



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:56 pm BST

PDB ID : 6YP7 / pdb\_00006yp7  
EMDB ID : EMD-10865  
Title : PSII-LHCII C2S2 supercomplex from *Pisum sativum* grown in high light conditions  
Authors : Grinzato, A.; Albanese, P.; Zanutti, G.; Pagliano, C.  
Deposited on : 2020-04-15  
Resolution : 3.80 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:

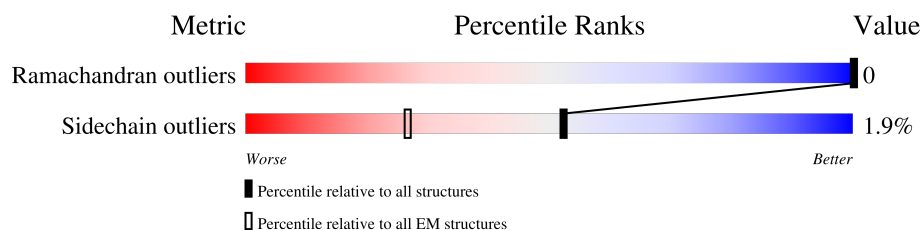
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | G     | 219    | <div> <div>33%</div> <div>98%</div> </div> |
| 1   | N     | 219    | <div> <div>25%</div> <div>98%</div> </div> |
| 1   | Y     | 219    | <div> <div>13%</div> <div>98%</div> </div> |
| 1   | g     | 219    | <div> <div>34%</div> <div>98%</div> </div> |
| 1   | n     | 219    | <div> <div>22%</div> <div>98%</div> </div> |
| 1   | y     | 219    | <div> <div>11%</div> <div>98%</div> </div> |
| 2   | A     | 334    | <div> <div>5%</div> <div>99%</div> </div>  |
| 2   | a     | 334    | <div> <div>•</div> <div>99%</div> </div>   |
| 3   | B     | 503    | <div> <div>7%</div> <div>99%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | b     | 503    | 7%<br>99%        |
| 4   | C     | 450    | 6%<br>98%        |
| 4   | c     | 450    | 5%<br>98%        |
| 5   | D     | 341    | 8%<br>99%        |
| 5   | d     | 341    | 8%<br>99%        |
| 6   | E     | 75     | 17%<br>100%      |
| 6   | e     | 75     | 8%<br>100%       |
| 7   | F     | 30     | 10%<br>97%       |
| 7   | f     | 30     | 10%<br>97%       |
| 8   | H     | 60     | 18%<br>100%      |
| 8   | h     | 60     | 20%<br>100%      |
| 9   | I     | 34     | 6%<br>100%       |
| 9   | i     | 34     | 6%<br>100%       |
| 10  | J     | 35     | 74%<br>100%      |
| 10  | j     | 35     | 69%<br>100%      |
| 11  | K     | 37     | 16%<br>100%      |
| 11  | k     | 37     | 16%<br>100%      |
| 12  | L     | 37     | 14%<br>100%      |
| 12  | l     | 37     | 16%<br>100%      |
| 13  | M     | 33     | 36%<br>100%      |
| 13  | m     | 33     | 39%<br>100%      |
| 14  | O     | 248    | 23%<br>99%       |
| 14  | o     | 248    | 27%<br>99%       |
| 15  | T     | 32     | 25%<br>100%      |
| 15  | t     | 32     | 25%<br>100%      |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 16  | W     | 54     | <div> <div>44%</div> <div>94%</div> <div>6%</div> </div> |
| 16  | w     | 54     | <div> <div>31%</div> <div>94%</div> <div>6%</div> </div> |
| 17  | X     | 39     | <div> <div>23%</div> <div>100%</div> </div>              |
| 17  | x     | 39     | <div> <div>23%</div> <div>100%</div> </div>              |
| 18  | Z     | 62     | <div> <div>21%</div> <div>98%</div> <div>.</div> </div>  |
| 18  | z     | 62     | <div> <div>18%</div> <div>98%</div> <div>.</div> </div>  |
| 19  | R     | 222    | <div> <div>34%</div> <div>98%</div> <div>.</div> </div>  |
| 19  | r     | 222    | <div> <div>32%</div> <div>98%</div> <div>.</div> </div>  |
| 20  | S     | 218    | <div> <div>24%</div> <div>97%</div> <div>.</div> </div>  |
| 20  | s     | 218    | <div> <div>24%</div> <div>97%</div> <div>.</div> </div>  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CHL  | G     | 601 | X         | -        | -       | -                |
| 21  | CHL  | G     | 605 | X         | -        | -       | -                |
| 21  | CHL  | G     | 606 | X         | -        | -       | -                |
| 21  | CHL  | G     | 607 | X         | -        | -       | -                |
| 21  | CHL  | G     | 608 | X         | -        | -       | -                |
| 21  | CHL  | G     | 609 | X         | -        | -       | -                |
| 21  | CHL  | N     | 601 | X         | -        | -       | -                |
| 21  | CHL  | N     | 605 | X         | -        | -       | -                |
| 21  | CHL  | N     | 606 | X         | -        | -       | -                |
| 21  | CHL  | N     | 607 | X         | -        | -       | -                |
| 21  | CHL  | N     | 608 | X         | -        | -       | -                |
| 21  | CHL  | R     | 305 | X         | -        | -       | -                |
| 21  | CHL  | R     | 306 | X         | -        | -       | -                |
| 21  | CHL  | R     | 307 | X         | -        | -       | -                |
| 21  | CHL  | S     | 301 | X         | -        | -       | -                |
| 21  | CHL  | S     | 302 | X         | -        | -       | -                |
| 21  | CHL  | S     | 306 | X         | -        | -       | -                |
| 21  | CHL  | S     | 307 | X         | -        | -       | -                |
| 21  | CHL  | Y     | 601 | X         | -        | -       | -                |
| 21  | CHL  | Y     | 605 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CHL  | Y     | 606 | X         | -        | -       | -                |
| 21  | CHL  | Y     | 607 | X         | -        | -       | -                |
| 21  | CHL  | Y     | 608 | X         | -        | -       | -                |
| 21  | CHL  | g     | 601 | X         | -        | -       | -                |
| 21  | CHL  | g     | 605 | X         | -        | -       | -                |
| 21  | CHL  | g     | 606 | X         | -        | -       | -                |
| 21  | CHL  | g     | 607 | X         | -        | -       | -                |
| 21  | CHL  | g     | 608 | X         | -        | -       | -                |
| 21  | CHL  | g     | 609 | X         | -        | -       | -                |
| 21  | CHL  | n     | 601 | X         | -        | -       | -                |
| 21  | CHL  | n     | 605 | X         | -        | -       | -                |
| 21  | CHL  | n     | 606 | X         | -        | -       | -                |
| 21  | CHL  | n     | 607 | X         | -        | -       | -                |
| 21  | CHL  | n     | 608 | X         | -        | -       | -                |
| 21  | CHL  | r     | 301 | X         | -        | -       | -                |
| 21  | CHL  | r     | 306 | X         | -        | -       | -                |
| 21  | CHL  | r     | 307 | X         | -        | -       | -                |
| 21  | CHL  | r     | 308 | X         | -        | -       | -                |
| 21  | CHL  | s     | 301 | X         | -        | -       | -                |
| 21  | CHL  | s     | 302 | X         | -        | -       | -                |
| 21  | CHL  | s     | 306 | X         | -        | -       | -                |
| 21  | CHL  | s     | 307 | X         | -        | -       | -                |
| 21  | CHL  | y     | 601 | X         | -        | -       | -                |
| 21  | CHL  | y     | 605 | X         | -        | -       | -                |
| 21  | CHL  | y     | 606 | X         | -        | -       | -                |
| 21  | CHL  | y     | 607 | X         | -        | -       | -                |
| 21  | CHL  | y     | 608 | X         | -        | -       | -                |
| 21  | CHL  | y     | 609 | X         | -        | -       | -                |
| 22  | CLA  | A     | 405 | X         | -        | -       | -                |
| 22  | CLA  | A     | 406 | X         | -        | -       | -                |
| 22  | CLA  | A     | 407 | X         | -        | -       | -                |
| 22  | CLA  | A     | 409 | X         | -        | -       | -                |
| 22  | CLA  | B     | 603 | X         | -        | -       | -                |
| 22  | CLA  | B     | 604 | X         | -        | -       | -                |
| 22  | CLA  | B     | 605 | X         | -        | -       | -                |
| 22  | CLA  | B     | 606 | X         | -        | -       | -                |
| 22  | CLA  | B     | 607 | X         | -        | -       | -                |
| 22  | CLA  | B     | 608 | X         | -        | -       | -                |
| 22  | CLA  | B     | 609 | X         | -        | -       | -                |
| 22  | CLA  | B     | 610 | X         | -        | -       | -                |
| 22  | CLA  | B     | 611 | X         | -        | -       | -                |
| 22  | CLA  | B     | 612 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | B     | 613 | X         | -        | -       | -                |
| 22  | CLA  | B     | 614 | X         | -        | -       | -                |
| 22  | CLA  | B     | 615 | X         | -        | -       | -                |
| 22  | CLA  | B     | 616 | X         | -        | -       | -                |
| 22  | CLA  | B     | 617 | X         | -        | -       | -                |
| 22  | CLA  | B     | 618 | X         | -        | -       | -                |
| 22  | CLA  | C     | 503 | X         | -        | -       | -                |
| 22  | CLA  | C     | 504 | X         | -        | -       | -                |
| 22  | CLA  | C     | 505 | X         | -        | -       | -                |
| 22  | CLA  | C     | 506 | X         | -        | -       | -                |
| 22  | CLA  | C     | 507 | X         | -        | -       | -                |
| 22  | CLA  | C     | 508 | X         | -        | -       | -                |
| 22  | CLA  | C     | 509 | X         | -        | -       | -                |
| 22  | CLA  | C     | 510 | X         | -        | -       | -                |
| 22  | CLA  | C     | 511 | X         | -        | -       | -                |
| 22  | CLA  | C     | 512 | X         | -        | -       | -                |
| 22  | CLA  | C     | 513 | X         | -        | -       | -                |
| 22  | CLA  | C     | 514 | X         | -        | -       | -                |
| 22  | CLA  | C     | 515 | X         | -        | -       | -                |
| 22  | CLA  | D     | 404 | X         | -        | -       | -                |
| 22  | CLA  | D     | 405 | X         | -        | -       | -                |
| 22  | CLA  | G     | 602 | X         | -        | -       | -                |
| 22  | CLA  | G     | 603 | X         | -        | -       | -                |
| 22  | CLA  | G     | 604 | X         | -        | -       | -                |
| 22  | CLA  | G     | 610 | X         | -        | -       | -                |
| 22  | CLA  | G     | 611 | X         | -        | -       | -                |
| 22  | CLA  | G     | 612 | X         | -        | -       | -                |
| 22  | CLA  | G     | 613 | X         | -        | -       | -                |
| 22  | CLA  | G     | 614 | X         | -        | -       | -                |
| 22  | CLA  | N     | 602 | X         | -        | -       | -                |
| 22  | CLA  | N     | 603 | X         | -        | -       | -                |
| 22  | CLA  | N     | 604 | X         | -        | -       | -                |
| 22  | CLA  | N     | 609 | X         | -        | -       | -                |
| 22  | CLA  | N     | 610 | X         | -        | -       | -                |
| 22  | CLA  | N     | 611 | X         | -        | -       | -                |
| 22  | CLA  | N     | 612 | X         | -        | -       | -                |
| 22  | CLA  | N     | 613 | X         | -        | -       | -                |
| 22  | CLA  | R     | 302 | X         | -        | -       | -                |
| 22  | CLA  | R     | 303 | X         | -        | -       | -                |
| 22  | CLA  | R     | 304 | X         | -        | -       | -                |
| 22  | CLA  | R     | 308 | X         | -        | -       | -                |
| 22  | CLA  | R     | 309 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | R     | 310 | X         | -        | -       | -                |
| 22  | CLA  | R     | 311 | X         | -        | -       | -                |
| 22  | CLA  | S     | 303 | X         | -        | -       | -                |
| 22  | CLA  | S     | 304 | X         | -        | -       | -                |
| 22  | CLA  | S     | 305 | X         | -        | -       | -                |
| 22  | CLA  | S     | 309 | X         | -        | -       | -                |
| 22  | CLA  | S     | 310 | X         | -        | -       | -                |
| 22  | CLA  | S     | 311 | X         | -        | -       | -                |
| 22  | CLA  | S     | 312 | X         | -        | -       | -                |
| 22  | CLA  | S     | 313 | X         | -        | -       | -                |
| 22  | CLA  | W     | 101 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 602 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 603 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 604 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 609 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 610 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 611 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 612 | X         | -        | -       | -                |
| 22  | CLA  | a     | 404 | X         | -        | -       | -                |
| 22  | CLA  | a     | 405 | X         | -        | -       | -                |
| 22  | CLA  | a     | 406 | X         | -        | -       | -                |
| 22  | CLA  | a     | 408 | X         | -        | -       | -                |
| 22  | CLA  | b     | 601 | X         | -        | -       | -                |
| 22  | CLA  | b     | 602 | X         | -        | -       | -                |
| 22  | CLA  | b     | 603 | X         | -        | -       | -                |
| 22  | CLA  | b     | 604 | X         | -        | -       | -                |
| 22  | CLA  | b     | 605 | X         | -        | -       | -                |
| 22  | CLA  | b     | 606 | X         | -        | -       | -                |
| 22  | CLA  | b     | 607 | X         | -        | -       | -                |
| 22  | CLA  | b     | 608 | X         | -        | -       | -                |
| 22  | CLA  | b     | 609 | X         | -        | -       | -                |
| 22  | CLA  | b     | 610 | X         | -        | -       | -                |
| 22  | CLA  | b     | 611 | X         | -        | -       | -                |
| 22  | CLA  | b     | 612 | X         | -        | -       | -                |
| 22  | CLA  | b     | 613 | X         | -        | -       | -                |
| 22  | CLA  | b     | 614 | X         | -        | -       | -                |
| 22  | CLA  | b     | 615 | X         | -        | -       | -                |
| 22  | CLA  | c     | 502 | X         | -        | -       | -                |
| 22  | CLA  | c     | 503 | X         | -        | -       | -                |
| 22  | CLA  | c     | 504 | X         | -        | -       | -                |
| 22  | CLA  | c     | 505 | X         | -        | -       | -                |
| 22  | CLA  | c     | 506 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | c     | 507 | X         | -        | -       | -                |
| 22  | CLA  | c     | 508 | X         | -        | -       | -                |
| 22  | CLA  | c     | 509 | X         | -        | -       | -                |
| 22  | CLA  | c     | 510 | X         | -        | -       | -                |
| 22  | CLA  | c     | 511 | X         | -        | -       | -                |
| 22  | CLA  | c     | 512 | X         | -        | -       | -                |
| 22  | CLA  | c     | 513 | X         | -        | -       | -                |
| 22  | CLA  | c     | 514 | X         | -        | -       | -                |
| 22  | CLA  | d     | 403 | X         | -        | -       | -                |
| 22  | CLA  | d     | 404 | X         | -        | -       | -                |
| 22  | CLA  | g     | 602 | X         | -        | -       | -                |
| 22  | CLA  | g     | 603 | X         | -        | -       | -                |
| 22  | CLA  | g     | 604 | X         | -        | -       | -                |
| 22  | CLA  | g     | 610 | X         | -        | -       | -                |
| 22  | CLA  | g     | 611 | X         | -        | -       | -                |
| 22  | CLA  | g     | 612 | X         | -        | -       | -                |
| 22  | CLA  | g     | 613 | X         | -        | -       | -                |
| 22  | CLA  | g     | 614 | X         | -        | -       | -                |
| 22  | CLA  | n     | 602 | X         | -        | -       | -                |
| 22  | CLA  | n     | 603 | X         | -        | -       | -                |
| 22  | CLA  | n     | 604 | X         | -        | -       | -                |
| 22  | CLA  | n     | 609 | X         | -        | -       | -                |
| 22  | CLA  | n     | 610 | X         | -        | -       | -                |
| 22  | CLA  | n     | 611 | X         | -        | -       | -                |
| 22  | CLA  | n     | 612 | X         | -        | -       | -                |
| 22  | CLA  | n     | 613 | X         | -        | -       | -                |
| 22  | CLA  | r     | 303 | X         | -        | -       | -                |
| 22  | CLA  | r     | 304 | X         | -        | -       | -                |
| 22  | CLA  | r     | 305 | X         | -        | -       | -                |
| 22  | CLA  | r     | 309 | X         | -        | -       | -                |
| 22  | CLA  | r     | 310 | X         | -        | -       | -                |
| 22  | CLA  | r     | 311 | X         | -        | -       | -                |
| 22  | CLA  | r     | 312 | X         | -        | -       | -                |
| 22  | CLA  | s     | 303 | X         | -        | -       | -                |
| 22  | CLA  | s     | 304 | X         | -        | -       | -                |
| 22  | CLA  | s     | 305 | X         | -        | -       | -                |
| 22  | CLA  | s     | 309 | X         | -        | -       | -                |
| 22  | CLA  | s     | 310 | X         | -        | -       | -                |
| 22  | CLA  | s     | 311 | X         | -        | -       | -                |
| 22  | CLA  | s     | 312 | X         | -        | -       | -                |
| 22  | CLA  | s     | 313 | X         | -        | -       | -                |
| 22  | CLA  | w     | 101 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | x     | 101 | X         | -        | -       | -                |
| 22  | CLA  | y     | 602 | X         | -        | -       | -                |
| 22  | CLA  | y     | 603 | X         | -        | -       | -                |
| 22  | CLA  | y     | 604 | X         | -        | -       | -                |
| 22  | CLA  | y     | 610 | X         | -        | -       | -                |
| 22  | CLA  | y     | 611 | X         | -        | -       | -                |
| 22  | CLA  | y     | 612 | X         | -        | -       | -                |
| 22  | CLA  | y     | 613 | X         | -        | -       | -                |
| 24  | XAT  | G     | 617 | X         | -        | -       | -                |
| 24  | XAT  | N     | 616 | X         | -        | -       | -                |
| 24  | XAT  | R     | 313 | X         | -        | -       | -                |
| 24  | XAT  | Y     | 615 | X         | -        | -       | -                |
| 24  | XAT  | g     | 617 | X         | -        | -       | -                |
| 24  | XAT  | n     | 615 | X         | -        | -       | -                |
| 24  | XAT  | r     | 314 | X         | -        | -       | -                |
| 24  | XAT  | y     | 615 | X         | -        | -       | -                |
| 25  | NEX  | N     | 617 | X         | -        | -       | -                |
| 25  | NEX  | Y     | 616 | X         | -        | -       | -                |
| 25  | NEX  | g     | 618 | X         | -        | -       | -                |
| 25  | NEX  | n     | 616 | X         | -        | -       | -                |
| 25  | NEX  | r     | 315 | X         | -        | -       | -                |
| 25  | NEX  | y     | 616 | X         | -        | -       | -                |
| 25  | NEX  | y     | 618 | X         | -        | -       | -                |
| 33  | SQD  | D     | 402 | X         | -        | -       | -                |
| 33  | SQD  | d     | 402 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 71784 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 Chlorophyll a-b binding protein 8, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | g     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | n     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | y     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | G     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | N     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | Y     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |

- Molecule 2 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | a     | 334      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2616  | 1708 | 431 | 464 | 13 |         |       |
| 2   | A     | 334      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2616  | 1708 | 431 | 464 | 13 |         |       |

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | b     | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3948  | 2581 | 669 | 686 | 12 |         |       |
| 3   | B     | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3948  | 2581 | 669 | 686 | 12 |         |       |

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | c     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3497  | 2300 | 583 | 604 | 10 |         |       |
| 4   | C     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3497  | 2300 | 583 | 604 | 10 |         |       |

- Molecule 5 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | d     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1790 | 444 | 466 | 12 |         |       |
| 5   | D     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1790 | 444 | 466 | 12 |         |       |

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | e     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 400 | 100 | 112 |         |       |
| 6   | E     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 400 | 100 | 112 |         |       |

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | f     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 41 | 37 | 1 |         |       |
| 7   | F     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 41 | 37 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| f     | 26      | PHE      | SER    | conflict | UNP P62096 |
| F     | 26      | PHE      | SER    | conflict | UNP P62096 |

- Molecule 8 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | h     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 296 | 72 | 81 | 3 |         |       |
| 8   | H     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 296 | 72 | 81 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | i     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 278   | 191 | 43 | 43 | 1 |         |       |
| 9   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 278   | 191 | 43 | 43 | 1 |         |       |

- Molecule 10 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | j     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 256   | 174 | 39 | 43 |         |       |
| 10  | J     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 256   | 174 | 39 | 43 |         |       |

- Molecule 11 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | k     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 306   | 215 | 44 | 46 | 1 |         |       |
| 11  | K     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 306   | 215 | 44 | 46 | 1 |         |       |

- Molecule 12 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 12  | l     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 311   | 205 | 49 | 57 |         |       |
| 12  | L     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 311   | 205 | 49 | 57 |         |       |

- Molecule 13 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | m     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 176 | 36 | 43 | 1 |         |       |
| 13  | M     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 176 | 36 | 43 | 1 |         |       |

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | o     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1179 | 306 | 382 | 3 |         |       |
| 14  | O     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1179 | 306 | 382 | 3 |         |       |

- Molecule 15 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | t     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 261   | 182 | 37 | 41 | 1 |         |       |
| 15  | T     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 261   | 182 | 37 | 41 | 1 |         |       |

- Molecule 16 is a protein called Photosystem II reaction center protein W.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | w     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 275 | 61 | 82 | 1 |         |       |
| 16  | W     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 275 | 61 | 82 | 1 |         |       |

- Molecule 17 is a protein called Ultraviolet-B-repressible protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | x     | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 180 | 46 | 50 |         |       |
| 17  | X     | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 180 | 46 | 50 |         |       |

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 312 | 69 | 82 | 1 |         |       |
| 18  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 312 | 69 | 82 | 1 |         |       |

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4.3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | r     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1732  | 1133 | 281 | 314 | 4 |         |       |

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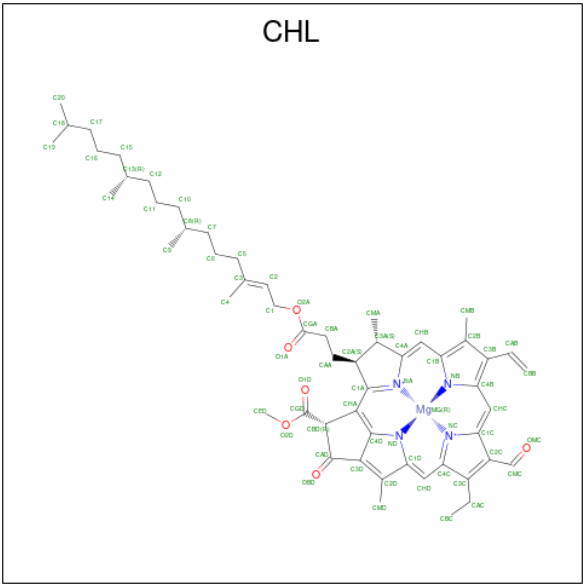
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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | R     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1732  | 1133 | 281 | 314 | 4 |         |       |

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | s     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1688  | 1105 | 271 | 308 | 4 |         |       |
| 20  | S     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1688  | 1105 | 271 | 308 | 4 |         |       |

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



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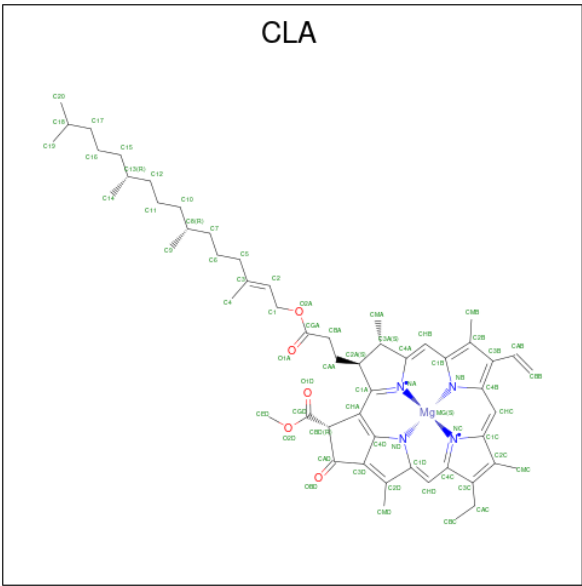
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>56 | C<br>45 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>56 | C<br>45 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | n     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | w     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | x     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | W     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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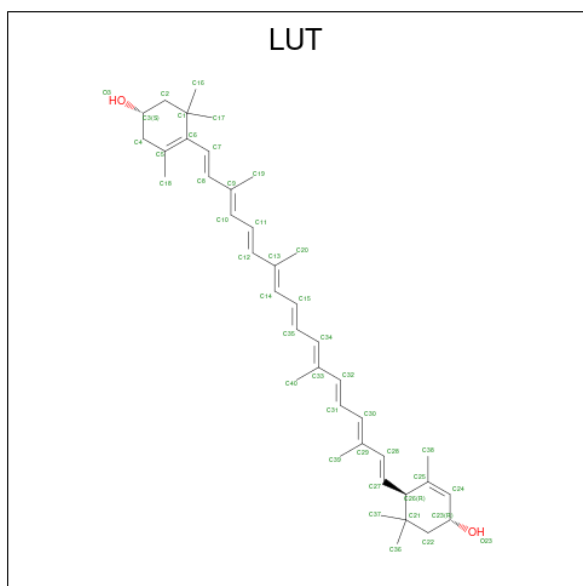
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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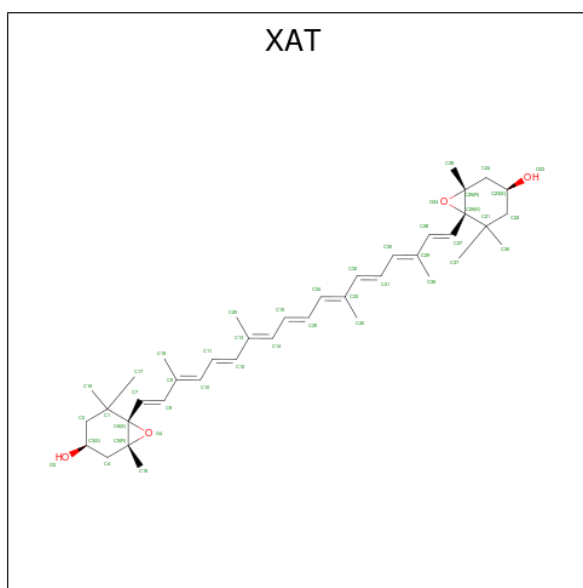
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ).



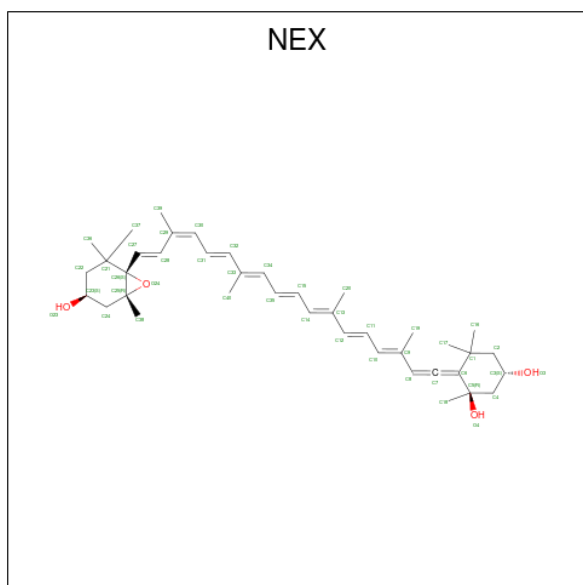
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 25 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



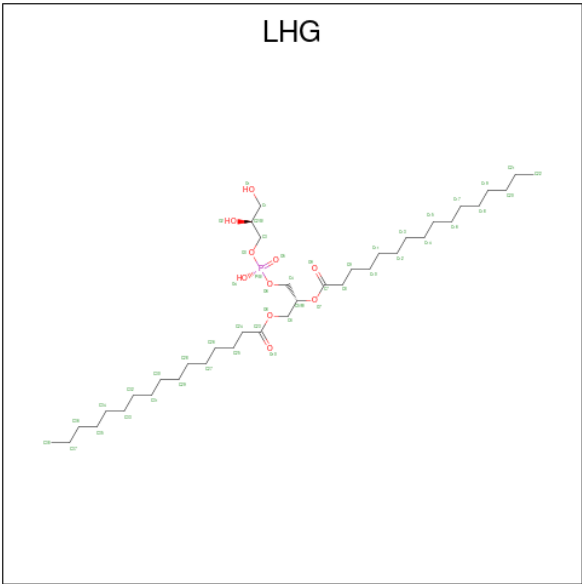
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

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



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | g     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | Y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

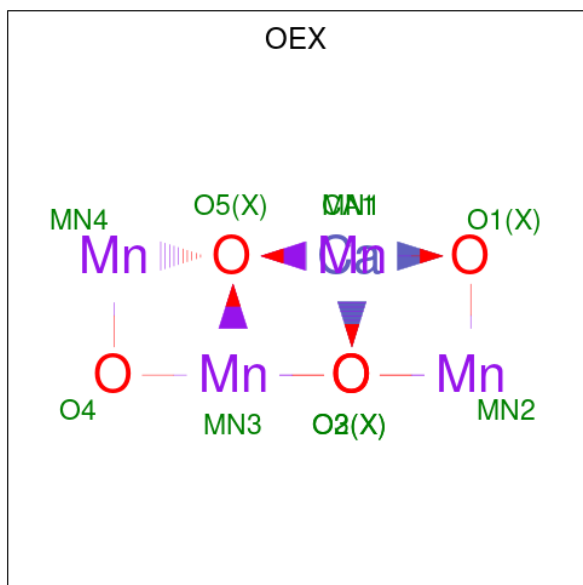
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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 26  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 26  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 26  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 26  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 26  | s     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | S     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | R     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).





| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27  | a     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |
| 27  | A     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |

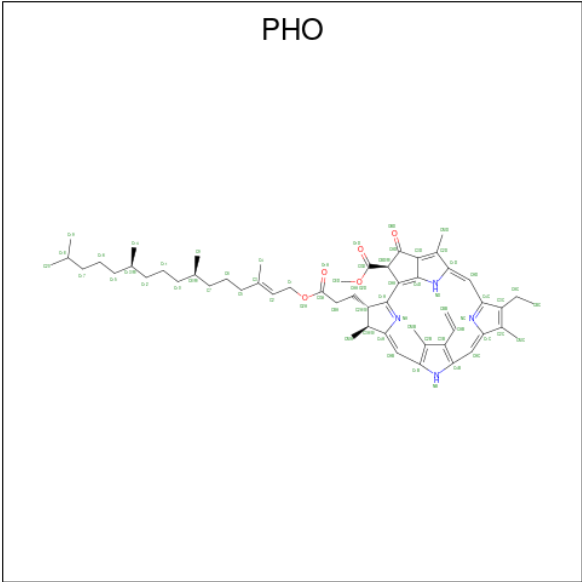
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | a     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 28  | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

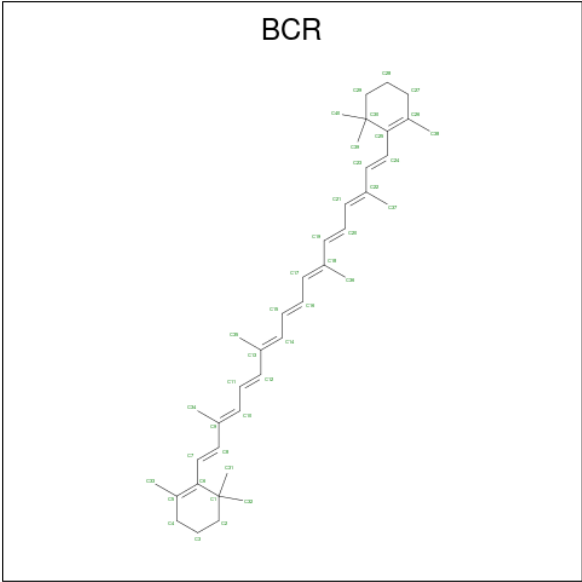
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 29  | a     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | c     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | A     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | C     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



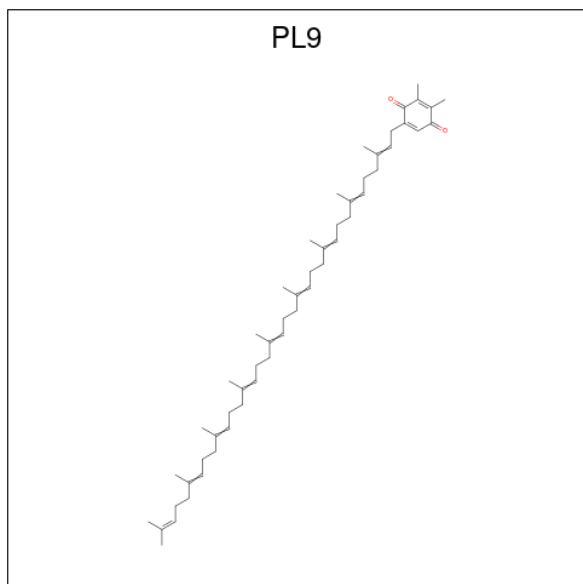
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 30  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | d     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



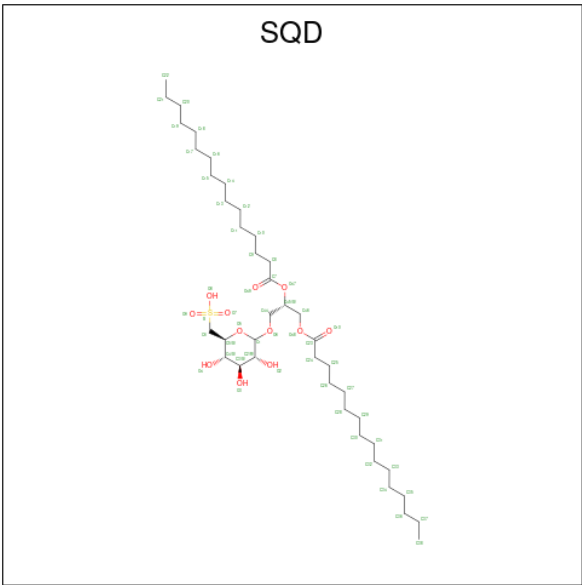
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 31  | a     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | c     | 1        | Total C<br>40 40 | 0       |
| 31  | c     | 1        | Total C<br>40 40 | 0       |
| 31  | d     | 1        | Total C<br>40 40 | 0       |
| 31  | h     | 1        | Total C<br>40 40 | 0       |
| 31  | k     | 1        | Total C<br>40 40 | 0       |
| 31  | k     | 1        | Total C<br>40 40 | 0       |
| 31  | A     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | C     | 1        | Total C<br>40 40 | 0       |
| 31  | C     | 1        | Total C<br>40 40 | 0       |
| 31  | D     | 1        | Total C<br>40 40 | 0       |
| 31  | H     | 1        | Total C<br>40 40 | 0       |
| 31  | K     | 1        | Total C<br>40 40 | 0       |
| 31  | K     | 1        | Total C<br>40 40 | 0       |
| 31  | T     | 1        | Total C<br>40 40 | 0       |

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



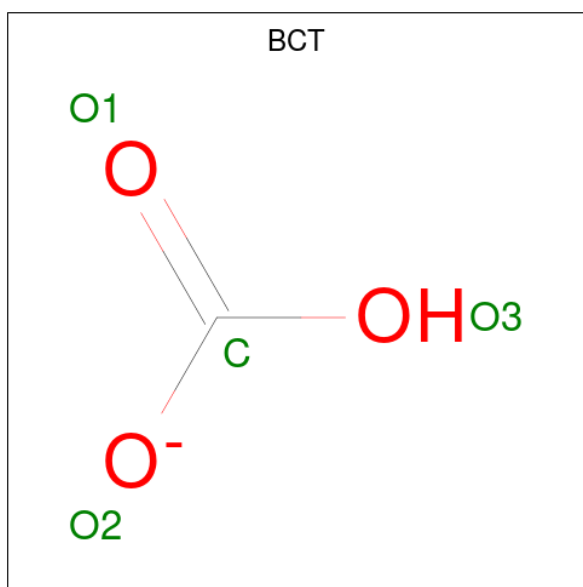
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 32  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 32  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



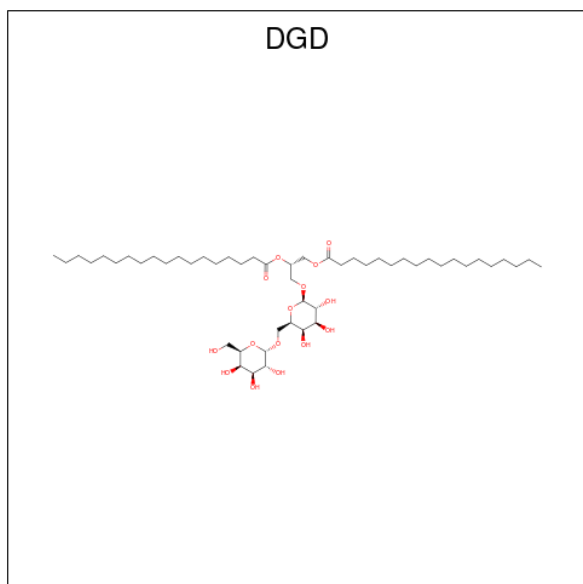
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 33  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | d     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 50    | 37 | 12 | 1 |         |
| 33  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 42    | 29 | 12 | 1 |         |
| 33  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | D     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 50    | 37 | 12 | 1 |         |
| 33  | L     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | L     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 42    | 29 | 12 | 1 |         |

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 34  | a     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |
| 34  | D     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



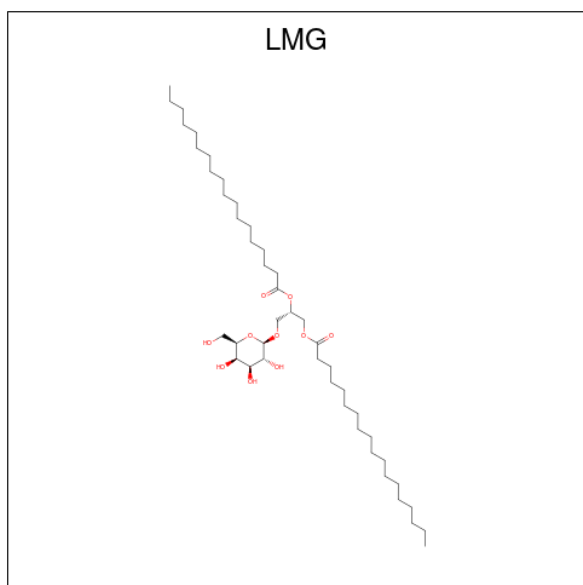
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |
| 35  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



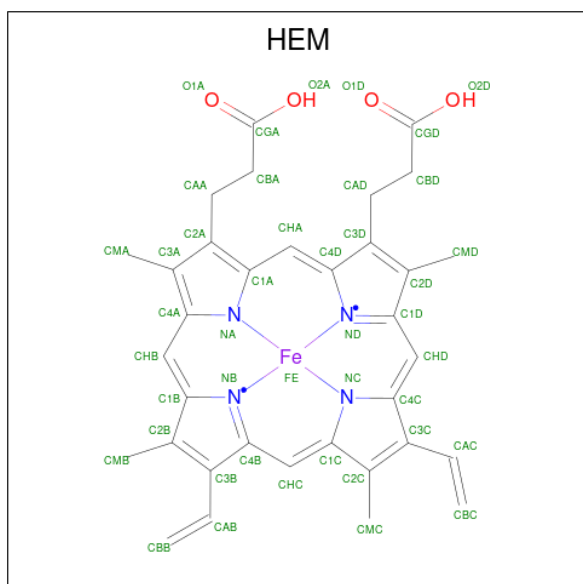
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 36  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 36  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |

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| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 36  | d     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 36  | k     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | w     | 1        | Total<br>48 | C<br>38 | O<br>10 | 0       |
| 36  | B     | 1        | Total<br>40 | C<br>30 | O<br>10 | 0       |
| 36  | B     | 1        | Total<br>55 | C<br>45 | O<br>10 | 0       |
| 36  | C     | 1        | Total<br>48 | C<br>38 | O<br>10 | 0       |
| 36  | C     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | D     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 36  | I     | 1        | Total<br>40 | C<br>30 | O<br>10 | 0       |
| 36  | K     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | M     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | T     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



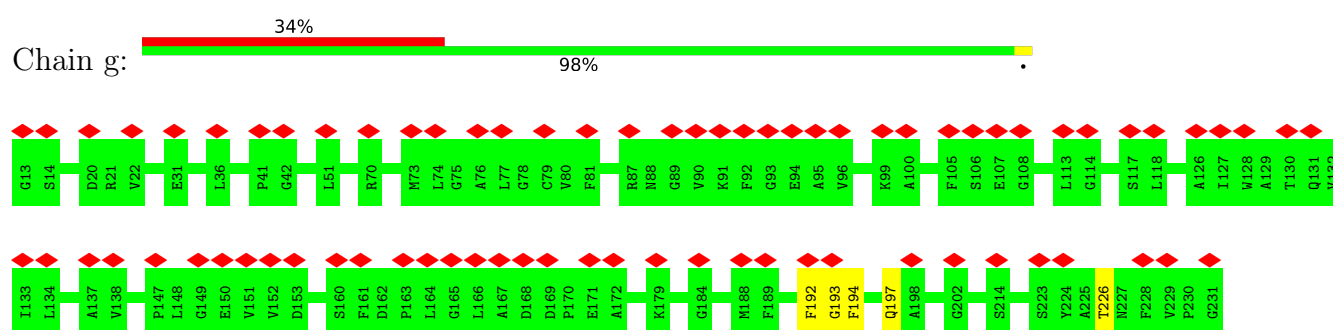


| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 37  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

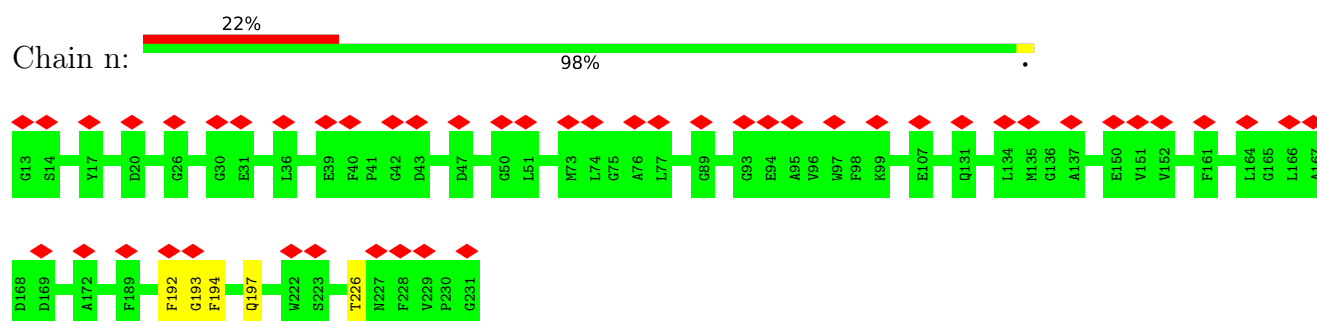
### 3 Residue-property plots

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

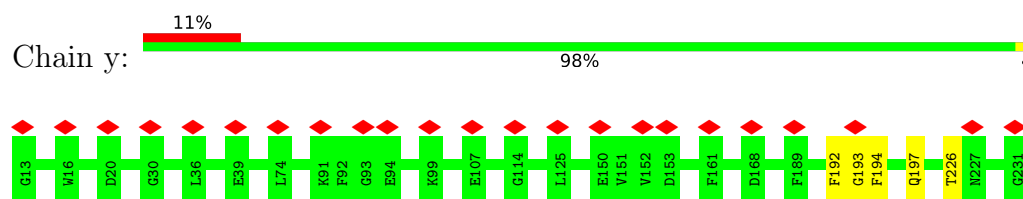
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



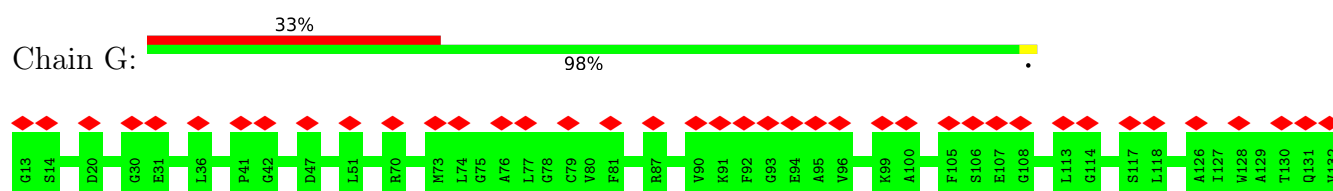
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

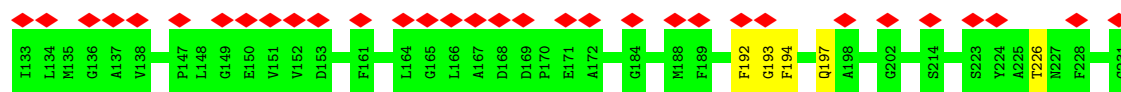


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

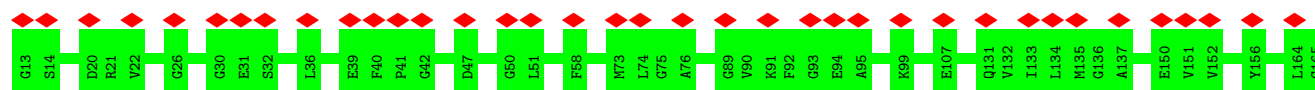


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

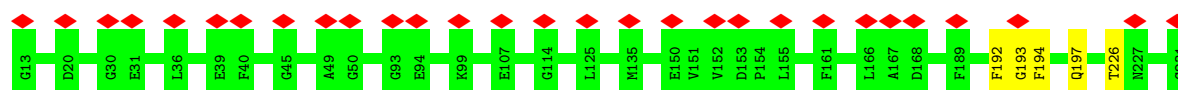




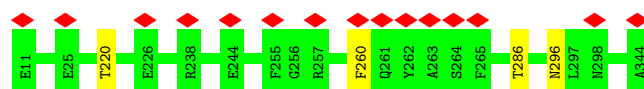
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



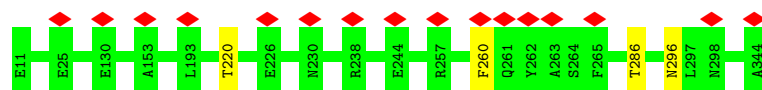
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



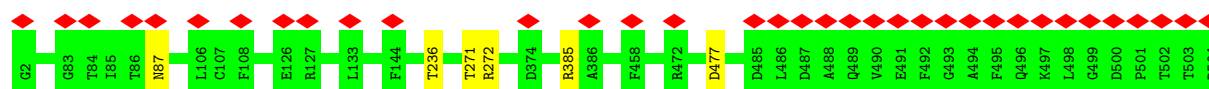
- Molecule 2: Photosystem II protein D1



- Molecule 2: Photosystem II protein D1

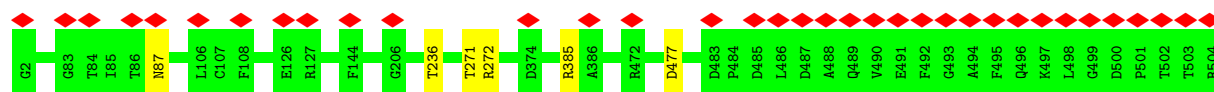


- Molecule 3: Photosystem II CP47 reaction center protein

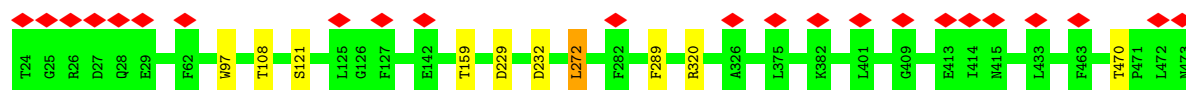


- Molecule 3: Photosystem II CP47 reaction center protein

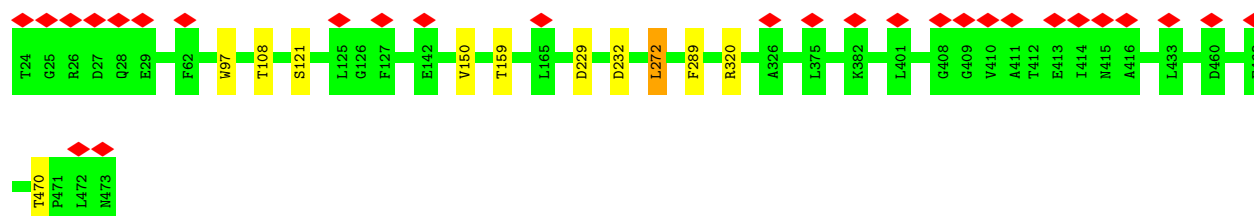




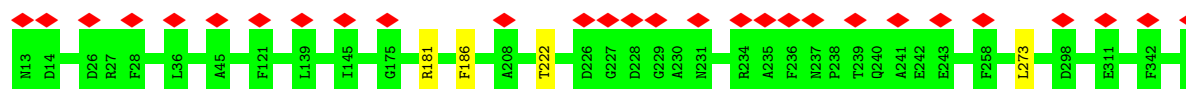
- Molecule 4: Photosystem II CP43 reaction center protein



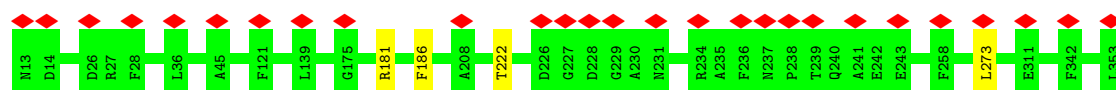
- Molecule 4: Photosystem II CP43 reaction center protein



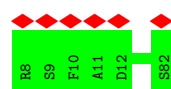
- Molecule 5: Photosystem II D2 protein



- Molecule 5: Photosystem II D2 protein

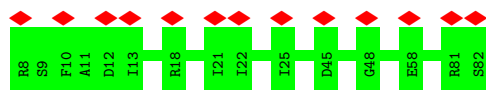


- Molecule 6: Cytochrome b559 subunit alpha

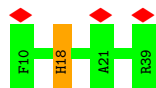


- Molecule 6: Cytochrome b559 subunit alpha

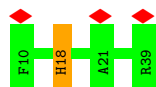




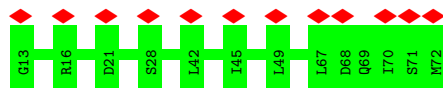
- Molecule 7: Cytochrome b559 subunit beta



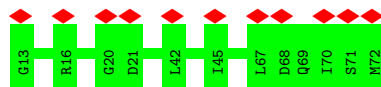
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H



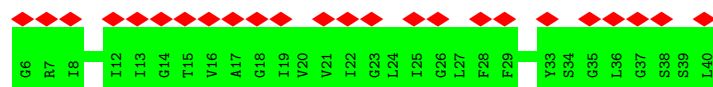
- Molecule 9: Photosystem II reaction center protein I



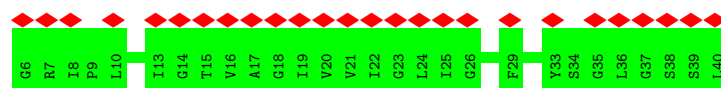
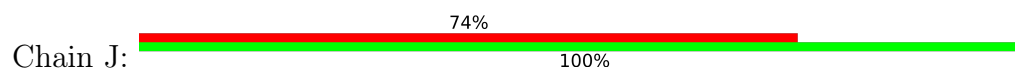
- Molecule 9: Photosystem II reaction center protein I



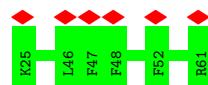
- Molecule 10: Photosystem II reaction center protein J



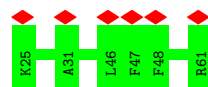
• Molecule 10: Photosystem II reaction center protein J



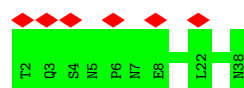
• Molecule 11: Photosystem II reaction center protein K



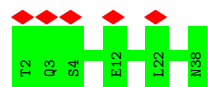
• Molecule 11: Photosystem II reaction center protein K



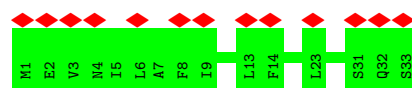
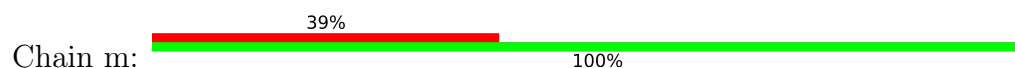
• Molecule 12: Photosystem II reaction center protein L



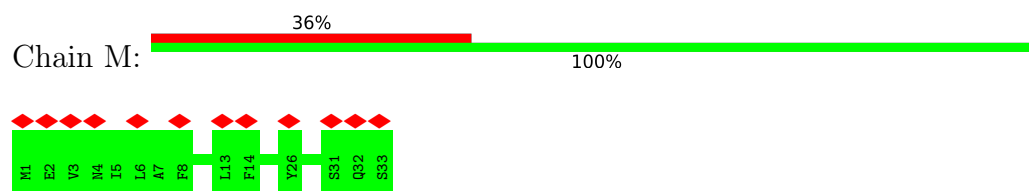
• Molecule 12: Photosystem II reaction center protein L



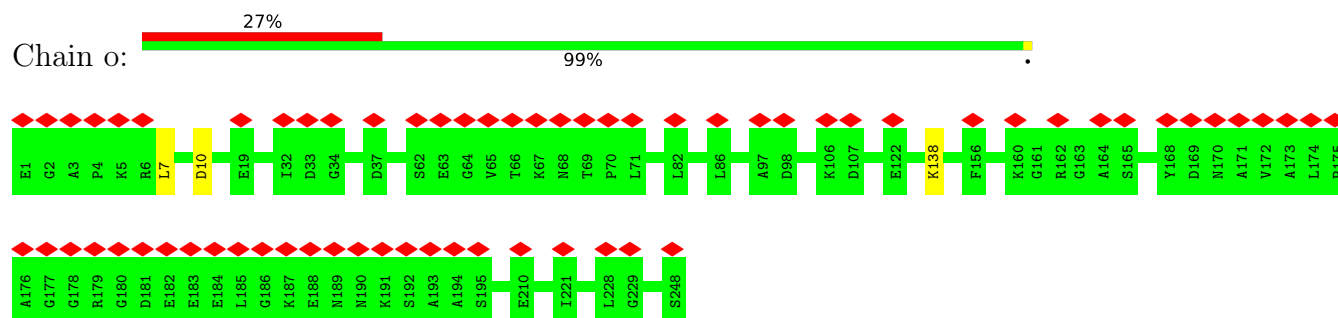
• Molecule 13: Photosystem II reaction center protein M



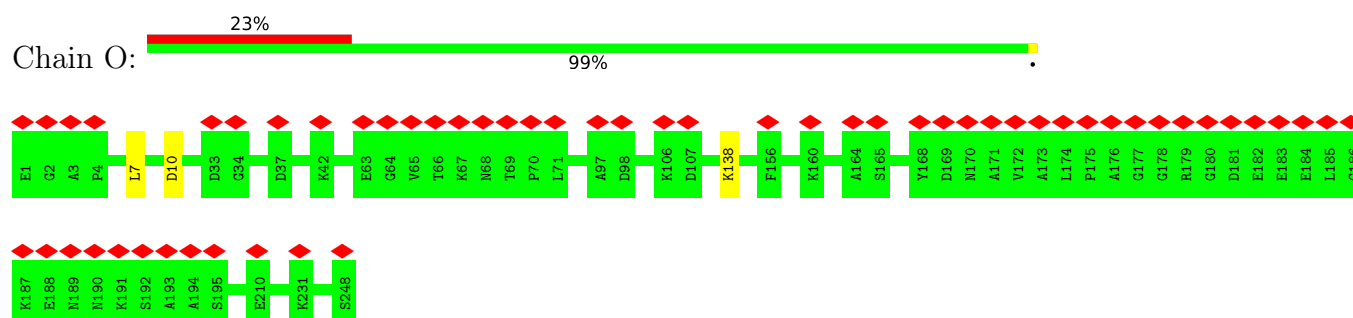
- Molecule 13: Photosystem II reaction center protein M



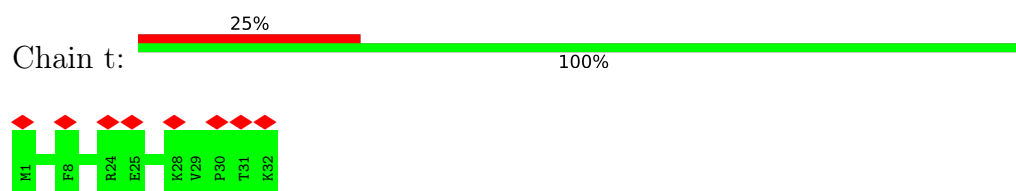
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



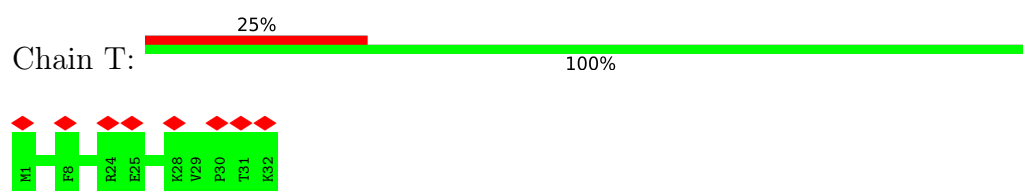
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

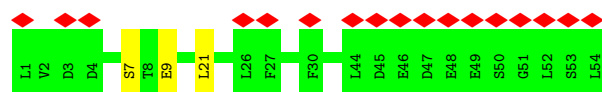


- Molecule 15: Photosystem II reaction center protein T

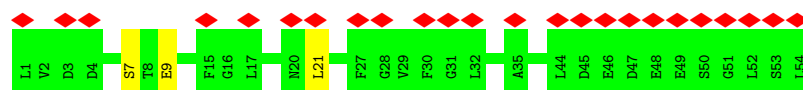
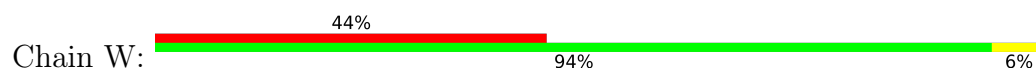


- Molecule 16: Photosystem II reaction center protein W

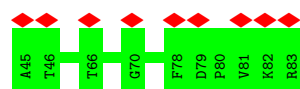




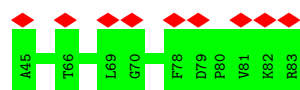
- Molecule 16: Photosystem II reaction center protein W



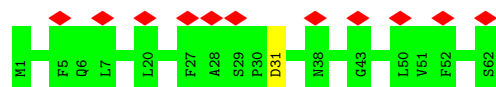
- Molecule 17: Ultraviolet-B-repressible protein



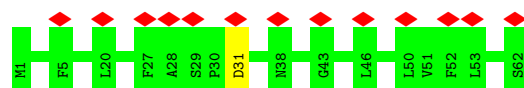
- Molecule 17: Ultraviolet-B-repressible protein



- Molecule 18: Photosystem II reaction center protein Z



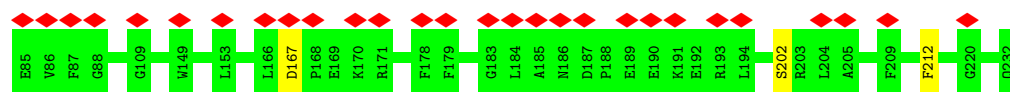
- Molecule 18: Photosystem II reaction center protein Z



- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

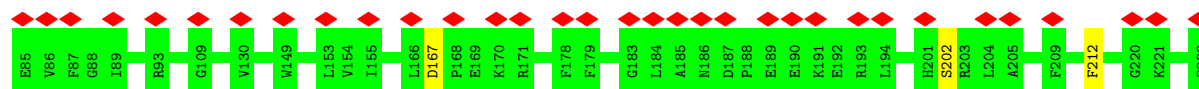
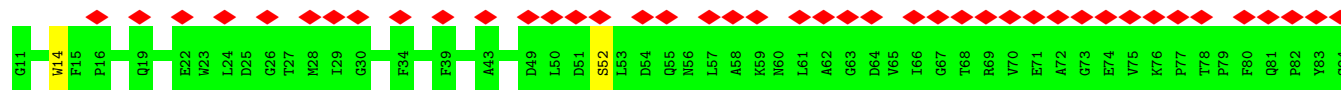






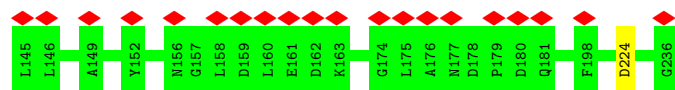
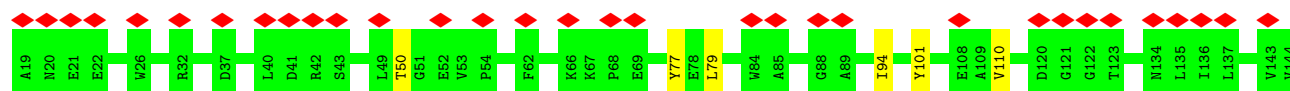
- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

Chain R: .



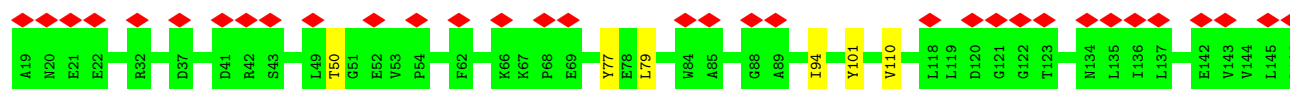
- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain s: .



- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S: .



## 4 Experimental information

| Property                             | Value  | Source    |
|--------------------------------------|--|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                  | Depositor |
| Imposed symmetry                     | POINT, C2  | Depositor |
| Number of particles used             | 27942  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                | Depositor |
| CTF correction method                | NONE   | Depositor |
| Microscope                           | FEI TITAN KRIOS                                  | Depositor |
| Voltage (kV)                         | 300  | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40, 40   | Depositor |
| Minimum defocus (nm)                 | Not provided                                     |           |
| Maximum defocus (nm)                 | Not provided                                     |           |
| Magnification                        | Not provided                                     |           |
| Image detector                       | GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k) | Depositor |
| Maximum map value                    | 1.923  | Depositor |
| Minimum map value                    | -0.630   | Depositor |
| Average map value                    | 0.055  | Depositor |
| Map value standard deviation         | 0.166  | Depositor |
| Recommended contour level            | 0.85   | Depositor |
| Map size (Å)                         | 374.0, 374.0, 374.0                              | wwPDB     |
| Map dimensions                       | 340, 340, 340                                    | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                    | 1.1, 1.1, 1.1                                    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, PHO, DGD, LHG, NEX, FE2, CHL, PL9, CL, HEM, LMG, XAT, CLA, BCR, OEX, LUT, BCT

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   | G     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 1   | N     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 1   | Y     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 1   | g     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 1   | n     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 1   | y     | 0.30         | 0/1720        | 0.43        | 0/2342        |
| 2   | A     | 0.31         | 0/2697        | 0.43        | 0/3677        |
| 2   | a     | 0.31         | 0/2697        | 0.43        | 0/3677        |
| 3   | B     | 0.31         | 0/4081        | 0.41        | 0/5556        |
| 3   | b     | 0.31         | 0/4081        | 0.41        | 0/5556        |
| 4   | C     | 0.82         | 1/3614 (0.0%) | 0.48        | 3/4922 (0.1%) |
| 4   | c     | 0.82         | 1/3614 (0.0%) | 0.48        | 3/4922 (0.1%) |
| 5   | D     | 0.31         | 0/2804        | 0.42        | 0/3823        |
| 5   | d     | 0.31         | 0/2804        | 0.42        | 0/3823        |
| 6   | E     | 0.28         | 0/630         | 0.39        | 0/857         |
| 6   | e     | 0.28         | 0/630         | 0.39        | 0/857         |
| 7   | F     | 0.56         | 1/248 (0.4%)  | 0.47        | 0/335         |
| 7   | f     | 0.56         | 1/248 (0.4%)  | 0.47        | 0/335         |
| 8   | H     | 0.29         | 0/461         | 0.43        | 0/626         |
| 8   | h     | 0.29         | 0/461         | 0.43        | 0/626         |
| 9   | I     | 0.33         | 0/286         | 0.40        | 0/386         |
| 9   | i     | 0.33         | 0/286         | 0.41        | 0/386         |
| 10  | J     | 0.27         | 0/262         | 0.40        | 0/354         |
| 10  | j     | 0.27         | 0/262         | 0.40        | 0/354         |
| 11  | K     | 0.32         | 0/318         | 0.43        | 0/434         |
| 11  | k     | 0.32         | 0/318         | 0.43        | 0/434         |
| 12  | L     | 0.31         | 0/319         | 0.40        | 0/434         |
| 12  | l     | 0.31         | 0/319         | 0.40        | 0/434         |
| 13  | M     | 0.30         | 0/260         | 0.39        | 0/355         |
| 13  | m     | 0.30         | 0/260         | 0.39        | 0/355         |
| 14  | O     | 0.28         | 0/1906        | 0.45        | 0/2575        |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 14  | o     | 0.28         | 0/1906         | 0.45        | 0/2575         |
| 15  | T     | 0.35         | 0/269          | 0.39        | 0/365          |
| 15  | t     | 0.35         | 0/269          | 0.39        | 0/365          |
| 16  | W     | 0.36         | 0/429          | 0.43        | 0/581          |
| 16  | w     | 0.36         | 0/429          | 0.42        | 0/581          |
| 17  | X     | 0.28         | 0/279          | 0.40        | 0/380          |
| 17  | x     | 0.28         | 0/279          | 0.39        | 0/380          |
| 18  | Z     | 0.27         | 0/474          | 0.35        | 0/648          |
| 18  | z     | 0.27         | 0/474          | 0.35        | 0/648          |
| 19  | R     | 0.28         | 0/1780         | 0.40        | 0/2417         |
| 19  | r     | 0.29         | 0/1780         | 0.40        | 0/2417         |
| 20  | S     | 0.31         | 0/1737         | 0.42        | 0/2361         |
| 20  | s     | 0.31         | 0/1737         | 0.42        | 0/2361         |
| All | All   | 0.41         | 4/56028 (0.0%) | 0.43        | 6/76224 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 2                   |
| 1   | N     | 0                   | 2                   |
| 1   | Y     | 0                   | 2                   |
| 1   | g     | 0                   | 2                   |
| 1   | n     | 0                   | 2                   |
| 1   | y     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | c     | 272 | LEU  | CG-CD1 | 45.67 | 3.20        | 1.51     |
| 4   | C     | 272 | LEU  | CG-CD1 | 45.67 | 3.20        | 1.51     |
| 7   | F     | 18  | HIS  | CB-CG  | 7.21  | 1.63        | 1.50     |
| 7   | f     | 18  | HIS  | CB-CG  | 7.19  | 1.62        | 1.50     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | c     | 272 | LEU  | CB-CG-CD1 | 12.88 | 132.89      | 111.00   |
| 4   | C     | 272 | LEU  | CB-CG-CD1 | 12.87 | 132.87      | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | c     | 272 | LEU  | CA-CB-CG  | 7.25  | 131.97      | 115.30   |
| 4   | C     | 272 | LEU  | CA-CB-CG  | 7.24  | 131.96      | 115.30   |
| 4   | C     | 272 | LEU  | CB-CG-CD2 | -6.80 | 99.44       | 111.00   |
| 4   | c     | 272 | LEU  | CB-CG-CD2 | -6.78 | 99.47       | 111.00   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 193 | GLY  | Mainchain |
| 1   | G     | 197 | GLN  | Sidechain |
| 1   | N     | 193 | GLY  | Mainchain |
| 1   | N     | 197 | GLN  | Sidechain |
| 1   | Y     | 193 | GLY  | Mainchain |
| 1   | Y     | 197 | GLN  | Sidechain |
| 1   | g     | 193 | GLY  | Mainchain |
| 1   | g     | 197 | GLN  | Sidechain |
| 1   | n     | 193 | GLY  | Mainchain |
| 1   | n     | 197 | GLN  | Sidechain |
| 1   | y     | 193 | GLY  | Mainchain |
| 1   | y     | 197 | GLN  | Sidechain |

## 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   | G     | 217/219 (99%) | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | N     | 217/219 (99%) | 202 (93%) | 15 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | Y     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | g     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | n     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | y     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 2   | A     | 332/334 (99%)  | 320 (96%) | 12 (4%) | 0        | 100         | 100 |
| 2   | a     | 332/334 (99%)  | 320 (96%) | 12 (4%) | 0        | 100         | 100 |
| 3   | B     | 501/503 (100%) | 485 (97%) | 16 (3%) | 0        | 100         | 100 |
| 3   | b     | 501/503 (100%) | 485 (97%) | 16 (3%) | 0        | 100         | 100 |
| 4   | C     | 448/450 (100%) | 428 (96%) | 20 (4%) | 0        | 100         | 100 |
| 4   | c     | 448/450 (100%) | 428 (96%) | 20 (4%) | 0        | 100         | 100 |
| 5   | D     | 339/341 (99%)  | 326 (96%) | 13 (4%) | 0        | 100         | 100 |
| 5   | d     | 339/341 (99%)  | 327 (96%) | 12 (4%) | 0        | 100         | 100 |
| 6   | E     | 73/75 (97%)    | 73 (100%) | 0       | 0        | 100         | 100 |
| 6   | e     | 73/75 (97%)    | 73 (100%) | 0       | 0        | 100         | 100 |
| 7   | F     | 28/30 (93%)    | 25 (89%)  | 3 (11%) | 0        | 100         | 100 |
| 7   | f     | 28/30 (93%)    | 25 (89%)  | 3 (11%) | 0        | 100         | 100 |
| 8   | H     | 58/60 (97%)    | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 8   | h     | 58/60 (97%)    | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 9   | I     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 9   | i     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 10  | J     | 33/35 (94%)    | 33 (100%) | 0       | 0        | 100         | 100 |
| 10  | j     | 33/35 (94%)    | 33 (100%) | 0       | 0        | 100         | 100 |
| 11  | K     | 35/37 (95%)    | 32 (91%)  | 3 (9%)  | 0        | 100         | 100 |
| 11  | k     | 35/37 (95%)    | 32 (91%)  | 3 (9%)  | 0        | 100         | 100 |
| 12  | L     | 35/37 (95%)    | 34 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 12  | l     | 35/37 (95%)    | 34 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 13  | M     | 31/33 (94%)    | 31 (100%) | 0       | 0        | 100         | 100 |
| 13  | m     | 31/33 (94%)    | 31 (100%) | 0       | 0        | 100         | 100 |
| 14  | O     | 246/248 (99%)  | 230 (94%) | 16 (6%) | 0        | 100         | 100 |
| 14  | o     | 246/248 (99%)  | 230 (94%) | 16 (6%) | 0        | 100         | 100 |
| 15  | T     | 30/32 (94%)    | 29 (97%)  | 1 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 15  | t     | 30/32 (94%)     | 29 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 16  | W     | 52/54 (96%)     | 48 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 16  | w     | 52/54 (96%)     | 48 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 17  | X     | 37/39 (95%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 17  | x     | 37/39 (95%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 18  | Z     | 60/62 (97%)     | 60 (100%)  | 0        | 0        | 100         | 100 |
| 18  | z     | 60/62 (97%)     | 60 (100%)  | 0        | 0        | 100         | 100 |
| 19  | R     | 220/222 (99%)   | 207 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 19  | r     | 220/222 (99%)   | 207 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 20  | S     | 216/218 (99%)   | 198 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 20  | s     | 216/218 (99%)   | 198 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| All | All   | 6914/7002 (99%) | 6583 (95%) | 331 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | G     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 1   | N     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 1   | Y     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 1   | g     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 1   | n     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 1   | y     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 54          | 71 |
| 2   | A     | 270/270 (100%) | 266 (98%) | 4 (2%)   | 60          | 74 |
| 2   | a     | 270/270 (100%) | 266 (98%) | 4 (2%)   | 60          | 74 |
| 3   | B     | 400/400 (100%) | 394 (98%) | 6 (2%)   | 60          | 74 |
| 3   | b     | 400/400 (100%) | 394 (98%) | 6 (2%)   | 60          | 74 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4   | C     | 352/352 (100%) | 341 (97%) | 11 (3%)  | 35          | 56  |
| 4   | c     | 352/352 (100%) | 342 (97%) | 10 (3%)  | 38          | 59  |
| 5   | D     | 275/275 (100%) | 271 (98%) | 4 (2%)   | 60          | 74  |
| 5   | d     | 275/275 (100%) | 271 (98%) | 4 (2%)   | 60          | 74  |
| 6   | E     | 67/67 (100%)   | 67 (100%) | 0        | 100         | 100 |
| 6   | e     | 67/67 (100%)   | 67 (100%) | 0        | 100         | 100 |
| 7   | F     | 25/25 (100%)   | 24 (96%)  | 1 (4%)   | 27          | 50  |
| 7   | f     | 25/25 (100%)   | 24 (96%)  | 1 (4%)   | 27          | 50  |
| 8   | H     | 49/49 (100%)   | 49 (100%) | 0        | 100         | 100 |
| 8   | h     | 49/49 (100%)   | 49 (100%) | 0        | 100         | 100 |
| 9   | I     | 31/31 (100%)   | 31 (100%) | 0        | 100         | 100 |
| 9   | i     | 31/31 (100%)   | 31 (100%) | 0        | 100         | 100 |
| 10  | J     | 26/26 (100%)   | 26 (100%) | 0        | 100         | 100 |
| 10  | j     | 26/26 (100%)   | 26 (100%) | 0        | 100         | 100 |
| 11  | K     | 32/32 (100%)   | 32 (100%) | 0        | 100         | 100 |
| 11  | k     | 32/32 (100%)   | 32 (100%) | 0        | 100         | 100 |
| 12  | L     | 35/35 (100%)   | 35 (100%) | 0        | 100         | 100 |
| 12  | l     | 35/35 (100%)   | 35 (100%) | 0        | 100         | 100 |
| 13  | M     | 29/29 (100%)   | 29 (100%) | 0        | 100         | 100 |
| 13  | m     | 29/29 (100%)   | 29 (100%) | 0        | 100         | 100 |
| 14  | O     | 204/204 (100%) | 201 (98%) | 3 (2%)   | 60          | 74  |
| 14  | o     | 204/204 (100%) | 201 (98%) | 3 (2%)   | 60          | 74  |
| 15  | T     | 29/29 (100%)   | 29 (100%) | 0        | 100         | 100 |
| 15  | t     | 29/29 (100%)   | 29 (100%) | 0        | 100         | 100 |
| 16  | W     | 44/44 (100%)   | 41 (93%)  | 3 (7%)   | 13          | 38  |
| 16  | w     | 44/44 (100%)   | 41 (93%)  | 3 (7%)   | 13          | 38  |
| 17  | X     | 32/32 (100%)   | 32 (100%) | 0        | 100         | 100 |
| 17  | x     | 32/32 (100%)   | 32 (100%) | 0        | 100         | 100 |
| 18  | Z     | 54/54 (100%)   | 53 (98%)  | 1 (2%)   | 52          | 69  |
| 18  | z     | 54/54 (100%)   | 53 (98%)  | 1 (2%)   | 52          | 69  |
| 19  | R     | 175/175 (100%) | 170 (97%) | 5 (3%)   | 37          | 58  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 19  | r     | 175/175 (100%)   | 170 (97%)  | 5 (3%)   | 37          | 58 |
| 20  | S     | 169/169 (100%)   | 162 (96%)  | 7 (4%)   | 26          | 50 |
| 20  | s     | 169/169 (100%)   | 162 (96%)  | 7 (4%)   | 26          | 50 |
| All | All   | 5622/5622 (100%) | 5515 (98%) | 107 (2%) | 52          | 69 |

