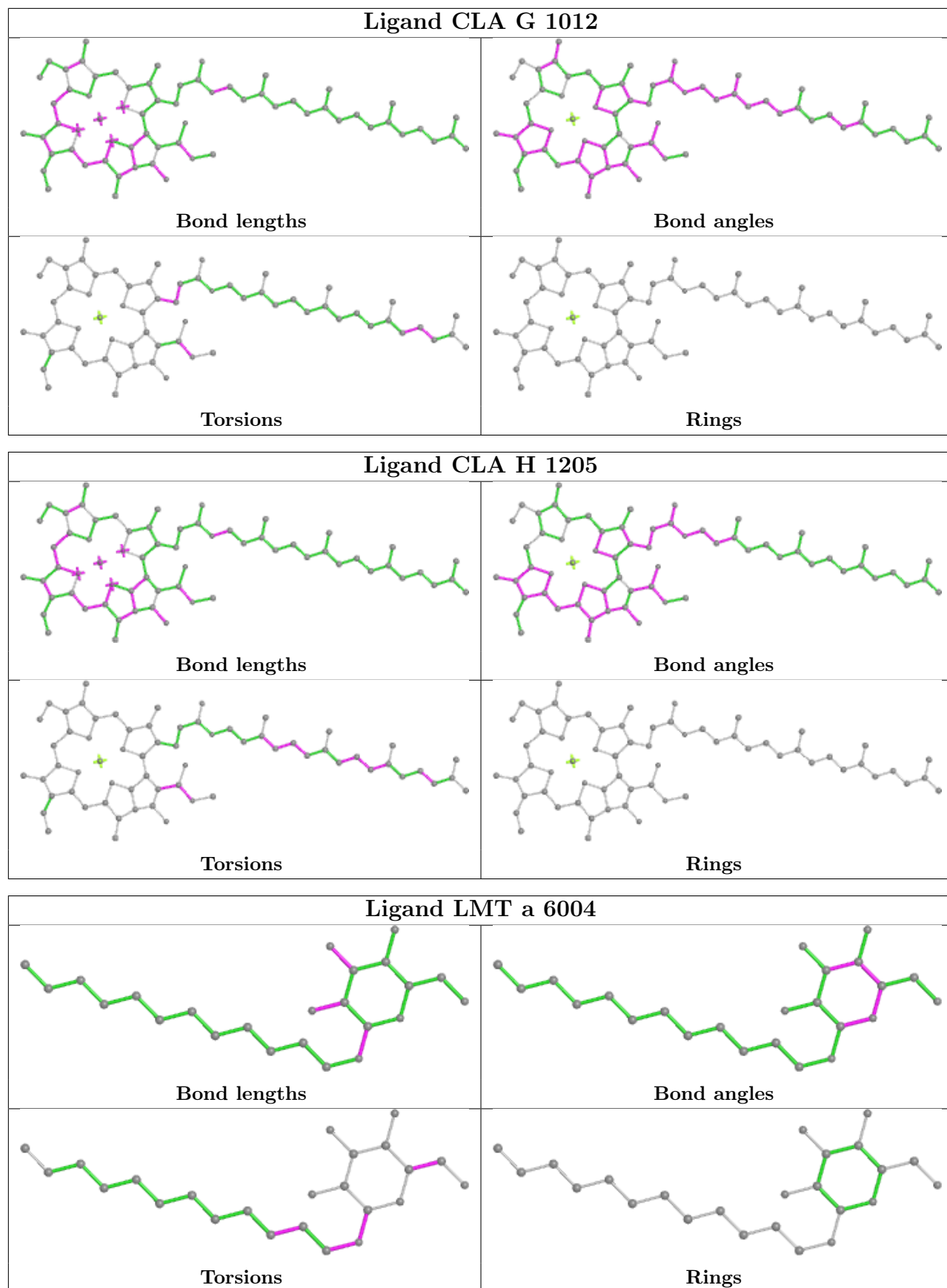


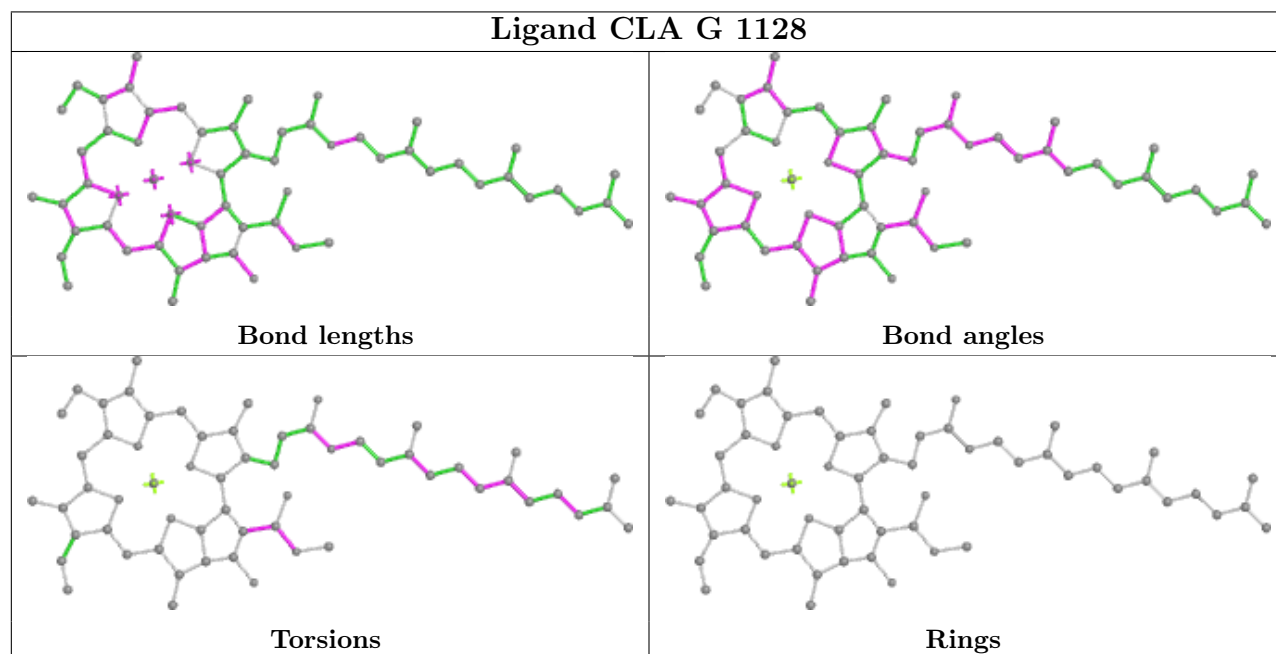
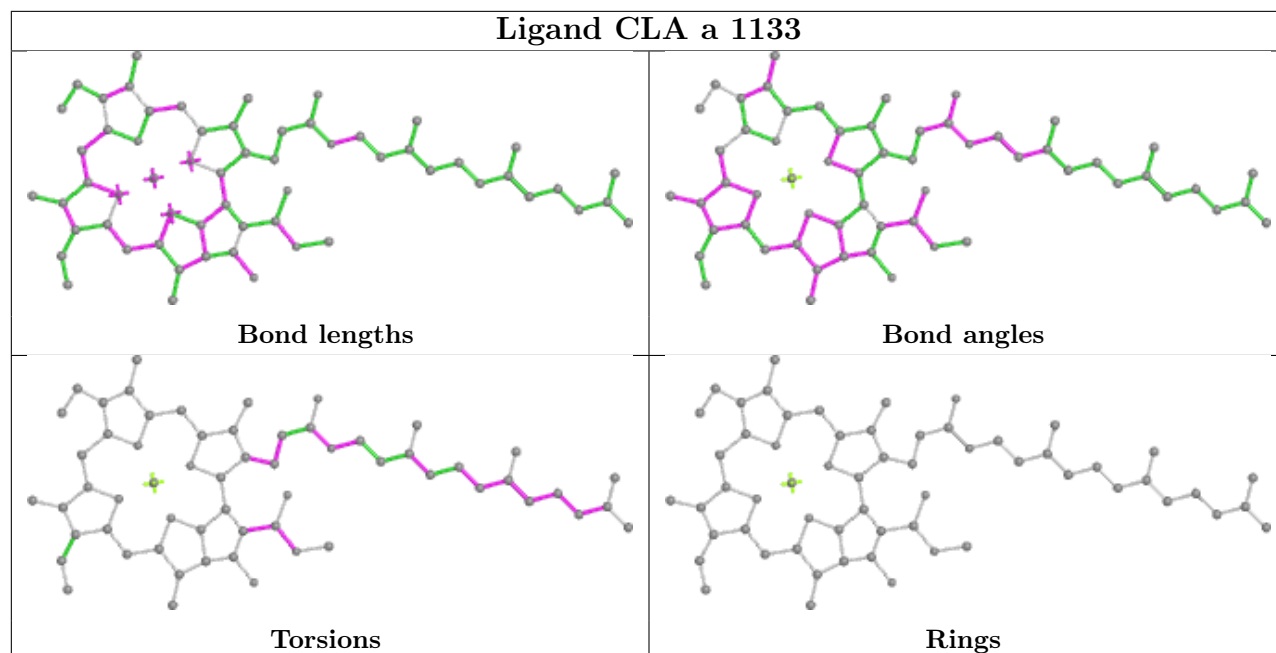


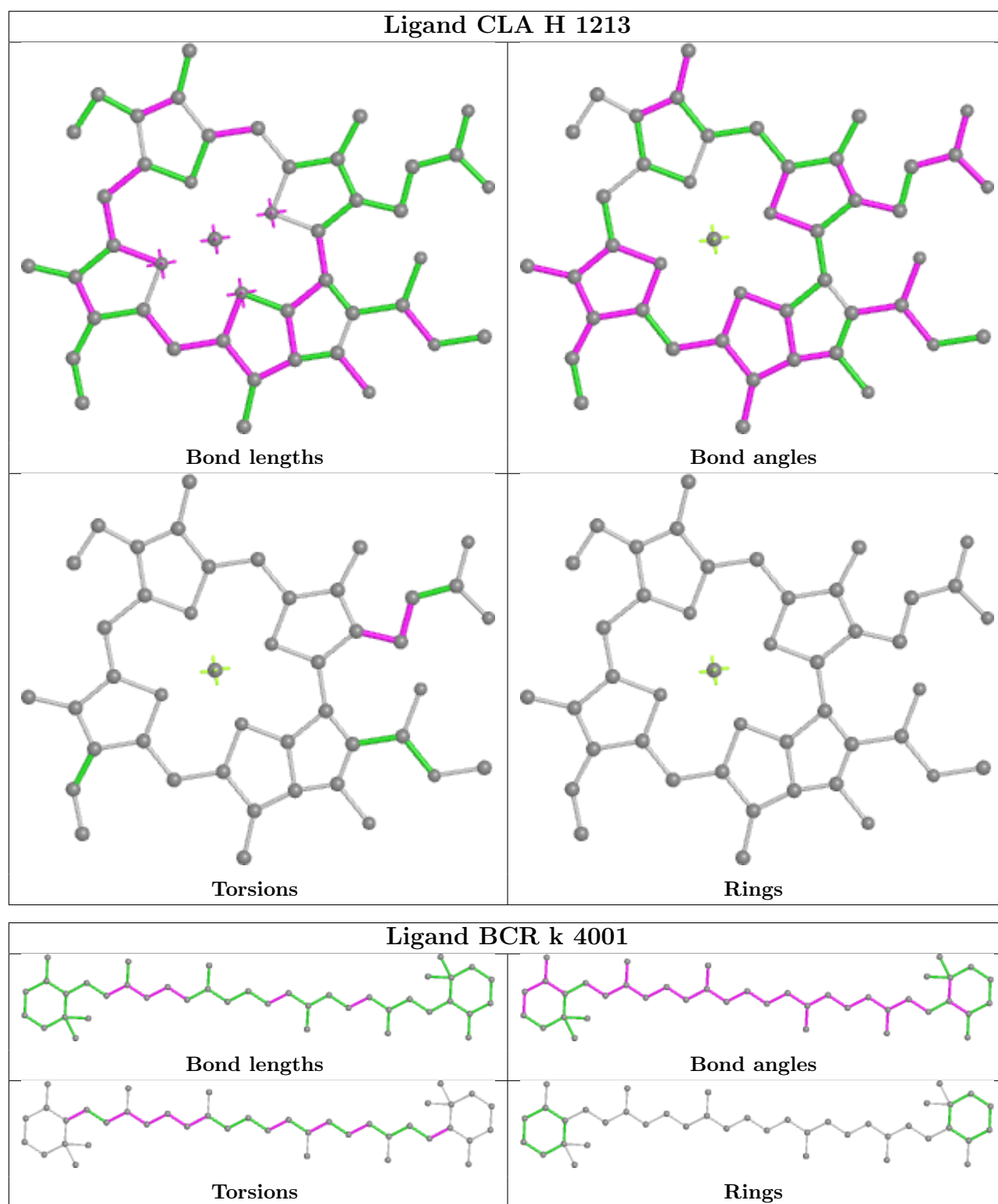


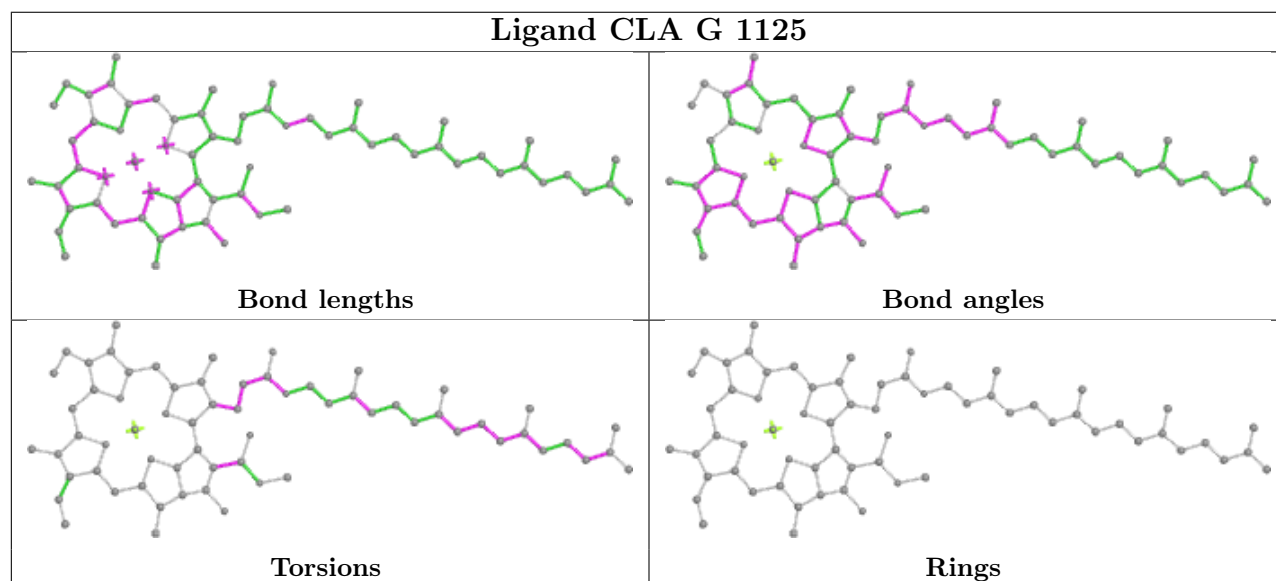
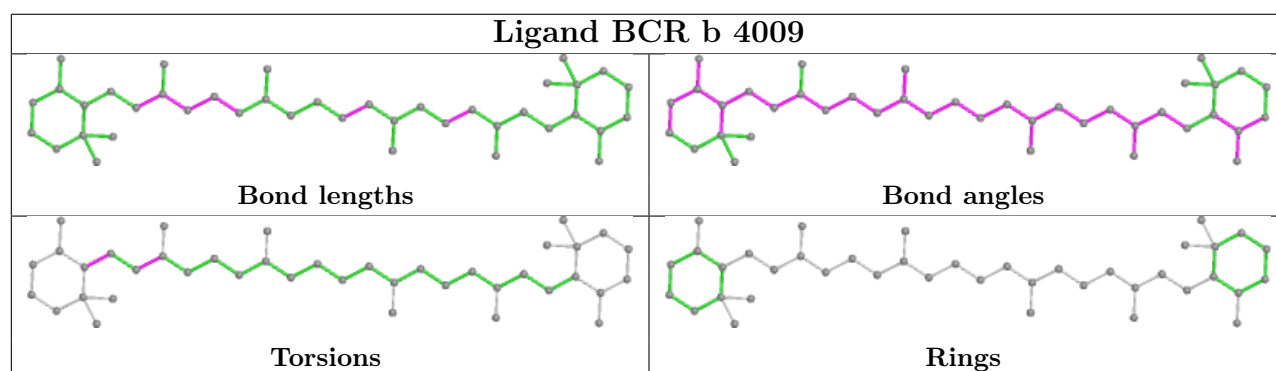
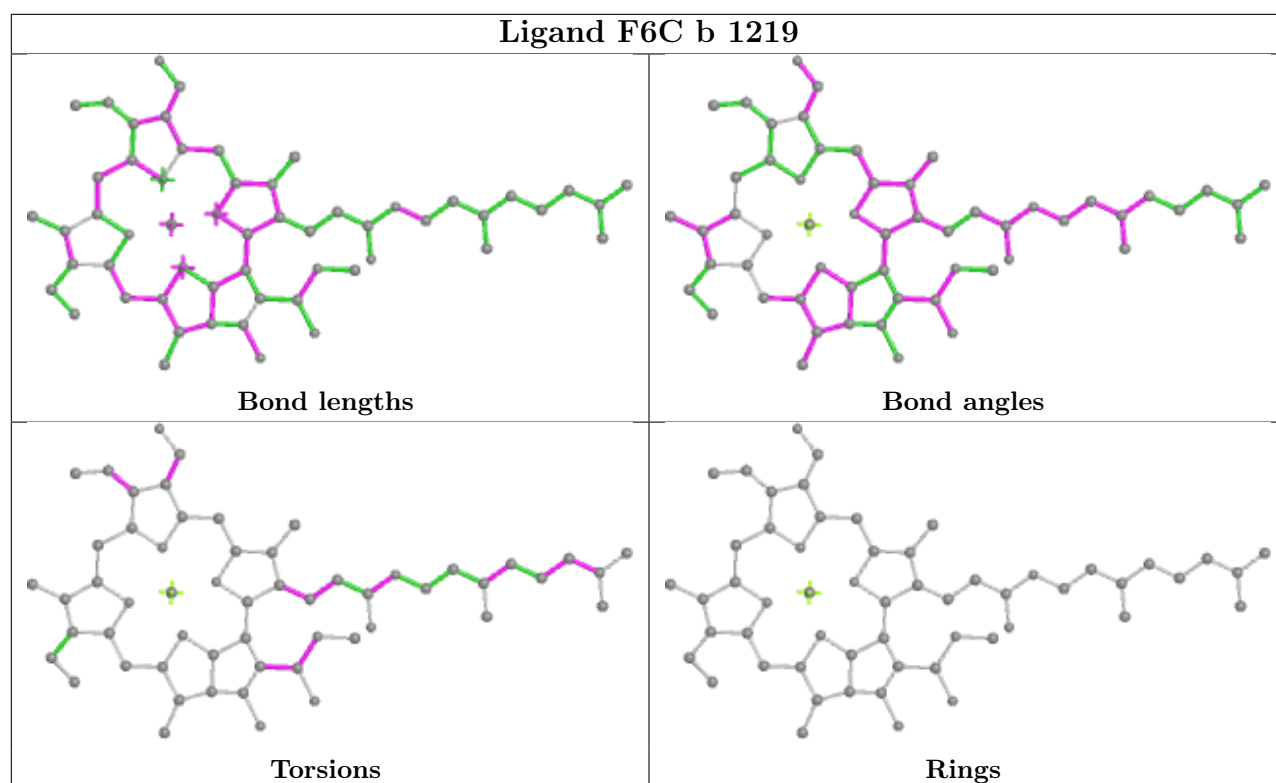