All (107) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | g     | 192 | PHE  |
| 1   | g     | 194 | PHE  |
| 1   | g     | 226 | THR  |
| 1   | n     | 192 | PHE  |
| 1   | n     | 194 | PHE  |
| 1   | n     | 226 | THR  |
| 1   | y     | 192 | PHE  |
| 1   | y     | 194 | PHE  |
| 1   | y     | 226 | THR  |
| 1   | G     | 192 | PHE  |
| 1   | G     | 194 | PHE  |
| 1   | G     | 226 | THR  |
| 1   | N     | 192 | PHE  |
| 1   | N     | 194 | PHE  |
| 1   | N     | 226 | THR  |
| 1   | Y     | 192 | PHE  |
| 1   | Y     | 194 | PHE  |
| 1   | Y     | 226 | THR  |
| 2   | a     | 220 | THR  |
| 2   | a     | 260 | PHE  |
| 2   | a     | 286 | THR  |
| 2   | a     | 296 | ASN  |
| 3   | b     | 87  | ASN  |
| 3   | b     | 236 | THR  |
| 3   | b     | 271 | THR  |
| 3   | b     | 272 | ARG  |
| 3   | b     | 385 | ARG  |
| 3   | b     | 477 | ASP  |
| 4   | c     | 97  | TRP  |
| 4   | c     | 108 | THR  |
| 4   | c     | 121 | SER  |
| 4   | c     | 159 | THR  |
| 4   | c     | 229 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | c     | 232 | ASP  |
| 4   | c     | 272 | LEU  |
| 4   | c     | 289 | PHE  |
| 4   | c     | 320 | ARG  |
| 4   | c     | 470 | THR  |
| 5   | d     | 181 | ARG  |
| 5   | d     | 186 | PHE  |
| 5   | d     | 222 | THR  |
| 5   | d     | 273 | LEU  |
| 7   | f     | 18  | HIS  |
| 14  | o     | 7   | LEU  |
| 14  | o     | 10  | ASP  |
| 14  | o     | 138 | LYS  |
| 16  | w     | 7   | SER  |
| 16  | w     | 9   | GLU  |
| 16  | w     | 21  | LEU  |
| 18  | z     | 31  | ASP  |
| 2   | A     | 220 | THR  |
| 2   | A     | 260 | PHE  |
| 2   | A     | 286 | THR  |
| 2   | A     | 296 | ASN  |
| 3   | B     | 87  | ASN  |
| 3   | B     | 236 | THR  |
| 3   | B     | 271 | THR  |
| 3   | B     | 272 | ARG  |
| 3   | B     | 385 | ARG  |
| 3   | B     | 477 | ASP  |
| 4   | C     | 97  | TRP  |
| 4   | C     | 108 | THR  |
| 4   | C     | 121 | SER  |
| 4   | C     | 150 | VAL  |
| 4   | C     | 159 | THR  |
| 4   | C     | 229 | ASP  |
| 4   | C     | 232 | ASP  |
| 4   | C     | 272 | LEU  |
| 4   | C     | 289 | PHE  |
| 4   | C     | 320 | ARG  |
| 4   | C     | 470 | THR  |
| 5   | D     | 181 | ARG  |
| 5   | D     | 186 | PHE  |
| 5   | D     | 222 | THR  |
| 5   | D     | 273 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | F     | 18  | HIS  |
| 14  | O     | 7   | LEU  |
| 14  | O     | 10  | ASP  |
| 14  | O     | 138 | LYS  |
| 16  | W     | 7   | SER  |
| 16  | W     | 9   | GLU  |
| 16  | W     | 21  | LEU  |
| 18  | Z     | 31  | ASP  |
| 19  | r     | 14  | TRP  |
| 19  | r     | 52  | SER  |
| 19  | r     | 167 | ASP  |
| 19  | r     | 202 | SER  |
| 19  | r     | 212 | PHE  |
| 20  | s     | 50  | THR  |
| 20  | s     | 77  | TYR  |
| 20  | s     | 79  | LEU  |
| 20  | s     | 94  | ILE  |
| 20  | s     | 101 | TYR  |
| 20  | s     | 110 | VAL  |
| 20  | s     | 224 | ASP  |
| 20  | S     | 50  | THR  |
| 20  | S     | 77  | TYR  |
| 20  | S     | 79  | LEU  |
| 20  | S     | 94  | ILE  |
| 20  | S     | 101 | TYR  |
| 20  | S     | 110 | VAL  |
| 20  | S     | 224 | ASP  |
| 19  | R     | 14  | TRP  |
| 19  | R     | 52  | SER  |
| 19  | R     | 167 | ASP  |
| 19  | R     | 202 | SER  |
| 19  | R     | 212 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | g     | 122 | GLN  |
| 1   | g     | 131 | GLN  |
| 1   | g     | 197 | GLN  |
| 1   | g     | 208 | ASN  |
| 1   | g     | 219 | ASN  |
| 1   | n     | 122 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | n     | 131 | GLN  |
| 1   | n     | 208 | ASN  |
| 1   | n     | 219 | ASN  |
| 1   | y     | 122 | GLN  |
| 1   | y     | 131 | GLN  |
| 1   | y     | 208 | ASN  |
| 1   | y     | 219 | ASN  |
| 1   | G     | 122 | GLN  |
| 1   | G     | 131 | GLN  |
| 1   | G     | 197 | GLN  |
| 1   | G     | 208 | ASN  |
| 1   | G     | 219 | ASN  |
| 1   | N     | 122 | GLN  |
| 1   | N     | 131 | GLN  |
| 1   | N     | 197 | GLN  |
| 1   | N     | 208 | ASN  |
| 1   | N     | 219 | ASN  |
| 1   | Y     | 122 | GLN  |
| 1   | Y     | 131 | GLN  |
| 1   | Y     | 197 | GLN  |
| 1   | Y     | 208 | ASN  |
| 1   | Y     | 219 | ASN  |
| 2   | a     | 187 | GLN  |
| 2   | a     | 325 | ASN  |
| 3   | b     | 9   | HIS  |
| 3   | b     | 216 | HIS  |
| 4   | c     | 322 | GLN  |
| 4   | c     | 415 | ASN  |
| 4   | c     | 418 | ASN  |
| 5   | d     | 62  | HIS  |
| 5   | d     | 143 | ASN  |
| 5   | d     | 221 | ASN  |
| 5   | d     | 351 | ASN  |
| 6   | e     | 75  | GLN  |
| 12  | l     | 34  | ASN  |
| 14  | o     | 74  | GLN  |
| 14  | o     | 222 | GLN  |
| 18  | z     | 58  | ASN  |
| 2   | A     | 187 | GLN  |
| 2   | A     | 325 | ASN  |
| 3   | B     | 9   | HIS  |
| 3   | B     | 216 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 322 | GLN  |
| 4   | C     | 418 | ASN  |
| 5   | D     | 62  | HIS  |
| 5   | D     | 143 | ASN  |
| 5   | D     | 221 | ASN  |
| 5   | D     | 351 | ASN  |
| 6   | E     | 75  | GLN  |
| 12  | L     | 34  | ASN  |
| 13  | M     | 32  | GLN  |
| 14  | O     | 74  | GLN  |
| 14  | O     | 222 | GLN  |
| 18  | Z     | 58  | ASN  |
| 19  | r     | 47  | GLN  |
| 19  | r     | 56  | ASN  |
| 19  | r     | 231 | ASN  |
| 20  | s     | 81  | HIS  |
| 20  | s     | 125 | ASN  |
| 20  | S     | 81  | HIS  |
| 20  | S     | 125 | ASN  |
| 19  | R     | 47  | GLN  |
| 19  | R     | 231 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 325 ligands modelled in this entry, 6 are monoatomic - leaving 319 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 |
| 21  | CHL  | R     | 305 | -    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 22  | CLA  | S     | 313 | 22   | 55,63,73     | 1.59 | 6 (10%)  | 64,101,113  | 1.49  | 6 (9%)   |
| 21  | CHL  | y     | 605 | -    | 48,56,74     | 2.49 | 17 (35%) | 51,92,114   | 2.83  | 17 (33%) |
| 33  | SQD  | d     | 402 | -    | 49,50,54     | 1.01 | 5 (10%)  | 58,61,65    | 1.56  | 10 (17%) |
| 21  | CHL  | y     | 606 | -    | 50,58,74     | 2.45 | 16 (32%) | 52,94,114   | 2.82  | 17 (32%) |
| 22  | CLA  | Y     | 602 | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.38  | 9 (11%)  |
| 22  | CLA  | b     | 610 | -    | 65,73,73     | 1.47 | 8 (12%)  | 76,113,113  | 1.38  | 7 (9%)   |
| 24  | XAT  | n     | 615 | -    | 39,47,47     | 5.22 | 20 (51%) | 54,74,74    | 13.59 | 30 (55%) |
| 33  | SQD  | a     | 411 | -    | 53,54,54     | 0.97 | 5 (9%)   | 62,65,65    | 1.60  | 12 (19%) |
| 23  | LUT  | Y     | 613 | -    | 42,43,43     | 5.87 | 19 (45%) | 51,60,60    | 5.44  | 25 (49%) |
| 26  | LHG  | L     | 103 | -    | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.29  | 7 (13%)  |
| 22  | CLA  | W     | 101 | -    | 60,68,73     | 1.56 | 6 (10%)  | 70,107,113  | 1.39  | 7 (10%)  |
| 30  | PHO  | a     | 407 | -    | 51,69,69     | 1.06 | 5 (9%)   | 47,99,99    | 1.11  | 4 (8%)   |
| 26  | LHG  | d     | 409 | -    | 42,42,48     | 0.67 | 1 (2%)   | 45,48,54    | 1.26  | 5 (11%)  |
| 22  | CLA  | b     | 604 | -    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.36  | 6 (7%)   |
| 21  | CHL  | Y     | 601 | 1    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 22  | CLA  | B     | 604 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.37  | 7 (9%)   |
| 22  | CLA  | B     | 614 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.41  | 6 (7%)   |
| 31  | BCR  | B     | 620 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.25  | 6 (10%)  |
| 36  | LMG  | k     | 103 | -    | 51,51,55     | 0.73 | 0        | 59,59,63    | 1.34  | 6 (10%)  |
| 23  | LUT  | n     | 614 | -    | 42,43,43     | 5.88 | 19 (45%) | 51,60,60    | 5.44  | 25 (49%) |
| 22  | CLA  | N     | 610 | -    | 60,68,73     | 1.52 | 6 (10%)  | 70,107,113  | 1.40  | 8 (11%)  |
| 21  | CHL  | S     | 301 | -    | 48,56,74     | 2.50 | 16 (33%) | 51,92,114   | 2.84  | 17 (33%) |
| 22  | CLA  | a     | 404 | -    | 65,73,73     | 1.47 | 8 (12%)  | 76,113,113  | 1.40  | 8 (10%)  |
| 22  | CLA  | B     | 605 | -    | 65,73,73     | 1.43 | 8 (12%)  | 76,113,113  | 1.40  | 8 (10%)  |
| 21  | CHL  | N     | 606 | -    | 66,74,74     | 2.14 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 23  | LUT  | N     | 614 | -    | 42,43,43     | 5.88 | 19 (45%) | 51,60,60    | 5.44  | 25 (49%) |
| 22  | CLA  | b     | 612 | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.35  | 6 (7%)   |
| 21  | CHL  | N     | 605 | -    | 50,58,74     | 2.44 | 16 (32%) | 52,94,114   | 2.81  | 17 (32%) |
| 22  | CLA  | G     | 603 | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.35  | 7 (9%)   |
| 31  | BCR  | h     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.31  | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 36  | LMG  | B     | 601 | -    | 40,40,55     | 0.84 | 0        | 48,48,63    | 1.30  | 5 (10%)  |
| 22  | CLA  | S     | 305 | 20   | 50,58,73     | 1.66 | 6 (12%)  | 58,95,113   | 1.60  | 8 (13%)  |
| 26  | LHG  | G     | 618 | -    | 48,48,48     | 0.64 | 1 (2%)   | 51,54,54    | 1.28  | 7 (13%)  |
| 22  | CLA  | c     | 512 | 4    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.42  | 8 (10%)  |
| 21  | CHL  | n     | 608 | -    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 24  | XAT  | G     | 617 | -    | 39,47,47     | 5.24 | 20 (51%) | 54,74,74    | 13.43 | 30 (55%) |
| 32  | PL9  | A     | 411 | -    | 13,13,55     | 1.59 | 2 (15%)  | 17,17,69    | 1.64  | 4 (23%)  |
| 22  | CLA  | s     | 313 | 22   | 55,63,73     | 1.58 | 6 (10%)  | 64,101,113  | 1.50  | 7 (10%)  |
| 22  | CLA  | B     | 612 | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.39  | 7 (9%)   |
| 22  | CLA  | C     | 513 | 4    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.42  | 8 (10%)  |
| 37  | HEM  | f     | 101 | 7    | 41,50,50     | 4.46 | 10 (24%) | 45,82,82    | 3.70  | 22 (48%) |
| 22  | CLA  | N     | 612 | 1    | 60,68,73     | 1.88 | 12 (20%) | 70,107,113  | 1.95  | 15 (21%) |
| 21  | CHL  | n     | 607 | -    | 66,74,74     | 2.14 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 21  | CHL  | G     | 609 | -    | 61,69,74     | 2.21 | 16 (26%) | 67,108,114  | 2.57  | 19 (28%) |
| 35  | DGD  | a     | 413 | -    | 60,60,67     | 0.88 | 2 (3%)   | 74,74,81    | 1.44  | 12 (16%) |
| 35  | DGD  | J     | 101 | -    | 61,61,67     | 0.98 | 5 (8%)   | 75,75,81    | 1.53  | 10 (13%) |
| 22  | CLA  | C     | 514 | 22   | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.31  | 6 (7%)   |
| 22  | CLA  | n     | 613 | -    | 48,56,73     | 1.71 | 6 (12%)  | 55,92,113   | 1.51  | 8 (14%)  |
| 21  | CHL  | S     | 307 | 20   | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.87  | 16 (32%) |
| 33  | SQD  | A     | 412 | -    | 53,54,54     | 0.97 | 5 (9%)   | 62,65,65    | 1.60  | 12 (19%) |
| 22  | CLA  | B     | 615 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.36  | 6 (7%)   |
| 31  | BCR  | A     | 410 | -    | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.26  | 7 (12%)  |
| 21  | CHL  | G     | 605 | -    | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.87  | 16 (32%) |
| 26  | LHG  | B     | 622 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.26  | 6 (11%)  |
| 21  | CHL  | n     | 601 | 1    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 31  | BCR  | C     | 517 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.29  | 7 (12%)  |
| 22  | CLA  | Y     | 610 | 26   | 60,68,73     | 1.53 | 7 (11%)  | 70,107,113  | 1.40  | 7 (10%)  |
| 22  | CLA  | c     | 502 | -    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.35  | 6 (7%)   |
| 22  | CLA  | s     | 305 | 20   | 50,58,73     | 1.66 | 6 (12%)  | 58,95,113   | 1.59  | 8 (13%)  |
| 31  | BCR  | B     | 602 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.24  | 6 (10%)  |
| 23  | LUT  | G     | 615 | -    | 42,43,43     | 5.88 | 19 (45%) | 51,60,60    | 5.45  | 25 (49%) |
| 23  | LUT  | Y     | 614 | -    | 42,43,43     | 6.05 | 20 (47%) | 51,60,60    | 4.89  | 22 (43%) |
| 22  | CLA  | n     | 604 | 25   | 50,58,73     | 1.64 | 8 (16%)  | 58,95,113   | 1.57  | 8 (13%)  |
| 22  | CLA  | Y     | 604 | 25   | 50,58,73     | 1.63 | 8 (16%)  | 58,95,113   | 1.58  | 8 (13%)  |
| 22  | CLA  | C     | 512 | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.37  | 8 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | S     | 304 | 20   | 45,53,73     | 1.80 | 6 (13%)  | 52,89,113   | 1.55 | 7 (13%)  |
| 22  | CLA  | R     | 303 | -    | 60,68,73     | 1.53 | 6 (10%)  | 70,107,113  | 1.42 | 7 (10%)  |
| 22  | CLA  | N     | 613 | -    | 48,56,73     | 1.71 | 5 (10%)  | 55,92,113   | 1.50 | 8 (14%)  |
| 22  | CLA  | c     | 506 | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.37 | 7 (9%)   |
| 22  | CLA  | g     | 603 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.35 | 7 (9%)   |
| 22  | CLA  | C     | 515 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.42 | 7 (9%)   |
| 25  | NEX  | g     | 618 | 22   | 38,46,46     | 5.10 | 15 (39%) | 50,70,70    | 8.41 | 27 (54%) |
| 22  | CLA  | c     | 511 | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.36 | 8 (10%)  |
| 25  | NEX  | N     | 617 | 22   | 38,46,46     | 5.17 | 15 (39%) | 50,70,70    | 8.67 | 26 (52%) |
| 22  | CLA  | c     | 503 | -    | 65,73,73     | 1.43 | 8 (12%)  | 76,113,113  | 1.39 | 8 (10%)  |
| 22  | CLA  | c     | 509 | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.36 | 8 (10%)  |
| 22  | CLA  | y     | 603 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.34 | 7 (9%)   |
| 22  | CLA  | C     | 505 | -    | 65,73,73     | 1.42 | 6 (9%)   | 76,113,113  | 1.44 | 6 (7%)   |
| 26  | LHG  | C     | 520 | 22   | 48,48,48     | 0.81 | 4 (8%)   | 51,54,54    | 1.30 | 7 (13%)  |
| 31  | BCR  | B     | 619 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 22  | CLA  | B     | 618 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.34 | 7 (9%)   |
| 26  | LHG  | D     | 408 | -    | 45,45,48     | 0.65 | 1 (2%)   | 48,51,54    | 1.23 | 4 (8%)   |
| 35  | DGD  | c     | 517 | -    | 56,56,67     | 1.00 | 4 (7%)   | 70,70,81    | 1.56 | 12 (17%) |
| 21  | CHL  | g     | 609 | -    | 61,69,74     | 2.22 | 16 (26%) | 67,108,114  | 2.57 | 19 (28%) |
| 31  | BCR  | k     | 102 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 22  | CLA  | b     | 608 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.38 | 6 (7%)   |
| 22  | CLA  | r     | 312 | 19   | 60,68,73     | 1.53 | 6 (10%)  | 70,107,113  | 1.42 | 6 (8%)   |
| 36  | LMG  | b     | 620 | -    | 55,55,55     | 0.85 | 3 (5%)   | 63,63,63    | 1.36 | 9 (14%)  |
| 34  | BCT  | a     | 412 | -    | 2,3,3        | 1.33 | 0        | 2,3,3       | 2.75 | 2 (100%) |
| 22  | CLA  | s     | 304 | 20   | 45,53,73     | 1.80 | 6 (13%)  | 52,89,113   | 1.54 | 7 (13%)  |
| 22  | CLA  | b     | 607 | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.42 | 8 (10%)  |
| 36  | LMG  | c     | 523 | -    | 51,51,55     | 0.72 | 1 (1%)   | 59,59,63    | 1.38 | 7 (11%)  |
| 22  | CLA  | a     | 406 | -    | 50,58,73     | 1.67 | 8 (16%)  | 58,95,113   | 1.51 | 8 (13%)  |
| 22  | CLA  | B     | 607 | -    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.37 | 6 (7%)   |
| 31  | BCR  | D     | 406 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 21  | CHL  | n     | 606 | -    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 26  | LHG  | c     | 520 | 22   | 48,48,48     | 0.81 | 4 (8%)   | 51,54,54    | 1.30 | 7 (13%)  |
| 22  | CLA  | r     | 303 | -    | 60,68,73     | 1.53 | 5 (8%)   | 70,107,113  | 1.41 | 8 (11%)  |
| 35  | DGD  | c     | 518 | -    | 63,63,67     | 0.93 | 3 (4%)   | 77,77,81    | 1.47 | 10 (12%) |
| 21  | CHL  | r     | 307 | -    | 56,64,74     | 2.32 | 17 (30%) | 61,102,114  | 2.68 | 19 (31%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | CHL  | G     | 601 | 1    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 23  | LUT  | g     | 615 | -    | 42,43,43     | 5.88 | 19 (45%) | 51,60,60    | 5.45 | 25 (49%) |
| 22  | CLA  | c     | 514 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.42 | 7 (9%)   |
| 26  | LHG  | l     | 102 | -    | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.28 | 7 (13%)  |
| 22  | CLA  | G     | 611 | -    | 60,68,73     | 1.53 | 7 (11%)  | 70,107,113  | 1.41 | 7 (10%)  |
| 22  | CLA  | c     | 504 | -    | 65,73,73     | 1.43 | 7 (10%)  | 76,113,113  | 1.44 | 6 (7%)   |
| 22  | CLA  | b     | 601 | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.37 | 7 (9%)   |
| 22  | CLA  | s     | 310 | 26   | 55,63,73     | 1.57 | 7 (12%)  | 64,101,113  | 1.47 | 7 (10%)  |
| 23  | LUT  | R     | 312 | 22   | 42,43,43     | 5.91 | 19 (45%) | 51,60,60    | 5.17 | 28 (54%) |
| 22  | CLA  | B     | 610 | -    | 65,73,73     | 1.43 | 7 (10%)  | 76,113,113  | 1.42 | 8 (10%)  |
| 23  | LUT  | N     | 615 | -    | 42,43,43     | 6.10 | 20 (47%) | 51,60,60    | 4.66 | 27 (52%) |
| 36  | LMG  | D     | 411 | -    | 46,46,55     | 0.81 | 3 (6%)   | 54,54,63    | 1.39 | 7 (12%)  |
| 22  | CLA  | G     | 602 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.38 | 8 (10%)  |
| 22  | CLA  | n     | 612 | 1    | 60,68,73     | 1.87 | 12 (20%) | 70,107,113  | 1.95 | 14 (20%) |
| 31  | BCR  | c     | 515 | -    | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 22  | CLA  | g     | 610 | -    | 64,72,73     | 1.50 | 6 (9%)   | 74,111,113  | 1.42 | 6 (8%)   |
| 26  | LHG  | N     | 618 | -    | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.23 | 7 (13%)  |
| 35  | DGD  | A     | 401 | -    | 60,60,67     | 0.88 | 2 (3%)   | 74,74,81    | 1.44 | 12 (16%) |
| 25  | NEX  | r     | 315 | -    | 38,46,46     | 5.12 | 16 (42%) | 50,70,70    | 7.87 | 27 (54%) |
| 23  | LUT  | y     | 614 | -    | 42,43,43     | 5.89 | 19 (45%) | 51,60,60    | 5.45 | 25 (49%) |
| 26  | LHG  | C     | 522 | -    | 48,48,48     | 0.60 | 1 (2%)   | 51,54,54    | 1.29 | 8 (15%)  |
| 22  | CLA  | R     | 304 | -    | 48,56,73     | 1.70 | 7 (14%)  | 55,92,113   | 1.52 | 8 (14%)  |
| 21  | CHL  | y     | 608 | -    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 31  | BCR  | T     | 102 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 26  | LHG  | d     | 408 | -    | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.29 | 6 (11%)  |
| 22  | CLA  | D     | 405 | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.39 | 8 (10%)  |
| 26  | LHG  | S     | 314 | 22   | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.27 | 6 (11%)  |
| 22  | CLA  | B     | 603 | -    | 65,73,73     | 1.48 | 8 (12%)  | 76,113,113  | 1.35 | 8 (10%)  |
| 21  | CHL  | N     | 608 | -    | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 35  | DGD  | C     | 518 | -    | 56,56,67     | 0.99 | 3 (5%)   | 70,70,81    | 1.56 | 13 (18%) |
| 36  | LMG  | M     | 101 | -    | 51,51,55     | 0.75 | 1 (1%)   | 59,59,63    | 1.35 | 7 (11%)  |
| 22  | CLA  | c     | 513 | 22   | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.32 | 6 (7%)   |
| 22  | CLA  | B     | 609 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.41 | 7 (9%)   |
| 22  | CLA  | y     | 604 | 25   | 50,58,73     | 1.64 | 8 (16%)  | 58,95,113   | 1.57 | 7 (12%)  |
| 22  | CLA  | c     | 505 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.46 | 7 (9%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 21  | CHL  | R     | 307 | 19    | 61,69,74     | 2.22 | 17 (27%) | 67,108,114  | 2.57  | 19 (28%) |
| 32  | PL9  | a     | 410 | -     | 13,13,55     | 1.57 | 2 (15%)  | 17,17,69    | 1.66  | 4 (23%)  |
| 22  | CLA  | n     | 609 | -     | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.39  | 6 (7%)   |
| 26  | LHG  | y     | 617 | -     | 48,48,48     | 0.64 | 1 (2%)   | 51,54,54    | 1.29  | 7 (13%)  |
| 21  | CHL  | s     | 302 | -     | 46,54,74     | 2.56 | 16 (34%) | 49,90,114   | 2.87  | 16 (32%) |
| 24  | XAT  | Y     | 615 | -     | 39,47,47     | 5.30 | 20 (51%) | 54,74,74    | 13.38 | 30 (55%) |
| 22  | CLA  | R     | 308 | -     | 58,66,73     | 1.57 | 7 (12%)  | 67,104,113  | 1.42  | 7 (10%)  |
| 22  | CLA  | g     | 611 | -     | 60,68,73     | 1.53 | 7 (11%)  | 70,107,113  | 1.40  | 8 (11%)  |
| 22  | CLA  | C     | 508 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.40  | 6 (7%)   |
| 25  | NEX  | Y     | 616 | 22    | 38,46,46     | 5.13 | 15 (39%) | 50,70,70    | 8.19  | 27 (54%) |
| 33  | SQD  | l     | 103 | 12    | 53,54,54     | 0.97 | 5 (9%)   | 62,65,65    | 1.61  | 11 (17%) |
| 22  | CLA  | S     | 309 | 20,22 | 55,63,73     | 1.59 | 5 (9%)   | 64,101,113  | 1.49  | 9 (14%)  |
| 25  | NEX  | y     | 616 | 22    | 38,46,46     | 5.17 | 14 (36%) | 50,70,70    | 8.58  | 27 (54%) |
| 22  | CLA  | b     | 606 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.42  | 7 (9%)   |
| 30  | PHO  | D     | 401 | -     | 51,69,69     | 1.02 | 4 (7%)   | 47,99,99    | 1.17  | 5 (10%)  |
| 22  | CLA  | g     | 602 | -     | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.38  | 7 (9%)   |
| 22  | CLA  | C     | 506 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.45  | 7 (9%)   |
| 22  | CLA  | g     | 614 | -     | 48,56,73     | 1.71 | 6 (12%)  | 55,92,113   | 1.51  | 8 (14%)  |
| 21  | CHL  | G     | 608 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 22  | CLA  | N     | 611 | -     | 60,68,73     | 1.58 | 6 (10%)  | 70,107,113  | 1.40  | 7 (10%)  |
| 31  | BCR  | c     | 516 | -     | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.28  | 7 (12%)  |
| 30  | PHO  | A     | 408 | -     | 51,69,69     | 1.07 | 5 (9%)   | 47,99,99    | 1.12  | 4 (8%)   |
| 26  | LHG  | s     | 314 | 22    | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.26  | 6 (11%)  |
| 22  | CLA  | b     | 615 | -     | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.35  | 7 (9%)   |
| 36  | LMG  | C     | 523 | -     | 51,51,55     | 0.72 | 1 (1%)   | 59,59,63    | 1.38  | 7 (11%)  |
| 24  | XAT  | R     | 313 | -     | 39,47,47     | 5.20 | 17 (43%) | 54,74,74    | 13.47 | 28 (51%) |
| 37  | HEM  | F     | 101 | 7     | 41,50,50     | 4.46 | 10 (24%) | 45,82,82    | 3.69  | 22 (48%) |
| 24  | XAT  | r     | 314 | -     | 39,47,47     | 5.21 | 19 (48%) | 54,74,74    | 13.48 | 28 (51%) |
| 22  | CLA  | N     | 602 | -     | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.38  | 8 (10%)  |
| 24  | XAT  | N     | 616 | -     | 39,47,47     | 5.20 | 20 (51%) | 54,74,74    | 13.62 | 31 (57%) |
| 24  | XAT  | y     | 615 | -     | 39,47,47     | 5.28 | 20 (51%) | 54,74,74    | 13.37 | 29 (53%) |
| 22  | CLA  | b     | 611 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.41  | 6 (7%)   |
| 33  | SQD  | L     | 102 | -     | 41,42,54     | 1.08 | 5 (12%)  | 50,53,65    | 1.61  | 9 (18%)  |
| 22  | CLA  | B     | 611 | -     | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.38  | 6 (7%)   |
| 21  | CHL  | g     | 601 | 1     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | S     | 312 | 20    | 49,57,73     | 1.70 | 7 (14%)  | 55,93,113   | 1.50 | 6 (10%)  |
| 31  | BCR  | k     | 101 | -     | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 33  | SQD  | l     | 101 | -     | 41,42,54     | 1.08 | 5 (12%)  | 50,53,65    | 1.61 | 9 (18%)  |
| 26  | LHG  | n     | 617 | 22    | 48,48,48     | 0.64 | 1 (2%)   | 51,54,54    | 1.29 | 7 (13%)  |
| 22  | CLA  | G     | 613 | 1     | 65,73,73     | 1.80 | 12 (18%) | 76,113,113  | 1.88 | 15 (19%) |
| 22  | CLA  | d     | 403 | -     | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 22  | CLA  | b     | 614 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.39 | 6 (7%)   |
| 26  | LHG  | r     | 302 | 19    | 46,46,48     | 0.64 | 1 (2%)   | 49,52,54    | 1.28 | 7 (14%)  |
| 36  | LMG  | T     | 101 | -     | 51,51,55     | 0.74 | 1 (1%)   | 59,59,63    | 1.35 | 7 (11%)  |
| 22  | CLA  | n     | 603 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 22  | CLA  | d     | 404 | -     | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.39 | 8 (10%)  |
| 21  | CHL  | N     | 601 | 1     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 32  | PL9  | D     | 407 | -     | 55,55,55     | 1.34 | 5 (9%)   | 68,69,69    | 1.54 | 13 (19%) |
| 26  | LHG  | R     | 301 | 19    | 46,46,48     | 0.64 | 1 (2%)   | 49,52,54    | 1.28 | 7 (14%)  |
| 22  | CLA  | s     | 309 | 20,22 | 55,63,73     | 1.58 | 5 (9%)   | 64,101,113  | 1.49 | 9 (14%)  |
| 22  | CLA  | C     | 503 | -     | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.35 | 6 (7%)   |
| 22  | CLA  | s     | 303 | 20    | 61,69,73     | 1.54 | 7 (11%)  | 71,108,113  | 1.43 | 8 (11%)  |
| 22  | CLA  | A     | 406 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.37 | 6 (7%)   |
| 22  | CLA  | b     | 603 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.38 | 7 (9%)   |
| 22  | CLA  | B     | 608 | -     | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.38 | 7 (9%)   |
| 26  | LHG  | c     | 522 | -     | 48,48,48     | 0.60 | 1 (2%)   | 51,54,54    | 1.29 | 8 (15%)  |
| 31  | BCR  | b     | 617 | -     | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 36  | LMG  | I     | 101 | -     | 40,40,55     | 0.85 | 0        | 48,48,63    | 1.30 | 5 (10%)  |
| 26  | LHG  | D     | 410 | -     | 42,42,48     | 0.67 | 1 (2%)   | 45,48,54    | 1.26 | 5 (11%)  |
| 22  | CLA  | b     | 613 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 27  | OEX  | A     | 402 | 2,4   | 0,15,15      | -    | -        | -           | -    | -        |
| 22  | CLA  | C     | 504 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.39 | 8 (10%)  |
| 23  | LUT  | G     | 616 | -     | 42,43,43     | 6.08 | 19 (45%) | 51,60,60    | 4.93 | 22 (43%) |
| 34  | BCT  | D     | 403 | -     | 2,3,3        | 1.33 | 0        | 2,3,3       | 2.74 | 2 (100%) |
| 22  | CLA  | a     | 408 | -     | 60,68,73     | 1.50 | 7 (11%)  | 70,107,113  | 1.45 | 8 (11%)  |
| 31  | BCR  | a     | 409 | -     | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 22  | CLA  | Y     | 611 | 1     | 65,73,73     | 1.80 | 12 (18%) | 76,113,113  | 1.89 | 15 (19%) |
| 22  | CLA  | B     | 606 | -     | 65,73,73     | 1.44 | 6 (9%)   | 76,113,113  | 1.39 | 7 (9%)   |
| 22  | CLA  | B     | 616 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 21  | CHL  | g     | 608 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 30  | PHO  | d     | 401 | -     | 51,69,69     | 1.03 | 4 (7%)   | 47,99,99    | 1.17 | 6 (12%)  |
| 23  | LUT  | r     | 313 | 22    | 42,43,43     | 5.90 | 19 (45%) | 51,60,60    | 5.16 | 28 (54%) |
| 21  | CHL  | Y     | 605 | -     | 50,58,74     | 2.45 | 16 (32%) | 52,94,114   | 2.81 | 17 (32%) |
| 22  | CLA  | G     | 604 | -     | 50,58,73     | 1.64 | 8 (16%)  | 58,95,113   | 1.57 | 7 (12%)  |
| 22  | CLA  | G     | 614 | -     | 48,56,73     | 1.70 | 5 (10%)  | 55,92,113   | 1.51 | 8 (14%)  |
| 22  | CLA  | y     | 612 | 1     | 65,73,73     | 1.80 | 12 (18%) | 76,113,113  | 1.88 | 15 (19%) |
| 22  | CLA  | g     | 612 | -     | 60,68,73     | 1.56 | 6 (10%)  | 70,107,113  | 1.39 | 7 (10%)  |
| 21  | CHL  | y     | 601 | 1     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 21  | CHL  | s     | 307 | 20    | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.88 | 16 (32%) |
| 22  | CLA  | s     | 311 | 20,22 | 56,64,73     | 1.58 | 6 (10%)  | 65,102,113  | 1.40 | 7 (10%)  |
| 25  | NEX  | n     | 616 | 22    | 38,46,46     | 5.17 | 15 (39%) | 50,70,70    | 8.46 | 26 (52%) |
| 26  | LHG  | d     | 407 | -     | 45,45,48     | 0.64 | 1 (2%)   | 48,51,54    | 1.23 | 4 (8%)   |
| 21  | CHL  | R     | 306 | -     | 56,64,74     | 2.31 | 17 (30%) | 61,102,114  | 2.67 | 19 (31%) |
| 22  | CLA  | s     | 312 | 20    | 49,57,73     | 1.71 | 7 (14%)  | 55,93,113   | 1.51 | 6 (10%)  |
| 22  | CLA  | r     | 309 | -     | 58,66,73     | 1.56 | 8 (13%)  | 67,104,113  | 1.42 | 7 (10%)  |
| 33  | SQD  | D     | 402 | -     | 49,50,54     | 1.01 | 5 (10%)  | 58,61,65    | 1.56 | 10 (17%) |
| 22  | CLA  | b     | 605 | -     | 65,73,73     | 1.44 | 6 (9%)   | 76,113,113  | 1.38 | 7 (9%)   |
| 21  | CHL  | n     | 605 | -     | 50,58,74     | 2.45 | 16 (32%) | 52,94,114   | 2.81 | 17 (32%) |
| 21  | CHL  | S     | 302 | -     | 46,54,74     | 2.55 | 17 (36%) | 49,90,114   | 2.88 | 16 (32%) |
| 21  | CHL  | g     | 606 | -     | 50,58,74     | 2.45 | 17 (34%) | 52,94,114   | 2.82 | 17 (32%) |
| 22  | CLA  | b     | 602 | -     | 65,73,73     | 1.43 | 8 (12%)  | 76,113,113  | 1.40 | 8 (10%)  |
| 22  | CLA  | y     | 613 | -     | 48,56,73     | 1.71 | 5 (10%)  | 55,92,113   | 1.50 | 8 (14%)  |
| 22  | CLA  | A     | 409 | -     | 60,68,73     | 1.50 | 7 (11%)  | 70,107,113  | 1.46 | 8 (11%)  |
| 22  | CLA  | r     | 311 | 23,19 | 49,57,73     | 1.74 | 7 (14%)  | 55,93,113   | 1.43 | 4 (7%)   |
| 35  | DGD  | h     | 102 | -     | 63,63,67     | 0.94 | 3 (4%)   | 77,77,81    | 1.48 | 14 (18%) |
| 21  | CHL  | y     | 609 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 26  | LHG  | D     | 409 | -     | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.28 | 6 (11%)  |
| 21  | CHL  | Y     | 608 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 27  | OEX  | a     | 401 | 2,4   | 0,15,15      | -    | -        | -           | -    | -        |
| 22  | CLA  | B     | 617 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.38 | 6 (7%)   |
| 21  | CHL  | y     | 607 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 36  | LMG  | C     | 502 | -     | 48,48,55     | 0.78 | 2 (4%)   | 56,56,63    | 1.42 | 8 (14%)  |
| 21  | CHL  | g     | 607 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 25  | NEX  | y     | 618 | -     | 38,46,46     | 5.13 | 16 (42%) | 50,70,70    | 7.86 | 27 (54%) |
| 31  | BCR  | b     | 618 | -     | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.23 | 3 (5%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | A     | 405 | -     | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.41 | 7 (9%)   |
| 26  | LHG  | C     | 521 | -     | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.23 | 7 (13%)  |
| 22  | CLA  | c     | 510 | -     | 65,73,73     | 3.57 | 12 (18%) | 76,113,113  | 2.58 | 18 (23%) |
| 22  | CLA  | g     | 613 | 1     | 65,73,73     | 1.80 | 11 (16%) | 76,113,113  | 1.89 | 15 (19%) |
| 22  | CLA  | S     | 308 | 20    | 45,53,73     | 1.82 | 6 (13%)  | 52,89,113   | 1.54 | 7 (13%)  |
| 22  | CLA  | R     | 310 | 23,19 | 49,57,73     | 1.75 | 7 (14%)  | 55,93,113   | 1.44 | 4 (7%)   |
| 23  | LUT  | g     | 616 | -     | 42,43,43     | 6.10 | 19 (45%) | 51,60,60    | 4.92 | 22 (43%) |
| 22  | CLA  | G     | 610 | -     | 64,72,73     | 1.50 | 6 (9%)   | 74,111,113  | 1.44 | 8 (10%)  |
| 22  | CLA  | R     | 311 | 19    | 60,68,73     | 1.52 | 6 (10%)  | 70,107,113  | 1.40 | 6 (8%)   |
| 21  | CHL  | G     | 606 | -     | 50,58,74     | 2.45 | 16 (32%) | 52,94,114   | 2.81 | 17 (32%) |
| 32  | PL9  | d     | 406 | -     | 55,55,55     | 1.33 | 4 (7%)   | 68,69,69    | 1.54 | 13 (19%) |
| 26  | LHG  | g     | 619 | -     | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.30 | 8 (15%)  |
| 22  | CLA  | g     | 604 | 25    | 50,58,73     | 1.64 | 8 (16%)  | 58,95,113   | 1.57 | 8 (13%)  |
| 22  | CLA  | N     | 609 | -     | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.40 | 6 (7%)   |
| 21  | CHL  | s     | 301 | -     | 48,56,74     | 2.50 | 16 (33%) | 51,92,114   | 2.83 | 17 (33%) |
| 31  | BCR  | b     | 616 | -     | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 33  | SQD  | L     | 101 | 12    | 53,54,54     | 0.97 | 5 (9%)   | 62,65,65    | 1.61 | 11 (17%) |
| 26  | LHG  | c     | 521 | -     | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.23 | 7 (13%)  |
| 21  | CHL  | N     | 607 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 22  | CLA  | n     | 611 | -     | 60,68,73     | 1.57 | 6 (10%)  | 70,107,113  | 1.39 | 7 (10%)  |
| 21  | CHL  | Y     | 606 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 22  | CLA  | w     | 101 | 16    | 60,68,73     | 1.57 | 6 (10%)  | 70,107,113  | 1.39 | 7 (10%)  |
| 22  | CLA  | a     | 405 | -     | 65,73,73     | 1.44 | 10 (15%) | 76,113,113  | 1.37 | 6 (7%)   |
| 22  | CLA  | r     | 304 | -     | 60,68,73     | 1.53 | 6 (10%)  | 70,107,113  | 1.42 | 7 (10%)  |
| 22  | CLA  | G     | 612 | -     | 60,68,73     | 1.58 | 6 (10%)  | 70,107,113  | 1.39 | 7 (10%)  |
| 22  | CLA  | N     | 604 | 25    | 50,58,73     | 1.64 | 8 (16%)  | 58,95,113   | 1.59 | 7 (12%)  |
| 22  | CLA  | b     | 609 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 21  | CHL  | G     | 607 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47 | 19 (26%) |
| 22  | CLA  | n     | 602 | -     | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.38 | 7 (9%)   |
| 21  | CHL  | r     | 301 | 19    | 48,56,74     | 2.49 | 16 (33%) | 51,92,114   | 2.83 | 17 (33%) |
| 22  | CLA  | y     | 602 | -     | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.38 | 8 (10%)  |
| 36  | LMG  | d     | 410 | -     | 46,46,55     | 0.81 | 3 (6%)   | 54,54,63    | 1.38 | 7 (12%)  |
| 22  | CLA  | s     | 308 | 20    | 45,53,73     | 1.82 | 6 (13%)  | 52,89,113   | 1.55 | 7 (13%)  |
| 22  | CLA  | x     | 101 | -     | 65,73,73     | 1.49 | 7 (10%)  | 76,113,113  | 1.36 | 8 (10%)  |
| 26  | LHG  | b     | 619 | -     | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.26 | 6 (11%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 31  | BCR  | C     | 516 | -     | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.26  | 6 (10%)  |
| 22  | CLA  | C     | 511 | -     | 65,73,73     | 3.57 | 12 (18%) | 76,113,113  | 2.58  | 17 (22%) |
| 31  | BCR  | K     | 102 | -     | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.26  | 8 (14%)  |
| 22  | CLA  | Y     | 609 | -     | 60,68,73     | 1.54 | 6 (10%)  | 70,107,113  | 1.43  | 7 (10%)  |
| 22  | CLA  | r     | 305 | -     | 48,56,73     | 1.71 | 7 (14%)  | 55,92,113   | 1.52  | 8 (14%)  |
| 31  | BCR  | d     | 405 | -     | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.24  | 7 (12%)  |
| 35  | DGD  | H     | 102 | -     | 63,63,67     | 0.94 | 3 (4%)   | 77,77,81    | 1.48  | 14 (18%) |
| 22  | CLA  | Y     | 612 | -     | 48,56,73     | 1.70 | 6 (12%)  | 55,92,113   | 1.51  | 8 (14%)  |
| 22  | CLA  | N     | 603 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.35  | 7 (9%)   |
| 21  | CHL  | Y     | 607 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 31  | BCR  | B     | 621 | -     | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.23  | 3 (5%)   |
| 36  | LMG  | B     | 623 | -     | 55,55,55     | 0.85 | 3 (5%)   | 63,63,63    | 1.36  | 9 (14%)  |
| 21  | CHL  | S     | 306 | 20    | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.87  | 16 (32%) |
| 22  | CLA  | S     | 310 | 26    | 55,63,73     | 1.58 | 7 (12%)  | 64,101,113  | 1.47  | 7 (10%)  |
| 22  | CLA  | C     | 507 | -     | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.37  | 7 (9%)   |
| 22  | CLA  | Y     | 603 | -     | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.35  | 7 (9%)   |
| 22  | CLA  | S     | 311 | 20,22 | 56,64,73     | 1.59 | 6 (10%)  | 65,102,113  | 1.42  | 7 (10%)  |
| 24  | XAT  | g     | 617 | -     | 39,47,47     | 5.24 | 20 (51%) | 54,74,74    | 13.43 | 29 (53%) |
| 22  | CLA  | r     | 310 | 19    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.40  | 6 (7%)   |
| 36  | LMG  | K     | 103 | -     | 51,51,55     | 0.72 | 0        | 59,59,63    | 1.34  | 6 (10%)  |
| 22  | CLA  | R     | 309 | 19    | 65,73,73     | 1.48 | 6 (9%)   | 76,113,113  | 1.40  | 6 (7%)   |
| 35  | DGD  | c     | 519 | -     | 61,61,67     | 0.98 | 5 (8%)   | 75,75,81    | 1.53  | 10 (13%) |
| 31  | BCR  | H     | 101 | -     | 41,41,41     | 1.19 | 3 (7%)   | 56,56,56    | 1.30  | 6 (10%)  |
| 22  | CLA  | c     | 507 | -     | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.41  | 7 (9%)   |
| 21  | CHL  | s     | 306 | 20    | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.88  | 16 (32%) |
| 21  | CHL  | r     | 306 | -     | 66,74,74     | 2.13 | 16 (24%) | 73,114,114  | 2.47  | 19 (26%) |
| 22  | CLA  | A     | 407 | -     | 50,58,73     | 1.67 | 8 (16%)  | 58,95,113   | 1.50  | 8 (13%)  |
| 22  | CLA  | R     | 302 | -     | 60,68,73     | 1.53 | 5 (8%)   | 70,107,113  | 1.42  | 8 (11%)  |
| 22  | CLA  | C     | 509 | -     | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.38  | 7 (9%)   |
| 31  | BCR  | K     | 101 | -     | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.23  | 7 (12%)  |
| 22  | CLA  | y     | 610 | -     | 60,68,73     | 1.54 | 7 (11%)  | 70,107,113  | 1.43  | 6 (8%)   |
| 36  | LMG  | w     | 102 | -     | 48,48,55     | 0.78 | 2 (4%)   | 56,56,63    | 1.41  | 8 (14%)  |
| 21  | CHL  | r     | 308 | 19    | 61,69,74     | 2.22 | 16 (26%) | 67,108,114  | 2.57  | 19 (28%) |
| 22  | CLA  | c     | 508 | -     | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.38  | 7 (9%)   |
| 26  | LHG  | Y     | 617 | 22    | 48,48,48     | 0.66 | 1 (2%)   | 51,54,54    | 1.26  | 7 (13%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | y     | 611 | -    | 60,68,73     | 1.53 | 7 (11%)  | 70,107,113  | 1.40 | 7 (10%)  |
| 22  | CLA  | C     | 510 | -    | 65,73,73     | 1.47 | 8 (12%)  | 76,113,113  | 1.37 | 8 (10%)  |
| 22  | CLA  | n     | 610 | 26   | 60,68,73     | 1.53 | 6 (10%)  | 70,107,113  | 1.40 | 7 (10%)  |
| 35  | DGD  | C     | 519 | -    | 63,63,67     | 0.93 | 3 (4%)   | 77,77,81    | 1.47 | 10 (12%) |
| 22  | CLA  | S     | 303 | 20   | 61,69,73     | 1.54 | 6 (9%)   | 71,108,113  | 1.43 | 8 (11%)  |
| 22  | CLA  | D     | 404 | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 22  | CLA  | B     | 613 | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.38 | 7 (9%)   |
| 21  | CHL  | g     | 605 | -    | 46,54,74     | 2.55 | 16 (34%) | 49,90,114   | 2.88 | 16 (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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | CHL  | R     | 305 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 22  | CLA  | S     | 313 | 22   | 1/1/13/20 | 12/25/103/115 | -       |
| 21  | CHL  | y     | 605 | -    | 3/3/16/26 | 11/18/116/137 | -       |
| 33  | SQD  | d     | 402 | -    | 1/1/9/9   | 18/45/65/69   | 0/1/1/1 |
| 21  | CHL  | y     | 606 | -    | 3/3/16/26 | 13/20/118/137 | -       |
| 22  | CLA  | Y     | 602 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | b     | 610 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 24  | XAT  | n     | 615 | -    | 2/2/12/26 | 16/31/93/93   | 0/4/4/4 |
| 33  | SQD  | a     | 411 | -    | -         | 23/49/69/69   | 0/1/1/1 |
| 23  | LUT  | Y     | 613 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 26  | LHG  | L     | 103 | -    | -         | 19/53/53/53   | -       |
| 22  | CLA  | W     | 101 | -    | 1/1/14/20 | 12/31/109/115 | -       |
| 30  | PHO  | a     | 407 | -    | -         | 13/37/103/103 | 0/5/6/6 |
| 26  | LHG  | d     | 409 | -    | -         | 19/47/47/53   | -       |
| 22  | CLA  | b     | 604 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 21  | CHL  | Y     | 601 | 1    | 4/4/20/26 | 24/39/137/137 | -       |
| 22  | CLA  | B     | 604 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | B     | 614 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 31  | BCR  | B     | 620 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 36  | LMG  | k     | 103 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 23  | LUT  | n     | 614 | -    | -         | 17/29/67/67   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | N     | 610 | -    | 1/1/14/20 | 8/31/109/115  | -       |
| 21  | CHL  | S     | 301 | -    | 3/3/16/26 | 10/18/116/137 | -       |
| 22  | CLA  | a     | 404 | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 22  | CLA  | B     | 605 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 21  | CHL  | N     | 606 | -    | 4/4/20/26 | 18/39/137/137 | -       |
| 23  | LUT  | N     | 614 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 22  | CLA  | b     | 612 | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 21  | CHL  | N     | 605 | -    | 3/3/16/26 | 13/20/118/137 | -       |
| 22  | CLA  | G     | 603 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 31  | BCR  | h     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 36  | LMG  | B     | 601 | -    | -         | 18/35/55/70   | 0/1/1/1 |
| 22  | CLA  | S     | 305 | 20   | 1/1/12/20 | 9/19/97/115   | -       |
| 26  | LHG  | G     | 618 | -    | -         | 28/53/53/53   | -       |
| 22  | CLA  | c     | 512 | 4    | 1/1/15/20 | 14/37/115/115 | -       |
| 21  | CHL  | n     | 608 | -    | 4/4/20/26 | 15/39/137/137 | -       |
| 24  | XAT  | G     | 617 | -    | 3/3/12/26 | 17/31/93/93   | 0/4/4/4 |
| 32  | PL9  | A     | 411 | -    | -         | 3/5/18/73     | 0/1/1/1 |
| 22  | CLA  | s     | 313 | 22   | 1/1/13/20 | 12/25/103/115 | -       |
| 22  | CLA  | B     | 612 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 22  | CLA  | C     | 513 | 4    | 1/1/15/20 | 14/37/115/115 | -       |
| 37  | HEM  | f     | 101 | 7    | -         | 4/12/54/54    | -       |
| 22  | CLA  | N     | 612 | 1    | 1/1/14/20 | 16/31/109/115 | -       |
| 21  | CHL  | n     | 607 | -    | 4/4/20/26 | 23/39/137/137 | -       |
| 21  | CHL  | G     | 609 | -    | 4/4/19/26 | 10/33/131/137 | -       |
| 35  | DGD  | a     | 413 | -    | -         | 21/48/88/95   | 0/2/2/2 |
| 35  | DGD  | J     | 101 | -    | -         | 16/49/89/95   | 0/2/2/2 |
| 22  | CLA  | C     | 514 | 22   | 1/1/15/20 | 21/37/115/115 | -       |
| 22  | CLA  | n     | 613 | -    | 1/1/11/20 | 9/17/95/115   | -       |
| 21  | CHL  | S     | 307 | 20   | 3/3/16/26 | 12/15/113/137 | -       |
| 33  | SQD  | A     | 412 | -    | -         | 23/49/69/69   | 0/1/1/1 |
| 22  | CLA  | B     | 615 | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 31  | BCR  | A     | 410 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 21  | CHL  | G     | 605 | -    | 3/3/16/26 | 9/15/113/137  | -       |
| 26  | LHG  | B     | 622 | -    | -         | 28/53/53/53   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | CHL  | n     | 601 | 1    | 4/4/20/26 | 24/39/137/137 | -       |
| 31  | BCR  | C     | 517 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 22  | CLA  | Y     | 610 | 26   | 1/1/14/20 | 8/31/109/115  | -       |
| 22  | CLA  | c     | 502 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | s     | 305 | 20   | 1/1/12/20 | 9/19/97/115   | -       |
| 31  | BCR  | B     | 602 | -    | -         | 20/29/63/63   | 0/2/2/2 |
| 23  | LUT  | G     | 615 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 23  | LUT  | Y     | 614 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 22  | CLA  | n     | 604 | 25   | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | Y     | 604 | 25   | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | C     | 512 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 22  | CLA  | S     | 304 | 20   | 1/1/11/20 | 7/13/91/115   | -       |
| 22  | CLA  | R     | 303 | -    | 1/1/14/20 | 9/31/109/115  | -       |
| 22  | CLA  | N     | 613 | -    | 1/1/11/20 | 9/17/95/115   | -       |
| 22  | CLA  | c     | 506 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 22  | CLA  | g     | 603 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 22  | CLA  | C     | 515 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 25  | NEX  | g     | 618 | 22   | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | c     | 511 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 25  | NEX  | N     | 617 | 22   | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | c     | 503 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 22  | CLA  | c     | 509 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | y     | 603 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 22  | CLA  | C     | 505 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 26  | LHG  | C     | 520 | 22   | -         | 31/53/53/53   | -       |
| 31  | BCR  | B     | 619 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 618 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 26  | LHG  | D     | 408 | -    | -         | 25/50/50/53   | -       |
| 35  | DGD  | c     | 517 | -    | -         | 18/44/84/95   | 0/2/2/2 |
| 21  | CHL  | g     | 609 | -    | 4/4/19/26 | 10/33/131/137 | -       |
| 31  | BCR  | k     | 102 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | b     | 608 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 22  | CLA  | r     | 312 | 19   | 1/1/14/20 | 12/31/109/115 | -       |
| 36  | LMG  | b     | 620 | -    | -         | 22/50/70/70   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | s     | 304 | 20   | 1/1/11/20 | 7/13/91/115   | -       |
| 22  | CLA  | b     | 607 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 36  | LMG  | c     | 523 | -    | -         | 20/46/66/70   | 0/1/1/1 |
| 22  | CLA  | a     | 406 | -    | 1/1/12/20 | 8/19/97/115   | -       |
| 22  | CLA  | B     | 607 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 31  | BCR  | D     | 406 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 21  | CHL  | n     | 606 | -    | 4/4/20/26 | 18/39/137/137 | -       |
| 26  | LHG  | c     | 520 | 22   | -         | 31/53/53/53   | -       |
| 22  | CLA  | r     | 303 | -    | 1/1/14/20 | 8/31/109/115  | -       |
| 35  | DGD  | c     | 518 | -    | -         | 26/51/91/95   | 0/2/2/2 |
| 21  | CHL  | r     | 307 | -    | 4/4/18/26 | 16/27/125/137 | -       |
| 21  | CHL  | G     | 601 | 1    | 4/4/20/26 | 24/39/137/137 | -       |
| 23  | LUT  | g     | 615 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 22  | CLA  | c     | 514 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 26  | LHG  | l     | 102 | -    | -         | 19/53/53/53   | -       |
| 22  | CLA  | G     | 611 | -    | 1/1/14/20 | 8/31/109/115  | -       |
| 22  | CLA  | c     | 504 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 22  | CLA  | b     | 601 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | s     | 310 | 26   | 1/1/13/20 | 16/25/103/115 | -       |
| 23  | LUT  | R     | 312 | 22   | -         | 18/29/67/67   | 0/2/2/2 |
| 22  | CLA  | B     | 610 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 23  | LUT  | N     | 615 | -    | -         | 15/29/67/67   | 0/2/2/2 |
| 36  | LMG  | D     | 411 | -    | -         | 12/41/61/70   | 0/1/1/1 |
| 22  | CLA  | G     | 602 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | n     | 612 | 1    | 1/1/14/20 | 16/31/109/115 | -       |
| 31  | BCR  | c     | 515 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | g     | 610 | -    | 1/1/14/20 | 16/36/114/115 | -       |
| 26  | LHG  | N     | 618 | -    | -         | 29/53/53/53   | -       |
| 35  | DGD  | A     | 401 | -    | -         | 21/48/88/95   | 0/2/2/2 |
| 25  | NEX  | r     | 315 | -    | 2/2/12/25 | 14/27/83/83   | 0/3/3/3 |
| 23  | LUT  | y     | 614 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 26  | LHG  | C     | 522 | -    | -         | 24/53/53/53   | -       |
| 22  | CLA  | R     | 304 | -    | 1/1/11/20 | 7/17/95/115   | -       |
| 21  | CHL  | y     | 608 | -    | 4/4/20/26 | 23/39/137/137 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 31  | BCR  | T     | 102 | -     | -         | 21/29/63/63   | 0/2/2/2 |
| 26  | LHG  | d     | 408 | -     | -         | 21/53/53/53   | -       |
| 22  | CLA  | D     | 405 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 26  | LHG  | S     | 314 | 22    | -         | 29/53/53/53   | -       |
| 22  | CLA  | B     | 603 | -     | 1/1/15/20 | 16/37/115/115 | -       |
| 21  | CHL  | N     | 608 | -     | 4/4/20/26 | 15/39/137/137 | -       |
| 35  | DGD  | C     | 518 | -     | -         | 18/44/84/95   | 0/2/2/2 |
| 36  | LMG  | M     | 101 | -     | -         | 23/46/66/70   | 0/1/1/1 |
| 22  | CLA  | c     | 513 | 22    | 1/1/15/20 | 21/37/115/115 | -       |
| 22  | CLA  | B     | 609 | -     | 1/1/15/20 | 6/37/115/115  | -       |
| 22  | CLA  | y     | 604 | 25    | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | c     | 505 | -     | 1/1/15/20 | 8/37/115/115  | -       |
| 21  | CHL  | R     | 307 | 19    | 4/4/19/26 | 17/33/131/137 | -       |
| 32  | PL9  | a     | 410 | -     | -         | 3/5/18/73     | 0/1/1/1 |
| 22  | CLA  | n     | 609 | -     | 1/1/15/20 | 18/37/115/115 | -       |
| 26  | LHG  | y     | 617 | -     | -         | 22/53/53/53   | -       |
| 21  | CHL  | s     | 302 | -     | 3/3/16/26 | 9/15/113/137  | -       |
| 24  | XAT  | Y     | 615 | -     | 2/2/12/26 | 18/31/93/93   | 0/4/4/4 |
| 22  | CLA  | R     | 308 | -     | 1/1/13/20 | 9/29/107/115  | -       |
| 22  | CLA  | g     | 611 | -     | 1/1/14/20 | 8/31/109/115  | -       |
| 22  | CLA  | C     | 508 | -     | 1/1/15/20 | 10/37/115/115 | -       |
| 25  | NEX  | Y     | 616 | 22    | 2/2/12/25 | 14/27/83/83   | 0/3/3/3 |
| 33  | SQD  | l     | 103 | 12    | -         | 18/49/69/69   | 0/1/1/1 |
| 22  | CLA  | S     | 309 | 20,22 | 1/1/13/20 | 7/25/103/115  | -       |
| 25  | NEX  | y     | 616 | 22    | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | b     | 606 | -     | 1/1/15/20 | 6/37/115/115  | -       |
| 30  | PHO  | D     | 401 | -     | -         | 15/37/103/103 | 0/5/6/6 |
| 22  | CLA  | g     | 602 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | C     | 506 | -     | 1/1/15/20 | 8/37/115/115  | -       |
| 22  | CLA  | g     | 614 | -     | 1/1/11/20 | 9/17/95/115   | -       |
| 21  | CHL  | G     | 608 | -     | 4/4/20/26 | 23/39/137/137 | -       |
| 22  | CLA  | N     | 611 | -     | 1/1/14/20 | 12/31/109/115 | -       |
| 31  | BCR  | c     | 516 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 30  | PHO  | A     | 408 | -     | -         | 13/37/103/103 | 0/5/6/6 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 26  | LHG  | s     | 314 | 22    | -         | 29/53/53/53   | -       |
| 22  | CLA  | b     | 615 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 36  | LMG  | C     | 523 | -     | -         | 20/46/66/70   | 0/1/1/1 |
| 24  | XAT  | R     | 313 | -     | 1/1/12/26 | 14/31/93/93   | 0/4/4/4 |
| 37  | HEM  | F     | 101 | 7     | -         | 4/12/54/54    | -       |
| 24  | XAT  | r     | 314 | -     | 1/1/12/26 | 14/31/93/93   | 0/4/4/4 |
| 22  | CLA  | N     | 602 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 24  | XAT  | N     | 616 | -     | 2/2/12/26 | 17/31/93/93   | 0/4/4/4 |
| 24  | XAT  | y     | 615 | -     | 2/2/12/26 | 18/31/93/93   | 0/4/4/4 |
| 22  | CLA  | b     | 611 | -     | 1/1/15/20 | 17/37/115/115 | -       |
| 33  | SQD  | L     | 102 | -     | -         | 13/37/57/69   | 0/1/1/1 |
| 22  | CLA  | B     | 611 | -     | 1/1/15/20 | 7/37/115/115  | -       |
| 21  | CHL  | g     | 601 | 1     | 4/4/20/26 | 24/39/137/137 | -       |
| 22  | CLA  | S     | 312 | 20    | 1/1/11/20 | 7/18/96/115   | -       |
| 31  | BCR  | k     | 101 | -     | -         | 16/29/63/63   | 0/2/2/2 |
| 33  | SQD  | l     | 101 | -     | -         | 13/37/57/69   | 0/1/1/1 |
| 26  | LHG  | n     | 617 | 22    | -         | 25/53/53/53   | -       |
| 22  | CLA  | G     | 613 | 1     | 1/1/15/20 | 20/37/115/115 | -       |
| 22  | CLA  | d     | 403 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | b     | 614 | -     | 1/1/15/20 | 20/37/115/115 | -       |
| 26  | LHG  | r     | 302 | 19    | -         | 27/51/51/53   | -       |
| 36  | LMG  | T     | 101 | -     | -         | 23/46/66/70   | 0/1/1/1 |
| 22  | CLA  | n     | 603 | -     | 1/1/15/20 | 17/37/115/115 | -       |
| 22  | CLA  | d     | 404 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 21  | CHL  | N     | 601 | 1     | 4/4/20/26 | 24/39/137/137 | -       |
| 32  | PL9  | D     | 407 | -     | -         | 17/53/73/73   | 0/1/1/1 |
| 26  | LHG  | R     | 301 | 19    | -         | 27/51/51/53   | -       |
| 22  | CLA  | s     | 309 | 20,22 | 1/1/13/20 | 7/25/103/115  | -       |
| 22  | CLA  | C     | 503 | -     | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | s     | 303 | 20    | 1/1/14/20 | 12/33/111/115 | -       |
| 22  | CLA  | A     | 406 | -     | 1/1/15/20 | 15/37/115/115 | -       |
| 22  | CLA  | b     | 603 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 22  | CLA  | B     | 608 | -     | 1/1/15/20 | 10/37/115/115 | -       |
| 26  | LHG  | c     | 522 | -     | -         | 23/53/53/53   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 31  | BCR  | b     | 617 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 36  | LMG  | I     | 101 | -     | -         | 18/35/55/70   | 0/1/1/1 |
| 26  | LHG  | D     | 410 | -     | -         | 19/47/47/53   | -       |
| 22  | CLA  | b     | 613 | -     | 1/1/15/20 | 14/37/115/115 | -       |
| 22  | CLA  | C     | 504 | -     | 1/1/15/20 | 17/37/115/115 | -       |
| 23  | LUT  | G     | 616 | -     | -         | 16/29/67/67   | 0/2/2/2 |
| 22  | CLA  | a     | 408 | -     | 1/1/14/20 | 3/31/109/115  | -       |
| 31  | BCR  | a     | 409 | -     | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | Y     | 611 | 1     | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | B     | 606 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 22  | CLA  | B     | 616 | -     | 1/1/15/20 | 14/37/115/115 | -       |
| 21  | CHL  | g     | 608 | -     | 4/4/20/26 | 23/39/137/137 | -       |
| 30  | PHO  | d     | 401 | -     | -         | 15/37/103/103 | 0/5/6/6 |
| 23  | LUT  | r     | 313 | 22    | -         | 18/29/67/67   | 0/2/2/2 |
| 21  | CHL  | Y     | 605 | -     | 3/3/16/26 | 13/20/118/137 | -       |
| 22  | CLA  | G     | 604 | -     | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | G     | 614 | -     | 1/1/11/20 | 9/17/95/115   | -       |
| 22  | CLA  | y     | 612 | 1     | 1/1/15/20 | 20/37/115/115 | -       |
| 22  | CLA  | g     | 612 | -     | 1/1/14/20 | 12/31/109/115 | -       |
| 21  | CHL  | y     | 601 | 1     | 4/4/20/26 | 24/39/137/137 | -       |
| 21  | CHL  | s     | 307 | 20    | 3/3/16/26 | 12/15/113/137 | -       |
| 22  | CLA  | s     | 311 | 20,22 | 1/1/13/20 | 13/27/105/115 | -       |
| 25  | NEX  | n     | 616 | 22    | 2/2/12/25 | 16/27/83/83   | 0/3/3/3 |
| 26  | LHG  | d     | 407 | -     | -         | 25/50/50/53   | -       |
| 21  | CHL  | R     | 306 | -     | 4/4/18/26 | 16/27/125/137 | -       |
| 22  | CLA  | s     | 312 | 20    | 1/1/11/20 | 7/18/96/115   | -       |
| 22  | CLA  | r     | 309 | -     | 1/1/13/20 | 9/29/107/115  | -       |
| 33  | SQD  | D     | 402 | -     | 1/1/9/9   | 18/45/65/69   | 0/1/1/1 |
| 22  | CLA  | b     | 605 | -     | 1/1/15/20 | 10/37/115/115 | -       |
| 21  | CHL  | n     | 605 | -     | 3/3/16/26 | 13/20/118/137 | -       |
| 21  | CHL  | S     | 302 | -     | 3/3/16/26 | 9/15/113/137  | -       |
| 21  | CHL  | g     | 606 | -     | 3/3/16/26 | 13/20/118/137 | -       |
| 22  | CLA  | b     | 602 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | y     | 613 | -     | 1/1/11/20 | 9/17/95/115   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 22  | CLA  | A     | 409 | -     | 1/1/14/20 | 3/31/109/115  | -       |
| 22  | CLA  | r     | 311 | 23,19 | 1/1/11/20 | 11/18/96/115  | -       |
| 35  | DGD  | h     | 102 | -     | -         | 19/51/91/95   | 0/2/2/2 |
| 21  | CHL  | y     | 609 | -     | 4/4/20/26 | 14/39/137/137 | -       |
| 26  | LHG  | D     | 409 | -     | -         | 21/53/53/53   | -       |
| 21  | CHL  | Y     | 608 | -     | 4/4/20/26 | 12/39/137/137 | -       |
| 22  | CLA  | B     | 617 | -     | 1/1/15/20 | 20/37/115/115 | -       |
| 21  | CHL  | y     | 607 | -     | 4/4/20/26 | 18/39/137/137 | -       |
| 36  | LMG  | C     | 502 | -     | -         | 16/43/63/70   | 0/1/1/1 |
| 21  | CHL  | g     | 607 | -     | 4/4/20/26 | 18/39/137/137 | -       |
| 25  | NEX  | y     | 618 | -     | 2/2/12/25 | 14/27/83/83   | 0/3/3/3 |
| 31  | BCR  | b     | 618 | -     | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | A     | 405 | -     | 1/1/15/20 | 4/37/115/115  | -       |
| 26  | LHG  | C     | 521 | -     | -         | 21/53/53/53   | -       |
| 22  | CLA  | c     | 510 | -     | 1/1/15/20 | 11/37/115/115 | -       |
| 22  | CLA  | g     | 613 | 1     | 1/1/15/20 | 18/37/115/115 | -       |
| 22  | CLA  | S     | 308 | 20    | -         | 8/13/91/115   | -       |
| 22  | CLA  | R     | 310 | 23,19 | 1/1/11/20 | 11/18/96/115  | -       |
| 23  | LUT  | g     | 616 | -     | -         | 15/29/67/67   | 0/2/2/2 |
| 22  | CLA  | G     | 610 | -     | 1/1/14/20 | 19/36/114/115 | -       |
| 22  | CLA  | R     | 311 | 19    | 1/1/14/20 | 12/31/109/115 | -       |
| 21  | CHL  | G     | 606 | -     | 3/3/16/26 | 13/20/118/137 | -       |
| 32  | PL9  | d     | 406 | -     | -         | 17/53/73/73   | 0/1/1/1 |
| 26  | LHG  | g     | 619 | -     | -         | 22/53/53/53   | -       |
| 22  | CLA  | g     | 604 | 25    | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | N     | 609 | -     | 1/1/15/20 | 16/37/115/115 | -       |
| 21  | CHL  | s     | 301 | -     | 3/3/16/26 | 10/18/116/137 | -       |
| 31  | BCR  | b     | 616 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 33  | SQD  | L     | 101 | 12    | -         | 18/49/69/69   | 0/1/1/1 |
| 26  | LHG  | c     | 521 | -     | -         | 21/53/53/53   | -       |
| 21  | CHL  | N     | 607 | -     | 4/4/20/26 | 23/39/137/137 | -       |
| 22  | CLA  | n     | 611 | -     | 1/1/14/20 | 12/31/109/115 | -       |
| 21  | CHL  | Y     | 606 | -     | 4/4/20/26 | 18/39/137/137 | -       |
| 22  | CLA  | w     | 101 | 16    | 1/1/14/20 | 12/31/109/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 22  | CLA  | a     | 405 | -     | 1/1/15/20 | 15/37/115/115 | -       |
| 22  | CLA  | r     | 304 | -     | 1/1/14/20 | 9/31/109/115  | -       |
| 22  | CLA  | G     | 612 | -     | 1/1/14/20 | 12/31/109/115 | -       |
| 22  | CLA  | N     | 604 | 25    | 1/1/12/20 | 6/19/97/115   | -       |
| 22  | CLA  | b     | 609 | -     | 1/1/15/20 | 11/37/115/115 | -       |
| 21  | CHL  | G     | 607 | -     | 4/4/20/26 | 18/39/137/137 | -       |
| 22  | CLA  | n     | 602 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 21  | CHL  | r     | 301 | 19    | 3/3/16/26 | 8/18/116/137  | -       |
| 22  | CLA  | y     | 602 | -     | 1/1/15/20 | 13/37/115/115 | -       |
| 36  | LMG  | d     | 410 | -     | -         | 11/41/61/70   | 0/1/1/1 |
| 22  | CLA  | s     | 308 | 20    | -         | 8/13/91/115   | -       |
| 22  | CLA  | x     | 101 | -     | 1/1/15/20 | 16/37/115/115 | -       |
| 26  | LHG  | b     | 619 | -     | -         | 28/53/53/53   | -       |
| 31  | BCR  | C     | 516 | -     | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | C     | 511 | -     | 1/1/15/20 | 11/37/115/115 | -       |
| 31  | BCR  | K     | 102 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 22  | CLA  | Y     | 609 | -     | 1/1/14/20 | 15/31/109/115 | -       |
| 22  | CLA  | r     | 305 | -     | 1/1/11/20 | 7/17/95/115   | -       |
| 31  | BCR  | d     | 405 | -     | -         | 8/29/63/63    | 0/2/2/2 |
| 35  | DGD  | H     | 102 | -     | -         | 19/51/91/95   | 0/2/2/2 |
| 22  | CLA  | Y     | 612 | -     | 1/1/11/20 | 9/17/95/115   | -       |
| 22  | CLA  | N     | 603 | -     | 1/1/15/20 | 17/37/115/115 | -       |
| 21  | CHL  | Y     | 607 | -     | 4/4/20/26 | 23/39/137/137 | -       |
| 31  | BCR  | B     | 621 | -     | -         | 5/29/63/63    | 0/2/2/2 |
| 36  | LMG  | B     | 623 | -     | -         | 22/50/70/70   | 0/1/1/1 |
| 21  | CHL  | S     | 306 | 20    | 3/3/16/26 | 10/15/113/137 | -       |
| 22  | CLA  | S     | 310 | 26    | 1/1/13/20 | 16/25/103/115 | -       |
| 22  | CLA  | C     | 507 | -     | 1/1/15/20 | 14/37/115/115 | -       |
| 22  | CLA  | Y     | 603 | -     | 1/1/15/20 | 17/37/115/115 | -       |
| 22  | CLA  | S     | 311 | 20,22 | 1/1/13/20 | 13/27/105/115 | -       |
| 24  | XAT  | g     | 617 | -     | 2/2/12/26 | 17/31/93/93   | 0/4/4/4 |
| 22  | CLA  | r     | 310 | 19    | 1/1/15/20 | 18/37/115/115 | -       |
| 36  | LMG  | K     | 103 | -     | -         | 26/46/66/70   | 0/1/1/1 |
| 22  | CLA  | R     | 309 | 19    | 1/1/15/20 | 18/37/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 35  | DGD  | c     | 519 | -    | -         | 16/49/89/95   | 0/2/2/2 |
| 31  | BCR  | H     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | c     | 507 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 21  | CHL  | s     | 306 | 20   | 3/3/16/26 | 10/15/113/137 | -       |
| 21  | CHL  | r     | 306 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 22  | CLA  | A     | 407 | -    | 1/1/12/20 | 8/19/97/115   | -       |
| 22  | CLA  | R     | 302 | -    | 1/1/14/20 | 8/31/109/115  | -       |
| 22  | CLA  | C     | 509 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 31  | BCR  | K     | 101 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | y     | 610 | -    | 1/1/14/20 | 15/31/109/115 | -       |
| 36  | LMG  | w     | 102 | -    | -         | 16/43/63/70   | 0/1/1/1 |
| 21  | CHL  | r     | 308 | 19   | 4/4/19/26 | 17/33/131/137 | -       |
| 22  | CLA  | c     | 508 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 26  | LHG  | Y     | 617 | 22   | -         | 29/53/53/53   | -       |
| 22  | CLA  | y     | 611 | -    | 1/1/14/20 | 8/31/109/115  | -       |
| 22  | CLA  | C     | 510 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | n     | 610 | 26   | 1/1/14/20 | 8/31/109/115  | -       |
| 35  | DGD  | C     | 519 | -    | -         | 26/51/91/95   | 0/2/2/2 |
| 22  | CLA  | S     | 303 | 20   | 1/1/14/20 | 12/33/111/115 | -       |
| 22  | CLA  | D     | 404 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 22  | CLA  | B     | 613 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 21  | CHL  | g     | 605 | -    | 3/3/16/26 | 9/15/113/137  | -       |