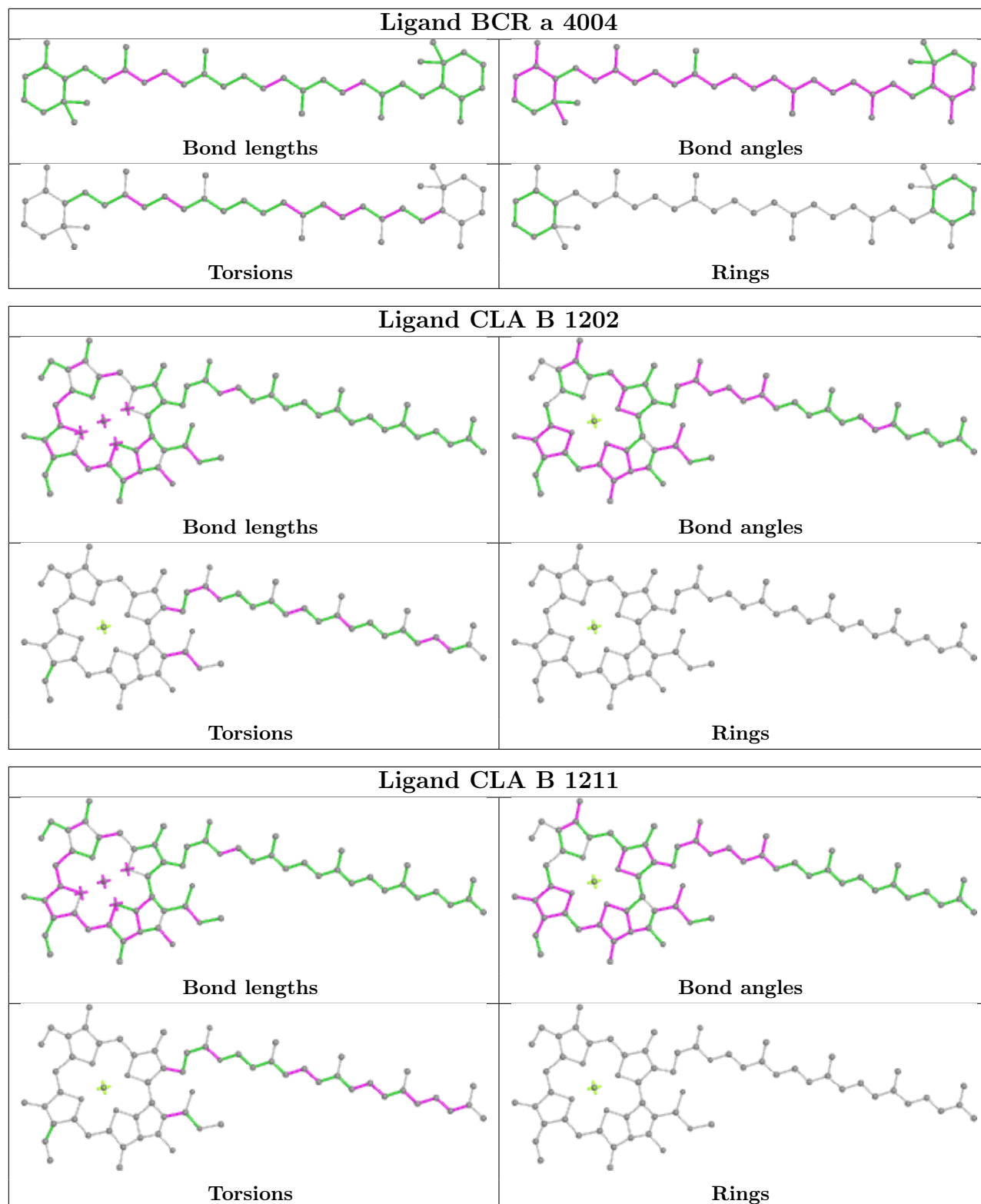


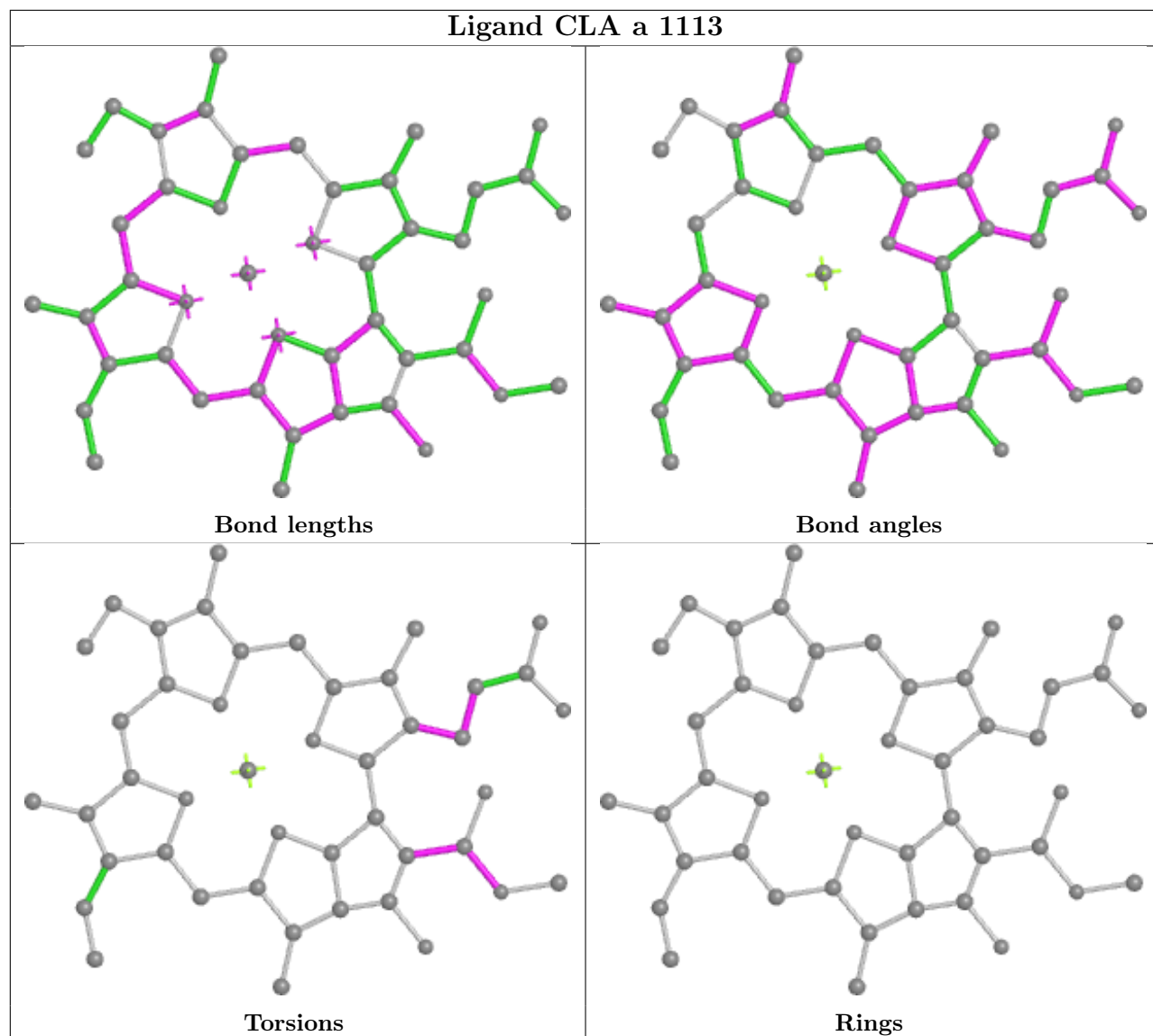


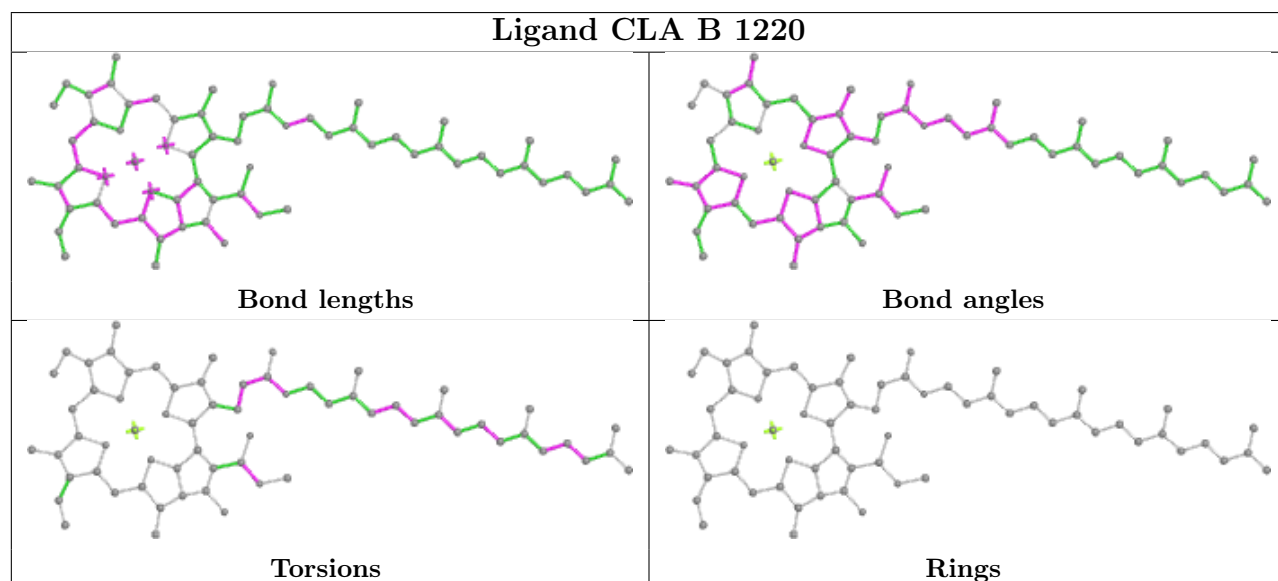
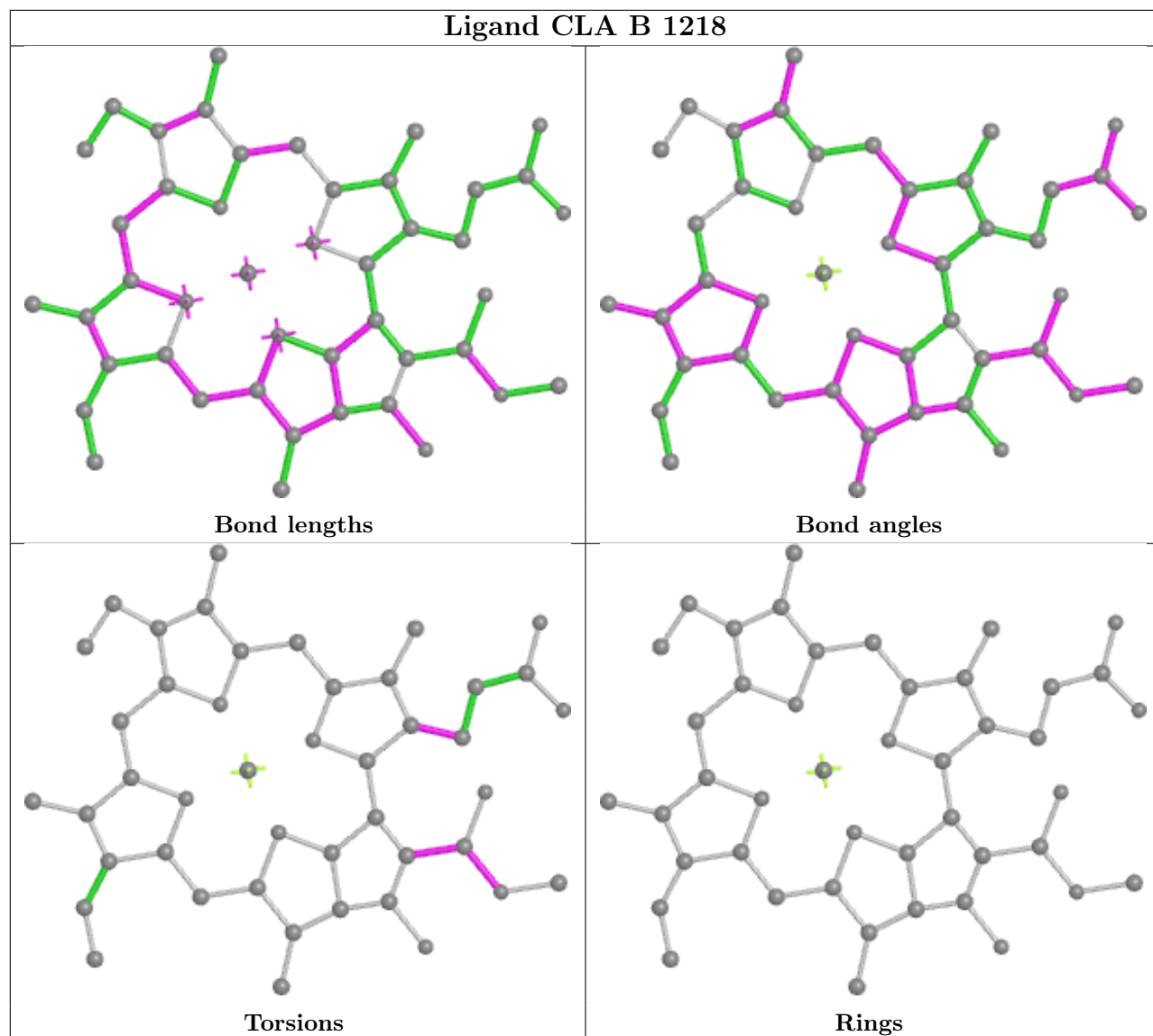