All (2557) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 37  | f     | 101 | HEM  | FE-NB   | 25.25 | 3.21        | 1.96     |
| 37  | F     | 101 | HEM  | FE-NB   | 25.23 | 3.21        | 1.96     |
| 23  | N     | 615 | LUT  | C24-C25 | 17.30 | 1.54        | 1.33     |
| 23  | N     | 614 | LUT  | C24-C25 | 17.28 | 1.54        | 1.33     |
| 23  | n     | 614 | LUT  | C24-C25 | 17.28 | 1.54        | 1.33     |
| 23  | G     | 615 | LUT  | C24-C25 | 17.27 | 1.54        | 1.33     |
| 23  | Y     | 613 | LUT  | C24-C25 | 17.27 | 1.54        | 1.33     |
| 23  | g     | 615 | LUT  | C24-C25 | 17.25 | 1.54        | 1.33     |
| 23  | y     | 614 | LUT  | C24-C25 | 17.25 | 1.54        | 1.33     |
| 23  | g     | 616 | LUT  | C24-C25 | 17.20 | 1.54        | 1.33     |
| 23  | r     | 313 | LUT  | C24-C25 | 17.08 | 1.54        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | R     | 312 | LUT  | C24-C25 | 17.08 | 1.54        | 1.33     |
| 23  | G     | 616 | LUT  | C24-C25 | 17.06 | 1.54        | 1.33     |
| 23  | Y     | 614 | LUT  | C24-C25 | 16.83 | 1.54        | 1.33     |
| 22  | c     | 510 | CLA  | C1D-ND  | 16.62 | 1.58        | 1.37     |
| 22  | C     | 511 | CLA  | C1D-ND  | 16.60 | 1.58        | 1.37     |
| 23  | g     | 616 | LUT  | C14-C13 | 15.83 | 1.56        | 1.35     |
| 23  | N     | 615 | LUT  | C14-C13 | 15.77 | 1.56        | 1.35     |
| 23  | G     | 616 | LUT  | C14-C13 | 15.74 | 1.56        | 1.35     |
| 23  | Y     | 614 | LUT  | C14-C13 | 15.45 | 1.56        | 1.35     |
| 23  | R     | 312 | LUT  | C14-C13 | 15.40 | 1.56        | 1.35     |
| 23  | Y     | 614 | LUT  | C10-C9  | 15.36 | 1.56        | 1.35     |
| 23  | r     | 313 | LUT  | C14-C13 | 15.34 | 1.56        | 1.35     |
| 23  | G     | 616 | LUT  | C10-C9  | 15.21 | 1.55        | 1.35     |
| 23  | G     | 616 | LUT  | C34-C33 | 15.19 | 1.55        | 1.35     |
| 23  | g     | 616 | LUT  | C10-C9  | 15.19 | 1.55        | 1.35     |
| 23  | g     | 616 | LUT  | C34-C33 | 15.17 | 1.55        | 1.35     |
| 23  | N     | 615 | LUT  | C10-C9  | 15.12 | 1.55        | 1.35     |
| 23  | y     | 614 | LUT  | C10-C9  | 15.12 | 1.55        | 1.35     |
| 23  | g     | 615 | LUT  | C10-C9  | 15.08 | 1.55        | 1.35     |
| 23  | N     | 615 | LUT  | C34-C33 | 15.07 | 1.55        | 1.35     |
| 23  | G     | 615 | LUT  | C10-C9  | 15.06 | 1.55        | 1.35     |
| 23  | Y     | 613 | LUT  | C10-C9  | 15.05 | 1.55        | 1.35     |
| 23  | Y     | 614 | LUT  | C34-C33 | 15.05 | 1.55        | 1.35     |
| 23  | y     | 614 | LUT  | C14-C13 | 15.05 | 1.55        | 1.35     |
| 23  | Y     | 613 | LUT  | C14-C13 | 15.04 | 1.55        | 1.35     |
| 23  | N     | 614 | LUT  | C10-C9  | 15.04 | 1.55        | 1.35     |
| 23  | g     | 615 | LUT  | C14-C13 | 15.03 | 1.55        | 1.35     |
| 23  | n     | 614 | LUT  | C10-C9  | 15.03 | 1.55        | 1.35     |
| 23  | n     | 614 | LUT  | C14-C13 | 15.01 | 1.55        | 1.35     |
| 23  | N     | 614 | LUT  | C14-C13 | 15.01 | 1.55        | 1.35     |
| 23  | G     | 615 | LUT  | C14-C13 | 15.01 | 1.55        | 1.35     |
| 23  | N     | 615 | LUT  | C30-C29 | 14.96 | 1.55        | 1.35     |
| 24  | Y     | 615 | XAT  | C30-C29 | 14.82 | 1.55        | 1.35     |
| 24  | Y     | 615 | XAT  | C34-C33 | 14.78 | 1.55        | 1.35     |
| 24  | y     | 615 | XAT  | C30-C29 | 14.77 | 1.55        | 1.35     |
| 24  | y     | 615 | XAT  | C34-C33 | 14.69 | 1.55        | 1.35     |
| 24  | Y     | 615 | XAT  | C14-C13 | 14.69 | 1.55        | 1.35     |
| 24  | y     | 615 | XAT  | C14-C13 | 14.68 | 1.55        | 1.35     |
| 24  | r     | 314 | XAT  | C30-C29 | 14.66 | 1.55        | 1.35     |
| 24  | N     | 616 | XAT  | C30-C29 | 14.66 | 1.55        | 1.35     |
| 23  | R     | 312 | LUT  | C34-C33 | 14.62 | 1.55        | 1.35     |
| 24  | r     | 314 | XAT  | C10-C9  | 14.59 | 1.55        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | R     | 312 | LUT  | C10-C9  | 14.59 | 1.55        | 1.35     |
| 23  | r     | 313 | LUT  | C34-C33 | 14.59 | 1.55        | 1.35     |
| 24  | G     | 617 | XAT  | C30-C29 | 14.58 | 1.55        | 1.35     |
| 24  | g     | 617 | XAT  | C30-C29 | 14.58 | 1.55        | 1.35     |
| 24  | Y     | 615 | XAT  | C10-C9  | 14.58 | 1.55        | 1.35     |
| 24  | R     | 313 | XAT  | C30-C29 | 14.57 | 1.55        | 1.35     |
| 25  | y     | 616 | NEX  | C10-C9  | 14.56 | 1.55        | 1.35     |
| 23  | g     | 616 | LUT  | C30-C29 | 14.56 | 1.55        | 1.35     |
| 23  | Y     | 614 | LUT  | C30-C29 | 14.56 | 1.55        | 1.35     |
| 24  | n     | 615 | XAT  | C30-C29 | 14.55 | 1.55        | 1.35     |
| 23  | r     | 313 | LUT  | C10-C9  | 14.55 | 1.55        | 1.35     |
| 24  | r     | 314 | XAT  | C34-C33 | 14.54 | 1.55        | 1.35     |
| 24  | g     | 617 | XAT  | C34-C33 | 14.54 | 1.55        | 1.35     |
| 24  | R     | 313 | XAT  | C10-C9  | 14.54 | 1.55        | 1.35     |
| 24  | G     | 617 | XAT  | C34-C33 | 14.53 | 1.55        | 1.35     |
| 24  | G     | 617 | XAT  | C10-C9  | 14.53 | 1.55        | 1.35     |
| 24  | R     | 313 | XAT  | C34-C33 | 14.53 | 1.55        | 1.35     |
| 24  | g     | 617 | XAT  | C10-C9  | 14.52 | 1.55        | 1.35     |
| 24  | G     | 617 | XAT  | C14-C13 | 14.52 | 1.55        | 1.35     |
| 23  | g     | 615 | LUT  | C34-C33 | 14.51 | 1.55        | 1.35     |
| 24  | n     | 615 | XAT  | C34-C33 | 14.50 | 1.55        | 1.35     |
| 23  | G     | 616 | LUT  | C30-C29 | 14.50 | 1.55        | 1.35     |
| 23  | n     | 614 | LUT  | C34-C33 | 14.50 | 1.55        | 1.35     |
| 23  | G     | 615 | LUT  | C34-C33 | 14.50 | 1.55        | 1.35     |
| 23  | N     | 614 | LUT  | C34-C33 | 14.48 | 1.55        | 1.35     |
| 23  | y     | 614 | LUT  | C34-C33 | 14.47 | 1.55        | 1.35     |
| 25  | y     | 616 | NEX  | C14-C13 | 14.46 | 1.54        | 1.35     |
| 24  | R     | 313 | XAT  | C14-C13 | 14.44 | 1.54        | 1.35     |
| 25  | N     | 617 | NEX  | C10-C9  | 14.44 | 1.54        | 1.35     |
| 24  | y     | 615 | XAT  | C10-C9  | 14.44 | 1.54        | 1.35     |
| 24  | n     | 615 | XAT  | C10-C9  | 14.43 | 1.54        | 1.35     |
| 25  | n     | 616 | NEX  | C14-C13 | 14.43 | 1.54        | 1.35     |
| 23  | Y     | 613 | LUT  | C34-C33 | 14.42 | 1.54        | 1.35     |
| 25  | Y     | 616 | NEX  | C10-C9  | 14.42 | 1.54        | 1.35     |
| 24  | N     | 616 | XAT  | C34-C33 | 14.42 | 1.54        | 1.35     |
| 24  | n     | 615 | XAT  | C14-C13 | 14.40 | 1.54        | 1.35     |
| 24  | g     | 617 | XAT  | C14-C13 | 14.40 | 1.54        | 1.35     |
| 24  | N     | 616 | XAT  | C10-C9  | 14.39 | 1.54        | 1.35     |
| 24  | r     | 314 | XAT  | C14-C13 | 14.39 | 1.54        | 1.35     |
| 25  | n     | 616 | NEX  | C10-C9  | 14.37 | 1.54        | 1.35     |
| 25  | N     | 617 | NEX  | C34-C33 | 14.36 | 1.54        | 1.35     |
| 25  | Y     | 616 | NEX  | C34-C33 | 14.36 | 1.54        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | y     | 614 | LUT  | C30-C29 | 14.33 | 1.54        | 1.35     |
| 25  | N     | 617 | NEX  | C14-C13 | 14.32 | 1.54        | 1.35     |
| 25  | g     | 618 | NEX  | C10-C9  | 14.31 | 1.54        | 1.35     |
| 25  | y     | 616 | NEX  | C34-C33 | 14.31 | 1.54        | 1.35     |
| 23  | n     | 614 | LUT  | C30-C29 | 14.30 | 1.54        | 1.35     |
| 23  | G     | 615 | LUT  | C30-C29 | 14.30 | 1.54        | 1.35     |
| 25  | Y     | 616 | NEX  | C14-C13 | 14.29 | 1.54        | 1.35     |
| 25  | y     | 618 | NEX  | C10-C9  | 14.28 | 1.54        | 1.35     |
| 23  | g     | 615 | LUT  | C30-C29 | 14.27 | 1.54        | 1.35     |
| 25  | n     | 616 | NEX  | C30-C29 | 14.26 | 1.54        | 1.35     |
| 25  | n     | 616 | NEX  | C34-C33 | 14.25 | 1.54        | 1.35     |
| 24  | N     | 616 | XAT  | C14-C13 | 14.24 | 1.54        | 1.35     |
| 23  | N     | 614 | LUT  | C30-C29 | 14.23 | 1.54        | 1.35     |
| 23  | Y     | 613 | LUT  | C30-C29 | 14.23 | 1.54        | 1.35     |
| 25  | N     | 617 | NEX  | C30-C29 | 14.22 | 1.54        | 1.35     |
| 25  | r     | 315 | NEX  | C10-C9  | 14.21 | 1.54        | 1.35     |
| 25  | y     | 618 | NEX  | C14-C13 | 14.19 | 1.54        | 1.35     |
| 25  | r     | 315 | NEX  | C14-C13 | 14.19 | 1.54        | 1.35     |
| 25  | g     | 618 | NEX  | C14-C13 | 14.18 | 1.54        | 1.35     |
| 25  | r     | 315 | NEX  | C34-C33 | 14.17 | 1.54        | 1.35     |
| 25  | y     | 616 | NEX  | C30-C29 | 14.15 | 1.54        | 1.35     |
| 25  | y     | 618 | NEX  | C34-C33 | 14.12 | 1.54        | 1.35     |
| 25  | g     | 618 | NEX  | C34-C33 | 14.04 | 1.54        | 1.35     |
| 25  | g     | 618 | NEX  | C30-C29 | 14.02 | 1.54        | 1.35     |
| 25  | y     | 618 | NEX  | C30-C29 | 13.98 | 1.54        | 1.35     |
| 23  | R     | 312 | LUT  | C30-C29 | 13.93 | 1.54        | 1.35     |
| 25  | r     | 315 | NEX  | C30-C29 | 13.93 | 1.54        | 1.35     |
| 23  | r     | 313 | LUT  | C30-C29 | 13.92 | 1.54        | 1.35     |
| 25  | Y     | 616 | NEX  | C30-C29 | 13.89 | 1.54        | 1.35     |
| 23  | G     | 616 | LUT  | C5-C6   | 11.87 | 1.55        | 1.34     |
| 23  | R     | 312 | LUT  | C5-C6   | 11.84 | 1.55        | 1.34     |
| 23  | g     | 616 | LUT  | C5-C6   | 11.84 | 1.54        | 1.34     |
| 23  | r     | 313 | LUT  | C5-C6   | 11.78 | 1.54        | 1.34     |
| 23  | Y     | 614 | LUT  | C5-C6   | 11.71 | 1.54        | 1.34     |
| 23  | N     | 615 | LUT  | C5-C6   | 11.33 | 1.54        | 1.34     |
| 22  | c     | 510 | CLA  | MG-NC   | 11.29 | 2.33        | 2.06     |
| 22  | C     | 511 | CLA  | MG-NC   | 11.27 | 2.33        | 2.06     |
| 23  | y     | 614 | LUT  | C5-C6   | 10.85 | 1.53        | 1.34     |
| 23  | N     | 614 | LUT  | C5-C6   | 10.82 | 1.53        | 1.34     |
| 23  | G     | 615 | LUT  | C5-C6   | 10.79 | 1.53        | 1.34     |
| 23  | n     | 614 | LUT  | C5-C6   | 10.78 | 1.53        | 1.34     |
| 23  | g     | 615 | LUT  | C5-C6   | 10.78 | 1.53        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | Y     | 613 | LUT  | C5-C6   | 10.76 | 1.53        | 1.34     |
| 22  | C     | 511 | CLA  | CHD-C1D | 9.51  | 1.56        | 1.38     |
| 22  | c     | 510 | CLA  | CHD-C1D | 9.50  | 1.56        | 1.38     |
| 22  | C     | 511 | CLA  | MG-ND   | 9.19  | 2.24        | 2.05     |
| 22  | c     | 510 | CLA  | MG-ND   | 9.17  | 2.24        | 2.05     |
| 22  | c     | 510 | CLA  | CHD-C4C | 8.80  | 1.59        | 1.39     |
| 22  | C     | 511 | CLA  | CHD-C4C | 8.76  | 1.59        | 1.39     |
| 22  | C     | 511 | CLA  | C4B-NB  | 8.40  | 1.42        | 1.35     |
| 22  | c     | 510 | CLA  | C4B-NB  | 8.36  | 1.42        | 1.35     |
| 22  | s     | 308 | CLA  | C4B-NB  | 7.65  | 1.42        | 1.35     |
| 22  | N     | 611 | CLA  | C4B-NB  | 7.59  | 1.42        | 1.35     |
| 22  | w     | 101 | CLA  | C4B-NB  | 7.58  | 1.42        | 1.35     |
| 22  | S     | 308 | CLA  | C4B-NB  | 7.58  | 1.42        | 1.35     |
| 22  | G     | 612 | CLA  | C4B-NB  | 7.58  | 1.42        | 1.35     |
| 22  | S     | 304 | CLA  | C4B-NB  | 7.57  | 1.42        | 1.35     |
| 22  | s     | 304 | CLA  | C4B-NB  | 7.57  | 1.42        | 1.35     |
| 22  | n     | 611 | CLA  | C4B-NB  | 7.55  | 1.41        | 1.35     |
| 22  | R     | 310 | CLA  | C4B-NB  | 7.54  | 1.41        | 1.35     |
| 22  | s     | 303 | CLA  | C4B-NB  | 7.52  | 1.41        | 1.35     |
| 22  | W     | 101 | CLA  | C4B-NB  | 7.50  | 1.41        | 1.35     |
| 22  | g     | 610 | CLA  | C4B-NB  | 7.48  | 1.41        | 1.35     |
| 22  | G     | 610 | CLA  | C4B-NB  | 7.46  | 1.41        | 1.35     |
| 22  | N     | 609 | CLA  | C4B-NB  | 7.46  | 1.41        | 1.35     |
| 22  | r     | 311 | CLA  | C4B-NB  | 7.46  | 1.41        | 1.35     |
| 22  | g     | 612 | CLA  | C4B-NB  | 7.45  | 1.41        | 1.35     |
| 22  | S     | 303 | CLA  | C4B-NB  | 7.45  | 1.41        | 1.35     |
| 22  | R     | 309 | CLA  | C4B-NB  | 7.41  | 1.41        | 1.35     |
| 22  | x     | 101 | CLA  | C4B-NB  | 7.40  | 1.41        | 1.35     |
| 22  | y     | 610 | CLA  | C4B-NB  | 7.39  | 1.41        | 1.35     |
| 22  | s     | 312 | CLA  | C4B-NB  | 7.36  | 1.41        | 1.35     |
| 22  | Y     | 609 | CLA  | C4B-NB  | 7.36  | 1.41        | 1.35     |
| 22  | B     | 603 | CLA  | C4B-NB  | 7.36  | 1.41        | 1.35     |
| 22  | r     | 310 | CLA  | C4B-NB  | 7.32  | 1.41        | 1.35     |
| 22  | S     | 312 | CLA  | C4B-NB  | 7.32  | 1.41        | 1.35     |
| 22  | n     | 609 | CLA  | C4B-NB  | 7.32  | 1.41        | 1.35     |
| 22  | r     | 312 | CLA  | C4B-NB  | 7.31  | 1.41        | 1.35     |
| 22  | R     | 311 | CLA  | C4B-NB  | 7.27  | 1.41        | 1.35     |
| 22  | B     | 611 | CLA  | C4B-NB  | 7.26  | 1.41        | 1.35     |
| 22  | S     | 311 | CLA  | C4B-NB  | 7.25  | 1.41        | 1.35     |
| 22  | s     | 305 | CLA  | C4B-NB  | 7.23  | 1.41        | 1.35     |
| 22  | g     | 614 | CLA  | C4B-NB  | 7.22  | 1.41        | 1.35     |
| 22  | r     | 304 | CLA  | C4B-NB  | 7.21  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 22  | d     | 404 | CLA  | C4B-NB | 7.19 | 1.41        | 1.35     |
| 22  | y     | 613 | CLA  | C4B-NB | 7.19 | 1.41        | 1.35     |
| 22  | G     | 611 | CLA  | C4B-NB | 7.18 | 1.41        | 1.35     |
| 22  | a     | 406 | CLA  | C4B-NB | 7.17 | 1.41        | 1.35     |
| 22  | R     | 308 | CLA  | C4B-NB | 7.17 | 1.41        | 1.35     |
| 22  | n     | 613 | CLA  | C4B-NB | 7.17 | 1.41        | 1.35     |
| 22  | D     | 405 | CLA  | C4B-NB | 7.17 | 1.41        | 1.35     |
| 22  | b     | 608 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 22  | N     | 613 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 22  | s     | 311 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 22  | Y     | 610 | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 22  | R     | 302 | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 22  | R     | 303 | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 22  | N     | 603 | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 22  | r     | 303 | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 22  | g     | 611 | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 22  | c     | 511 | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 22  | n     | 610 | CLA  | C4B-NB | 7.13 | 1.41        | 1.35     |
| 22  | Y     | 612 | CLA  | C4B-NB | 7.12 | 1.41        | 1.35     |
| 22  | A     | 407 | CLA  | C4B-NB | 7.12 | 1.41        | 1.35     |
| 22  | g     | 603 | CLA  | C4B-NB | 7.11 | 1.41        | 1.35     |
| 22  | y     | 602 | CLA  | C4B-NB | 7.11 | 1.41        | 1.35     |
| 22  | S     | 305 | CLA  | C4B-NB | 7.11 | 1.41        | 1.35     |
| 22  | y     | 611 | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 22  | N     | 612 | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 22  | Y     | 602 | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 22  | G     | 602 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | C     | 512 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | r     | 309 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | G     | 603 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | S     | 309 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | N     | 602 | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 22  | d     | 403 | CLA  | C4B-NB | 7.08 | 1.41        | 1.35     |
| 22  | n     | 603 | CLA  | C4B-NB | 7.08 | 1.41        | 1.35     |
| 22  | y     | 603 | CLA  | C4B-NB | 7.08 | 1.41        | 1.35     |
| 22  | n     | 612 | CLA  | C4B-NB | 7.08 | 1.41        | 1.35     |
| 22  | G     | 614 | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 22  | C     | 506 | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 22  | Y     | 603 | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 22  | s     | 309 | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 22  | c     | 506 | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 22  | N     | 610 | CLA  | C4B-NB | 7.05 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | r     | 305 | CLA  | C4B-NB  | 7.05 | 1.41        | 1.35     |
| 22  | y     | 612 | CLA  | C4B-NB  | 7.05 | 1.41        | 1.35     |
| 22  | C     | 507 | CLA  | C4B-NB  | 7.05 | 1.41        | 1.35     |
| 22  | B     | 618 | CLA  | C4B-NB  | 7.05 | 1.41        | 1.35     |
| 22  | g     | 613 | CLA  | C4B-NB  | 7.04 | 1.41        | 1.35     |
| 22  | B     | 615 | CLA  | C4B-NB  | 7.04 | 1.41        | 1.35     |
| 22  | b     | 612 | CLA  | C4B-NB  | 7.04 | 1.41        | 1.35     |
| 22  | S     | 313 | CLA  | C4B-NB  | 7.04 | 1.41        | 1.35     |
| 22  | Y     | 611 | CLA  | C4B-NB  | 7.04 | 1.41        | 1.35     |
| 22  | G     | 613 | CLA  | C4B-NB  | 7.03 | 1.41        | 1.35     |
| 22  | b     | 610 | CLA  | C4B-NB  | 7.02 | 1.41        | 1.35     |
| 22  | C     | 515 | CLA  | C4B-NB  | 7.02 | 1.41        | 1.35     |
| 22  | a     | 404 | CLA  | C4B-NB  | 7.01 | 1.41        | 1.35     |
| 22  | B     | 613 | CLA  | C4B-NB  | 7.01 | 1.41        | 1.35     |
| 22  | D     | 404 | CLA  | C4B-NB  | 7.01 | 1.41        | 1.35     |
| 22  | n     | 602 | CLA  | C4B-NB  | 7.01 | 1.41        | 1.35     |
| 22  | c     | 509 | CLA  | C4B-NB  | 7.01 | 1.41        | 1.35     |
| 22  | g     | 602 | CLA  | C4B-NB  | 6.99 | 1.41        | 1.35     |
| 22  | B     | 617 | CLA  | C4B-NB  | 6.99 | 1.41        | 1.35     |
| 22  | s     | 313 | CLA  | C4B-NB  | 6.99 | 1.41        | 1.35     |
| 22  | B     | 608 | CLA  | C4B-NB  | 6.98 | 1.41        | 1.35     |
| 22  | c     | 505 | CLA  | C4B-NB  | 6.98 | 1.41        | 1.35     |
| 22  | c     | 514 | CLA  | C4B-NB  | 6.98 | 1.41        | 1.35     |
| 22  | R     | 304 | CLA  | C4B-NB  | 6.97 | 1.41        | 1.35     |
| 22  | B     | 607 | CLA  | C4B-NB  | 6.97 | 1.41        | 1.35     |
| 22  | C     | 510 | CLA  | C4B-NB  | 6.97 | 1.41        | 1.35     |
| 22  | b     | 605 | CLA  | C4B-NB  | 6.96 | 1.41        | 1.35     |
| 22  | b     | 614 | CLA  | C4B-NB  | 6.96 | 1.41        | 1.35     |
| 22  | y     | 612 | CLA  | CHC-C1C | 6.96 | 1.52        | 1.35     |
| 22  | c     | 507 | CLA  | C4B-NB  | 6.95 | 1.41        | 1.35     |
| 22  | b     | 606 | CLA  | C4B-NB  | 6.95 | 1.41        | 1.35     |
| 22  | g     | 613 | CLA  | CHC-C1C | 6.95 | 1.52        | 1.35     |
| 22  | b     | 611 | CLA  | C4B-NB  | 6.94 | 1.41        | 1.35     |
| 22  | A     | 405 | CLA  | C4B-NB  | 6.94 | 1.41        | 1.35     |
| 22  | B     | 609 | CLA  | C4B-NB  | 6.94 | 1.41        | 1.35     |
| 22  | n     | 612 | CLA  | CHC-C1C | 6.94 | 1.52        | 1.35     |
| 22  | N     | 612 | CLA  | CHC-C1C | 6.94 | 1.52        | 1.35     |
| 22  | C     | 513 | CLA  | C4B-NB  | 6.94 | 1.41        | 1.35     |
| 22  | C     | 503 | CLA  | C4B-NB  | 6.93 | 1.41        | 1.35     |
| 22  | G     | 613 | CLA  | CHC-C1C | 6.93 | 1.52        | 1.35     |
| 22  | Y     | 611 | CLA  | CHC-C1C | 6.93 | 1.52        | 1.35     |
| 22  | B     | 616 | CLA  | C4B-NB  | 6.92 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | B     | 614 | CLA  | C4B-NB  | 6.92 | 1.41        | 1.35     |
| 22  | b     | 603 | CLA  | C4B-NB  | 6.92 | 1.41        | 1.35     |
| 22  | B     | 606 | CLA  | C4B-NB  | 6.92 | 1.41        | 1.35     |
| 22  | b     | 613 | CLA  | C4B-NB  | 6.92 | 1.41        | 1.35     |
| 22  | S     | 310 | CLA  | C4B-NB  | 6.90 | 1.41        | 1.35     |
| 22  | a     | 408 | CLA  | C4B-NB  | 6.89 | 1.41        | 1.35     |
| 22  | b     | 615 | CLA  | C4B-NB  | 6.88 | 1.41        | 1.35     |
| 22  | b     | 607 | CLA  | C4B-NB  | 6.88 | 1.41        | 1.35     |
| 22  | c     | 513 | CLA  | C4B-NB  | 6.86 | 1.41        | 1.35     |
| 22  | C     | 508 | CLA  | C4B-NB  | 6.86 | 1.41        | 1.35     |
| 22  | b     | 604 | CLA  | C4B-NB  | 6.85 | 1.41        | 1.35     |
| 22  | c     | 508 | CLA  | C4B-NB  | 6.84 | 1.41        | 1.35     |
| 22  | c     | 512 | CLA  | C4B-NB  | 6.82 | 1.41        | 1.35     |
| 22  | b     | 609 | CLA  | C4B-NB  | 6.81 | 1.41        | 1.35     |
| 22  | b     | 601 | CLA  | C4B-NB  | 6.81 | 1.41        | 1.35     |
| 22  | B     | 612 | CLA  | C4B-NB  | 6.81 | 1.41        | 1.35     |
| 22  | C     | 504 | CLA  | C4B-NB  | 6.80 | 1.41        | 1.35     |
| 22  | A     | 406 | CLA  | C4B-NB  | 6.79 | 1.41        | 1.35     |
| 22  | B     | 604 | CLA  | C4B-NB  | 6.78 | 1.41        | 1.35     |
| 22  | A     | 409 | CLA  | C4B-NB  | 6.78 | 1.41        | 1.35     |
| 22  | C     | 509 | CLA  | C4B-NB  | 6.78 | 1.41        | 1.35     |
| 22  | s     | 310 | CLA  | C4B-NB  | 6.78 | 1.41        | 1.35     |
| 22  | B     | 610 | CLA  | C4B-NB  | 6.77 | 1.41        | 1.35     |
| 22  | c     | 502 | CLA  | C4B-NB  | 6.76 | 1.41        | 1.35     |
| 22  | C     | 514 | CLA  | C4B-NB  | 6.76 | 1.41        | 1.35     |
| 22  | a     | 405 | CLA  | C4B-NB  | 6.75 | 1.41        | 1.35     |
| 22  | c     | 504 | CLA  | C4B-NB  | 6.72 | 1.41        | 1.35     |
| 22  | c     | 503 | CLA  | C4B-NB  | 6.71 | 1.41        | 1.35     |
| 22  | B     | 605 | CLA  | C4B-NB  | 6.68 | 1.41        | 1.35     |
| 22  | C     | 505 | CLA  | C4B-NB  | 6.67 | 1.41        | 1.35     |
| 22  | b     | 602 | CLA  | C4B-NB  | 6.66 | 1.41        | 1.35     |
| 22  | y     | 604 | CLA  | C4B-NB  | 6.58 | 1.41        | 1.35     |
| 22  | N     | 604 | CLA  | C4B-NB  | 6.57 | 1.41        | 1.35     |
| 22  | Y     | 604 | CLA  | C4B-NB  | 6.55 | 1.41        | 1.35     |
| 22  | n     | 604 | CLA  | C4B-NB  | 6.55 | 1.41        | 1.35     |
| 22  | G     | 604 | CLA  | C4B-NB  | 6.54 | 1.41        | 1.35     |
| 22  | g     | 604 | CLA  | C4B-NB  | 6.54 | 1.41        | 1.35     |
| 25  | n     | 616 | NEX  | C24-C25 | 6.24 | 1.60        | 1.52     |
| 25  | g     | 618 | NEX  | C24-C25 | 6.21 | 1.60        | 1.52     |
| 25  | y     | 618 | NEX  | C24-C25 | 6.11 | 1.60        | 1.52     |
| 25  | r     | 315 | NEX  | C24-C25 | 6.07 | 1.60        | 1.52     |
| 25  | Y     | 616 | NEX  | C24-C25 | 6.03 | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | N     | 617 | NEX  | C24-C25 | 6.02  | 1.60        | 1.52     |
| 25  | y     | 616 | NEX  | C24-C25 | 5.83  | 1.60        | 1.52     |
| 37  | F     | 101 | HEM  | FE-ND   | -5.82 | 1.68        | 1.96     |
| 37  | f     | 101 | HEM  | FE-ND   | -5.82 | 1.68        | 1.96     |
| 24  | g     | 617 | XAT  | C24-C25 | 5.71  | 1.60        | 1.52     |
| 21  | N     | 606 | CHL  | C3B-C2B | 5.69  | 1.48        | 1.40     |
| 21  | y     | 606 | CHL  | C3B-C2B | 5.69  | 1.48        | 1.40     |
| 21  | g     | 605 | CHL  | C3B-C2B | 5.68  | 1.48        | 1.40     |
| 21  | S     | 307 | CHL  | C3B-C2B | 5.68  | 1.48        | 1.40     |
| 21  | Y     | 608 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | Y     | 607 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | s     | 301 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | G     | 601 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | Y     | 601 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | N     | 601 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 21  | g     | 609 | CHL  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 21  | s     | 302 | CHL  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 21  | Y     | 605 | CHL  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 21  | S     | 301 | CHL  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 21  | g     | 601 | CHL  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 21  | N     | 607 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | y     | 609 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | G     | 608 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | s     | 307 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | G     | 605 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | Y     | 606 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | n     | 608 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | R     | 307 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | R     | 306 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 21  | y     | 608 | CHL  | C3B-C2B | 5.64  | 1.48        | 1.40     |
| 21  | n     | 605 | CHL  | C3B-C2B | 5.64  | 1.48        | 1.40     |
| 21  | n     | 607 | CHL  | C3B-C2B | 5.64  | 1.48        | 1.40     |
| 21  | y     | 601 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | N     | 605 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | r     | 307 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | s     | 306 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | g     | 608 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | n     | 606 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 21  | r     | 301 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 21  | y     | 607 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 21  | S     | 302 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 21  | g     | 606 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | g     | 607 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 21  | G     | 606 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 21  | N     | 608 | CHL  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 21  | r     | 308 | CHL  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 21  | y     | 605 | CHL  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 21  | n     | 601 | CHL  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 21  | G     | 607 | CHL  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 21  | R     | 305 | CHL  | C3B-C2B | 5.60  | 1.48        | 1.40     |
| 21  | G     | 609 | CHL  | C3B-C2B | 5.60  | 1.48        | 1.40     |
| 24  | R     | 313 | XAT  | C24-C25 | 5.59  | 1.60        | 1.52     |
| 21  | r     | 306 | CHL  | C3B-C2B | 5.58  | 1.48        | 1.40     |
| 21  | S     | 306 | CHL  | C3B-C2B | 5.56  | 1.48        | 1.40     |
| 24  | Y     | 615 | XAT  | C24-C25 | 5.50  | 1.59        | 1.52     |
| 24  | r     | 314 | XAT  | C24-C25 | 5.50  | 1.59        | 1.52     |
| 24  | y     | 615 | XAT  | C24-C25 | 5.49  | 1.59        | 1.52     |
| 21  | R     | 306 | CHL  | CHC-C1C | 5.47  | 1.49        | 1.35     |
| 21  | Y     | 601 | CHL  | CHC-C1C | 5.46  | 1.49        | 1.35     |
| 21  | S     | 306 | CHL  | CHC-C1C | 5.46  | 1.49        | 1.35     |
| 21  | n     | 601 | CHL  | CHC-C1C | 5.46  | 1.49        | 1.35     |
| 21  | r     | 306 | CHL  | CHC-C1C | 5.46  | 1.49        | 1.35     |
| 21  | S     | 307 | CHL  | CHC-C1C | 5.45  | 1.49        | 1.35     |
| 21  | Y     | 605 | CHL  | CHC-C1C | 5.45  | 1.48        | 1.35     |
| 21  | r     | 308 | CHL  | CHC-C1C | 5.45  | 1.48        | 1.35     |
| 21  | n     | 608 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | n     | 607 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | G     | 608 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | y     | 609 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | G     | 605 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | R     | 307 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | N     | 601 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | g     | 601 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | S     | 301 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | r     | 301 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 21  | R     | 305 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 22  | C     | 511 | CLA  | C4D-ND  | -5.43 | 1.30        | 1.37     |
| 21  | N     | 607 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | g     | 606 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | g     | 608 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | N     | 606 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | s     | 307 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | g     | 607 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | r     | 307 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | G     | 606 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | G     | 609 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | y     | 608 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | y     | 601 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | Y     | 607 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | N     | 608 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | y     | 605 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | y     | 606 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | Y     | 606 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 21  | G     | 607 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | Y     | 608 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | s     | 306 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | s     | 302 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | g     | 609 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | S     | 302 | CHL  | CHC-C1C | 5.42  | 1.48        | 1.35     |
| 21  | n     | 605 | CHL  | CHC-C1C | 5.41  | 1.48        | 1.35     |
| 21  | n     | 606 | CHL  | CHC-C1C | 5.41  | 1.48        | 1.35     |
| 21  | g     | 605 | CHL  | CHC-C1C | 5.41  | 1.48        | 1.35     |
| 21  | s     | 301 | CHL  | CHC-C1C | 5.41  | 1.48        | 1.35     |
| 21  | y     | 607 | CHL  | CHC-C1C | 5.41  | 1.48        | 1.35     |
| 22  | N     | 612 | CLA  | C1C-C2C | 5.41  | 1.55        | 1.44     |
| 22  | g     | 613 | CLA  | C1C-C2C | 5.40  | 1.55        | 1.44     |
| 21  | G     | 601 | CHL  | CHC-C1C | 5.40  | 1.48        | 1.35     |
| 21  | N     | 605 | CHL  | CHC-C1C | 5.39  | 1.48        | 1.35     |
| 22  | y     | 612 | CLA  | C1C-C2C | 5.38  | 1.55        | 1.44     |
| 22  | G     | 613 | CLA  | C1C-C2C | 5.37  | 1.55        | 1.44     |
| 22  | c     | 510 | CLA  | C4D-ND  | -5.36 | 1.30        | 1.37     |
| 22  | n     | 612 | CLA  | C1C-C2C | 5.36  | 1.54        | 1.44     |
| 22  | Y     | 611 | CLA  | C1C-C2C | 5.35  | 1.54        | 1.44     |
| 37  | f     | 101 | HEM  | C4B-NB  | 5.34  | 1.49        | 1.38     |
| 37  | F     | 101 | HEM  | C4B-NB  | 5.31  | 1.49        | 1.38     |
| 21  | G     | 601 | CHL  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 21  | G     | 607 | CHL  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 21  | N     | 606 | CHL  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 21  | g     | 605 | CHL  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 21  | g     | 607 | CHL  | CHD-C1D | 5.22  | 1.48        | 1.38     |
| 21  | g     | 609 | CHL  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 21  | n     | 607 | CHL  | O2D-CGD | 5.21  | 1.45        | 1.33     |
| 21  | g     | 608 | CHL  | O2D-CGD | 5.21  | 1.45        | 1.33     |
| 21  | G     | 605 | CHL  | O2D-CGD | 5.21  | 1.45        | 1.33     |
| 21  | y     | 609 | CHL  | O2D-CGD | 5.21  | 1.45        | 1.33     |
| 21  | Y     | 607 | CHL  | O2D-CGD | 5.21  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | R     | 307 | CHL  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 21  | S     | 301 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | G     | 608 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | S     | 307 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | Y     | 605 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | g     | 601 | CHL  | CHD-C1D | 5.20 | 1.48        | 1.38     |
| 21  | s     | 302 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | y     | 605 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | N     | 605 | CHL  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 21  | s     | 301 | CHL  | CHD-C1D | 5.20 | 1.48        | 1.38     |
| 21  | n     | 607 | CHL  | CHD-C1D | 5.20 | 1.48        | 1.38     |
| 21  | y     | 607 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | Y     | 606 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | s     | 301 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | N     | 601 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | r     | 307 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | g     | 606 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 21  | r     | 301 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | N     | 608 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 21  | s     | 302 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 21  | R     | 305 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | r     | 307 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 21  | s     | 307 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 21  | s     | 306 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | Y     | 601 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | r     | 308 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | s     | 306 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | S     | 302 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | y     | 606 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | R     | 307 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | g     | 607 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 24  | n     | 615 | XAT  | C24-C25 | 5.18 | 1.59        | 1.52     |
| 21  | y     | 608 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | G     | 601 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | n     | 608 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | r     | 306 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | Y     | 605 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | n     | 606 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | G     | 609 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | R     | 306 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 21  | G     | 608 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | G     | 605 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | s     | 307 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | y     | 606 | CHL  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 21  | g     | 609 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 21  | n     | 601 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | y     | 608 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | Y     | 608 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 21  | g     | 605 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 21  | S     | 306 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 21  | S     | 306 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | y     | 601 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | g     | 606 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | g     | 601 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | n     | 605 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | Y     | 606 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 21  | Y     | 608 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 21  | G     | 606 | CHL  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 21  | S     | 302 | CHL  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 21  | n     | 608 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | n     | 605 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | S     | 301 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | N     | 605 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | N     | 608 | CHL  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 21  | R     | 306 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | y     | 601 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | r     | 308 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | N     | 607 | CHL  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 21  | y     | 607 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | G     | 606 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | n     | 601 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | G     | 609 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | R     | 305 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 21  | r     | 306 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 24  | G     | 617 | XAT  | C24-C25 | 5.15 | 1.59        | 1.52     |
| 21  | S     | 307 | CHL  | CHD-C1D | 5.15 | 1.48        | 1.38     |
| 21  | G     | 607 | CHL  | CHD-C1D | 5.15 | 1.48        | 1.38     |
| 21  | g     | 608 | CHL  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 21  | N     | 606 | CHL  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 21  | N     | 601 | CHL  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 21  | n     | 606 | CHL  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 21  | y     | 606 | CHL  | C2C-C3C | 5.13 | 1.47        | 1.36     |
| 21  | Y     | 601 | CHL  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 21  | N     | 601 | CHL  | C2C-C3C | 5.13 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | y     | 609 | CHL  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 21  | g     | 607 | CHL  | C2C-C3C | 5.13 | 1.47        | 1.36     |
| 21  | g     | 608 | CHL  | C2C-C3C | 5.12 | 1.47        | 1.36     |
| 21  | N     | 607 | CHL  | CHD-C1D | 5.12 | 1.48        | 1.38     |
| 21  | r     | 301 | CHL  | CHD-C1D | 5.12 | 1.48        | 1.38     |
| 21  | y     | 605 | CHL  | CHD-C1D | 5.12 | 1.48        | 1.38     |
| 21  | N     | 606 | CHL  | C2C-C3C | 5.12 | 1.47        | 1.36     |
| 21  | s     | 302 | CHL  | C2C-C3C | 5.12 | 1.47        | 1.36     |
| 21  | N     | 607 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | y     | 607 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | G     | 608 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | S     | 307 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 24  | N     | 616 | XAT  | C24-C25 | 5.11 | 1.59        | 1.52     |
| 21  | Y     | 607 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | S     | 301 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | N     | 605 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | n     | 606 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | S     | 302 | CHL  | C2C-C3C | 5.11 | 1.47        | 1.36     |
| 21  | r     | 307 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | Y     | 607 | CHL  | CHD-C1D | 5.10 | 1.48        | 1.38     |
| 21  | Y     | 606 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | y     | 605 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | g     | 601 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | r     | 301 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | y     | 608 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | g     | 605 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | S     | 306 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | R     | 307 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | R     | 305 | CHL  | C2C-C3C | 5.10 | 1.47        | 1.36     |
| 21  | n     | 607 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | g     | 606 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | G     | 606 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | Y     | 608 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | s     | 306 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | y     | 601 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | r     | 306 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | G     | 607 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | y     | 609 | CHL  | C2C-C3C | 5.09 | 1.47        | 1.36     |
| 21  | n     | 601 | CHL  | C2C-C3C | 5.08 | 1.47        | 1.36     |
| 21  | G     | 605 | CHL  | C2C-C3C | 5.08 | 1.47        | 1.36     |
| 21  | s     | 307 | CHL  | C2C-C3C | 5.08 | 1.47        | 1.36     |
| 21  | N     | 608 | CHL  | C2C-C3C | 5.08 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | n     | 608 | CHL  | C2C-C3C | 5.08  | 1.47        | 1.36     |
| 21  | G     | 601 | CHL  | C2C-C3C | 5.08  | 1.47        | 1.36     |
| 21  | g     | 609 | CHL  | C2C-C3C | 5.08  | 1.47        | 1.36     |
| 21  | s     | 301 | CHL  | C2C-C3C | 5.08  | 1.47        | 1.36     |
| 21  | n     | 605 | CHL  | C2C-C3C | 5.07  | 1.47        | 1.36     |
| 21  | Y     | 601 | CHL  | C2C-C3C | 5.07  | 1.47        | 1.36     |
| 21  | R     | 306 | CHL  | C2C-C3C | 5.07  | 1.47        | 1.36     |
| 21  | G     | 609 | CHL  | C2C-C3C | 5.06  | 1.47        | 1.36     |
| 21  | r     | 308 | CHL  | C2C-C3C | 5.06  | 1.47        | 1.36     |
| 21  | Y     | 605 | CHL  | C2C-C3C | 5.06  | 1.47        | 1.36     |
| 23  | N     | 615 | LUT  | C26-C27 | 4.93  | 1.57        | 1.50     |
| 21  | s     | 302 | CHL  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 23  | N     | 615 | LUT  | C28-C29 | 4.76  | 1.56        | 1.45     |
| 21  | R     | 307 | CHL  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 21  | N     | 607 | CHL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 21  | G     | 606 | CHL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 21  | N     | 606 | CHL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 21  | r     | 307 | CHL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 21  | G     | 609 | CHL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 21  | Y     | 608 | CHL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 21  | n     | 607 | CHL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 21  | g     | 605 | CHL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 21  | s     | 306 | CHL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 21  | y     | 609 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | Y     | 606 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | s     | 307 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 23  | Y     | 614 | LUT  | C26-C27 | 4.73  | 1.57        | 1.50     |
| 21  | N     | 605 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | R     | 306 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | y     | 606 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | Y     | 601 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 21  | y     | 605 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | S     | 306 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | G     | 607 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | G     | 605 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | S     | 307 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | N     | 601 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | s     | 301 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | S     | 301 | CHL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 21  | N     | 608 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | y     | 608 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | S     | 302 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | G     | 608 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | Y     | 607 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | g     | 609 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | G     | 601 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | g     | 608 | CHL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 21  | r     | 306 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | g     | 606 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | r     | 301 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | y     | 607 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | Y     | 605 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | n     | 605 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | n     | 606 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | y     | 601 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | r     | 308 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | g     | 601 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 21  | n     | 608 | CHL  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 21  | n     | 601 | CHL  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 21  | R     | 305 | CHL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 32  | D     | 407 | PL9  | C7-C3   | -4.68 | 1.46        | 1.51     |
| 21  | g     | 607 | CHL  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 23  | Y     | 614 | LUT  | C28-C29 | 4.61  | 1.55        | 1.45     |
| 23  | R     | 312 | LUT  | C12-C13 | 4.57  | 1.55        | 1.45     |
| 21  | n     | 606 | CHL  | CHD-C4C | 4.56  | 1.49        | 1.39     |
| 21  | n     | 605 | CHL  | CHD-C4C | 4.55  | 1.49        | 1.39     |
| 21  | G     | 605 | CHL  | CHD-C4C | 4.55  | 1.49        | 1.39     |
| 21  | S     | 307 | CHL  | CHD-C4C | 4.55  | 1.49        | 1.39     |
| 21  | r     | 306 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | y     | 606 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | N     | 607 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | r     | 301 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | Y     | 607 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | R     | 305 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | s     | 307 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | G     | 601 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 23  | G     | 616 | LUT  | C28-C29 | 4.54  | 1.55        | 1.45     |
| 21  | g     | 608 | CHL  | CHD-C4C | 4.54  | 1.49        | 1.39     |
| 21  | r     | 308 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | R     | 306 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | G     | 609 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | n     | 601 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | Y     | 601 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | n     | 607 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | y     | 607 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 23  | r     | 313 | LUT  | C12-C13 | 4.53  | 1.55        | 1.45     |
| 21  | g     | 605 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | y     | 605 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | N     | 601 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | n     | 608 | CHL  | CHD-C4C | 4.53  | 1.49        | 1.39     |
| 21  | N     | 608 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | G     | 605 | CHL  | O2A-CGA | 4.52  | 1.45        | 1.30     |
| 21  | r     | 307 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | g     | 606 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | Y     | 608 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | s     | 306 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | y     | 609 | CHL  | CHD-C4C | 4.52  | 1.49        | 1.39     |
| 21  | g     | 609 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | g     | 605 | CHL  | O2A-CGA | 4.51  | 1.45        | 1.30     |
| 32  | d     | 406 | PL9  | C7-C3   | -4.51 | 1.46        | 1.51     |
| 21  | s     | 302 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | G     | 606 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | N     | 606 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | N     | 605 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | S     | 302 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | R     | 307 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | y     | 601 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | G     | 607 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | g     | 601 | CHL  | CHD-C4C | 4.51  | 1.49        | 1.39     |
| 21  | S     | 306 | CHL  | CHD-C4C | 4.50  | 1.49        | 1.39     |
| 21  | G     | 608 | CHL  | CHD-C4C | 4.50  | 1.49        | 1.39     |
| 21  | s     | 302 | CHL  | O2A-CGA | 4.50  | 1.45        | 1.30     |
| 21  | y     | 608 | CHL  | CHD-C4C | 4.50  | 1.49        | 1.39     |
| 24  | N     | 616 | XAT  | C4-C5   | 4.50  | 1.58        | 1.52     |
| 21  | g     | 607 | CHL  | CHD-C4C | 4.50  | 1.49        | 1.39     |
| 21  | S     | 306 | CHL  | O2A-CGA | 4.50  | 1.45        | 1.30     |
| 21  | Y     | 606 | CHL  | CHD-C4C | 4.49  | 1.49        | 1.39     |
| 21  | s     | 301 | CHL  | CHD-C4C | 4.49  | 1.49        | 1.39     |
| 24  | n     | 615 | XAT  | C4-C5   | 4.49  | 1.58        | 1.52     |
| 21  | Y     | 605 | CHL  | CHD-C4C | 4.49  | 1.49        | 1.39     |
| 21  | S     | 307 | CHL  | O2A-CGA | 4.49  | 1.45        | 1.30     |
| 21  | S     | 301 | CHL  | CHD-C4C | 4.49  | 1.49        | 1.39     |
| 21  | s     | 307 | CHL  | O2A-CGA | 4.48  | 1.45        | 1.30     |
| 21  | s     | 306 | CHL  | O2A-CGA | 4.47  | 1.45        | 1.30     |
| 21  | S     | 302 | CHL  | O2A-CGA | 4.46  | 1.45        | 1.30     |
| 23  | g     | 616 | LUT  | C28-C29 | 4.46  | 1.55        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 23  | g     | 616 | LUT  | C26-C27 | 4.44 | 1.56        | 1.50     |
| 23  | g     | 616 | LUT  | C12-C13 | 4.39 | 1.55        | 1.45     |
| 25  | Y     | 616 | NEX  | C28-C29 | 4.37 | 1.55        | 1.45     |
| 23  | G     | 616 | LUT  | C26-C27 | 4.36 | 1.56        | 1.50     |
| 23  | Y     | 614 | LUT  | C12-C13 | 4.35 | 1.55        | 1.45     |
| 23  | G     | 616 | LUT  | C12-C13 | 4.34 | 1.55        | 1.45     |
| 21  | N     | 605 | CHL  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 24  | y     | 615 | XAT  | C15-C14 | 4.30 | 1.56        | 1.43     |
| 21  | R     | 306 | CHL  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 21  | n     | 605 | CHL  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 21  | Y     | 606 | CHL  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 21  | g     | 601 | CHL  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 21  | r     | 308 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | y     | 609 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | R     | 307 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | N     | 608 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | Y     | 607 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | g     | 607 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | y     | 605 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 24  | Y     | 615 | XAT  | C15-C14 | 4.29 | 1.56        | 1.43     |
| 21  | Y     | 601 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | G     | 606 | CHL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 21  | g     | 606 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | n     | 606 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | G     | 601 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 23  | N     | 615 | LUT  | C12-C13 | 4.28 | 1.55        | 1.45     |
| 21  | n     | 608 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | r     | 307 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | r     | 306 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | r     | 301 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | S     | 301 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | y     | 606 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | N     | 607 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | Y     | 605 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | g     | 608 | CHL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 21  | n     | 607 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 24  | Y     | 615 | XAT  | C31-C30 | 4.27 | 1.56        | 1.43     |
| 21  | g     | 609 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 21  | y     | 607 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 21  | G     | 609 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 21  | Y     | 608 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 21  | y     | 601 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | s     | 301 | CHL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 21  | N     | 606 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 21  | G     | 608 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 21  | G     | 607 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 21  | y     | 608 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 24  | y     | 615 | XAT  | C31-C30 | 4.26 | 1.56        | 1.43     |
| 23  | N     | 614 | LUT  | C28-C29 | 4.26 | 1.55        | 1.45     |
| 21  | n     | 601 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 21  | R     | 305 | CHL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 23  | Y     | 613 | LUT  | C28-C29 | 4.25 | 1.55        | 1.45     |
| 24  | Y     | 615 | XAT  | C35-C34 | 4.25 | 1.56        | 1.43     |
| 23  | r     | 313 | LUT  | C28-C29 | 4.25 | 1.55        | 1.45     |
| 21  | N     | 601 | CHL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 24  | G     | 617 | XAT  | C15-C14 | 4.25 | 1.56        | 1.43     |
| 25  | r     | 315 | NEX  | C28-C29 | 4.24 | 1.55        | 1.45     |
| 23  | G     | 615 | LUT  | C28-C29 | 4.24 | 1.55        | 1.45     |
| 25  | N     | 617 | NEX  | C28-C29 | 4.23 | 1.55        | 1.45     |
| 23  | n     | 614 | LUT  | C28-C29 | 4.22 | 1.55        | 1.45     |
| 25  | y     | 618 | NEX  | C28-C29 | 4.22 | 1.55        | 1.45     |
| 24  | g     | 617 | XAT  | C15-C14 | 4.22 | 1.56        | 1.43     |
| 23  | g     | 615 | LUT  | C28-C29 | 4.22 | 1.55        | 1.45     |
| 23  | y     | 614 | LUT  | C28-C29 | 4.22 | 1.55        | 1.45     |
| 23  | R     | 312 | LUT  | C28-C29 | 4.22 | 1.55        | 1.45     |
| 24  | G     | 617 | XAT  | C35-C34 | 4.21 | 1.56        | 1.43     |
| 24  | Y     | 615 | XAT  | C11-C10 | 4.20 | 1.56        | 1.43     |
| 23  | n     | 614 | LUT  | C12-C13 | 4.19 | 1.55        | 1.45     |
| 23  | N     | 615 | LUT  | C8-C9   | 4.19 | 1.55        | 1.45     |
| 24  | y     | 615 | XAT  | C35-C34 | 4.19 | 1.56        | 1.43     |
| 25  | y     | 616 | NEX  | C11-C10 | 4.19 | 1.56        | 1.43     |
| 24  | y     | 615 | XAT  | C11-C10 | 4.19 | 1.56        | 1.43     |
| 24  | g     | 617 | XAT  | C4-C5   | 4.19 | 1.58        | 1.52     |
| 24  | G     | 617 | XAT  | C11-C10 | 4.19 | 1.56        | 1.43     |
| 25  | N     | 617 | NEX  | C11-C10 | 4.18 | 1.56        | 1.43     |
| 24  | G     | 617 | XAT  | C31-C30 | 4.18 | 1.56        | 1.43     |
| 25  | n     | 616 | NEX  | C28-C29 | 4.18 | 1.54        | 1.45     |
| 23  | Y     | 613 | LUT  | C12-C13 | 4.18 | 1.54        | 1.45     |
| 23  | G     | 615 | LUT  | C12-C13 | 4.18 | 1.54        | 1.45     |
| 24  | R     | 313 | XAT  | C11-C10 | 4.18 | 1.56        | 1.43     |
| 23  | N     | 614 | LUT  | C12-C13 | 4.18 | 1.54        | 1.45     |
| 24  | g     | 617 | XAT  | C11-C10 | 4.18 | 1.56        | 1.43     |
| 25  | Y     | 616 | NEX  | C11-C10 | 4.17 | 1.56        | 1.43     |
| 24  | n     | 615 | XAT  | C15-C14 | 4.17 | 1.56        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 23  | Y     | 614 | LUT  | C8-C9   | 4.17 | 1.54        | 1.45     |
| 23  | g     | 616 | LUT  | C15-C14 | 4.17 | 1.56        | 1.43     |
| 24  | g     | 617 | XAT  | C31-C30 | 4.16 | 1.56        | 1.43     |
| 24  | r     | 314 | XAT  | C11-C10 | 4.16 | 1.56        | 1.43     |
| 25  | g     | 618 | NEX  | C28-C29 | 4.16 | 1.54        | 1.45     |
| 25  | n     | 616 | NEX  | C11-C10 | 4.16 | 1.56        | 1.43     |
| 24  | g     | 617 | XAT  | C35-C34 | 4.16 | 1.56        | 1.43     |
| 23  | g     | 615 | LUT  | C12-C13 | 4.16 | 1.54        | 1.45     |
| 23  | y     | 614 | LUT  | C12-C13 | 4.16 | 1.54        | 1.45     |
| 24  | n     | 615 | XAT  | C31-C30 | 4.15 | 1.56        | 1.43     |
| 23  | G     | 616 | LUT  | C15-C14 | 4.15 | 1.56        | 1.43     |
| 24  | G     | 617 | XAT  | C4-C5   | 4.15 | 1.58        | 1.52     |
| 24  | R     | 313 | XAT  | C31-C30 | 4.14 | 1.56        | 1.43     |
| 24  | N     | 616 | XAT  | C15-C14 | 4.14 | 1.56        | 1.43     |
| 24  | r     | 314 | XAT  | C31-C30 | 4.14 | 1.56        | 1.43     |
| 24  | n     | 615 | XAT  | C11-C10 | 4.13 | 1.56        | 1.43     |
| 25  | y     | 618 | NEX  | C11-C10 | 4.13 | 1.56        | 1.43     |
| 24  | N     | 616 | XAT  | C31-C30 | 4.13 | 1.56        | 1.43     |
| 23  | g     | 616 | LUT  | C8-C9   | 4.12 | 1.54        | 1.45     |
| 25  | r     | 315 | NEX  | C11-C10 | 4.12 | 1.56        | 1.43     |
| 24  | N     | 616 | XAT  | C11-C10 | 4.12 | 1.56        | 1.43     |
| 25  | N     | 617 | NEX  | C15-C14 | 4.12 | 1.56        | 1.43     |
| 24  | n     | 615 | XAT  | C35-C34 | 4.11 | 1.56        | 1.43     |
| 25  | n     | 616 | NEX  | C15-C14 | 4.11 | 1.56        | 1.43     |
| 25  | N     | 617 | NEX  | C35-C34 | 4.11 | 1.56        | 1.43     |
| 25  | g     | 618 | NEX  | C11-C10 | 4.10 | 1.56        | 1.43     |
| 25  | y     | 616 | NEX  | C35-C34 | 4.10 | 1.56        | 1.43     |
| 25  | y     | 616 | NEX  | C15-C14 | 4.09 | 1.56        | 1.43     |
| 25  | Y     | 616 | NEX  | C35-C34 | 4.09 | 1.56        | 1.43     |
| 23  | N     | 615 | LUT  | C15-C14 | 4.08 | 1.56        | 1.43     |
| 24  | r     | 314 | XAT  | C15-C14 | 4.08 | 1.56        | 1.43     |
| 25  | n     | 616 | NEX  | C35-C34 | 4.07 | 1.56        | 1.43     |
| 25  | y     | 616 | NEX  | C28-C29 | 4.07 | 1.54        | 1.45     |
| 24  | R     | 313 | XAT  | C15-C14 | 4.07 | 1.56        | 1.43     |
| 23  | G     | 616 | LUT  | C8-C9   | 4.06 | 1.54        | 1.45     |
| 23  | Y     | 614 | LUT  | C15-C14 | 4.06 | 1.56        | 1.43     |
| 25  | y     | 618 | NEX  | C35-C34 | 4.05 | 1.56        | 1.43     |
| 25  | Y     | 616 | NEX  | C15-C14 | 4.05 | 1.56        | 1.43     |
| 25  | g     | 618 | NEX  | C35-C34 | 4.04 | 1.56        | 1.43     |
| 25  | r     | 315 | NEX  | C35-C34 | 4.04 | 1.56        | 1.43     |
| 25  | g     | 618 | NEX  | C15-C14 | 4.03 | 1.55        | 1.43     |
| 24  | R     | 313 | XAT  | C35-C34 | 4.02 | 1.55        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | N     | 616 | XAT  | C35-C34 | 4.02  | 1.55        | 1.43     |
| 25  | r     | 315 | NEX  | C15-C14 | 4.02  | 1.55        | 1.43     |
| 24  | r     | 314 | XAT  | C35-C34 | 4.01  | 1.55        | 1.43     |
| 25  | y     | 618 | NEX  | C15-C14 | 4.00  | 1.55        | 1.43     |
| 24  | y     | 615 | XAT  | C4-C5   | 3.99  | 1.57        | 1.52     |
| 24  | y     | 615 | XAT  | C32-C33 | 3.98  | 1.54        | 1.45     |
| 25  | N     | 617 | NEX  | C31-C30 | 3.98  | 1.55        | 1.43     |
| 32  | A     | 411 | PL9  | C7-C3   | -3.98 | 1.47        | 1.51     |
| 25  | r     | 315 | NEX  | C31-C30 | 3.97  | 1.55        | 1.43     |
| 25  | y     | 618 | NEX  | C31-C30 | 3.97  | 1.55        | 1.43     |
| 25  | n     | 616 | NEX  | C31-C30 | 3.97  | 1.55        | 1.43     |
| 24  | Y     | 615 | XAT  | C32-C33 | 3.96  | 1.54        | 1.45     |
| 23  | r     | 313 | LUT  | C26-C27 | 3.96  | 1.56        | 1.50     |
| 24  | N     | 616 | XAT  | C28-C29 | 3.94  | 1.54        | 1.45     |
| 22  | r     | 311 | CLA  | C1D-ND  | 3.94  | 1.42        | 1.37     |
| 24  | Y     | 615 | XAT  | C4-C5   | 3.94  | 1.57        | 1.52     |
| 23  | R     | 312 | LUT  | C26-C27 | 3.94  | 1.56        | 1.50     |
| 25  | g     | 618 | NEX  | C31-C30 | 3.93  | 1.55        | 1.43     |
| 24  | r     | 314 | XAT  | C4-C5   | 3.93  | 1.57        | 1.52     |
| 23  | Y     | 613 | LUT  | C26-C27 | 3.92  | 1.56        | 1.50     |
| 23  | G     | 616 | LUT  | C35-C34 | 3.92  | 1.55        | 1.43     |
| 24  | R     | 313 | XAT  | C4-C5   | 3.92  | 1.57        | 1.52     |
| 25  | y     | 616 | NEX  | C31-C30 | 3.92  | 1.55        | 1.43     |
| 37  | f     | 101 | HEM  | CHB-C1B | 3.92  | 1.45        | 1.35     |
| 32  | a     | 410 | PL9  | C7-C3   | -3.91 | 1.47        | 1.51     |
| 24  | Y     | 615 | XAT  | C8-C9   | 3.91  | 1.54        | 1.45     |
| 24  | Y     | 615 | XAT  | C12-C13 | 3.91  | 1.54        | 1.45     |
| 37  | F     | 101 | HEM  | CHB-C1B | 3.91  | 1.45        | 1.35     |
| 24  | G     | 617 | XAT  | C32-C33 | 3.91  | 1.54        | 1.45     |
| 24  | n     | 615 | XAT  | C32-C33 | 3.90  | 1.54        | 1.45     |
| 24  | Y     | 615 | XAT  | C28-C29 | 3.89  | 1.54        | 1.45     |
| 23  | g     | 616 | LUT  | C35-C34 | 3.89  | 1.55        | 1.43     |
| 23  | G     | 615 | LUT  | C26-C27 | 3.89  | 1.56        | 1.50     |
| 23  | n     | 614 | LUT  | C26-C27 | 3.89  | 1.56        | 1.50     |
| 24  | G     | 617 | XAT  | C28-C29 | 3.89  | 1.54        | 1.45     |
| 24  | y     | 615 | XAT  | C28-C29 | 3.89  | 1.54        | 1.45     |
| 25  | n     | 616 | NEX  | C32-C33 | 3.88  | 1.54        | 1.45     |
| 31  | c     | 515 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 24  | y     | 615 | XAT  | C12-C13 | 3.88  | 1.54        | 1.45     |
| 23  | y     | 614 | LUT  | C15-C14 | 3.88  | 1.55        | 1.43     |
| 32  | d     | 406 | PL9  | C3-C4   | -3.88 | 1.43        | 1.49     |
| 31  | C     | 516 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | g     | 615 | LUT  | C26-C27 | 3.87  | 1.56        | 1.50     |
| 23  | n     | 614 | LUT  | C15-C14 | 3.87  | 1.55        | 1.43     |
| 23  | N     | 614 | LUT  | C15-C14 | 3.87  | 1.55        | 1.43     |
| 24  | G     | 617 | XAT  | C8-C9   | 3.87  | 1.54        | 1.45     |
| 24  | R     | 313 | XAT  | C28-C29 | 3.86  | 1.54        | 1.45     |
| 24  | g     | 617 | XAT  | C32-C33 | 3.86  | 1.54        | 1.45     |
| 23  | r     | 313 | LUT  | C15-C14 | 3.86  | 1.55        | 1.43     |
| 25  | y     | 616 | NEX  | C32-C33 | 3.86  | 1.54        | 1.45     |
| 23  | y     | 614 | LUT  | C26-C27 | 3.86  | 1.56        | 1.50     |
| 24  | g     | 617 | XAT  | C28-C29 | 3.86  | 1.54        | 1.45     |
| 24  | r     | 314 | XAT  | C28-C29 | 3.85  | 1.54        | 1.45     |
| 23  | G     | 615 | LUT  | C15-C14 | 3.85  | 1.55        | 1.43     |
| 23  | Y     | 614 | LUT  | C35-C34 | 3.85  | 1.55        | 1.43     |
| 23  | g     | 615 | LUT  | C15-C14 | 3.85  | 1.55        | 1.43     |
| 23  | N     | 614 | LUT  | C26-C27 | 3.85  | 1.55        | 1.50     |
| 32  | D     | 407 | PL9  | C3-C4   | -3.85 | 1.43        | 1.49     |
| 24  | g     | 617 | XAT  | C8-C9   | 3.85  | 1.54        | 1.45     |
| 23  | G     | 616 | LUT  | C7-C6   | 3.84  | 1.58        | 1.45     |
| 24  | n     | 615 | XAT  | C28-C29 | 3.84  | 1.54        | 1.45     |
| 23  | Y     | 613 | LUT  | C15-C14 | 3.84  | 1.55        | 1.43     |
| 24  | y     | 615 | XAT  | C8-C9   | 3.84  | 1.54        | 1.45     |
| 24  | N     | 616 | XAT  | C32-C33 | 3.84  | 1.54        | 1.45     |
| 23  | g     | 616 | LUT  | C7-C6   | 3.84  | 1.58        | 1.45     |
| 24  | G     | 617 | XAT  | C12-C13 | 3.83  | 1.54        | 1.45     |
| 22  | R     | 310 | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 22  | S     | 308 | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 23  | R     | 312 | LUT  | C15-C14 | 3.83  | 1.55        | 1.43     |
| 25  | Y     | 616 | NEX  | C31-C30 | 3.83  | 1.55        | 1.43     |
| 23  | N     | 615 | LUT  | C35-C34 | 3.82  | 1.55        | 1.43     |
| 24  | R     | 313 | XAT  | C32-C33 | 3.81  | 1.54        | 1.45     |
| 31  | c     | 516 | BCR  | C1-C6   | -3.81 | 1.48        | 1.53     |
| 24  | r     | 314 | XAT  | C32-C33 | 3.80  | 1.54        | 1.45     |
| 21  | s     | 301 | CHL  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 23  | Y     | 614 | LUT  | C7-C6   | 3.80  | 1.58        | 1.45     |
| 21  | g     | 609 | CHL  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 21  | G     | 601 | CHL  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 24  | g     | 617 | XAT  | C12-C13 | 3.79  | 1.54        | 1.45     |
| 21  | n     | 605 | CHL  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 25  | y     | 618 | NEX  | C32-C33 | 3.79  | 1.54        | 1.45     |
| 22  | s     | 308 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 21  | y     | 609 | CHL  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 21  | G     | 609 | CHL  | OBD-CAD | 3.78  | 1.29        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | C     | 517 | BCR  | C1-C6   | -3.78 | 1.48        | 1.53     |
| 21  | n     | 606 | CHL  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 21  | G     | 606 | CHL  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 31  | a     | 409 | BCR  | C1-C6   | -3.78 | 1.48        | 1.53     |
| 21  | n     | 601 | CHL  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 21  | g     | 607 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | S     | 301 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | s     | 307 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 25  | r     | 315 | NEX  | C32-C33 | 3.77  | 1.54        | 1.45     |
| 21  | n     | 607 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | N     | 607 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | y     | 607 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | Y     | 605 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 21  | r     | 308 | CHL  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 24  | N     | 616 | XAT  | C12-C13 | 3.76  | 1.54        | 1.45     |
| 21  | g     | 606 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | s     | 306 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | y     | 605 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 31  | K     | 102 | BCR  | C1-C6   | -3.76 | 1.48        | 1.53     |
| 25  | g     | 618 | NEX  | C32-C33 | 3.76  | 1.54        | 1.45     |
| 21  | G     | 605 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | y     | 601 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | N     | 608 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | S     | 302 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 21  | R     | 306 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 25  | N     | 617 | NEX  | C12-C13 | 3.75  | 1.54        | 1.45     |
| 21  | Y     | 601 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 21  | R     | 307 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 21  | R     | 305 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 21  | n     | 608 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 24  | n     | 615 | XAT  | C12-C13 | 3.75  | 1.54        | 1.45     |
| 24  | r     | 314 | XAT  | C12-C13 | 3.75  | 1.54        | 1.45     |
| 21  | S     | 306 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 21  | G     | 608 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 21  | N     | 606 | CHL  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 31  | k     | 102 | BCR  | C1-C6   | -3.75 | 1.48        | 1.53     |
| 21  | N     | 601 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 21  | y     | 606 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 25  | n     | 616 | NEX  | C12-C13 | 3.74  | 1.54        | 1.45     |
| 21  | y     | 608 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 21  | S     | 307 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 21  | G     | 607 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | Y     | 608 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 21  | g     | 601 | CHL  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 21  | s     | 302 | CHL  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 21  | g     | 605 | CHL  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 21  | Y     | 606 | CHL  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 25  | Y     | 616 | NEX  | C12-C13 | 3.73  | 1.54        | 1.45     |
| 25  | y     | 616 | NEX  | C12-C13 | 3.73  | 1.54        | 1.45     |
| 31  | H     | 101 | BCR  | C1-C6   | -3.72 | 1.48        | 1.53     |
| 22  | r     | 309 | CLA  | C1D-ND  | 3.72  | 1.42        | 1.37     |
| 21  | r     | 301 | CHL  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 31  | C     | 516 | BCR  | C30-C25 | -3.72 | 1.48        | 1.53     |
| 24  | n     | 615 | XAT  | C8-C9   | 3.72  | 1.53        | 1.45     |
| 21  | r     | 307 | CHL  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 24  | R     | 313 | XAT  | C12-C13 | 3.72  | 1.53        | 1.45     |
| 31  | b     | 616 | BCR  | C1-C6   | -3.72 | 1.48        | 1.53     |
| 31  | b     | 616 | BCR  | C30-C25 | -3.72 | 1.48        | 1.53     |
| 31  | A     | 410 | BCR  | C1-C6   | -3.72 | 1.48        | 1.53     |
| 21  | g     | 608 | CHL  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 21  | N     | 605 | CHL  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 22  | C     | 513 | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 24  | N     | 616 | XAT  | C8-C9   | 3.71  | 1.53        | 1.45     |
| 21  | r     | 306 | CHL  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 21  | Y     | 607 | CHL  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 31  | c     | 515 | BCR  | C30-C25 | -3.70 | 1.48        | 1.53     |
| 22  | n     | 611 | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 31  | B     | 619 | BCR  | C30-C25 | -3.69 | 1.48        | 1.53     |
| 31  | B     | 619 | BCR  | C1-C6   | -3.69 | 1.48        | 1.53     |
| 22  | N     | 609 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 25  | N     | 617 | NEX  | C32-C33 | 3.68  | 1.53        | 1.45     |
| 22  | s     | 309 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 24  | r     | 314 | XAT  | C8-C9   | 3.68  | 1.53        | 1.45     |
| 22  | S     | 309 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 24  | R     | 313 | XAT  | C8-C9   | 3.67  | 1.53        | 1.45     |
| 37  | f     | 101 | HEM  | CHC-C4B | 3.67  | 1.51        | 1.41     |
| 23  | N     | 614 | LUT  | C35-C34 | 3.66  | 1.54        | 1.43     |
| 23  | n     | 614 | LUT  | C35-C34 | 3.66  | 1.54        | 1.43     |
| 22  | G     | 612 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | r     | 303 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 31  | D     | 406 | BCR  | C1-C6   | -3.66 | 1.48        | 1.53     |
| 22  | c     | 512 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 23  | y     | 614 | LUT  | C35-C34 | 3.66  | 1.54        | 1.43     |
| 37  | F     | 101 | HEM  | CHC-C4B | 3.66  | 1.51        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | R     | 302 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 23  | R     | 312 | LUT  | C35-C34 | 3.65  | 1.54        | 1.43     |
| 22  | g     | 610 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | y     | 611 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 23  | g     | 615 | LUT  | C35-C34 | 3.65  | 1.54        | 1.43     |
| 23  | G     | 615 | LUT  | C35-C34 | 3.65  | 1.54        | 1.43     |
| 22  | r     | 310 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | N     | 611 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | Y     | 612 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | W     | 101 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 25  | Y     | 616 | NEX  | C32-C33 | 3.65  | 1.53        | 1.45     |
| 22  | N     | 613 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | Y     | 602 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 37  | f     | 101 | HEM  | C4A-NA  | 3.65  | 1.43        | 1.36     |
| 25  | r     | 315 | NEX  | C12-C13 | 3.64  | 1.53        | 1.45     |
| 22  | Y     | 609 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 37  | F     | 101 | HEM  | C4A-NA  | 3.64  | 1.43        | 1.36     |
| 31  | h     | 101 | BCR  | C1-C6   | -3.64 | 1.48        | 1.53     |
| 22  | R     | 308 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 22  | R     | 309 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 22  | S     | 303 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 31  | b     | 617 | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 23  | N     | 615 | LUT  | C7-C6   | 3.63  | 1.58        | 1.45     |
| 23  | Y     | 613 | LUT  | C35-C34 | 3.63  | 1.54        | 1.43     |
| 31  | d     | 405 | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 22  | G     | 610 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 25  | y     | 618 | NEX  | C12-C13 | 3.63  | 1.53        | 1.45     |
| 22  | n     | 609 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 22  | y     | 613 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 22  | G     | 614 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 31  | c     | 516 | BCR  | C30-C25 | -3.62 | 1.48        | 1.53     |
| 23  | r     | 313 | LUT  | C35-C34 | 3.62  | 1.54        | 1.43     |
| 22  | n     | 613 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 23  | N     | 615 | LUT  | C31-C30 | 3.62  | 1.54        | 1.43     |
| 22  | w     | 101 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 22  | y     | 610 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 31  | K     | 101 | BCR  | C1-C6   | -3.61 | 1.48        | 1.53     |
| 22  | S     | 313 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 22  | r     | 312 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 25  | g     | 618 | NEX  | C12-C13 | 3.61  | 1.53        | 1.45     |
| 31  | C     | 517 | BCR  | C30-C25 | -3.60 | 1.48        | 1.53     |
| 22  | S     | 305 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | y     | 602 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | s     | 303 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 22  | S     | 304 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 22  | Y     | 610 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 31  | B     | 620 | BCR  | C1-C6   | -3.59 | 1.48        | 1.53     |
| 22  | g     | 614 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 22  | n     | 610 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 22  | g     | 611 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | g     | 602 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | s     | 313 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | N     | 602 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 25  | y     | 618 | NEX  | C7-C8   | 3.58  | 1.37        | 1.32     |
| 22  | C     | 515 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | g     | 612 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | G     | 604 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | R     | 303 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 31  | k     | 101 | BCR  | C1-C6   | -3.57 | 1.48        | 1.53     |
| 22  | N     | 610 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | s     | 310 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | s     | 304 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | c     | 507 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | G     | 611 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | c     | 514 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 25  | r     | 315 | NEX  | C7-C8   | 3.56  | 1.37        | 1.32     |
| 22  | S     | 310 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | s     | 312 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 22  | R     | 311 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 23  | g     | 616 | LUT  | C11-C10 | 3.55  | 1.54        | 1.43     |
| 22  | B     | 612 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 22  | C     | 508 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 31  | A     | 410 | BCR  | C30-C25 | -3.54 | 1.48        | 1.53     |
| 23  | Y     | 613 | LUT  | C8-C9   | 3.54  | 1.53        | 1.45     |
| 22  | S     | 311 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 23  | G     | 615 | LUT  | C8-C9   | 3.53  | 1.53        | 1.45     |
| 23  | Y     | 614 | LUT  | C11-C10 | 3.53  | 1.54        | 1.43     |
| 23  | G     | 616 | LUT  | C31-C30 | 3.53  | 1.54        | 1.43     |
| 22  | N     | 604 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 22  | s     | 305 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 23  | G     | 616 | LUT  | C11-C10 | 3.53  | 1.54        | 1.43     |
| 22  | G     | 602 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 22  | n     | 602 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 23  | N     | 614 | LUT  | C8-C9   | 3.52  | 1.53        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | y     | 614 | LUT  | C8-C9   | 3.52  | 1.53        | 1.45     |
| 31  | a     | 409 | BCR  | C30-C25 | -3.51 | 1.48        | 1.53     |
| 22  | C     | 512 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 31  | d     | 405 | BCR  | C30-C25 | -3.51 | 1.48        | 1.53     |
| 23  | n     | 614 | LUT  | C8-C9   | 3.51  | 1.53        | 1.45     |
| 37  | F     | 101 | HEM  | C3C-C2C | -3.51 | 1.35        | 1.40     |
| 22  | S     | 312 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 23  | g     | 616 | LUT  | C31-C30 | 3.51  | 1.54        | 1.43     |
| 22  | C     | 509 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | r     | 304 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | A     | 409 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | b     | 613 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 23  | g     | 615 | LUT  | C8-C9   | 3.50  | 1.53        | 1.45     |
| 22  | b     | 606 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 22  | b     | 607 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 22  | A     | 407 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 22  | C     | 507 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 22  | n     | 604 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | c     | 511 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | c     | 508 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | s     | 311 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | B     | 609 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | x     | 101 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | y     | 604 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 23  | Y     | 614 | LUT  | C31-C30 | 3.47  | 1.54        | 1.43     |
| 37  | f     | 101 | HEM  | C3C-C2C | -3.47 | 1.35        | 1.40     |
| 22  | a     | 404 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 22  | c     | 506 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 22  | B     | 616 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 22  | b     | 609 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 22  | D     | 405 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 22  | a     | 406 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 31  | D     | 406 | BCR  | C30-C25 | -3.46 | 1.49        | 1.53     |
| 22  | g     | 604 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 37  | F     | 101 | HEM  | C3C-CAC | 3.45  | 1.54        | 1.47     |
| 23  | r     | 313 | LUT  | C8-C9   | 3.45  | 1.53        | 1.45     |
| 23  | R     | 312 | LUT  | C8-C9   | 3.45  | 1.53        | 1.45     |
| 22  | B     | 603 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 22  | b     | 601 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 22  | r     | 305 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 22  | b     | 608 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 37  | f     | 101 | HEM  | C3C-CAC | 3.44  | 1.54        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | c     | 505 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 22  | D     | 404 | CLA  | C4D-ND  | -3.44 | 1.33        | 1.37     |
| 22  | b     | 611 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 22  | a     | 408 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 22  | B     | 617 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | T     | 102 | BCR  | C1-C6   | -3.43 | 1.49        | 1.53     |
| 22  | Y     | 604 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 22  | b     | 604 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 22  | B     | 610 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 22  | c     | 502 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 22  | B     | 604 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 21  | N     | 606 | CHL  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 22  | C     | 505 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 22  | B     | 607 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 22  | b     | 614 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 22  | c     | 509 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 21  | R     | 306 | CHL  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 22  | d     | 404 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | b     | 610 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | B     | 614 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | a     | 405 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | B     | 605 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 21  | g     | 601 | CHL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 21  | y     | 609 | CHL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 22  | B     | 606 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | C     | 514 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 22  | b     | 614 | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 21  | g     | 609 | CHL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 22  | S     | 308 | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 31  | B     | 602 | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 21  | N     | 605 | CHL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 22  | B     | 615 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 21  | g     | 607 | CHL  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 22  | B     | 618 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 21  | G     | 601 | CHL  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 21  | G     | 605 | CHL  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 22  | B     | 613 | CLA  | C1D-ND  | 3.39  | 1.41        | 1.37     |
| 21  | R     | 307 | CHL  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 22  | b     | 602 | CLA  | C1D-ND  | 3.39  | 1.41        | 1.37     |
| 22  | A     | 405 | CLA  | C1D-ND  | 3.39  | 1.41        | 1.37     |
| 21  | s     | 302 | CHL  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 21  | G     | 606 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | s     | 307 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | n     | 605 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | y     | 601 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | G     | 609 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | r     | 308 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 22  | b     | 615 | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 21  | y     | 607 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | y     | 608 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 31  | b     | 618 | BCR  | C1-C6   | -3.38 | 1.49        | 1.53     |
| 21  | n     | 608 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | r     | 301 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | S     | 301 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 21  | N     | 601 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 22  | g     | 603 | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 22  | c     | 513 | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 23  | N     | 615 | LUT  | C32-C33 | 3.38  | 1.53        | 1.45     |
| 21  | g     | 608 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 22  | A     | 406 | CLA  | C4D-ND  | -3.38 | 1.33        | 1.37     |
| 21  | g     | 606 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 22  | c     | 504 | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 23  | g     | 615 | LUT  | C31-C30 | 3.37  | 1.53        | 1.43     |
| 22  | c     | 512 | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 21  | Y     | 608 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | y     | 605 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 22  | C     | 503 | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 21  | S     | 306 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | N     | 607 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | s     | 301 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 23  | Y     | 613 | LUT  | C31-C30 | 3.37  | 1.53        | 1.43     |
| 31  | B     | 620 | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 21  | n     | 606 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | Y     | 605 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | G     | 608 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 21  | R     | 305 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 22  | A     | 406 | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 21  | n     | 607 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 23  | N     | 614 | LUT  | C31-C30 | 3.37  | 1.53        | 1.43     |
| 22  | b     | 607 | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 22  | d     | 403 | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 21  | r     | 306 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 22  | b     | 612 | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 21  | S     | 307 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | g     | 605 | CHL  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 22  | C     | 514 | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 21  | n     | 601 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 21  | S     | 302 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 22  | c     | 513 | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 21  | s     | 306 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 22  | b     | 603 | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |
| 22  | C     | 506 | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |
| 31  | b     | 617 | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 21  | Y     | 601 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 22  | B     | 608 | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |
| 22  | C     | 513 | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 21  | G     | 607 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 22  | Y     | 603 | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |
| 21  | y     | 606 | CHL  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 21  | Y     | 606 | CHL  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 23  | R     | 312 | LUT  | C11-C10 | 3.35  | 1.53        | 1.43     |
| 22  | b     | 604 | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 21  | N     | 608 | CHL  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 22  | B     | 611 | CLA  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 22  | b     | 605 | CLA  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 21  | r     | 307 | CHL  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 22  | C     | 510 | CLA  | C1D-ND  | 3.34  | 1.41        | 1.37     |
| 22  | B     | 604 | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 23  | n     | 614 | LUT  | C31-C30 | 3.34  | 1.53        | 1.43     |
| 21  | Y     | 607 | CHL  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 22  | a     | 404 | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 22  | B     | 610 | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 21  | r     | 301 | CHL  | C1D-C2D | 3.34  | 1.51        | 1.45     |
| 21  | n     | 608 | CHL  | C1D-C2D | 3.34  | 1.51        | 1.45     |
| 22  | a     | 405 | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 23  | G     | 616 | LUT  | C32-C33 | 3.34  | 1.53        | 1.45     |
| 22  | n     | 603 | CLA  | C1D-ND  | 3.34  | 1.41        | 1.37     |
| 23  | G     | 615 | LUT  | C31-C30 | 3.34  | 1.53        | 1.43     |
| 22  | C     | 503 | CLA  | C4D-ND  | -3.33 | 1.33        | 1.37     |
| 22  | R     | 304 | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 23  | y     | 614 | LUT  | C31-C30 | 3.33  | 1.53        | 1.43     |
| 22  | C     | 504 | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 23  | g     | 616 | LUT  | C32-C33 | 3.33  | 1.53        | 1.45     |
| 22  | s     | 308 | CLA  | C4D-ND  | -3.33 | 1.33        | 1.37     |
| 21  | Y     | 607 | CHL  | C1D-C2D | 3.33  | 1.51        | 1.45     |
| 23  | r     | 313 | LUT  | C11-C10 | 3.33  | 1.53        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | n     | 606 | CHL  | C1D-C2D | 3.32  | 1.51        | 1.45     |
| 21  | G     | 606 | CHL  | C1D-C2D | 3.32  | 1.51        | 1.45     |
| 21  | n     | 605 | CHL  | C1D-C2D | 3.32  | 1.51        | 1.45     |
| 22  | N     | 603 | CLA  | C1D-ND  | 3.32  | 1.41        | 1.37     |
| 22  | c     | 503 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 21  | Y     | 601 | CHL  | C1D-C2D | 3.32  | 1.51        | 1.45     |
| 22  | C     | 511 | CLA  | CHC-C1C | 3.32  | 1.43        | 1.35     |
| 22  | B     | 617 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 21  | N     | 607 | CHL  | C1D-C2D | 3.31  | 1.51        | 1.45     |
| 22  | D     | 404 | CLA  | C1D-ND  | 3.31  | 1.41        | 1.37     |
| 21  | y     | 601 | CHL  | C1D-C2D | 3.31  | 1.51        | 1.45     |
| 21  | S     | 302 | CHL  | C1D-C2D | 3.31  | 1.51        | 1.45     |
| 22  | b     | 610 | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 22  | B     | 618 | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 22  | B     | 613 | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 21  | Y     | 608 | CHL  | C1D-C2D | 3.31  | 1.51        | 1.45     |
| 22  | C     | 504 | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 22  | n     | 613 | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 21  | G     | 601 | CHL  | C1D-C2D | 3.31  | 1.51        | 1.45     |
| 22  | B     | 607 | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 21  | r     | 306 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 21  | y     | 609 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 21  | N     | 606 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 22  | c     | 503 | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 21  | n     | 607 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 23  | N     | 615 | LUT  | C11-C10 | 3.30  | 1.53        | 1.43     |
| 21  | y     | 605 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 21  | G     | 609 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 22  | n     | 611 | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 21  | s     | 302 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 23  | R     | 312 | LUT  | C31-C30 | 3.30  | 1.53        | 1.43     |
| 22  | G     | 603 | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 21  | N     | 601 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 21  | y     | 608 | CHL  | C1D-C2D | 3.30  | 1.51        | 1.45     |
| 22  | b     | 611 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 21  | s     | 301 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | N     | 605 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | y     | 607 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 22  | S     | 313 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | g     | 612 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | G     | 612 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | R     | 304 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | S     | 306 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | g     | 606 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | g     | 609 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | S     | 307 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 22  | c     | 502 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | C     | 505 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | s     | 310 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 21  | s     | 306 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 21  | g     | 608 | CHL  | C1D-C2D | 3.29  | 1.51        | 1.45     |
| 22  | c     | 510 | CLA  | CHC-C1C | 3.29  | 1.43        | 1.35     |
| 21  | Y     | 605 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | r     | 307 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 22  | b     | 601 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 22  | A     | 405 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 23  | r     | 313 | LUT  | C7-C6   | 3.28  | 1.56        | 1.45     |
| 21  | s     | 307 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | g     | 605 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | n     | 601 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | S     | 301 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 22  | w     | 101 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 21  | g     | 607 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | y     | 606 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 23  | R     | 312 | LUT  | C7-C6   | 3.28  | 1.56        | 1.45     |
| 22  | d     | 403 | CLA  | C1D-ND  | 3.28  | 1.41        | 1.37     |
| 22  | b     | 609 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 22  | S     | 310 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 21  | R     | 306 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 21  | Y     | 606 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 22  | r     | 305 | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 21  | R     | 307 | CHL  | C1D-C2D | 3.28  | 1.51        | 1.45     |
| 22  | B     | 615 | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 21  | G     | 607 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 21  | R     | 305 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 22  | N     | 604 | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 21  | g     | 601 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 21  | r     | 308 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 22  | C     | 512 | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 21  | G     | 608 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 21  | N     | 608 | CHL  | C1D-C2D | 3.27  | 1.51        | 1.45     |
| 22  | R     | 302 | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 22  | y     | 613 | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 22  | B     | 608 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 509 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 23  | r     | 313 | LUT  | C31-C30 | 3.26  | 1.53        | 1.43     |
| 22  | c     | 508 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 21  | G     | 605 | CHL  | C1D-C2D | 3.26  | 1.51        | 1.45     |
| 22  | b     | 615 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 22  | y     | 603 | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 22  | B     | 614 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 23  | G     | 615 | LUT  | C11-C10 | 3.26  | 1.53        | 1.43     |
| 22  | N     | 613 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 31  | B     | 621 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 22  | c     | 514 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | R     | 310 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 23  | g     | 615 | LUT  | C11-C10 | 3.25  | 1.53        | 1.43     |
| 31  | K     | 101 | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 22  | c     | 504 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | B     | 606 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | B     | 605 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | W     | 101 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | r     | 311 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | b     | 602 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | s     | 313 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | a     | 406 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | B     | 612 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 23  | n     | 614 | LUT  | C11-C10 | 3.24  | 1.53        | 1.43     |
| 22  | b     | 603 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | A     | 409 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 23  | Y     | 613 | LUT  | C11-C10 | 3.24  | 1.53        | 1.43     |
| 31  | B     | 602 | BCR  | C30-C25 | -3.24 | 1.49        | 1.53     |
| 22  | N     | 611 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | n     | 610 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | G     | 614 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | A     | 407 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 23  | Y     | 614 | LUT  | C32-C33 | 3.23  | 1.52        | 1.45     |
| 22  | c     | 511 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 32  | A     | 411 | PL9  | C3-C4   | -3.23 | 1.44        | 1.49     |
| 22  | y     | 611 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 23  | g     | 615 | LUT  | C7-C6   | 3.23  | 1.56        | 1.45     |
| 23  | N     | 614 | LUT  | C11-C10 | 3.23  | 1.53        | 1.43     |
| 22  | Y     | 612 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 22  | y     | 604 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 22  | b     | 606 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 23  | G     | 615 | LUT  | C7-C6   | 3.23  | 1.56        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 507 | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 23  | y     | 614 | LUT  | C11-C10 | 3.22  | 1.53        | 1.43     |
| 22  | b     | 605 | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 22  | B     | 603 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 23  | N     | 614 | LUT  | C7-C6   | 3.21  | 1.56        | 1.45     |
| 22  | g     | 614 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | b     | 612 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | s     | 311 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | S     | 311 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 32  | a     | 410 | PL9  | C3-C4   | -3.21 | 1.44        | 1.49     |
| 22  | C     | 515 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | g     | 604 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | x     | 101 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | c     | 506 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 23  | Y     | 613 | LUT  | C7-C6   | 3.21  | 1.56        | 1.45     |
| 23  | n     | 614 | LUT  | C7-C6   | 3.20  | 1.56        | 1.45     |
| 22  | Y     | 610 | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 22  | r     | 303 | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 31  | k     | 101 | BCR  | C30-C25 | -3.20 | 1.49        | 1.53     |
| 23  | y     | 614 | LUT  | C7-C6   | 3.20  | 1.56        | 1.45     |
| 22  | N     | 612 | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 31  | T     | 102 | BCR  | C30-C25 | -3.19 | 1.49        | 1.53     |
| 22  | b     | 613 | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 22  | g     | 603 | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 31  | H     | 101 | BCR  | C30-C25 | -3.19 | 1.49        | 1.53     |
| 22  | G     | 604 | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 22  | B     | 609 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | n     | 604 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | Y     | 604 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | y     | 612 | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 22  | N     | 610 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 21  | y     | 606 | CHL  | MG-NA   | -3.18 | 1.98        | 2.06     |
| 31  | k     | 102 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 22  | Y     | 602 | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 21  | G     | 605 | CHL  | MG-NA   | -3.17 | 1.98        | 2.06     |
| 22  | n     | 612 | CLA  | C1D-ND  | 3.17  | 1.41        | 1.37     |
| 21  | n     | 606 | CHL  | MG-NA   | -3.17 | 1.98        | 2.06     |
| 22  | c     | 509 | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 21  | r     | 308 | CHL  | MG-NA   | -3.17 | 1.98        | 2.06     |
| 21  | s     | 301 | CHL  | MG-NA   | -3.17 | 1.98        | 2.06     |
| 31  | K     | 102 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 22  | G     | 611 | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | R     | 307 | CHL  | MG-NA   | -3.17 | 1.98        | 2.06     |
| 21  | r     | 301 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 25  | N     | 617 | NEX  | C7-C8   | 3.16  | 1.37        | 1.32     |
| 33  | l     | 103 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 22  | Y     | 611 | CLA  | C1D-ND  | 3.16  | 1.41        | 1.37     |
| 21  | G     | 607 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 22  | g     | 613 | CLA  | C1D-ND  | 3.16  | 1.41        | 1.37     |
| 33  | D     | 402 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 21  | n     | 605 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 21  | g     | 605 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 21  | r     | 306 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 33  | L     | 101 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 22  | C     | 510 | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 22  | r     | 309 | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 21  | N     | 605 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 21  | y     | 608 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 21  | G     | 609 | CHL  | MG-NA   | -3.16 | 1.98        | 2.06     |
| 21  | S     | 306 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 22  | B     | 611 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 21  | g     | 608 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 22  | c     | 505 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 21  | N     | 608 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 21  | r     | 307 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 21  | s     | 302 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 21  | N     | 601 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 21  | S     | 302 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 22  | b     | 608 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 22  | n     | 603 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 21  | G     | 606 | CHL  | MG-NA   | -3.15 | 1.98        | 2.06     |
| 23  | G     | 615 | LUT  | C32-C33 | 3.15  | 1.52        | 1.45     |
| 22  | B     | 616 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 22  | N     | 602 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 33  | d     | 402 | SQD  | O48-C23 | 3.14  | 1.42        | 1.33     |
| 21  | y     | 607 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | g     | 607 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 22  | g     | 611 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 21  | Y     | 605 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | g     | 601 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | G     | 601 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | S     | 301 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | Y     | 606 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | Y     | 607 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | n     | 601 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 21  | n     | 607 | CHL  | MG-NA   | -3.14 | 1.98        | 2.06     |
| 31  | B     | 621 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 22  | Y     | 603 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 22  | S     | 304 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 21  | n     | 608 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | Y     | 601 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 22  | R     | 309 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 21  | s     | 306 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | R     | 306 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | R     | 305 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | S     | 307 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | y     | 605 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 21  | s     | 307 | CHL  | MG-NA   | -3.13 | 1.98        | 2.06     |
| 22  | y     | 603 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 22  | y     | 602 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | s     | 312 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | R     | 303 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | D     | 405 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | n     | 602 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | G     | 603 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 21  | y     | 609 | CHL  | MG-NA   | -3.12 | 1.98        | 2.06     |
| 21  | G     | 608 | CHL  | MG-NA   | -3.12 | 1.98        | 2.06     |
| 21  | g     | 609 | CHL  | MG-NA   | -3.12 | 1.98        | 2.06     |
| 21  | Y     | 608 | CHL  | MG-NA   | -3.12 | 1.98        | 2.06     |
| 23  | Y     | 613 | LUT  | C32-C33 | 3.12  | 1.52        | 1.45     |
| 22  | G     | 602 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 21  | g     | 606 | CHL  | MG-NA   | -3.12 | 1.98        | 2.06     |
| 22  | R     | 308 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 22  | a     | 408 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 21  | N     | 607 | CHL  | MG-NA   | -3.11 | 1.98        | 2.06     |
| 22  | g     | 602 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 21  | y     | 601 | CHL  | MG-NA   | -3.11 | 1.98        | 2.06     |
| 22  | C     | 506 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 31  | h     | 101 | BCR  | C30-C25 | -3.11 | 1.49        | 1.53     |
| 23  | N     | 614 | LUT  | C32-C33 | 3.11  | 1.52        | 1.45     |
| 22  | S     | 312 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 22  | s     | 304 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 23  | y     | 614 | LUT  | C32-C33 | 3.11  | 1.52        | 1.45     |
| 31  | b     | 618 | BCR  | C30-C25 | -3.11 | 1.49        | 1.53     |
| 22  | G     | 613 | CLA  | C1D-ND  | 3.11  | 1.41        | 1.37     |
| 21  | N     | 606 | CHL  | MG-NA   | -3.10 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | r     | 304 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 23  | g     | 615 | LUT  | C32-C33 | 3.10  | 1.52        | 1.45     |
| 22  | S     | 311 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 22  | C     | 508 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 22  | S     | 309 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 22  | r     | 303 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 22  | s     | 311 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 22  | r     | 310 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 23  | n     | 614 | LUT  | C32-C33 | 3.09  | 1.52        | 1.45     |
| 22  | G     | 602 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 22  | N     | 609 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 22  | c     | 507 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 22  | g     | 614 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 22  | Y     | 602 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 22  | b     | 601 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 22  | d     | 404 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | s     | 309 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 22  | N     | 603 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | y     | 610 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | S     | 305 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 22  | n     | 602 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 22  | s     | 310 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 22  | S     | 303 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 22  | R     | 302 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 22  | A     | 407 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 22  | y     | 602 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 33  | L     | 102 | SQD  | O48-C23 | 3.06  | 1.42        | 1.33     |
| 22  | Y     | 612 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 22  | G     | 610 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 22  | n     | 613 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 22  | S     | 309 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 33  | l     | 101 | SQD  | O48-C23 | 3.06  | 1.42        | 1.33     |
| 22  | s     | 304 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 33  | a     | 411 | SQD  | O48-C23 | 3.06  | 1.42        | 1.33     |
| 22  | N     | 602 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 33  | A     | 412 | SQD  | O48-C23 | 3.06  | 1.42        | 1.33     |
| 22  | y     | 613 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 22  | s     | 303 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | g     | 602 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | b     | 607 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | B     | 605 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | g     | 610 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | N     | 613 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | B     | 617 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 22  | B     | 604 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | s     | 309 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | R     | 308 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | S     | 310 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | a     | 406 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | r     | 309 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | S     | 304 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | S     | 303 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | y     | 610 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | d     | 403 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 22  | b     | 609 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 22  | g     | 603 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 22  | G     | 614 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 22  | g     | 610 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | b     | 614 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | r     | 312 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 22  | n     | 603 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | G     | 610 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | N     | 609 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | Y     | 609 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 22  | b     | 602 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | c     | 512 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | B     | 611 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | n     | 609 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 22  | R     | 303 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 22  | D     | 404 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | B     | 614 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | C     | 508 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | b     | 613 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | C     | 513 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | Y     | 609 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | c     | 511 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | b     | 608 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | s     | 305 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 22  | y     | 603 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | N     | 610 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | d     | 404 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | c     | 503 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 22  | s     | 303 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 22  | C     | 515 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | Y     | 603 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | S     | 313 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | n     | 609 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | B     | 610 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | C     | 512 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | C     | 504 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | B     | 607 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | Y     | 610 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | b     | 610 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | c     | 502 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 30  | a     | 407 | PHO  | CAC-C3C | -3.00 | 1.46        | 1.52     |
| 22  | C     | 503 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | r     | 311 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 22  | R     | 311 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 22  | n     | 610 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | N     | 603 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | R     | 310 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | B     | 612 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | g     | 611 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 30  | A     | 408 | PHO  | CAC-C3C | -2.99 | 1.46        | 1.52     |
| 22  | b     | 604 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | G     | 603 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | c     | 507 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | c     | 504 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | c     | 513 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | w     | 101 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | b     | 611 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | G     | 611 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | c     | 514 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 22  | g     | 612 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 25  | n     | 616 | NEX  | C7-C8   | 2.98  | 1.36        | 1.32     |
| 22  | G     | 612 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | B     | 618 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | r     | 304 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | s     | 313 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | n     | 611 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | b     | 615 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | N     | 611 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | B     | 616 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 25  | y     | 616 | NEX  | C7-C8   | 2.98  | 1.36        | 1.32     |
| 22  | C     | 507 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 22  | s     | 308 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 608 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | B     | 615 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | b     | 603 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | c     | 509 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | b     | 605 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | y     | 611 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | B     | 603 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | W     | 101 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | D     | 405 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | b     | 612 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | C     | 514 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 22  | A     | 405 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 22  | C     | 510 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 22  | B     | 606 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 22  | B     | 613 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 22  | x     | 101 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 22  | r     | 310 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 22  | r     | 312 | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 22  | a     | 404 | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 23  | r     | 313 | LUT  | C32-C33 | 2.94  | 1.52        | 1.45     |
| 22  | s     | 305 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 22  | c     | 506 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 22  | a     | 405 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 22  | A     | 409 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 22  | S     | 305 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 25  | Y     | 616 | NEX  | C7-C8   | 2.94  | 1.36        | 1.32     |
| 22  | C     | 505 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 22  | c     | 508 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 22  | A     | 406 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 22  | S     | 308 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 22  | R     | 311 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 22  | R     | 309 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 22  | b     | 606 | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 32  | d     | 406 | PL9  | C6-C1   | -2.92 | 1.43        | 1.48     |
| 22  | a     | 408 | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 22  | C     | 509 | CLA  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 22  | B     | 609 | CLA  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 23  | R     | 312 | LUT  | C32-C33 | 2.90  | 1.52        | 1.45     |
| 22  | C     | 506 | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 32  | D     | 407 | PL9  | C6-C1   | -2.89 | 1.43        | 1.48     |
| 22  | C     | 510 | CLA  | CMB-C2B | -2.89 | 1.45        | 1.51     |
| 22  | c     | 505 | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | S     | 312 | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 22  | s     | 312 | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 33  | l     | 103 | SQD  | O47-C7  | 2.87  | 1.42        | 1.34     |
| 22  | r     | 305 | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 33  | L     | 101 | SQD  | O47-C7  | 2.86  | 1.42        | 1.34     |
| 33  | D     | 402 | SQD  | O47-C7  | 2.85  | 1.42        | 1.34     |
| 30  | d     | 401 | PHO  | CAC-C3C | -2.85 | 1.47        | 1.52     |
| 33  | A     | 412 | SQD  | O47-C7  | 2.85  | 1.42        | 1.34     |
| 22  | R     | 304 | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 33  | d     | 402 | SQD  | O47-C7  | 2.84  | 1.42        | 1.34     |
| 22  | c     | 509 | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 24  | n     | 615 | XAT  | C2-C1   | -2.82 | 1.50        | 1.54     |
| 33  | a     | 411 | SQD  | O47-C7  | 2.82  | 1.42        | 1.34     |
| 25  | g     | 618 | NEX  | C7-C8   | 2.81  | 1.36        | 1.32     |
| 22  | n     | 604 | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 24  | G     | 617 | XAT  | C2-C1   | -2.81 | 1.50        | 1.54     |
| 22  | g     | 604 | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 22  | G     | 604 | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 30  | D     | 401 | PHO  | CAC-C3C | -2.80 | 1.47        | 1.52     |
| 37  | F     | 101 | HEM  | CAB-C3B | 2.80  | 1.55        | 1.47     |
| 22  | y     | 604 | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 24  | g     | 617 | XAT  | C2-C1   | -2.80 | 1.50        | 1.54     |
| 35  | J     | 101 | DGD  | O2G-C2G | -2.79 | 1.39        | 1.46     |
| 22  | G     | 613 | CLA  | C3B-C2B | -2.79 | 1.36        | 1.40     |
| 22  | N     | 612 | CLA  | C3B-C2B | -2.78 | 1.36        | 1.40     |
| 22  | N     | 604 | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 22  | Y     | 604 | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 22  | g     | 613 | CLA  | C3B-C2B | -2.78 | 1.36        | 1.40     |
| 35  | c     | 519 | DGD  | O2G-C2G | -2.78 | 1.39        | 1.46     |
| 22  | y     | 612 | CLA  | C3B-C2B | -2.78 | 1.36        | 1.40     |
| 22  | n     | 612 | CLA  | C3B-C2B | -2.76 | 1.36        | 1.40     |
| 22  | Y     | 611 | CLA  | C3B-C2B | -2.76 | 1.36        | 1.40     |
| 37  | f     | 101 | HEM  | CAB-C3B | 2.76  | 1.54        | 1.47     |
| 33  | l     | 101 | SQD  | O47-C7  | 2.75  | 1.42        | 1.34     |
| 23  | N     | 615 | LUT  | C8-C7   | 2.73  | 1.41        | 1.33     |
| 33  | L     | 102 | SQD  | O47-C7  | 2.73  | 1.42        | 1.34     |
| 22  | R     | 304 | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 24  | y     | 615 | XAT  | C2-C1   | -2.73 | 1.50        | 1.54     |
| 21  | g     | 608 | CHL  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 24  | r     | 314 | XAT  | C2-C1   | -2.72 | 1.50        | 1.54     |
| 21  | g     | 606 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 21  | Y     | 608 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | G     | 607 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 21  | g     | 601 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 22  | r     | 305 | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 35  | C     | 518 | DGD  | O2G-C2G | -2.70 | 1.39        | 1.46     |
| 35  | c     | 517 | DGD  | O2G-C2G | -2.70 | 1.39        | 1.46     |
| 21  | Y     | 601 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | n     | 607 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | S     | 306 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 24  | Y     | 615 | XAT  | C2-C1   | -2.70 | 1.50        | 1.54     |
| 21  | g     | 609 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | G     | 605 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | s     | 306 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | R     | 307 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | y     | 607 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | S     | 302 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | r     | 301 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | r     | 307 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 21  | n     | 608 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | y     | 601 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | G     | 601 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | n     | 606 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | N     | 605 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | N     | 606 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | s     | 302 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | y     | 605 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | n     | 605 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | y     | 606 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | S     | 301 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | n     | 601 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | y     | 609 | CHL  | C4C-C3C | 2.69  | 1.49        | 1.45     |
| 21  | N     | 608 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | Y     | 605 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | s     | 307 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | N     | 601 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | s     | 301 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | g     | 605 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | G     | 606 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | Y     | 606 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 21  | r     | 307 | CHL  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 21  | S     | 306 | CHL  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 21  | y     | 605 | CHL  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 21  | G     | 608 | CHL  | C4B-CHC | 2.68  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | R     | 306 | CHL  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 26  | Y     | 617 | LHG  | O7-C5   | -2.68 | 1.39        | 1.46     |
| 21  | R     | 305 | CHL  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 21  | g     | 607 | CHL  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 21  | r     | 308 | CHL  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 21  | G     | 609 | CHL  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 21  | R     | 305 | CHL  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 21  | Y     | 607 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 22  | y     | 604 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 21  | G     | 601 | CHL  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 21  | r     | 308 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 21  | s     | 302 | CHL  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 21  | N     | 607 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 22  | N     | 604 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 21  | y     | 608 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 21  | y     | 609 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 21  | r     | 306 | CHL  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 21  | S     | 302 | CHL  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 21  | S     | 301 | CHL  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 21  | R     | 307 | CHL  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 32  | D     | 407 | PL9  | C53-C6  | -2.66 | 1.45        | 1.50     |
| 22  | g     | 604 | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 21  | g     | 609 | CHL  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 21  | N     | 606 | CHL  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 21  | G     | 608 | CHL  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 22  | Y     | 604 | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 21  | S     | 307 | CHL  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 22  | n     | 604 | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 21  | N     | 608 | CHL  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 21  | n     | 601 | CHL  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 21  | g     | 601 | CHL  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 21  | y     | 608 | CHL  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 21  | Y     | 605 | CHL  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 21  | s     | 307 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 24  | N     | 616 | XAT  | C2-C1   | -2.64 | 1.50        | 1.54     |
| 21  | n     | 607 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 21  | Y     | 601 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 22  | G     | 604 | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 21  | g     | 606 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 21  | y     | 606 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 32  | d     | 406 | PL9  | C53-C6  | -2.64 | 1.45        | 1.50     |
| 21  | Y     | 607 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | R     | 313 | XAT  | C2-C1   | -2.64 | 1.50        | 1.54     |
| 21  | s     | 306 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 21  | g     | 605 | CHL  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 22  | C     | 503 | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 21  | N     | 601 | CHL  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 21  | r     | 301 | CHL  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 35  | c     | 518 | DGD  | O2G-C2G | -2.63 | 1.40        | 1.46     |
| 21  | Y     | 608 | CHL  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 21  | N     | 607 | CHL  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 21  | n     | 605 | CHL  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 21  | G     | 605 | CHL  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 22  | A     | 407 | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 21  | G     | 606 | CHL  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 22  | b     | 610 | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 21  | R     | 306 | CHL  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 21  | s     | 301 | CHL  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 21  | r     | 306 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 21  | n     | 608 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 21  | N     | 605 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 21  | y     | 601 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 21  | Y     | 606 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 22  | a     | 406 | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 22  | A     | 405 | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 21  | g     | 608 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 22  | c     | 502 | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 21  | G     | 609 | CHL  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 21  | n     | 606 | CHL  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 21  | S     | 301 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 21  | g     | 607 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 21  | G     | 607 | CHL  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 21  | g     | 607 | CHL  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 25  | r     | 315 | NEX  | C38-C25 | 2.60  | 1.55        | 1.51     |
| 22  | c     | 511 | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 21  | g     | 601 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 35  | C     | 519 | DGD  | O2G-C2G | -2.60 | 1.40        | 1.46     |
| 21  | G     | 606 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 21  | N     | 607 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 22  | c     | 508 | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 21  | n     | 608 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 21  | n     | 607 | CHL  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 22  | B     | 613 | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 21  | r     | 301 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | s     | 307 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | y     | 607 | CHL  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 21  | s     | 302 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 22  | C     | 509 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 22  | a     | 404 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 22  | C     | 512 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 21  | G     | 605 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | y     | 601 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | G     | 609 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | R     | 307 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | y     | 605 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | N     | 606 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | S     | 306 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 21  | g     | 608 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | y     | 607 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | G     | 607 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 22  | B     | 614 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 22  | B     | 618 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 21  | Y     | 605 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | n     | 601 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | R     | 305 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | N     | 601 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | r     | 306 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 22  | n     | 603 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 22  | b     | 611 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 22  | g     | 603 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 23  | G     | 616 | LUT  | C8-C7   | 2.58  | 1.40        | 1.33     |
| 22  | C     | 511 | CLA  | C3C-C2C | 2.58  | 1.42        | 1.36     |
| 21  | y     | 606 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | y     | 609 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | G     | 608 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 22  | D     | 405 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 21  | s     | 301 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | Y     | 601 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | g     | 606 | CHL  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 21  | S     | 307 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 22  | b     | 613 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 21  | r     | 308 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | S     | 302 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 22  | y     | 603 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 21  | R     | 306 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | Y     | 606 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | s     | 306 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | G     | 601 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 22  | B     | 615 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 21  | y     | 608 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | r     | 307 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | g     | 609 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 21  | Y     | 608 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 22  | d     | 404 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 22  | R     | 303 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 23  | Y     | 614 | LUT  | C8-C7   | 2.57  | 1.40        | 1.33     |
| 35  | h     | 102 | DGD  | O2G-C2G | -2.57 | 1.40        | 1.46     |
| 21  | S     | 307 | CHL  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 22  | Y     | 603 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 22  | G     | 603 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 21  | N     | 605 | CHL  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 22  | b     | 605 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 22  | d     | 403 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 21  | g     | 605 | CHL  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 22  | c     | 510 | CLA  | C3C-C2C | 2.56  | 1.42        | 1.36     |
| 21  | Y     | 607 | CHL  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 21  | n     | 605 | CHL  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 22  | B     | 616 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 35  | c     | 517 | DGD  | O1G-C1G | -2.56 | 1.39        | 1.45     |
| 22  | r     | 304 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 22  | b     | 612 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 22  | B     | 608 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 21  | N     | 608 | CHL  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 26  | y     | 617 | LHG  | O7-C5   | -2.55 | 1.40        | 1.46     |
| 22  | b     | 615 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 22  | N     | 603 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 22  | a     | 405 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 35  | c     | 519 | DGD  | O1G-C1G | -2.55 | 1.39        | 1.45     |
| 23  | g     | 616 | LUT  | C8-C7   | 2.55  | 1.40        | 1.33     |
| 22  | A     | 406 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 21  | n     | 606 | CHL  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 35  | J     | 101 | DGD  | O1G-C1G | -2.54 | 1.39        | 1.45     |
| 35  | H     | 102 | DGD  | O2G-C2G | -2.54 | 1.40        | 1.46     |
| 22  | a     | 408 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | D     | 404 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 25  | y     | 618 | NEX  | C38-C25 | 2.54  | 1.55        | 1.51     |
| 22  | B     | 603 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | b     | 604 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 409 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | c     | 506 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | c     | 513 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | S     | 303 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 22  | S     | 312 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 36  | b     | 620 | LMG  | C21-C20 | 2.53  | 1.65        | 1.51     |
| 26  | d     | 408 | LHG  | O7-C5   | -2.53 | 1.40        | 1.46     |
| 22  | S     | 313 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 26  | n     | 617 | LHG  | O7-C5   | -2.53 | 1.40        | 1.46     |
| 35  | C     | 518 | DGD  | O1G-C1G | -2.53 | 1.39        | 1.45     |
| 22  | B     | 607 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 22  | C     | 511 | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 26  | D     | 409 | LHG  | O7-C5   | -2.52 | 1.40        | 1.46     |
| 36  | B     | 623 | LMG  | C21-C20 | 2.52  | 1.65        | 1.51     |
| 22  | B     | 617 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 25  | Y     | 616 | NEX  | C38-C25 | 2.52  | 1.55        | 1.51     |
| 22  | s     | 309 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | C     | 514 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | B     | 605 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | g     | 610 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | n     | 611 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | x     | 101 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | r     | 309 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | B     | 606 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | s     | 313 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | Y     | 609 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | Y     | 612 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | B     | 604 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | Y     | 602 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | R     | 308 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 23  | r     | 313 | LUT  | C4-C5   | 2.51  | 1.55        | 1.51     |
| 22  | B     | 612 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | c     | 505 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | S     | 305 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | b     | 602 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | s     | 303 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | y     | 610 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | G     | 610 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | b     | 603 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | N     | 609 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | W     | 101 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | c     | 510 | CLA  | CMD-C2D | -2.50 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | G     | 612 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | g     | 602 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | C     | 507 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | n     | 609 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | N     | 611 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | C     | 504 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | N     | 613 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | G     | 602 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | b     | 601 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | r     | 310 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 26  | l     | 102 | LHG  | O7-C5   | -2.50 | 1.40        | 1.46     |
| 26  | G     | 618 | LHG  | O7-C5   | -2.49 | 1.40        | 1.46     |
| 22  | B     | 611 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | C     | 515 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 35  | h     | 102 | DGD  | O5D-C6D | -2.49 | 1.39        | 1.43     |
| 22  | N     | 602 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 36  | w     | 102 | LMG  | O7-C8   | -2.49 | 1.40        | 1.46     |
| 22  | c     | 514 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | b     | 614 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | n     | 602 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | b     | 606 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | b     | 607 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | S     | 309 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 35  | c     | 518 | DGD  | O1G-C1G | -2.48 | 1.39        | 1.45     |
| 22  | r     | 303 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | G     | 611 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | s     | 304 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 37  | f     | 101 | HEM  | CHA-C4D | 2.48  | 1.41        | 1.35     |
| 22  | w     | 101 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 36  | C     | 502 | LMG  | O7-C8   | -2.48 | 1.40        | 1.46     |
| 23  | R     | 312 | LUT  | C4-C5   | 2.48  | 1.54        | 1.51     |
| 22  | n     | 610 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | C     | 506 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | b     | 609 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | g     | 611 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | y     | 602 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | Y     | 610 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | s     | 305 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | S     | 311 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 26  | L     | 103 | LHG  | O7-C5   | -2.47 | 1.40        | 1.46     |
| 22  | R     | 309 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 37  | F     | 101 | HEM  | CHA-C4D | 2.47  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | g     | 612 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | y     | 613 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 35  | H     | 102 | DGD  | O1G-C1G | -2.47 | 1.39        | 1.45     |
| 22  | n     | 613 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | s     | 312 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | c     | 507 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | s     | 311 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 35  | C     | 519 | DGD  | O1G-C1G | -2.46 | 1.39        | 1.45     |
| 22  | R     | 311 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | y     | 611 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 35  | H     | 102 | DGD  | O5D-C6D | -2.46 | 1.39        | 1.43     |
| 22  | G     | 614 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | R     | 302 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | N     | 610 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | c     | 503 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | b     | 608 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | B     | 609 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | S     | 304 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 26  | d     | 409 | LHG  | O7-C5   | -2.45 | 1.40        | 1.46     |
| 22  | g     | 614 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | B     | 610 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 26  | C     | 520 | LHG  | C6-C5   | 2.45  | 1.58        | 1.50     |
| 23  | g     | 616 | LUT  | C23-C24 | 2.44  | 1.53        | 1.50     |
| 22  | C     | 505 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | C     | 513 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | S     | 308 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 26  | D     | 410 | LHG  | O7-C5   | -2.44 | 1.40        | 1.46     |
| 22  | C     | 508 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | G     | 613 | CLA  | C3D-C4D | 2.44  | 1.49        | 1.44     |
| 22  | r     | 312 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | g     | 613 | CLA  | C3D-C4D | 2.44  | 1.49        | 1.44     |
| 22  | s     | 308 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | y     | 612 | CLA  | C3D-C4D | 2.43  | 1.49        | 1.44     |
| 35  | h     | 102 | DGD  | O1G-C1G | -2.43 | 1.39        | 1.45     |
| 22  | c     | 504 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 26  | D     | 408 | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 22  | c     | 510 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 26  | c     | 520 | LHG  | C6-C5   | 2.43  | 1.58        | 1.50     |
| 22  | s     | 310 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 26  | d     | 407 | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 23  | n     | 614 | LUT  | C8-C7   | 2.42  | 1.40        | 1.33     |
| 22  | Y     | 611 | CLA  | C3D-C4D | 2.42  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | N     | 612 | CLA  | C3D-C4D | 2.42  | 1.49        | 1.44     |
| 23  | y     | 614 | LUT  | C8-C7   | 2.42  | 1.40        | 1.33     |
| 22  | n     | 612 | CLA  | C3D-C4D | 2.42  | 1.49        | 1.44     |
| 23  | N     | 615 | LUT  | C23-C24 | 2.41  | 1.53        | 1.50     |
| 22  | c     | 512 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 22  | C     | 511 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 22  | S     | 310 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 22  | g     | 613 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 23  | N     | 614 | LUT  | C8-C7   | 2.40  | 1.40        | 1.33     |
| 23  | Y     | 613 | LUT  | C8-C7   | 2.39  | 1.40        | 1.33     |
| 23  | g     | 615 | LUT  | C8-C7   | 2.39  | 1.40        | 1.33     |
| 26  | c     | 521 | LHG  | O7-C5   | -2.39 | 1.40        | 1.46     |
| 23  | G     | 615 | LUT  | C8-C7   | 2.38  | 1.40        | 1.33     |
| 23  | N     | 614 | LUT  | C4-C5   | 2.38  | 1.54        | 1.51     |
| 22  | Y     | 611 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 22  | N     | 612 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 23  | g     | 615 | LUT  | C4-C5   | 2.37  | 1.54        | 1.51     |
| 22  | G     | 613 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 26  | C     | 521 | LHG  | O7-C5   | -2.36 | 1.40        | 1.46     |
| 26  | C     | 520 | LHG  | O8-C23  | 2.35  | 1.40        | 1.33     |
| 35  | a     | 413 | DGD  | O2G-C2G | -2.35 | 1.40        | 1.46     |
| 22  | n     | 612 | CLA  | CMB-C2B | -2.35 | 1.46        | 1.51     |
| 26  | c     | 520 | LHG  | O8-C23  | 2.34  | 1.40        | 1.33     |
| 22  | y     | 612 | CLA  | CMB-C2B | -2.34 | 1.46        | 1.51     |
| 35  | A     | 401 | DGD  | O2G-C2G | -2.34 | 1.40        | 1.46     |
| 22  | N     | 612 | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 22  | G     | 613 | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 26  | c     | 520 | LHG  | O8-C6   | 2.34  | 1.50        | 1.45     |
| 21  | n     | 605 | CHL  | C1D-ND  | -2.33 | 1.34        | 1.37     |
| 22  | y     | 612 | CLA  | CMC-C2C | -2.33 | 1.45        | 1.50     |
| 25  | y     | 616 | NEX  | C38-C25 | 2.33  | 1.55        | 1.51     |
| 22  | g     | 613 | CLA  | CMC-C2C | -2.32 | 1.45        | 1.50     |
| 23  | n     | 614 | LUT  | C4-C5   | 2.32  | 1.54        | 1.51     |
| 21  | g     | 607 | CHL  | C1D-ND  | -2.32 | 1.34        | 1.37     |
| 26  | C     | 520 | LHG  | O8-C6   | 2.32  | 1.50        | 1.45     |
| 23  | Y     | 613 | LUT  | C4-C5   | 2.32  | 1.54        | 1.51     |
| 21  | r     | 307 | CHL  | C1D-ND  | -2.32 | 1.34        | 1.37     |
| 22  | n     | 612 | CLA  | CMC-C2C | -2.31 | 1.45        | 1.50     |
| 24  | R     | 313 | XAT  | C8-C7   | 2.31  | 1.37        | 1.32     |
| 24  | G     | 617 | XAT  | C18-C5  | 2.31  | 1.55        | 1.51     |
| 23  | Y     | 614 | LUT  | C23-C24 | 2.31  | 1.53        | 1.50     |
| 21  | y     | 606 | CHL  | C1D-ND  | -2.31 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | y     | 614 | LUT  | C4-C5   | 2.31  | 1.54        | 1.51     |
| 21  | s     | 306 | CHL  | C1D-ND  | -2.31 | 1.34        | 1.37     |
| 21  | G     | 606 | CHL  | C1D-ND  | -2.31 | 1.34        | 1.37     |
| 21  | r     | 306 | CHL  | C1D-ND  | -2.30 | 1.35        | 1.37     |
| 23  | G     | 615 | LUT  | C4-C5   | 2.30  | 1.54        | 1.51     |
| 21  | s     | 301 | CHL  | C1D-ND  | -2.30 | 1.35        | 1.37     |
| 22  | Y     | 611 | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 23  | G     | 616 | LUT  | C23-C24 | 2.29  | 1.53        | 1.50     |
| 22  | c     | 509 | CLA  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 21  | N     | 606 | CHL  | C1D-ND  | -2.29 | 1.35        | 1.37     |
| 21  | Y     | 601 | CHL  | C1D-ND  | -2.29 | 1.35        | 1.37     |
| 24  | g     | 617 | XAT  | C18-C5  | 2.28  | 1.55        | 1.51     |
| 22  | g     | 604 | CLA  | C3B-CAB | -2.28 | 1.43        | 1.47     |
| 24  | G     | 617 | XAT  | O24-C25 | 2.28  | 1.49        | 1.46     |
| 21  | N     | 605 | CHL  | C1D-ND  | -2.28 | 1.35        | 1.37     |
| 22  | g     | 613 | CLA  | C2A-C1A | 2.28  | 1.57        | 1.52     |
| 21  | S     | 307 | CHL  | C1D-ND  | -2.28 | 1.35        | 1.37     |
| 21  | Y     | 605 | CHL  | C1D-ND  | -2.27 | 1.35        | 1.37     |
| 21  | S     | 302 | CHL  | C1D-ND  | -2.27 | 1.35        | 1.37     |
| 21  | G     | 605 | CHL  | C1D-ND  | -2.27 | 1.35        | 1.37     |
| 22  | N     | 604 | CLA  | C3B-CAB | -2.27 | 1.43        | 1.47     |
| 24  | n     | 615 | XAT  | O24-C25 | 2.27  | 1.49        | 1.46     |
| 21  | N     | 601 | CHL  | C1D-ND  | -2.27 | 1.35        | 1.37     |
| 21  | g     | 609 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 24  | r     | 314 | XAT  | C8-C7   | 2.26  | 1.37        | 1.32     |
| 21  | R     | 307 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 30  | a     | 407 | PHO  | CMC-C2C | -2.26 | 1.46        | 1.51     |
| 21  | g     | 606 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 21  | y     | 607 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 30  | A     | 408 | PHO  | CMC-C2C | -2.26 | 1.46        | 1.51     |
| 21  | G     | 608 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 21  | s     | 307 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 21  | R     | 305 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 22  | C     | 510 | CLA  | C3B-C2B | -2.26 | 1.37        | 1.40     |
| 24  | y     | 615 | XAT  | C18-C5  | 2.26  | 1.55        | 1.51     |
| 21  | s     | 302 | CHL  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 22  | G     | 604 | CLA  | C3B-CAB | -2.25 | 1.43        | 1.47     |
| 22  | g     | 603 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 21  | g     | 601 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 21  | r     | 308 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 21  | n     | 608 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 22  | D     | 404 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | g     | 617 | XAT  | O24-C25 | 2.25  | 1.49        | 1.46     |
| 21  | n     | 606 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 22  | y     | 612 | CLA  | C2A-C1A | 2.25  | 1.57        | 1.52     |
| 22  | s     | 304 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 35  | A     | 401 | DGD  | O1G-C1G | -2.25 | 1.40        | 1.45     |
| 24  | G     | 617 | XAT  | C38-C25 | 2.25  | 1.55        | 1.51     |
| 21  | g     | 605 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 21  | R     | 306 | CHL  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 26  | s     | 314 | LHG  | O7-C5   | -2.25 | 1.41        | 1.46     |
| 22  | R     | 310 | CLA  | CMB-C2B | -2.25 | 1.47        | 1.51     |
| 21  | g     | 608 | CHL  | C1D-ND  | -2.24 | 1.35        | 1.37     |
| 21  | n     | 607 | CHL  | C1D-ND  | -2.24 | 1.35        | 1.37     |
| 21  | y     | 601 | CHL  | C1D-ND  | -2.24 | 1.35        | 1.37     |
| 21  | r     | 301 | CHL  | C1D-ND  | -2.24 | 1.35        | 1.37     |
| 22  | n     | 612 | CLA  | C2A-C1A | 2.24  | 1.57        | 1.52     |
| 22  | n     | 604 | CLA  | C3B-CAB | -2.24 | 1.43        | 1.47     |
| 26  | R     | 301 | LHG  | O7-C5   | -2.24 | 1.41        | 1.46     |
| 22  | r     | 311 | CLA  | CMB-C2B | -2.24 | 1.47        | 1.51     |
| 30  | A     | 408 | PHO  | C3B-C2B | -2.24 | 1.37        | 1.40     |
| 26  | S     | 314 | LHG  | O7-C5   | -2.23 | 1.41        | 1.46     |
| 22  | N     | 612 | CLA  | C2A-C1A | 2.23  | 1.57        | 1.52     |
| 26  | r     | 302 | LHG  | O7-C5   | -2.23 | 1.41        | 1.46     |
| 22  | y     | 604 | CLA  | C3B-CAB | -2.23 | 1.43        | 1.47     |
| 21  | G     | 601 | CHL  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 21  | Y     | 606 | CHL  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 22  | B     | 613 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 33  | d     | 402 | SQD  | O2-C2   | -2.23 | 1.37        | 1.43     |
| 24  | g     | 617 | XAT  | C38-C25 | 2.23  | 1.55        | 1.51     |
| 22  | C     | 507 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 22  | R     | 303 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 21  | N     | 608 | CHL  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 22  | G     | 603 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 21  | S     | 301 | CHL  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 22  | B     | 611 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 22  | C     | 503 | CLA  | C3B-C2B | -2.23 | 1.37        | 1.40     |
| 35  | a     | 413 | DGD  | O1G-C1G | -2.23 | 1.40        | 1.45     |
| 30  | a     | 407 | PHO  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 30  | D     | 401 | PHO  | CMC-C2C | -2.22 | 1.46        | 1.51     |
| 30  | d     | 401 | PHO  | CMC-C2C | -2.22 | 1.46        | 1.51     |
| 23  | G     | 616 | LUT  | C4-C5   | 2.22  | 1.54        | 1.51     |
| 22  | c     | 506 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 22  | Y     | 604 | CLA  | C3B-CAB | -2.22 | 1.43        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | n     | 603 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 21  | y     | 609 | CHL  | C1D-ND  | -2.22 | 1.35        | 1.37     |
| 21  | n     | 601 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 22  | Y     | 611 | CLA  | C2A-C1A | 2.21  | 1.57        | 1.52     |
| 24  | n     | 615 | XAT  | C18-C5  | 2.21  | 1.55        | 1.51     |
| 22  | y     | 603 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 22  | d     | 403 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 21  | Y     | 608 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 24  | n     | 615 | XAT  | C8-C7   | 2.21  | 1.37        | 1.32     |
| 22  | B     | 608 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 21  | G     | 609 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 21  | S     | 306 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 22  | N     | 612 | CLA  | C4D-CHA | 2.21  | 1.46        | 1.38     |
| 21  | N     | 607 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 22  | N     | 603 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 22  | A     | 409 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 24  | Y     | 615 | XAT  | C8-C7   | 2.21  | 1.37        | 1.32     |
| 22  | G     | 613 | CLA  | C2A-C1A | 2.20  | 1.57        | 1.52     |
| 24  | N     | 616 | XAT  | C28-C27 | 2.20  | 1.37        | 1.32     |
| 23  | R     | 312 | LUT  | C23-C24 | 2.20  | 1.53        | 1.50     |
| 23  | R     | 312 | LUT  | C8-C7   | 2.20  | 1.39        | 1.33     |
| 24  | Y     | 615 | XAT  | C18-C5  | 2.20  | 1.55        | 1.51     |
| 33  | L     | 102 | SQD  | O2-C2   | -2.20 | 1.37        | 1.43     |
| 22  | Y     | 611 | CLA  | C4D-CHA | 2.20  | 1.46        | 1.38     |
| 24  | y     | 615 | XAT  | C38-C25 | 2.20  | 1.55        | 1.51     |
| 22  | Y     | 603 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 22  | S     | 304 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 26  | c     | 522 | LHG  | O7-C5   | -2.20 | 1.41        | 1.46     |
| 33  | D     | 402 | SQD  | O2-C2   | -2.20 | 1.37        | 1.43     |
| 22  | c     | 502 | CLA  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 22  | s     | 312 | CLA  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 21  | y     | 605 | CHL  | C1D-ND  | -2.20 | 1.35        | 1.37     |
| 21  | y     | 608 | CHL  | C1D-ND  | -2.20 | 1.35        | 1.37     |
| 26  | C     | 522 | LHG  | O7-C5   | -2.19 | 1.41        | 1.46     |
| 24  | N     | 616 | XAT  | C38-C25 | 2.19  | 1.55        | 1.51     |
| 23  | N     | 615 | LUT  | C28-C27 | 2.19  | 1.37        | 1.32     |
| 22  | n     | 604 | CLA  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 30  | A     | 408 | PHO  | CMD-C2D | -2.19 | 1.46        | 1.51     |
| 22  | B     | 604 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 23  | r     | 313 | LUT  | C8-C7   | 2.19  | 1.39        | 1.33     |
| 22  | G     | 613 | CLA  | C4D-CHA | 2.19  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | n     | 615 | XAT  | C38-C25 | 2.19  | 1.55        | 1.51     |
| 22  | R     | 304 | CLA  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 22  | c     | 504 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 22  | b     | 605 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 22  | B     | 609 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 22  | y     | 612 | CLA  | C4D-CHA | 2.18  | 1.46        | 1.38     |
| 22  | r     | 305 | CLA  | C3B-C2B | -2.18 | 1.37        | 1.40     |
| 24  | N     | 616 | XAT  | C18-C5  | 2.18  | 1.55        | 1.51     |
| 35  | c     | 517 | DGD  | O6D-C5D | -2.18 | 1.39        | 1.44     |
| 22  | c     | 510 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 22  | C     | 511 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 33  | l     | 101 | SQD  | O2-C2   | -2.18 | 1.37        | 1.43     |
| 24  | g     | 617 | XAT  | C8-C7   | 2.18  | 1.37        | 1.32     |
| 22  | b     | 611 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 30  | a     | 407 | PHO  | CMB-C2B | -2.17 | 1.46        | 1.51     |
| 22  | n     | 612 | CLA  | C4D-CHA | 2.17  | 1.46        | 1.38     |
| 26  | g     | 619 | LHG  | O7-C5   | -2.17 | 1.41        | 1.46     |
| 22  | r     | 304 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | Y     | 604 | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 22  | C     | 504 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | A     | 406 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | g     | 613 | CLA  | C4D-CHA | 2.17  | 1.46        | 1.38     |
| 22  | a     | 408 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | B     | 616 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 25  | n     | 616 | NEX  | C38-C25 | 2.17  | 1.55        | 1.51     |
| 22  | c     | 505 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 21  | Y     | 607 | CHL  | C1D-ND  | -2.17 | 1.35        | 1.37     |
| 24  | Y     | 615 | XAT  | C38-C25 | 2.17  | 1.55        | 1.51     |
| 22  | b     | 604 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 24  | y     | 615 | XAT  | C28-C27 | 2.17  | 1.37        | 1.32     |
| 22  | x     | 101 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 22  | b     | 614 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 30  | a     | 407 | PHO  | C3B-C2B | -2.16 | 1.37        | 1.40     |
| 23  | r     | 313 | LUT  | C23-C24 | 2.16  | 1.53        | 1.50     |
| 24  | Y     | 615 | XAT  | C28-C27 | 2.16  | 1.37        | 1.32     |
| 22  | a     | 405 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 25  | g     | 618 | NEX  | C38-C25 | 2.16  | 1.55        | 1.51     |
| 36  | C     | 523 | LMG  | O7-C8   | -2.16 | 1.41        | 1.46     |
| 22  | b     | 606 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 22  | G     | 604 | CLA  | C3B-C2B | -2.16 | 1.37        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 613 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 22  | C     | 505 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 24  | y     | 615 | XAT  | C8-C7   | 2.16  | 1.37        | 1.32     |
| 22  | c     | 503 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 22  | c     | 507 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 21  | G     | 607 | CHL  | C1D-ND  | -2.16 | 1.35        | 1.37     |
| 22  | B     | 613 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 35  | C     | 518 | DGD  | O6D-C5D | -2.16 | 1.39        | 1.44     |
| 36  | M     | 101 | LMG  | O7-C8   | -2.16 | 1.41        | 1.46     |
| 22  | B     | 606 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 33  | A     | 412 | SQD  | O2-C2   | -2.15 | 1.37        | 1.43     |
| 36  | c     | 523 | LMG  | O7-C8   | -2.15 | 1.41        | 1.46     |
| 30  | d     | 401 | PHO  | CMD-C2D | -2.15 | 1.46        | 1.51     |
| 22  | b     | 610 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 22  | B     | 617 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 22  | b     | 612 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 33  | l     | 103 | SQD  | O2-C2   | -2.15 | 1.37        | 1.43     |
| 22  | B     | 603 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 22  | s     | 313 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 22  | S     | 312 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 22  | b     | 601 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 22  | c     | 513 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 24  | G     | 617 | XAT  | C8-C7   | 2.14  | 1.37        | 1.32     |
| 25  | Y     | 616 | NEX  | C28-C27 | 2.14  | 1.37        | 1.32     |
| 22  | D     | 405 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 22  | y     | 604 | CLA  | C3B-C2B | -2.14 | 1.37        | 1.40     |
| 22  | c     | 511 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | c     | 514 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 24  | y     | 615 | XAT  | O24-C25 | 2.13  | 1.49        | 1.46     |
| 22  | d     | 404 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | B     | 610 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | B     | 615 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | B     | 618 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | C     | 514 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 36  | D     | 411 | LMG  | O7-C8   | -2.13 | 1.41        | 1.46     |
| 22  | b     | 607 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | a     | 404 | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 23  | Y     | 614 | LUT  | C4-C5   | 2.13  | 1.54        | 1.51     |
| 22  | g     | 604 | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 22  | C     | 503 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 36  | B     | 623 | LMG  | C22-C21 | 2.13  | 1.63        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | S     | 312 | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 36  | b     | 620 | LMG  | C22-C21 | 2.13  | 1.63        | 1.51     |
| 22  | c     | 508 | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 22  | S     | 313 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 33  | L     | 101 | SQD  | O4-C4   | -2.13 | 1.38        | 1.43     |
| 22  | C     | 507 | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 23  | g     | 616 | LUT  | C4-C5   | 2.13  | 1.54        | 1.51     |
| 22  | a     | 404 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 33  | a     | 411 | SQD  | O2-C2   | -2.12 | 1.38        | 1.43     |
| 24  | N     | 616 | XAT  | C8-C7   | 2.12  | 1.37        | 1.32     |
| 30  | D     | 401 | PHO  | CMD-C2D | -2.12 | 1.46        | 1.51     |
| 35  | C     | 519 | DGD  | O6D-C5D | -2.12 | 1.39        | 1.44     |
| 36  | B     | 623 | LMG  | O7-C8   | -2.12 | 1.41        | 1.46     |
| 35  | c     | 518 | DGD  | O6D-C5D | -2.12 | 1.39        | 1.44     |
| 22  | c     | 502 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 33  | L     | 101 | SQD  | O3-C3   | -2.12 | 1.38        | 1.43     |
| 22  | a     | 406 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 22  | N     | 604 | CLA  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 22  | A     | 405 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 22  | C     | 515 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 24  | Y     | 615 | XAT  | O24-C25 | 2.12  | 1.49        | 1.46     |
| 22  | C     | 506 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 36  | T     | 101 | LMG  | O7-C8   | -2.11 | 1.41        | 1.46     |
| 22  | B     | 607 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | A     | 407 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 22  | B     | 614 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 23  | n     | 614 | LUT  | C23-C24 | 2.11  | 1.53        | 1.50     |
| 33  | D     | 402 | SQD  | O3-C3   | -2.11 | 1.38        | 1.43     |
| 22  | A     | 405 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | n     | 604 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | B     | 607 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 33  | l     | 101 | SQD  | O4-C4   | -2.11 | 1.38        | 1.43     |
| 22  | c     | 508 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 26  | N     | 618 | LHG  | P-O6    | 2.11  | 1.67        | 1.59     |
| 22  | C     | 512 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 33  | D     | 402 | SQD  | O4-C4   | -2.11 | 1.38        | 1.43     |
| 30  | A     | 408 | PHO  | CMB-C2B | -2.11 | 1.46        | 1.51     |
| 22  | a     | 406 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 33  | L     | 101 | SQD  | O2-C2   | -2.11 | 1.38        | 1.43     |
| 22  | b     | 603 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 24  | R     | 313 | XAT  | C28-C27 | 2.11  | 1.37        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | Y     | 604 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 22  | b     | 601 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 33  | l     | 103 | SQD  | O4-C4   | -2.10 | 1.38        | 1.43     |
| 26  | b     | 619 | LHG  | O7-C5   | -2.10 | 1.41        | 1.46     |
| 22  | a     | 406 | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 24  | r     | 314 | XAT  | C28-C27 | 2.10  | 1.37        | 1.32     |
| 22  | S     | 305 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 35  | c     | 519 | DGD  | C4E-C3E | 2.10  | 1.57        | 1.52     |
| 33  | l     | 103 | SQD  | O3-C3   | -2.10 | 1.38        | 1.43     |
| 33  | A     | 412 | SQD  | O4-C4   | -2.10 | 1.38        | 1.43     |
| 36  | d     | 410 | LMG  | O7-C8   | -2.10 | 1.41        | 1.46     |
| 22  | g     | 613 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 25  | n     | 616 | NEX  | C28-C27 | 2.09  | 1.37        | 1.32     |
| 22  | A     | 407 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | Y     | 609 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | r     | 309 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | s     | 312 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | S     | 310 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 23  | N     | 615 | LUT  | C31-C32 | 2.09  | 1.40        | 1.34     |
| 23  | y     | 614 | LUT  | C23-C24 | 2.09  | 1.53        | 1.50     |
| 22  | g     | 604 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 22  | w     | 101 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 33  | a     | 411 | SQD  | O4-C4   | -2.09 | 1.38        | 1.43     |
| 22  | W     | 101 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 33  | d     | 402 | SQD  | O3-C3   | -2.09 | 1.38        | 1.43     |
| 22  | G     | 612 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | b     | 604 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | r     | 309 | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 22  | R     | 311 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | s     | 303 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | g     | 611 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | D     | 404 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 25  | y     | 618 | NEX  | C4-C3   | 2.08  | 1.55        | 1.52     |
| 22  | B     | 609 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 23  | G     | 615 | LUT  | C23-C24 | 2.08  | 1.53        | 1.50     |
| 22  | G     | 604 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | B     | 604 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | C     | 510 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | R     | 304 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | Y     | 610 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 33  | l     | 101 | SQD  | O3-C3   | -2.08 | 1.38        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | a     | 404 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | s     | 310 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 24  | g     | 617 | XAT  | C28-C27 | 2.08  | 1.37        | 1.32     |
| 35  | J     | 101 | DGD  | C4E-C5E | 2.07  | 1.57        | 1.53     |
| 22  | N     | 612 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 35  | J     | 101 | DGD  | C4E-C3E | 2.07  | 1.57        | 1.52     |
| 33  | L     | 102 | SQD  | O3-C3   | -2.07 | 1.38        | 1.43     |
| 22  | r     | 310 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 36  | b     | 620 | LMG  | O7-C8   | -2.07 | 1.41        | 1.46     |
| 33  | d     | 402 | SQD  | O4-C4   | -2.07 | 1.38        | 1.43     |
| 26  | B     | 622 | LHG  | O7-C5   | -2.07 | 1.41        | 1.46     |
| 22  | y     | 612 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 36  | C     | 502 | LMG  | O8-C9   | -2.07 | 1.40        | 1.45     |
| 22  | r     | 312 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | b     | 602 | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 22  | R     | 310 | CLA  | C1B-NB  | 2.07  | 1.37        | 1.35     |
| 22  | d     | 404 | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 22  | r     | 311 | CLA  | C1B-NB  | 2.07  | 1.37        | 1.35     |
| 22  | b     | 602 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 36  | w     | 102 | LMG  | O8-C9   | -2.07 | 1.40        | 1.45     |
| 30  | D     | 401 | PHO  | CMB-C2B | -2.07 | 1.46        | 1.51     |
| 33  | L     | 102 | SQD  | O4-C4   | -2.07 | 1.38        | 1.43     |
| 22  | B     | 605 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | R     | 309 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | c     | 513 | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 22  | D     | 404 | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 22  | N     | 611 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | Y     | 602 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | c     | 506 | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 22  | B     | 616 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 22  | d     | 403 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 22  | n     | 612 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | G     | 610 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | N     | 602 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 25  | N     | 617 | NEX  | C28-C27 | 2.06  | 1.37        | 1.32     |
| 22  | d     | 403 | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 22  | g     | 612 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | r     | 305 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 23  | g     | 615 | LUT  | C23-C24 | 2.06  | 1.53        | 1.50     |
| 33  | a     | 411 | SQD  | O3-C3   | -2.06 | 1.38        | 1.43     |
| 24  | N     | 616 | XAT  | O24-C25 | 2.06  | 1.49        | 1.46     |
| 22  | C     | 509 | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | J     | 101 | DGD  | O6D-C5D | -2.06 | 1.39        | 1.44     |
| 36  | d     | 410 | LMG  | O1-C7   | -2.06 | 1.40        | 1.43     |
| 22  | y     | 611 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | N     | 609 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | B     | 605 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | C3B-CAB | -2.06 | 1.43        | 1.47     |
| 24  | G     | 617 | XAT  | C28-C27 | 2.06  | 1.37        | 1.32     |
| 33  | A     | 412 | SQD  | O3-C3   | -2.06 | 1.38        | 1.43     |
| 22  | B     | 613 | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 22  | n     | 609 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | n     | 610 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | y     | 604 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | B     | 614 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 22  | S     | 303 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | C     | 509 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | b     | 611 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 22  | N     | 604 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 26  | c     | 520 | LHG  | P-O6    | 2.05  | 1.67        | 1.59     |
| 22  | G     | 602 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 24  | n     | 615 | XAT  | C28-C27 | 2.05  | 1.37        | 1.32     |
| 35  | c     | 519 | DGD  | C4E-C5E | 2.05  | 1.57        | 1.53     |
| 22  | S     | 310 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 22  | C     | 514 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 22  | G     | 613 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | C     | 510 | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 22  | s     | 305 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | s     | 311 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | n     | 613 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | C     | 514 | CLA  | MG-ND   | -2.05 | 2.01        | 2.05     |
| 22  | g     | 610 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | G     | 611 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | Y     | 611 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | Y     | 611 | CLA  | C4D-ND  | -2.05 | 1.34        | 1.37     |
| 22  | R     | 308 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | B     | 607 | CLA  | MG-ND   | -2.05 | 2.01        | 2.05     |
| 22  | c     | 507 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 22  | b     | 607 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 30  | d     | 401 | PHO  | CMB-C2B | -2.05 | 1.46        | 1.51     |
| 22  | y     | 602 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | A     | 407 | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 22  | A     | 405 | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 26  | C     | 520 | LHG  | P-O6    | 2.04  | 1.67        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | N     | 610 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 36  | D     | 411 | LMG  | O8-C9   | -2.04 | 1.40        | 1.45     |
| 22  | n     | 611 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | y     | 612 | CLA  | C4D-ND  | -2.04 | 1.34        | 1.37     |
| 22  | s     | 308 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | R     | 308 | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 22  | b     | 606 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | n     | 602 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | B     | 612 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | C     | 503 | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 22  | c     | 504 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | a     | 408 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | c     | 508 | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 22  | A     | 406 | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 22  | b     | 609 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | c     | 506 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | c     | 505 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 25  | g     | 618 | NEX  | C28-C27 | 2.03  | 1.37        | 1.32     |
| 36  | d     | 410 | LMG  | O8-C9   | -2.03 | 1.40        | 1.45     |
| 22  | s     | 310 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | c     | 503 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | S     | 311 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | a     | 405 | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 25  | r     | 315 | NEX  | C4-C3   | 2.03  | 1.55        | 1.52     |
| 22  | C     | 503 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | b     | 602 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | C     | 504 | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 22  | R     | 310 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 35  | c     | 519 | DGD  | O6D-C5D | -2.03 | 1.39        | 1.44     |
| 22  | B     | 612 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | B     | 603 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | N     | 612 | CLA  | C4D-ND  | -2.03 | 1.34        | 1.37     |
| 22  | b     | 604 | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 22  | y     | 610 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | B     | 610 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 23  | N     | 614 | LUT  | C23-C24 | 2.03  | 1.53        | 1.50     |
| 32  | D     | 407 | PL9  | C31-C29 | -2.03 | 1.47        | 1.51     |
| 23  | Y     | 613 | LUT  | C23-C24 | 2.03  | 1.53        | 1.50     |
| 22  | c     | 502 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 515 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | c     | 514 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | N     | 617 | NEX  | C38-C25 | 2.02  | 1.55        | 1.51     |
| 22  | a     | 405 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 22  | C     | 509 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 36  | D     | 411 | LMG  | O1-C7   | -2.02 | 1.40        | 1.43     |
| 22  | Y     | 610 | CLA  | C3B-C2B | -2.02 | 1.37        | 1.40     |
| 24  | r     | 314 | XAT  | O24-C25 | 2.02  | 1.49        | 1.46     |
| 22  | r     | 309 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 22  | b     | 614 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | G     | 613 | CLA  | C4D-ND  | -2.02 | 1.34        | 1.37     |
| 22  | n     | 603 | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 22  | B     | 603 | CLA  | C3B-C2B | -2.02 | 1.37        | 1.40     |
| 22  | B     | 617 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 506 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 22  | B     | 607 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 22  | y     | 603 | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 22  | B     | 611 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 512 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 513 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 512 | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 22  | a     | 405 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 24  | r     | 314 | XAT  | C18-C5  | 2.01  | 1.55        | 1.51     |
| 22  | g     | 611 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | r     | 311 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | c     | 512 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | c     | 513 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 25  | y     | 618 | NEX  | C28-C27 | 2.01  | 1.37        | 1.32     |
| 22  | b     | 601 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 22  | a     | 405 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 22  | g     | 602 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | S     | 308 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | x     | 101 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | G     | 611 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | c     | 503 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 22  | C     | 513 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | c     | 502 | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 21  | g     | 606 | CHL  | C4D-CHA | 2.01  | 1.45        | 1.38     |
| 22  | s     | 303 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 22  | c     | 512 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 23  | Y     | 614 | LUT  | C28-C27 | 2.01  | 1.37        | 1.32     |
| 22  | c     | 511 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 22  | c     | 509 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | c     | 517 | DGD  | O5D-C6D | -2.01 | 1.40        | 1.43     |
| 22  | y     | 610 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | c     | 508 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | c     | 513 | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 22  | Y     | 603 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 31  | H     | 101 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 22  | C     | 509 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 25  | r     | 315 | NEX  | C28-C27 | 2.01  | 1.37        | 1.32     |
| 22  | C     | 512 | CLA  | C3B-C2B | -2.00 | 1.37        | 1.40     |
| 22  | b     | 613 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 22  | b     | 604 | CLA  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 22  | n     | 612 | CLA  | C4D-ND  | -2.00 | 1.34        | 1.37     |
| 22  | B     | 605 | CLA  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 22  | Y     | 612 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 22  | A     | 409 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 21  | R     | 306 | CHL  | C4D-CHA | 2.00  | 1.45        | 1.38     |
| 22  | D     | 405 | CLA  | C3B-C2B | -2.00 | 1.37        | 1.40     |
| 22  | B     | 613 | CLA  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 21  | y     | 605 | CHL  | C4D-CHA | 2.00  | 1.45        | 1.38     |
| 21  | S     | 302 | CHL  | C4D-CHA | 2.00  | 1.45        | 1.38     |
| 22  | y     | 611 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 22  | b     | 603 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 21  | r     | 307 | CHL  | C4D-CHA | 2.00  | 1.45        | 1.38     |
| 22  | g     | 614 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | N     | 603 | CLA  | MG-ND   | -2.00 | 2.01        | 2.05     |
| 21  | R     | 307 | CHL  | C4D-CHA | 2.00  | 1.45        | 1.38     |