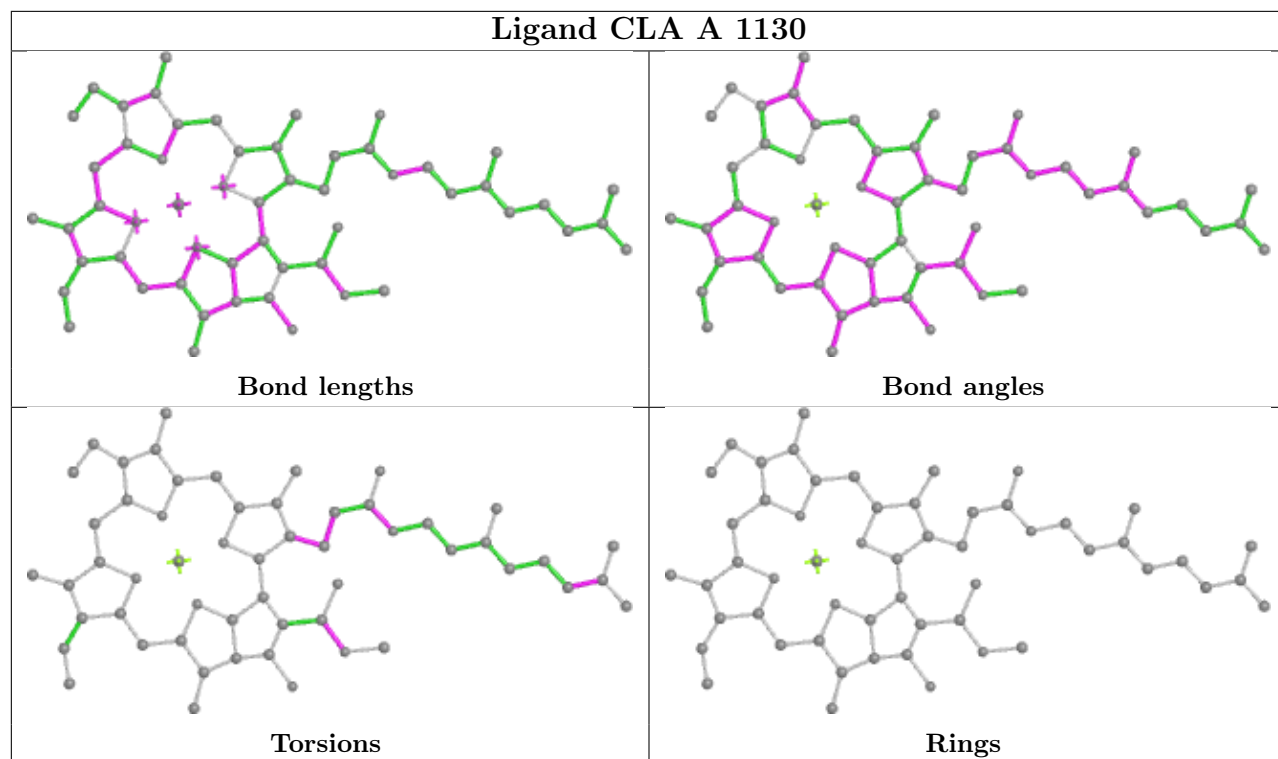


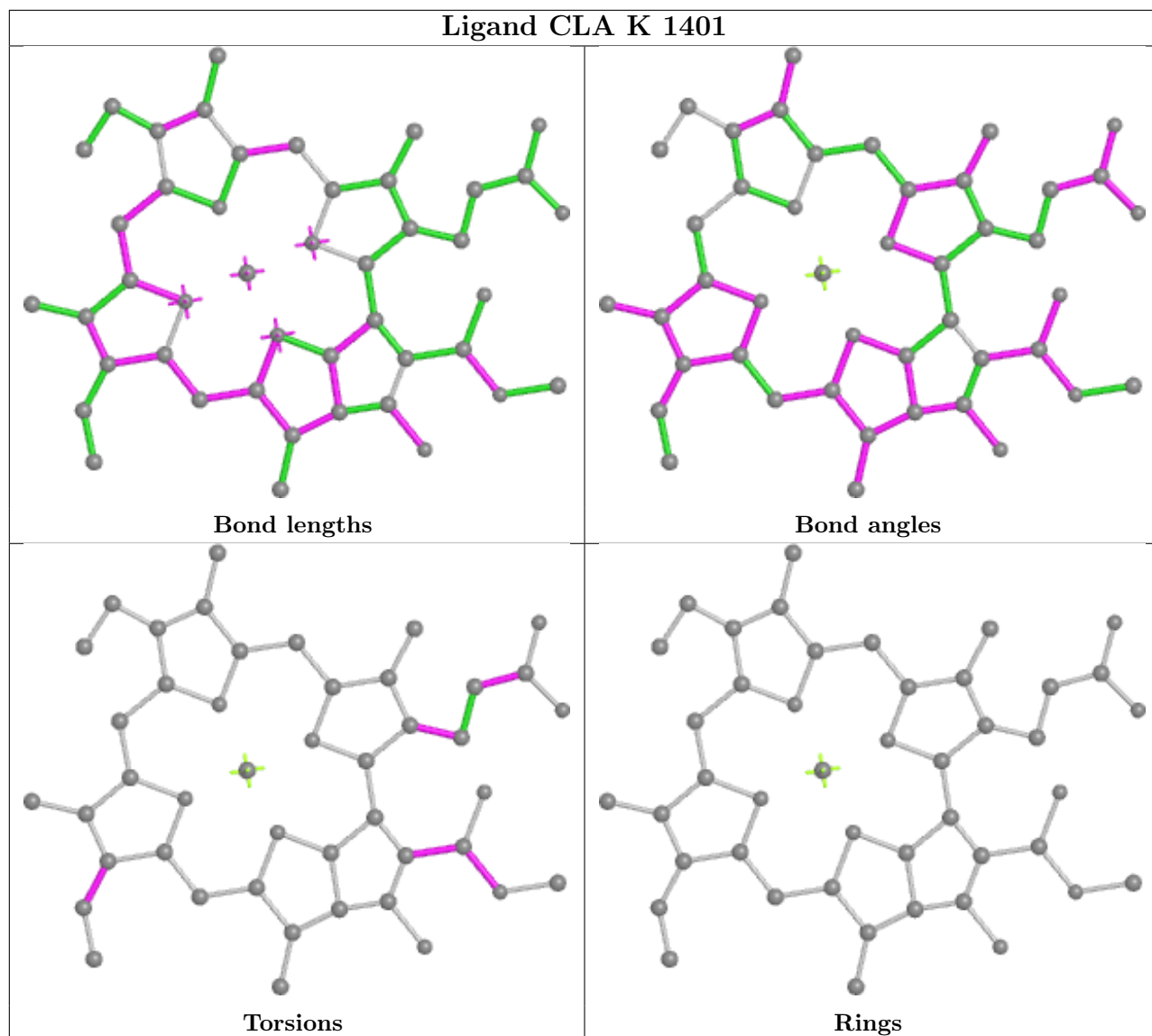


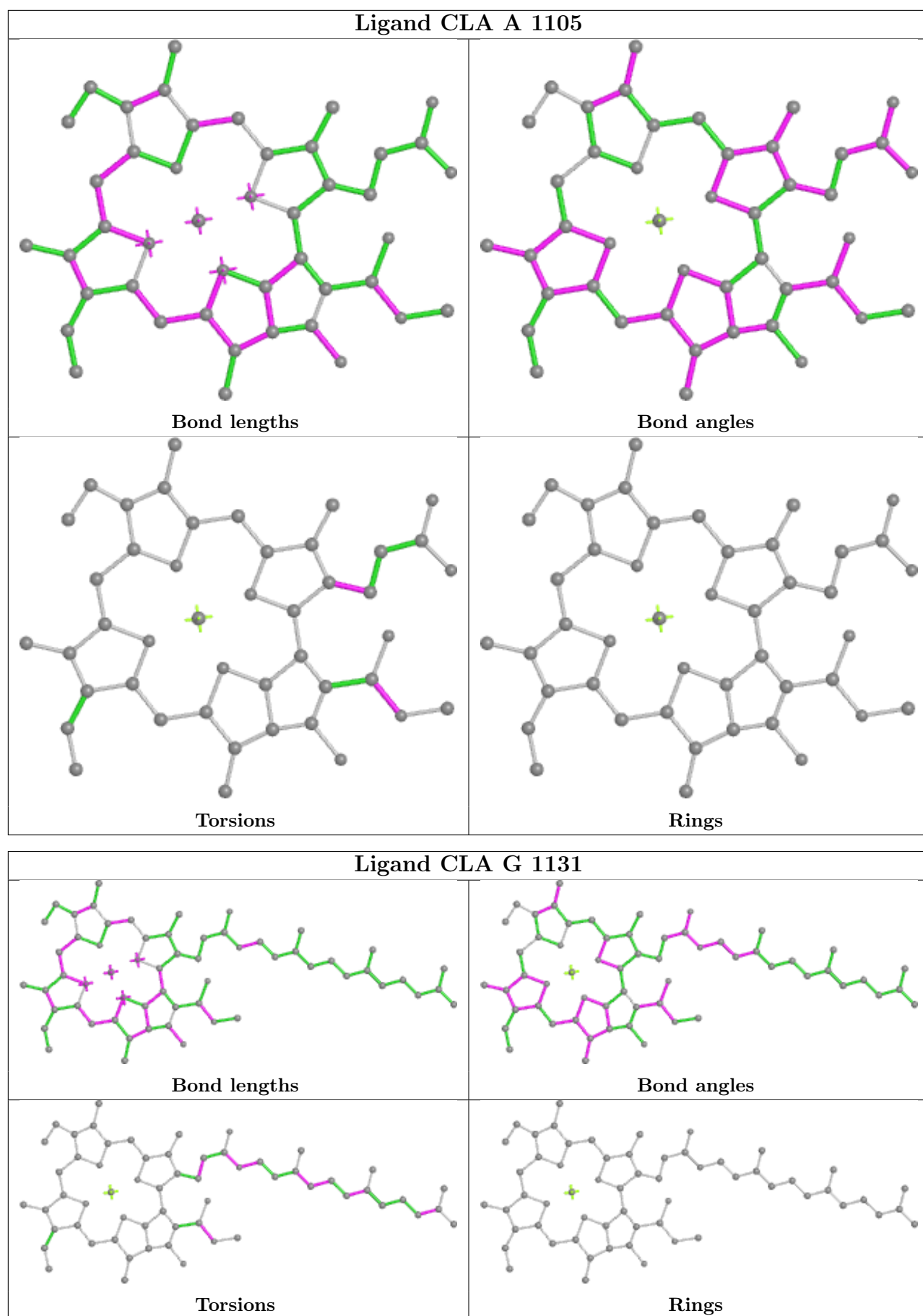


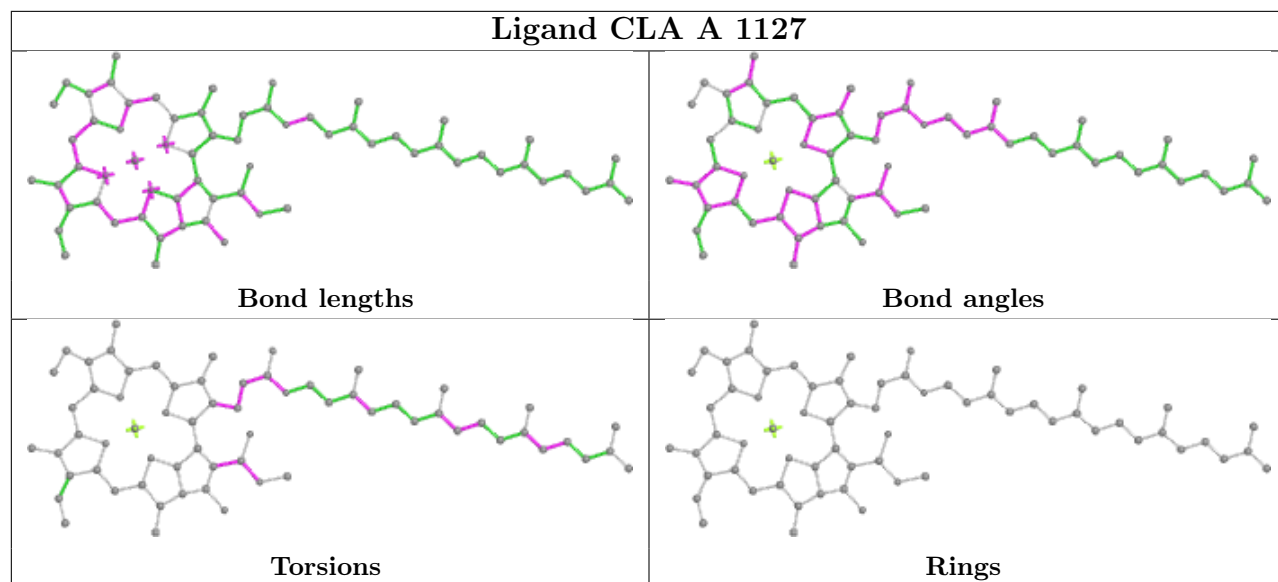