All (3429) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24  | G     | 617 | XAT  | O24-C25-C24 | -78.18 | 54.66       | 113.38   |
| 24  | N     | 616 | XAT  | O24-C25-C24 | -78.01 | 54.78       | 113.38   |
| 24  | R     | 313 | XAT  | O24-C25-C24 | -77.64 | 55.06       | 113.38   |
| 24  | r     | 314 | XAT  | O24-C25-C24 | -77.61 | 55.08       | 113.38   |
| 24  | g     | 617 | XAT  | O24-C25-C24 | -77.46 | 55.19       | 113.38   |
| 24  | n     | 615 | XAT  | O24-C25-C24 | -77.08 | 55.48       | 113.38   |
| 24  | y     | 615 | XAT  | O24-C25-C24 | -77.08 | 55.48       | 113.38   |
| 24  | Y     | 615 | XAT  | O24-C25-C24 | -77.05 | 55.50       | 113.38   |
| 25  | N     | 617 | NEX  | O24-C25-C24 | -51.71 | 74.53       | 113.38   |
| 25  | y     | 616 | NEX  | O24-C25-C24 | -50.97 | 75.09       | 113.38   |
| 24  | n     | 615 | XAT  | O4-C5-C4    | 50.84  | 151.57      | 113.38   |
| 25  | n     | 616 | NEX  | O24-C25-C24 | -49.94 | 75.86       | 113.38   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24  | N     | 616 | XAT  | O4-C5-C4    | 49.53  | 150.59      | 113.38   |
| 24  | r     | 314 | XAT  | O4-C5-C4    | 49.05  | 150.23      | 113.38   |
| 25  | g     | 618 | NEX  | O24-C25-C24 | -49.04 | 76.54       | 113.38   |
| 24  | R     | 313 | XAT  | O4-C5-C4    | 49.01  | 150.20      | 113.38   |
| 24  | g     | 617 | XAT  | O4-C5-C4    | 48.45  | 149.78      | 113.38   |
| 24  | Y     | 615 | XAT  | O4-C5-C4    | 47.95  | 149.41      | 113.38   |
| 24  | y     | 615 | XAT  | O4-C5-C4    | 47.81  | 149.30      | 113.38   |
| 24  | G     | 617 | XAT  | O4-C5-C4    | 47.48  | 149.05      | 113.38   |
| 25  | Y     | 616 | NEX  | O24-C25-C24 | -47.30 | 77.85       | 113.38   |
| 25  | y     | 618 | NEX  | O24-C25-C24 | -43.55 | 80.67       | 113.38   |
| 25  | r     | 315 | NEX  | O24-C25-C24 | -43.55 | 80.67       | 113.38   |
| 24  | N     | 616 | XAT  | C31-C30-C29 | -12.76 | 109.10      | 127.31   |
| 22  | c     | 510 | CLA  | C2D-C1D-ND  | -12.71 | 100.74      | 110.10   |
| 22  | C     | 511 | CLA  | C2D-C1D-ND  | -12.68 | 100.76      | 110.10   |
| 23  | R     | 312 | LUT  | C18-C5-C6   | -12.28 | 110.74      | 124.53   |
| 23  | r     | 313 | LUT  | C18-C5-C6   | -12.25 | 110.77      | 124.53   |
| 23  | Y     | 613 | LUT  | C18-C5-C6   | -12.06 | 110.98      | 124.53   |
| 23  | n     | 614 | LUT  | C18-C5-C6   | -12.06 | 110.99      | 124.53   |
| 23  | y     | 614 | LUT  | C18-C5-C6   | -12.06 | 110.99      | 124.53   |
| 23  | G     | 615 | LUT  | C18-C5-C6   | -12.05 | 111.00      | 124.53   |
| 23  | N     | 614 | LUT  | C18-C5-C6   | -12.05 | 111.00      | 124.53   |
| 23  | g     | 615 | LUT  | C18-C5-C6   | -12.05 | 111.00      | 124.53   |
| 24  | Y     | 615 | XAT  | C11-C10-C9  | -12.01 | 110.17      | 127.31   |
| 24  | G     | 617 | XAT  | C31-C30-C29 | -11.62 | 110.73      | 127.31   |
| 23  | Y     | 613 | LUT  | C20-C13-C14 | -11.58 | 106.71      | 122.92   |
| 23  | y     | 614 | LUT  | C20-C13-C14 | -11.56 | 106.73      | 122.92   |
| 23  | N     | 614 | LUT  | C20-C13-C14 | -11.56 | 106.73      | 122.92   |
| 23  | g     | 615 | LUT  | C20-C13-C14 | -11.55 | 106.74      | 122.92   |
| 23  | n     | 614 | LUT  | C20-C13-C14 | -11.53 | 106.77      | 122.92   |
| 23  | G     | 615 | LUT  | C20-C13-C14 | -11.53 | 106.78      | 122.92   |
| 24  | g     | 617 | XAT  | C31-C30-C29 | -11.49 | 110.92      | 127.31   |
| 24  | y     | 615 | XAT  | C11-C10-C9  | -11.42 | 111.01      | 127.31   |
| 23  | n     | 614 | LUT  | C35-C34-C33 | -11.41 | 111.02      | 127.31   |
| 24  | n     | 615 | XAT  | C31-C30-C29 | -11.41 | 111.02      | 127.31   |
| 23  | g     | 615 | LUT  | C35-C34-C33 | -11.41 | 111.02      | 127.31   |
| 23  | G     | 615 | LUT  | C35-C34-C33 | -11.41 | 111.03      | 127.31   |
| 23  | y     | 614 | LUT  | C35-C34-C33 | -11.40 | 111.05      | 127.31   |
| 23  | N     | 614 | LUT  | C35-C34-C33 | -11.39 | 111.05      | 127.31   |
| 23  | Y     | 613 | LUT  | C35-C34-C33 | -11.38 | 111.07      | 127.31   |
| 23  | y     | 614 | LUT  | C1-C6-C5    | -11.27 | 106.73      | 122.61   |
| 23  | N     | 614 | LUT  | C1-C6-C5    | -11.27 | 106.73      | 122.61   |
| 23  | g     | 615 | LUT  | C1-C6-C5    | -11.27 | 106.74      | 122.61   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 23  | Y     | 613 | LUT  | C1-C6-C5    | -11.27 | 106.74      | 122.61   |
| 23  | G     | 615 | LUT  | C1-C6-C5    | -11.27 | 106.74      | 122.61   |
| 23  | n     | 614 | LUT  | C1-C6-C5    | -11.25 | 106.76      | 122.61   |
| 24  | n     | 615 | XAT  | C35-C34-C33 | -11.18 | 111.36      | 127.31   |
| 23  | Y     | 614 | LUT  | C18-C5-C6   | -11.08 | 112.09      | 124.53   |
| 24  | Y     | 615 | XAT  | C31-C30-C29 | -11.04 | 111.55      | 127.31   |
| 24  | y     | 615 | XAT  | C31-C30-C29 | -10.95 | 111.68      | 127.31   |
| 24  | N     | 616 | XAT  | C35-C34-C33 | -10.93 | 111.71      | 127.31   |
| 23  | R     | 312 | LUT  | C15-C14-C13 | -10.83 | 111.85      | 127.31   |
| 23  | G     | 616 | LUT  | C19-C9-C10  | -10.82 | 107.77      | 122.92   |
| 23  | r     | 313 | LUT  | C15-C14-C13 | -10.80 | 111.89      | 127.31   |
| 23  | G     | 616 | LUT  | C18-C5-C6   | -10.67 | 112.55      | 124.53   |
| 37  | f     | 101 | HEM  | C1B-NB-C4B  | 10.66  | 116.09      | 105.07   |
| 37  | F     | 101 | HEM  | C1B-NB-C4B  | 10.66  | 116.09      | 105.07   |
| 24  | r     | 314 | XAT  | C35-C34-C33 | -10.66 | 112.10      | 127.31   |
| 25  | n     | 616 | NEX  | C40-C33-C34 | -10.66 | 108.00      | 122.92   |
| 25  | N     | 617 | NEX  | C31-C30-C29 | -10.64 | 112.12      | 127.31   |
| 24  | R     | 313 | XAT  | C35-C34-C33 | -10.64 | 112.12      | 127.31   |
| 23  | g     | 616 | LUT  | C18-C5-C6   | -10.63 | 112.59      | 124.53   |
| 23  | r     | 313 | LUT  | C31-C30-C29 | -10.60 | 112.19      | 127.31   |
| 23  | R     | 312 | LUT  | C31-C30-C29 | -10.59 | 112.20      | 127.31   |
| 23  | Y     | 614 | LUT  | C19-C9-C10  | -10.55 | 108.14      | 122.92   |
| 25  | Y     | 616 | NEX  | C39-C29-C30 | -10.54 | 108.16      | 122.92   |
| 23  | g     | 616 | LUT  | C19-C9-C10  | -10.54 | 108.16      | 122.92   |
| 25  | g     | 618 | NEX  | C15-C14-C13 | -10.53 | 112.28      | 127.31   |
| 23  | G     | 615 | LUT  | C31-C30-C29 | -10.52 | 112.29      | 127.31   |
| 23  | N     | 614 | LUT  | C31-C30-C29 | -10.52 | 112.30      | 127.31   |
| 23  | y     | 614 | LUT  | C31-C30-C29 | -10.51 | 112.30      | 127.31   |
| 23  | n     | 614 | LUT  | C31-C30-C29 | -10.51 | 112.31      | 127.31   |
| 23  | g     | 615 | LUT  | C31-C30-C29 | -10.51 | 112.32      | 127.31   |
| 24  | N     | 616 | XAT  | C11-C10-C9  | -10.50 | 112.32      | 127.31   |
| 23  | Y     | 613 | LUT  | C31-C30-C29 | -10.50 | 112.33      | 127.31   |
| 25  | g     | 618 | NEX  | C40-C33-C34 | -10.43 | 108.31      | 122.92   |
| 24  | g     | 617 | XAT  | C35-C34-C33 | -10.42 | 112.44      | 127.31   |
| 23  | g     | 615 | LUT  | C11-C10-C9  | -10.38 | 112.49      | 127.31   |
| 23  | Y     | 613 | LUT  | C11-C10-C9  | -10.38 | 112.50      | 127.31   |
| 23  | G     | 615 | LUT  | C11-C10-C9  | -10.38 | 112.50      | 127.31   |
| 25  | Y     | 616 | NEX  | C15-C14-C13 | -10.37 | 112.50      | 127.31   |
| 23  | n     | 614 | LUT  | C11-C10-C9  | -10.37 | 112.51      | 127.31   |
| 23  | y     | 614 | LUT  | C11-C10-C9  | -10.36 | 112.52      | 127.31   |
| 25  | N     | 617 | NEX  | C11-C10-C9  | -10.36 | 112.52      | 127.31   |
| 24  | r     | 314 | XAT  | C15-C14-C13 | -10.36 | 112.53      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 23  | N     | 614 | LUT  | C11-C10-C9  | -10.35 | 112.53      | 127.31   |
| 24  | R     | 313 | XAT  | C15-C14-C13 | -10.33 | 112.57      | 127.31   |
| 23  | R     | 312 | LUT  | C11-C10-C9  | -10.27 | 112.65      | 127.31   |
| 24  | r     | 314 | XAT  | C20-C13-C14 | -10.26 | 108.55      | 122.92   |
| 24  | R     | 313 | XAT  | C20-C13-C14 | -10.25 | 108.56      | 122.92   |
| 25  | g     | 618 | NEX  | C35-C34-C33 | -10.24 | 112.69      | 127.31   |
| 23  | R     | 312 | LUT  | C35-C34-C33 | -10.21 | 112.73      | 127.31   |
| 23  | r     | 313 | LUT  | C11-C10-C9  | -10.21 | 112.74      | 127.31   |
| 24  | n     | 615 | XAT  | C11-C10-C9  | -10.20 | 112.75      | 127.31   |
| 24  | Y     | 615 | XAT  | C19-C9-C10  | -10.19 | 108.65      | 122.92   |
| 23  | r     | 313 | LUT  | C35-C34-C33 | -10.19 | 112.77      | 127.31   |
| 24  | g     | 617 | XAT  | C11-C10-C9  | -10.12 | 112.86      | 127.31   |
| 24  | G     | 617 | XAT  | C35-C34-C33 | -10.08 | 112.93      | 127.31   |
| 24  | y     | 615 | XAT  | C19-C9-C10  | -10.07 | 108.81      | 122.92   |
| 24  | N     | 616 | XAT  | C39-C29-C30 | -10.06 | 108.83      | 122.92   |
| 25  | y     | 616 | NEX  | C40-C33-C34 | -10.06 | 108.84      | 122.92   |
| 25  | r     | 315 | NEX  | C15-C14-C13 | -10.03 | 113.00      | 127.31   |
| 25  | y     | 618 | NEX  | C39-C29-C30 | -10.02 | 108.89      | 122.92   |
| 25  | y     | 618 | NEX  | C15-C14-C13 | -10.01 | 113.03      | 127.31   |
| 24  | Y     | 615 | XAT  | C35-C34-C33 | -9.99  | 113.05      | 127.31   |
| 23  | y     | 614 | LUT  | C15-C14-C13 | -9.99  | 113.05      | 127.31   |
| 23  | n     | 614 | LUT  | C15-C14-C13 | -9.99  | 113.06      | 127.31   |
| 24  | R     | 313 | XAT  | C31-C30-C29 | -9.99  | 113.06      | 127.31   |
| 25  | r     | 315 | NEX  | C39-C29-C30 | -9.99  | 108.94      | 122.92   |
| 24  | r     | 314 | XAT  | C31-C30-C29 | -9.99  | 113.06      | 127.31   |
| 23  | g     | 615 | LUT  | C15-C14-C13 | -9.98  | 113.07      | 127.31   |
| 23  | G     | 615 | LUT  | C15-C14-C13 | -9.97  | 113.08      | 127.31   |
| 23  | Y     | 613 | LUT  | C15-C14-C13 | -9.96  | 113.09      | 127.31   |
| 23  | N     | 614 | LUT  | C15-C14-C13 | -9.94  | 113.12      | 127.31   |
| 24  | y     | 615 | XAT  | C35-C34-C33 | -9.91  | 113.16      | 127.31   |
| 24  | n     | 615 | XAT  | C40-C33-C34 | -9.88  | 109.09      | 122.92   |
| 25  | Y     | 616 | NEX  | C20-C13-C14 | -9.85  | 109.13      | 122.92   |
| 23  | R     | 312 | LUT  | C19-C9-C10  | -9.84  | 109.14      | 122.92   |
| 24  | G     | 617 | XAT  | C39-C29-C30 | -9.82  | 109.16      | 122.92   |
| 24  | n     | 615 | XAT  | C39-C29-C30 | -9.82  | 109.16      | 122.92   |
| 23  | r     | 313 | LUT  | C19-C9-C10  | -9.82  | 109.16      | 122.92   |
| 23  | R     | 312 | LUT  | C39-C29-C30 | -9.78  | 109.22      | 122.92   |
| 23  | r     | 313 | LUT  | C39-C29-C30 | -9.76  | 109.25      | 122.92   |
| 24  | g     | 617 | XAT  | C39-C29-C30 | -9.76  | 109.25      | 122.92   |
| 24  | Y     | 615 | XAT  | C40-C33-C34 | -9.75  | 109.27      | 122.92   |
| 25  | n     | 616 | NEX  | C20-C13-C14 | -9.74  | 109.28      | 122.92   |
| 24  | g     | 617 | XAT  | C40-C33-C34 | -9.73  | 109.29      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | N     | 616 | XAT  | C18-C5-C4   | -9.72 | 103.35      | 114.28   |
| 24  | y     | 615 | XAT  | C39-C29-C30 | -9.72 | 109.31      | 122.92   |
| 23  | y     | 614 | LUT  | C40-C33-C34 | -9.71 | 109.33      | 122.92   |
| 24  | n     | 615 | XAT  | C18-C5-C4   | -9.70 | 103.36      | 114.28   |
| 23  | N     | 614 | LUT  | C40-C33-C34 | -9.70 | 109.33      | 122.92   |
| 25  | r     | 315 | NEX  | C40-C33-C34 | -9.70 | 109.34      | 122.92   |
| 23  | g     | 615 | LUT  | C40-C33-C34 | -9.70 | 109.34      | 122.92   |
| 24  | r     | 314 | XAT  | C39-C29-C30 | -9.69 | 109.34      | 122.92   |
| 23  | n     | 614 | LUT  | C40-C33-C34 | -9.69 | 109.35      | 122.92   |
| 24  | Y     | 615 | XAT  | C39-C29-C30 | -9.68 | 109.36      | 122.92   |
| 24  | R     | 313 | XAT  | C40-C33-C34 | -9.68 | 109.36      | 122.92   |
| 25  | g     | 618 | NEX  | C20-C13-C14 | -9.68 | 109.37      | 122.92   |
| 24  | R     | 313 | XAT  | C39-C29-C30 | -9.66 | 109.40      | 122.92   |
| 23  | G     | 615 | LUT  | C40-C33-C34 | -9.65 | 109.40      | 122.92   |
| 23  | Y     | 613 | LUT  | C40-C33-C34 | -9.65 | 109.40      | 122.92   |
| 24  | y     | 615 | XAT  | C40-C33-C34 | -9.65 | 109.41      | 122.92   |
| 24  | r     | 314 | XAT  | C40-C33-C34 | -9.65 | 109.41      | 122.92   |
| 25  | y     | 616 | NEX  | C15-C14-C13 | -9.64 | 113.55      | 127.31   |
| 25  | N     | 617 | NEX  | C20-C13-C14 | -9.64 | 109.42      | 122.92   |
| 25  | y     | 618 | NEX  | C40-C33-C34 | -9.64 | 109.42      | 122.92   |
| 25  | y     | 618 | NEX  | C11-C10-C9  | -9.64 | 113.56      | 127.31   |
| 24  | G     | 617 | XAT  | C11-C10-C9  | -9.62 | 113.58      | 127.31   |
| 25  | r     | 315 | NEX  | C11-C10-C9  | -9.61 | 113.59      | 127.31   |
| 24  | G     | 617 | XAT  | C40-C33-C34 | -9.61 | 109.46      | 122.92   |
| 24  | N     | 616 | XAT  | C15-C14-C13 | -9.59 | 113.63      | 127.31   |
| 25  | n     | 616 | NEX  | C15-C14-C13 | -9.57 | 113.65      | 127.31   |
| 25  | y     | 618 | NEX  | C19-C9-C10  | -9.56 | 109.53      | 122.92   |
| 24  | g     | 617 | XAT  | C19-C9-C10  | -9.56 | 109.53      | 122.92   |
| 25  | r     | 315 | NEX  | C19-C9-C10  | -9.56 | 109.53      | 122.92   |
| 25  | y     | 616 | NEX  | C20-C13-C14 | -9.56 | 109.53      | 122.92   |
| 25  | g     | 618 | NEX  | C31-C30-C29 | -9.55 | 113.67      | 127.31   |
| 25  | g     | 618 | NEX  | C39-C29-C30 | -9.55 | 109.54      | 122.92   |
| 23  | R     | 312 | LUT  | C40-C33-C34 | -9.54 | 109.55      | 122.92   |
| 24  | y     | 615 | XAT  | C20-C13-C14 | -9.54 | 109.55      | 122.92   |
| 25  | N     | 617 | NEX  | C19-C9-C10  | -9.54 | 109.56      | 122.92   |
| 24  | Y     | 615 | XAT  | C20-C13-C14 | -9.54 | 109.56      | 122.92   |
| 23  | N     | 615 | LUT  | C19-C9-C10  | -9.53 | 109.58      | 122.92   |
| 24  | N     | 616 | XAT  | C19-C9-C10  | -9.53 | 109.58      | 122.92   |
| 25  | y     | 618 | NEX  | C20-C13-C14 | -9.52 | 109.58      | 122.92   |
| 25  | r     | 315 | NEX  | C20-C13-C14 | -9.52 | 109.58      | 122.92   |
| 25  | r     | 315 | NEX  | C35-C34-C33 | -9.52 | 113.73      | 127.31   |
| 23  | r     | 313 | LUT  | C40-C33-C34 | -9.51 | 109.60      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | N     | 615 | LUT  | C20-C13-C14 | -9.51 | 109.60      | 122.92   |
| 23  | Y     | 614 | LUT  | C20-C13-C14 | -9.50 | 109.61      | 122.92   |
| 24  | N     | 616 | XAT  | C40-C33-C34 | -9.50 | 109.62      | 122.92   |
| 24  | r     | 314 | XAT  | C18-C5-C4   | -9.49 | 103.60      | 114.28   |
| 25  | y     | 618 | NEX  | C35-C34-C33 | -9.49 | 113.76      | 127.31   |
| 24  | R     | 313 | XAT  | C18-C5-C4   | -9.48 | 103.61      | 114.28   |
| 23  | g     | 616 | LUT  | C15-C14-C13 | -9.48 | 113.79      | 127.31   |
| 24  | G     | 617 | XAT  | C18-C5-C4   | -9.47 | 103.62      | 114.28   |
| 24  | g     | 617 | XAT  | C20-C13-C14 | -9.47 | 109.66      | 122.92   |
| 24  | N     | 616 | XAT  | C20-C13-C14 | -9.47 | 109.66      | 122.92   |
| 24  | G     | 617 | XAT  | C15-C14-C13 | -9.46 | 113.81      | 127.31   |
| 24  | g     | 617 | XAT  | C18-C5-C4   | -9.46 | 103.64      | 114.28   |
| 24  | n     | 615 | XAT  | C19-C9-C10  | -9.44 | 109.70      | 122.92   |
| 24  | n     | 615 | XAT  | C20-C13-C14 | -9.43 | 109.72      | 122.92   |
| 24  | y     | 615 | XAT  | C18-C5-C4   | -9.42 | 103.68      | 114.28   |
| 23  | Y     | 614 | LUT  | C35-C34-C33 | -9.40 | 113.89      | 127.31   |
| 24  | G     | 617 | XAT  | C20-C13-C14 | -9.39 | 109.77      | 122.92   |
| 24  | g     | 617 | XAT  | C15-C14-C13 | -9.38 | 113.92      | 127.31   |
| 25  | r     | 315 | NEX  | C31-C30-C29 | -9.38 | 113.93      | 127.31   |
| 25  | y     | 618 | NEX  | C31-C30-C29 | -9.37 | 113.93      | 127.31   |
| 25  | N     | 617 | NEX  | C15-C14-C13 | -9.36 | 113.95      | 127.31   |
| 23  | g     | 616 | LUT  | C39-C29-C30 | -9.35 | 109.83      | 122.92   |
| 23  | N     | 615 | LUT  | C1-C6-C5    | -9.34 | 109.45      | 122.61   |
| 24  | y     | 615 | XAT  | C15-C14-C13 | -9.33 | 113.99      | 127.31   |
| 25  | N     | 617 | NEX  | C40-C33-C34 | -9.33 | 109.86      | 122.92   |
| 23  | Y     | 614 | LUT  | C15-C14-C13 | -9.31 | 114.03      | 127.31   |
| 23  | G     | 616 | LUT  | C35-C34-C33 | -9.30 | 114.04      | 127.31   |
| 24  | n     | 615 | XAT  | C15-C14-C13 | -9.29 | 114.05      | 127.31   |
| 25  | Y     | 616 | NEX  | C31-C30-C29 | -9.26 | 114.09      | 127.31   |
| 23  | g     | 615 | LUT  | C19-C9-C10  | -9.26 | 109.95      | 122.92   |
| 24  | G     | 617 | XAT  | C19-C9-C10  | -9.25 | 109.97      | 122.92   |
| 24  | Y     | 615 | XAT  | C18-C5-C4   | -9.23 | 103.89      | 114.28   |
| 23  | G     | 615 | LUT  | C19-C9-C10  | -9.23 | 109.99      | 122.92   |
| 23  | N     | 614 | LUT  | C19-C9-C10  | -9.23 | 110.00      | 122.92   |
| 23  | y     | 614 | LUT  | C19-C9-C10  | -9.23 | 110.00      | 122.92   |
| 23  | Y     | 613 | LUT  | C19-C9-C10  | -9.23 | 110.00      | 122.92   |
| 23  | n     | 614 | LUT  | C19-C9-C10  | -9.22 | 110.01      | 122.92   |
| 23  | G     | 616 | LUT  | C39-C29-C30 | -9.22 | 110.01      | 122.92   |
| 23  | g     | 615 | LUT  | C39-C29-C30 | -9.21 | 110.02      | 122.92   |
| 23  | G     | 615 | LUT  | C39-C29-C30 | -9.21 | 110.02      | 122.92   |
| 23  | Y     | 613 | LUT  | C39-C29-C30 | -9.21 | 110.02      | 122.92   |
| 23  | G     | 616 | LUT  | C11-C10-C9  | -9.21 | 114.17      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | r     | 314 | XAT  | C19-C9-C10  | -9.20 | 110.03      | 122.92   |
| 23  | y     | 614 | LUT  | C39-C29-C30 | -9.19 | 110.05      | 122.92   |
| 23  | g     | 616 | LUT  | C31-C30-C29 | -9.19 | 114.20      | 127.31   |
| 23  | n     | 614 | LUT  | C39-C29-C30 | -9.19 | 110.06      | 122.92   |
| 24  | R     | 313 | XAT  | C19-C9-C10  | -9.18 | 110.07      | 122.92   |
| 25  | y     | 616 | NEX  | C35-C34-C33 | -9.17 | 114.22      | 127.31   |
| 25  | n     | 616 | NEX  | C35-C34-C33 | -9.17 | 114.22      | 127.31   |
| 23  | N     | 614 | LUT  | C39-C29-C30 | -9.16 | 110.09      | 122.92   |
| 25  | Y     | 616 | NEX  | C11-C10-C9  | -9.16 | 114.24      | 127.31   |
| 25  | N     | 617 | NEX  | C39-C29-C30 | -9.15 | 110.10      | 122.92   |
| 25  | n     | 616 | NEX  | C19-C9-C10  | -9.15 | 110.11      | 122.92   |
| 25  | Y     | 616 | NEX  | C40-C33-C34 | -9.14 | 110.11      | 122.92   |
| 25  | n     | 616 | NEX  | C31-C30-C29 | -9.14 | 114.26      | 127.31   |
| 25  | n     | 616 | NEX  | C39-C29-C30 | -9.14 | 110.12      | 122.92   |
| 23  | Y     | 614 | LUT  | C39-C29-C30 | -9.11 | 110.16      | 122.92   |
| 23  | N     | 615 | LUT  | C15-C14-C13 | -9.07 | 114.36      | 127.31   |
| 23  | g     | 616 | LUT  | C35-C34-C33 | -9.07 | 114.36      | 127.31   |
| 37  | f     | 101 | HEM  | C4D-ND-C1D  | 9.06  | 114.43      | 105.07   |
| 23  | G     | 616 | LUT  | C15-C14-C13 | -9.05 | 114.40      | 127.31   |
| 23  | Y     | 614 | LUT  | C40-C33-C34 | -9.04 | 110.26      | 122.92   |
| 23  | G     | 616 | LUT  | C20-C13-C14 | -9.03 | 110.28      | 122.92   |
| 23  | g     | 616 | LUT  | C40-C33-C34 | -9.01 | 110.30      | 122.92   |
| 37  | F     | 101 | HEM  | C4D-ND-C1D  | 9.01  | 114.38      | 105.07   |
| 25  | n     | 616 | NEX  | C11-C10-C9  | -9.00 | 114.46      | 127.31   |
| 24  | Y     | 615 | XAT  | C15-C14-C13 | -8.99 | 114.48      | 127.31   |
| 25  | y     | 616 | NEX  | C31-C30-C29 | -8.97 | 114.51      | 127.31   |
| 25  | y     | 616 | NEX  | C19-C9-C10  | -8.97 | 110.36      | 122.92   |
| 23  | G     | 616 | LUT  | C31-C30-C29 | -8.93 | 114.56      | 127.31   |
| 23  | g     | 616 | LUT  | C20-C13-C14 | -8.93 | 110.41      | 122.92   |
| 23  | N     | 615 | LUT  | C35-C34-C33 | -8.93 | 114.57      | 127.31   |
| 23  | N     | 615 | LUT  | C18-C5-C6   | -8.92 | 114.51      | 124.53   |
| 25  | Y     | 616 | NEX  | C19-C9-C10  | -8.92 | 110.43      | 122.92   |
| 25  | g     | 618 | NEX  | C11-C10-C9  | -8.92 | 114.58      | 127.31   |
| 23  | G     | 616 | LUT  | C40-C33-C34 | -8.88 | 110.48      | 122.92   |
| 25  | r     | 315 | NEX  | O24-C25-C38 | -8.85 | 104.46      | 115.06   |
| 25  | y     | 618 | NEX  | O24-C25-C38 | -8.81 | 104.50      | 115.06   |
| 25  | g     | 618 | NEX  | C19-C9-C10  | -8.81 | 110.58      | 122.92   |
| 23  | Y     | 614 | LUT  | C1-C6-C5    | -8.74 | 110.30      | 122.61   |
| 25  | y     | 616 | NEX  | C39-C29-C30 | -8.71 | 110.72      | 122.92   |
| 23  | g     | 616 | LUT  | C11-C10-C9  | -8.69 | 114.91      | 127.31   |
| 25  | y     | 616 | NEX  | C11-C10-C9  | -8.67 | 114.93      | 127.31   |
| 23  | Y     | 614 | LUT  | C11-C10-C9  | -8.66 | 114.96      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | N     | 615 | LUT  | C40-C33-C34 | -8.65 | 110.81      | 122.92   |
| 23  | R     | 312 | LUT  | C20-C13-C14 | -8.60 | 110.87      | 122.92   |
| 23  | r     | 313 | LUT  | C20-C13-C14 | -8.60 | 110.88      | 122.92   |
| 23  | N     | 615 | LUT  | C39-C29-C30 | -8.53 | 110.98      | 122.92   |
| 24  | N     | 616 | XAT  | C18-C5-C6   | -8.50 | 108.01      | 122.26   |
| 24  | n     | 615 | XAT  | O4-C5-C18   | -8.47 | 104.91      | 115.06   |
| 24  | y     | 615 | XAT  | C18-C5-C6   | -8.41 | 108.17      | 122.26   |
| 24  | G     | 617 | XAT  | C18-C5-C6   | -8.35 | 108.27      | 122.26   |
| 24  | r     | 314 | XAT  | C11-C10-C9  | -8.32 | 115.44      | 127.31   |
| 24  | R     | 313 | XAT  | C11-C10-C9  | -8.31 | 115.45      | 127.31   |
| 23  | N     | 615 | LUT  | C38-C25-C24 | -8.31 | 105.79      | 123.56   |
| 23  | g     | 616 | LUT  | C1-C6-C5    | -8.30 | 110.92      | 122.61   |
| 25  | Y     | 616 | NEX  | C35-C34-C33 | -8.28 | 115.50      | 127.31   |
| 23  | G     | 616 | LUT  | C1-C6-C5    | -8.25 | 111.00      | 122.61   |
| 24  | g     | 617 | XAT  | C18-C5-C6   | -8.11 | 108.67      | 122.26   |
| 21  | Y     | 606 | CHL  | CHD-C1D-ND  | -8.10 | 117.01      | 124.45   |
| 21  | r     | 308 | CHL  | CHD-C1D-ND  | -8.10 | 117.01      | 124.45   |
| 21  | G     | 605 | CHL  | CHD-C1D-ND  | -8.10 | 117.01      | 124.45   |
| 21  | S     | 301 | CHL  | CHD-C1D-ND  | -8.09 | 117.02      | 124.45   |
| 21  | g     | 601 | CHL  | CHD-C1D-ND  | -8.09 | 117.02      | 124.45   |
| 21  | y     | 608 | CHL  | CHD-C1D-ND  | -8.09 | 117.02      | 124.45   |
| 21  | r     | 307 | CHL  | CHD-C1D-ND  | -8.08 | 117.03      | 124.45   |
| 21  | s     | 307 | CHL  | CHD-C1D-ND  | -8.08 | 117.03      | 124.45   |
| 21  | g     | 607 | CHL  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 21  | N     | 608 | CHL  | CHD-C1D-ND  | -8.07 | 117.04      | 124.45   |
| 21  | s     | 306 | CHL  | CHD-C1D-ND  | -8.07 | 117.04      | 124.45   |
| 21  | R     | 307 | CHL  | CHD-C1D-ND  | -8.07 | 117.04      | 124.45   |
| 21  | N     | 605 | CHL  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 21  | N     | 606 | CHL  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 21  | y     | 601 | CHL  | CMD-C2D-C1D | 8.07  | 138.94      | 124.71   |
| 21  | s     | 307 | CHL  | CMD-C2D-C1D | 8.07  | 138.93      | 124.71   |
| 21  | y     | 607 | CHL  | CHD-C1D-ND  | -8.07 | 117.04      | 124.45   |
| 21  | R     | 306 | CHL  | CMD-C2D-C1D | 8.07  | 138.93      | 124.71   |
| 21  | s     | 302 | CHL  | CMD-C2D-C1D | 8.06  | 138.93      | 124.71   |
| 21  | n     | 607 | CHL  | CMD-C2D-C1D | 8.06  | 138.93      | 124.71   |
| 21  | r     | 308 | CHL  | CMD-C2D-C1D | 8.06  | 138.93      | 124.71   |
| 21  | g     | 606 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 21  | s     | 301 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 21  | g     | 609 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 21  | G     | 608 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 23  | G     | 616 | LUT  | C38-C25-C24 | -8.06 | 106.31      | 123.56   |
| 21  | S     | 302 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | n     | 601 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 21  | G     | 609 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 21  | Y     | 605 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 25  | N     | 617 | NEX  | C35-C34-C33 | -8.06 | 115.81      | 127.31   |
| 21  | G     | 605 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 21  | n     | 605 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 21  | g     | 607 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 21  | g     | 601 | CHL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.71   |
| 21  | G     | 607 | CHL  | CHD-C1D-ND  | -8.06 | 117.05      | 124.45   |
| 21  | R     | 307 | CHL  | CMD-C2D-C1D | 8.06  | 138.91      | 124.71   |
| 21  | g     | 609 | CHL  | CMD-C2D-C1D | 8.05  | 138.91      | 124.71   |
| 21  | S     | 301 | CHL  | CMD-C2D-C1D | 8.05  | 138.91      | 124.71   |
| 21  | s     | 301 | CHL  | CHD-C1D-ND  | -8.05 | 117.05      | 124.45   |
| 21  | g     | 605 | CHL  | CHD-C1D-ND  | -8.05 | 117.06      | 124.45   |
| 21  | S     | 306 | CHL  | CHD-C1D-ND  | -8.05 | 117.06      | 124.45   |
| 21  | Y     | 605 | CHL  | CMD-C2D-C1D | 8.05  | 138.90      | 124.71   |
| 21  | S     | 307 | CHL  | CMD-C2D-C1D | 8.05  | 138.90      | 124.71   |
| 21  | R     | 305 | CHL  | CMD-C2D-C1D | 8.05  | 138.90      | 124.71   |
| 21  | G     | 601 | CHL  | CHD-C1D-ND  | -8.05 | 117.06      | 124.45   |
| 21  | n     | 608 | CHL  | CMD-C2D-C1D | 8.05  | 138.90      | 124.71   |
| 21  | G     | 606 | CHL  | CMD-C2D-C1D | 8.05  | 138.89      | 124.71   |
| 21  | y     | 606 | CHL  | CMD-C2D-C1D | 8.05  | 138.89      | 124.71   |
| 21  | N     | 605 | CHL  | CHD-C1D-ND  | -8.04 | 117.06      | 124.45   |
| 21  | S     | 302 | CHL  | CHD-C1D-ND  | -8.04 | 117.06      | 124.45   |
| 21  | G     | 609 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | g     | 608 | CHL  | CHD-C1D-ND  | -8.04 | 117.06      | 124.45   |
| 21  | y     | 607 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | y     | 609 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | r     | 307 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | y     | 605 | CHL  | CHD-C1D-ND  | -8.04 | 117.06      | 124.45   |
| 21  | r     | 301 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | y     | 608 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | s     | 306 | CHL  | CMD-C2D-C1D | 8.04  | 138.89      | 124.71   |
| 21  | g     | 608 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | G     | 607 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | g     | 605 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | N     | 601 | CHL  | CHD-C1D-ND  | -8.04 | 117.07      | 124.45   |
| 21  | Y     | 607 | CHL  | CHD-C1D-ND  | -8.04 | 117.07      | 124.45   |
| 21  | r     | 306 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | Y     | 606 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | S     | 306 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | n     | 606 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | N     | 607 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | n     | 607 | CHL  | CHD-C1D-ND  | -8.04 | 117.07      | 124.45   |
| 21  | G     | 608 | CHL  | CMD-C2D-C1D | 8.04  | 138.88      | 124.71   |
| 21  | n     | 601 | CHL  | CMD-C2D-C1D | 8.04  | 138.87      | 124.71   |
| 21  | N     | 606 | CHL  | CHD-C1D-ND  | -8.03 | 117.07      | 124.45   |
| 21  | R     | 306 | CHL  | CHD-C1D-ND  | -8.03 | 117.07      | 124.45   |
| 21  | y     | 606 | CHL  | CHD-C1D-ND  | -8.03 | 117.07      | 124.45   |
| 21  | N     | 608 | CHL  | CMD-C2D-C1D | 8.03  | 138.87      | 124.71   |
| 21  | G     | 601 | CHL  | CMD-C2D-C1D | 8.03  | 138.86      | 124.71   |
| 21  | Y     | 601 | CHL  | CMD-C2D-C1D | 8.03  | 138.86      | 124.71   |
| 21  | Y     | 608 | CHL  | CHD-C1D-ND  | -8.03 | 117.08      | 124.45   |
| 21  | S     | 307 | CHL  | CHD-C1D-ND  | -8.03 | 117.08      | 124.45   |
| 21  | N     | 601 | CHL  | CMD-C2D-C1D | 8.03  | 138.86      | 124.71   |
| 21  | g     | 606 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | r     | 301 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | s     | 302 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | y     | 605 | CHL  | CMD-C2D-C1D | 8.02  | 138.85      | 124.71   |
| 21  | G     | 606 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | n     | 606 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | n     | 605 | CHL  | CHD-C1D-ND  | -8.02 | 117.08      | 124.45   |
| 21  | y     | 601 | CHL  | CHD-C1D-ND  | -8.02 | 117.09      | 124.45   |
| 21  | Y     | 607 | CHL  | CMD-C2D-C1D | 8.02  | 138.84      | 124.71   |
| 21  | Y     | 608 | CHL  | CMD-C2D-C1D | 8.01  | 138.83      | 124.71   |
| 21  | r     | 306 | CHL  | CHD-C1D-ND  | -8.01 | 117.09      | 124.45   |
| 21  | N     | 607 | CHL  | CHD-C1D-ND  | -8.01 | 117.10      | 124.45   |
| 21  | y     | 609 | CHL  | CHD-C1D-ND  | -8.00 | 117.10      | 124.45   |
| 24  | n     | 615 | XAT  | C18-C5-C6   | -8.00 | 108.86      | 122.26   |
| 21  | R     | 305 | CHL  | CHD-C1D-ND  | -7.99 | 117.11      | 124.45   |
| 21  | Y     | 601 | CHL  | CHD-C1D-ND  | -7.99 | 117.11      | 124.45   |
| 21  | n     | 608 | CHL  | CHD-C1D-ND  | -7.98 | 117.12      | 124.45   |
| 23  | g     | 616 | LUT  | C38-C25-C24 | -7.94 | 106.57      | 123.56   |
| 24  | Y     | 615 | XAT  | C18-C5-C6   | -7.89 | 109.03      | 122.26   |
| 22  | c     | 510 | CLA  | C3C-C4C-NC  | -7.89 | 101.72      | 110.57   |
| 22  | C     | 511 | CLA  | C3C-C4C-NC  | -7.87 | 101.74      | 110.57   |
| 24  | r     | 314 | XAT  | O4-C5-C18   | -7.79 | 105.72      | 115.06   |
| 24  | R     | 313 | XAT  | O4-C5-C18   | -7.78 | 105.74      | 115.06   |
| 24  | r     | 314 | XAT  | C18-C5-C6   | -7.76 | 109.26      | 122.26   |
| 23  | Y     | 614 | LUT  | C38-C25-C24 | -7.73 | 107.03      | 123.56   |
| 24  | R     | 313 | XAT  | C18-C5-C6   | -7.72 | 109.33      | 122.26   |
| 24  | N     | 616 | XAT  | O4-C5-C18   | -7.66 | 105.88      | 115.06   |
| 25  | y     | 618 | NEX  | C16-C1-C6   | 7.66  | 117.32      | 110.47   |
| 25  | r     | 315 | NEX  | C16-C1-C6   | 7.66  | 117.32      | 110.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | Y     | 614 | LUT  | C31-C30-C29 | -7.52 | 116.57      | 127.31   |
| 24  | Y     | 615 | XAT  | C7-C8-C9    | -7.45 | 113.96      | 125.53   |
| 22  | g     | 613 | CLA  | C4A-NA-C1A  | 7.32  | 110.00      | 106.71   |
| 37  | f     | 101 | HEM  | C3B-C2B-C1B | 7.31  | 111.91      | 106.49   |
| 24  | Y     | 615 | XAT  | O4-C5-C18   | -7.30 | 106.31      | 115.06   |
| 37  | F     | 101 | HEM  | C3B-C2B-C1B | 7.29  | 111.89      | 106.49   |
| 23  | R     | 312 | LUT  | C38-C25-C24 | -7.28 | 107.98      | 123.56   |
| 24  | g     | 617 | XAT  | O4-C5-C18   | -7.28 | 106.34      | 115.06   |
| 22  | c     | 510 | CLA  | C4A-NA-C1A  | 7.28  | 109.98      | 106.71   |
| 23  | r     | 313 | LUT  | C38-C25-C24 | -7.26 | 108.03      | 123.56   |
| 22  | Y     | 611 | CLA  | C4A-NA-C1A  | 7.26  | 109.97      | 106.71   |
| 22  | y     | 612 | CLA  | C4A-NA-C1A  | 7.25  | 109.97      | 106.71   |
| 22  | G     | 613 | CLA  | C4A-NA-C1A  | 7.25  | 109.97      | 106.71   |
| 22  | N     | 612 | CLA  | C4A-NA-C1A  | 7.22  | 109.95      | 106.71   |
| 22  | n     | 612 | CLA  | C4A-NA-C1A  | 7.20  | 109.94      | 106.71   |
| 22  | c     | 514 | CLA  | C4A-NA-C1A  | 7.14  | 109.92      | 106.71   |
| 22  | C     | 511 | CLA  | C4A-NA-C1A  | 7.11  | 109.90      | 106.71   |
| 23  | G     | 615 | LUT  | C38-C25-C24 | -7.11 | 108.36      | 123.56   |
| 23  | n     | 614 | LUT  | C38-C25-C24 | -7.11 | 108.36      | 123.56   |
| 23  | Y     | 613 | LUT  | C38-C25-C24 | -7.10 | 108.37      | 123.56   |
| 22  | g     | 610 | CLA  | C4A-NA-C1A  | 7.10  | 109.90      | 106.71   |
| 23  | y     | 614 | LUT  | C38-C25-C24 | -7.09 | 108.39      | 123.56   |
| 23  | g     | 615 | LUT  | C38-C25-C24 | -7.09 | 108.39      | 123.56   |
| 23  | N     | 614 | LUT  | C38-C25-C24 | -7.09 | 108.40      | 123.56   |
| 22  | C     | 515 | CLA  | C4A-NA-C1A  | 7.08  | 109.89      | 106.71   |
| 24  | y     | 615 | XAT  | C7-C8-C9    | -7.06 | 114.58      | 125.53   |
| 22  | n     | 609 | CLA  | C4A-NA-C1A  | 7.06  | 109.88      | 106.71   |
| 22  | G     | 610 | CLA  | C4A-NA-C1A  | 7.05  | 109.88      | 106.71   |
| 21  | g     | 605 | CHL  | C2C-C3C-C4C | -7.05 | 101.46      | 106.49   |
| 21  | Y     | 608 | CHL  | C2C-C3C-C4C | -7.05 | 101.47      | 106.49   |
| 21  | y     | 605 | CHL  | C2C-C3C-C4C | -7.04 | 101.47      | 106.49   |
| 22  | N     | 609 | CLA  | C4A-NA-C1A  | 7.04  | 109.87      | 106.71   |
| 21  | N     | 601 | CHL  | C2C-C3C-C4C | -7.03 | 101.48      | 106.49   |
| 21  | s     | 302 | CHL  | C2C-C3C-C4C | -7.03 | 101.48      | 106.49   |
| 21  | g     | 609 | CHL  | C2C-C3C-C4C | -7.02 | 101.48      | 106.49   |
| 21  | y     | 606 | CHL  | C2C-C3C-C4C | -7.02 | 101.48      | 106.49   |
| 21  | n     | 605 | CHL  | C2C-C3C-C4C | -7.02 | 101.49      | 106.49   |
| 37  | f     | 101 | HEM  | C2B-C1B-NB  | -7.02 | 101.52      | 109.84   |
| 21  | r     | 308 | CHL  | C2C-C3C-C4C | -7.02 | 101.49      | 106.49   |
| 21  | R     | 305 | CHL  | C2C-C3C-C4C | -7.01 | 101.49      | 106.49   |
| 21  | r     | 306 | CHL  | C2C-C3C-C4C | -7.00 | 101.50      | 106.49   |
| 21  | r     | 301 | CHL  | C2C-C3C-C4C | -7.00 | 101.50      | 106.49   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | F     | 101 | HEM  | C2B-C1B-NB  | -7.00 | 101.55      | 109.84   |
| 21  | s     | 306 | CHL  | C2C-C3C-C4C | -7.00 | 101.50      | 106.49   |
| 21  | g     | 606 | CHL  | C2C-C3C-C4C | -7.00 | 101.50      | 106.49   |
| 21  | n     | 606 | CHL  | C2C-C3C-C4C | -7.00 | 101.50      | 106.49   |
| 24  | y     | 615 | XAT  | O4-C5-C18   | -6.99 | 106.67      | 115.06   |
| 21  | G     | 608 | CHL  | C2C-C3C-C4C | -6.99 | 101.50      | 106.49   |
| 21  | y     | 609 | CHL  | C2C-C3C-C4C | -6.99 | 101.51      | 106.49   |
| 21  | S     | 302 | CHL  | C2C-C3C-C4C | -6.99 | 101.51      | 106.49   |
| 21  | G     | 601 | CHL  | C2C-C3C-C4C | -6.99 | 101.51      | 106.49   |
| 21  | r     | 307 | CHL  | C2C-C3C-C4C | -6.99 | 101.51      | 106.49   |
| 21  | Y     | 607 | CHL  | C2C-C3C-C4C | -6.98 | 101.51      | 106.49   |
| 21  | R     | 307 | CHL  | C2C-C3C-C4C | -6.98 | 101.51      | 106.49   |
| 21  | N     | 607 | CHL  | C2C-C3C-C4C | -6.98 | 101.51      | 106.49   |
| 21  | n     | 607 | CHL  | C2C-C3C-C4C | -6.98 | 101.51      | 106.49   |
| 21  | S     | 306 | CHL  | C2C-C3C-C4C | -6.98 | 101.51      | 106.49   |
| 21  | S     | 301 | CHL  | C2C-C3C-C4C | -6.98 | 101.52      | 106.49   |
| 21  | y     | 601 | CHL  | C2C-C3C-C4C | -6.97 | 101.52      | 106.49   |
| 21  | y     | 607 | CHL  | C2C-C3C-C4C | -6.97 | 101.52      | 106.49   |
| 21  | G     | 606 | CHL  | C2C-C3C-C4C | -6.97 | 101.52      | 106.49   |
| 21  | N     | 606 | CHL  | C2C-C3C-C4C | -6.97 | 101.52      | 106.49   |
| 21  | N     | 608 | CHL  | C2C-C3C-C4C | -6.96 | 101.53      | 106.49   |
| 21  | N     | 605 | CHL  | C2C-C3C-C4C | -6.96 | 101.53      | 106.49   |
| 21  | Y     | 606 | CHL  | C2C-C3C-C4C | -6.96 | 101.53      | 106.49   |
| 21  | g     | 601 | CHL  | C2C-C3C-C4C | -6.96 | 101.53      | 106.49   |
| 21  | G     | 609 | CHL  | C2C-C3C-C4C | -6.95 | 101.54      | 106.49   |
| 21  | Y     | 601 | CHL  | C2C-C3C-C4C | -6.95 | 101.54      | 106.49   |
| 21  | n     | 601 | CHL  | C2C-C3C-C4C | -6.95 | 101.54      | 106.49   |
| 21  | S     | 307 | CHL  | C2C-C3C-C4C | -6.94 | 101.54      | 106.49   |
| 22  | y     | 610 | CLA  | C4A-NA-C1A  | 6.94  | 109.83      | 106.71   |
| 22  | N     | 604 | CLA  | C4A-NA-C1A  | 6.94  | 109.83      | 106.71   |
| 22  | Y     | 609 | CLA  | C4A-NA-C1A  | 6.94  | 109.83      | 106.71   |
| 21  | s     | 307 | CHL  | C2C-C3C-C4C | -6.94 | 101.54      | 106.49   |
| 21  | n     | 608 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | y     | 608 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | G     | 605 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | G     | 607 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | g     | 608 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | s     | 301 | CHL  | C2C-C3C-C4C | -6.93 | 101.55      | 106.49   |
| 21  | g     | 607 | CHL  | C2C-C3C-C4C | -6.92 | 101.56      | 106.49   |
| 22  | c     | 505 | CLA  | C4A-NA-C1A  | 6.92  | 109.82      | 106.71   |
| 21  | R     | 306 | CHL  | C2C-C3C-C4C | -6.91 | 101.56      | 106.49   |
| 21  | Y     | 605 | CHL  | C2C-C3C-C4C | -6.90 | 101.57      | 106.49   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 611 | CLA  | C4A-NA-C1A  | 6.90  | 109.81      | 106.71   |
| 22  | Y     | 604 | CLA  | C4A-NA-C1A  | 6.90  | 109.81      | 106.71   |
| 22  | S     | 305 | CLA  | C4A-NA-C1A  | 6.90  | 109.81      | 106.71   |
| 22  | n     | 604 | CLA  | C4A-NA-C1A  | 6.84  | 109.78      | 106.71   |
| 22  | y     | 604 | CLA  | C4A-NA-C1A  | 6.84  | 109.78      | 106.71   |
| 22  | G     | 612 | CLA  | C4A-NA-C1A  | 6.83  | 109.78      | 106.71   |
| 22  | s     | 305 | CLA  | C4A-NA-C1A  | 6.83  | 109.78      | 106.71   |
| 23  | N     | 615 | LUT  | C31-C30-C29 | -6.82 | 117.58      | 127.31   |
| 22  | G     | 604 | CLA  | C4A-NA-C1A  | 6.79  | 109.76      | 106.71   |
| 25  | y     | 616 | NEX  | O24-C25-C38 | -6.78 | 106.94      | 115.06   |
| 22  | g     | 612 | CLA  | C4A-NA-C1A  | 6.77  | 109.75      | 106.71   |
| 22  | C     | 506 | CLA  | C4A-NA-C1A  | 6.77  | 109.75      | 106.71   |
| 22  | g     | 604 | CLA  | C4A-NA-C1A  | 6.76  | 109.75      | 106.71   |
| 22  | s     | 313 | CLA  | C4A-NA-C1A  | 6.76  | 109.75      | 106.71   |
| 22  | c     | 507 | CLA  | C4A-NA-C1A  | 6.76  | 109.74      | 106.71   |
| 24  | r     | 314 | XAT  | C38-C25-C26 | -6.75 | 110.94      | 122.26   |
| 22  | r     | 312 | CLA  | C4A-NA-C1A  | 6.75  | 109.74      | 106.71   |
| 22  | w     | 101 | CLA  | C4A-NA-C1A  | 6.74  | 109.74      | 106.71   |
| 22  | C     | 508 | CLA  | C4A-NA-C1A  | 6.74  | 109.73      | 106.71   |
| 24  | R     | 313 | XAT  | C38-C25-C26 | -6.73 | 110.97      | 122.26   |
| 22  | b     | 611 | CLA  | C4A-NA-C1A  | 6.73  | 109.73      | 106.71   |
| 22  | n     | 611 | CLA  | C4A-NA-C1A  | 6.72  | 109.73      | 106.71   |
| 22  | b     | 606 | CLA  | C4A-NA-C1A  | 6.72  | 109.73      | 106.71   |
| 22  | W     | 101 | CLA  | C4A-NA-C1A  | 6.72  | 109.73      | 106.71   |
| 22  | d     | 404 | CLA  | C4A-NA-C1A  | 6.71  | 109.72      | 106.71   |
| 22  | S     | 313 | CLA  | C4A-NA-C1A  | 6.70  | 109.72      | 106.71   |
| 22  | D     | 405 | CLA  | C4A-NA-C1A  | 6.70  | 109.72      | 106.71   |
| 24  | G     | 617 | XAT  | O4-C5-C18   | -6.69 | 107.04      | 115.06   |
| 22  | R     | 303 | CLA  | C4A-NA-C1A  | 6.69  | 109.71      | 106.71   |
| 22  | r     | 304 | CLA  | C4A-NA-C1A  | 6.68  | 109.71      | 106.71   |
| 22  | A     | 406 | CLA  | C4A-NA-C1A  | 6.67  | 109.71      | 106.71   |
| 22  | B     | 614 | CLA  | C4A-NA-C1A  | 6.67  | 109.70      | 106.71   |
| 22  | y     | 602 | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 22  | R     | 302 | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 22  | B     | 611 | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 22  | G     | 602 | CLA  | C4A-NA-C1A  | 6.64  | 109.69      | 106.71   |
| 22  | B     | 609 | CLA  | C4A-NA-C1A  | 6.64  | 109.69      | 106.71   |
| 22  | r     | 310 | CLA  | C4A-NA-C1A  | 6.62  | 109.68      | 106.71   |
| 23  | y     | 614 | LUT  | C8-C9-C10   | -6.61 | 108.79      | 118.94   |
| 22  | g     | 602 | CLA  | C4A-NA-C1A  | 6.61  | 109.68      | 106.71   |
| 23  | N     | 615 | LUT  | C11-C10-C9  | -6.60 | 117.89      | 127.31   |
| 22  | r     | 303 | CLA  | C4A-NA-C1A  | 6.59  | 109.67      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 602 | CLA  | C4A-NA-C1A  | 6.59  | 109.67      | 106.71   |
| 22  | A     | 409 | CLA  | C4A-NA-C1A  | 6.59  | 109.67      | 106.71   |
| 22  | b     | 608 | CLA  | C4A-NA-C1A  | 6.58  | 109.67      | 106.71   |
| 24  | y     | 615 | XAT  | C19-C9-C8   | -6.58 | 107.70      | 118.08   |
| 22  | c     | 506 | CLA  | C4A-NA-C1A  | 6.58  | 109.66      | 106.71   |
| 22  | B     | 608 | CLA  | C4A-NA-C1A  | 6.58  | 109.66      | 106.71   |
| 22  | n     | 602 | CLA  | C4A-NA-C1A  | 6.58  | 109.66      | 106.71   |
| 23  | N     | 614 | LUT  | C8-C9-C10   | -6.57 | 108.85      | 118.94   |
| 23  | g     | 616 | LUT  | C20-C13-C12 | -6.57 | 107.72      | 118.08   |
| 23  | G     | 615 | LUT  | C8-C9-C10   | -6.57 | 108.86      | 118.94   |
| 24  | Y     | 615 | XAT  | C19-C9-C8   | -6.57 | 107.73      | 118.08   |
| 22  | R     | 311 | CLA  | C4A-NA-C1A  | 6.56  | 109.66      | 106.71   |
| 22  | b     | 605 | CLA  | C4A-NA-C1A  | 6.56  | 109.66      | 106.71   |
| 23  | Y     | 613 | LUT  | C8-C9-C10   | -6.56 | 108.88      | 118.94   |
| 25  | Y     | 616 | NEX  | O24-C25-C38 | -6.56 | 107.20      | 115.06   |
| 22  | R     | 304 | CLA  | C4A-NA-C1A  | 6.56  | 109.65      | 106.71   |
| 22  | R     | 308 | CLA  | C4A-NA-C1A  | 6.56  | 109.65      | 106.71   |
| 23  | g     | 615 | LUT  | C8-C9-C10   | -6.55 | 108.89      | 118.94   |
| 23  | n     | 614 | LUT  | C8-C9-C10   | -6.55 | 108.89      | 118.94   |
| 24  | R     | 313 | XAT  | C8-C9-C10   | -6.55 | 108.89      | 118.94   |
| 22  | s     | 312 | CLA  | C4A-NA-C1A  | 6.55  | 109.65      | 106.71   |
| 22  | a     | 405 | CLA  | C4A-NA-C1A  | 6.55  | 109.65      | 106.71   |
| 22  | B     | 604 | CLA  | C4A-NA-C1A  | 6.55  | 109.65      | 106.71   |
| 22  | b     | 601 | CLA  | C4A-NA-C1A  | 6.54  | 109.64      | 106.71   |
| 22  | Y     | 602 | CLA  | C4A-NA-C1A  | 6.53  | 109.64      | 106.71   |
| 22  | B     | 606 | CLA  | C4A-NA-C1A  | 6.53  | 109.64      | 106.71   |
| 24  | r     | 314 | XAT  | C8-C9-C10   | -6.53 | 108.93      | 118.94   |
| 22  | x     | 101 | CLA  | C4A-NA-C1A  | 6.52  | 109.64      | 106.71   |
| 22  | r     | 305 | CLA  | C4A-NA-C1A  | 6.52  | 109.64      | 106.71   |
| 22  | r     | 309 | CLA  | C4A-NA-C1A  | 6.51  | 109.63      | 106.71   |
| 25  | Y     | 616 | NEX  | C32-C33-C34 | -6.51 | 108.96      | 118.94   |
| 22  | b     | 610 | CLA  | C4A-NA-C1A  | 6.51  | 109.63      | 106.71   |
| 22  | R     | 309 | CLA  | C4A-NA-C1A  | 6.51  | 109.63      | 106.71   |
| 22  | B     | 613 | CLA  | C4A-NA-C1A  | 6.50  | 109.63      | 106.71   |
| 22  | b     | 613 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 22  | b     | 602 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 22  | b     | 615 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 22  | a     | 408 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 22  | d     | 403 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 22  | S     | 312 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 22  | B     | 607 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 22  | C     | 507 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 509 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 22  | b     | 603 | CLA  | C4A-NA-C1A  | 6.45  | 109.60      | 106.71   |
| 22  | B     | 618 | CLA  | C4A-NA-C1A  | 6.44  | 109.60      | 106.71   |
| 22  | C     | 505 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 22  | D     | 404 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 22  | B     | 616 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 22  | B     | 605 | CLA  | C4A-NA-C1A  | 6.42  | 109.59      | 106.71   |
| 23  | G     | 616 | LUT  | C20-C13-C12 | -6.42 | 107.97      | 118.08   |
| 22  | a     | 406 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 22  | c     | 502 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 22  | A     | 407 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 22  | b     | 607 | CLA  | C4A-NA-C1A  | 6.38  | 109.58      | 106.71   |
| 22  | c     | 508 | CLA  | C4A-NA-C1A  | 6.38  | 109.58      | 106.71   |
| 22  | B     | 603 | CLA  | C4A-NA-C1A  | 6.38  | 109.57      | 106.71   |
| 22  | c     | 504 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 22  | G     | 614 | CLA  | C4A-NA-C1A  | 6.36  | 109.57      | 106.71   |
| 22  | C     | 504 | CLA  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 22  | B     | 612 | CLA  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 22  | C     | 510 | CLA  | C4A-NA-C1A  | 6.35  | 109.56      | 106.71   |
| 22  | c     | 503 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | S     | 309 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | b     | 604 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | B     | 610 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | c     | 509 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | C     | 503 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 22  | A     | 405 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 23  | Y     | 614 | LUT  | C28-C29-C30 | -6.32 | 109.24      | 118.94   |
| 22  | s     | 309 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 22  | R     | 310 | CLA  | C4A-NA-C1A  | 6.31  | 109.54      | 106.71   |
| 22  | Y     | 612 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 22  | B     | 615 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 22  | g     | 614 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 22  | G     | 611 | CLA  | C4A-NA-C1A  | 6.29  | 109.54      | 106.71   |
| 23  | G     | 616 | LUT  | C40-C33-C32 | -6.29 | 108.16      | 118.08   |
| 22  | n     | 613 | CLA  | C4A-NA-C1A  | 6.29  | 109.53      | 106.71   |
| 22  | b     | 609 | CLA  | C4A-NA-C1A  | 6.29  | 109.53      | 106.71   |
| 24  | g     | 617 | XAT  | C38-C25-C26 | -6.28 | 111.74      | 122.26   |
| 25  | N     | 617 | NEX  | C32-C33-C34 | -6.27 | 109.32      | 118.94   |
| 22  | N     | 613 | CLA  | C4A-NA-C1A  | 6.26  | 109.52      | 106.71   |
| 22  | a     | 404 | CLA  | C4A-NA-C1A  | 6.26  | 109.52      | 106.71   |
| 22  | g     | 611 | CLA  | C4A-NA-C1A  | 6.25  | 109.52      | 106.71   |
| 22  | y     | 611 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | r     | 311 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 23  | g     | 616 | LUT  | C40-C33-C32 | -6.23 | 108.27      | 118.08   |
| 22  | C     | 511 | CLA  | C1D-ND-C4D  | 6.23  | 110.76      | 106.33   |
| 22  | n     | 610 | CLA  | C4A-NA-C1A  | 6.23  | 109.50      | 106.71   |
| 22  | y     | 613 | CLA  | C4A-NA-C1A  | 6.22  | 109.50      | 106.71   |
| 25  | n     | 616 | NEX  | C32-C33-C34 | -6.22 | 109.40      | 118.94   |
| 25  | g     | 618 | NEX  | O24-C25-C38 | -6.21 | 107.61      | 115.06   |
| 23  | Y     | 614 | LUT  | C40-C33-C32 | -6.21 | 108.30      | 118.08   |
| 24  | N     | 616 | XAT  | C38-C25-C26 | -6.21 | 111.86      | 122.26   |
| 22  | c     | 510 | CLA  | C1D-ND-C4D  | 6.20  | 110.74      | 106.33   |
| 22  | b     | 612 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 24  | Y     | 615 | XAT  | C20-C13-C12 | -6.19 | 108.32      | 118.08   |
| 22  | N     | 610 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 22  | Y     | 610 | CLA  | C4A-NA-C1A  | 6.18  | 109.48      | 106.71   |
| 22  | C     | 513 | CLA  | C4A-NA-C1A  | 6.17  | 109.48      | 106.71   |
| 24  | N     | 616 | XAT  | C19-C9-C8   | -6.16 | 108.37      | 118.08   |
| 24  | Y     | 615 | XAT  | C40-C33-C32 | -6.16 | 108.38      | 118.08   |
| 25  | Y     | 616 | NEX  | C2-C1-C6    | 6.15  | 115.19      | 109.21   |
| 23  | R     | 312 | LUT  | C28-C29-C30 | -6.14 | 109.52      | 118.94   |
| 22  | g     | 613 | CLA  | CMC-C2C-C1C | 6.14  | 134.39      | 125.04   |
| 24  | Y     | 615 | XAT  | C39-C29-C28 | -6.13 | 108.41      | 118.08   |
| 24  | y     | 615 | XAT  | C38-C25-C26 | -6.13 | 111.98      | 122.26   |
| 22  | n     | 612 | CLA  | CMC-C2C-C1C | 6.13  | 134.38      | 125.04   |
| 22  | y     | 612 | CLA  | CMC-C2C-C1C | 6.13  | 134.37      | 125.04   |
| 22  | c     | 512 | CLA  | C4A-NA-C1A  | 6.13  | 109.46      | 106.71   |
| 22  | N     | 612 | CLA  | CMC-C2C-C1C | 6.13  | 134.37      | 125.04   |
| 22  | G     | 613 | CLA  | CMC-C2C-C1C | 6.13  | 134.37      | 125.04   |
| 23  | Y     | 614 | LUT  | C20-C13-C12 | -6.13 | 108.43      | 118.08   |
| 23  | r     | 313 | LUT  | C28-C29-C30 | -6.12 | 109.55      | 118.94   |
| 22  | C     | 512 | CLA  | C4A-NA-C1A  | 6.12  | 109.46      | 106.71   |
| 22  | n     | 603 | CLA  | C4A-NA-C1A  | 6.11  | 109.45      | 106.71   |
| 22  | s     | 303 | CLA  | C4A-NA-C1A  | 6.11  | 109.45      | 106.71   |
| 22  | c     | 511 | CLA  | C4A-NA-C1A  | 6.10  | 109.45      | 106.71   |
| 22  | Y     | 611 | CLA  | CMC-C2C-C1C | 6.10  | 134.32      | 125.04   |
| 24  | y     | 615 | XAT  | C39-C29-C28 | -6.09 | 108.48      | 118.08   |
| 22  | b     | 614 | CLA  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 22  | B     | 617 | CLA  | C4A-NA-C1A  | 6.08  | 109.44      | 106.71   |
| 22  | g     | 603 | CLA  | C4A-NA-C1A  | 6.08  | 109.44      | 106.71   |
| 22  | N     | 603 | CLA  | C4A-NA-C1A  | 6.07  | 109.43      | 106.71   |
| 24  | N     | 616 | XAT  | C27-C28-C29 | -6.06 | 116.12      | 125.53   |
| 22  | c     | 513 | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 22  | S     | 304 | CLA  | C4A-NA-C1A  | 6.05  | 109.43      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Y     | 603 | CLA  | C4A-NA-C1A  | 6.05  | 109.43      | 106.71   |
| 22  | G     | 603 | CLA  | C4A-NA-C1A  | 6.05  | 109.42      | 106.71   |
| 22  | S     | 303 | CLA  | C4A-NA-C1A  | 6.05  | 109.42      | 106.71   |
| 24  | g     | 617 | XAT  | C39-C29-C28 | -6.04 | 108.57      | 118.08   |
| 21  | G     | 609 | CHL  | C1B-CHB-C4A | -6.02 | 118.19      | 130.12   |
| 21  | g     | 605 | CHL  | C1B-CHB-C4A | -6.02 | 118.19      | 130.12   |
| 24  | Y     | 615 | XAT  | C38-C25-C26 | -6.02 | 112.17      | 122.26   |
| 21  | R     | 307 | CHL  | C1B-CHB-C4A | -6.02 | 118.20      | 130.12   |
| 24  | n     | 615 | XAT  | C19-C9-C8   | -6.01 | 108.60      | 118.08   |
| 21  | r     | 307 | CHL  | C1B-CHB-C4A | -6.01 | 118.21      | 130.12   |
| 22  | s     | 310 | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 21  | g     | 606 | CHL  | C1B-CHB-C4A | -6.00 | 118.23      | 130.12   |
| 21  | g     | 607 | CHL  | C1B-CHB-C4A | -6.00 | 118.23      | 130.12   |
| 21  | G     | 607 | CHL  | C1B-CHB-C4A | -6.00 | 118.23      | 130.12   |
| 21  | s     | 306 | CHL  | C1B-CHB-C4A | -6.00 | 118.23      | 130.12   |
| 21  | G     | 601 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 21  | N     | 601 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 24  | y     | 615 | XAT  | C40-C33-C32 | -6.00 | 108.62      | 118.08   |
| 21  | g     | 608 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 21  | n     | 601 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 22  | S     | 310 | CLA  | C4A-NA-C1A  | 6.00  | 109.40      | 106.71   |
| 21  | Y     | 601 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 21  | S     | 301 | CHL  | C1B-CHB-C4A | -6.00 | 118.24      | 130.12   |
| 21  | S     | 306 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 22  | C     | 514 | CLA  | C4A-NA-C1A  | 5.99  | 109.40      | 106.71   |
| 21  | Y     | 605 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | S     | 302 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | N     | 608 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | r     | 306 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | s     | 307 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | N     | 607 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | n     | 608 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | r     | 308 | CHL  | C1B-CHB-C4A | -5.99 | 118.25      | 130.12   |
| 21  | N     | 605 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | n     | 605 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | R     | 306 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | n     | 607 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | Y     | 607 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | y     | 607 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | G     | 608 | CHL  | C1B-CHB-C4A | -5.99 | 118.26      | 130.12   |
| 21  | y     | 605 | CHL  | C1B-CHB-C4A | -5.98 | 118.27      | 130.12   |
| 21  | y     | 601 | CHL  | C1B-CHB-C4A | -5.98 | 118.27      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | s     | 304 | CLA  | C4A-NA-C1A  | 5.98  | 109.40      | 106.71   |
| 21  | s     | 302 | CHL  | C1B-CHB-C4A | -5.98 | 118.27      | 130.12   |
| 21  | y     | 606 | CHL  | C1B-CHB-C4A | -5.98 | 118.27      | 130.12   |
| 21  | R     | 305 | CHL  | C1B-CHB-C4A | -5.98 | 118.27      | 130.12   |
| 21  | g     | 609 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | G     | 606 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | S     | 307 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | y     | 608 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | s     | 301 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | Y     | 608 | CHL  | C1B-CHB-C4A | -5.98 | 118.28      | 130.12   |
| 21  | g     | 601 | CHL  | C1B-CHB-C4A | -5.97 | 118.29      | 130.12   |
| 21  | r     | 301 | CHL  | C1B-CHB-C4A | -5.97 | 118.29      | 130.12   |
| 24  | G     | 617 | XAT  | C39-C29-C28 | -5.97 | 108.67      | 118.08   |
| 21  | y     | 609 | CHL  | C1B-CHB-C4A | -5.97 | 118.30      | 130.12   |
| 21  | G     | 605 | CHL  | C1B-CHB-C4A | -5.97 | 118.30      | 130.12   |
| 21  | n     | 606 | CHL  | C1B-CHB-C4A | -5.97 | 118.30      | 130.12   |
| 21  | N     | 606 | CHL  | C1B-CHB-C4A | -5.96 | 118.31      | 130.12   |
| 21  | Y     | 606 | CHL  | C1B-CHB-C4A | -5.96 | 118.31      | 130.12   |
| 37  | F     | 101 | HEM  | C4C-CHD-C1D | 5.95  | 130.41      | 122.56   |
| 24  | y     | 615 | XAT  | C20-C13-C12 | -5.94 | 108.71      | 118.08   |
| 25  | y     | 616 | NEX  | C2-C1-C6    | 5.94  | 114.99      | 109.21   |
| 22  | s     | 308 | CLA  | C4A-NA-C1A  | 5.94  | 109.38      | 106.71   |
| 21  | s     | 307 | CHL  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 22  | y     | 603 | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 22  | S     | 311 | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 21  | g     | 606 | CHL  | C4A-NA-C1A  | 5.92  | 109.37      | 106.71   |
| 24  | G     | 617 | XAT  | C38-C25-C26 | -5.92 | 112.34      | 122.26   |
| 21  | R     | 306 | CHL  | C4A-NA-C1A  | 5.92  | 109.37      | 106.71   |
| 37  | f     | 101 | HEM  | C4C-CHD-C1D | 5.91  | 130.36      | 122.56   |
| 21  | r     | 307 | CHL  | C4A-NA-C1A  | 5.90  | 109.36      | 106.71   |
| 21  | G     | 601 | CHL  | C4A-NA-C1A  | 5.89  | 109.35      | 106.71   |
| 21  | Y     | 608 | CHL  | C4A-NA-C1A  | 5.89  | 109.35      | 106.71   |
| 23  | g     | 615 | LUT  | C12-C13-C14 | -5.88 | 109.91      | 118.94   |
| 21  | S     | 307 | CHL  | C4A-NA-C1A  | 5.88  | 109.35      | 106.71   |
| 23  | N     | 614 | LUT  | C12-C13-C14 | -5.88 | 109.92      | 118.94   |
| 23  | G     | 615 | LUT  | C12-C13-C14 | -5.87 | 109.93      | 118.94   |
| 23  | n     | 614 | LUT  | C12-C13-C14 | -5.87 | 109.93      | 118.94   |
| 21  | S     | 306 | CHL  | C4A-NA-C1A  | 5.87  | 109.35      | 106.71   |
| 23  | y     | 614 | LUT  | C12-C13-C14 | -5.87 | 109.93      | 118.94   |
| 21  | g     | 609 | CHL  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |
| 21  | y     | 601 | CHL  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |
| 21  | G     | 609 | CHL  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | g     | 607 | CHL  | C4A-NA-C1A  | 5.86  | 109.34      | 106.71   |
| 23  | r     | 313 | LUT  | C40-C33-C32 | -5.86 | 108.84      | 118.08   |
| 23  | Y     | 613 | LUT  | C12-C13-C14 | -5.86 | 109.95      | 118.94   |
| 25  | g     | 618 | NEX  | C32-C33-C34 | -5.86 | 109.95      | 118.94   |
| 21  | g     | 601 | CHL  | C4A-NA-C1A  | 5.85  | 109.34      | 106.71   |
| 21  | s     | 306 | CHL  | C4A-NA-C1A  | 5.85  | 109.34      | 106.71   |
| 25  | n     | 616 | NEX  | O24-C25-C38 | -5.85 | 108.05      | 115.06   |
| 21  | y     | 607 | CHL  | C4A-NA-C1A  | 5.85  | 109.33      | 106.71   |
| 21  | N     | 605 | CHL  | C4A-NA-C1A  | 5.85  | 109.33      | 106.71   |
| 21  | R     | 307 | CHL  | C4A-NA-C1A  | 5.85  | 109.33      | 106.71   |
| 23  | R     | 312 | LUT  | C40-C33-C32 | -5.84 | 108.87      | 118.08   |
| 21  | g     | 605 | CHL  | C4A-NA-C1A  | 5.84  | 109.33      | 106.71   |
| 21  | G     | 606 | CHL  | C4A-NA-C1A  | 5.84  | 109.33      | 106.71   |
| 21  | N     | 601 | CHL  | C4A-NA-C1A  | 5.84  | 109.33      | 106.71   |
| 22  | C     | 511 | CLA  | CHD-C4C-C3C | 5.84  | 133.42      | 124.84   |
| 21  | r     | 308 | CHL  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 21  | y     | 609 | CHL  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 21  | y     | 606 | CHL  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 21  | N     | 607 | CHL  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 21  | Y     | 607 | CHL  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 21  | Y     | 606 | CHL  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 21  | n     | 608 | CHL  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 21  | G     | 608 | CHL  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 21  | Y     | 605 | CHL  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 22  | c     | 510 | CLA  | CHD-C4C-C3C | 5.81  | 133.39      | 124.84   |
| 21  | N     | 606 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 21  | R     | 305 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 23  | r     | 313 | LUT  | C19-C9-C8   | -5.81 | 108.92      | 118.08   |
| 21  | r     | 301 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 21  | y     | 605 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 21  | s     | 301 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 25  | y     | 616 | NEX  | C32-C33-C34 | -5.81 | 110.03      | 118.94   |
| 21  | Y     | 601 | CHL  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 23  | R     | 312 | LUT  | C19-C9-C8   | -5.81 | 108.93      | 118.08   |
| 21  | N     | 608 | CHL  | C4A-NA-C1A  | 5.80  | 109.31      | 106.71   |
| 24  | n     | 615 | XAT  | C39-C29-C28 | -5.80 | 108.94      | 118.08   |
| 21  | n     | 601 | CHL  | C4A-NA-C1A  | 5.80  | 109.31      | 106.71   |
| 22  | s     | 311 | CLA  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |
| 37  | F     | 101 | HEM  | C3D-C4D-ND  | -5.79 | 103.72      | 110.17   |
| 21  | n     | 605 | CHL  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |
| 37  | f     | 101 | HEM  | C3D-C4D-ND  | -5.79 | 103.72      | 110.17   |
| 21  | S     | 302 | CHL  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | g     | 617 | XAT  | C19-C9-C8   | -5.78 | 108.97      | 118.08   |
| 21  | r     | 306 | CHL  | C4A-NA-C1A  | 5.78  | 109.30      | 106.71   |
| 22  | S     | 308 | CLA  | C4A-NA-C1A  | 5.78  | 109.30      | 106.71   |
| 21  | S     | 301 | CHL  | C4A-NA-C1A  | 5.78  | 109.30      | 106.71   |
| 24  | n     | 615 | XAT  | C38-C25-C26 | -5.77 | 112.59      | 122.26   |
| 25  | r     | 315 | NEX  | C40-C33-C32 | -5.76 | 109.00      | 118.08   |
| 23  | N     | 615 | LUT  | C20-C13-C12 | -5.76 | 109.00      | 118.08   |
| 24  | r     | 314 | XAT  | C20-C13-C12 | -5.76 | 109.01      | 118.08   |
| 21  | n     | 606 | CHL  | C4A-NA-C1A  | 5.75  | 109.29      | 106.71   |
| 24  | G     | 617 | XAT  | C40-C33-C32 | -5.75 | 109.02      | 118.08   |
| 23  | r     | 313 | LUT  | C32-C33-C34 | -5.75 | 110.12      | 118.94   |
| 23  | R     | 312 | LUT  | C32-C33-C34 | -5.74 | 110.13      | 118.94   |
| 21  | g     | 608 | CHL  | C4A-NA-C1A  | 5.74  | 109.29      | 106.71   |
| 24  | N     | 616 | XAT  | C12-C13-C14 | -5.74 | 110.14      | 118.94   |
| 25  | N     | 617 | NEX  | C20-C13-C12 | -5.74 | 109.04      | 118.08   |
| 25  | y     | 618 | NEX  | C40-C33-C32 | -5.73 | 109.04      | 118.08   |
| 21  | n     | 607 | CHL  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 21  | G     | 605 | CHL  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 24  | n     | 615 | XAT  | C40-C33-C32 | -5.73 | 109.04      | 118.08   |
| 21  | y     | 608 | CHL  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 25  | g     | 618 | NEX  | C2-C1-C6    | 5.72  | 114.77      | 109.21   |
| 25  | r     | 315 | NEX  | C12-C13-C14 | -5.72 | 110.16      | 118.94   |
| 21  | G     | 607 | CHL  | C4A-NA-C1A  | 5.72  | 109.28      | 106.71   |
| 21  | s     | 302 | CHL  | C4A-NA-C1A  | 5.71  | 109.27      | 106.71   |
| 24  | R     | 313 | XAT  | C20-C13-C12 | -5.70 | 109.10      | 118.08   |
| 24  | n     | 615 | XAT  | C12-C13-C14 | -5.69 | 110.20      | 118.94   |
| 25  | y     | 616 | NEX  | C28-C29-C30 | -5.69 | 110.21      | 118.94   |
| 23  | G     | 615 | LUT  | C28-C29-C30 | -5.69 | 110.22      | 118.94   |
| 23  | Y     | 613 | LUT  | C28-C29-C30 | -5.69 | 110.22      | 118.94   |
| 24  | R     | 313 | XAT  | C39-C29-C28 | -5.68 | 109.12      | 118.08   |
| 23  | y     | 614 | LUT  | C28-C29-C30 | -5.68 | 110.22      | 118.94   |
| 23  | N     | 614 | LUT  | C28-C29-C30 | -5.68 | 110.22      | 118.94   |
| 23  | n     | 614 | LUT  | C28-C29-C30 | -5.68 | 110.22      | 118.94   |
| 25  | y     | 618 | NEX  | C12-C13-C14 | -5.68 | 110.22      | 118.94   |
| 24  | g     | 617 | XAT  | C40-C33-C32 | -5.68 | 109.13      | 118.08   |
| 23  | g     | 615 | LUT  | C28-C29-C30 | -5.68 | 110.23      | 118.94   |
| 23  | N     | 615 | LUT  | C32-C33-C34 | -5.67 | 110.23      | 118.94   |
| 23  | g     | 616 | LUT  | C28-C29-C30 | -5.66 | 110.26      | 118.94   |
| 25  | Y     | 616 | NEX  | C40-C33-C32 | -5.65 | 109.17      | 118.08   |
| 24  | G     | 617 | XAT  | C19-C9-C8   | -5.64 | 109.19      | 118.08   |
| 24  | r     | 314 | XAT  | C39-C29-C28 | -5.64 | 109.20      | 118.08   |
| 23  | g     | 616 | LUT  | C7-C8-C9    | -5.63 | 117.72      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | N     | 616 | XAT  | C20-C13-C12 | -5.63 | 109.21      | 118.08   |
| 23  | G     | 616 | LUT  | C28-C29-C30 | -5.62 | 110.31      | 118.94   |
| 24  | n     | 615 | XAT  | C27-C28-C29 | -5.61 | 116.83      | 125.53   |
| 37  | F     | 101 | HEM  | C4B-C3B-C2B | 5.61  | 111.57      | 107.11   |
| 37  | f     | 101 | HEM  | CHC-C4B-C3B | 5.61  | 133.16      | 124.57   |
| 37  | f     | 101 | HEM  | C4B-C3B-C2B | 5.61  | 111.57      | 107.11   |
| 37  | f     | 101 | HEM  | C2D-C1D-ND  | -5.61 | 103.16      | 109.88   |
| 37  | F     | 101 | HEM  | C2D-C1D-ND  | -5.61 | 103.17      | 109.88   |
| 24  | R     | 313 | XAT  | C19-C9-C8   | -5.61 | 109.24      | 118.08   |
| 37  | F     | 101 | HEM  | CHC-C4B-C3B | 5.60  | 133.14      | 124.57   |
| 24  | r     | 314 | XAT  | C19-C9-C8   | -5.59 | 109.27      | 118.08   |
| 24  | n     | 615 | XAT  | C20-C13-C12 | -5.58 | 109.28      | 118.08   |
| 25  | n     | 616 | NEX  | C2-C1-C6    | 5.58  | 114.63      | 109.21   |
| 23  | G     | 615 | LUT  | C39-C29-C28 | -5.57 | 109.30      | 118.08   |
| 23  | g     | 615 | LUT  | C39-C29-C28 | -5.57 | 109.30      | 118.08   |
| 24  | G     | 617 | XAT  | C27-C28-C29 | -5.57 | 116.89      | 125.53   |
| 23  | Y     | 613 | LUT  | C39-C29-C28 | -5.57 | 109.31      | 118.08   |
| 23  | N     | 614 | LUT  | C39-C29-C28 | -5.56 | 109.31      | 118.08   |
| 25  | Y     | 616 | NEX  | C20-C13-C12 | -5.56 | 109.32      | 118.08   |
| 24  | g     | 617 | XAT  | C12-C13-C14 | -5.56 | 110.42      | 118.94   |
| 23  | n     | 614 | LUT  | C39-C29-C28 | -5.55 | 109.33      | 118.08   |
| 23  | y     | 614 | LUT  | C39-C29-C28 | -5.55 | 109.34      | 118.08   |
| 24  | g     | 617 | XAT  | C20-C13-C12 | -5.55 | 109.34      | 118.08   |
| 25  | r     | 315 | NEX  | C39-C29-C28 | -5.53 | 109.36      | 118.08   |
| 25  | y     | 618 | NEX  | C39-C29-C28 | -5.53 | 109.37      | 118.08   |
| 25  | Y     | 616 | NEX  | C39-C29-C28 | -5.52 | 109.38      | 118.08   |
| 25  | n     | 616 | NEX  | C20-C13-C12 | -5.52 | 109.38      | 118.08   |
| 25  | g     | 618 | NEX  | C28-C29-C30 | -5.52 | 110.47      | 118.94   |
| 25  | y     | 618 | NEX  | C20-C13-C12 | -5.49 | 109.43      | 118.08   |
| 23  | G     | 616 | LUT  | C7-C8-C9    | -5.48 | 117.95      | 126.23   |
| 24  | R     | 313 | XAT  | C40-C33-C32 | -5.48 | 109.45      | 118.08   |
| 25  | N     | 617 | NEX  | C40-C33-C32 | -5.47 | 109.45      | 118.08   |
| 25  | g     | 618 | NEX  | C20-C13-C12 | -5.47 | 109.45      | 118.08   |
| 24  | r     | 314 | XAT  | C40-C33-C32 | -5.46 | 109.48      | 118.08   |
| 25  | r     | 315 | NEX  | C20-C13-C12 | -5.46 | 109.48      | 118.08   |
| 25  | y     | 616 | NEX  | C20-C13-C12 | -5.45 | 109.49      | 118.08   |
| 24  | G     | 617 | XAT  | C20-C13-C12 | -5.43 | 109.52      | 118.08   |
| 23  | N     | 614 | LUT  | C20-C13-C12 | -5.41 | 109.55      | 118.08   |
| 23  | N     | 615 | LUT  | C39-C29-C28 | -5.40 | 109.57      | 118.08   |
| 23  | y     | 614 | LUT  | C20-C13-C12 | -5.40 | 109.58      | 118.08   |
| 23  | Y     | 613 | LUT  | C20-C13-C12 | -5.39 | 109.58      | 118.08   |
| 23  | n     | 614 | LUT  | C20-C13-C12 | -5.39 | 109.58      | 118.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | G     | 615 | LUT  | C20-C13-C12 | -5.39 | 109.59      | 118.08   |
| 23  | g     | 615 | LUT  | C20-C13-C12 | -5.38 | 109.60      | 118.08   |
| 23  | N     | 615 | LUT  | C28-C29-C30 | -5.37 | 110.70      | 118.94   |
| 24  | N     | 616 | XAT  | C40-C33-C32 | -5.35 | 109.64      | 118.08   |
| 23  | g     | 616 | LUT  | C39-C29-C28 | -5.35 | 109.64      | 118.08   |
| 25  | N     | 617 | NEX  | C39-C29-C28 | -5.35 | 109.64      | 118.08   |
| 25  | y     | 618 | NEX  | C32-C33-C34 | -5.31 | 110.79      | 118.94   |
| 25  | r     | 315 | NEX  | C32-C33-C34 | -5.30 | 110.81      | 118.94   |
| 25  | g     | 618 | NEX  | C39-C29-C28 | -5.29 | 109.74      | 118.08   |
| 23  | N     | 614 | LUT  | C32-C33-C34 | -5.29 | 110.82      | 118.94   |
| 23  | g     | 615 | LUT  | C32-C33-C34 | -5.28 | 110.84      | 118.94   |
| 23  | G     | 615 | LUT  | C32-C33-C34 | -5.28 | 110.84      | 118.94   |
| 25  | y     | 616 | NEX  | C39-C29-C28 | -5.28 | 109.76      | 118.08   |
| 25  | n     | 616 | NEX  | C39-C29-C28 | -5.27 | 109.78      | 118.08   |
| 23  | y     | 614 | LUT  | C32-C33-C34 | -5.27 | 110.86      | 118.94   |
| 23  | n     | 614 | LUT  | C32-C33-C34 | -5.27 | 110.86      | 118.94   |
| 23  | G     | 616 | LUT  | C39-C29-C28 | -5.26 | 109.79      | 118.08   |
| 23  | Y     | 613 | LUT  | C40-C33-C32 | -5.25 | 109.80      | 118.08   |
| 23  | R     | 312 | LUT  | C8-C9-C10   | -5.25 | 110.89      | 118.94   |
| 23  | Y     | 613 | LUT  | C32-C33-C34 | -5.25 | 110.89      | 118.94   |
| 23  | N     | 615 | LUT  | C40-C33-C32 | -5.24 | 109.81      | 118.08   |
| 25  | y     | 616 | NEX  | C12-C13-C14 | -5.24 | 110.90      | 118.94   |
| 23  | g     | 615 | LUT  | C40-C33-C32 | -5.24 | 109.83      | 118.08   |
| 23  | r     | 313 | LUT  | C8-C9-C10   | -5.24 | 110.91      | 118.94   |
| 23  | N     | 614 | LUT  | C40-C33-C32 | -5.23 | 109.83      | 118.08   |
| 25  | n     | 616 | NEX  | C12-C13-C14 | -5.23 | 110.92      | 118.94   |
| 23  | G     | 615 | LUT  | C40-C33-C32 | -5.22 | 109.84      | 118.08   |
| 25  | y     | 616 | NEX  | C40-C33-C32 | -5.22 | 109.85      | 118.08   |
| 23  | y     | 614 | LUT  | C40-C33-C32 | -5.22 | 109.85      | 118.08   |
| 23  | n     | 614 | LUT  | C40-C33-C32 | -5.20 | 109.88      | 118.08   |
| 24  | n     | 615 | XAT  | C8-C9-C10   | -5.20 | 110.96      | 118.94   |
| 24  | Y     | 615 | XAT  | C27-C28-C29 | -5.20 | 117.47      | 125.53   |
| 23  | r     | 313 | LUT  | C39-C29-C28 | -5.19 | 109.89      | 118.08   |
| 23  | R     | 312 | LUT  | C39-C29-C28 | -5.16 | 109.94      | 118.08   |
| 25  | g     | 618 | NEX  | C12-C13-C14 | -5.15 | 111.04      | 118.94   |
| 25  | N     | 617 | NEX  | C28-C29-C30 | -5.15 | 111.04      | 118.94   |
| 24  | g     | 617 | XAT  | C27-C28-C29 | -5.15 | 117.55      | 125.53   |
| 24  | g     | 617 | XAT  | C7-C8-C9    | -5.13 | 117.56      | 125.53   |
| 25  | N     | 617 | NEX  | C12-C13-C14 | -5.13 | 111.07      | 118.94   |
| 24  | N     | 616 | XAT  | C7-C8-C9    | -5.11 | 117.61      | 125.53   |
| 22  | Y     | 611 | CLA  | CHC-C1C-NC  | -5.10 | 116.46      | 124.20   |
| 24  | G     | 617 | XAT  | C7-C8-C9    | -5.10 | 117.62      | 125.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | y     | 612 | CLA  | CHC-C1C-NC  | -5.10 | 116.47      | 124.20   |
| 22  | G     | 613 | CLA  | CHC-C1C-NC  | -5.10 | 116.47      | 124.20   |
| 22  | n     | 612 | CLA  | CHC-C1C-NC  | -5.08 | 116.50      | 124.20   |
| 22  | g     | 613 | CLA  | CHC-C1C-NC  | -5.08 | 116.50      | 124.20   |
| 24  | y     | 615 | XAT  | C27-C28-C29 | -5.06 | 117.68      | 125.53   |
| 24  | G     | 617 | XAT  | C12-C13-C14 | -5.06 | 111.18      | 118.94   |
| 22  | N     | 612 | CLA  | CHC-C1C-NC  | -5.06 | 116.53      | 124.20   |
| 24  | G     | 617 | XAT  | O24-C25-C38 | -5.05 | 109.00      | 115.06   |
| 25  | g     | 618 | NEX  | C40-C33-C32 | -5.04 | 110.14      | 118.08   |
| 25  | Y     | 616 | NEX  | C12-C13-C14 | -5.04 | 111.21      | 118.94   |
| 21  | s     | 307 | CHL  | O2D-CGD-CBD | 5.03  | 120.21      | 111.27   |
| 21  | R     | 306 | CHL  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 21  | G     | 608 | CHL  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 21  | G     | 601 | CHL  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 21  | y     | 606 | CHL  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 21  | n     | 605 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | G     | 606 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | S     | 302 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | Y     | 601 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | g     | 601 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | N     | 601 | CHL  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 21  | y     | 608 | CHL  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 21  | s     | 302 | CHL  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 21  | n     | 606 | CHL  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 21  | R     | 307 | CHL  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 21  | s     | 306 | CHL  | O2D-CGD-CBD | 5.01  | 120.18      | 111.27   |
| 21  | s     | 301 | CHL  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 21  | Y     | 607 | CHL  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 23  | r     | 313 | LUT  | C7-C6-C5    | -5.01 | 109.33      | 121.46   |
| 21  | g     | 609 | CHL  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 25  | n     | 616 | NEX  | C28-C29-C30 | -5.01 | 111.26      | 118.94   |
| 21  | n     | 607 | CHL  | O2D-CGD-CBD | 5.01  | 120.16      | 111.27   |
| 23  | Y     | 614 | LUT  | C12-C13-C14 | -5.00 | 111.26      | 118.94   |
| 21  | N     | 606 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | Y     | 606 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | Y     | 608 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | S     | 307 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | G     | 607 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | y     | 601 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | r     | 301 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 21  | n     | 601 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | r     | 307 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | y     | 609 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | g     | 606 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 23  | R     | 312 | LUT  | C7-C6-C5    | -5.00 | 109.36      | 121.46   |
| 21  | g     | 605 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | n     | 608 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | N     | 608 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | Y     | 605 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | r     | 306 | CHL  | O2D-CGD-CBD | 5.00  | 120.15      | 111.27   |
| 21  | g     | 607 | CHL  | O2D-CGD-CBD | 5.00  | 120.14      | 111.27   |
| 21  | r     | 308 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | G     | 609 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | S     | 306 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | N     | 605 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | R     | 305 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | N     | 607 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | S     | 301 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | G     | 605 | CHL  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 21  | y     | 607 | CHL  | O2D-CGD-CBD | 4.99  | 120.13      | 111.27   |
| 21  | g     | 608 | CHL  | O2D-CGD-CBD | 4.98  | 120.11      | 111.27   |
| 24  | r     | 314 | XAT  | C32-C33-C34 | -4.97 | 111.32      | 118.94   |
| 21  | y     | 605 | CHL  | O2D-CGD-CBD | 4.97  | 120.09      | 111.27   |
| 24  | N     | 616 | XAT  | C39-C29-C28 | -4.96 | 110.26      | 118.08   |
| 25  | r     | 315 | NEX  | C28-C29-C30 | -4.96 | 111.33      | 118.94   |
| 32  | D     | 407 | PL9  | C7-C3-C4    | 4.96  | 120.91      | 116.88   |
| 25  | y     | 618 | NEX  | C28-C29-C30 | -4.96 | 111.33      | 118.94   |
| 24  | R     | 313 | XAT  | C12-C13-C14 | -4.95 | 111.34      | 118.94   |
| 24  | R     | 313 | XAT  | C32-C33-C34 | -4.95 | 111.34      | 118.94   |
| 32  | d     | 406 | PL9  | C7-C3-C4    | 4.95  | 120.90      | 116.88   |
| 24  | r     | 314 | XAT  | C12-C13-C14 | -4.95 | 111.35      | 118.94   |
| 23  | g     | 616 | LUT  | C19-C9-C8   | -4.94 | 110.30      | 118.08   |
| 25  | N     | 617 | NEX  | C5-C6-C1    | -4.93 | 114.81      | 119.70   |
| 24  | r     | 314 | XAT  | C28-C29-C30 | -4.91 | 111.41      | 118.94   |
| 24  | R     | 313 | XAT  | C28-C29-C30 | -4.91 | 111.41      | 118.94   |
| 24  | N     | 616 | XAT  | C8-C9-C10   | -4.90 | 111.42      | 118.94   |
| 23  | g     | 616 | LUT  | C32-C33-C34 | -4.90 | 111.43      | 118.94   |
| 24  | n     | 615 | XAT  | O24-C25-C38 | -4.89 | 109.20      | 115.06   |
| 25  | N     | 617 | NEX  | C37-C21-C26 | 4.87  | 123.19      | 110.05   |
| 35  | C     | 518 | DGD  | O3G-C3G-C2G | -4.86 | 99.17       | 110.90   |
| 25  | y     | 616 | NEX  | C37-C21-C26 | 4.86  | 123.16      | 110.05   |
| 23  | R     | 312 | LUT  | C1-C6-C5    | -4.86 | 115.77      | 122.61   |
| 23  | Y     | 614 | LUT  | C39-C29-C28 | -4.85 | 110.44      | 118.08   |
| 35  | c     | 517 | DGD  | O3G-C3G-C2G | -4.84 | 99.22       | 110.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 510 | CLA  | CHD-C1D-C2D | 4.83  | 135.61      | 125.48   |
| 23  | N     | 615 | LUT  | C8-C9-C10   | -4.83 | 111.54      | 118.94   |
| 22  | C     | 511 | CLA  | CHD-C1D-C2D | 4.82  | 135.60      | 125.48   |
| 23  | r     | 313 | LUT  | C1-C6-C5    | -4.82 | 115.83      | 122.61   |
| 25  | n     | 616 | NEX  | C40-C33-C32 | -4.80 | 110.52      | 118.08   |
| 23  | Y     | 614 | LUT  | C32-C33-C34 | -4.80 | 111.58      | 118.94   |
| 23  | G     | 616 | LUT  | C19-C9-C8   | -4.77 | 110.56      | 118.08   |
| 25  | N     | 617 | NEX  | O24-C25-C38 | -4.77 | 109.34      | 115.06   |
| 24  | y     | 615 | XAT  | C12-C13-C14 | -4.76 | 111.64      | 118.94   |
| 23  | Y     | 614 | LUT  | C7-C8-C9    | -4.75 | 119.05      | 126.23   |
| 25  | Y     | 616 | NEX  | C25-C24-C23 | 4.74  | 122.13      | 112.75   |
| 23  | r     | 313 | LUT  | C12-C13-C14 | -4.74 | 111.67      | 118.94   |
| 23  | R     | 312 | LUT  | C12-C13-C14 | -4.73 | 111.69      | 118.94   |
| 23  | y     | 614 | LUT  | C4-C5-C6    | -4.72 | 110.34      | 120.85   |
| 24  | G     | 617 | XAT  | C8-C9-C10   | -4.71 | 111.71      | 118.94   |
| 23  | N     | 614 | LUT  | C4-C5-C6    | -4.70 | 110.38      | 120.85   |
| 23  | g     | 615 | LUT  | C4-C5-C6    | -4.69 | 110.39      | 120.85   |
| 23  | n     | 614 | LUT  | C4-C5-C6    | -4.69 | 110.39      | 120.85   |
| 25  | N     | 617 | NEX  | C19-C9-C8   | -4.69 | 108.06      | 118.93   |
| 23  | Y     | 613 | LUT  | C4-C5-C6    | -4.69 | 110.40      | 120.85   |
| 23  | G     | 615 | LUT  | C4-C5-C6    | -4.68 | 110.43      | 120.85   |
| 23  | Y     | 614 | LUT  | C19-C9-C8   | -4.65 | 110.75      | 118.08   |
| 23  | G     | 616 | LUT  | C32-C33-C34 | -4.65 | 111.81      | 118.94   |
| 23  | N     | 615 | LUT  | C12-C13-C14 | -4.64 | 111.83      | 118.94   |
| 23  | G     | 616 | LUT  | C12-C13-C14 | -4.62 | 111.85      | 118.94   |
| 35  | c     | 519 | DGD  | O3G-C3G-C2G | -4.61 | 99.79       | 110.90   |
| 35  | J     | 101 | DGD  | O3G-C3G-C2G | -4.59 | 99.83       | 110.90   |
| 24  | y     | 615 | XAT  | O24-C25-C38 | -4.59 | 109.56      | 115.06   |
| 24  | Y     | 615 | XAT  | O24-C25-C38 | -4.58 | 109.57      | 115.06   |
| 23  | Y     | 613 | LUT  | C19-C9-C8   | -4.58 | 110.86      | 118.08   |
| 24  | n     | 615 | XAT  | C7-C8-C9    | -4.57 | 118.44      | 125.53   |
| 23  | n     | 614 | LUT  | C19-C9-C8   | -4.57 | 110.88      | 118.08   |
| 23  | G     | 615 | LUT  | C19-C9-C8   | -4.56 | 110.89      | 118.08   |
| 37  | F     | 101 | HEM  | C2C-C3C-C4C | 4.54  | 110.07      | 106.90   |
| 24  | g     | 617 | XAT  | C8-C9-C10   | -4.53 | 111.99      | 118.94   |
| 23  | g     | 615 | LUT  | C19-C9-C8   | -4.53 | 110.95      | 118.08   |
| 23  | y     | 614 | LUT  | C19-C9-C8   | -4.52 | 110.95      | 118.08   |
| 23  | N     | 614 | LUT  | C19-C9-C8   | -4.52 | 110.96      | 118.08   |
| 25  | n     | 616 | NEX  | C37-C21-C26 | 4.51  | 122.23      | 110.05   |
| 24  | g     | 617 | XAT  | O24-C25-C38 | -4.51 | 109.65      | 115.06   |
| 35  | c     | 518 | DGD  | O3G-C3G-C2G | -4.50 | 100.04      | 110.90   |
| 24  | N     | 616 | XAT  | C32-C33-C34 | -4.50 | 112.04      | 118.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | C     | 519 | DGD  | O3G-C3G-C2G | -4.50 | 100.05      | 110.90   |
| 37  | f     | 101 | HEM  | C4A-C3A-C2A | 4.48  | 110.11      | 107.00   |
| 24  | R     | 313 | XAT  | O24-C25-C38 | -4.47 | 109.70      | 115.06   |
| 35  | A     | 401 | DGD  | O3G-C3G-C2G | -4.47 | 100.11      | 110.90   |
| 37  | f     | 101 | HEM  | C2C-C3C-C4C | 4.46  | 110.01      | 106.90   |
| 35  | a     | 413 | DGD  | O3G-C3G-C2G | -4.46 | 100.15      | 110.90   |
| 24  | r     | 314 | XAT  | O24-C25-C38 | -4.44 | 109.74      | 115.06   |
| 37  | F     | 101 | HEM  | C4A-C3A-C2A | 4.42  | 110.07      | 107.00   |
| 24  | Y     | 615 | XAT  | C12-C13-C14 | -4.42 | 112.16      | 118.94   |
| 22  | B     | 610 | CLA  | CMB-C2B-C1B | -4.40 | 121.70      | 128.46   |
| 22  | b     | 607 | CLA  | CMB-C2B-C1B | -4.40 | 121.71      | 128.46   |
| 25  | g     | 618 | NEX  | C25-C24-C23 | 4.37  | 121.39      | 112.75   |
| 24  | r     | 314 | XAT  | C5-C4-C3    | -4.34 | 104.16      | 112.75   |
| 24  | g     | 617 | XAT  | C32-C33-C34 | -4.33 | 112.29      | 118.94   |
| 24  | N     | 616 | XAT  | O24-C25-C38 | -4.33 | 109.87      | 115.06   |
| 33  | D     | 402 | SQD  | O9-S-C6     | 4.31  | 112.06      | 106.94   |
| 24  | R     | 313 | XAT  | C5-C4-C3    | -4.31 | 104.22      | 112.75   |
| 33  | d     | 402 | SQD  | O9-S-C6     | 4.30  | 112.05      | 106.94   |
| 35  | h     | 102 | DGD  | O3G-C3G-C2G | -4.29 | 100.54      | 110.90   |
| 25  | Y     | 616 | NEX  | C19-C9-C8   | -4.29 | 108.98      | 118.93   |
| 35  | H     | 102 | DGD  | O3G-C3G-C2G | -4.28 | 100.58      | 110.90   |
| 24  | G     | 617 | XAT  | C32-C33-C34 | -4.27 | 112.38      | 118.94   |
| 26  | d     | 407 | LHG  | O4-P-O5     | 4.25  | 133.27      | 112.24   |
| 26  | D     | 408 | LHG  | O4-P-O5     | 4.25  | 133.25      | 112.24   |
| 26  | G     | 618 | LHG  | O4-P-O5     | 4.25  | 133.24      | 112.24   |
| 26  | g     | 619 | LHG  | O4-P-O5     | 4.25  | 133.23      | 112.24   |
| 26  | D     | 409 | LHG  | O4-P-O5     | 4.24  | 133.21      | 112.24   |
| 26  | S     | 314 | LHG  | O4-P-O5     | 4.24  | 133.19      | 112.24   |
| 25  | y     | 616 | NEX  | C25-C24-C23 | 4.24  | 121.13      | 112.75   |
| 26  | d     | 408 | LHG  | O4-P-O5     | 4.24  | 133.19      | 112.24   |
| 26  | C     | 522 | LHG  | O4-P-O5     | 4.23  | 133.16      | 112.24   |
| 26  | c     | 522 | LHG  | O4-P-O5     | 4.23  | 133.14      | 112.24   |
| 25  | y     | 616 | NEX  | C19-C9-C8   | -4.23 | 109.13      | 118.93   |
| 26  | s     | 314 | LHG  | O4-P-O5     | 4.22  | 133.12      | 112.24   |
| 26  | y     | 617 | LHG  | O4-P-O5     | 4.22  | 133.11      | 112.24   |
| 26  | c     | 520 | LHG  | O4-P-O5     | 4.22  | 133.11      | 112.24   |
| 26  | C     | 520 | LHG  | O4-P-O5     | 4.20  | 133.02      | 112.24   |
| 26  | n     | 617 | LHG  | O4-P-O5     | 4.20  | 133.02      | 112.24   |
| 26  | L     | 103 | LHG  | O4-P-O5     | 4.20  | 133.01      | 112.24   |
| 26  | d     | 409 | LHG  | O4-P-O5     | 4.20  | 133.01      | 112.24   |
| 26  | D     | 410 | LHG  | O4-P-O5     | 4.20  | 133.01      | 112.24   |
| 26  | l     | 102 | LHG  | O4-P-O5     | 4.20  | 133.00      | 112.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | n     | 615 | XAT  | C32-C33-C34 | -4.20 | 112.50      | 118.94   |
| 26  | b     | 619 | LHG  | O4-P-O5     | 4.19  | 132.98      | 112.24   |
| 24  | R     | 313 | XAT  | C6-C7-C8    | -4.19 | 117.13      | 125.99   |
| 25  | g     | 618 | NEX  | C19-C9-C8   | -4.19 | 109.21      | 118.93   |
| 26  | B     | 622 | LHG  | O4-P-O5     | 4.19  | 132.96      | 112.24   |
| 23  | N     | 615 | LUT  | C4-C5-C6    | -4.19 | 111.51      | 120.85   |
| 26  | c     | 521 | LHG  | O4-P-O5     | 4.19  | 132.95      | 112.24   |
| 26  | C     | 521 | LHG  | O4-P-O5     | 4.18  | 132.91      | 112.24   |
| 26  | Y     | 617 | LHG  | O4-P-O5     | 4.18  | 132.89      | 112.24   |
| 24  | r     | 314 | XAT  | C6-C7-C8    | -4.17 | 117.17      | 125.99   |
| 25  | g     | 618 | NEX  | C37-C21-C26 | 4.17  | 121.31      | 110.05   |
| 25  | r     | 315 | NEX  | C19-C9-C8   | -4.16 | 109.28      | 118.93   |
| 26  | R     | 301 | LHG  | O4-P-O5     | 4.16  | 132.79      | 112.24   |
| 26  | r     | 302 | LHG  | O4-P-O5     | 4.16  | 132.79      | 112.24   |
| 25  | n     | 616 | NEX  | C25-C24-C23 | 4.16  | 120.97      | 112.75   |
| 21  | s     | 302 | CHL  | C3D-C2D-C1D | -4.15 | 100.17      | 105.83   |
| 25  | y     | 618 | NEX  | C19-C9-C8   | -4.15 | 109.32      | 118.93   |
| 26  | N     | 618 | LHG  | O4-P-O5     | 4.15  | 132.74      | 112.24   |
| 21  | S     | 302 | CHL  | C3D-C2D-C1D | -4.14 | 100.18      | 105.83   |
| 21  | n     | 607 | CHL  | C3D-C2D-C1D | -4.13 | 100.19      | 105.83   |
| 21  | s     | 306 | CHL  | C3D-C2D-C1D | -4.13 | 100.19      | 105.83   |
| 21  | G     | 601 | CHL  | C3D-C2D-C1D | -4.13 | 100.20      | 105.83   |
| 21  | N     | 606 | CHL  | C3D-C2D-C1D | -4.13 | 100.20      | 105.83   |
| 21  | R     | 306 | CHL  | C3D-C2D-C1D | -4.13 | 100.20      | 105.83   |
| 21  | s     | 301 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 21  | g     | 607 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 21  | R     | 307 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 25  | N     | 617 | NEX  | C2-C1-C6    | 4.12  | 113.22      | 109.21   |
| 22  | C     | 511 | CLA  | CMB-C2B-C1B | -4.12 | 122.13      | 128.46   |
| 21  | g     | 601 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 21  | N     | 607 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 21  | s     | 307 | CHL  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 21  | G     | 605 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | n     | 605 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | N     | 605 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | G     | 609 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | Y     | 601 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | r     | 307 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 21  | n     | 608 | CHL  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 25  | N     | 617 | NEX  | C25-C24-C23 | 4.12  | 120.89      | 112.75   |
| 21  | y     | 601 | CHL  | C3D-C2D-C1D | -4.12 | 100.22      | 105.83   |
| 21  | n     | 606 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | y     | 608 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 21  | G     | 606 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 21  | S     | 307 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 24  | G     | 617 | XAT  | C38-C25-C24 | -4.11 | 109.66      | 114.28   |
| 21  | N     | 601 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 21  | r     | 308 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 21  | r     | 301 | CHL  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 21  | y     | 607 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | g     | 606 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | g     | 609 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | y     | 605 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | Y     | 605 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | y     | 606 | CHL  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 21  | Y     | 606 | CHL  | C3D-C2D-C1D | -4.10 | 100.23      | 105.83   |
| 22  | c     | 510 | CLA  | CMB-C2B-C1B | -4.10 | 122.16      | 128.46   |
| 21  | y     | 609 | CHL  | C3D-C2D-C1D | -4.10 | 100.23      | 105.83   |
| 21  | N     | 608 | CHL  | C3D-C2D-C1D | -4.10 | 100.23      | 105.83   |
| 21  | Y     | 608 | CHL  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 21  | g     | 605 | CHL  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 21  | G     | 608 | CHL  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 21  | g     | 608 | CHL  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 21  | Y     | 607 | CHL  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 21  | S     | 301 | CHL  | C3D-C2D-C1D | -4.09 | 100.24      | 105.83   |
| 21  | S     | 306 | CHL  | C3D-C2D-C1D | -4.09 | 100.24      | 105.83   |
| 21  | r     | 306 | CHL  | C3D-C2D-C1D | -4.09 | 100.25      | 105.83   |
| 25  | n     | 616 | NEX  | C17-C1-C6   | -4.09 | 106.81      | 110.47   |
| 21  | n     | 601 | CHL  | C3D-C2D-C1D | -4.09 | 100.25      | 105.83   |
| 21  | G     | 607 | CHL  | C3D-C2D-C1D | -4.08 | 100.26      | 105.83   |
| 21  | R     | 305 | CHL  | C3D-C2D-C1D | -4.08 | 100.27      | 105.83   |
| 25  | y     | 618 | NEX  | C25-C24-C23 | 4.05  | 120.77      | 112.75   |
| 25  | r     | 315 | NEX  | C25-C24-C23 | 4.05  | 120.76      | 112.75   |
| 25  | r     | 315 | NEX  | C5-C6-C1    | -4.04 | 115.69      | 119.70   |
| 24  | y     | 615 | XAT  | C32-C33-C34 | -4.03 | 112.75      | 118.94   |
| 23  | N     | 615 | LUT  | C19-C9-C8   | -4.03 | 111.73      | 118.08   |
| 25  | n     | 616 | NEX  | C19-C9-C8   | -4.02 | 109.61      | 118.93   |