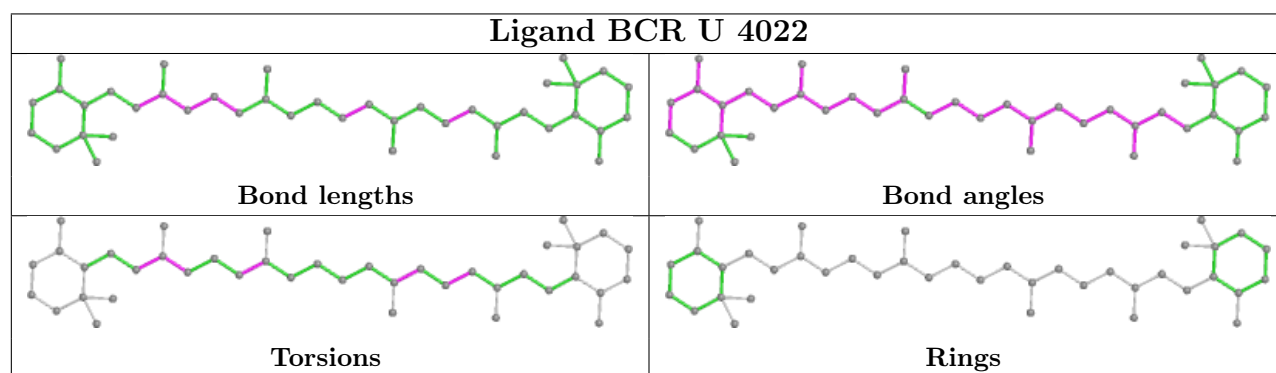
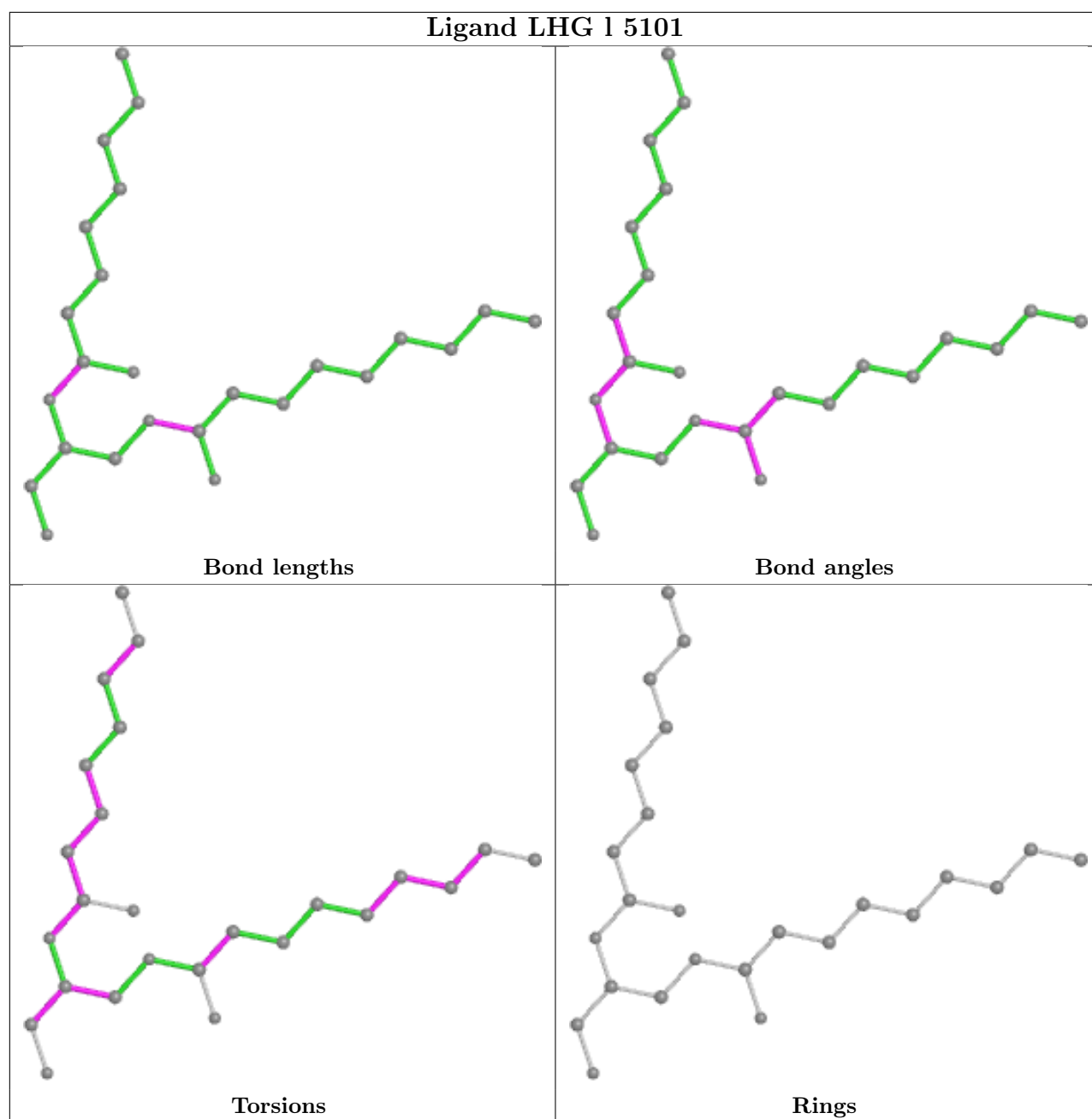


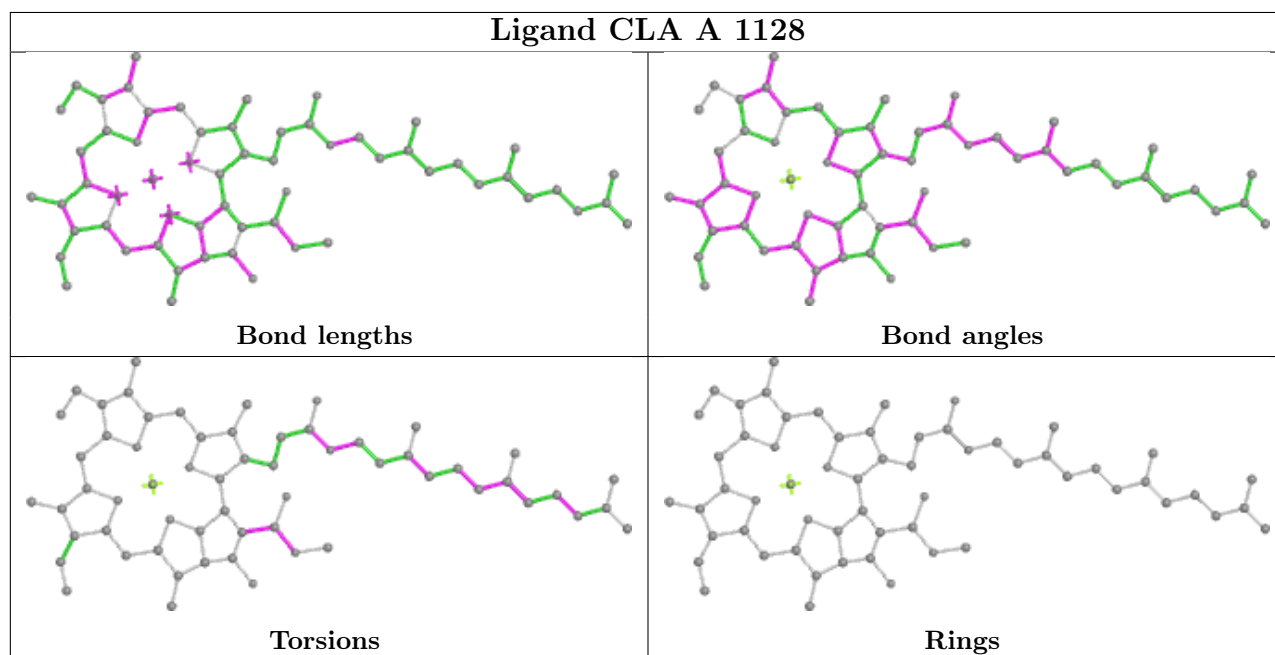
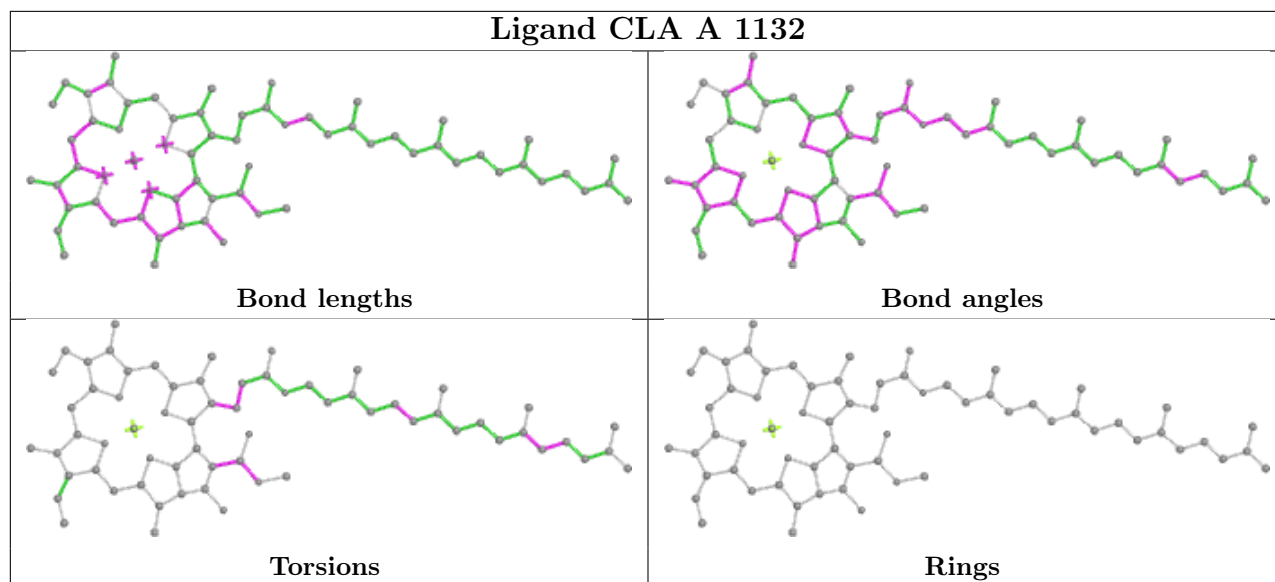


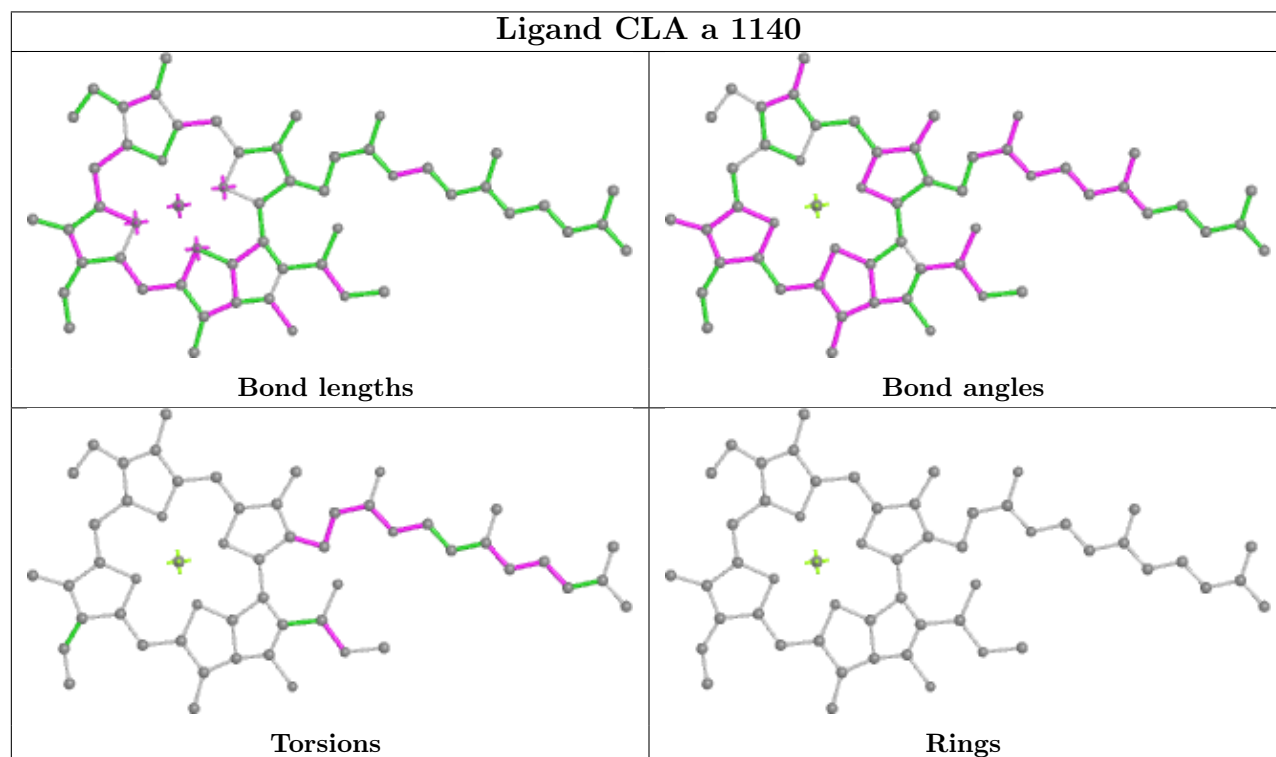
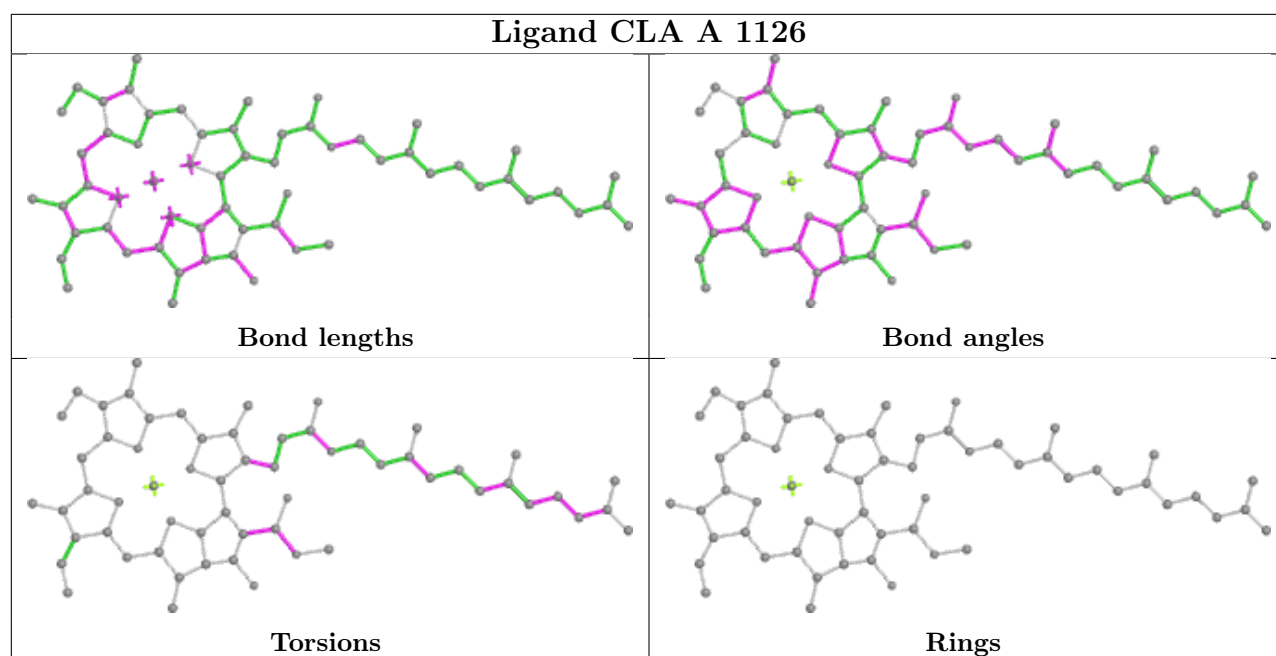












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

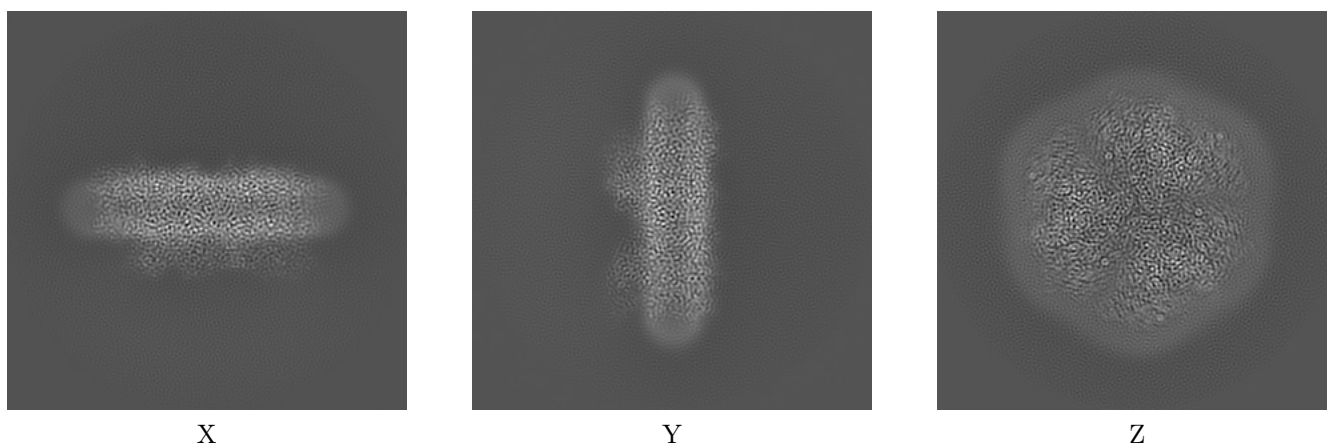
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24821. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

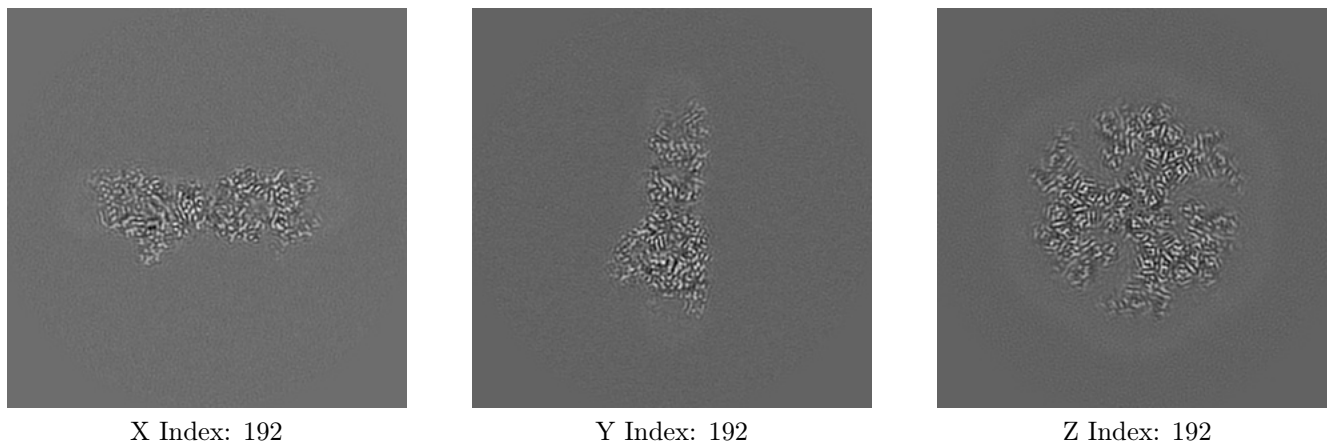
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

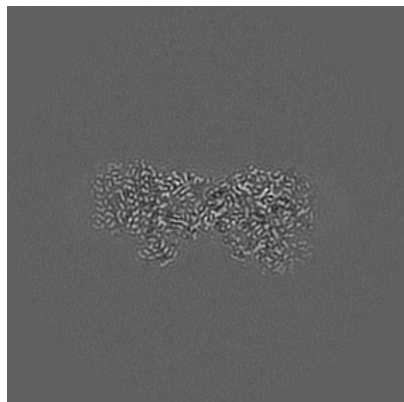




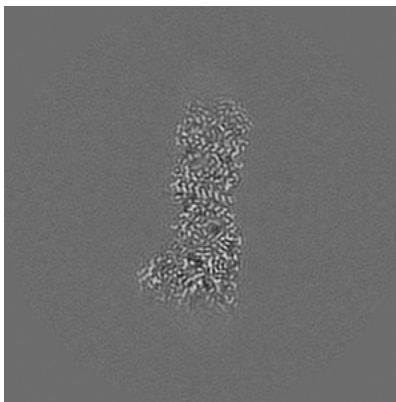
The images above show central slices of the map in three orthogonal directions.

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

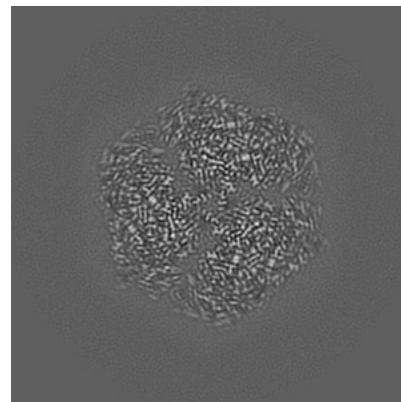
### 6.3.1 Primary map



X Index: 212



Y Index: 180

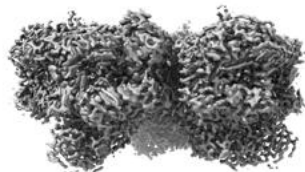


Z Index: 212

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

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

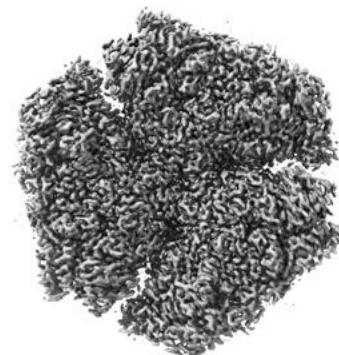
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