| 22  | S     | 311 | CLA  | CMB-C2B-C1B | -4.02 | 122.29      | 128.46   |
| 37  | F     | 101 | HEM  | C3C-C4C-NC  | -4.02 | 103.36      | 110.94   |
| 37  | f     | 101 | HEM  | C3C-C4C-NC  | -4.02 | 103.36      | 110.94   |
| 22  | c     | 504 | CLA  | CMB-C2B-C1B | -4.00 | 122.31      | 128.46   |
| 22  | c     | 512 | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 22  | C     | 505 | CLA  | CMB-C2B-C1B | -3.99 | 122.33      | 128.46   |
| 22  | C     | 513 | CLA  | CMB-C2B-C1B | -3.98 | 122.34      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | A     | 412 | SQD  | O7-S-C6     | 3.97  | 111.66      | 106.94   |
| 25  | y     | 618 | NEX  | C5-C6-C1    | -3.97 | 115.75      | 119.70   |
| 33  | a     | 411 | SQD  | O7-S-C6     | 3.97  | 111.66      | 106.94   |
| 22  | s     | 311 | CLA  | CMB-C2B-C1B | -3.96 | 122.37      | 128.46   |
| 33  | l     | 101 | SQD  | O9-S-C6     | 3.95  | 111.64      | 106.94   |
| 23  | N     | 614 | LUT  | C7-C6-C5    | -3.95 | 111.89      | 121.46   |
| 23  | y     | 614 | LUT  | C7-C6-C5    | -3.94 | 111.91      | 121.46   |
| 22  | B     | 616 | CLA  | CMB-C2B-C1B | -3.94 | 122.41      | 128.46   |
| 24  | y     | 615 | XAT  | C38-C25-C24 | -3.94 | 109.85      | 114.28   |
| 23  | Y     | 613 | LUT  | C7-C6-C5    | -3.94 | 111.92      | 121.46   |
| 23  | G     | 615 | LUT  | C7-C6-C5    | -3.94 | 111.93      | 121.46   |
| 22  | g     | 613 | CLA  | C1B-CHB-C4A | -3.93 | 122.33      | 130.12   |
| 23  | g     | 615 | LUT  | C7-C6-C5    | -3.93 | 111.94      | 121.46   |
| 23  | n     | 614 | LUT  | C7-C6-C5    | -3.93 | 111.94      | 121.46   |
| 22  | n     | 612 | CLA  | C1B-CHB-C4A | -3.92 | 122.35      | 130.12   |
| 22  | a     | 408 | CLA  | CMB-C2B-C1B | -3.92 | 122.44      | 128.46   |
| 22  | b     | 613 | CLA  | CMB-C2B-C1B | -3.92 | 122.45      | 128.46   |
| 22  | b     | 603 | CLA  | CMB-C2B-C1B | -3.91 | 122.45      | 128.46   |
| 22  | y     | 612 | CLA  | C1B-CHB-C4A | -3.91 | 122.37      | 130.12   |
| 22  | R     | 309 | CLA  | CMB-C2B-C1B | -3.91 | 122.45      | 128.46   |
| 22  | r     | 310 | CLA  | CMB-C2B-C1B | -3.90 | 122.46      | 128.46   |
| 33  | L     | 102 | SQD  | O9-S-C6     | 3.90  | 111.58      | 106.94   |
| 22  | N     | 612 | CLA  | C1B-CHB-C4A | -3.90 | 122.39      | 130.12   |
| 22  | A     | 409 | CLA  | CMB-C2B-C1B | -3.90 | 122.48      | 128.46   |
| 22  | Y     | 611 | CLA  | C1B-CHB-C4A | -3.89 | 122.42      | 130.12   |
| 33  | l     | 103 | SQD  | O47-C7-C8   | 3.88  | 119.87      | 111.50   |
| 22  | G     | 613 | CLA  | C1B-CHB-C4A | -3.88 | 122.43      | 130.12   |
| 22  | B     | 606 | CLA  | CMB-C2B-C1B | -3.88 | 122.50      | 128.46   |
| 23  | R     | 312 | LUT  | C20-C13-C12 | -3.87 | 111.98      | 118.08   |
| 24  | Y     | 615 | XAT  | C38-C25-C24 | -3.87 | 109.93      | 114.28   |
| 33  | L     | 101 | SQD  | O47-C7-C8   | 3.86  | 119.82      | 111.50   |
| 23  | r     | 313 | LUT  | C20-C13-C12 | -3.85 | 112.01      | 118.08   |
| 22  | c     | 507 | CLA  | CMB-C2B-C1B | -3.85 | 122.55      | 128.46   |
| 22  | b     | 614 | CLA  | CMB-C2B-C1B | -3.84 | 122.57      | 128.46   |
| 22  | B     | 617 | CLA  | CMB-C2B-C1B | -3.84 | 122.57      | 128.46   |
| 22  | C     | 508 | CLA  | CMB-C2B-C1B | -3.84 | 122.57      | 128.46   |
| 24  | N     | 616 | XAT  | C28-C29-C30 | -3.84 | 113.06      | 118.94   |
| 25  | Y     | 616 | NEX  | C17-C1-C6   | -3.83 | 107.04      | 110.47   |
| 25  | Y     | 616 | NEX  | C37-C21-C26 | 3.83  | 120.38      | 110.05   |
| 25  | r     | 315 | NEX  | C37-C21-C26 | 3.82  | 120.35      | 110.05   |
| 24  | n     | 615 | XAT  | C28-C29-C30 | -3.82 | 113.08      | 118.94   |
| 22  | s     | 303 | CLA  | CMB-C2B-C1B | -3.81 | 122.60      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | S     | 303 | CLA  | CMB-C2B-C1B | -3.81 | 122.61      | 128.46   |
| 23  | g     | 616 | LUT  | C12-C13-C14 | -3.81 | 113.09      | 118.94   |
| 33  | L     | 102 | SQD  | O7-S-C6     | 3.81  | 111.47      | 106.94   |
| 33  | l     | 101 | SQD  | O7-S-C6     | 3.81  | 111.47      | 106.94   |
| 25  | g     | 618 | NEX  | C17-C1-C6   | -3.81 | 107.06      | 110.47   |
| 25  | Y     | 616 | NEX  | C28-C29-C30 | -3.81 | 113.10      | 118.94   |
| 22  | B     | 614 | CLA  | CMB-C2B-C1B | -3.80 | 122.62      | 128.46   |
| 23  | R     | 312 | LUT  | C21-C26-C27 | -3.80 | 107.90      | 112.70   |
| 25  | y     | 618 | NEX  | C37-C21-C26 | 3.80  | 120.29      | 110.05   |
| 24  | r     | 314 | XAT  | C27-C28-C29 | -3.80 | 119.64      | 125.53   |
| 25  | y     | 616 | NEX  | C17-C1-C6   | -3.79 | 107.08      | 110.47   |
| 24  | g     | 617 | XAT  | C38-C25-C24 | -3.78 | 110.03      | 114.28   |
| 22  | b     | 611 | CLA  | CMB-C2B-C1B | -3.78 | 122.66      | 128.46   |
| 24  | R     | 313 | XAT  | C27-C28-C29 | -3.78 | 119.67      | 125.53   |
| 33  | L     | 101 | SQD  | C44-O6-C1   | 3.78  | 121.12      | 113.74   |
| 23  | r     | 313 | LUT  | C21-C26-C27 | -3.77 | 107.93      | 112.70   |
| 33  | l     | 103 | SQD  | O9-S-O7     | -3.77 | 100.91      | 113.95   |
| 33  | A     | 412 | SQD  | C44-O6-C1   | 3.76  | 121.09      | 113.74   |
| 33  | D     | 402 | SQD  | O9-S-O7     | -3.76 | 100.94      | 113.95   |
| 33  | L     | 101 | SQD  | O9-S-O7     | -3.76 | 100.94      | 113.95   |
| 22  | G     | 603 | CLA  | CMB-C2B-C1B | -3.76 | 122.69      | 128.46   |
| 33  | A     | 412 | SQD  | O9-S-O7     | -3.76 | 100.95      | 113.95   |
| 33  | d     | 402 | SQD  | O9-S-O7     | -3.76 | 100.95      | 113.95   |
| 33  | a     | 411 | SQD  | O9-S-O7     | -3.76 | 100.95      | 113.95   |
| 25  | Y     | 616 | NEX  | C27-C28-C29 | -3.75 | 119.71      | 125.53   |
| 22  | s     | 310 | CLA  | CMB-C2B-C1B | -3.75 | 122.70      | 128.46   |
| 33  | a     | 411 | SQD  | C44-O6-C1   | 3.75  | 121.06      | 113.74   |
| 22  | N     | 603 | CLA  | CMB-C2B-C1B | -3.74 | 122.71      | 128.46   |
| 22  | n     | 603 | CLA  | CMB-C2B-C1B | -3.74 | 122.72      | 128.46   |
| 22  | B     | 613 | CLA  | CMB-C2B-C1B | -3.74 | 122.72      | 128.46   |
| 22  | c     | 503 | CLA  | CMB-C2B-C1B | -3.74 | 122.72      | 128.46   |
| 33  | l     | 103 | SQD  | C44-O6-C1   | 3.74  | 121.04      | 113.74   |
| 22  | g     | 603 | CLA  | CMB-C2B-C1B | -3.73 | 122.73      | 128.46   |
| 33  | l     | 103 | SQD  | O7-S-C6     | 3.73  | 111.37      | 106.94   |
| 22  | C     | 504 | CLA  | CMB-C2B-C1B | -3.73 | 122.73      | 128.46   |
| 33  | L     | 101 | SQD  | O7-S-C6     | 3.73  | 111.37      | 106.94   |
| 22  | y     | 603 | CLA  | CMB-C2B-C1B | -3.73 | 122.74      | 128.46   |
| 22  | Y     | 603 | CLA  | CMB-C2B-C1B | -3.73 | 122.74      | 128.46   |
| 22  | S     | 310 | CLA  | CMB-C2B-C1B | -3.72 | 122.75      | 128.46   |
| 22  | b     | 607 | CLA  | CMB-C2B-C3B | 3.72  | 131.64      | 124.68   |
| 22  | b     | 610 | CLA  | CMB-C2B-C1B | -3.71 | 122.76      | 128.46   |
| 22  | b     | 605 | CLA  | CMB-C2B-C1B | -3.70 | 122.77      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | n     | 615 | XAT  | C38-C25-C24 | -3.70 | 110.12      | 114.28   |
| 22  | B     | 608 | CLA  | CMB-C2B-C1B | -3.70 | 122.78      | 128.46   |
| 33  | L     | 102 | SQD  | O9-S-O7     | -3.70 | 101.15      | 113.95   |
| 24  | N     | 616 | XAT  | C38-C25-C24 | -3.70 | 110.12      | 114.28   |
| 22  | B     | 615 | CLA  | CMB-C2B-C1B | -3.69 | 122.78      | 128.46   |
| 35  | J     | 101 | DGD  | O6D-C1D-O3G | -3.69 | 101.23      | 109.97   |
| 22  | B     | 610 | CLA  | CMB-C2B-C3B | 3.69  | 131.58      | 124.68   |
| 35  | c     | 519 | DGD  | O6D-C1D-O3G | -3.69 | 101.24      | 109.97   |
| 33  | l     | 101 | SQD  | O9-S-O7     | -3.69 | 101.19      | 113.95   |
| 22  | b     | 609 | CLA  | CMB-C2B-C1B | -3.68 | 122.81      | 128.46   |
| 22  | b     | 612 | CLA  | CMB-C2B-C1B | -3.68 | 122.81      | 128.46   |
| 22  | C     | 506 | CLA  | CMB-C2B-C1B | -3.68 | 122.81      | 128.46   |
| 22  | B     | 612 | CLA  | CMB-C2B-C1B | -3.67 | 122.82      | 128.46   |
| 25  | r     | 315 | NEX  | C27-C28-C29 | -3.67 | 119.84      | 125.53   |
| 22  | A     | 406 | CLA  | CMB-C2B-C1B | -3.67 | 122.83      | 128.46   |
| 22  | S     | 313 | CLA  | CMB-C2B-C1B | -3.67 | 122.83      | 128.46   |
| 22  | a     | 405 | CLA  | CMB-C2B-C1B | -3.67 | 122.83      | 128.46   |
| 33  | l     | 103 | SQD  | O9-S-C6     | 3.67  | 111.30      | 106.94   |
| 22  | c     | 505 | CLA  | CMB-C2B-C1B | -3.66 | 122.84      | 128.46   |
| 22  | s     | 313 | CLA  | CMB-C2B-C1B | -3.66 | 122.84      | 128.46   |
| 22  | b     | 602 | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 22  | B     | 605 | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 24  | y     | 615 | XAT  | C28-C29-C30 | -3.65 | 113.34      | 118.94   |
| 22  | d     | 403 | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 24  | g     | 617 | XAT  | C28-C29-C30 | -3.65 | 113.34      | 118.94   |
| 33  | L     | 101 | SQD  | O9-S-C6     | 3.65  | 111.28      | 106.94   |
| 22  | c     | 509 | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 22  | C     | 514 | CLA  | CMB-C2B-C1B | -3.65 | 122.86      | 128.46   |
| 25  | y     | 618 | NEX  | C27-C28-C29 | -3.65 | 119.87      | 125.53   |
| 37  | f     | 101 | HEM  | CHB-C1B-C2B | 3.65  | 136.81      | 126.72   |
| 33  | D     | 402 | SQD  | O7-S-C6     | 3.64  | 111.26      | 106.94   |
| 35  | c     | 517 | DGD  | O6D-C1D-O3G | -3.64 | 101.36      | 109.97   |
| 33  | L     | 102 | SQD  | O47-C7-C8   | 3.63  | 119.33      | 111.50   |
| 33  | d     | 402 | SQD  | O7-S-C6     | 3.63  | 111.25      | 106.94   |
| 22  | C     | 511 | CLA  | CMB-C2B-C3B | 3.63  | 131.47      | 124.68   |
| 22  | S     | 305 | CLA  | CMB-C2B-C1B | -3.63 | 122.89      | 128.46   |
| 37  | F     | 101 | HEM  | CHB-C1B-C2B | 3.63  | 136.75      | 126.72   |
| 35  | C     | 518 | DGD  | O6D-C1D-O3G | -3.63 | 101.39      | 109.97   |
| 24  | Y     | 615 | XAT  | C32-C33-C34 | -3.62 | 113.38      | 118.94   |
| 22  | D     | 404 | CLA  | CMB-C2B-C1B | -3.62 | 122.89      | 128.46   |
| 23  | G     | 615 | LUT  | C21-C26-C27 | -3.62 | 108.12      | 112.70   |
| 23  | g     | 616 | LUT  | C4-C5-C6    | -3.62 | 112.78      | 120.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | Y     | 613 | LUT  | C21-C26-C27 | -3.62 | 108.13      | 112.70   |
| 22  | c     | 513 | CLA  | CMB-C2B-C1B | -3.62 | 122.90      | 128.46   |
| 33  | l     | 101 | SQD  | O47-C7-C8   | 3.62  | 119.29      | 111.50   |
| 23  | y     | 614 | LUT  | C21-C26-C27 | -3.61 | 108.13      | 112.70   |
| 23  | N     | 614 | LUT  | C21-C26-C27 | -3.61 | 108.14      | 112.70   |
| 22  | c     | 510 | CLA  | CMB-C2B-C3B | 3.61  | 131.43      | 124.68   |
| 22  | C     | 510 | CLA  | CMB-C2B-C1B | -3.61 | 122.92      | 128.46   |
| 24  | R     | 313 | XAT  | C38-C25-C24 | -3.59 | 110.24      | 114.28   |
| 22  | R     | 310 | CLA  | C1B-CHB-C4A | -3.59 | 123.00      | 130.12   |
| 33  | a     | 411 | SQD  | O47-C7-C8   | 3.59  | 119.24      | 111.50   |
| 23  | n     | 614 | LUT  | C21-C26-C27 | -3.59 | 108.16      | 112.70   |
| 22  | s     | 308 | CLA  | CMB-C2B-C1B | -3.59 | 122.95      | 128.46   |
| 22  | s     | 305 | CLA  | CMB-C2B-C1B | -3.59 | 122.95      | 128.46   |
| 23  | g     | 615 | LUT  | C21-C26-C27 | -3.59 | 108.17      | 112.70   |
| 22  | r     | 312 | CLA  | CMB-C2B-C1B | -3.59 | 122.95      | 128.46   |
| 22  | R     | 303 | CLA  | CMB-C2B-C1B | -3.59 | 122.95      | 128.46   |
| 22  | B     | 607 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 22  | r     | 311 | CLA  | C1B-CHB-C4A | -3.58 | 123.03      | 130.12   |
| 22  | S     | 308 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 33  | D     | 402 | SQD  | O47-C7-C8   | 3.58  | 119.21      | 111.50   |
| 33  | d     | 402 | SQD  | O47-C7-C8   | 3.57  | 119.20      | 111.50   |
| 22  | b     | 604 | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 22  | r     | 304 | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 22  | R     | 311 | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 22  | C     | 515 | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 33  | A     | 412 | SQD  | O47-C7-C8   | 3.57  | 119.19      | 111.50   |
| 23  | G     | 616 | LUT  | C4-C5-C6    | -3.56 | 112.91      | 120.85   |
| 22  | c     | 514 | CLA  | CMB-C2B-C1B | -3.55 | 123.01      | 128.46   |
| 22  | b     | 615 | CLA  | CMB-C2B-C1B | -3.55 | 123.01      | 128.46   |
| 22  | B     | 603 | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 22  | B     | 618 | CLA  | CMB-C2B-C1B | -3.53 | 123.04      | 128.46   |
| 23  | n     | 614 | LUT  | C1-C6-C7    | -3.53 | 105.79      | 115.78   |
| 24  | r     | 314 | XAT  | C38-C25-C24 | -3.53 | 110.31      | 114.28   |
| 22  | x     | 101 | CLA  | CMB-C2B-C1B | -3.53 | 123.04      | 128.46   |
| 23  | G     | 615 | LUT  | C1-C6-C7    | -3.52 | 105.81      | 115.78   |
| 22  | g     | 602 | CLA  | CMB-C2B-C1B | -3.52 | 123.05      | 128.46   |
| 22  | C     | 512 | CLA  | CMB-C2B-C1B | -3.52 | 123.05      | 128.46   |
| 23  | g     | 615 | LUT  | C1-C6-C7    | -3.52 | 105.83      | 115.78   |
| 22  | b     | 606 | CLA  | CMB-C2B-C1B | -3.52 | 123.06      | 128.46   |
| 24  | G     | 617 | XAT  | C28-C29-C30 | -3.52 | 113.55      | 118.94   |
| 23  | Y     | 613 | LUT  | C1-C6-C7    | -3.51 | 105.84      | 115.78   |
| 23  | N     | 614 | LUT  | C1-C6-C7    | -3.51 | 105.84      | 115.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 602 | CLA  | CMB-C2B-C1B | -3.51 | 123.07      | 128.46   |
| 22  | n     | 602 | CLA  | CMB-C2B-C1B | -3.51 | 123.07      | 128.46   |
| 23  | y     | 614 | LUT  | C1-C6-C7    | -3.51 | 105.86      | 115.78   |
| 33  | A     | 412 | SQD  | C1-O5-C5    | 3.50  | 120.57      | 113.69   |
| 21  | n     | 606 | CHL  | C3C-C4C-NC  | 3.50  | 114.50      | 110.57   |
| 21  | g     | 605 | CHL  | C3C-C4C-NC  | 3.50  | 114.50      | 110.57   |
| 24  | Y     | 615 | XAT  | C28-C29-C30 | -3.50 | 113.58      | 118.94   |
| 22  | Y     | 602 | CLA  | CMB-C2B-C1B | -3.50 | 123.09      | 128.46   |
| 22  | c     | 511 | CLA  | CMB-C2B-C1B | -3.49 | 123.09      | 128.46   |
| 22  | y     | 602 | CLA  | CMB-C2B-C1B | -3.49 | 123.10      | 128.46   |
| 21  | y     | 607 | CHL  | C3C-C4C-NC  | 3.49  | 114.48      | 110.57   |
| 22  | B     | 609 | CLA  | CMB-C2B-C1B | -3.49 | 123.10      | 128.46   |
| 23  | Y     | 614 | LUT  | C4-C5-C6    | -3.49 | 113.07      | 120.85   |
| 35  | a     | 413 | DGD  | O6D-C1D-O3G | -3.49 | 101.72      | 109.97   |
| 33  | a     | 411 | SQD  | C1-O5-C5    | 3.49  | 120.53      | 113.69   |
| 21  | S     | 307 | CHL  | C3C-C4C-NC  | 3.48  | 114.48      | 110.57   |
| 21  | n     | 605 | CHL  | C3C-C4C-NC  | 3.48  | 114.48      | 110.57   |
| 21  | y     | 606 | CHL  | C3C-C4C-NC  | 3.48  | 114.47      | 110.57   |
| 21  | n     | 608 | CHL  | C3C-C4C-NC  | 3.47  | 114.47      | 110.57   |
| 21  | Y     | 608 | CHL  | C3C-C4C-NC  | 3.47  | 114.47      | 110.57   |
| 21  | R     | 305 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | N     | 601 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | g     | 609 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | G     | 609 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | N     | 607 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | r     | 301 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | g     | 608 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 35  | A     | 401 | DGD  | O6D-C1D-O3G | -3.47 | 101.76      | 109.97   |
| 22  | N     | 609 | CLA  | CMB-C2B-C1B | -3.47 | 123.14      | 128.46   |
| 21  | G     | 607 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | Y     | 607 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 21  | s     | 306 | CHL  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 22  | G     | 602 | CLA  | CMB-C2B-C1B | -3.46 | 123.14      | 128.46   |
| 22  | S     | 309 | CLA  | CMB-C2B-C1B | -3.46 | 123.14      | 128.46   |
| 21  | r     | 306 | CHL  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 22  | y     | 610 | CLA  | CMB-C2B-C1B | -3.46 | 123.15      | 128.46   |
| 22  | s     | 309 | CLA  | CMB-C2B-C1B | -3.46 | 123.15      | 128.46   |
| 21  | G     | 606 | CHL  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 21  | G     | 608 | CHL  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 21  | n     | 601 | CHL  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 22  | c     | 504 | CLA  | CMB-C2B-C3B | 3.46  | 131.15      | 124.68   |
| 36  | w     | 102 | LMG  | O6-C1-O1    | -3.46 | 101.79      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | N     | 608 | CHL  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 21  | G     | 605 | CHL  | C3C-C4C-NC  | 3.45  | 114.44      | 110.57   |
| 21  | s     | 302 | CHL  | C3C-C4C-NC  | 3.45  | 114.44      | 110.57   |
| 21  | n     | 606 | CHL  | CAC-C3C-C4C | 3.45  | 129.29      | 124.81   |
| 21  | y     | 605 | CHL  | C3C-C4C-NC  | 3.45  | 114.44      | 110.57   |
| 22  | N     | 610 | CLA  | CMB-C2B-C1B | -3.45 | 123.16      | 128.46   |
| 21  | G     | 601 | CHL  | C3C-C4C-NC  | 3.45  | 114.44      | 110.57   |
| 21  | N     | 605 | CHL  | C3C-C4C-NC  | 3.45  | 114.44      | 110.57   |
| 22  | C     | 505 | CLA  | CMB-C2B-C3B | 3.45  | 131.13      | 124.68   |
| 22  | G     | 610 | CLA  | CMB-C2B-C1B | -3.45 | 123.17      | 128.46   |
| 21  | y     | 606 | CHL  | CAC-C3C-C4C | 3.44  | 129.28      | 124.81   |
| 21  | n     | 607 | CHL  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 22  | a     | 406 | CLA  | CMB-C2B-C1B | -3.44 | 123.18      | 128.46   |
| 36  | C     | 502 | LMG  | O6-C1-O1    | -3.44 | 101.83      | 109.97   |
| 32  | d     | 406 | PL9  | C7-C3-C2    | -3.44 | 118.78      | 123.30   |
| 21  | g     | 606 | CHL  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 21  | r     | 307 | CHL  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 21  | R     | 307 | CHL  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 21  | y     | 607 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 22  | b     | 608 | CLA  | CMB-C2B-C1B | -3.44 | 123.18      | 128.46   |
| 21  | N     | 601 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 21  | R     | 306 | CHL  | C3C-C4C-NC  | 3.44  | 114.42      | 110.57   |
| 21  | g     | 606 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 21  | S     | 307 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 21  | g     | 605 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 21  | G     | 608 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 21  | N     | 607 | CHL  | CAC-C3C-C4C | 3.43  | 129.27      | 124.81   |
| 21  | S     | 302 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | Y     | 606 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | g     | 607 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | y     | 601 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | y     | 601 | CHL  | CAC-C3C-C4C | 3.43  | 129.26      | 124.81   |
| 32  | D     | 407 | PL9  | C7-C3-C2    | -3.43 | 118.79      | 123.30   |
| 21  | r     | 308 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 22  | Y     | 610 | CLA  | CMB-C2B-C1B | -3.43 | 123.19      | 128.46   |
| 22  | B     | 611 | CLA  | CMB-C2B-C1B | -3.43 | 123.19      | 128.46   |
| 21  | s     | 307 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | g     | 601 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | S     | 302 | CHL  | CAC-C3C-C4C | 3.43  | 129.26      | 124.81   |
| 21  | y     | 608 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | Y     | 605 | CHL  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 21  | G     | 607 | CHL  | CAC-C3C-C4C | 3.43  | 129.26      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | N     | 608 | CHL  | CAC-C3C-C4C | 3.43  | 129.26      | 124.81   |
| 21  | Y     | 607 | CHL  | CAC-C3C-C4C | 3.43  | 129.26      | 124.81   |
| 21  | r     | 301 | CHL  | CAC-C3C-C4C | 3.43  | 129.25      | 124.81   |
| 22  | g     | 610 | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 21  | r     | 306 | CHL  | CAC-C3C-C4C | 3.42  | 129.25      | 124.81   |
| 21  | y     | 609 | CHL  | C3C-C4C-NC  | 3.42  | 114.41      | 110.57   |
| 21  | S     | 301 | CHL  | C3C-C4C-NC  | 3.42  | 114.41      | 110.57   |
| 22  | n     | 610 | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 22  | A     | 407 | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 22  | G     | 611 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 22  | S     | 304 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 21  | Y     | 601 | CHL  | C3C-C4C-NC  | 3.42  | 114.41      | 110.57   |
| 21  | N     | 606 | CHL  | C3C-C4C-NC  | 3.42  | 114.41      | 110.57   |
| 21  | g     | 608 | CHL  | CAC-C3C-C4C | 3.42  | 129.25      | 124.81   |
| 21  | Y     | 606 | CHL  | CAC-C3C-C4C | 3.42  | 129.25      | 124.81   |
| 21  | Y     | 608 | CHL  | CAC-C3C-C4C | 3.42  | 129.25      | 124.81   |
| 21  | g     | 607 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | G     | 606 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | N     | 606 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | S     | 306 | CHL  | C3C-C4C-NC  | 3.42  | 114.40      | 110.57   |
| 21  | g     | 609 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | n     | 605 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | s     | 306 | CHL  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 21  | s     | 301 | CHL  | C3C-C4C-NC  | 3.41  | 114.40      | 110.57   |
| 21  | n     | 607 | CHL  | CAC-C3C-C4C | 3.41  | 129.24      | 124.81   |
| 22  | n     | 609 | CLA  | CMB-C2B-C1B | -3.41 | 123.22      | 128.46   |
| 22  | g     | 611 | CLA  | CMB-C2B-C1B | -3.41 | 123.23      | 128.46   |
| 22  | y     | 611 | CLA  | CMB-C2B-C1B | -3.41 | 123.23      | 128.46   |
| 21  | y     | 605 | CHL  | CAC-C3C-C4C | 3.41  | 129.23      | 124.81   |
| 21  | y     | 609 | CHL  | CAC-C3C-C4C | 3.41  | 129.23      | 124.81   |
| 21  | N     | 605 | CHL  | CAC-C3C-C4C | 3.41  | 129.23      | 124.81   |
| 21  | y     | 608 | CHL  | CAC-C3C-C4C | 3.41  | 129.23      | 124.81   |
| 21  | s     | 301 | CHL  | CAC-C3C-C4C | 3.41  | 129.23      | 124.81   |
| 21  | r     | 308 | CHL  | CAC-C3C-C4C | 3.40  | 129.23      | 124.81   |
| 22  | Y     | 609 | CLA  | CMB-C2B-C1B | -3.40 | 123.23      | 128.46   |
| 25  | y     | 616 | NEX  | C5-C6-C1    | -3.40 | 116.32      | 119.70   |
| 21  | Y     | 601 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 32  | a     | 410 | PL9  | C7-C3-C2    | -3.40 | 118.83      | 123.30   |
| 21  | s     | 302 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 21  | R     | 305 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 21  | S     | 301 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 22  | C     | 509 | CLA  | CMB-C2B-C1B | -3.40 | 123.24      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | G     | 605 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 33  | A     | 412 | SQD  | O9-S-C6     | 3.40  | 110.98      | 106.94   |
| 21  | n     | 601 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 21  | r     | 307 | CHL  | CAC-C3C-C4C | 3.40  | 129.22      | 124.81   |
| 33  | a     | 411 | SQD  | O9-S-C6     | 3.40  | 110.97      | 106.94   |
| 22  | c     | 508 | CLA  | CMB-C2B-C1B | -3.40 | 123.25      | 128.46   |
| 22  | b     | 601 | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 21  | n     | 608 | CHL  | CAC-C3C-C4C | 3.39  | 129.21      | 124.81   |
| 21  | G     | 609 | CHL  | CAC-C3C-C4C | 3.39  | 129.21      | 124.81   |
| 22  | c     | 512 | CLA  | CMB-C2B-C3B | 3.39  | 131.02      | 124.68   |
| 21  | S     | 306 | CHL  | CAC-C3C-C4C | 3.39  | 129.21      | 124.81   |
| 22  | C     | 513 | CLA  | CMB-C2B-C3B | 3.39  | 131.01      | 124.68   |
| 21  | G     | 601 | CHL  | CAC-C3C-C4C | 3.38  | 129.20      | 124.81   |
| 22  | s     | 304 | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 22  | g     | 614 | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 21  | R     | 307 | CHL  | CAC-C3C-C4C | 3.38  | 129.20      | 124.81   |
| 22  | n     | 613 | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 21  | g     | 601 | CHL  | CAC-C3C-C4C | 3.38  | 129.19      | 124.81   |
| 22  | d     | 404 | CLA  | CMB-C2B-C1B | -3.38 | 123.27      | 128.46   |
| 22  | D     | 405 | CLA  | CMB-C2B-C1B | -3.38 | 123.27      | 128.46   |
| 21  | R     | 306 | CHL  | CAC-C3C-C4C | 3.37  | 129.19      | 124.81   |
| 21  | s     | 307 | CHL  | CAC-C3C-C4C | 3.37  | 129.19      | 124.81   |
| 21  | Y     | 605 | CHL  | CAC-C3C-C4C | 3.37  | 129.18      | 124.81   |
| 35  | c     | 518 | DGD  | O6D-C1D-O3G | -3.37 | 102.00      | 109.97   |
| 22  | G     | 614 | CLA  | CMB-C2B-C1B | -3.37 | 123.29      | 128.46   |
| 32  | A     | 411 | PL9  | C7-C3-C2    | -3.36 | 118.88      | 123.30   |
| 22  | B     | 604 | CLA  | CMB-C2B-C1B | -3.36 | 123.30      | 128.46   |
| 22  | y     | 613 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 22  | Y     | 612 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 35  | C     | 519 | DGD  | O6D-C1D-O3G | -3.35 | 102.05      | 109.97   |
| 22  | N     | 613 | CLA  | CMB-C2B-C1B | -3.33 | 123.34      | 128.46   |
| 33  | L     | 101 | SQD  | C1-O5-C5    | 3.33  | 120.23      | 113.69   |
| 35  | h     | 102 | DGD  | O6D-C1D-O3G | -3.32 | 102.11      | 109.97   |
| 22  | c     | 507 | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 22  | C     | 507 | CLA  | CMB-C2B-C1B | -3.31 | 123.37      | 128.46   |
| 22  | a     | 404 | CLA  | CMB-C2B-C1B | -3.31 | 123.37      | 128.46   |
| 33  | l     | 103 | SQD  | C1-O5-C5    | 3.31  | 120.18      | 113.69   |
| 35  | H     | 102 | DGD  | O6D-C1D-O3G | -3.31 | 102.14      | 109.97   |
| 22  | c     | 506 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 22  | R     | 302 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 22  | C     | 503 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 22  | r     | 309 | CLA  | CMB-C2B-C1B | -3.30 | 123.40      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 508 | CLA  | CMB-C2B-C3B | 3.29  | 130.84      | 124.68   |
| 22  | s     | 310 | CLA  | CMB-C2B-C3B | 3.29  | 130.83      | 124.68   |
| 22  | S     | 311 | CLA  | CMB-C2B-C3B | 3.29  | 130.83      | 124.68   |
| 22  | c     | 502 | CLA  | CMB-C2B-C1B | -3.29 | 123.41      | 128.46   |
| 33  | D     | 402 | SQD  | C1-O5-C5    | 3.28  | 120.13      | 113.69   |
| 22  | r     | 303 | CLA  | CMB-C2B-C1B | -3.27 | 123.43      | 128.46   |
| 24  | N     | 616 | XAT  | C31-C32-C33 | -3.27 | 117.22      | 126.42   |
| 22  | A     | 405 | CLA  | CMB-C2B-C1B | -3.27 | 123.44      | 128.46   |
| 22  | B     | 616 | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 22  | g     | 613 | CLA  | C4D-CHA-C1A | -3.27 | 117.28      | 121.25   |
| 37  | F     | 101 | HEM  | CHC-C4B-NB  | 3.26  | 127.98      | 124.43   |
| 22  | Y     | 611 | CLA  | C4D-CHA-C1A | -3.26 | 117.28      | 121.25   |
| 22  | r     | 310 | CLA  | CMB-C2B-C3B | 3.26  | 130.78      | 124.68   |
| 22  | S     | 310 | CLA  | CMB-C2B-C3B | 3.26  | 130.77      | 124.68   |
| 33  | d     | 402 | SQD  | C1-O5-C5    | 3.26  | 120.08      | 113.69   |
| 22  | b     | 603 | CLA  | CMB-C2B-C3B | 3.26  | 130.77      | 124.68   |
| 25  | N     | 617 | NEX  | C16-C1-C6   | 3.25  | 113.38      | 110.47   |
| 22  | R     | 309 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 22  | s     | 303 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 22  | B     | 606 | CLA  | CMB-C2B-C3B | 3.25  | 130.75      | 124.68   |
| 22  | G     | 613 | CLA  | C4D-CHA-C1A | -3.25 | 117.30      | 121.25   |
| 37  | f     | 101 | HEM  | CHC-C4B-NB  | 3.25  | 127.96      | 124.43   |
| 22  | y     | 612 | CLA  | C4D-CHA-C1A | -3.25 | 117.30      | 121.25   |
| 22  | b     | 613 | CLA  | CMB-C2B-C3B | 3.25  | 130.75      | 124.68   |
| 23  | R     | 312 | LUT  | C7-C8-C9    | -3.24 | 121.33      | 126.23   |
| 22  | S     | 303 | CLA  | CMB-C2B-C3B | 3.24  | 130.75      | 124.68   |
| 22  | N     | 612 | CLA  | C4D-CHA-C1A | -3.24 | 117.31      | 121.25   |
| 21  | y     | 601 | CHL  | C1-C2-C3    | -3.24 | 120.44      | 126.04   |
| 22  | s     | 312 | CLA  | CMB-C2B-C1B | -3.24 | 123.49      | 128.46   |
| 22  | s     | 311 | CLA  | CMB-C2B-C3B | 3.24  | 130.74      | 124.68   |
| 22  | R     | 308 | CLA  | CMB-C2B-C1B | -3.24 | 123.49      | 128.46   |
| 21  | R     | 305 | CHL  | C1-C2-C3    | -3.23 | 120.45      | 126.04   |
| 23  | r     | 313 | LUT  | C7-C8-C9    | -3.23 | 121.35      | 126.23   |
| 21  | N     | 607 | CHL  | C1-C2-C3    | -3.23 | 120.46      | 126.04   |
| 22  | S     | 312 | CLA  | CMB-C2B-C1B | -3.23 | 123.50      | 128.46   |
| 21  | Y     | 601 | CHL  | C1-C2-C3    | -3.23 | 120.46      | 126.04   |
| 22  | b     | 614 | CLA  | CMB-C2B-C3B | 3.23  | 130.71      | 124.68   |
| 21  | r     | 307 | CHL  | C1-C2-C3    | -3.23 | 120.46      | 126.04   |
| 21  | r     | 308 | CHL  | C1-C2-C3    | -3.22 | 120.47      | 126.04   |
| 22  | B     | 617 | CLA  | CMB-C2B-C3B | 3.22  | 130.70      | 124.68   |
| 21  | G     | 609 | CHL  | C1-C2-C3    | -3.22 | 120.47      | 126.04   |
| 22  | n     | 612 | CLA  | C4D-CHA-C1A | -3.22 | 117.34      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | g     | 609 | CHL  | C1-C2-C3    | -3.21 | 120.48      | 126.04   |
| 34  | a     | 412 | BCT  | O2-C-O1     | -3.21 | 111.21      | 119.55   |
| 25  | y     | 616 | NEX  | C27-C28-C29 | -3.21 | 120.55      | 125.53   |
| 21  | n     | 601 | CHL  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 21  | G     | 607 | CHL  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 21  | g     | 601 | CHL  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 21  | r     | 306 | CHL  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 21  | n     | 608 | CHL  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 21  | y     | 608 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 34  | D     | 403 | BCT  | O2-C-O1     | -3.20 | 111.23      | 119.55   |
| 21  | N     | 608 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 21  | Y     | 607 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 21  | Y     | 606 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 21  | N     | 601 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 22  | A     | 409 | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 22  | a     | 408 | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 21  | g     | 607 | CHL  | C1-C2-C3    | -3.20 | 120.51      | 126.04   |
| 21  | R     | 307 | CHL  | C1-C2-C3    | -3.20 | 120.51      | 126.04   |
| 22  | B     | 614 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 22  | b     | 611 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 21  | y     | 609 | CHL  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |
| 21  | n     | 607 | CHL  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |
| 21  | g     | 608 | CHL  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |
| 21  | N     | 606 | CHL  | C1-C2-C3    | -3.19 | 120.53      | 126.04   |
| 21  | R     | 306 | CHL  | C1-C2-C3    | -3.19 | 120.53      | 126.04   |
| 25  | r     | 315 | NEX  | C17-C1-C6   | -3.19 | 107.62      | 110.47   |
| 21  | Y     | 608 | CHL  | C1-C2-C3    | -3.19 | 120.53      | 126.04   |
| 23  | Y     | 614 | LUT  | C8-C9-C10   | -3.18 | 114.06      | 118.94   |
| 37  | F     | 101 | HEM  | CHD-C1D-C2D | 3.18  | 129.95      | 124.98   |
| 22  | N     | 611 | CLA  | CMB-C2B-C1B | -3.18 | 123.57      | 128.46   |
| 22  | N     | 612 | CLA  | CMB-C2B-C1B | -3.18 | 123.58      | 128.46   |
| 22  | g     | 613 | CLA  | CMB-C2B-C1B | -3.17 | 123.59      | 128.46   |
| 22  | s     | 308 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 21  | n     | 606 | CHL  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 22  | G     | 613 | CLA  | CMB-C2B-C1B | -3.17 | 123.59      | 128.46   |
| 22  | C     | 510 | CLA  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 21  | y     | 607 | CHL  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 22  | S     | 309 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 22  | n     | 612 | CLA  | CMB-C2B-C1B | -3.17 | 123.59      | 128.46   |
| 21  | G     | 601 | CHL  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 21  | G     | 608 | CHL  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 22  | s     | 309 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | g     | 612 | CLA  | CMB-C2B-C1B | -3.16 | 123.60      | 128.46   |
| 22  | C     | 514 | CLA  | CMB-C2B-C3B | 3.16  | 130.60      | 124.68   |
| 22  | W     | 101 | CLA  | CMB-C2B-C1B | -3.16 | 123.60      | 128.46   |
| 25  | y     | 618 | NEX  | C17-C1-C6   | -3.16 | 107.64      | 110.47   |
| 22  | Y     | 611 | CLA  | CMB-C2B-C1B | -3.16 | 123.60      | 128.46   |
| 22  | c     | 509 | CLA  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |
| 22  | w     | 101 | CLA  | CMB-C2B-C1B | -3.16 | 123.61      | 128.46   |
| 25  | n     | 616 | NEX  | C5-C6-C1    | -3.16 | 116.56      | 119.70   |
| 22  | y     | 612 | CLA  | CMB-C2B-C1B | -3.16 | 123.61      | 128.46   |
| 22  | C     | 504 | CLA  | CMB-C2B-C3B | 3.15  | 130.58      | 124.68   |
| 22  | S     | 308 | CLA  | C1B-CHB-C4A | -3.15 | 123.87      | 130.12   |
| 37  | f     | 101 | HEM  | CHD-C1D-C2D | 3.15  | 129.90      | 124.98   |
| 22  | c     | 503 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 22  | s     | 308 | CLA  | C1B-CHB-C4A | -3.15 | 123.88      | 130.12   |
| 22  | S     | 308 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 23  | N     | 615 | LUT  | C3-C4-C5    | -3.15 | 105.58      | 111.85   |
| 33  | L     | 101 | SQD  | O8-S-C6     | 3.15  | 110.75      | 105.74   |
| 22  | G     | 612 | CLA  | CMB-C2B-C1B | -3.14 | 123.63      | 128.46   |
| 22  | c     | 513 | CLA  | CMB-C2B-C3B | 3.14  | 130.55      | 124.68   |
| 30  | D     | 401 | PHO  | O1D-CGD-CBD | 3.14  | 129.96      | 124.74   |
| 33  | l     | 103 | SQD  | O8-S-C6     | 3.14  | 110.74      | 105.74   |
| 22  | n     | 611 | CLA  | CMB-C2B-C1B | -3.13 | 123.65      | 128.46   |
| 22  | G     | 613 | CLA  | C3A-C2A-C1A | 3.13  | 106.03      | 101.34   |
| 25  | y     | 616 | NEX  | C5-C4-C3    | 3.11  | 115.43      | 111.75   |
| 23  | R     | 312 | LUT  | C18-C5-C4   | -3.11 | 108.59      | 114.36   |
| 23  | r     | 313 | LUT  | C18-C5-C4   | -3.11 | 108.59      | 114.36   |
| 30  | d     | 401 | PHO  | O1D-CGD-CBD | 3.11  | 129.91      | 124.74   |
| 22  | g     | 613 | CLA  | CMB-C2B-C3B | 3.10  | 130.48      | 124.68   |
| 22  | Y     | 611 | CLA  | C3A-C2A-C1A | 3.10  | 105.98      | 101.34   |
| 22  | n     | 612 | CLA  | C3A-C2A-C1A | 3.10  | 105.98      | 101.34   |
| 22  | B     | 612 | CLA  | CMB-C2B-C3B | 3.10  | 130.47      | 124.68   |
| 22  | B     | 605 | CLA  | CMB-C2B-C3B | 3.10  | 130.47      | 124.68   |
| 22  | g     | 613 | CLA  | C3A-C2A-C1A | 3.09  | 105.97      | 101.34   |
| 22  | b     | 602 | CLA  | CMB-C2B-C3B | 3.09  | 130.46      | 124.68   |
| 22  | y     | 612 | CLA  | C3A-C2A-C1A | 3.09  | 105.97      | 101.34   |
| 22  | b     | 609 | CLA  | CMB-C2B-C3B | 3.09  | 130.45      | 124.68   |
| 22  | N     | 612 | CLA  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 22  | S     | 305 | CLA  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 25  | Y     | 616 | NEX  | C5-C4-C3    | 3.08  | 115.39      | 111.75   |
| 22  | B     | 613 | CLA  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 22  | A     | 406 | CLA  | CMB-C2B-C3B | 3.07  | 130.43      | 124.68   |
| 22  | y     | 612 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | n     | 612 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 24  | n     | 615 | XAT  | C25-C24-C23 | -3.07 | 106.68      | 112.75   |
| 22  | Y     | 611 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 22  | Y     | 604 | CLA  | CMB-C2B-C1B | -3.07 | 123.75      | 128.46   |
| 22  | s     | 313 | CLA  | CMB-C2B-C3B | 3.07  | 130.41      | 124.68   |
| 22  | b     | 610 | CLA  | CMB-C2B-C3B | 3.06  | 130.41      | 124.68   |
| 22  | y     | 604 | CLA  | CMB-C2B-C1B | -3.06 | 123.76      | 128.46   |
| 22  | S     | 313 | CLA  | CMB-C2B-C3B | 3.06  | 130.41      | 124.68   |
| 22  | G     | 613 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 22  | N     | 604 | CLA  | CMB-C2B-C1B | -3.06 | 123.76      | 128.46   |
| 22  | N     | 612 | CLA  | C3A-C2A-C1A | 3.06  | 105.92      | 101.34   |
| 25  | Y     | 616 | NEX  | C5-C6-C1    | -3.06 | 116.66      | 119.70   |
| 22  | a     | 405 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 22  | G     | 604 | CLA  | CMB-C2B-C1B | -3.06 | 123.76      | 128.46   |
| 22  | S     | 304 | CLA  | C1B-CHB-C4A | -3.05 | 124.07      | 130.12   |
| 22  | n     | 604 | CLA  | CMB-C2B-C1B | -3.05 | 123.77      | 128.46   |
| 33  | l     | 103 | SQD  | O5-C5-C4    | 3.05  | 115.23      | 109.69   |
| 22  | C     | 506 | CLA  | CMB-C2B-C3B | 3.05  | 130.38      | 124.68   |
| 22  | g     | 613 | CLA  | CHB-C4A-NA  | 3.04  | 128.72      | 124.51   |
| 22  | b     | 605 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 22  | B     | 608 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 24  | N     | 616 | XAT  | C25-C24-C23 | -3.04 | 106.73      | 112.75   |
| 35  | c     | 519 | DGD  | O5D-C6D-C5D | -3.04 | 103.42      | 109.05   |
| 22  | y     | 612 | CLA  | CHB-C4A-NA  | 3.04  | 128.71      | 124.51   |
| 22  | c     | 505 | CLA  | CMB-C2B-C3B | 3.04  | 130.36      | 124.68   |
| 22  | G     | 603 | CLA  | CMB-C2B-C3B | 3.04  | 130.36      | 124.68   |
| 33  | L     | 101 | SQD  | O5-C5-C4    | 3.03  | 115.20      | 109.69   |
| 22  | g     | 604 | CLA  | CMB-C2B-C1B | -3.03 | 123.80      | 128.46   |
| 22  | N     | 603 | CLA  | CMB-C2B-C3B | 3.03  | 130.35      | 124.68   |
| 22  | n     | 612 | CLA  | CHB-C4A-NA  | 3.03  | 128.70      | 124.51   |
| 22  | N     | 612 | CLA  | CHB-C4A-NA  | 3.03  | 128.70      | 124.51   |
| 22  | g     | 603 | CLA  | CMB-C2B-C3B | 3.02  | 130.34      | 124.68   |
| 22  | s     | 304 | CLA  | C1B-CHB-C4A | -3.02 | 124.13      | 130.12   |
| 35  | J     | 101 | DGD  | O5D-C6D-C5D | -3.02 | 103.46      | 109.05   |
| 22  | Y     | 611 | CLA  | CHB-C4A-NA  | 3.02  | 128.69      | 124.51   |
| 22  | n     | 603 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 32  | D     | 407 | PL9  | C40-C39-C41 | 3.02  | 120.35      | 115.27   |
| 22  | s     | 305 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 32  | a     | 410 | PL9  | O2-C1-C2    | -3.02 | 117.09      | 121.41   |
| 23  | G     | 616 | LUT  | C8-C9-C10   | -3.01 | 114.31      | 118.94   |
| 22  | y     | 603 | CLA  | CMB-C2B-C3B | 3.01  | 130.32      | 124.68   |
| 22  | G     | 613 | CLA  | CHB-C4A-NA  | 3.01  | 128.68      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Y     | 603 | CLA  | CMB-C2B-C3B | 3.01  | 130.31      | 124.68   |
| 22  | B     | 607 | CLA  | CMB-C2B-C3B | 3.01  | 130.31      | 124.68   |
| 22  | b     | 604 | CLA  | CMB-C2B-C3B | 3.01  | 130.31      | 124.68   |
| 24  | y     | 615 | XAT  | C8-C9-C10   | -3.00 | 114.33      | 118.94   |
| 22  | C     | 515 | CLA  | CMB-C2B-C3B | 3.00  | 130.30      | 124.68   |
| 32  | d     | 406 | PL9  | C40-C39-C41 | 3.00  | 120.32      | 115.27   |
| 30  | A     | 408 | PHO  | O1D-CGD-CBD | 3.00  | 129.74      | 124.74   |
| 25  | g     | 618 | NEX  | C5-C4-C3    | 3.00  | 115.29      | 111.75   |
| 23  | r     | 313 | LUT  | C4-C5-C6    | -2.99 | 114.17      | 120.85   |
| 25  | g     | 618 | NEX  | C27-C28-C29 | -2.99 | 120.89      | 125.53   |
| 22  | Y     | 602 | CLA  | CMB-C2B-C3B | 2.99  | 130.27      | 124.68   |
| 25  | n     | 616 | NEX  | C5-C4-C3    | 2.99  | 115.28      | 111.75   |
| 21  | G     | 607 | CHL  | CHD-C1D-C2D | 2.99  | 131.74      | 125.48   |
| 21  | Y     | 607 | CHL  | CHD-C1D-C2D | 2.98  | 131.74      | 125.48   |
| 21  | Y     | 606 | CHL  | CHD-C1D-C2D | 2.98  | 131.74      | 125.48   |
| 21  | Y     | 608 | CHL  | CHD-C1D-C2D | 2.98  | 131.73      | 125.48   |
| 23  | G     | 615 | LUT  | C21-C26-C25 | 2.98  | 116.75      | 111.42   |
| 21  | S     | 301 | CHL  | CHD-C1D-C2D | 2.98  | 131.73      | 125.48   |
| 22  | y     | 612 | CLA  | C1C-C2C-C3C | -2.98 | 103.83      | 106.96   |
| 21  | n     | 601 | CHL  | CHD-C1D-C2D | 2.98  | 131.72      | 125.48   |
| 22  | R     | 303 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 22  | n     | 602 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 22  | g     | 613 | CLA  | C1C-C2C-C3C | -2.97 | 103.83      | 106.96   |
| 23  | R     | 312 | LUT  | C4-C5-C6    | -2.97 | 114.22      | 120.85   |
| 21  | G     | 609 | CHL  | CHD-C1D-C2D | 2.97  | 131.72      | 125.48   |
| 22  | b     | 601 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 22  | D     | 404 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 21  | g     | 605 | CHL  | CHD-C1D-C2D | 2.97  | 131.71      | 125.48   |
| 32  | A     | 411 | PL9  | O2-C1-C2    | -2.97 | 117.16      | 121.41   |
| 21  | S     | 306 | CHL  | CHD-C1D-C2D | 2.97  | 131.71      | 125.48   |
| 24  | Y     | 615 | XAT  | C31-C32-C33 | -2.97 | 118.08      | 126.42   |
| 21  | N     | 608 | CHL  | CHD-C1D-C2D | 2.97  | 131.71      | 125.48   |
| 21  | y     | 608 | CHL  | CHD-C1D-C2D | 2.97  | 131.70      | 125.48   |
| 22  | g     | 602 | CLA  | CMB-C2B-C3B | 2.97  | 130.23      | 124.68   |
| 22  | c     | 514 | CLA  | CMB-C2B-C3B | 2.97  | 130.23      | 124.68   |
| 23  | g     | 615 | LUT  | C21-C26-C25 | 2.97  | 116.73      | 111.42   |
| 21  | N     | 601 | CHL  | CHD-C1D-C2D | 2.97  | 131.70      | 125.48   |
| 22  | B     | 604 | CLA  | CMB-C2B-C3B | 2.96  | 130.22      | 124.68   |
| 21  | y     | 605 | CHL  | CHD-C1D-C2D | 2.96  | 131.70      | 125.48   |
| 22  | C     | 512 | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 21  | N     | 605 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | s     | 306 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | a     | 407 | PHO  | O1D-CGD-CBD | 2.96  | 129.67      | 124.74   |
| 21  | R     | 306 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 23  | Y     | 613 | LUT  | C21-C26-C25 | 2.96  | 116.72      | 111.42   |
| 35  | J     | 101 | DGD  | C3D-C4D-C5D | -2.96 | 104.95      | 110.24   |
| 21  | g     | 608 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | y     | 609 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | r     | 301 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | r     | 308 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | y     | 607 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | Y     | 605 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | g     | 601 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | G     | 608 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | S     | 307 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 21  | r     | 307 | CHL  | CHD-C1D-C2D | 2.96  | 131.69      | 125.48   |
| 23  | g     | 616 | LUT  | C8-C9-C10   | -2.96 | 114.40      | 118.94   |
| 21  | y     | 606 | CHL  | CHD-C1D-C2D | 2.96  | 131.68      | 125.48   |
| 21  | N     | 607 | CHL  | CHD-C1D-C2D | 2.96  | 131.68      | 125.48   |
| 21  | G     | 605 | CHL  | CHD-C1D-C2D | 2.96  | 131.68      | 125.48   |
| 33  | A     | 412 | SQD  | O8-S-C6     | 2.96  | 110.45      | 105.74   |
| 21  | R     | 307 | CHL  | CHD-C1D-C2D | 2.96  | 131.68      | 125.48   |
| 22  | N     | 612 | CLA  | C1C-C2C-C3C | -2.96 | 103.85      | 106.96   |
| 22  | r     | 304 | CLA  | CMB-C2B-C3B | 2.95  | 130.21      | 124.68   |
| 22  | N     | 602 | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 21  | G     | 606 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 23  | n     | 614 | LUT  | C21-C26-C25 | 2.95  | 116.71      | 111.42   |
| 21  | R     | 305 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 23  | N     | 614 | LUT  | C21-C26-C25 | 2.95  | 116.70      | 111.42   |
| 21  | n     | 608 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 21  | s     | 301 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 22  | G     | 613 | CLA  | C1C-C2C-C3C | -2.95 | 103.85      | 106.96   |
| 21  | G     | 601 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 21  | s     | 307 | CHL  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 22  | n     | 610 | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 21  | g     | 609 | CHL  | CHD-C1D-C2D | 2.95  | 131.66      | 125.48   |
| 21  | s     | 302 | CHL  | CHD-C1D-C2D | 2.95  | 131.66      | 125.48   |
| 22  | b     | 606 | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 22  | n     | 612 | CLA  | C1C-C2C-C3C | -2.95 | 103.86      | 106.96   |
| 31  | c     | 516 | BCR  | C15-C14-C13 | -2.95 | 123.10      | 127.31   |
| 21  | N     | 606 | CHL  | CHD-C1D-C2D | 2.95  | 131.66      | 125.48   |
| 33  | a     | 411 | SQD  | O8-S-C6     | 2.95  | 110.44      | 105.74   |
| 22  | G     | 611 | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 21  | g     | 606 | CHL  | CHD-C1D-C2D | 2.95  | 131.66      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 610 | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 21  | y     | 601 | CHL  | CHD-C1D-C2D | 2.95  | 131.66      | 125.48   |
| 21  | R     | 305 | CHL  | CMD-C2D-C3D | -2.95 | 120.84      | 127.61   |
| 21  | n     | 606 | CHL  | CHD-C1D-C2D | 2.94  | 131.66      | 125.48   |
| 21  | n     | 605 | CHL  | CHD-C1D-C2D | 2.94  | 131.66      | 125.48   |
| 21  | r     | 306 | CHL  | CHD-C1D-C2D | 2.94  | 131.66      | 125.48   |
| 22  | d     | 403 | CLA  | O2D-CGD-O1D | -2.94 | 118.08      | 123.84   |
| 22  | d     | 403 | CLA  | CMB-C2B-C3B | 2.94  | 130.19      | 124.68   |
| 21  | n     | 607 | CHL  | CHD-C1D-C2D | 2.94  | 131.65      | 125.48   |
| 21  | Y     | 601 | CHL  | CHD-C1D-C2D | 2.94  | 131.65      | 125.48   |
| 22  | Y     | 611 | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 22  | y     | 611 | CLA  | CMB-C2B-C3B | 2.94  | 130.18      | 124.68   |
| 21  | y     | 601 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 21  | S     | 301 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 21  | g     | 606 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 23  | y     | 614 | LUT  | C21-C26-C25 | 2.94  | 116.68      | 111.42   |
| 21  | N     | 605 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 21  | r     | 308 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 21  | S     | 302 | CHL  | CHD-C1D-C2D | 2.94  | 131.64      | 125.48   |
| 21  | g     | 607 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 21  | G     | 607 | CHL  | CMD-C2D-C3D | -2.94 | 120.85      | 127.61   |
| 22  | G     | 602 | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 22  | r     | 312 | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 35  | c     | 519 | DGD  | C3D-C4D-C5D | -2.94 | 105.00      | 110.24   |
| 31  | C     | 517 | BCR  | C11-C10-C9  | -2.94 | 123.12      | 127.31   |
| 21  | s     | 307 | CHL  | CMD-C2D-C3D | -2.94 | 120.86      | 127.61   |
| 22  | y     | 602 | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 21  | N     | 606 | CHL  | CMD-C2D-C3D | -2.94 | 120.86      | 127.61   |
| 21  | g     | 609 | CHL  | CMD-C2D-C3D | -2.93 | 120.86      | 127.61   |
| 21  | R     | 306 | CHL  | CMD-C2D-C3D | -2.93 | 120.86      | 127.61   |
| 22  | C     | 515 | CLA  | O2D-CGD-O1D | -2.93 | 118.10      | 123.84   |
| 22  | g     | 611 | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 21  | Y     | 605 | CHL  | CMD-C2D-C3D | -2.93 | 120.87      | 127.61   |
| 21  | r     | 306 | CHL  | CMD-C2D-C3D | -2.93 | 120.87      | 127.61   |
| 21  | g     | 607 | CHL  | CHD-C1D-C2D | 2.93  | 131.63      | 125.48   |
| 21  | n     | 601 | CHL  | CMD-C2D-C3D | -2.93 | 120.87      | 127.61   |
| 21  | g     | 608 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | n     | 605 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | G     | 605 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | s     | 301 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 22  | Y     | 610 | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 22  | B     | 609 | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | G     | 613 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 21  | g     | 601 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | S     | 306 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | g     | 605 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | y     | 609 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | y     | 606 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | n     | 607 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 22  | c     | 511 | CLA  | O2D-CGD-O1D | -2.93 | 118.12      | 123.84   |
| 31  | C     | 517 | BCR  | C15-C14-C13 | -2.93 | 123.13      | 127.31   |
| 21  | y     | 607 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | S     | 307 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | G     | 608 | CHL  | CMD-C2D-C3D | -2.93 | 120.88      | 127.61   |
| 21  | R     | 307 | CHL  | CMD-C2D-C3D | -2.93 | 120.89      | 127.61   |
| 22  | N     | 612 | CLA  | O2D-CGD-O1D | -2.93 | 118.12      | 123.84   |
| 21  | G     | 606 | CHL  | CMD-C2D-C3D | -2.92 | 120.89      | 127.61   |
| 22  | B     | 615 | CLA  | CMB-C2B-C3B | 2.92  | 130.15      | 124.68   |
| 21  | Y     | 606 | CHL  | CMD-C2D-C3D | -2.92 | 120.89      | 127.61   |
| 21  | r     | 301 | CHL  | CMD-C2D-C3D | -2.92 | 120.89      | 127.61   |
| 21  | n     | 608 | CHL  | CMD-C2D-C3D | -2.92 | 120.89      | 127.61   |
| 25  | n     | 616 | NEX  | C27-C28-C29 | -2.92 | 121.00      | 125.53   |
| 22  | Y     | 611 | CLA  | C1C-C2C-C3C | -2.92 | 103.89      | 106.96   |
| 35  | C     | 518 | DGD  | O5D-C6D-C5D | -2.92 | 103.64      | 109.05   |
| 21  | y     | 608 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 22  | R     | 304 | CLA  | CMB-C2B-C1B | -2.92 | 123.98      | 128.46   |
| 21  | G     | 609 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 21  | N     | 608 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 21  | r     | 307 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 21  | S     | 302 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 22  | y     | 612 | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 22  | c     | 504 | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 21  | n     | 606 | CHL  | CMD-C2D-C3D | -2.92 | 120.90      | 127.61   |
| 22  | c     | 514 | CLA  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |
| 21  | s     | 302 | CHL  | CMD-C2D-C3D | -2.92 | 120.91      | 127.61   |
| 22  | s     | 303 | CLA  | C1B-CHB-C4A | -2.91 | 124.35      | 130.12   |
| 35  | c     | 517 | DGD  | O5D-C6D-C5D | -2.91 | 103.66      | 109.05   |
| 22  | S     | 303 | CLA  | C1B-CHB-C4A | -2.91 | 124.35      | 130.12   |
| 22  | A     | 405 | CLA  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 21  | Y     | 607 | CHL  | CMD-C2D-C3D | -2.91 | 120.92      | 127.61   |
| 21  | N     | 607 | CHL  | CMD-C2D-C3D | -2.91 | 120.92      | 127.61   |
| 21  | y     | 605 | CHL  | CMD-C2D-C3D | -2.91 | 120.92      | 127.61   |
| 21  | N     | 601 | CHL  | CMD-C2D-C3D | -2.91 | 120.92      | 127.61   |
| 21  | s     | 306 | CHL  | CMD-C2D-C3D | -2.91 | 120.92      | 127.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | a     | 404 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 22  | b     | 612 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 33  | a     | 411 | SQD  | O5-C1-C2    | 2.91  | 116.50      | 110.35   |
| 33  | A     | 412 | SQD  | O5-C1-C2    | 2.91  | 116.50      | 110.35   |
| 36  | C     | 502 | LMG  | O1-C1-C2    | -2.91 | 103.77      | 108.30   |
| 21  | Y     | 608 | CHL  | CMD-C2D-C3D | -2.91 | 120.93      | 127.61   |
| 21  | g     | 609 | CHL  | C3D-C4D-ND  | 2.91  | 114.94      | 110.24   |
| 21  | Y     | 601 | CHL  | CMD-C2D-C3D | -2.90 | 120.93      | 127.61   |
| 22  | n     | 612 | CLA  | O2D-CGD-O1D | -2.90 | 118.16      | 123.84   |
| 31  | C     | 517 | BCR  | C7-C8-C9    | -2.90 | 121.85      | 126.23   |
| 22  | C     | 513 | CLA  | O2D-CGD-O1D | -2.90 | 118.16      | 123.84   |
| 22  | n     | 613 | CLA  | CMB-C2B-C3B | 2.90  | 130.11      | 124.68   |
| 22  | g     | 613 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 36  | b     | 620 | LMG  | O6-C1-O1    | -2.90 | 103.11      | 109.97   |
| 21  | G     | 601 | CHL  | CMD-C2D-C3D | -2.90 | 120.94      | 127.61   |
| 22  | D     | 404 | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 31  | H     | 101 | BCR  | C24-C23-C22 | -2.90 | 121.86      | 126.23   |
| 22  | R     | 311 | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 22  | r     | 305 | CLA  | CMB-C2B-C1B | -2.90 | 124.01      | 128.46   |
| 36  | B     | 623 | LMG  | O6-C1-O1    | -2.90 | 103.12      | 109.97   |
| 21  | y     | 608 | CHL  | C3D-C4D-ND  | 2.89  | 114.92      | 110.24   |
| 22  | B     | 611 | CLA  | CMB-C2B-C3B | 2.89  | 130.09      | 124.68   |
| 22  | C     | 509 | CLA  | CMB-C2B-C3B | 2.89  | 130.09      | 124.68   |
| 21  | y     | 605 | CHL  | C3D-C4D-ND  | 2.89  | 114.91      | 110.24   |
| 22  | c     | 512 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 31  | B     | 620 | BCR  | C15-C14-C13 | -2.89 | 123.19      | 127.31   |
| 36  | w     | 102 | LMG  | O1-C1-C2    | -2.89 | 103.79      | 108.30   |
| 21  | y     | 601 | CHL  | C3D-C4D-ND  | 2.89  | 114.91      | 110.24   |
| 22  | g     | 614 | CLA  | CMB-C2B-C3B | 2.89  | 130.08      | 124.68   |
| 22  | N     | 613 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 21  | y     | 609 | CHL  | C3D-C4D-ND  | 2.88  | 114.90      | 110.24   |
| 21  | R     | 307 | CHL  | C3D-C4D-ND  | 2.88  | 114.90      | 110.24   |
| 31  | b     | 617 | BCR  | C15-C14-C13 | -2.88 | 123.20      | 127.31   |
| 24  | n     | 615 | XAT  | C31-C32-C33 | -2.88 | 118.32      | 126.42   |
| 25  | y     | 616 | NEX  | C24-C23-C22 | 2.88  | 116.34      | 110.77   |
| 22  | y     | 613 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 31  | C     | 516 | BCR  | C15-C16-C17 | -2.88 | 117.58      | 123.47   |
| 21  | G     | 607 | CHL  | C3D-C4D-ND  | 2.88  | 114.90      | 110.24   |
| 21  | g     | 606 | CHL  | C3D-C4D-ND  | 2.88  | 114.89      | 110.24   |
| 22  | Y     | 612 | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 22  | s     | 309 | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 31  | h     | 101 | BCR  | C24-C23-C22 | -2.88 | 121.89      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | s     | 307 | CHL  | C3D-C4D-ND  | 2.88  | 114.89      | 110.24   |
| 21  | G     | 601 | CHL  | C3D-C4D-ND  | 2.88  | 114.89      | 110.24   |
| 21  | G     | 605 | CHL  | C3D-C4D-ND  | 2.87  | 114.89      | 110.24   |
| 22  | S     | 309 | CLA  | CMB-C2B-C3B | 2.87  | 130.06      | 124.68   |
| 21  | Y     | 606 | CHL  | C3D-C4D-ND  | 2.87  | 114.89      | 110.24   |
| 21  | N     | 606 | CHL  | C3D-C4D-ND  | 2.87  | 114.89      | 110.24   |
| 21  | G     | 606 | CHL  | C3D-C4D-ND  | 2.87  | 114.89      | 110.24   |
| 31  | c     | 516 | BCR  | C7-C8-C9    | -2.87 | 121.89      | 126.23   |
| 35  | c     | 519 | DGD  | O6E-C5E-C4E | 2.87  | 114.91      | 109.69   |
| 31  | k     | 102 | BCR  | C15-C16-C17 | -2.87 | 117.59      | 123.47   |
| 22  | c     | 508 | CLA  | CMB-C2B-C3B | 2.87  | 130.05      | 124.68   |
| 21  | S     | 302 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 31  | c     | 516 | BCR  | C11-C10-C9  | -2.87 | 123.21      | 127.31   |
| 31  | K     | 102 | BCR  | C15-C16-C17 | -2.87 | 117.59      | 123.47   |
| 21  | S     | 306 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 22  | b     | 609 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 21  | G     | 608 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 21  | G     | 609 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 22  | C     | 505 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 22  | b     | 608 | CLA  | CMB-C2B-C3B | 2.87  | 130.04      | 124.68   |
| 24  | G     | 617 | XAT  | C31-C32-C33 | -2.87 | 118.36      | 126.42   |
| 21  | g     | 605 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 21  | n     | 606 | CHL  | C3D-C4D-ND  | 2.87  | 114.88      | 110.24   |
| 21  | R     | 305 | CHL  | C3D-C4D-ND  | 2.87  | 114.87      | 110.24   |
| 22  | G     | 614 | CLA  | CMB-C2B-C3B | 2.87  | 130.04      | 124.68   |
| 22  | b     | 615 | CLA  | CMB-C2B-C3B | 2.86  | 130.04      | 124.68   |
| 21  | Y     | 601 | CHL  | C3D-C4D-ND  | 2.86  | 114.87      | 110.24   |
| 22  | B     | 612 | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 21  | y     | 607 | CHL  | C3D-C4D-ND  | 2.86  | 114.87      | 110.24   |
| 21  | n     | 607 | CHL  | C3D-C4D-ND  | 2.86  | 114.87      | 110.24   |
| 24  | g     | 617 | XAT  | C31-C32-C33 | -2.86 | 118.38      | 126.42   |
| 21  | n     | 608 | CHL  | C3D-C4D-ND  | 2.86  | 114.87      | 110.24   |
| 21  | g     | 601 | CHL  | C3D-C4D-ND  | 2.86  | 114.87      | 110.24   |
| 21  | N     | 608 | CHL  | C3D-C4D-ND  | 2.86  | 114.86      | 110.24   |
| 22  | s     | 303 | CLA  | O2D-CGD-O1D | -2.86 | 118.25      | 123.84   |
| 21  | r     | 301 | CHL  | C3D-C4D-ND  | 2.86  | 114.86      | 110.24   |
| 21  | R     | 306 | CHL  | C3D-C4D-ND  | 2.86  | 114.86      | 110.24   |
| 21  | r     | 306 | CHL  | C3D-C4D-ND  | 2.86  | 114.86      | 110.24   |
| 35  | J     | 101 | DGD  | O6E-C5E-C4E | 2.86  | 114.88      | 109.69   |
| 21  | S     | 301 | CHL  | C3D-C4D-ND  | 2.86  | 114.86      | 110.24   |
| 21  | N     | 607 | CHL  | C3D-C4D-ND  | 2.85  | 114.86      | 110.24   |
| 21  | r     | 308 | CHL  | C3D-C4D-ND  | 2.85  | 114.86      | 110.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | C     | 519 | DGD  | O5D-C6D-C5D | -2.85 | 103.77      | 109.05   |
| 21  | s     | 302 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 21  | r     | 307 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 36  | D     | 411 | LMG  | O6-C1-O1    | -2.85 | 103.22      | 109.97   |
| 21  | Y     | 605 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 21  | g     | 608 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 21  | n     | 605 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 21  | Y     | 607 | CHL  | C3D-C4D-ND  | 2.85  | 114.85      | 110.24   |
| 21  | g     | 607 | CHL  | C3D-C4D-ND  | 2.85  | 114.84      | 110.24   |
| 21  | Y     | 608 | CHL  | C3D-C4D-ND  | 2.85  | 114.84      | 110.24   |
| 21  | n     | 601 | CHL  | C3D-C4D-ND  | 2.85  | 114.84      | 110.24   |
| 22  | C     | 509 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 21  | R     | 307 | CHL  | C4-C3-C5    | 2.84  | 120.06      | 115.27   |
| 22  | C     | 512 | CLA  | CMB-C2B-C3B | 2.84  | 130.00      | 124.68   |
| 22  | B     | 618 | CLA  | CMB-C2B-C3B | 2.84  | 130.00      | 124.68   |
| 22  | c     | 508 | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 31  | c     | 515 | BCR  | C15-C16-C17 | -2.84 | 117.65      | 123.47   |
| 22  | b     | 615 | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 22  | B     | 603 | CLA  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 21  | n     | 608 | CHL  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 21  | N     | 605 | CHL  | C3D-C4D-ND  | 2.84  | 114.83      | 110.24   |
| 21  | S     | 307 | CHL  | C3D-C4D-ND  | 2.84  | 114.83      | 110.24   |
| 22  | B     | 611 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 31  | C     | 516 | BCR  | C24-C23-C22 | -2.84 | 121.95      | 126.23   |
| 22  | n     | 613 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 22  | b     | 613 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 22  | C     | 510 | CLA  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 22  | S     | 304 | CLA  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 22  | B     | 615 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 22  | c     | 509 | CLA  | CMB-C2B-C3B | 2.84  | 129.98      | 124.68   |
| 21  | N     | 601 | CHL  | C3D-C4D-ND  | 2.84  | 114.82      | 110.24   |
| 31  | c     | 515 | BCR  | C24-C23-C22 | -2.83 | 121.95      | 126.23   |
| 22  | S     | 303 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 22  | B     | 618 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 22  | s     | 304 | CLA  | CMB-C2B-C3B | 2.83  | 129.98      | 124.68   |
| 21  | Y     | 601 | CHL  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 21  | s     | 301 | CHL  | C3D-C4D-ND  | 2.83  | 114.82      | 110.24   |
| 22  | b     | 608 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 21  | s     | 306 | CHL  | C3D-C4D-ND  | 2.83  | 114.81      | 110.24   |
| 35  | c     | 518 | DGD  | O5D-C6D-C5D | -2.83 | 103.81      | 109.05   |
| 25  | y     | 618 | NEX  | C38-C25-C24 | 2.83  | 117.46      | 114.28   |
| 22  | B     | 616 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | y     | 606 | CHL  | C3D-C4D-ND  | 2.83  | 114.81      | 110.24   |
| 22  | c     | 510 | CLA  | C4D-C3D-CAD | -2.83 | 104.76      | 108.10   |
| 21  | Y     | 607 | CHL  | C4-C3-C5    | 2.83  | 120.02      | 115.27   |
| 21  | R     | 305 | CHL  | C4-C3-C5    | 2.83  | 120.02      | 115.27   |
| 36  | d     | 410 | LMG  | O6-C1-O1    | -2.83 | 103.28      | 109.97   |
| 21  | N     | 601 | CHL  | C4-C3-C5    | 2.82  | 120.02      | 115.27   |
| 21  | G     | 607 | CHL  | C4-C3-C5    | 2.82  | 120.02      | 115.27   |
| 22  | C     | 506 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 21  | g     | 609 | CHL  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 21  | N     | 607 | CHL  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 22  | y     | 613 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 21  | r     | 308 | CHL  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 21  | n     | 601 | CHL  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 30  | d     | 401 | PHO  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 22  | b     | 603 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 21  | G     | 609 | CHL  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 30  | D     | 401 | PHO  | CMB-C2B-C3B | 2.82  | 129.94      | 124.68   |
| 22  | c     | 505 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 35  | H     | 102 | DGD  | CDB-CCB-CBB | -2.81 | 100.15      | 114.42   |
| 25  | r     | 315 | NEX  | C38-C25-C24 | 2.81  | 117.44      | 114.28   |
| 21  | g     | 607 | CHL  | C4-C3-C5    | 2.81  | 120.00      | 115.27   |
| 22  | Y     | 609 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 21  | G     | 608 | CHL  | C4-C3-C5    | 2.81  | 120.00      | 115.27   |
| 35  | h     | 102 | DGD  | CDB-CCB-CBB | -2.81 | 100.16      | 114.42   |
| 33  | D     | 402 | SQD  | O8-S-C6     | 2.81  | 110.22      | 105.74   |
| 22  | C     | 507 | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 22  | R     | 302 | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 22  | g     | 614 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 22  | G     | 614 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 22  | C     | 511 | CLA  | C4D-C3D-CAD | -2.81 | 104.79      | 108.10   |
| 21  | y     | 607 | CHL  | C4-C3-C5    | 2.81  | 120.00      | 115.27   |
| 22  | c     | 511 | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 22  | s     | 309 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 21  | R     | 306 | CHL  | C4-C3-C5    | 2.81  | 119.99      | 115.27   |
| 21  | y     | 601 | CHL  | C4-C3-C5    | 2.81  | 119.99      | 115.27   |
| 22  | b     | 612 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 36  | C     | 523 | LMG  | O6-C1-O1    | -2.80 | 103.33      | 109.97   |
| 31  | B     | 619 | BCR  | C33-C5-C6   | -2.80 | 121.38      | 124.53   |
| 22  | r     | 303 | CLA  | CMB-C2B-C3B | 2.80  | 129.92      | 124.68   |
| 22  | N     | 609 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 22  | r     | 304 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 22  | R     | 303 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | n     | 607 | CHL  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 22  | Y     | 612 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 22  | N     | 613 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 21  | r     | 307 | CHL  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 22  | D     | 405 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 21  | G     | 601 | CHL  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 22  | c     | 506 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 21  | Y     | 608 | CHL  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 22  | C     | 507 | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 31  | B     | 620 | BCR  | C15-C16-C17 | -2.79 | 117.75      | 123.47   |
| 31  | B     | 621 | BCR  | C24-C23-C22 | -2.79 | 122.01      | 126.23   |
| 22  | B     | 606 | CLA  | O2D-CGD-O1D | -2.79 | 118.37      | 123.84   |
| 21  | g     | 601 | CHL  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 31  | b     | 616 | BCR  | C33-C5-C6   | -2.79 | 121.39      | 124.53   |
| 22  | G     | 610 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 35  | c     | 518 | DGD  | CDB-CCB-CBB | -2.79 | 100.24      | 114.42   |
| 22  | g     | 610 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 21  | g     | 608 | CHL  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 22  | y     | 610 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 31  | b     | 617 | BCR  | C15-C16-C17 | -2.79 | 117.76      | 123.47   |
| 21  | n     | 606 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 21  | y     | 608 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 33  | d     | 402 | SQD  | O8-S-C6     | 2.79  | 110.18      | 105.74   |
| 21  | r     | 306 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 26  | l     | 102 | LHG  | O8-C23-C24  | 2.79  | 120.65      | 111.91   |
| 21  | N     | 606 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 21  | N     | 608 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 22  | n     | 609 | CLA  | O2D-CGD-O1D | -2.78 | 118.39      | 123.84   |
| 26  | L     | 103 | LHG  | O8-C23-C24  | 2.78  | 120.64      | 111.91   |
| 31  | b     | 618 | BCR  | C24-C23-C22 | -2.78 | 122.03      | 126.23   |
| 22  | x     | 101 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 35  | C     | 519 | DGD  | CDB-CCB-CBB | -2.78 | 100.30      | 114.42   |
| 36  | c     | 523 | LMG  | O6-C1-O1    | -2.78 | 103.39      | 109.97   |
| 22  | d     | 404 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 22  | c     | 506 | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 32  | D     | 407 | PL9  | C22-C23-C24 | -2.78 | 120.97      | 127.66   |
| 22  | B     | 608 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 22  | S     | 309 | CLA  | O2D-CGD-O1D | -2.77 | 118.41      | 123.84   |
| 21  | y     | 609 | CHL  | C4-C3-C5    | 2.77  | 119.94      | 115.27   |
| 22  | B     | 610 | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 21  | Y     | 606 | CHL  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 22  | A     | 407 | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | C     | 516 | BCR  | C33-C5-C6   | -2.77 | 121.42      | 124.53   |
| 22  | a     | 406 | CLA  | CMB-C2B-C3B | 2.77  | 129.85      | 124.68   |
| 22  | b     | 607 | CLA  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 31  | D     | 406 | BCR  | C24-C23-C22 | -2.76 | 122.07      | 126.23   |
| 24  | y     | 615 | XAT  | C31-C32-C33 | -2.76 | 118.67      | 126.42   |
| 22  | s     | 310 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 22  | c     | 507 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 22  | r     | 309 | CLA  | CMB-C2B-C3B | 2.75  | 129.83      | 124.68   |
| 30  | A     | 408 | PHO  | CMB-C2B-C3B | 2.75  | 129.82      | 124.68   |
| 32  | d     | 406 | PL9  | C7-C8-C9    | -2.75 | 122.21      | 126.79   |
| 22  | N     | 609 | CLA  | CMB-C2B-C3B | 2.75  | 129.82      | 124.68   |
| 22  | A     | 407 | CLA  | CMB-C2B-C3B | 2.75  | 129.82      | 124.68   |
| 22  | g     | 611 | CLA  | O2D-CGD-O1D | -2.75 | 118.46      | 123.84   |
| 30  | a     | 407 | PHO  | CMB-C2B-C3B | 2.75  | 129.82      | 124.68   |
| 32  | d     | 406 | PL9  | C22-C23-C24 | -2.75 | 121.04      | 127.66   |
| 22  | S     | 304 | CLA  | O2D-CGD-O1D | -2.75 | 118.47      | 123.84   |
| 22  | a     | 406 | CLA  | O2D-CGD-O1D | -2.75 | 118.47      | 123.84   |
| 22  | s     | 313 | CLA  | O2D-CGD-O1D | -2.75 | 118.47      | 123.84   |
| 25  | g     | 618 | NEX  | C5-C6-C1    | -2.74 | 116.97      | 119.70   |
| 22  | b     | 605 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 22  | G     | 610 | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 22  | d     | 404 | CLA  | CHB-C4A-NA  | 2.74  | 128.30      | 124.51   |
| 33  | L     | 102 | SQD  | O5-C5-C4    | 2.74  | 114.67      | 109.69   |
| 22  | R     | 308 | CLA  | CMB-C2B-C3B | 2.74  | 129.80      | 124.68   |
| 22  | s     | 304 | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 22  | S     | 313 | CLA  | O2D-CGD-O1D | -2.73 | 118.49      | 123.84   |
| 22  | G     | 611 | CLA  | O2D-CGD-O1D | -2.73 | 118.49      | 123.84   |
| 22  | C     | 508 | CLA  | O2D-CGD-O1D | -2.73 | 118.49      | 123.84   |
| 22  | Y     | 610 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 22  | n     | 610 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 31  | D     | 406 | BCR  | C33-C5-C6   | -2.73 | 121.46      | 124.53   |
| 22  | C     | 503 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 22  | r     | 311 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 22  | g     | 610 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 26  | S     | 314 | LHG  | O8-C23-C24  | 2.73  | 120.47      | 111.91   |
| 22  | G     | 602 | CLA  | CHB-C4A-NA  | 2.73  | 128.28      | 124.51   |
| 22  | s     | 312 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 22  | N     | 610 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 22  | R     | 311 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 31  | d     | 405 | BCR  | C33-C5-C6   | -2.73 | 121.47      | 124.53   |
| 31  | k     | 101 | BCR  | C24-C23-C22 | -2.73 | 122.12      | 126.23   |
| 22  | R     | 309 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | y     | 610 | CLA  | CMB-C2B-C3B | 2.72  | 129.78      | 124.68   |
| 22  | R     | 310 | CLA  | O2D-CGD-O1D | -2.72 | 118.51      | 123.84   |
| 22  | g     | 602 | CLA  | CHB-C4A-NA  | 2.72  | 128.28      | 124.51   |
| 35  | a     | 413 | DGD  | CDB-CCB-CBB | -2.72 | 100.61      | 114.42   |
| 31  | c     | 515 | BCR  | C33-C5-C6   | -2.72 | 121.47      | 124.53   |
| 32  | D     | 407 | PL9  | C7-C8-C9    | -2.72 | 122.26      | 126.79   |
| 35  | A     | 401 | DGD  | CDB-CCB-CBB | -2.72 | 100.62      | 114.42   |
| 22  | S     | 312 | CLA  | CMB-C2B-C3B | 2.72  | 129.76      | 124.68   |
| 26  | R     | 301 | LHG  | O8-C23-C24  | 2.71  | 120.42      | 111.91   |
| 31  | d     | 405 | BCR  | C24-C23-C22 | -2.71 | 122.14      | 126.23   |
| 33  | l     | 101 | SQD  | O5-C5-C4    | 2.71  | 114.62      | 109.69   |
| 22  | y     | 604 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 22  | g     | 610 | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 22  | c     | 502 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 22  | b     | 606 | CLA  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |
| 26  | s     | 314 | LHG  | O8-C23-C24  | 2.71  | 120.41      | 111.91   |
| 22  | Y     | 604 | CLA  | C1B-CHB-C4A | -2.71 | 124.75      | 130.12   |
| 22  | r     | 310 | CLA  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |
| 22  | D     | 405 | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 31  | c     | 516 | BCR  | C15-C16-C17 | -2.71 | 117.92      | 123.47   |
| 22  | S     | 310 | CLA  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |
| 21  | N     | 607 | CHL  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 22  | S     | 305 | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 35  | c     | 517 | DGD  | CDB-CCB-CBB | -2.71 | 100.68      | 114.42   |
| 22  | N     | 609 | CLA  | CHB-C4A-NA  | 2.71  | 128.25      | 124.51   |
| 22  | n     | 609 | CLA  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 22  | B     | 609 | CLA  | O2D-CGD-O1D | -2.71 | 118.55      | 123.84   |
| 26  | r     | 302 | LHG  | O8-C23-C24  | 2.71  | 120.40      | 111.91   |
| 21  | y     | 601 | CHL  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 21  | G     | 607 | CHL  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 21  | S     | 306 | CHL  | CMB-C2B-C3B | 2.70  | 129.74      | 124.68   |
| 31  | K     | 101 | BCR  | C24-C23-C22 | -2.70 | 122.15      | 126.23   |
| 21  | N     | 601 | CHL  | CMB-C2B-C3B | 2.70  | 129.74      | 124.68   |
| 22  | N     | 604 | CLA  | CHB-C4A-NA  | 2.70  | 128.25      | 124.51   |
| 21  | S     | 307 | CHL  | CMB-C2B-C3B | 2.70  | 129.74      | 124.68   |
| 21  | s     | 301 | CHL  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 22  | Y     | 609 | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 21  | S     | 301 | CHL  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 22  | Y     | 604 | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 22  | r     | 312 | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 22  | Y     | 602 | CLA  | CHB-C4A-NA  | 2.70  | 128.25      | 124.51   |
| 26  | C     | 521 | LHG  | O8-C23-C24  | 2.70  | 120.38      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | r     | 308 | CHL  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 21  | n     | 601 | CHL  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 21  | R     | 305 | CHL  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 22  | y     | 611 | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 22  | n     | 602 | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 26  | y     | 617 | LHG  | C11-C10-C9  | -2.70 | 100.74      | 114.42   |
| 22  | n     | 609 | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 21  | y     | 608 | CHL  | CMB-C2B-C3B | 2.70  | 129.72      | 124.68   |
| 21  | r     | 301 | CHL  | CMB-C2B-C3B | 2.70  | 129.72      | 124.68   |
| 22  | y     | 602 | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 35  | C     | 518 | DGD  | CDB-CCB-CBB | -2.69 | 100.75      | 114.42   |
| 21  | n     | 607 | CHL  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 21  | s     | 306 | CHL  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 21  | G     | 608 | CHL  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 22  | N     | 604 | CLA  | C1B-CHB-C4A | -2.69 | 124.78      | 130.12   |
| 21  | r     | 306 | CHL  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 21  | y     | 605 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 22  | n     | 604 | CLA  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 21  | g     | 601 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 22  | r     | 312 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 21  | S     | 302 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 21  | n     | 605 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 22  | B     | 605 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 21  | g     | 608 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 21  | s     | 307 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 22  | Y     | 604 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 21  | N     | 605 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 21  | N     | 608 | CHL  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 22  | b     | 614 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 22  | g     | 604 | CLA  | CMB-C2B-C3B | 2.69  | 129.70      | 124.68   |
| 21  | y     | 606 | CHL  | CMB-C2B-C3B | 2.69  | 129.70      | 124.68   |
| 21  | Y     | 607 | CHL  | CMB-C2B-C3B | 2.69  | 129.70      | 124.68   |
| 21  | R     | 307 | CHL  | CMB-C2B-C3B | 2.69  | 129.70      | 124.68   |
| 22  | r     | 305 | CLA  | O2D-CGD-O1D | -2.69 | 118.59      | 123.84   |
| 33  | l     | 101 | SQD  | O8-S-C6     | 2.69  | 110.02      | 105.74   |
| 22  | N     | 603 | CLA  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 22  | S     | 305 | CLA  | C1-C2-C3    | -2.68 | 122.41      | 126.75   |
| 22  | N     | 604 | CLA  | CMB-C2B-C3B | 2.68  | 129.70      | 124.68   |
| 21  | R     | 306 | CHL  | CMB-C2B-C3B | 2.68  | 129.70      | 124.68   |
| 21  | G     | 605 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | g     | 606 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | G     | 609 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | G     | 604 | CLA  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | Y     | 601 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | s     | 302 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 22  | b     | 602 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 22  | y     | 610 | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 22  | N     | 602 | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 22  | n     | 603 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 22  | c     | 502 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 21  | g     | 605 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | Y     | 608 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 26  | c     | 521 | LHG  | O8-C23-C24  | 2.68  | 120.31      | 111.91   |
| 21  | n     | 606 | CHL  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 22  | r     | 303 | CLA  | O2D-CGD-O1D | -2.68 | 118.61      | 123.84   |
| 22  | R     | 302 | CLA  | O2D-CGD-O1D | -2.68 | 118.61      | 123.84   |
| 33  | L     | 102 | SQD  | O8-S-C6     | 2.68  | 110.00      | 105.74   |
| 22  | Y     | 609 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 22  | n     | 604 | CLA  | C1B-CHB-C4A | -2.67 | 124.82      | 130.12   |
| 22  | G     | 610 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 30  | D     | 401 | PHO  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 21  | N     | 606 | CHL  | CMB-C2B-C3B | 2.67  | 129.68      | 124.68   |
| 21  | n     | 608 | CHL  | CMB-C2B-C3B | 2.67  | 129.68      | 124.68   |
| 22  | s     | 305 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 21  | Y     | 606 | CHL  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 22  | R     | 304 | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 21  | g     | 607 | CHL  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 22  | g     | 604 | CLA  | C1B-CHB-C4A | -2.67 | 124.83      | 130.12   |
| 22  | G     | 604 | CLA  | C1B-CHB-C4A | -2.67 | 124.83      | 130.12   |
| 21  | g     | 609 | CHL  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 26  | d     | 409 | LHG  | O8-C23-C24  | 2.67  | 120.28      | 111.91   |
| 31  | C     | 517 | BCR  | C15-C16-C17 | -2.67 | 118.01      | 123.47   |
| 36  | C     | 502 | LMG  | O3-C3-C2    | -2.67 | 104.19      | 110.35   |
| 21  | y     | 607 | CHL  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 21  | G     | 606 | CHL  | CMB-C2B-C3B | 2.67  | 129.66      | 124.68   |
| 21  | y     | 609 | CHL  | CMB-C2B-C3B | 2.66  | 129.66      | 124.68   |
| 22  | y     | 604 | CLA  | C1B-CHB-C4A | -2.66 | 124.84      | 130.12   |
| 22  | s     | 305 | CLA  | C1-C2-C3    | -2.66 | 122.44      | 126.75   |
| 22  | g     | 603 | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 22  | B     | 617 | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 22  | C     | 503 | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 22  | a     | 405 | CLA  | O2D-CGD-O1D | -2.66 | 118.64      | 123.84   |
| 22  | y     | 603 | CLA  | O2D-CGD-O1D | -2.66 | 118.64      | 123.84   |
| 21  | G     | 601 | CHL  | CMB-C2B-C3B | 2.66  | 129.65      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | Y     | 605 | CHL  | CMB-C2B-C3B | 2.66  | 129.65      | 124.68   |
| 26  | D     | 410 | LHG  | O8-C23-C24  | 2.65  | 120.24      | 111.91   |
| 21  | r     | 307 | CHL  | CMB-C2B-C3B | 2.65  | 129.64      | 124.68   |
| 22  | g     | 614 | CLA  | C1B-CHB-C4A | -2.65 | 124.86      | 130.12   |
| 22  | r     | 309 | CLA  | O2D-CGD-O1D | -2.65 | 118.65      | 123.84   |
| 31  | a     | 409 | BCR  | C15-C14-C13 | -2.65 | 123.53      | 127.31   |
| 22  | n     | 613 | CLA  | C1B-CHB-C4A | -2.65 | 124.87      | 130.12   |
| 22  | y     | 604 | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 31  | A     | 410 | BCR  | C15-C14-C13 | -2.65 | 123.53      | 127.31   |
| 21  | N     | 606 | CHL  | O2A-CGA-CBA | 2.65  | 120.22      | 111.91   |
| 22  | G     | 603 | CLA  | O2D-CGD-O1D | -2.65 | 118.66      | 123.84   |
| 22  | n     | 604 | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 22  | A     | 406 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 22  | B     | 614 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 22  | G     | 604 | CLA  | CHB-C4A-NA  | 2.64  | 128.17      | 124.51   |
| 22  | b     | 611 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 21  | g     | 601 | CHL  | O2A-CGA-CBA | 2.64  | 120.20      | 111.91   |
| 22  | N     | 613 | CLA  | C1B-CHB-C4A | -2.64 | 124.88      | 130.12   |
| 22  | a     | 404 | CLA  | CMB-C2B-C3B | 2.64  | 129.62      | 124.68   |
| 26  | D     | 409 | LHG  | O8-C23-C24  | 2.64  | 120.20      | 111.91   |
| 22  | R     | 309 | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 22  | G     | 614 | CLA  | C1B-CHB-C4A | -2.64 | 124.89      | 130.12   |
| 22  | C     | 505 | CLA  | C1B-CHB-C4A | -2.64 | 124.89      | 130.12   |
| 22  | s     | 312 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 22  | Y     | 612 | CLA  | C1B-CHB-C4A | -2.64 | 124.89      | 130.12   |
| 21  | r     | 308 | CHL  | O2A-CGA-CBA | 2.64  | 120.20      | 111.91   |
| 22  | Y     | 603 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 22  | c     | 503 | CLA  | O2D-CGD-O1D | -2.64 | 118.67      | 123.84   |
| 22  | G     | 611 | CLA  | C1B-CHB-C4A | -2.64 | 124.89      | 130.12   |
| 21  | y     | 606 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 21  | N     | 607 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 22  | c     | 502 | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 21  | g     | 609 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 21  | y     | 601 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 22  | S     | 305 | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 21  | N     | 601 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 22  | R     | 308 | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 26  | g     | 619 | LHG  | C11-C10-C9  | -2.64 | 101.03      | 114.42   |
| 22  | A     | 405 | CLA  | CMB-C2B-C3B | 2.64  | 129.61      | 124.68   |
| 21  | y     | 608 | CHL  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 26  | d     | 408 | LHG  | O8-C23-C24  | 2.64  | 120.19      | 111.91   |
| 21  | N     | 608 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 604 | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 21  | G     | 608 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 21  | n     | 607 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 21  | n     | 608 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 22  | s     | 305 | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 30  | d     | 401 | PHO  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 33  | D     | 402 | SQD  | O5-C5-C4    | 2.64  | 114.48      | 109.69   |
| 21  | y     | 607 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 33  | d     | 402 | SQD  | O5-C5-C4    | 2.64  | 114.48      | 109.69   |
| 22  | B     | 613 | CLA  | O2D-CGD-O1D | -2.64 | 118.69      | 123.84   |
| 22  | g     | 611 | CLA  | C1B-CHB-C4A | -2.64 | 124.90      | 130.12   |
| 21  | G     | 601 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 22  | g     | 604 | CLA  | CHB-C4A-NA  | 2.63  | 128.16      | 124.51   |
| 21  | y     | 609 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 21  | n     | 601 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 21  | R     | 307 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 21  | G     | 606 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 35  | C     | 519 | DGD  | C3G-C2G-C1G | -2.63 | 105.56      | 111.79   |
| 21  | r     | 301 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 22  | y     | 613 | CLA  | C1B-CHB-C4A | -2.63 | 124.90      | 130.12   |
| 21  | Y     | 607 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 21  | Y     | 608 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 21  | r     | 307 | CHL  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 36  | w     | 102 | LMG  | O3-C3-C2    | -2.63 | 104.27      | 110.35   |
| 21  | G     | 609 | CHL  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 22  | R     | 311 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 21  | R     | 305 | CHL  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 21  | R     | 306 | CHL  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 31  | C     | 516 | BCR  | C27-C26-C25 | 2.63  | 126.55      | 122.73   |
| 21  | n     | 606 | CHL  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 35  | c     | 518 | DGD  | C3G-C2G-C1G | -2.63 | 105.57      | 111.79   |
| 21  | g     | 608 | CHL  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 21  | G     | 607 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 22  | b     | 610 | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 31  | a     | 409 | BCR  | C27-C26-C25 | 2.63  | 126.55      | 122.73   |
| 26  | Y     | 617 | LHG  | O8-C23-C24  | 2.63  | 120.15      | 111.91   |
| 21  | y     | 605 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 21  | Y     | 601 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 21  | S     | 301 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 21  | r     | 306 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 21  | n     | 605 | CHL  | O2A-CGA-CBA | 2.62  | 120.14      | 111.91   |
| 22  | c     | 505 | CLA  | CHB-C4A-NA  | 2.62  | 128.14      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Y     | 610 | CLA  | C1B-CHB-C4A | -2.62 | 124.92      | 130.12   |
| 21  | g     | 607 | CHL  | O2A-CGA-CBA | 2.62  | 120.14      | 111.91   |
| 21  | s     | 301 | CHL  | O2A-CGA-CBA | 2.62  | 120.14      | 111.91   |
| 22  | B     | 604 | CLA  | C1B-CHB-C4A | -2.62 | 124.93      | 130.12   |
| 22  | n     | 604 | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 32  | d     | 406 | PL9  | C27-C28-C29 | -2.62 | 121.35      | 127.66   |
| 31  | b     | 616 | BCR  | C27-C26-C25 | 2.62  | 126.53      | 122.73   |
| 21  | N     | 605 | CHL  | O2A-CGA-CBA | 2.62  | 120.13      | 111.91   |
| 22  | N     | 604 | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 22  | S     | 312 | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 21  | g     | 606 | CHL  | O2A-CGA-CBA | 2.62  | 120.12      | 111.91   |
| 22  | A     | 409 | CLA  | CHB-C4A-NA  | 2.62  | 128.13      | 124.51   |
| 22  | C     | 503 | CLA  | CHB-C4A-NA  | 2.62  | 128.13      | 124.51   |
| 21  | Y     | 605 | CHL  | O2A-CGA-CBA | 2.62  | 120.11      | 111.91   |
| 22  | b     | 611 | CLA  | CHB-C4A-NA  | 2.61  | 128.13      | 124.51   |
| 21  | Y     | 606 | CHL  | O2A-CGA-CBA | 2.61  | 120.11      | 111.91   |
| 22  | c     | 504 | CLA  | C1B-CHB-C4A | -2.61 | 124.94      | 130.12   |
| 22  | x     | 101 | CLA  | O2D-CGD-O1D | -2.61 | 118.73      | 123.84   |
| 22  | a     | 408 | CLA  | O2D-CGD-O1D | -2.61 | 118.73      | 123.84   |
| 22  | C     | 506 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 22  | b     | 601 | CLA  | C1B-CHB-C4A | -2.61 | 124.95      | 130.12   |
| 22  | y     | 604 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 31  | K     | 102 | BCR  | C24-C23-C22 | -2.61 | 122.30      | 126.23   |
| 22  | G     | 604 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 22  | B     | 603 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 22  | b     | 601 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 22  | y     | 611 | CLA  | C1B-CHB-C4A | -2.60 | 124.96      | 130.12   |
| 22  | C     | 504 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 32  | D     | 407 | PL9  | C27-C28-C29 | -2.60 | 121.39      | 127.66   |
| 22  | r     | 310 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | b     | 606 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | c     | 510 | CLA  | C3D-C2D-C1D | 2.60  | 109.38      | 105.83   |
| 22  | c     | 507 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | Y     | 604 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | B     | 614 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | Y     | 602 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 35  | C     | 518 | DGD  | C3G-C2G-C1G | -2.60 | 105.64      | 111.79   |
| 22  | y     | 602 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | G     | 602 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | g     | 604 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | A     | 409 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | C     | 508 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 604 | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 22  | n     | 602 | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 22  | N     | 610 | CLA  | C1B-CHB-C4A | -2.60 | 124.97      | 130.12   |
| 31  | A     | 410 | BCR  | C27-C26-C25 | 2.60  | 126.50      | 122.73   |
| 36  | M     | 101 | LMG  | O6-C1-O1    | -2.59 | 103.83      | 109.97   |
| 31  | k     | 102 | BCR  | C24-C23-C22 | -2.59 | 122.32      | 126.23   |
| 35  | c     | 517 | DGD  | C3G-C2G-C1G | -2.59 | 105.66      | 111.79   |
| 22  | d     | 404 | CLA  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 22  | n     | 610 | CLA  | C1B-CHB-C4A | -2.59 | 124.99      | 130.12   |
| 35  | c     | 519 | DGD  | C3G-C2G-C1G | -2.59 | 105.66      | 111.79   |
| 36  | T     | 101 | LMG  | O6-C1-O1    | -2.59 | 103.84      | 109.97   |
| 31  | B     | 619 | BCR  | C27-C26-C25 | 2.59  | 126.49      | 122.73   |
| 26  | y     | 617 | LHG  | O8-C23-C24  | 2.59  | 120.03      | 111.91   |
| 22  | r     | 309 | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 33  | L     | 102 | SQD  | C4-C3-C2    | 2.59  | 115.34      | 110.82   |
| 31  | K     | 102 | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 31  | c     | 515 | BCR  | C27-C26-C25 | 2.58  | 126.48      | 122.73   |
| 35  | J     | 101 | DGD  | C3G-C2G-C1G | -2.58 | 105.69      | 111.79   |
| 22  | c     | 508 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 22  | D     | 405 | CLA  | O2D-CGD-O1D | -2.58 | 118.80      | 123.84   |
| 22  | R     | 308 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 31  | A     | 410 | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 22  | C     | 509 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 22  | D     | 404 | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 22  | B     | 607 | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 26  | n     | 617 | LHG  | C11-C10-C9  | -2.57 | 101.36      | 114.42   |
| 22  | C     | 511 | CLA  | C3D-C2D-C1D | 2.57  | 109.34      | 105.83   |
| 22  | g     | 602 | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 30  | A     | 408 | PHO  | O2D-CGD-O1D | -2.57 | 118.82      | 123.84   |
| 31  | C     | 517 | BCR  | C33-C5-C6   | -2.57 | 121.64      | 124.53   |
| 31  | c     | 516 | BCR  | C33-C5-C6   | -2.57 | 121.65      | 124.53   |
| 33  | l     | 101 | SQD  | C4-C3-C2    | 2.57  | 115.30      | 110.82   |
| 22  | a     | 408 | CLA  | CHB-C4A-NA  | 2.57  | 128.06      | 124.51   |
| 22  | c     | 513 | CLA  | CHB-C4A-NA  | 2.56  | 128.06      | 124.51   |
| 31  | b     | 616 | BCR  | C11-C10-C9  | -2.56 | 123.65      | 127.31   |
| 22  | r     | 305 | CLA  | C1B-CHB-C4A | -2.56 | 125.04      | 130.12   |
| 23  | r     | 313 | LUT  | C21-C26-C25 | 2.56  | 116.00      | 111.42   |
| 22  | B     | 611 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 23  | R     | 312 | LUT  | C21-C26-C25 | 2.56  | 116.00      | 111.42   |
| 24  | Y     | 615 | XAT  | C11-C12-C13 | -2.56 | 119.23      | 126.42   |
| 31  | k     | 102 | BCR  | C33-C5-C6   | -2.56 | 121.66      | 124.53   |
| 31  | C     | 517 | BCR  | C27-C26-C25 | 2.56  | 126.44      | 122.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 409 | BCR  | C11-C10-C9  | -2.56 | 123.66      | 127.31   |
| 35  | C     | 518 | DGD  | O3G-C1D-C2D | -2.56 | 104.31      | 108.30   |
| 22  | B     | 606 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 22  | C     | 514 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | N     | 602 | CLA  | O2D-CGD-O1D | -2.55 | 118.84      | 123.84   |
| 22  | r     | 304 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 26  | G     | 618 | LHG  | O8-C23-C24  | 2.55  | 119.92      | 111.91   |
| 22  | c     | 514 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | S     | 310 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | r     | 303 | CLA  | C1B-CHB-C4A | -2.55 | 125.06      | 130.12   |
| 22  | b     | 608 | CLA  | C1B-CHB-C4A | -2.55 | 125.06      | 130.12   |
| 22  | R     | 303 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | d     | 403 | CLA  | C1B-CHB-C4A | -2.55 | 125.07      | 130.12   |
| 22  | C     | 515 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | B     | 609 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | c     | 502 | CLA  | C1B-CHB-C4A | -2.55 | 125.07      | 130.12   |
| 22  | R     | 304 | CLA  | C1B-CHB-C4A | -2.55 | 125.07      | 130.12   |
| 22  | s     | 310 | CLA  | CHB-C4A-NA  | 2.55  | 128.03      | 124.51   |
| 31  | a     | 409 | BCR  | C33-C5-C6   | -2.55 | 121.67      | 124.53   |
| 22  | g     | 602 | CLA  | C1B-CHB-C4A | -2.55 | 125.07      | 130.12   |
| 31  | B     | 602 | BCR  | C15-C16-C17 | -2.55 | 118.26      | 123.47   |
| 22  | S     | 312 | CLA  | C1B-CHB-C4A | -2.55 | 125.08      | 130.12   |
| 22  | A     | 406 | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 22  | S     | 313 | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 22  | G     | 602 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 22  | Y     | 602 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 22  | C     | 503 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 25  | Y     | 616 | NEX  | C36-C21-C22 | -2.54 | 104.56      | 108.98   |
| 26  | g     | 619 | LHG  | O8-C23-C24  | 2.54  | 119.89      | 111.91   |
| 31  | B     | 619 | BCR  | C11-C10-C9  | -2.54 | 123.68      | 127.31   |
| 31  | T     | 102 | BCR  | C15-C14-C13 | -2.54 | 123.68      | 127.31   |
| 23  | N     | 614 | LUT  | C31-C32-C33 | -2.54 | 119.27      | 126.42   |
| 31  | B     | 602 | BCR  | C15-C14-C13 | -2.54 | 123.68      | 127.31   |
| 21  | Y     | 605 | CHL  | OMC-CMC-C2C | -2.54 | 119.94      | 125.69   |
| 23  | G     | 615 | LUT  | C31-C32-C33 | -2.54 | 119.28      | 126.42   |
| 22  | r     | 303 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 26  | D     | 409 | LHG  | C11-C10-C9  | -2.54 | 101.53      | 114.42   |
| 22  | n     | 602 | CLA  | C1B-CHB-C4A | -2.54 | 125.09      | 130.12   |
| 21  | G     | 607 | CHL  | OMC-CMC-C2C | -2.54 | 119.94      | 125.69   |
| 22  | s     | 312 | CLA  | C1B-CHB-C4A | -2.54 | 125.09      | 130.12   |
| 21  | R     | 306 | CHL  | OMC-CMC-C2C | -2.54 | 119.95      | 125.69   |
| 36  | c     | 523 | LMG  | O1-C7-C8    | -2.54 | 104.78      | 110.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | L     | 103 | LHG  | C11-C10-C9  | -2.54 | 101.55      | 114.42   |
| 26  | d     | 408 | LHG  | C11-C10-C9  | -2.54 | 101.55      | 114.42   |
| 21  | n     | 601 | CHL  | OMC-CMC-C2C | -2.54 | 119.95      | 125.69   |
| 30  | a     | 407 | PHO  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 35  | c     | 517 | DGD  | O3G-C1D-C2D | -2.54 | 104.34      | 108.30   |
| 36  | C     | 523 | LMG  | O1-C7-C8    | -2.54 | 104.78      | 110.90   |
| 22  | C     | 505 | CLA  | CHB-C4A-NA  | 2.53  | 128.02      | 124.51   |
| 21  | s     | 307 | CHL  | OMC-CMC-C2C | -2.53 | 119.96      | 125.69   |
| 22  | s     | 313 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 23  | n     | 614 | LUT  | C31-C32-C33 | -2.53 | 119.30      | 126.42   |
| 22  | R     | 302 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 22  | c     | 513 | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 23  | g     | 615 | LUT  | C31-C32-C33 | -2.53 | 119.30      | 126.42   |
| 21  | r     | 307 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 21  | R     | 305 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 22  | b     | 603 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 26  | l     | 102 | LHG  | C11-C10-C9  | -2.53 | 101.59      | 114.42   |
| 23  | R     | 312 | LUT  | C8-C7-C6    | -2.53 | 120.10      | 127.20   |
| 21  | N     | 607 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 25  | r     | 315 | NEX  | C36-C21-C22 | -2.53 | 104.59      | 108.98   |
| 21  | g     | 609 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 21  | y     | 607 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 21  | y     | 608 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 22  | b     | 608 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 21  | g     | 608 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 21  | r     | 301 | CHL  | OMC-CMC-C2C | -2.53 | 119.97      | 125.69   |
| 21  | N     | 601 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 23  | y     | 614 | LUT  | C31-C32-C33 | -2.52 | 119.33      | 126.42   |
| 31  | A     | 410 | BCR  | C11-C10-C9  | -2.52 | 123.71      | 127.31   |
| 21  | G     | 609 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 21  | N     | 606 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 21  | S     | 306 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 22  | a     | 405 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 21  | y     | 605 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 21  | r     | 308 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 21  | S     | 301 | CHL  | OMC-CMC-C2C | -2.52 | 119.98      | 125.69   |
| 22  | C     | 504 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 21  | S     | 302 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 21  | S     | 307 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 31  | c     | 516 | BCR  | C27-C26-C25 | 2.52  | 126.39      | 122.73   |
| 21  | g     | 606 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 21  | n     | 605 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | n     | 606 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 21  | N     | 608 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 31  | T     | 102 | BCR  | C15-C16-C17 | -2.52 | 118.32      | 123.47   |
| 22  | y     | 602 | CLA  | C1B-CHB-C4A | -2.52 | 125.13      | 130.12   |
| 21  | g     | 607 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 21  | R     | 307 | CHL  | OMC-CMC-C2C | -2.52 | 119.99      | 125.69   |
| 21  | y     | 601 | CHL  | OMC-CMC-C2C | -2.52 | 120.00      | 125.69   |
| 21  | s     | 306 | CHL  | OMC-CMC-C2C | -2.52 | 120.00      | 125.69   |
| 22  | N     | 611 | CLA  | CMB-C2B-C3B | 2.52  | 129.38      | 124.68   |
| 21  | g     | 601 | CHL  | OMC-CMC-C2C | -2.52 | 120.00      | 125.69   |
| 33  | L     | 102 | SQD  | C44-O6-C1   | 2.52  | 118.65      | 113.74   |
| 22  | B     | 611 | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 22  | b     | 613 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 22  | s     | 303 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 33  | l     | 101 | SQD  | C44-O6-C1   | 2.51  | 118.65      | 113.74   |
| 22  | n     | 611 | CLA  | CMB-C2B-C3B | 2.51  | 129.38      | 124.68   |
| 23  | r     | 313 | LUT  | C8-C7-C6    | -2.51 | 120.14      | 127.20   |
| 26  | n     | 617 | LHG  | O8-C23-C24  | 2.51  | 119.80      | 111.91   |
| 22  | b     | 607 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 21  | G     | 608 | CHL  | OMC-CMC-C2C | -2.51 | 120.00      | 125.69   |
| 21  | N     | 605 | CHL  | OMC-CMC-C2C | -2.51 | 120.00      | 125.69   |
| 21  | y     | 606 | CHL  | OMC-CMC-C2C | -2.51 | 120.00      | 125.69   |
| 22  | C     | 514 | CLA  | O2D-CGD-O1D | -2.51 | 118.92      | 123.84   |
| 23  | Y     | 613 | LUT  | C31-C32-C33 | -2.51 | 119.36      | 126.42   |
| 21  | Y     | 607 | CHL  | OMC-CMC-C2C | -2.51 | 120.01      | 125.69   |
| 22  | c     | 503 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 21  | n     | 607 | CHL  | OMC-CMC-C2C | -2.51 | 120.01      | 125.69   |
| 22  | B     | 616 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 21  | G     | 605 | CHL  | OMC-CMC-C2C | -2.51 | 120.01      | 125.69   |
| 25  | y     | 618 | NEX  | C36-C21-C22 | -2.51 | 104.62      | 108.98   |
| 31  | T     | 102 | BCR  | C33-C5-C6   | -2.51 | 121.71      | 124.53   |
| 22  | C     | 507 | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 24  | Y     | 615 | XAT  | C8-C9-C10   | -2.51 | 115.09      | 118.94   |
| 22  | N     | 602 | CLA  | C1B-CHB-C4A | -2.51 | 125.15      | 130.12   |
| 22  | s     | 303 | CLA  | CHD-C1D-ND  | -2.51 | 122.15      | 124.45   |
| 21  | y     | 609 | CHL  | OMC-CMC-C2C | -2.51 | 120.01      | 125.69   |
| 22  | W     | 101 | CLA  | CMB-C2B-C3B | 2.51  | 129.37      | 124.68   |
| 31  | d     | 405 | BCR  | C27-C26-C25 | 2.51  | 126.37      | 122.73   |
| 21  | r     | 306 | CHL  | OMC-CMC-C2C | -2.51 | 120.02      | 125.69   |
| 22  | s     | 311 | CLA  | O2D-CGD-O1D | -2.51 | 118.94      | 123.84   |
| 22  | S     | 311 | CLA  | O2D-CGD-O1D | -2.51 | 118.94      | 123.84   |
| 31  | h     | 101 | BCR  | C33-C5-C6   | -2.51 | 121.71      | 124.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | k     | 102 | BCR  | C15-C14-C13 | -2.50 | 123.73      | 127.31   |
| 21  | Y     | 601 | CHL  | OMC-CMC-C2C | -2.50 | 120.03      | 125.69   |
| 22  | B     | 607 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 22  | R     | 302 | CLA  | C1B-CHB-C4A | -2.50 | 125.16      | 130.12   |
| 22  | G     | 610 | CLA  | C16-C15-C13 | -2.50 | 107.83      | 115.92   |
| 22  | g     | 612 | CLA  | CMB-C2B-C3B | 2.50  | 129.36      | 124.68   |
| 36  | b     | 620 | LMG  | O1-C7-C8    | -2.50 | 104.86      | 110.90   |
| 21  | s     | 302 | CHL  | OMC-CMC-C2C | -2.50 | 120.03      | 125.69   |
| 22  | S     | 310 | CLA  | C1B-CHB-C4A | -2.50 | 125.16      | 130.12   |
| 22  | c     | 506 | CLA  | C1B-CHB-C4A | -2.50 | 125.17      | 130.12   |
| 31  | a     | 409 | BCR  | C24-C23-C22 | -2.50 | 122.46      | 126.23   |
| 22  | C     | 506 | CLA  | C1-C2-C3    | -2.50 | 121.72      | 126.04   |
| 21  | G     | 601 | CHL  | OMC-CMC-C2C | -2.50 | 120.04      | 125.69   |
| 31  | k     | 101 | BCR  | C33-C5-C6   | -2.50 | 121.72      | 124.53   |
| 22  | c     | 504 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 31  | K     | 102 | BCR  | C15-C14-C13 | -2.50 | 123.75      | 127.31   |
| 22  | B     | 607 | CLA  | C1B-CHB-C4A | -2.50 | 125.17      | 130.12   |
| 22  | S     | 303 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 21  | n     | 608 | CHL  | OMC-CMC-C2C | -2.49 | 120.05      | 125.69   |
| 21  | Y     | 608 | CHL  | OMC-CMC-C2C | -2.49 | 120.05      | 125.69   |
| 21  | g     | 605 | CHL  | OMC-CMC-C2C | -2.49 | 120.05      | 125.69   |
| 31  | K     | 101 | BCR  | C33-C5-C6   | -2.49 | 121.73      | 124.53   |
| 22  | S     | 313 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |
| 36  | B     | 623 | LMG  | O1-C7-C8    | -2.49 | 104.88      | 110.90   |
| 22  | c     | 505 | CLA  | C1-C2-C3    | -2.49 | 121.73      | 126.04   |
| 22  | w     | 101 | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 21  | Y     | 606 | CHL  | OMC-CMC-C2C | -2.49 | 120.06      | 125.69   |
| 22  | b     | 602 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 21  | s     | 301 | CHL  | OMC-CMC-C2C | -2.49 | 120.06      | 125.69   |
| 22  | G     | 612 | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 22  | b     | 604 | CLA  | C1B-CHB-C4A | -2.49 | 125.19      | 130.12   |
| 21  | G     | 606 | CHL  | OMC-CMC-C2C | -2.49 | 120.06      | 125.69   |
| 31  | B     | 602 | BCR  | C24-C23-C22 | -2.49 | 122.48      | 126.23   |
| 22  | G     | 611 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 22  | b     | 605 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 37  | F     | 101 | HEM  | C1D-C2D-C3D | 2.49  | 109.57      | 106.96   |
| 22  | B     | 610 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 26  | n     | 617 | LHG  | C20-C19-C18 | -2.48 | 101.81      | 114.42   |
| 22  | s     | 313 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 22  | S     | 305 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 22  | R     | 304 | CLA  | O2A-CGA-O1A | -2.48 | 117.33      | 123.59   |
| 26  | b     | 619 | LHG  | C11-C10-C9  | -2.48 | 101.83      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | b     | 619 | LHG  | O8-C23-C24  | 2.48  | 119.69      | 111.91   |
| 22  | s     | 305 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 22  | n     | 612 | CLA  | C2A-C1A-CHA | 2.48  | 128.20      | 123.86   |
| 26  | c     | 520 | LHG  | C11-C10-C9  | -2.48 | 101.84      | 114.42   |
| 36  | k     | 103 | LMG  | O6-C1-O1    | -2.48 | 104.10      | 109.97   |
| 22  | B     | 608 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 22  | A     | 405 | CLA  | C1B-CHB-C4A | -2.48 | 125.21      | 130.12   |
| 26  | C     | 520 | LHG  | C11-C10-C9  | -2.48 | 101.85      | 114.42   |
| 26  | B     | 622 | LHG  | C11-C10-C9  | -2.48 | 101.86      | 114.42   |
| 22  | G     | 613 | CLA  | C2A-C1A-CHA | 2.48  | 128.19      | 123.86   |
| 22  | g     | 613 | CLA  | C2A-C1A-CHA | 2.47  | 128.19      | 123.86   |
| 31  | T     | 102 | BCR  | C24-C23-C22 | -2.47 | 122.50      | 126.23   |
| 31  | C     | 516 | BCR  | C15-C14-C13 | -2.47 | 123.78      | 127.31   |
| 31  | b     | 617 | BCR  | C11-C10-C9  | -2.47 | 123.78      | 127.31   |
| 22  | s     | 310 | CLA  | C1B-CHB-C4A | -2.47 | 125.22      | 130.12   |
| 22  | R     | 309 | CLA  | C1B-CHB-C4A | -2.47 | 125.22      | 130.12   |
| 22  | c     | 509 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 36  | K     | 103 | LMG  | O6-C1-O1    | -2.47 | 104.12      | 109.97   |
| 31  | B     | 620 | BCR  | C11-C10-C9  | -2.47 | 123.78      | 127.31   |
| 31  | D     | 406 | BCR  | C27-C26-C25 | 2.47  | 126.32      | 122.73   |
| 26  | D     | 410 | LHG  | C11-C10-C9  | -2.47 | 101.89      | 114.42   |
| 31  | c     | 515 | BCR  | C15-C14-C13 | -2.47 | 123.79      | 127.31   |
| 31  | A     | 410 | BCR  | C24-C23-C22 | -2.47 | 122.51      | 126.23   |
| 22  | Y     | 611 | CLA  | C2A-C1A-CHA | 2.47  | 128.17      | 123.86   |
| 31  | B     | 602 | BCR  | C33-C5-C6   | -2.47 | 121.76      | 124.53   |
| 22  | c     | 508 | CLA  | C1B-CHB-C4A | -2.47 | 125.23      | 130.12   |
| 22  | c     | 509 | CLA  | C1B-CHB-C4A | -2.47 | 125.23      | 130.12   |
| 22  | b     | 602 | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 22  | B     | 605 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 22  | C     | 510 | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 26  | d     | 409 | LHG  | C11-C10-C9  | -2.46 | 101.93      | 114.42   |
| 22  | C     | 510 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 26  | B     | 622 | LHG  | O8-C23-C24  | 2.46  | 119.63      | 111.91   |
| 22  | s     | 309 | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 36  | b     | 620 | LMG  | O3-C3-C2    | -2.46 | 104.66      | 110.35   |
| 26  | d     | 408 | LHG  | C20-C19-C18 | -2.46 | 101.93      | 114.42   |
| 37  | f     | 101 | HEM  | C1D-C2D-C3D | 2.46  | 109.54      | 106.96   |
| 26  | D     | 408 | LHG  | O8-C23-C24  | 2.46  | 119.63      | 111.91   |
| 36  | C     | 523 | LMG  | C38-C37-C36 | -2.46 | 101.94      | 114.42   |
| 22  | r     | 312 | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 22  | S     | 308 | CLA  | O2D-CGD-O1D | -2.46 | 119.03      | 123.84   |
| 26  | d     | 407 | LHG  | O8-C23-C24  | 2.46  | 119.62      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 615 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 24  | y     | 615 | XAT  | C11-C12-C13 | -2.45 | 119.52      | 126.42   |
| 22  | a     | 404 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | r     | 305 | CLA  | O2A-CGA-O1A | -2.45 | 117.40      | 123.59   |
| 22  | b     | 604 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 22  | y     | 612 | CLA  | C2A-C1A-CHA | 2.45  | 128.15      | 123.86   |
| 22  | c     | 511 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | C     | 509 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | Y     | 611 | CLA  | CHC-C1C-C2C | 2.45  | 133.51      | 126.72   |
| 22  | B     | 618 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 22  | S     | 309 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | s     | 308 | CLA  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 22  | B     | 604 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 22  | y     | 612 | CLA  | CHC-C1C-C2C | 2.45  | 133.50      | 126.72   |
| 22  | N     | 612 | CLA  | C2A-C1A-CHA | 2.45  | 128.14      | 123.86   |
| 22  | Y     | 610 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 25  | N     | 617 | NEX  | C27-C28-C29 | -2.45 | 121.73      | 125.53   |
| 36  | c     | 523 | LMG  | C38-C37-C36 | -2.45 | 101.99      | 114.42   |
| 22  | y     | 611 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 22  | c     | 510 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 26  | D     | 409 | LHG  | C20-C19-C18 | -2.45 | 102.00      | 114.42   |
| 22  | C     | 507 | CLA  | CHB-C4A-NA  | 2.45  | 127.89      | 124.51   |
| 22  | A     | 409 | CLA  | C1-C2-C3    | -2.45 | 121.81      | 126.04   |
| 22  | b     | 611 | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 26  | G     | 618 | LHG  | C20-C19-C18 | -2.45 | 102.01      | 114.42   |
| 22  | G     | 613 | CLA  | CHC-C1C-C2C | 2.45  | 133.49      | 126.72   |
| 22  | c     | 506 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 22  | x     | 101 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 22  | b     | 614 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | B     | 605 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | g     | 611 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 22  | r     | 310 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | C     | 511 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | B     | 603 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 22  | B     | 610 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 36  | K     | 103 | LMG  | C40-C39-C38 | -2.44 | 102.04      | 114.42   |
| 22  | A     | 405 | CLA  | CHB-C4A-NA  | 2.44  | 127.88      | 124.51   |
| 22  | A     | 407 | CLA  | CHB-C4A-NA  | 2.44  | 127.88      | 124.51   |
| 22  | x     | 101 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 22  | R     | 311 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 31  | H     | 101 | BCR  | C33-C5-C6   | -2.44 | 121.79      | 124.53   |
| 22  | B     | 617 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | c     | 523 | LMG  | C40-C39-C38 | -2.44 | 102.06      | 114.42   |
| 22  | S     | 303 | CLA  | CHD-C1D-ND  | -2.44 | 122.22      | 124.45   |
| 24  | G     | 617 | XAT  | C11-C12-C13 | -2.44 | 119.58      | 126.42   |
| 22  | c     | 510 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 36  | k     | 103 | LMG  | C40-C39-C38 | -2.43 | 102.06      | 114.42   |
| 22  | B     | 614 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 36  | B     | 623 | LMG  | O3-C3-C2    | -2.43 | 104.72      | 110.35   |
| 26  | c     | 520 | LHG  | O8-C6-C5    | -2.43 | 101.35      | 108.43   |
| 22  | b     | 606 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 22  | r     | 305 | CLA  | CHB-C4A-NA  | 2.43  | 127.88      | 124.51   |
| 22  | d     | 404 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 36  | D     | 411 | LMG  | O3-C3-C2    | -2.43 | 104.72      | 110.35   |
| 22  | n     | 612 | CLA  | CHC-C1C-C2C | 2.43  | 133.45      | 126.72   |
| 22  | b     | 601 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 22  | C     | 513 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 36  | k     | 103 | LMG  | C38-C37-C36 | -2.43 | 102.08      | 114.42   |
| 22  | g     | 613 | CLA  | CHC-C1C-C2C | 2.43  | 133.45      | 126.72   |
| 22  | a     | 406 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 22  | N     | 612 | CLA  | CHC-C1C-C2C | 2.43  | 133.44      | 126.72   |
| 37  | F     | 101 | HEM  | CHA-C4D-C3D | 2.43  | 129.88      | 125.33   |
| 31  | b     | 618 | BCR  | C33-C5-C6   | -2.43 | 121.80      | 124.53   |
| 36  | C     | 523 | LMG  | C40-C39-C38 | -2.43 | 102.10      | 114.42   |
| 26  | C     | 520 | LHG  | O8-C6-C5    | -2.43 | 101.37      | 108.43   |
| 22  | b     | 607 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 31  | b     | 616 | BCR  | C24-C23-C22 | -2.43 | 122.57      | 126.23   |
| 22  | C     | 513 | CLA  | CHD-C1D-ND  | -2.43 | 122.22      | 124.45   |
| 22  | B     | 615 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 22  | C     | 511 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 31  | b     | 618 | BCR  | C27-C26-C25 | 2.42  | 126.25      | 122.73   |
| 26  | r     | 302 | LHG  | C20-C19-C18 | -2.42 | 102.12      | 114.42   |
| 23  | N     | 615 | LUT  | C7-C8-C9    | -2.42 | 122.57      | 126.23   |
| 22  | b     | 610 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 26  | G     | 618 | LHG  | C11-C10-C9  | -2.42 | 102.12      | 114.42   |
| 25  | g     | 618 | NEX  | C11-C12-C13 | -2.42 | 119.61      | 126.42   |
| 22  | R     | 304 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 22  | r     | 304 | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 22  | R     | 303 | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 31  | B     | 621 | BCR  | C33-C5-C6   | -2.42 | 121.81      | 124.53   |
| 36  | K     | 103 | LMG  | C38-C37-C36 | -2.42 | 102.13      | 114.42   |
| 22  | g     | 603 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 22  | S     | 311 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 26  | c     | 520 | LHG  | O8-C23-C24  | 2.42  | 119.50      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | d     | 410 | LMG  | O3-C3-C2    | -2.42 | 104.76      | 110.35   |
| 26  | s     | 314 | LHG  | C11-C10-C9  | -2.42 | 102.14      | 114.42   |
| 22  | Y     | 603 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 22  | n     | 603 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 25  | N     | 617 | NEX  | C36-C21-C26 | -2.42 | 103.52      | 110.05   |
| 22  | c     | 513 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 31  | B     | 619 | BCR  | C24-C23-C22 | -2.42 | 122.58      | 126.23   |
| 22  | b     | 609 | CLA  | CHB-C4A-NA  | 2.42  | 127.85      | 124.51   |
| 22  | N     | 603 | CLA  | CHB-C4A-NA  | 2.42  | 127.85      | 124.51   |
| 31  | B     | 621 | BCR  | C27-C26-C25 | 2.41  | 126.24      | 122.73   |
| 22  | N     | 610 | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 36  | d     | 410 | LMG  | O1-C7-C8    | -2.41 | 105.08      | 110.90   |
| 36  | B     | 601 | LMG  | C40-C39-C38 | -2.41 | 102.17      | 114.42   |
| 36  | I     | 101 | LMG  | C40-C39-C38 | -2.41 | 102.17      | 114.42   |
| 22  | C     | 512 | CLA  | C1B-CHB-C4A | -2.41 | 125.34      | 130.12   |
| 26  | S     | 314 | LHG  | C11-C10-C9  | -2.41 | 102.18      | 114.42   |
| 26  | R     | 301 | LHG  | C20-C19-C18 | -2.41 | 102.18      | 114.42   |
| 31  | T     | 102 | BCR  | C11-C10-C9  | -2.41 | 123.87      | 127.31   |
| 36  | D     | 411 | LMG  | O1-C7-C8    | -2.41 | 105.08      | 110.90   |
| 22  | a     | 408 | CLA  | C1-C2-C3    | -2.41 | 121.87      | 126.04   |
| 37  | f     | 101 | HEM  | CHA-C4D-C3D | 2.41  | 129.85      | 125.33   |
| 21  | g     | 605 | CHL  | O2D-CGD-O1D | -2.41 | 119.12      | 123.84   |
| 26  | S     | 314 | LHG  | C20-C19-C18 | -2.41 | 102.19      | 114.42   |
| 21  | G     | 601 | CHL  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 22  | a     | 404 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 22  | s     | 311 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 22  | n     | 610 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 22  | B     | 612 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 26  | C     | 520 | LHG  | O8-C23-C24  | 2.41  | 119.46      | 111.91   |
| 22  | b     | 612 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 21  | N     | 601 | CHL  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 21  | G     | 608 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 26  | s     | 314 | LHG  | C20-C19-C18 | -2.40 | 102.22      | 114.42   |
| 21  | R     | 306 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 22  | s     | 309 | CLA  | CHB-C4A-NA  | 2.40  | 127.84      | 124.51   |
| 22  | b     | 605 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 37  | f     | 101 | HEM  | CMA-C3A-C4A | -2.40 | 124.77      | 128.46   |
| 26  | Y     | 617 | LHG  | C11-C10-C9  | -2.40 | 102.22      | 114.42   |
| 33  | D     | 402 | SQD  | C44-O6-C1   | 2.40  | 118.43      | 113.74   |
| 26  | r     | 302 | LHG  | C11-C10-C9  | -2.40 | 102.22      | 114.42   |
| 22  | y     | 603 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 26  | c     | 522 | LHG  | C11-C10-C9  | -2.40 | 102.23      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | n     | 606 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 22  | C     | 514 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 31  | B     | 602 | BCR  | C11-C10-C9  | -2.40 | 123.88      | 127.31   |
| 36  | C     | 502 | LMG  | C40-C39-C38 | -2.40 | 102.24      | 114.42   |
| 21  | n     | 605 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 21  | n     | 607 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 21  | S     | 302 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 36  | B     | 623 | LMG  | C40-C39-C38 | -2.40 | 102.24      | 114.42   |
| 21  | R     | 307 | CHL  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 26  | R     | 301 | LHG  | C11-C10-C9  | -2.40 | 102.24      | 114.42   |
| 21  | n     | 601 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 21  | Y     | 601 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 21  | Y     | 606 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 21  | Y     | 605 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 22  | c     | 511 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 26  | C     | 522 | LHG  | C11-C10-C9  | -2.40 | 102.26      | 114.42   |
| 36  | w     | 102 | LMG  | C40-C39-C38 | -2.40 | 102.26      | 114.42   |
| 26  | c     | 520 | LHG  | C20-C19-C18 | -2.40 | 102.26      | 114.42   |
| 22  | c     | 512 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 22  | B     | 613 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 21  | s     | 301 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 22  | R     | 308 | CLA  | C1B-CHB-C4A | -2.40 | 125.37      | 130.12   |
| 26  | L     | 103 | LHG  | C20-C19-C18 | -2.40 | 102.26      | 114.42   |
| 21  | s     | 307 | CHL  | O2D-CGD-O1D | -2.40 | 119.16      | 123.84   |
| 21  | R     | 305 | CHL  | O2D-CGD-O1D | -2.40 | 119.16      | 123.84   |
| 21  | r     | 307 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 22  | b     | 610 | CLA  | C1B-CHB-C4A | -2.39 | 125.37      | 130.12   |
| 22  | R     | 310 | CLA  | CAA-C2A-C3A | -2.39 | 106.22      | 112.78   |
| 22  | D     | 405 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 22  | C     | 513 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 22  | B     | 603 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 36  | b     | 620 | LMG  | C40-C39-C38 | -2.39 | 102.27      | 114.42   |
| 21  | G     | 607 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 21  | N     | 606 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 21  | g     | 609 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 26  | l     | 102 | LHG  | C20-C19-C18 | -2.39 | 102.28      | 114.42   |
| 21  | Y     | 601 | CHL  | C3B-C4B-NB  | 2.39  | 112.30      | 109.21   |
| 21  | g     | 601 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 21  | r     | 301 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 33  | d     | 402 | SQD  | C44-O6-C1   | 2.39  | 118.41      | 113.74   |
| 26  | C     | 520 | LHG  | C20-C19-C18 | -2.39 | 102.29      | 114.42   |
| 21  | g     | 608 | CHL  | C3B-C4B-NB  | 2.39  | 112.30      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | y     | 606 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 21  | Y     | 608 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 21  | G     | 609 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 22  | G     | 614 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 21  | N     | 605 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 22  | B     | 609 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 21  | g     | 608 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 21  | Y     | 607 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 21  | g     | 601 | CHL  | C3B-C4B-NB  | 2.39  | 112.30      | 109.21   |
| 22  | B     | 608 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 22  | c     | 512 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 26  | g     | 619 | LHG  | C5-O7-C7    | -2.39 | 111.92      | 117.79   |
| 21  | N     | 608 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 21  | r     | 308 | CHL  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 36  | c     | 523 | LMG  | O1-C1-C2    | -2.39 | 104.58      | 108.30   |
| 21  | g     | 606 | CHL  | O2D-CGD-O1D | -2.38 | 119.17      | 123.84   |
| 21  | G     | 606 | CHL  | O2D-CGD-O1D | -2.38 | 119.17      | 123.84   |
| 21  | G     | 608 | CHL  | C3B-C4B-NB  | 2.38  | 112.29      | 109.21   |
| 21  | Y     | 606 | CHL  | C3B-C4B-NB  | 2.38  | 112.29      | 109.21   |
| 21  | s     | 306 | CHL  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 21  | s     | 302 | CHL  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 22  | G     | 604 | CLA  | C1-C2-C3    | -2.38 | 122.90      | 126.75   |
| 22  | S     | 311 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 22  | B     | 615 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 21  | g     | 607 | CHL  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 21  | S     | 307 | CHL  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 21  | R     | 307 | CHL  | C3B-C4B-NB  | 2.38  | 112.29      | 109.21   |
| 31  | H     | 101 | BCR  | C11-C10-C9  | -2.38 | 123.92      | 127.31   |
| 31  | B     | 620 | BCR  | C33-C5-C6   | -2.38 | 121.86      | 124.53   |
| 22  | c     | 512 | CLA  | CHD-C1D-ND  | -2.38 | 122.27      | 124.45   |
| 22  | B     | 618 | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 22  | b     | 614 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 21  | g     | 605 | CHL  | C3B-C4B-NB  | 2.38  | 112.28      | 109.21   |
| 22  | b     | 609 | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 22  | r     | 309 | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 22  | r     | 311 | CLA  | CAA-C2A-C3A | -2.37 | 106.28      | 112.78   |
| 31  | A     | 410 | BCR  | C15-C16-C17 | -2.37 | 118.61      | 123.47   |
| 22  | G     | 603 | CLA  | CHB-C4A-NA  | 2.37  | 127.80      | 124.51   |
| 22  | S     | 309 | CLA  | CHB-C4A-NA  | 2.37  | 127.80      | 124.51   |
| 26  | B     | 622 | LHG  | C20-C19-C18 | -2.37 | 102.37      | 114.42   |
| 31  | a     | 409 | BCR  | C15-C16-C17 | -2.37 | 118.61      | 123.47   |
| 31  | h     | 101 | BCR  | C11-C10-C9  | -2.37 | 123.92      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | N     | 601 | CHL  | C3B-C4B-NB  | 2.37  | 112.28      | 109.21   |
| 21  | R     | 306 | CHL  | C3B-C4B-NB  | 2.37  | 112.28      | 109.21   |
| 21  | s     | 307 | CHL  | C3B-C4B-NB  | 2.37  | 112.28      | 109.21   |
| 22  | A     | 406 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 37  | F     | 101 | HEM  | CMA-C3A-C4A | -2.37 | 124.82      | 128.46   |
| 22  | g     | 614 | CLA  | CHB-C4A-NA  | 2.37  | 127.79      | 124.51   |
| 31  | b     | 617 | BCR  | C27-C26-C25 | 2.37  | 126.17      | 122.73   |
| 36  | D     | 411 | LMG  | O2-C2-C1    | -2.37 | 104.28      | 110.05   |
| 26  | c     | 522 | LHG  | C20-C19-C18 | -2.37 | 102.38      | 114.42   |
| 21  | r     | 306 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 21  | N     | 608 | CHL  | C3B-C4B-NB  | 2.37  | 112.28      | 109.21   |
| 21  | G     | 605 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 23  | R     | 312 | LUT  | C31-C32-C33 | -2.37 | 119.76      | 126.42   |
| 36  | C     | 502 | LMG  | O2-C2-C1    | -2.37 | 104.29      | 110.05   |
| 21  | S     | 306 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 21  | y     | 605 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 21  | y     | 609 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 21  | Y     | 608 | CHL  | C3B-C4B-NB  | 2.37  | 112.27      | 109.21   |
| 21  | y     | 607 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 36  | w     | 102 | LMG  | O2-C2-C1    | -2.37 | 104.29      | 110.05   |
| 21  | y     | 601 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 26  | y     | 617 | LHG  | C5-O7-C7    | -2.37 | 111.96      | 117.79   |
| 22  | B     | 612 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 21  | n     | 608 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 22  | A     | 407 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 26  | b     | 619 | LHG  | C20-C19-C18 | -2.37 | 102.41      | 114.42   |
| 21  | s     | 302 | CHL  | C3B-C4B-NB  | 2.37  | 112.27      | 109.21   |
| 22  | n     | 613 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 21  | y     | 608 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 36  | d     | 410 | LMG  | O2-C2-C1    | -2.37 | 104.30      | 110.05   |
| 22  | C     | 512 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 21  | S     | 301 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 26  | C     | 522 | LHG  | C20-C19-C18 | -2.37 | 102.42      | 114.42   |
| 21  | G     | 606 | CHL  | C3B-C4B-NB  | 2.37  | 112.27      | 109.21   |
| 21  | N     | 607 | CHL  | O2D-CGD-O1D | -2.37 | 119.21      | 123.84   |
| 22  | W     | 101 | CLA  | C1B-CHB-C4A | -2.36 | 125.43      | 130.12   |
| 22  | b     | 612 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 21  | G     | 607 | CHL  | C3B-C4B-NB  | 2.36  | 112.27      | 109.21   |
| 21  | S     | 302 | CHL  | C3B-C4B-NB  | 2.36  | 112.27      | 109.21   |
| 31  | H     | 101 | BCR  | C15-C14-C13 | -2.36 | 123.94      | 127.31   |
| 22  | b     | 615 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 21  | g     | 609 | CHL  | C3B-C4B-NB  | 2.36  | 112.27      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | a     | 413 | DGD  | C3G-C2G-C1G | -2.36 | 106.20      | 111.79   |
| 22  | a     | 406 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 26  | N     | 618 | LHG  | C5-O7-C7    | -2.36 | 111.98      | 117.79   |
| 22  | y     | 604 | CLA  | C1-C2-C3    | -2.36 | 122.93      | 126.75   |
| 22  | g     | 612 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 22  | n     | 603 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 35  | A     | 401 | DGD  | C3G-C2G-C1G | -2.36 | 106.20      | 111.79   |
| 21  | n     | 607 | CHL  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 21  | N     | 606 | CHL  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 21  | S     | 301 | CHL  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 31  | B     | 602 | BCR  | C27-C26-C25 | 2.36  | 126.16      | 122.73   |
| 22  | B     | 617 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 36  | C     | 523 | LMG  | O1-C1-C2    | -2.36 | 104.62      | 108.30   |
| 26  | d     | 407 | LHG  | C11-C10-C9  | -2.36 | 102.44      | 114.42   |
| 22  | S     | 308 | CLA  | CHD-C1D-ND  | -2.36 | 122.29      | 124.45   |
| 22  | Y     | 612 | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 36  | M     | 101 | LMG  | C38-C37-C36 | -2.36 | 102.45      | 114.42   |
| 21  | n     | 608 | CHL  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 22  | B     | 613 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 26  | c     | 521 | LHG  | C11-C10-C9  | -2.36 | 102.46      | 114.42   |
| 33  | d     | 402 | SQD  | O48-C23-C24 | 2.36  | 119.31      | 111.91   |
| 31  | d     | 405 | BCR  | C11-C10-C9  | -2.36 | 123.95      | 127.31   |
| 22  | N     | 611 | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 22  | G     | 612 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 21  | y     | 606 | CHL  | C3B-C4B-NB  | 2.36  | 112.25      | 109.21   |
| 21  | N     | 607 | CHL  | C3B-C4B-NB  | 2.36  | 112.25      | 109.21   |
| 36  | T     | 101 | LMG  | C38-C37-C36 | -2.36 | 102.47      | 114.42   |
| 22  | a     | 405 | CLA  | C1B-CHB-C4A | -2.35 | 125.45      | 130.12   |
| 21  | g     | 606 | CHL  | C3B-C4B-NB  | 2.35  | 112.25      | 109.21   |
| 21  | n     | 601 | CHL  | C3B-C4B-NB  | 2.35  | 112.25      | 109.21   |
| 24  | N     | 616 | XAT  | C11-C12-C13 | -2.35 | 119.80      | 126.42   |
| 25  | Y     | 616 | NEX  | C36-C21-C26 | -2.35 | 103.69      | 110.05   |
| 22  | N     | 604 | CLA  | C1-C2-C3    | -2.35 | 122.94      | 126.75   |
| 22  | g     | 603 | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 31  | A     | 410 | BCR  | C7-C8-C9    | -2.35 | 122.68      | 126.23   |
| 36  | B     | 601 | LMG  | C38-C37-C36 | -2.35 | 102.49      | 114.42   |
| 22  | Y     | 603 | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 21  | y     | 609 | CHL  | C3B-C4B-NB  | 2.35  | 112.25      | 109.21   |
| 26  | D     | 408 | LHG  | C11-C10-C9  | -2.35 | 102.49      | 114.42   |
| 22  | N     | 613 | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 21  | s     | 306 | CHL  | C3B-C4B-NB  | 2.35  | 112.25      | 109.21   |
| 36  | C     | 502 | LMG  | O7-C10-O9   | -2.35 | 118.03      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | D     | 402 | SQD  | O48-C23-C24 | 2.35  | 119.28      | 111.91   |
| 21  | y     | 601 | CHL  | C3B-C4B-NB  | 2.35  | 112.25      | 109.21   |
| 22  | c     | 503 | CLA  | O2A-CGA-O1A | -2.35 | 117.67      | 123.59   |
| 21  | y     | 608 | CHL  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 22  | n     | 604 | CLA  | C1-C2-C3    | -2.35 | 122.95      | 126.75   |
| 31  | B     | 620 | BCR  | C27-C26-C25 | 2.35  | 126.14      | 122.73   |
| 21  | r     | 301 | CHL  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 21  | r     | 307 | CHL  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 31  | T     | 102 | BCR  | C27-C26-C25 | 2.35  | 126.14      | 122.73   |
| 22  | y     | 603 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 21  | G     | 605 | CHL  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 22  | g     | 612 | CLA  | CHB-C4A-NA  | 2.35  | 127.75      | 124.51   |
| 23  | r     | 313 | LUT  | C31-C32-C33 | -2.35 | 119.83      | 126.42   |
| 36  | B     | 623 | LMG  | C38-C37-C36 | -2.34 | 102.53      | 114.42   |
| 22  | N     | 603 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 36  | b     | 620 | LMG  | C38-C37-C36 | -2.34 | 102.53      | 114.42   |
| 22  | n     | 611 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 21  | G     | 601 | CHL  | C3B-C4B-NB  | 2.34  | 112.24      | 109.21   |
| 21  | S     | 307 | CHL  | C3B-C4B-NB  | 2.34  | 112.24      | 109.21   |
| 22  | B     | 606 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 26  | C     | 521 | LHG  | C11-C10-C9  | -2.34 | 102.54      | 114.42   |
| 21  | r     | 308 | CHL  | C3B-C4B-NB  | 2.34  | 112.24      | 109.21   |
| 26  | g     | 619 | LHG  | C20-C19-C18 | -2.34 | 102.55      | 114.42   |
| 36  | I     | 101 | LMG  | C38-C37-C36 | -2.34 | 102.55      | 114.42   |
| 22  | G     | 612 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 22  | c     | 503 | CLA  | C1-C2-C3    | -2.34 | 122.00      | 126.04   |
| 31  | h     | 101 | BCR  | C15-C14-C13 | -2.34 | 123.97      | 127.31   |
| 22  | W     | 101 | CLA  | CHD-C1D-ND  | -2.34 | 122.31      | 124.45   |
| 22  | w     | 101 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 21  | n     | 605 | CHL  | C3B-C4B-NB  | 2.34  | 112.23      | 109.21   |
| 21  | r     | 306 | CHL  | C3B-C4B-NB  | 2.34  | 112.23      | 109.21   |
| 22  | N     | 611 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 36  | c     | 523 | LMG  | O3-C3-C2    | -2.34 | 104.95      | 110.35   |
| 21  | N     | 605 | CHL  | C3B-C4B-NB  | 2.34  | 112.23      | 109.21   |
| 22  | w     | 101 | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 22  | s     | 311 | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 22  | c     | 503 | CLA  | C1B-CHB-C4A | -2.33 | 125.49      | 130.12   |
| 22  | C     | 504 | CLA  | O2A-CGA-O1A | -2.33 | 117.70      | 123.59   |
| 21  | n     | 606 | CHL  | C3B-C4B-NB  | 2.33  | 112.23      | 109.21   |
| 21  | R     | 305 | CHL  | C3B-C4B-NB  | 2.33  | 112.23      | 109.21   |
| 22  | y     | 613 | CLA  | CHB-C4A-NA  | 2.33  | 127.74      | 124.51   |
| 36  | C     | 523 | LMG  | O3-C3-C2    | -2.33 | 104.96      | 110.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 504 | CLA  | C1B-CHB-C4A | -2.33 | 125.50      | 130.12   |
| 22  | W     | 101 | CLA  | CHB-C4A-NA  | 2.33  | 127.74      | 124.51   |
| 21  | g     | 607 | CHL  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 21  | Y     | 605 | CHL  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 26  | C     | 522 | LHG  | C5-O7-C7    | -2.33 | 112.05      | 117.79   |
| 36  | d     | 410 | LMG  | O1-C1-C2    | -2.33 | 104.66      | 108.30   |
| 31  | b     | 617 | BCR  | C33-C5-C6   | -2.33 | 121.91      | 124.53   |
| 21  | S     | 306 | CHL  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 36  | D     | 411 | LMG  | O1-C1-C2    | -2.33 | 104.67      | 108.30   |
| 22  | g     | 604 | CLA  | C1-C2-C3    | -2.33 | 122.98      | 126.75   |
| 26  | y     | 617 | LHG  | C20-C19-C18 | -2.33 | 102.61      | 114.42   |
| 36  | w     | 102 | LMG  | O7-C10-O9   | -2.33 | 118.08      | 123.70   |
| 21  | s     | 301 | CHL  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 31  | D     | 406 | BCR  | C11-C10-C9  | -2.33 | 123.99      | 127.31   |
| 22  | B     | 616 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 31  | K     | 102 | BCR  | C27-C26-C25 | 2.33  | 126.11      | 122.73   |
| 21  | y     | 605 | CHL  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 22  | s     | 308 | CLA  | CHD-C1D-ND  | -2.33 | 122.32      | 124.45   |
| 26  | N     | 618 | LHG  | O8-C23-C24  | 2.33  | 119.20      | 111.91   |
| 22  | n     | 609 | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 35  | H     | 102 | DGD  | O2D-C2D-C1D | -2.32 | 104.40      | 110.05   |
| 26  | c     | 522 | LHG  | C5-O7-C7    | -2.32 | 112.07      | 117.79   |
| 21  | Y     | 607 | CHL  | C3B-C4B-NB  | 2.32  | 112.21      | 109.21   |
| 36  | C     | 502 | LMG  | C38-C37-C36 | -2.32 | 102.64      | 114.42   |
| 31  | h     | 101 | BCR  | C27-C26-C25 | 2.32  | 126.10      | 122.73   |
| 22  | G     | 603 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 36  | w     | 102 | LMG  | C38-C37-C36 | -2.32 | 102.65      | 114.42   |
| 35  | h     | 102 | DGD  | C1D-C2D-C3D | -2.32 | 105.17      | 110.00   |
| 25  | N     | 617 | NEX  | C11-C12-C13 | -2.32 | 119.90      | 126.42   |
| 21  | G     | 609 | CHL  | C3B-C4B-NB  | 2.32  | 112.21      | 109.21   |
| 22  | n     | 611 | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 22  | Y     | 604 | CLA  | C1-C2-C3    | -2.32 | 123.00      | 126.75   |
| 22  | b     | 603 | CLA  | C1B-CHB-C4A | -2.31 | 125.53      | 130.12   |
| 22  | C     | 506 | CLA  | C1B-CHB-C4A | -2.31 | 125.53      | 130.12   |
| 31  | a     | 409 | BCR  | C7-C8-C9    | -2.31 | 122.74      | 126.23   |
| 22  | C     | 504 | CLA  | C1-C2-C3    | -2.31 | 122.04      | 126.04   |
| 35  | H     | 102 | DGD  | C1D-C2D-C3D | -2.31 | 105.18      | 110.00   |
| 31  | K     | 101 | BCR  | C27-C26-C25 | 2.31  | 126.09      | 122.73   |
| 22  | N     | 609 | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 22  | g     | 612 | CLA  | O2D-CGD-O1D | -2.31 | 119.32      | 123.84   |
| 26  | Y     | 617 | LHG  | C20-C19-C18 | -2.31 | 102.70      | 114.42   |
| 21  | y     | 607 | CHL  | C3B-C4B-NB  | 2.31  | 112.19      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | d     | 406 | PL9  | O1-C4-C3    | -2.31 | 118.18      | 120.72   |
| 31  | k     | 102 | BCR  | C27-C26-C25 | 2.31  | 126.08      | 122.73   |
| 22  | c     | 505 | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |
| 33  | l     | 103 | SQD  | O6-C1-C2    | 2.31  | 111.91      | 108.30   |
| 22  | G     | 612 | CLA  | O2D-CGD-O1D | -2.31 | 119.33      | 123.84   |
| 22  | b     | 613 | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |
| 22  | b     | 605 | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 35  | h     | 102 | DGD  | C3G-C2G-C1G | -2.31 | 106.33      | 111.79   |
| 22  | R     | 304 | CLA  | CHD-C1D-ND  | -2.30 | 122.34      | 124.45   |
| 37  | f     | 101 | HEM  | CHD-C1D-ND  | 2.30  | 126.93      | 124.43   |
| 32  | D     | 407 | PL9  | O1-C4-C3    | -2.30 | 118.19      | 120.72   |
| 22  | g     | 610 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 22  | Y     | 609 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 35  | h     | 102 | DGD  | O2D-C2D-C1D | -2.30 | 104.46      | 110.05   |
| 23  | N     | 615 | LUT  | C10-C11-C12 | -2.30 | 116.04      | 123.22   |
| 22  | B     | 606 | CLA  | O2A-CGA-O1A | -2.30 | 117.79      | 123.59   |
| 25  | g     | 618 | NEX  | C36-C21-C22 | -2.30 | 104.99      | 108.98   |
| 22  | B     | 608 | CLA  | O2A-CGA-O1A | -2.30 | 117.79      | 123.59   |
| 30  | d     | 401 | PHO  | C1-C2-C3    | -2.30 | 122.07      | 126.04   |
| 33  | L     | 101 | SQD  | O48-C23-C24 | 2.30  | 119.12      | 111.91   |
| 26  | D     | 409 | LHG  | C18-C17-C16 | -2.30 | 102.76      | 114.42   |
| 35  | A     | 401 | DGD  | C4E-C3E-C2E | -2.30 | 106.81      | 110.82   |
| 22  | W     | 101 | CLA  | O2D-CGD-O1D | -2.29 | 119.35      | 123.84   |
| 26  | d     | 408 | LHG  | C18-C17-C16 | -2.29 | 102.79      | 114.42   |
| 24  | g     | 617 | XAT  | C11-C12-C13 | -2.29 | 119.98      | 126.42   |
| 22  | y     | 610 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 22  | n     | 611 | CLA  | CHD-C1D-ND  | -2.29 | 122.35      | 124.45   |
| 24  | r     | 314 | XAT  | C31-C32-C33 | -2.29 | 119.99      | 126.42   |
| 31  | k     | 101 | BCR  | C27-C26-C25 | 2.29  | 126.05      | 122.73   |
| 22  | A     | 409 | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 35  | h     | 102 | DGD  | O5D-C6D-C5D | -2.28 | 104.82      | 109.05   |
| 24  | y     | 615 | XAT  | O4-C5-C6    | 2.28  | 60.85       | 58.96    |
| 35  | a     | 413 | DGD  | C4E-C3E-C2E | -2.28 | 106.83      | 110.82   |
| 22  | Y     | 612 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 24  | g     | 617 | XAT  | O4-C5-C6    | 2.28  | 60.85       | 58.96    |
| 24  | R     | 313 | XAT  | C31-C32-C33 | -2.28 | 120.00      | 126.42   |
| 22  | c     | 507 | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 36  | B     | 601 | LMG  | O3-C3-C2    | -2.28 | 105.07      | 110.35   |
| 35  | H     | 102 | DGD  | O5D-C6D-C5D | -2.28 | 104.82      | 109.05   |
| 23  | R     | 312 | LUT  | C1-C6-C7    | -2.28 | 109.32      | 115.78   |
| 22  | G     | 612 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 33  | l     | 103 | SQD  | O48-C23-C24 | 2.28  | 119.07      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 511 | CLA  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 22  | G     | 610 | CLA  | C1B-CHB-C4A | -2.28 | 125.60      | 130.12   |
| 26  | G     | 618 | LHG  | C5-O7-C7    | -2.28 | 112.18      | 117.79   |
| 22  | b     | 603 | CLA  | O2A-CGA-O1A | -2.28 | 117.84      | 123.59   |
| 26  | l     | 102 | LHG  | C18-C17-C16 | -2.28 | 102.86      | 114.42   |
| 26  | D     | 409 | LHG  | C27-C26-C25 | -2.28 | 102.86      | 114.42   |
| 23  | r     | 313 | LUT  | C1-C6-C7    | -2.28 | 109.34      | 115.78   |
| 22  | c     | 510 | CLA  | O2D-CGD-O1D | -2.28 | 119.39      | 123.84   |
| 26  | d     | 408 | LHG  | C27-C26-C25 | -2.28 | 102.87      | 114.42   |
| 22  | N     | 611 | CLA  | O2D-CGD-O1D | -2.28 | 119.39      | 123.84   |
| 22  | g     | 612 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 22  | R     | 304 | CLA  | CMB-C2B-C3B | 2.28  | 128.94      | 124.68   |
| 22  | C     | 515 | CLA  | C1B-CHB-C4A | -2.27 | 125.61      | 130.12   |
| 22  | n     | 611 | CLA  | O2D-CGD-O1D | -2.27 | 119.39      | 123.84   |
| 22  | w     | 101 | CLA  | O2D-CGD-O1D | -2.27 | 119.39      | 123.84   |
| 31  | H     | 101 | BCR  | C27-C26-C25 | 2.27  | 126.03      | 122.73   |
| 22  | d     | 403 | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 22  | s     | 312 | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 26  | L     | 103 | LHG  | C18-C17-C16 | -2.27 | 102.89      | 114.42   |
| 35  | H     | 102 | DGD  | C3G-C2G-C1G | -2.27 | 106.42      | 111.79   |
| 36  | I     | 101 | LMG  | O3-C3-C2    | -2.27 | 105.11      | 110.35   |
| 30  | D     | 401 | PHO  | C1-C2-C3    | -2.27 | 122.12      | 126.04   |
| 26  | N     | 618 | LHG  | C20-C19-C18 | -2.26 | 102.93      | 114.42   |
| 22  | D     | 404 | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 33  | L     | 101 | SQD  | O6-C1-C2    | 2.26  | 111.84      | 108.30   |
| 36  | k     | 103 | LMG  | C1-C2-C3    | -2.26 | 105.28      | 110.00   |
| 36  | K     | 103 | LMG  | C1-C2-C3    | -2.26 | 105.28      | 110.00   |
| 22  | a     | 408 | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 22  | w     | 101 | CLA  | CHD-C1D-ND  | -2.26 | 122.38      | 124.45   |
| 24  | n     | 615 | XAT  | C11-C12-C13 | -2.26 | 120.06      | 126.42   |
| 31  | H     | 101 | BCR  | C20-C21-C22 | -2.26 | 124.08      | 127.31   |
| 25  | y     | 618 | NEX  | C36-C21-C26 | -2.26 | 103.94      | 110.05   |
| 22  | r     | 305 | CLA  | CMB-C2B-C3B | 2.26  | 128.91      | 124.68   |
| 22  | C     | 508 | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 37  | F     | 101 | HEM  | CHD-C1D-ND  | 2.26  | 126.88      | 124.43   |
| 26  | c     | 522 | LHG  | O8-C6-C5    | -2.26 | 101.86      | 108.43   |
| 22  | s     | 303 | CLA  | O2A-CGA-O1A | -2.26 | 117.89      | 123.59   |
| 22  | S     | 303 | CLA  | O2A-CGA-O1A | -2.26 | 117.89      | 123.59   |
| 25  | r     | 315 | NEX  | C36-C21-C26 | -2.26 | 103.95      | 110.05   |
| 35  | c     | 517 | DGD  | O2D-C2D-C1D | -2.26 | 104.56      | 110.05   |
| 22  | a     | 406 | CLA  | O2A-CGA-O1A | -2.25 | 117.90      | 123.59   |
| 25  | N     | 617 | NEX  | C38-C25-C26 | -2.25 | 118.48      | 122.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | d     | 405 | BCR  | C15-C16-C17 | -2.25 | 118.86      | 123.47   |
| 26  | r     | 302 | LHG  | C5-O7-C7    | -2.25 | 112.25      | 117.79   |
| 22  | C     | 512 | CLA  | O2A-CGA-O1A | -2.25 | 117.91      | 123.59   |
| 22  | b     | 601 | CLA  | C1-C2-C3    | -2.25 | 122.15      | 126.04   |
| 22  | S     | 312 | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 26  | n     | 617 | LHG  | C18-C17-C16 | -2.25 | 103.01      | 114.42   |
| 26  | C     | 522 | LHG  | O8-C6-C5    | -2.25 | 101.89      | 108.43   |
| 36  | T     | 101 | LMG  | C40-C39-C38 | -2.25 | 103.02      | 114.42   |
| 22  | c     | 514 | CLA  | C1B-CHB-C4A | -2.24 | 125.67      | 130.12   |
| 36  | M     | 101 | LMG  | C40-C39-C38 | -2.24 | 103.03      | 114.42   |
| 22  | r     | 305 | CLA  | CHD-C1D-ND  | -2.24 | 122.39      | 124.45   |
| 24  | Y     | 615 | XAT  | O4-C5-C6    | 2.24  | 60.81       | 58.96    |
| 22  | c     | 511 | CLA  | O2A-CGA-O1A | -2.24 | 117.93      | 123.59   |
| 35  | C     | 518 | DGD  | O2D-C2D-C1D | -2.24 | 104.60      | 110.05   |
| 36  | M     | 101 | LMG  | O3-C3-C2    | -2.24 | 105.17      | 110.35   |
| 35  | C     | 519 | DGD  | CBB-CAB-C9B | -2.24 | 103.06      | 114.42   |
| 31  | B     | 619 | BCR  | C7-C8-C9    | -2.24 | 122.86      | 126.23   |
| 22  | A     | 407 | CLA  | O2A-CGA-O1A | -2.24 | 117.95      | 123.59   |
| 31  | h     | 101 | BCR  | C20-C21-C22 | -2.24 | 124.12      | 127.31   |
| 26  | C     | 522 | LHG  | O8-C23-C24  | 2.23  | 118.92      | 111.91   |
| 22  | g     | 614 | CLA  | CHD-C1D-ND  | -2.23 | 122.40      | 124.45   |
| 22  | N     | 613 | CLA  | CHD-C1D-ND  | -2.23 | 122.40      | 124.45   |
| 35  | C     | 519 | DGD  | C1D-C2D-C3D | -2.23 | 105.35      | 110.00   |
| 26  | c     | 522 | LHG  | C18-C17-C16 | -2.23 | 103.09      | 114.42   |
| 35  | c     | 518 | DGD  | C1D-C2D-C3D | -2.23 | 105.35      | 110.00   |
| 22  | C     | 511 | CLA  | C4D-CHA-C1A | 2.23  | 123.96      | 121.25   |
| 26  | R     | 301 | LHG  | C5-O7-C7    | -2.23 | 112.30      | 117.79   |
| 26  | C     | 520 | LHG  | C18-C17-C16 | -2.23 | 103.10      | 114.42   |
| 36  | B     | 623 | LMG  | C42-C41-C40 | -2.23 | 103.10      | 114.42   |
| 22  | N     | 611 | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 26  | N     | 618 | LHG  | C11-C10-C9  | -2.23 | 103.11      | 114.42   |
| 35  | c     | 518 | DGD  | CBB-CAB-C9B | -2.23 | 103.11      | 114.42   |
| 36  | b     | 620 | LMG  | C42-C41-C40 | -2.23 | 103.12      | 114.42   |
| 22  | B     | 604 | CLA  | C1-C2-C3    | -2.23 | 122.19      | 126.04   |
| 22  | r     | 303 | CLA  | C1-C2-C3    | -2.23 | 122.19      | 126.04   |
| 22  | C     | 515 | CLA  | C1-C2-C3    | -2.23 | 122.19      | 126.04   |
| 36  | T     | 101 | LMG  | O3-C3-C2    | -2.23 | 105.20      | 110.35   |
| 22  | s     | 304 | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 26  | c     | 520 | LHG  | C18-C17-C16 | -2.22 | 103.14      | 114.42   |
| 31  | B     | 619 | BCR  | C15-C14-C13 | -2.22 | 124.14      | 127.31   |
| 31  | b     | 616 | BCR  | C7-C8-C9    | -2.22 | 122.88      | 126.23   |
| 22  | c     | 514 | CLA  | C1-C2-C3    | -2.22 | 122.20      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | R     | 302 | CLA  | C1-C2-C3    | -2.22 | 122.20      | 126.04   |
| 31  | D     | 406 | BCR  | C15-C16-C17 | -2.22 | 118.93      | 123.47   |
| 26  | C     | 522 | LHG  | C18-C17-C16 | -2.22 | 103.16      | 114.42   |
| 31  | C     | 517 | BCR  | C24-C23-C22 | -2.22 | 122.88      | 126.23   |
| 26  | r     | 302 | LHG  | C18-C17-C16 | -2.22 | 103.16      | 114.42   |
| 22  | y     | 613 | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 26  | c     | 522 | LHG  | O8-C23-C24  | 2.22  | 118.87      | 111.91   |
| 26  | R     | 301 | LHG  | C18-C17-C16 | -2.21 | 103.19      | 114.42   |
| 35  | C     | 518 | DGD  | CBB-CAB-C9B | -2.21 | 103.19      | 114.42   |
| 26  | Y     | 617 | LHG  | C27-C26-C25 | -2.21 | 103.20      | 114.42   |
| 22  | S     | 310 | CLA  | O2A-CGA-O1A | -2.21 | 118.01      | 123.59   |
| 35  | c     | 517 | DGD  | CBB-CAB-C9B | -2.21 | 103.20      | 114.42   |
| 22  | G     | 614 | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 25  | Y     | 616 | NEX  | C11-C12-C13 | -2.21 | 120.21      | 126.42   |
| 37  | f     | 101 | HEM  | CHB-C1B-NB  | -2.21 | 121.65      | 124.38   |
| 31  | b     | 616 | BCR  | C15-C14-C13 | -2.20 | 124.16      | 127.31   |
| 22  | n     | 613 | CLA  | CHD-C1D-ND  | -2.20 | 122.43      | 124.45   |
| 35  | c     | 519 | DGD  | C5B-C4B-C3B | -2.20 | 103.25      | 114.42   |
| 22  | C     | 513 | CLA  | O2A-CGA-O1A | -2.20 | 118.04      | 123.59   |
| 35  | H     | 102 | DGD  | CBB-CAB-C9B | -2.20 | 103.26      | 114.42   |
| 22  | g     | 614 | CLA  | O2A-CGA-O1A | -2.20 | 118.04      | 123.59   |
| 35  | J     | 101 | DGD  | C5B-C4B-C3B | -2.20 | 103.27      | 114.42   |
| 31  | c     | 516 | BCR  | C24-C23-C22 | -2.20 | 122.92      | 126.23   |
| 32  | a     | 410 | PL9  | C7-C3-C4    | 2.20  | 120.85      | 118.08   |
| 22  | c     | 512 | CLA  | O2A-CGA-O1A | -2.20 | 118.05      | 123.59   |
| 26  | b     | 619 | LHG  | C18-C17-C16 | -2.20 | 103.28      | 114.42   |
| 26  | R     | 301 | LHG  | C27-C26-C25 | -2.20 | 103.28      | 114.42   |
| 22  | c     | 510 | CLA  | C4D-CHA-C1A | 2.19  | 123.92      | 121.25   |
| 26  | r     | 302 | LHG  | C27-C26-C25 | -2.19 | 103.30      | 114.42   |
| 26  | g     | 619 | LHG  | C27-C26-C25 | -2.19 | 103.30      | 114.42   |
| 36  | I     | 101 | LMG  | O6-C1-O1    | -2.19 | 104.79      | 109.97   |
| 22  | a     | 404 | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 22  | B     | 605 | CLA  | O2A-CGA-O1A | -2.19 | 118.07      | 123.59   |
| 26  | B     | 622 | LHG  | C18-C17-C16 | -2.19 | 103.31      | 114.42   |
| 22  | N     | 613 | CLA  | O2A-CGA-O1A | -2.19 | 118.07      | 123.59   |
| 32  | a     | 410 | PL9  | C2-C3-C4    | 2.19  | 120.32      | 118.64   |
| 35  | h     | 102 | DGD  | CBB-CAB-C9B | -2.19 | 103.31      | 114.42   |
| 36  | B     | 601 | LMG  | O6-C1-O1    | -2.19 | 104.79      | 109.97   |
| 26  | G     | 618 | LHG  | C18-C17-C16 | -2.19 | 103.32      | 114.42   |
| 22  | b     | 602 | CLA  | O2A-CGA-O1A | -2.19 | 118.07      | 123.59   |
| 22  | n     | 613 | CLA  | O2A-CGA-O1A | -2.19 | 118.07      | 123.59   |
| 22  | A     | 405 | CLA  | C1-C2-C3    | -2.19 | 122.26      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Y     | 612 | CLA  | O2A-CGA-O1A | -2.19 | 118.08      | 123.59   |
| 22  | s     | 310 | CLA  | O2A-CGA-O1A | -2.19 | 118.08      | 123.59   |
| 34  | a     | 412 | BCT  | O3-C-O1     | -2.19 | 113.88      | 119.55   |
| 22  | C     | 511 | CLA  | CMC-C2C-C1C | -2.19 | 121.71      | 125.04   |
| 36  | M     | 101 | LMG  | O2-C2-C1    | -2.18 | 104.74      | 110.05   |
| 37  | F     | 101 | HEM  | CHB-C1B-NB  | -2.18 | 121.69      | 124.38   |
| 35  | J     | 101 | DGD  | CAB-C9B-C8B | -2.18 | 103.36      | 114.42   |
| 34  | D     | 403 | BCT  | O3-C-O1     | -2.18 | 113.89      | 119.55   |
| 22  | y     | 613 | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 22  | c     | 510 | CLA  | CMC-C2C-C1C | -2.18 | 121.72      | 125.04   |
| 24  | N     | 616 | XAT  | O4-C5-C6    | 2.18  | 60.76       | 58.96    |
| 22  | a     | 406 | CLA  | C1-C2-C3    | -2.17 | 123.23      | 126.75   |
| 35  | c     | 517 | DGD  | O3E-C3E-C2E | -2.17 | 105.32      | 110.35   |
| 32  | d     | 406 | PL9  | C37-C38-C39 | -2.17 | 122.43      | 127.66   |
| 24  | n     | 615 | XAT  | O4-C5-C6    | 2.17  | 60.76       | 58.96    |
| 22  | S     | 304 | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 33  | l     | 101 | SQD  | O48-C23-C24 | 2.17  | 118.73      | 111.91   |
| 35  | a     | 413 | DGD  | O5D-C6D-C5D | -2.17 | 105.03      | 109.05   |
| 33  | L     | 102 | SQD  | O48-C23-C24 | 2.17  | 118.72      | 111.91   |
| 35  | h     | 102 | DGD  | O3E-C3E-C2E | -2.17 | 105.33      | 110.35   |
| 32  | A     | 411 | PL9  | C2-C3-C4    | 2.17  | 120.31      | 118.64   |
| 35  | J     | 101 | DGD  | CBB-CAB-C9B | -2.17 | 103.41      | 114.42   |
| 36  | M     | 101 | LMG  | C1-C2-C3    | -2.17 | 105.48      | 110.00   |
| 26  | s     | 314 | LHG  | C18-C17-C16 | -2.17 | 103.41      | 114.42   |
| 24  | G     | 617 | XAT  | O4-C5-C6    | 2.17  | 60.75       | 58.96    |
| 35  | C     | 518 | DGD  | O3E-C3E-C2E | -2.17 | 105.34      | 110.35   |
| 26  | s     | 314 | LHG  | C27-C26-C25 | -2.17 | 103.42      | 114.42   |
| 22  | G     | 614 | CLA  | O2A-CGA-O1A | -2.17 | 118.12      | 123.59   |
| 26  | C     | 521 | LHG  | C27-C26-C25 | -2.17 | 103.42      | 114.42   |
| 36  | T     | 101 | LMG  | O2-C2-C1    | -2.17 | 104.78      | 110.05   |
| 32  | A     | 411 | PL9  | C7-C3-C4    | 2.17  | 120.81      | 118.08   |
| 26  | S     | 314 | LHG  | C27-C26-C25 | -2.17 | 103.43      | 114.42   |
| 36  | T     | 101 | LMG  | C1-C2-C3    | -2.17 | 105.49      | 110.00   |
| 35  | A     | 401 | DGD  | O5D-C6D-C5D | -2.16 | 105.04      | 109.05   |
| 26  | S     | 314 | LHG  | C18-C17-C16 | -2.16 | 103.44      | 114.42   |
| 35  | c     | 519 | DGD  | CBB-CAB-C9B | -2.16 | 103.44      | 114.42   |
| 26  | B     | 622 | LHG  | C27-C26-C25 | -2.16 | 103.45      | 114.42   |
| 22  | C     | 510 | CLA  | O2D-CGD-CBD | 2.16  | 115.11      | 111.27   |
| 26  | c     | 521 | LHG  | C27-C26-C25 | -2.16 | 103.45      | 114.42   |
| 35  | c     | 519 | DGD  | CAB-C9B-C8B | -2.16 | 103.46      | 114.42   |
| 31  | k     | 102 | BCR  | C11-C10-C9  | -2.16 | 124.23      | 127.31   |
| 22  | s     | 305 | CLA  | O2A-CGA-O1A | -2.16 | 118.14      | 123.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | y     | 617 | LHG  | C27-C26-C25 | -2.16 | 103.47      | 114.42   |
| 26  | n     | 617 | LHG  | C27-C26-C25 | -2.16 | 103.47      | 114.42   |
| 35  | c     | 517 | DGD  | C5B-C4B-C3B | -2.16 | 103.47      | 114.42   |
| 35  | c     | 518 | DGD  | C5B-C4B-C3B | -2.16 | 103.47      | 114.42   |
| 24  | N     | 616 | XAT  | C35-C15-C14 | -2.16 | 119.06      | 123.47   |
| 31  | K     | 102 | BCR  | C11-C10-C9  | -2.16 | 124.23      | 127.31   |
| 22  | r     | 304 | CLA  | O2A-CGA-O1A | -2.16 | 118.15      | 123.59   |
| 22  | S     | 311 | CLA  | O2A-CGA-O1A | -2.16 | 118.15      | 123.59   |
| 35  | H     | 102 | DGD  | O3E-C3E-C2E | -2.15 | 105.37      | 110.35   |
| 35  | C     | 519 | DGD  | C5B-C4B-C3B | -2.15 | 103.49      | 114.42   |
| 25  | y     | 618 | NEX  | C31-C32-C33 | -2.15 | 120.37      | 126.42   |
| 25  | r     | 315 | NEX  | C31-C32-C33 | -2.15 | 120.37      | 126.42   |
| 22  | A     | 407 | CLA  | C1-C2-C3    | -2.15 | 123.27      | 126.75   |
| 26  | b     | 619 | LHG  | C27-C26-C25 | -2.15 | 103.50      | 114.42   |
| 35  | h     | 102 | DGD  | C3D-C4D-C5D | -2.15 | 106.40      | 110.24   |
| 31  | k     | 101 | BCR  | C11-C10-C9  | -2.15 | 124.24      | 127.31   |
| 35  | C     | 518 | DGD  | C5B-C4B-C3B | -2.15 | 103.50      | 114.42   |
| 22  | S     | 305 | CLA  | O2A-CGA-O1A | -2.15 | 118.16      | 123.59   |
| 22  | b     | 606 | CLA  | C1-C2-C3    | -2.15 | 122.32      | 126.04   |
| 23  | N     | 615 | LUT  | C16-C1-C6   | -2.15 | 106.81      | 110.30   |
| 31  | K     | 102 | BCR  | C7-C8-C9    | -2.15 | 122.99      | 126.23   |
| 32  | D     | 407 | PL9  | O2-C1-C6    | 2.15  | 124.31      | 120.59   |
| 30  | d     | 401 | PHO  | CMC-C2C-C3C | 2.15  | 129.00      | 124.94   |
| 26  | C     | 520 | LHG  | C27-C26-C25 | -2.15 | 103.52      | 114.42   |
| 31  | b     | 616 | BCR  | C15-C16-C17 | -2.15 | 119.07      | 123.47   |
| 31  | B     | 619 | BCR  | C15-C16-C17 | -2.15 | 119.07      | 123.47   |
| 32  | D     | 407 | PL9  | C37-C38-C39 | -2.15 | 122.49      | 127.66   |
| 22  | R     | 303 | CLA  | O2A-CGA-O1A | -2.15 | 118.18      | 123.59   |
| 35  | H     | 102 | DGD  | C3D-C4D-C5D | -2.15 | 106.41      | 110.24   |
| 35  | a     | 413 | DGD  | C1D-C2D-C3D | -2.15 | 105.53      | 110.00   |
| 22  | s     | 311 | CLA  | O2A-CGA-O1A | -2.14 | 118.18      | 123.59   |
| 26  | Y     | 617 | LHG  | C18-C17-C16 | -2.14 | 103.54      | 114.42   |
| 32  | D     | 407 | PL9  | C20-C19-C21 | 2.14  | 118.88      | 115.27   |
| 32  | d     | 406 | PL9  | C20-C19-C21 | 2.14  | 118.88      | 115.27   |
| 26  | c     | 520 | LHG  | C27-C26-C25 | -2.14 | 103.55      | 114.42   |
| 26  | L     | 103 | LHG  | C27-C26-C25 | -2.14 | 103.55      | 114.42   |
| 22  | S     | 304 | CLA  | CHB-C4A-NA  | 2.14  | 127.47      | 124.51   |
| 22  | s     | 308 | CLA  | CED-O2D-CGD | 2.14  | 120.78      | 115.94   |
| 22  | G     | 613 | CLA  | CHD-C4C-C3C | -2.14 | 121.69      | 124.84   |
| 35  | A     | 401 | DGD  | O3E-C3E-C2E | -2.14 | 105.40      | 110.35   |
| 32  | d     | 406 | PL9  | O2-C1-C6    | 2.14  | 124.30      | 120.59   |
| 22  | B     | 609 | CLA  | C1-C2-C3    | -2.14 | 122.34      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | d     | 407 | LHG  | C27-C26-C25 | -2.14 | 103.56      | 114.42   |
| 26  | D     | 408 | LHG  | C27-C26-C25 | -2.14 | 103.56      | 114.42   |
| 30  | D     | 401 | PHO  | CMC-C2C-C3C | 2.14  | 128.97      | 124.94   |
| 22  | x     | 101 | CLA  | O2A-CGA-O1A | -2.14 | 118.20      | 123.59   |
| 33  | A     | 412 | SQD  | C1-C2-C3    | 2.14  | 114.45      | 110.00   |
| 35  | C     | 519 | DGD  | CAB-C9B-C8B | -2.14 | 103.58      | 114.42   |
| 35  | A     | 401 | DGD  | C1D-C2D-C3D | -2.14 | 105.55      | 110.00   |
| 22  | N     | 603 | CLA  | C1-C2-C3    | -2.13 | 122.35      | 126.04   |
| 26  | l     | 102 | LHG  | C27-C26-C25 | -2.13 | 103.59      | 114.42   |
| 22  | r     | 303 | CLA  | CHD-C1D-ND  | -2.13 | 122.49      | 124.45   |
| 22  | N     | 610 | CLA  | O2A-CGA-O1A | -2.13 | 118.21      | 123.59   |
| 22  | C     | 510 | CLA  | O2A-CGA-O1A | -2.13 | 118.21      | 123.59   |
| 35  | a     | 413 | DGD  | O3E-C3E-C2E | -2.13 | 105.42      | 110.35   |
| 22  | c     | 509 | CLA  | O2D-CGD-CBD | 2.13  | 115.05      | 111.27   |
| 26  | g     | 619 | LHG  | C18-C17-C16 | -2.13 | 103.62      | 114.42   |
| 22  | Y     | 610 | CLA  | O2A-CGA-O1A | -2.13 | 118.22      | 123.59   |
| 35  | H     | 102 | DGD  | O3D-C3D-C4D | -2.13 | 105.44      | 110.35   |
| 35  | h     | 102 | DGD  | O3D-C3D-C4D | -2.13 | 105.44      | 110.35   |
| 22  | c     | 509 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 35  | h     | 102 | DGD  | CAB-C9B-C8B | -2.12 | 103.64      | 114.42   |
| 22  | s     | 309 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 22  | S     | 309 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 26  | L     | 103 | LHG  | C5-O7-C7    | -2.12 | 112.56      | 117.79   |
| 22  | n     | 610 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 35  | c     | 518 | DGD  | CAB-C9B-C8B | -2.12 | 103.65      | 114.42   |
| 22  | n     | 602 | CLA  | CHD-C1D-ND  | -2.12 | 122.50      | 124.45   |
| 22  | G     | 602 | CLA  | CHD-C1D-ND  | -2.12 | 122.50      | 124.45   |
| 22  | N     | 602 | CLA  | CHD-C1D-ND  | -2.12 | 122.50      | 124.45   |
| 22  | g     | 613 | CLA  | CHD-C4C-C3C | -2.12 | 121.72      | 124.84   |
| 26  | D     | 410 | LHG  | C27-C26-C25 | -2.12 | 103.66      | 114.42   |
| 35  | a     | 413 | DGD  | CBB-CAB-C9B | -2.12 | 103.66      | 114.42   |
| 31  | k     | 101 | BCR  | C15-C14-C13 | -2.12 | 124.28      | 127.31   |
| 22  | Y     | 611 | CLA  | CHD-C4C-C3C | -2.12 | 121.72      | 124.84   |
| 26  | l     | 102 | LHG  | C5-O7-C7    | -2.12 | 112.57      | 117.79   |
| 26  | C     | 521 | LHG  | C20-C19-C18 | -2.12 | 103.67      | 114.42   |
| 30  | A     | 408 | PHO  | CMC-C2C-C3C | 2.12  | 128.94      | 124.94   |
| 22  | g     | 602 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 30  | a     | 407 | PHO  | CMC-C2C-C3C | 2.12  | 128.93      | 124.94   |
| 22  | Y     | 602 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 22  | G     | 611 | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 26  | g     | 619 | LHG  | O8-C6-C5    | -2.12 | 102.27      | 108.43   |
| 26  | G     | 618 | LHG  | C27-C26-C25 | -2.12 | 103.68      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | y     | 611 | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 33  | a     | 411 | SQD  | C1-C2-C3    | 2.11  | 114.40      | 110.00   |
| 22  | g     | 611 | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 35  | A     | 401 | DGD  | CBB-CAB-C9B | -2.11 | 103.70      | 114.42   |
| 35  | H     | 102 | DGD  | CAB-C9B-C8B | -2.11 | 103.70      | 114.42   |
| 26  | d     | 409 | LHG  | C27-C26-C25 | -2.11 | 103.70      | 114.42   |
| 26  | y     | 617 | LHG  | C18-C17-C16 | -2.11 | 103.71      | 114.42   |
| 26  | c     | 521 | LHG  | C20-C19-C18 | -2.11 | 103.71      | 114.42   |
| 36  | k     | 103 | LMG  | O3-C3-C2    | -2.11 | 105.47      | 110.35   |
| 22  | N     | 612 | CLA  | CHD-C4C-C3C | -2.11 | 121.74      | 124.84   |
| 22  | d     | 403 | CLA  | O2A-CGA-O1A | -2.11 | 118.27      | 123.59   |
| 35  | a     | 413 | DGD  | CAB-C9B-C8B | -2.11 | 103.72      | 114.42   |
| 31  | K     | 101 | BCR  | C15-C14-C13 | -2.11 | 124.30      | 127.31   |
| 36  | K     | 103 | LMG  | O3-C3-C2    | -2.11 | 105.47      | 110.35   |
| 31  | K     | 101 | BCR  | C11-C10-C9  | -2.11 | 124.30      | 127.31   |
| 22  | D     | 404 | CLA  | O2A-CGA-O1A | -2.10 | 118.28      | 123.59   |
| 23  | N     | 615 | LUT  | C7-C6-C5    | -2.10 | 116.36      | 121.46   |
| 22  | n     | 612 | CLA  | CHD-C4C-C3C | -2.10 | 121.75      | 124.84   |
| 31  | K     | 101 | BCR  | C15-C16-C17 | -2.10 | 119.17      | 123.47   |
| 22  | B     | 603 | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 22  | s     | 304 | CLA  | CHB-C4A-NA  | 2.10  | 127.42      | 124.51   |
| 24  | Y     | 615 | XAT  | C25-C24-C23 | -2.10 | 108.59      | 112.75   |
| 35  | A     | 401 | DGD  | CAB-C9B-C8B | -2.10 | 103.77      | 114.42   |
| 22  | D     | 405 | CLA  | C1-C2-C3    | -2.10 | 122.41      | 126.04   |
| 26  | c     | 521 | LHG  | C18-C17-C16 | -2.10 | 103.77      | 114.42   |
| 31  | K     | 101 | BCR  | C7-C8-C9    | -2.10 | 123.06      | 126.23   |
| 25  | g     | 618 | NEX  | C36-C21-C26 | -2.10 | 104.38      | 110.05   |
| 33  | a     | 411 | SQD  | O48-C23-O10 | -2.10 | 118.30      | 123.59   |
| 26  | C     | 521 | LHG  | C18-C17-C16 | -2.10 | 103.77      | 114.42   |
| 22  | S     | 308 | CLA  | CED-O2D-CGD | 2.10  | 120.68      | 115.94   |
| 25  | n     | 616 | NEX  | C36-C21-C26 | -2.10 | 104.38      | 110.05   |
| 31  | k     | 101 | BCR  | C15-C16-C17 | -2.10 | 119.18      | 123.47   |
| 31  | k     | 102 | BCR  | C7-C8-C9    | -2.09 | 123.07      | 126.23   |
| 22  | B     | 616 | CLA  | C1-C2-C3    | -2.09 | 122.42      | 126.04   |
| 22  | y     | 612 | CLA  | CHD-C4C-C3C | -2.09 | 121.76      | 124.84   |
| 23  | N     | 615 | LUT  | C15-C35-C34 | -2.09 | 119.19      | 123.47   |
| 22  | y     | 602 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 22  | G     | 603 | CLA  | C1-C2-C3    | -2.09 | 122.43      | 126.04   |
| 32  | d     | 406 | PL9  | C31-C32-C33 | -2.09 | 105.01      | 111.88   |
| 26  | n     | 617 | LHG  | C5-O7-C7    | -2.09 | 112.65      | 117.79   |
| 22  | s     | 309 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 23  | Y     | 614 | LUT  | C3-C4-C5    | -2.09 | 107.69      | 111.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | A     | 412 | SQD  | O48-C23-O10 | -2.09 | 118.32      | 123.59   |
| 22  | d     | 404 | CLA  | O2A-CGA-O1A | -2.09 | 118.32      | 123.59   |
| 32  | D     | 407 | PL9  | C31-C32-C33 | -2.09 | 105.03      | 111.88   |
| 22  | b     | 610 | CLA  | O2A-CGA-O1A | -2.09 | 118.33      | 123.59   |
| 32  | D     | 407 | PL9  | O2-C1-C2    | -2.08 | 117.00      | 121.78   |
| 23  | N     | 615 | LUT  | C1-C6-C7    | -2.08 | 109.88      | 115.78   |
| 22  | d     | 404 | CLA  | C1-C2-C3    | -2.08 | 122.44      | 126.04   |
| 36  | b     | 620 | LMG  | O2-C2-C1    | -2.08 | 104.99      | 110.05   |
| 22  | g     | 603 | CLA  | C1-C2-C3    | -2.08 | 122.44      | 126.04   |
| 35  | C     | 518 | DGD  | CAB-C9B-C8B | -2.08 | 103.85      | 114.42   |
| 26  | c     | 522 | LHG  | C27-C26-C25 | -2.08 | 103.85      | 114.42   |
| 22  | B     | 613 | CLA  | O2A-CGA-O1A | -2.08 | 118.34      | 123.59   |
| 22  | C     | 511 | CLA  | C1C-C2C-C3C | 2.08  | 109.14      | 106.96   |
| 22  | c     | 508 | CLA  | O2A-CGA-O1A | -2.08 | 118.34      | 123.59   |
| 36  | I     | 101 | LMG  | O2-C2-C1    | -2.08 | 105.00      | 110.05   |
| 22  | Y     | 603 | CLA  | C1-C2-C3    | -2.08 | 122.45      | 126.04   |
| 37  | F     | 101 | HEM  | C4B-CHC-C1C | 2.08  | 125.30      | 122.56   |
| 26  | C     | 522 | LHG  | C27-C26-C25 | -2.08 | 103.88      | 114.42   |
| 35  | c     | 517 | DGD  | CAB-C9B-C8B | -2.08 | 103.88      | 114.42   |
| 32  | d     | 406 | PL9  | O2-C1-C2    | -2.08 | 117.02      | 121.78   |
| 22  | b     | 602 | CLA  | C1-C2-C3    | -2.08 | 122.45      | 126.04   |
| 31  | D     | 406 | BCR  | C15-C14-C13 | -2.08 | 124.35      | 127.31   |
| 23  | g     | 616 | LUT  | C31-C32-C33 | -2.08 | 120.59      | 126.42   |
| 22  | y     | 603 | CLA  | C1-C2-C3    | -2.07 | 122.45      | 126.04   |
| 36  | c     | 523 | LMG  | O2-C2-C1    | -2.07 | 105.01      | 110.05   |
| 36  | B     | 601 | LMG  | O2-C2-C1    | -2.07 | 105.01      | 110.05   |
| 22  | A     | 409 | CLA  | O2A-CGA-O1A | -2.07 | 118.36      | 123.59   |
| 36  | C     | 502 | LMG  | C3-C4-C5    | -2.07 | 106.55      | 110.24   |
| 36  | B     | 623 | LMG  | O2-C2-C1    | -2.07 | 105.02      | 110.05   |
| 33  | d     | 402 | SQD  | O5-C1-C2    | 2.07  | 114.73      | 110.35   |
| 31  | D     | 406 | BCR  | C7-C8-C9    | -2.07 | 123.11      | 126.23   |
| 26  | N     | 618 | LHG  | C18-C17-C16 | -2.07 | 103.92      | 114.42   |
| 22  | D     | 405 | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 31  | k     | 101 | BCR  | C7-C8-C9    | -2.07 | 123.11      | 126.23   |
| 22  | a     | 408 | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 26  | Y     | 617 | LHG  | C5-O7-C7    | -2.06 | 112.71      | 117.79   |
| 32  | D     | 407 | PL9  | C32-C33-C34 | -2.06 | 122.69      | 127.66   |
| 35  | h     | 102 | DGD  | C5B-C4B-C3B | -2.06 | 103.96      | 114.42   |
| 22  | C     | 507 | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 33  | A     | 412 | SQD  | O48-C23-C24 | 2.06  | 118.38      | 111.91   |
| 35  | H     | 102 | DGD  | C5B-C4B-C3B | -2.06 | 103.96      | 114.42   |
| 22  | b     | 613 | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | C     | 523 | LMG  | O2-C2-C1    | -2.06 | 105.04      | 110.05   |
| 22  | B     | 605 | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |
| 26  | D     | 410 | LHG  | C5-O7-C7    | -2.06 | 112.73      | 117.79   |
| 33  | a     | 411 | SQD  | O48-C23-C24 | 2.06  | 118.36      | 111.91   |
| 33  | D     | 402 | SQD  | O5-C1-C2    | 2.06  | 114.70      | 110.35   |
| 22  | b     | 615 | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 22  | C     | 509 | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 22  | c     | 506 | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 25  | n     | 616 | NEX  | C38-C25-C26 | -2.05 | 118.82      | 122.26   |
| 37  | f     | 101 | HEM  | C4B-CHC-C1C | 2.05  | 125.27      | 122.56   |
| 22  | c     | 510 | CLA  | C1C-C2C-C3C | 2.05  | 109.11      | 106.96   |
| 31  | d     | 405 | BCR  | C7-C8-C9    | -2.05 | 123.13      | 126.23   |
| 23  | G     | 616 | LUT  | C31-C32-C33 | -2.05 | 120.65      | 126.42   |
| 35  | c     | 518 | DGD  | O2D-C2D-C1D | -2.05 | 105.06      | 110.05   |
| 24  | G     | 617 | XAT  | C25-C24-C23 | -2.05 | 108.69      | 112.75   |
| 31  | d     | 405 | BCR  | C15-C14-C13 | -2.05 | 124.38      | 127.31   |
| 26  | N     | 618 | LHG  | C27-C26-C25 | -2.05 | 104.02      | 114.42   |
| 22  | B     | 603 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 26  | C     | 521 | LHG  | C5-O7-C7    | -2.05 | 112.75      | 117.79   |
| 22  | B     | 610 | CLA  | C1-C2-C3    | -2.05 | 122.50      | 126.04   |
| 32  | d     | 406 | PL9  | C32-C33-C34 | -2.05 | 122.73      | 127.66   |
| 22  | b     | 607 | CLA  | C1-C2-C3    | -2.04 | 122.51      | 126.04   |
| 22  | C     | 512 | CLA  | O2D-CGD-CBD | 2.04  | 114.90      | 111.27   |
| 22  | n     | 603 | CLA  | C1-C2-C3    | -2.04 | 122.51      | 126.04   |
| 31  | b     | 617 | BCR  | C24-C23-C22 | -2.04 | 123.15      | 126.23   |
| 35  | c     | 519 | DGD  | O3E-C3E-C2E | -2.04 | 105.63      | 110.35   |
| 26  | c     | 521 | LHG  | C5-O7-C7    | -2.04 | 112.77      | 117.79   |
| 36  | w     | 102 | LMG  | C3-C4-C5    | -2.04 | 106.60      | 110.24   |
| 22  | R     | 302 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 25  | y     | 616 | NEX  | C36-C21-C22 | -2.04 | 105.44      | 108.98   |
| 33  | a     | 411 | SQD  | O5-C5-C4    | 2.04  | 113.39      | 109.69   |
| 22  | B     | 618 | CLA  | O2A-CGA-O1A | -2.04 | 118.45      | 123.59   |
| 35  | C     | 519 | DGD  | O2D-C2D-C1D | -2.04 | 105.10      | 110.05   |
| 36  | T     | 101 | LMG  | O1-C7-C8    | -2.04 | 105.99      | 110.90   |
| 22  | g     | 611 | CLA  | CHD-C1D-ND  | -2.03 | 122.58      | 124.45   |
| 33  | l     | 103 | SQD  | O5-C1-C2    | 2.03  | 114.66      | 110.35   |
| 22  | Y     | 602 | CLA  | O2A-CGA-O1A | -2.03 | 118.46      | 123.59   |
| 22  | c     | 510 | CLA  | CAC-C3C-C2C | -2.03 | 124.05      | 127.53   |
| 22  | B     | 610 | CLA  | O2A-CGA-O1A | -2.03 | 118.46      | 123.59   |
| 36  | D     | 411 | LMG  | C6-C5-C4    | -2.03 | 108.24      | 113.00   |
| 35  | H     | 102 | DGD  | C7B-C6B-C5B | -2.03 | 104.11      | 114.42   |
| 35  | a     | 413 | DGD  | C5B-C4B-C3B | -2.03 | 104.11      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | h     | 102 | DGD  | C7B-C6B-C5B | -2.03 | 104.11      | 114.42   |
| 36  | D     | 411 | LMG  | C1-C2-C3    | -2.03 | 105.77      | 110.00   |
| 36  | b     | 620 | LMG  | O7-C10-O9   | -2.03 | 118.79      | 123.70   |
| 36  | M     | 101 | LMG  | O1-C7-C8    | -2.03 | 106.00      | 110.90   |
| 36  | B     | 623 | LMG  | O7-C10-O9   | -2.03 | 118.80      | 123.70   |
| 35  | J     | 101 | DGD  | O3E-C3E-C2E | -2.03 | 105.66      | 110.35   |
| 35  | c     | 517 | DGD  | C3D-C4D-C5D | -2.03 | 106.62      | 110.24   |
| 22  | N     | 602 | CLA  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 35  | A     | 401 | DGD  | C5B-C4B-C3B | -2.02 | 104.15      | 114.42   |
| 22  | N     | 610 | CLA  | CHD-C1D-ND  | -2.02 | 122.59      | 124.45   |
| 22  | R     | 308 | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 25  | y     | 616 | NEX  | C36-C21-C26 | -2.02 | 104.58      | 110.05   |
| 22  | g     | 604 | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 22  | Y     | 611 | CLA  | CAA-CBA-CGA | -2.02 | 107.35      | 113.25   |
| 31  | B     | 620 | BCR  | C24-C23-C22 | -2.02 | 123.18      | 126.23   |
| 22  | c     | 511 | CLA  | O2D-CGD-CBD | 2.02  | 114.86      | 111.27   |
| 22  | b     | 607 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 22  | c     | 507 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 36  | d     | 410 | LMG  | C1-C2-C3    | -2.02 | 105.80      | 110.00   |
| 22  | N     | 612 | CLA  | CAA-CBA-CGA | -2.02 | 107.36      | 113.25   |
| 22  | a     | 404 | CLA  | O2A-CGA-O1A | -2.02 | 118.51      | 123.59   |
| 36  | b     | 620 | LMG  | C24-C23-C22 | -2.01 | 104.20      | 114.42   |
| 22  | y     | 602 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 22  | r     | 309 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 35  | a     | 413 | DGD  | O2D-C2D-C1D | -2.01 | 105.15      | 110.05   |
| 36  | K     | 103 | LMG  | O2-C2-C1    | -2.01 | 105.16      | 110.05   |
| 22  | G     | 602 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 22  | Y     | 604 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 22  | S     | 309 | CLA  | CHD-C1D-ND  | -2.01 | 122.60      | 124.45   |
| 26  | d     | 409 | LHG  | C5-O7-C7    | -2.01 | 112.83      | 117.79   |
| 22  | c     | 510 | CLA  | C3A-C2A-C1A | 2.01  | 104.35      | 101.34   |
| 33  | A     | 412 | SQD  | O5-C5-C4    | 2.01  | 113.35      | 109.69   |
| 22  | B     | 612 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 22  | s     | 313 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 31  | k     | 102 | BCR  | C35-C13-C14 | -2.01 | 120.11      | 122.92   |
| 22  | b     | 609 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 33  | L     | 101 | SQD  | O5-C1-C2    | 2.01  | 114.60      | 110.35   |
| 30  | d     | 401 | PHO  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 22  | n     | 604 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 36  | k     | 103 | LMG  | O2-C2-C1    | -2.01 | 105.17      | 110.05   |
| 22  | G     | 610 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 35  | C     | 518 | DGD  | C3D-C4D-C5D | -2.01 | 106.66      | 110.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | C     | 516 | BCR  | C11-C10-C9  | -2.01 | 124.45      | 127.31   |
| 31  | K     | 102 | BCR  | C35-C13-C14 | -2.01 | 120.11      | 122.92   |
| 22  | Y     | 609 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 35  | A     | 401 | DGD  | O2D-C2D-C1D | -2.00 | 105.18      | 110.05   |
| 22  | x     | 101 | CLA  | CHD-C1D-ND  | -2.00 | 122.61      | 124.45   |
| 22  | g     | 613 | CLA  | CAA-CBA-CGA | -2.00 | 107.40      | 113.25   |
| 36  | d     | 410 | LMG  | C6-C5-C4    | -2.00 | 108.31      | 113.00   |
| 22  | y     | 612 | CLA  | CAA-CBA-CGA | -2.00 | 107.40      | 113.25   |
| 37  | F     | 101 | HEM  | CAA-CBA-CGA | -2.00 | 108.14      | 113.76   |
| 22  | C     | 511 | CLA  | CAC-C3C-C2C | -2.00 | 124.11      | 127.53   |
| 36  | B     | 623 | LMG  | C24-C23-C22 | -2.00 | 104.27      | 114.42   |
| 22  | G     | 613 | CLA  | CAA-CBA-CGA | -2.00 | 107.41      | 113.25   |
| 22  | Y     | 602 | CLA  | C1-C2-C3    | -2.00 | 122.58      | 126.04   |
| 37  | f     | 101 | HEM  | CAA-CBA-CGA | -2.00 | 108.15      | 113.76   |
| 35  | C     | 518 | DGD  | O6E-C1E-O5D | -2.00 | 105.24      | 109.97   |