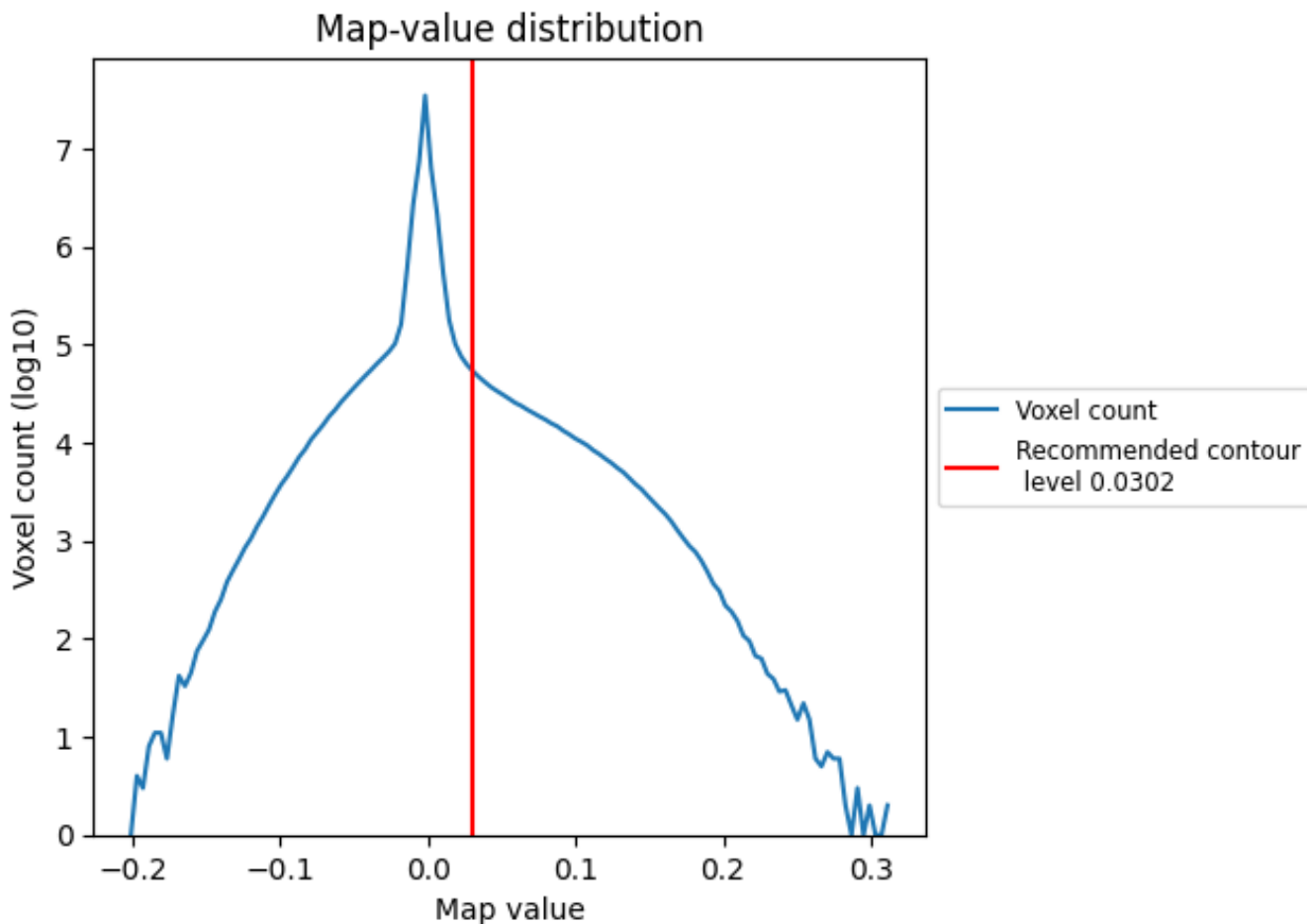
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

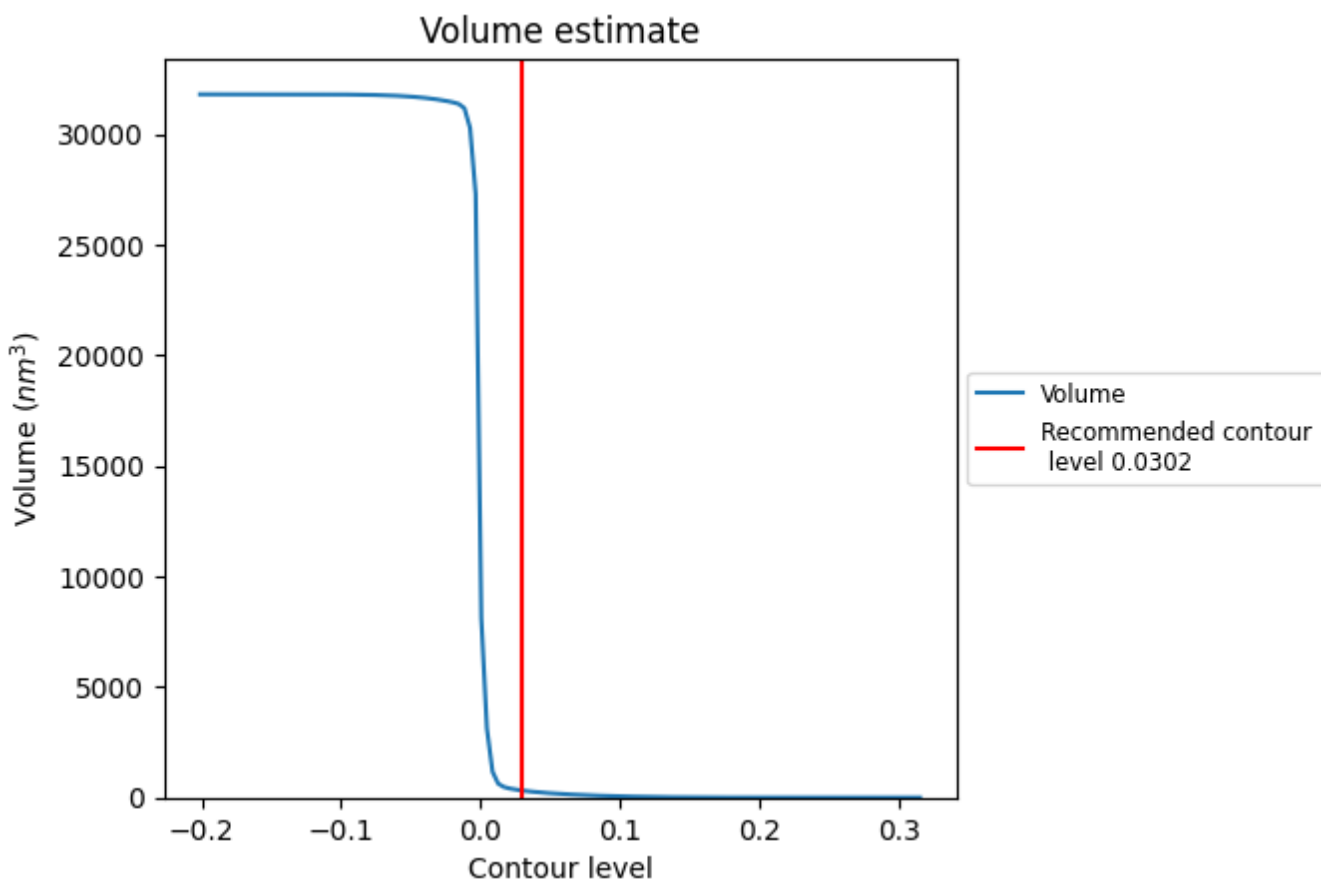
This section contains the results of statistical analysis of the map.

### 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.

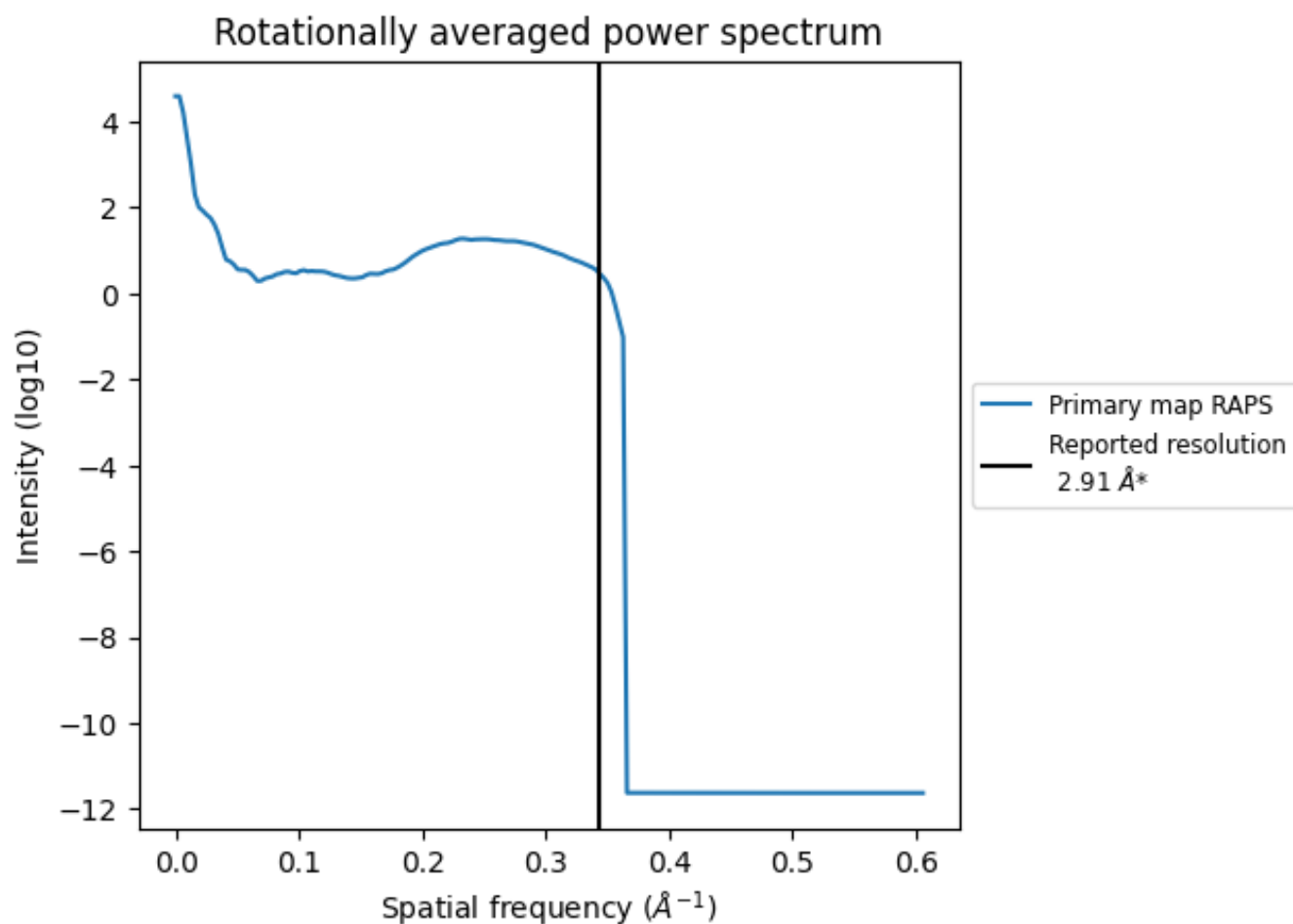
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm<sup>3</sup>; this corresponds to an approximate mass of 286 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