All (353) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | g     | 601 | CHL  | NC   |
| 21  | g     | 601 | CHL  | C8   |
| 21  | g     | 601 | CHL  | ND   |
| 21  | g     | 601 | CHL  | NA   |
| 21  | g     | 605 | CHL  | NC   |
| 21  | g     | 605 | CHL  | ND   |
| 21  | g     | 605 | CHL  | NA   |
| 21  | g     | 606 | CHL  | NC   |
| 21  | g     | 606 | CHL  | ND   |
| 21  | g     | 606 | CHL  | NA   |
| 21  | g     | 607 | CHL  | NC   |
| 21  | g     | 607 | CHL  | C8   |
| 21  | g     | 607 | CHL  | ND   |
| 21  | g     | 607 | CHL  | NA   |
| 21  | g     | 608 | CHL  | NC   |
| 21  | g     | 608 | CHL  | C8   |
| 21  | g     | 608 | CHL  | ND   |
| 21  | g     | 608 | CHL  | NA   |
| 21  | g     | 609 | CHL  | NC   |
| 21  | g     | 609 | CHL  | C8   |
| 21  | g     | 609 | CHL  | ND   |
| 21  | g     | 609 | CHL  | NA   |
| 21  | n     | 601 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | n     | 601 | CHL  | C8   |
| 21  | n     | 601 | CHL  | ND   |
| 21  | n     | 601 | CHL  | NA   |
| 21  | n     | 605 | CHL  | NC   |
| 21  | n     | 605 | CHL  | ND   |
| 21  | n     | 605 | CHL  | NA   |
| 21  | n     | 606 | CHL  | NC   |
| 21  | n     | 606 | CHL  | C8   |
| 21  | n     | 606 | CHL  | ND   |
| 21  | n     | 606 | CHL  | NA   |
| 21  | n     | 607 | CHL  | NC   |
| 21  | n     | 607 | CHL  | C8   |
| 21  | n     | 607 | CHL  | ND   |
| 21  | n     | 607 | CHL  | NA   |
| 21  | n     | 608 | CHL  | NC   |
| 21  | n     | 608 | CHL  | C8   |
| 21  | n     | 608 | CHL  | ND   |
| 21  | n     | 608 | CHL  | NA   |
| 21  | y     | 601 | CHL  | NC   |
| 21  | y     | 601 | CHL  | C8   |
| 21  | y     | 601 | CHL  | ND   |
| 21  | y     | 601 | CHL  | NA   |
| 21  | y     | 605 | CHL  | NC   |
| 21  | y     | 605 | CHL  | ND   |
| 21  | y     | 605 | CHL  | NA   |
| 21  | y     | 606 | CHL  | NC   |
| 21  | y     | 606 | CHL  | ND   |
| 21  | y     | 606 | CHL  | NA   |
| 21  | y     | 607 | CHL  | NC   |
| 21  | y     | 607 | CHL  | C8   |
| 21  | y     | 607 | CHL  | ND   |
| 21  | y     | 607 | CHL  | NA   |
| 21  | y     | 608 | CHL  | NC   |
| 21  | y     | 608 | CHL  | C8   |
| 21  | y     | 608 | CHL  | ND   |
| 21  | y     | 608 | CHL  | NA   |
| 21  | y     | 609 | CHL  | NC   |
| 21  | y     | 609 | CHL  | C8   |
| 21  | y     | 609 | CHL  | ND   |
| 21  | y     | 609 | CHL  | NA   |
| 21  | G     | 601 | CHL  | NC   |
| 21  | G     | 601 | CHL  | C8   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | G     | 601 | CHL  | ND   |
| 21  | G     | 601 | CHL  | NA   |
| 21  | G     | 605 | CHL  | NC   |
| 21  | G     | 605 | CHL  | ND   |
| 21  | G     | 605 | CHL  | NA   |
| 21  | G     | 606 | CHL  | NC   |
| 21  | G     | 606 | CHL  | ND   |
| 21  | G     | 606 | CHL  | NA   |
| 21  | G     | 607 | CHL  | NC   |
| 21  | G     | 607 | CHL  | C8   |
| 21  | G     | 607 | CHL  | ND   |
| 21  | G     | 607 | CHL  | NA   |
| 21  | G     | 608 | CHL  | NC   |
| 21  | G     | 608 | CHL  | C8   |
| 21  | G     | 608 | CHL  | ND   |
| 21  | G     | 608 | CHL  | NA   |
| 21  | G     | 609 | CHL  | NC   |
| 21  | G     | 609 | CHL  | C8   |
| 21  | G     | 609 | CHL  | ND   |
| 21  | G     | 609 | CHL  | NA   |
| 21  | N     | 601 | CHL  | NC   |
| 21  | N     | 601 | CHL  | C8   |
| 21  | N     | 601 | CHL  | ND   |
| 21  | N     | 601 | CHL  | NA   |
| 21  | N     | 605 | CHL  | NC   |
| 21  | N     | 605 | CHL  | ND   |
| 21  | N     | 605 | CHL  | NA   |
| 21  | N     | 606 | CHL  | NC   |
| 21  | N     | 606 | CHL  | C8   |
| 21  | N     | 606 | CHL  | ND   |
| 21  | N     | 606 | CHL  | NA   |
| 21  | N     | 607 | CHL  | NC   |
| 21  | N     | 607 | CHL  | C8   |
| 21  | N     | 607 | CHL  | ND   |
| 21  | N     | 607 | CHL  | NA   |
| 21  | N     | 608 | CHL  | NC   |
| 21  | N     | 608 | CHL  | C8   |
| 21  | N     | 608 | CHL  | ND   |
| 21  | N     | 608 | CHL  | NA   |
| 21  | Y     | 601 | CHL  | NC   |
| 21  | Y     | 601 | CHL  | C8   |
| 21  | Y     | 601 | CHL  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | Y     | 601 | CHL  | NA   |
| 21  | Y     | 605 | CHL  | NC   |
| 21  | Y     | 605 | CHL  | ND   |
| 21  | Y     | 605 | CHL  | NA   |
| 21  | Y     | 606 | CHL  | NC   |
| 21  | Y     | 606 | CHL  | C8   |
| 21  | Y     | 606 | CHL  | ND   |
| 21  | Y     | 606 | CHL  | NA   |
| 21  | Y     | 607 | CHL  | NC   |
| 21  | Y     | 607 | CHL  | C8   |
| 21  | Y     | 607 | CHL  | ND   |
| 21  | Y     | 607 | CHL  | NA   |
| 21  | Y     | 608 | CHL  | NC   |
| 21  | Y     | 608 | CHL  | C8   |
| 21  | Y     | 608 | CHL  | ND   |
| 21  | Y     | 608 | CHL  | NA   |
| 21  | r     | 301 | CHL  | NC   |
| 21  | r     | 301 | CHL  | ND   |
| 21  | r     | 301 | CHL  | NA   |
| 21  | r     | 306 | CHL  | NC   |
| 21  | r     | 306 | CHL  | C8   |
| 21  | r     | 306 | CHL  | ND   |
| 21  | r     | 306 | CHL  | NA   |
| 21  | r     | 307 | CHL  | NC   |
| 21  | r     | 307 | CHL  | C8   |
| 21  | r     | 307 | CHL  | ND   |
| 21  | r     | 307 | CHL  | NA   |
| 21  | r     | 308 | CHL  | NC   |
| 21  | r     | 308 | CHL  | C8   |
| 21  | r     | 308 | CHL  | ND   |
| 21  | r     | 308 | CHL  | NA   |
| 21  | s     | 301 | CHL  | NC   |
| 21  | s     | 301 | CHL  | ND   |
| 21  | s     | 301 | CHL  | NA   |
| 21  | s     | 302 | CHL  | NC   |
| 21  | s     | 302 | CHL  | ND   |
| 21  | s     | 302 | CHL  | NA   |
| 21  | s     | 306 | CHL  | NC   |
| 21  | s     | 306 | CHL  | ND   |
| 21  | s     | 306 | CHL  | NA   |
| 21  | s     | 307 | CHL  | NC   |
| 21  | s     | 307 | CHL  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | s     | 307 | CHL  | NA   |
| 21  | S     | 301 | CHL  | NC   |
| 21  | S     | 301 | CHL  | ND   |
| 21  | S     | 301 | CHL  | NA   |
| 21  | S     | 302 | CHL  | NC   |
| 21  | S     | 302 | CHL  | ND   |
| 21  | S     | 302 | CHL  | NA   |
| 21  | S     | 306 | CHL  | NC   |
| 21  | S     | 306 | CHL  | ND   |
| 21  | S     | 306 | CHL  | NA   |
| 21  | S     | 307 | CHL  | NC   |
| 21  | S     | 307 | CHL  | ND   |
| 21  | S     | 307 | CHL  | NA   |
| 21  | R     | 305 | CHL  | NC   |
| 21  | R     | 305 | CHL  | C8   |
| 21  | R     | 305 | CHL  | ND   |
| 21  | R     | 305 | CHL  | NA   |
| 21  | R     | 306 | CHL  | NC   |
| 21  | R     | 306 | CHL  | C8   |
| 21  | R     | 306 | CHL  | ND   |
| 21  | R     | 306 | CHL  | NA   |
| 21  | R     | 307 | CHL  | NC   |
| 21  | R     | 307 | CHL  | C8   |
| 21  | R     | 307 | CHL  | ND   |
| 21  | R     | 307 | CHL  | NA   |
| 22  | g     | 602 | CLA  | ND   |
| 22  | g     | 603 | CLA  | ND   |
| 22  | g     | 604 | CLA  | ND   |
| 22  | g     | 610 | CLA  | ND   |
| 22  | g     | 611 | CLA  | ND   |
| 22  | g     | 612 | CLA  | ND   |
| 22  | g     | 613 | CLA  | ND   |
| 22  | g     | 614 | CLA  | ND   |
| 22  | n     | 602 | CLA  | ND   |
| 22  | n     | 603 | CLA  | ND   |
| 22  | n     | 604 | CLA  | ND   |
| 22  | n     | 609 | CLA  | ND   |
| 22  | n     | 610 | CLA  | ND   |
| 22  | n     | 611 | CLA  | ND   |
| 22  | n     | 612 | CLA  | ND   |
| 22  | n     | 613 | CLA  | ND   |
| 22  | y     | 602 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | y     | 603 | CLA  | ND   |
| 22  | y     | 604 | CLA  | ND   |
| 22  | y     | 610 | CLA  | ND   |
| 22  | y     | 611 | CLA  | ND   |
| 22  | y     | 612 | CLA  | ND   |
| 22  | y     | 613 | CLA  | ND   |
| 22  | G     | 602 | CLA  | ND   |
| 22  | G     | 603 | CLA  | ND   |
| 22  | G     | 604 | CLA  | ND   |
| 22  | G     | 610 | CLA  | ND   |
| 22  | G     | 611 | CLA  | ND   |
| 22  | G     | 612 | CLA  | ND   |
| 22  | G     | 613 | CLA  | ND   |
| 22  | G     | 614 | CLA  | ND   |
| 22  | N     | 602 | CLA  | ND   |
| 22  | N     | 603 | CLA  | ND   |
| 22  | N     | 604 | CLA  | ND   |
| 22  | N     | 609 | CLA  | ND   |
| 22  | N     | 610 | CLA  | ND   |
| 22  | N     | 611 | CLA  | ND   |
| 22  | N     | 612 | CLA  | ND   |
| 22  | N     | 613 | CLA  | ND   |
| 22  | Y     | 602 | CLA  | ND   |
| 22  | Y     | 603 | CLA  | ND   |
| 22  | Y     | 604 | CLA  | ND   |
| 22  | Y     | 609 | CLA  | ND   |
| 22  | Y     | 610 | CLA  | ND   |
| 22  | Y     | 611 | CLA  | ND   |
| 22  | Y     | 612 | CLA  | ND   |
| 22  | a     | 404 | CLA  | ND   |
| 22  | a     | 405 | CLA  | ND   |
| 22  | a     | 406 | CLA  | ND   |
| 22  | a     | 408 | CLA  | ND   |
| 22  | b     | 601 | CLA  | ND   |
| 22  | b     | 602 | CLA  | ND   |
| 22  | b     | 603 | CLA  | ND   |
| 22  | b     | 604 | CLA  | ND   |
| 22  | b     | 605 | CLA  | ND   |
| 22  | b     | 606 | CLA  | ND   |
| 22  | b     | 607 | CLA  | ND   |
| 22  | b     | 608 | CLA  | ND   |
| 22  | b     | 609 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | b     | 610 | CLA  | ND   |
| 22  | b     | 611 | CLA  | ND   |
| 22  | b     | 612 | CLA  | ND   |
| 22  | b     | 613 | CLA  | ND   |
| 22  | b     | 614 | CLA  | ND   |
| 22  | b     | 615 | CLA  | ND   |
| 22  | c     | 502 | CLA  | ND   |
| 22  | c     | 503 | CLA  | ND   |
| 22  | c     | 504 | CLA  | ND   |
| 22  | c     | 505 | CLA  | ND   |
| 22  | c     | 506 | CLA  | ND   |
| 22  | c     | 507 | CLA  | ND   |
| 22  | c     | 508 | CLA  | ND   |
| 22  | c     | 509 | CLA  | ND   |
| 22  | c     | 510 | CLA  | ND   |
| 22  | c     | 511 | CLA  | ND   |
| 22  | c     | 512 | CLA  | ND   |
| 22  | c     | 513 | CLA  | ND   |
| 22  | c     | 514 | CLA  | ND   |
| 22  | d     | 403 | CLA  | ND   |
| 22  | d     | 404 | CLA  | ND   |
| 22  | w     | 101 | CLA  | ND   |
| 22  | x     | 101 | CLA  | ND   |
| 22  | A     | 405 | CLA  | ND   |
| 22  | A     | 406 | CLA  | ND   |
| 22  | A     | 407 | CLA  | ND   |
| 22  | A     | 409 | CLA  | ND   |
| 22  | B     | 603 | CLA  | ND   |
| 22  | B     | 604 | CLA  | ND   |
| 22  | B     | 605 | CLA  | ND   |
| 22  | B     | 606 | CLA  | ND   |
| 22  | B     | 607 | CLA  | ND   |
| 22  | B     | 608 | CLA  | ND   |
| 22  | B     | 609 | CLA  | ND   |
| 22  | B     | 610 | CLA  | ND   |
| 22  | B     | 611 | CLA  | ND   |
| 22  | B     | 612 | CLA  | ND   |
| 22  | B     | 613 | CLA  | ND   |
| 22  | B     | 614 | CLA  | ND   |
| 22  | B     | 615 | CLA  | ND   |
| 22  | B     | 616 | CLA  | ND   |
| 22  | B     | 617 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | B     | 618 | CLA  | ND   |
| 22  | C     | 503 | CLA  | ND   |
| 22  | C     | 504 | CLA  | ND   |
| 22  | C     | 505 | CLA  | ND   |
| 22  | C     | 506 | CLA  | ND   |
| 22  | C     | 507 | CLA  | ND   |
| 22  | C     | 508 | CLA  | ND   |
| 22  | C     | 509 | CLA  | ND   |
| 22  | C     | 510 | CLA  | ND   |
| 22  | C     | 511 | CLA  | ND   |
| 22  | C     | 512 | CLA  | ND   |
| 22  | C     | 513 | CLA  | ND   |
| 22  | C     | 514 | CLA  | ND   |
| 22  | C     | 515 | CLA  | ND   |
| 22  | D     | 404 | CLA  | ND   |
| 22  | D     | 405 | CLA  | ND   |
| 22  | W     | 101 | CLA  | ND   |
| 22  | r     | 303 | CLA  | ND   |
| 22  | r     | 304 | CLA  | ND   |
| 22  | r     | 305 | CLA  | ND   |
| 22  | r     | 309 | CLA  | ND   |
| 22  | r     | 310 | CLA  | ND   |
| 22  | r     | 311 | CLA  | ND   |
| 22  | r     | 312 | CLA  | ND   |
| 22  | s     | 303 | CLA  | ND   |
| 22  | s     | 304 | CLA  | ND   |
| 22  | s     | 305 | CLA  | ND   |
| 22  | s     | 309 | CLA  | ND   |
| 22  | s     | 310 | CLA  | ND   |
| 22  | s     | 311 | CLA  | ND   |
| 22  | s     | 312 | CLA  | ND   |
| 22  | s     | 313 | CLA  | ND   |
| 22  | S     | 303 | CLA  | ND   |
| 22  | S     | 304 | CLA  | ND   |
| 22  | S     | 305 | CLA  | ND   |
| 22  | S     | 309 | CLA  | ND   |
| 22  | S     | 310 | CLA  | ND   |
| 22  | S     | 311 | CLA  | ND   |
| 22  | S     | 312 | CLA  | ND   |
| 22  | S     | 313 | CLA  | ND   |
| 22  | R     | 302 | CLA  | ND   |
| 22  | R     | 303 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | R     | 304 | CLA  | ND   |
| 22  | R     | 308 | CLA  | ND   |
| 22  | R     | 309 | CLA  | ND   |
| 22  | R     | 310 | CLA  | ND   |
| 22  | R     | 311 | CLA  | ND   |
| 24  | g     | 617 | XAT  | C6   |
| 24  | g     | 617 | XAT  | C25  |
| 24  | n     | 615 | XAT  | C6   |
| 24  | n     | 615 | XAT  | C25  |
| 24  | y     | 615 | XAT  | C6   |
| 24  | y     | 615 | XAT  | C25  |
| 24  | G     | 617 | XAT  | C26  |
| 24  | G     | 617 | XAT  | C6   |
| 24  | G     | 617 | XAT  | C25  |
| 24  | N     | 616 | XAT  | C6   |
| 24  | N     | 616 | XAT  | C25  |
| 24  | Y     | 615 | XAT  | C6   |
| 24  | Y     | 615 | XAT  | C25  |
| 24  | r     | 314 | XAT  | C25  |
| 24  | R     | 313 | XAT  | C25  |
| 25  | g     | 618 | NEX  | C26  |
| 25  | g     | 618 | NEX  | C25  |
| 25  | n     | 616 | NEX  | C26  |
| 25  | n     | 616 | NEX  | C25  |
| 25  | y     | 616 | NEX  | C26  |
| 25  | y     | 616 | NEX  | C25  |
| 25  | y     | 618 | NEX  | C26  |
| 25  | y     | 618 | NEX  | C25  |
| 25  | N     | 617 | NEX  | C26  |
| 25  | N     | 617 | NEX  | C25  |
| 25  | Y     | 616 | NEX  | C26  |
| 25  | Y     | 616 | NEX  | C25  |
| 25  | r     | 315 | NEX  | C26  |
| 25  | r     | 315 | NEX  | C25  |
| 33  | d     | 402 | SQD  | C5   |
| 33  | D     | 402 | SQD  | C5   |