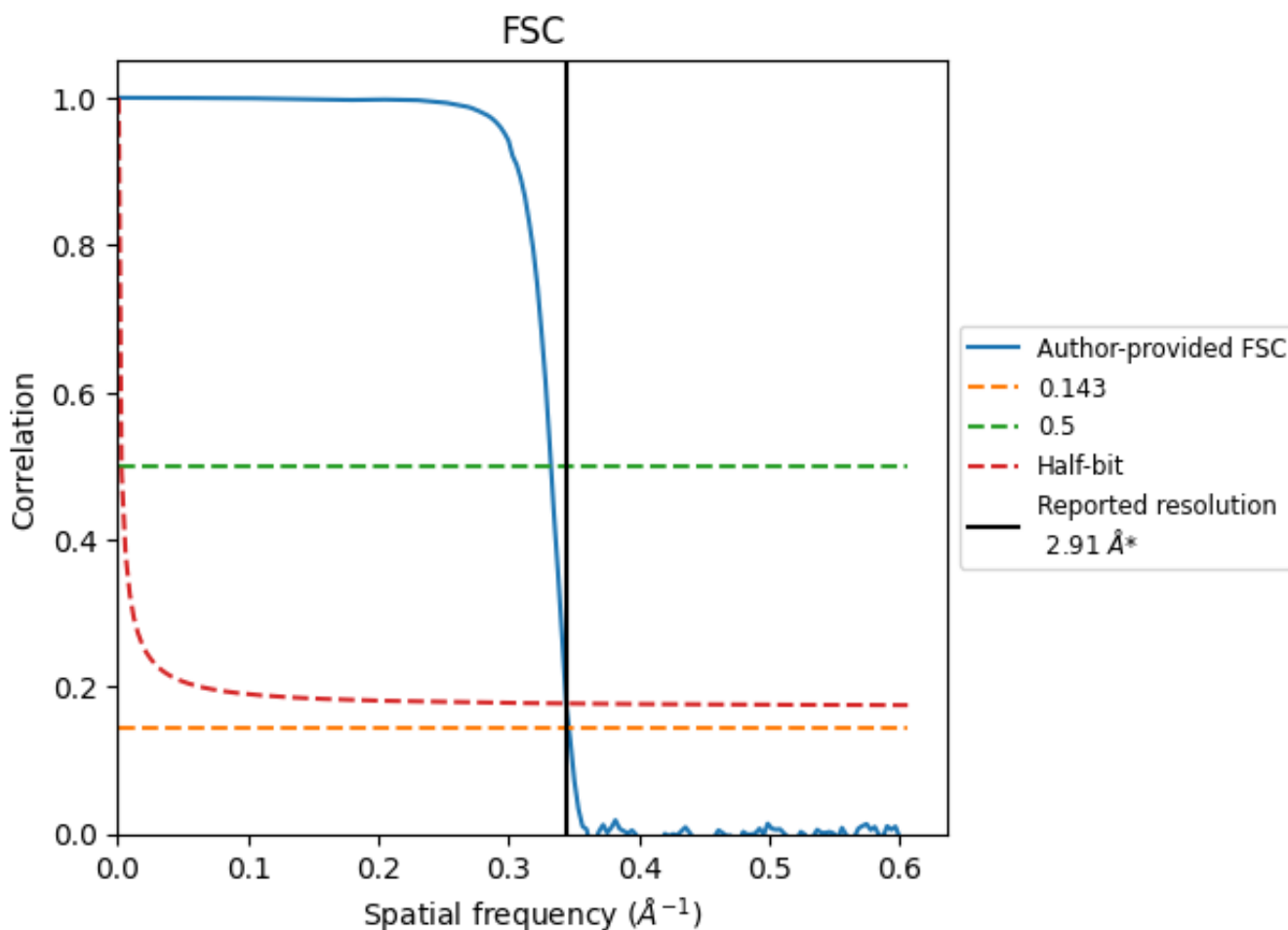


\*Reported resolution corresponds to spatial frequency of  $0.344 \text{\AA}^{-1}$

## 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 0.344 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

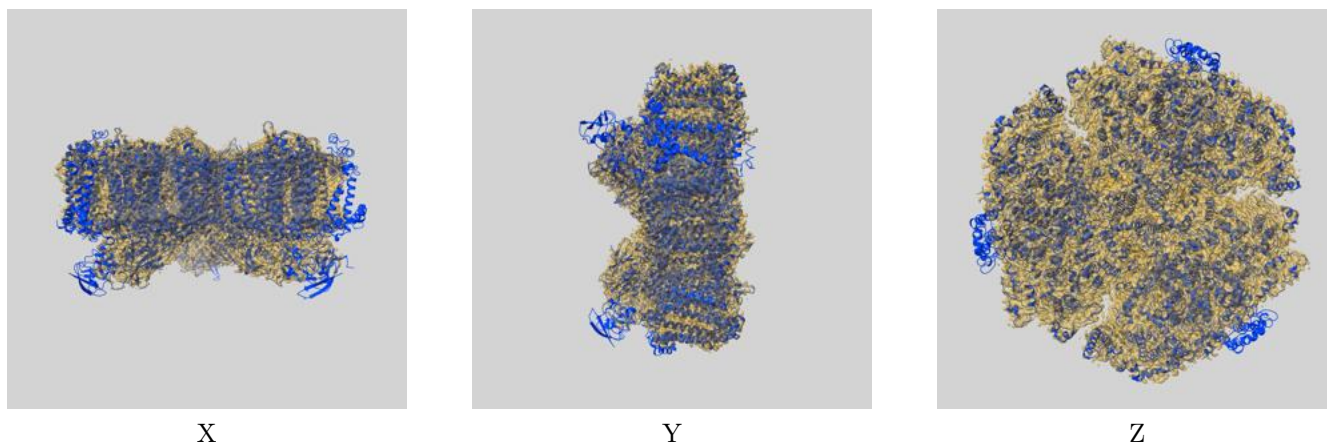
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.91                               | -    | -        |
| Author-provided FSC curve | 2.89                               | 3.01 | 2.91     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-24821 and PDB model 7S3D. Per-residue inclusion information can be found in section 3 on page 40.

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



The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

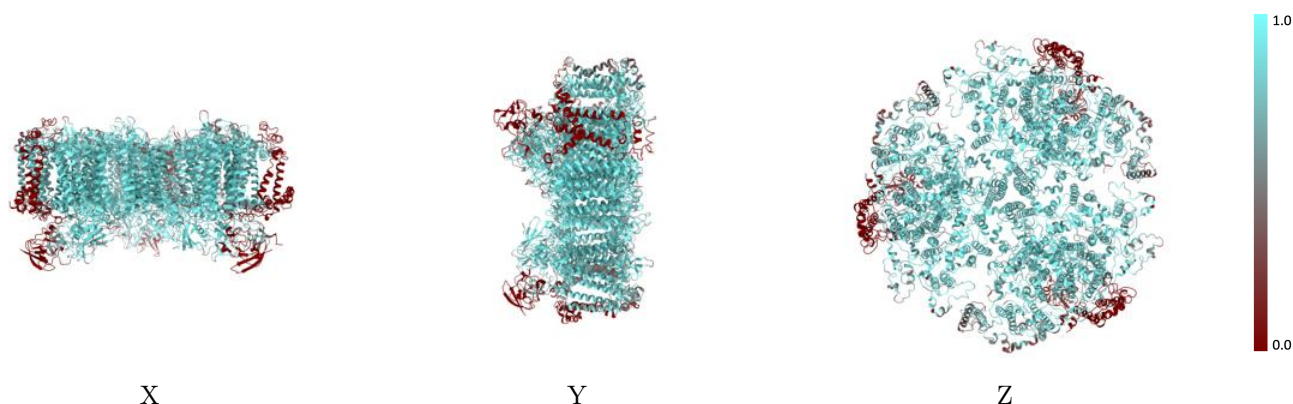


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



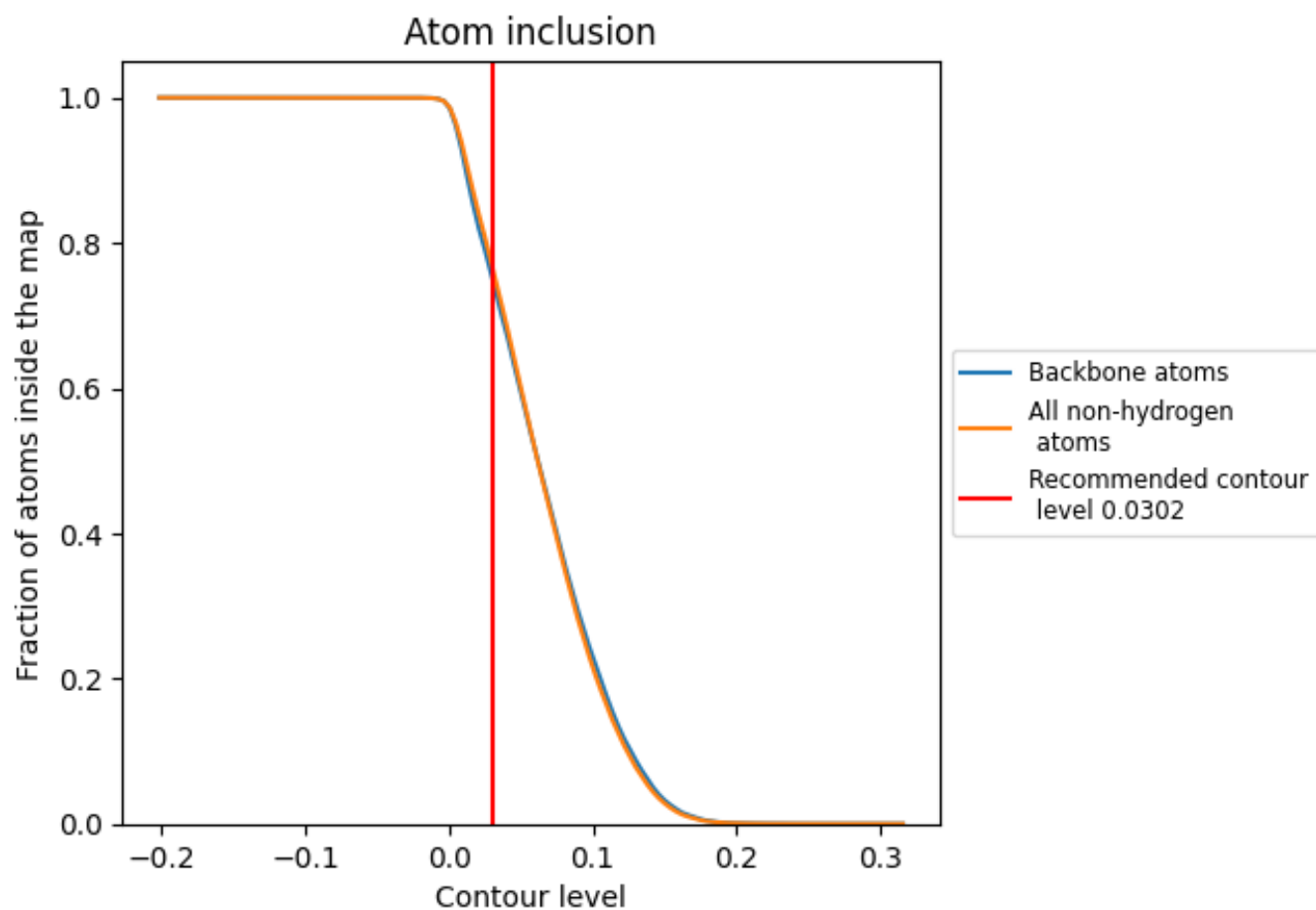
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0302).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.0302) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7668   |  0.5990   |
| A     |  0.8192   |  0.6180   |
| B     |  0.8493   |  0.6180   |
| C     |  0.9231   |  0.6330   |
| D     |  0.7655   |  0.5910   |
| E     |  0.5793   |  0.5940   |
| F     |  0.0061   |  0.4060   |
| G     |  0.8199   |  0.6180   |
| H     |  0.8486   |  0.6180   |
| I     |  0.8914   |  0.6310   |
| J     |  0.0068   |  0.4470   |
| K     |  0.4815   |  0.5480   |
| L     |  0.9186   |  0.6310   |
| M     |  0.8229   |  0.6080   |
| N     |  0.9147  |  0.6340  |
| O     |  0.7599 |  0.5920 |
| P     |  0.5813 |  0.5900 |
| Q     |  0.0049 |  0.4060 |
| R     |  0.8975 |  0.6320 |
| S     |  0.0068 |  0.4420 |
| T     |  0.4765 |  0.5470 |
| U     |  0.9192 |  0.6310 |
| V     |  0.8200 |  0.6090 |
| W     |  0.0000 |  0.3220 |
| X     |  0.0015 |  0.3220 |
| a     |  0.8207 |  0.6180 |
| b     |  0.8490 |  0.6160 |
| c     |  0.9214 |  0.6320 |
| d     |  0.7636 |  0.5910 |
| e     |  0.5711 |  0.5880 |
| f     |  0.0049 |  0.4080 |
| i     |  0.8955 |  0.6300 |
| j     |  0.0068 |  0.4380 |
| k     |  0.4832 |  0.5460 |
| l     |  0.9174 |  0.6310 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| m     |  0.8286 |  0.6040 |
| x     |  0.0015 |  0.3230 |