All (4559) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | g     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | g     | 601 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | g     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | g     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | g     | 605 | CHL  | O1D-CGD-O2D-CED |
| 21  | g     | 606 | CHL  | C2-C1-O2A-CGA   |
| 21  | g     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | g     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 21  | g     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 21  | g     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 21  | g     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | O1D-CGD-O2D-CED |
| 21  | g     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 608 | CHL  | C2-C3-C5-C6     |
| 21  | g     | 608 | CHL  | C4-C3-C5-C6     |
| 21  | g     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 21  | g     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 21  | n     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | n     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | n     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | n     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | n     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | n     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | n     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 21  | n     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 21  | n     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | n     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | n     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | n     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | n     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | n     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | n     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | n     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | y     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | y     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | y     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | y     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 21  | y     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 21  | y     | 605 | CHL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | y     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | y     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | y     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | y     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | y     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | y     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | y     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 21  | y     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 21  | y     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 21  | y     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | y     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | y     | 607 | CHL  | O1D-CGD-O2D-CED |
| 21  | y     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 21  | y     | 608 | CHL  | C2-C3-C5-C6     |
| 21  | y     | 608 | CHL  | C4-C3-C5-C6     |
| 21  | y     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 21  | y     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 21  | G     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | G     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | G     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | G     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | G     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | G     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | G     | 605 | CHL  | O1D-CGD-O2D-CED |
| 21  | G     | 606 | CHL  | C2-C1-O2A-CGA   |
| 21  | G     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | G     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | G     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | G     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 21  | G     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 21  | G     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 21  | G     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | G     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | G     | 607 | CHL  | O1D-CGD-O2D-CED |
| 21  | G     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 21  | G     | 608 | CHL  | C2-C3-C5-C6     |
| 21  | G     | 608 | CHL  | C4-C3-C5-C6     |
| 21  | G     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 21  | G     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 21  | N     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | N     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | N     | 601 | CHL  | C3C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | N     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | N     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | N     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | N     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 21  | N     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 21  | N     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | N     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | N     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | N     | 606 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | N     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | N     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | N     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | N     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | Y     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 21  | Y     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | Y     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | Y     | 605 | CHL  | C2-C1-O2A-CGA   |
| 21  | Y     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | Y     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 21  | Y     | 605 | CHL  | CBD-CGD-O2D-CED |
| 21  | Y     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 21  | Y     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 21  | Y     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 21  | Y     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 21  | Y     | 606 | CHL  | CBD-CGD-O2D-CED |
| 21  | Y     | 606 | CHL  | O1D-CGD-O2D-CED |
| 21  | Y     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 21  | Y     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | Y     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | Y     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | Y     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | r     | 301 | CHL  | C1A-C2A-CAA-CBA |
| 21  | r     | 301 | CHL  | C1C-C2C-CMC-OMC |
| 21  | r     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 21  | r     | 301 | CHL  | CBD-CGD-O2D-CED |
| 21  | r     | 306 | CHL  | CBD-CGD-O2D-CED |
| 21  | r     | 306 | CHL  | O1D-CGD-O2D-CED |
| 21  | r     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 21  | r     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 21  | r     | 307 | CHL  | CBD-CGD-O2D-CED |
| 21  | r     | 307 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | r     | 307 | CHL  | O2A-C1-C2-C3    |
| 21  | r     | 308 | CHL  | C1C-C2C-CMC-OMC |
| 21  | r     | 308 | CHL  | C3C-C2C-CMC-OMC |
| 21  | r     | 308 | CHL  | CBD-CGD-O2D-CED |
| 21  | r     | 308 | CHL  | O1D-CGD-O2D-CED |
| 21  | s     | 301 | CHL  | C1A-C2A-CAA-CBA |
| 21  | s     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 21  | s     | 301 | CHL  | C1C-C2C-CMC-OMC |
| 21  | s     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 21  | s     | 301 | CHL  | CBD-CGD-O2D-CED |
| 21  | s     | 301 | CHL  | O1D-CGD-O2D-CED |
| 21  | s     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 21  | s     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 21  | s     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 21  | s     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 21  | s     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 21  | S     | 301 | CHL  | C1A-C2A-CAA-CBA |
| 21  | S     | 301 | CHL  | C1C-C2C-CMC-OMC |
| 21  | S     | 301 | CHL  | C3C-C2C-CMC-OMC |
| 21  | S     | 301 | CHL  | CBD-CGD-O2D-CED |
| 21  | S     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 21  | S     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 21  | S     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 21  | S     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 21  | S     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 21  | R     | 305 | CHL  | CBD-CGD-O2D-CED |
| 21  | R     | 305 | CHL  | O1D-CGD-O2D-CED |
| 21  | R     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 21  | R     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 21  | R     | 306 | CHL  | CBD-CGD-O2D-CED |
| 21  | R     | 306 | CHL  | O1D-CGD-O2D-CED |
| 21  | R     | 306 | CHL  | O2A-C1-C2-C3    |
| 21  | R     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 21  | R     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 21  | R     | 307 | CHL  | CBD-CGD-O2D-CED |
| 21  | R     | 307 | CHL  | O1D-CGD-O2D-CED |
| 22  | g     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | g     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | g     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 22  | g     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | g     | 613 | CLA  | CHA-CBD-CGD-O1D |
| 22  | g     | 614 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | g     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 22  | n     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | n     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | n     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 22  | n     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | n     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 22  | n     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | n     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | y     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | y     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | y     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 22  | y     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | y     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 22  | y     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | y     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | G     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 22  | G     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | G     | 613 | CLA  | CHA-CBD-CGD-O1D |
| 22  | G     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 22  | G     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 22  | N     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | N     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | N     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 22  | N     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | N     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 22  | N     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | N     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Y     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Y     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Y     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Y     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Y     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 22  | Y     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Y     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 406 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 406 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 406 | CLA  | CHA-CBD-CGD-O1D |
| 22  | a     | 406 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 601 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 609 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 503 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 503 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 503 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 504 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 504 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 505 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 507 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 507 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 509 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 509 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 510 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 510 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 513 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 513 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 513 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 513 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 514 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 514 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 514 | CLA  | CAD-CBD-CGD-O2D |
| 22  | d     | 404 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 404 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 407 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 407 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 407 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 407 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 606 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 612 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 612 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 504 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 504 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 504 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 504 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 505 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 505 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 505 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 506 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 508 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 508 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 509 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 509 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 510 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 510 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 511 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 511 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 513 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 514 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 514 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 514 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 514 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 515 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 515 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 515 | CLA  | CAD-CBD-CGD-O2D |
| 22  | D     | 405 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 405 | CLA  | C4-C3-C5-C6     |
| 22  | r     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 22  | r     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | r     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 22  | r     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | r     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 22  | r     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | r     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | r     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 22  | s     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 22  | s     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 22  | s     | 305 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 22  | s     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 22  | s     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 22  | s     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 22  | s     | 310 | CLA  | CAD-CBD-CGD-O1D |
| 22  | s     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 312 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 22  | S     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 22  | S     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 22  | S     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 22  | S     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 22  | S     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 22  | S     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 22  | S     | 310 | CLA  | CAD-CBD-CGD-O1D |
| 22  | S     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 312 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 22  | R     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | R     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | R     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | R     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 22  | R     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | R     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 22  | R     | 310 | CLA  | CBD-CGD-O2D-CED |
| 23  | g     | 615 | LUT  | C11-C10-C9-C8   |
| 23  | g     | 615 | LUT  | C11-C10-C9-C19  |
| 23  | g     | 615 | LUT  | C11-C12-C13-C20 |
| 23  | g     | 615 | LUT  | C12-C13-C14-C15 |
| 23  | g     | 615 | LUT  | C20-C13-C14-C15 |
| 23  | g     | 615 | LUT  | C27-C28-C29-C39 |
| 23  | g     | 615 | LUT  | C39-C29-C30-C31 |
| 23  | g     | 615 | LUT  | C31-C32-C33-C40 |
| 23  | g     | 615 | LUT  | C32-C33-C34-C35 |
| 23  | g     | 615 | LUT  | C40-C33-C34-C35 |
| 23  | g     | 616 | LUT  | C5-C6-C7-C8     |
| 23  | g     | 616 | LUT  | C7-C8-C9-C19    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | g     | 616 | LUT  | C11-C10-C9-C8   |
| 23  | g     | 616 | LUT  | C11-C12-C13-C14 |
| 23  | g     | 616 | LUT  | C20-C13-C14-C15 |
| 23  | g     | 616 | LUT  | C39-C29-C30-C31 |
| 23  | g     | 616 | LUT  | C31-C32-C33-C34 |
| 23  | g     | 616 | LUT  | C31-C32-C33-C40 |
| 23  | g     | 616 | LUT  | C32-C33-C34-C35 |
| 23  | g     | 616 | LUT  | C40-C33-C34-C35 |
| 23  | n     | 614 | LUT  | C11-C10-C9-C8   |
| 23  | n     | 614 | LUT  | C11-C10-C9-C19  |
| 23  | n     | 614 | LUT  | C11-C12-C13-C20 |
| 23  | n     | 614 | LUT  | C12-C13-C14-C15 |
| 23  | n     | 614 | LUT  | C20-C13-C14-C15 |
| 23  | n     | 614 | LUT  | C27-C28-C29-C39 |
| 23  | n     | 614 | LUT  | C39-C29-C30-C31 |
| 23  | n     | 614 | LUT  | C31-C32-C33-C40 |
| 23  | n     | 614 | LUT  | C32-C33-C34-C35 |
| 23  | n     | 614 | LUT  | C40-C33-C34-C35 |
| 23  | y     | 614 | LUT  | C11-C10-C9-C8   |
| 23  | y     | 614 | LUT  | C11-C10-C9-C19  |
| 23  | y     | 614 | LUT  | C11-C12-C13-C20 |
| 23  | y     | 614 | LUT  | C12-C13-C14-C15 |
| 23  | y     | 614 | LUT  | C20-C13-C14-C15 |
| 23  | y     | 614 | LUT  | C27-C28-C29-C39 |
| 23  | y     | 614 | LUT  | C39-C29-C30-C31 |
| 23  | y     | 614 | LUT  | C31-C32-C33-C40 |
| 23  | y     | 614 | LUT  | C32-C33-C34-C35 |
| 23  | y     | 614 | LUT  | C40-C33-C34-C35 |
| 23  | G     | 615 | LUT  | C11-C10-C9-C8   |
| 23  | G     | 615 | LUT  | C11-C10-C9-C19  |
| 23  | G     | 615 | LUT  | C11-C12-C13-C20 |
| 23  | G     | 615 | LUT  | C12-C13-C14-C15 |
| 23  | G     | 615 | LUT  | C20-C13-C14-C15 |
| 23  | G     | 615 | LUT  | C27-C28-C29-C39 |
| 23  | G     | 615 | LUT  | C39-C29-C30-C31 |
| 23  | G     | 615 | LUT  | C31-C32-C33-C40 |
| 23  | G     | 615 | LUT  | C32-C33-C34-C35 |
| 23  | G     | 615 | LUT  | C40-C33-C34-C35 |
| 23  | G     | 616 | LUT  | C5-C6-C7-C8     |
| 23  | G     | 616 | LUT  | C7-C8-C9-C19    |
| 23  | G     | 616 | LUT  | C11-C10-C9-C8   |
| 23  | G     | 616 | LUT  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | G     | 616 | LUT  | C20-C13-C14-C15 |
| 23  | G     | 616 | LUT  | C39-C29-C30-C31 |
| 23  | G     | 616 | LUT  | C31-C32-C33-C34 |
| 23  | G     | 616 | LUT  | C32-C33-C34-C35 |
| 23  | G     | 616 | LUT  | C40-C33-C34-C35 |
| 23  | N     | 614 | LUT  | C11-C10-C9-C8   |
| 23  | N     | 614 | LUT  | C11-C10-C9-C19  |
| 23  | N     | 614 | LUT  | C11-C12-C13-C20 |
| 23  | N     | 614 | LUT  | C12-C13-C14-C15 |
| 23  | N     | 614 | LUT  | C20-C13-C14-C15 |
| 23  | N     | 614 | LUT  | C27-C28-C29-C39 |
| 23  | N     | 614 | LUT  | C39-C29-C30-C31 |
| 23  | N     | 614 | LUT  | C31-C32-C33-C40 |
| 23  | N     | 614 | LUT  | C32-C33-C34-C35 |
| 23  | N     | 614 | LUT  | C40-C33-C34-C35 |
| 23  | N     | 615 | LUT  | C11-C12-C13-C14 |
| 23  | N     | 615 | LUT  | C11-C12-C13-C20 |
| 23  | N     | 615 | LUT  | C20-C13-C14-C15 |
| 23  | N     | 615 | LUT  | C27-C28-C29-C39 |
| 23  | N     | 615 | LUT  | C39-C29-C30-C31 |
| 23  | N     | 615 | LUT  | C31-C32-C33-C40 |
| 23  | N     | 615 | LUT  | C40-C33-C34-C35 |
| 23  | Y     | 613 | LUT  | C11-C10-C9-C8   |
| 23  | Y     | 613 | LUT  | C11-C10-C9-C19  |
| 23  | Y     | 613 | LUT  | C11-C12-C13-C20 |
| 23  | Y     | 613 | LUT  | C12-C13-C14-C15 |
| 23  | Y     | 613 | LUT  | C20-C13-C14-C15 |
| 23  | Y     | 613 | LUT  | C27-C28-C29-C39 |
| 23  | Y     | 613 | LUT  | C39-C29-C30-C31 |
| 23  | Y     | 613 | LUT  | C31-C32-C33-C40 |
| 23  | Y     | 613 | LUT  | C32-C33-C34-C35 |
| 23  | Y     | 613 | LUT  | C40-C33-C34-C35 |
| 23  | Y     | 614 | LUT  | C5-C6-C7-C8     |
| 23  | Y     | 614 | LUT  | C7-C8-C9-C19    |
| 23  | Y     | 614 | LUT  | C11-C10-C9-C8   |
| 23  | Y     | 614 | LUT  | C11-C12-C13-C14 |
| 23  | Y     | 614 | LUT  | C11-C12-C13-C20 |
| 23  | Y     | 614 | LUT  | C20-C13-C14-C15 |
| 23  | Y     | 614 | LUT  | C39-C29-C30-C31 |
| 23  | Y     | 614 | LUT  | C31-C32-C33-C34 |
| 23  | Y     | 614 | LUT  | C32-C33-C34-C35 |
| 23  | Y     | 614 | LUT  | C40-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | r     | 313 | LUT  | C5-C6-C7-C8     |
| 23  | r     | 313 | LUT  | C7-C8-C9-C19    |
| 23  | r     | 313 | LUT  | C11-C10-C9-C8   |
| 23  | r     | 313 | LUT  | C11-C10-C9-C19  |
| 23  | r     | 313 | LUT  | C11-C12-C13-C14 |
| 23  | r     | 313 | LUT  | C20-C13-C14-C15 |
| 23  | r     | 313 | LUT  | C28-C29-C30-C31 |
| 23  | r     | 313 | LUT  | C32-C33-C34-C35 |
| 23  | r     | 313 | LUT  | C40-C33-C34-C35 |
| 23  | R     | 312 | LUT  | C5-C6-C7-C8     |
| 23  | R     | 312 | LUT  | C7-C8-C9-C19    |
| 23  | R     | 312 | LUT  | C11-C10-C9-C8   |
| 23  | R     | 312 | LUT  | C11-C10-C9-C19  |
| 23  | R     | 312 | LUT  | C11-C12-C13-C14 |
| 23  | R     | 312 | LUT  | C20-C13-C14-C15 |
| 23  | R     | 312 | LUT  | C28-C29-C30-C31 |
| 23  | R     | 312 | LUT  | C32-C33-C34-C35 |
| 23  | R     | 312 | LUT  | C40-C33-C34-C35 |
| 24  | g     | 617 | XAT  | C7-C8-C9-C19    |
| 24  | g     | 617 | XAT  | C11-C10-C9-C19  |
| 24  | g     | 617 | XAT  | C27-C28-C29-C30 |
| 24  | g     | 617 | XAT  | C27-C28-C29-C39 |
| 24  | g     | 617 | XAT  | C28-C29-C30-C31 |
| 24  | g     | 617 | XAT  | C39-C29-C30-C31 |
| 24  | g     | 617 | XAT  | C31-C32-C33-C40 |
| 24  | n     | 615 | XAT  | C7-C8-C9-C19    |
| 24  | n     | 615 | XAT  | C11-C10-C9-C19  |
| 24  | n     | 615 | XAT  | C11-C12-C13-C14 |
| 24  | n     | 615 | XAT  | C11-C12-C13-C20 |
| 24  | n     | 615 | XAT  | C20-C13-C14-C15 |
| 24  | n     | 615 | XAT  | C27-C28-C29-C30 |
| 24  | n     | 615 | XAT  | C27-C28-C29-C39 |
| 24  | n     | 615 | XAT  | C28-C29-C30-C31 |
| 24  | n     | 615 | XAT  | C39-C29-C30-C31 |
| 24  | n     | 615 | XAT  | C40-C33-C34-C35 |
| 24  | y     | 615 | XAT  | C11-C10-C9-C19  |
| 24  | y     | 615 | XAT  | C11-C12-C13-C20 |
| 24  | y     | 615 | XAT  | C20-C13-C14-C15 |
| 24  | y     | 615 | XAT  | C27-C28-C29-C30 |
| 24  | y     | 615 | XAT  | C27-C28-C29-C39 |
| 24  | y     | 615 | XAT  | C28-C29-C30-C31 |
| 24  | y     | 615 | XAT  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | y     | 615 | XAT  | C32-C33-C34-C35 |
| 24  | G     | 617 | XAT  | C7-C8-C9-C19    |
| 24  | G     | 617 | XAT  | C11-C10-C9-C19  |
| 24  | G     | 617 | XAT  | C20-C13-C14-C15 |
| 24  | G     | 617 | XAT  | C27-C28-C29-C30 |
| 24  | G     | 617 | XAT  | C27-C28-C29-C39 |
| 24  | G     | 617 | XAT  | C28-C29-C30-C31 |
| 24  | G     | 617 | XAT  | C39-C29-C30-C31 |
| 24  | G     | 617 | XAT  | C32-C33-C34-C35 |
| 24  | N     | 616 | XAT  | C7-C8-C9-C19    |
| 24  | N     | 616 | XAT  | C11-C10-C9-C19  |
| 24  | N     | 616 | XAT  | C11-C12-C13-C14 |
| 24  | N     | 616 | XAT  | C11-C12-C13-C20 |
| 24  | N     | 616 | XAT  | C20-C13-C14-C15 |
| 24  | N     | 616 | XAT  | C27-C28-C29-C30 |
| 24  | N     | 616 | XAT  | C27-C28-C29-C39 |
| 24  | N     | 616 | XAT  | C28-C29-C30-C31 |
| 24  | N     | 616 | XAT  | C39-C29-C30-C31 |
| 24  | N     | 616 | XAT  | C40-C33-C34-C35 |
| 24  | Y     | 615 | XAT  | C11-C10-C9-C19  |
| 24  | Y     | 615 | XAT  | C11-C12-C13-C14 |
| 24  | Y     | 615 | XAT  | C11-C12-C13-C20 |
| 24  | Y     | 615 | XAT  | C27-C28-C29-C30 |
| 24  | Y     | 615 | XAT  | C27-C28-C29-C39 |
| 24  | Y     | 615 | XAT  | C28-C29-C30-C31 |
| 24  | Y     | 615 | XAT  | C39-C29-C30-C31 |
| 24  | Y     | 615 | XAT  | C32-C33-C34-C35 |
| 24  | r     | 314 | XAT  | C7-C8-C9-C10    |
| 24  | r     | 314 | XAT  | C7-C8-C9-C19    |
| 24  | r     | 314 | XAT  | C11-C10-C9-C8   |
| 24  | r     | 314 | XAT  | C12-C13-C14-C15 |
| 24  | r     | 314 | XAT  | C20-C13-C14-C15 |
| 24  | r     | 314 | XAT  | C40-C33-C34-C35 |
| 24  | R     | 313 | XAT  | C7-C8-C9-C10    |
| 24  | R     | 313 | XAT  | C7-C8-C9-C19    |
| 24  | R     | 313 | XAT  | C11-C10-C9-C8   |
| 24  | R     | 313 | XAT  | C12-C13-C14-C15 |
| 24  | R     | 313 | XAT  | C20-C13-C14-C15 |
| 24  | R     | 313 | XAT  | C40-C33-C34-C35 |
| 25  | g     | 618 | NEX  | C7-C8-C9-C10    |
| 25  | g     | 618 | NEX  | C11-C10-C9-C8   |
| 25  | g     | 618 | NEX  | C11-C12-C13-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | g     | 618 | NEX  | C20-C13-C14-C15 |
| 25  | g     | 618 | NEX  | C21-C26-C27-C28 |
| 25  | g     | 618 | NEX  | C28-C29-C30-C31 |
| 25  | g     | 618 | NEX  | C39-C29-C30-C31 |
| 25  | g     | 618 | NEX  | C31-C32-C33-C40 |
| 25  | g     | 618 | NEX  | C40-C33-C34-C35 |
| 25  | n     | 616 | NEX  | C7-C8-C9-C19    |
| 25  | n     | 616 | NEX  | C11-C10-C9-C19  |
| 25  | n     | 616 | NEX  | C11-C12-C13-C14 |
| 25  | n     | 616 | NEX  | C11-C12-C13-C20 |
| 25  | n     | 616 | NEX  | C20-C13-C14-C15 |
| 25  | n     | 616 | NEX  | C21-C26-C27-C28 |
| 25  | n     | 616 | NEX  | C28-C29-C30-C31 |
| 25  | n     | 616 | NEX  | C39-C29-C30-C31 |
| 25  | n     | 616 | NEX  | C40-C33-C34-C35 |
| 25  | y     | 616 | NEX  | C11-C10-C9-C8   |
| 25  | y     | 616 | NEX  | C11-C12-C13-C14 |
| 25  | y     | 616 | NEX  | C20-C13-C14-C15 |
| 25  | y     | 616 | NEX  | C21-C26-C27-C28 |
| 25  | y     | 616 | NEX  | C28-C29-C30-C31 |
| 25  | y     | 616 | NEX  | C39-C29-C30-C31 |
| 25  | y     | 616 | NEX  | C31-C32-C33-C34 |
| 25  | y     | 616 | NEX  | C31-C32-C33-C40 |
| 25  | y     | 618 | NEX  | C11-C10-C9-C8   |
| 25  | y     | 618 | NEX  | C11-C10-C9-C19  |
| 25  | y     | 618 | NEX  | C11-C12-C13-C14 |
| 25  | y     | 618 | NEX  | C20-C13-C14-C15 |
| 25  | y     | 618 | NEX  | C27-C28-C29-C30 |
| 25  | y     | 618 | NEX  | C28-C29-C30-C31 |
| 25  | y     | 618 | NEX  | C39-C29-C30-C31 |
| 25  | N     | 617 | NEX  | C7-C8-C9-C19    |
| 25  | N     | 617 | NEX  | C11-C12-C13-C20 |
| 25  | N     | 617 | NEX  | C20-C13-C14-C15 |
| 25  | N     | 617 | NEX  | C21-C26-C27-C28 |
| 25  | N     | 617 | NEX  | C28-C29-C30-C31 |
| 25  | N     | 617 | NEX  | C39-C29-C30-C31 |
| 25  | N     | 617 | NEX  | C31-C32-C33-C34 |
| 25  | N     | 617 | NEX  | C31-C32-C33-C40 |
| 25  | N     | 617 | NEX  | C32-C33-C34-C35 |
| 25  | Y     | 616 | NEX  | C7-C8-C9-C10    |
| 25  | Y     | 616 | NEX  | C11-C10-C9-C8   |
| 25  | Y     | 616 | NEX  | C11-C12-C13-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | Y     | 616 | NEX  | C20-C13-C14-C15 |
| 25  | Y     | 616 | NEX  | C27-C28-C29-C30 |
| 25  | Y     | 616 | NEX  | C28-C29-C30-C31 |
| 25  | Y     | 616 | NEX  | C31-C32-C33-C34 |
| 25  | Y     | 616 | NEX  | C31-C32-C33-C40 |
| 25  | Y     | 616 | NEX  | C32-C33-C34-C35 |
| 25  | r     | 315 | NEX  | C11-C10-C9-C8   |
| 25  | r     | 315 | NEX  | C11-C10-C9-C19  |
| 25  | r     | 315 | NEX  | C11-C12-C13-C14 |
| 25  | r     | 315 | NEX  | C20-C13-C14-C15 |
| 25  | r     | 315 | NEX  | C27-C28-C29-C30 |
| 25  | r     | 315 | NEX  | C28-C29-C30-C31 |
| 25  | r     | 315 | NEX  | C39-C29-C30-C31 |
| 26  | g     | 619 | LHG  | O1-C1-C2-C3     |
| 26  | g     | 619 | LHG  | O2-C2-C3-O3     |
| 26  | g     | 619 | LHG  | C3-O3-P-O4      |
| 26  | n     | 617 | LHG  | O1-C1-C2-C3     |
| 26  | n     | 617 | LHG  | C1-C2-C3-O3     |
| 26  | n     | 617 | LHG  | O2-C2-C3-O3     |
| 26  | n     | 617 | LHG  | C3-O3-P-O4      |
| 26  | n     | 617 | LHG  | C3-O3-P-O6      |
| 26  | y     | 617 | LHG  | O2-C2-C3-O3     |
| 26  | y     | 617 | LHG  | C3-O3-P-O5      |
| 26  | y     | 617 | LHG  | C3-O3-P-O6      |
| 26  | G     | 618 | LHG  | O1-C1-C2-O2     |
| 26  | G     | 618 | LHG  | C4-O6-P-O5      |
| 26  | N     | 618 | LHG  | O1-C1-C2-C3     |
| 26  | N     | 618 | LHG  | O2-C2-C3-O3     |
| 26  | N     | 618 | LHG  | C3-O3-P-O4      |
| 26  | Y     | 617 | LHG  | C4-O6-P-O4      |
| 26  | Y     | 617 | LHG  | O7-C5-C6-O8     |
| 26  | b     | 619 | LHG  | C3-O3-P-O5      |
| 26  | b     | 619 | LHG  | C4-O6-P-O5      |
| 26  | c     | 520 | LHG  | C3-O3-P-O5      |
| 26  | c     | 520 | LHG  | C8-C7-O7-C5     |
| 26  | c     | 521 | LHG  | C3-O3-P-O5      |
| 26  | c     | 521 | LHG  | C4-O6-P-O5      |
| 26  | c     | 522 | LHG  | O1-C1-C2-C3     |
| 26  | d     | 407 | LHG  | C3-O3-P-O5      |
| 26  | d     | 407 | LHG  | C4-O6-P-O4      |
| 26  | d     | 408 | LHG  | O1-C1-C2-C3     |
| 26  | d     | 408 | LHG  | C4-O6-P-O5      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | d     | 409 | LHG  | C3-O3-P-O5      |
| 26  | d     | 409 | LHG  | C4-O6-P-O5      |
| 26  | l     | 102 | LHG  | O1-C1-C2-C3     |
| 26  | l     | 102 | LHG  | C3-O3-P-O4      |
| 26  | B     | 622 | LHG  | C3-O3-P-O5      |
| 26  | B     | 622 | LHG  | C4-O6-P-O5      |
| 26  | C     | 520 | LHG  | C3-O3-P-O5      |
| 26  | C     | 520 | LHG  | C8-C7-O7-C5     |
| 26  | C     | 521 | LHG  | C3-O3-P-O5      |
| 26  | C     | 521 | LHG  | C4-O6-P-O5      |
| 26  | C     | 522 | LHG  | O1-C1-C2-C3     |
| 26  | D     | 408 | LHG  | C3-O3-P-O5      |
| 26  | D     | 408 | LHG  | C4-O6-P-O4      |
| 26  | D     | 409 | LHG  | O1-C1-C2-C3     |
| 26  | D     | 409 | LHG  | C4-O6-P-O5      |
| 26  | D     | 410 | LHG  | C3-O3-P-O5      |
| 26  | D     | 410 | LHG  | C4-O6-P-O5      |
| 26  | L     | 103 | LHG  | O1-C1-C2-C3     |
| 26  | L     | 103 | LHG  | C3-O3-P-O4      |
| 26  | r     | 302 | LHG  | O1-C1-C2-C3     |
| 26  | s     | 314 | LHG  | C4-O6-P-O5      |
| 26  | S     | 314 | LHG  | C4-O6-P-O5      |
| 26  | R     | 301 | LHG  | O1-C1-C2-C3     |
| 30  | d     | 401 | PHO  | CBD-CGD-O2D-CED |
| 30  | D     | 401 | PHO  | CBD-CGD-O2D-CED |
| 31  | b     | 617 | BCR  | C7-C8-C9-C10    |
| 31  | b     | 617 | BCR  | C7-C8-C9-C34    |
| 31  | b     | 617 | BCR  | C37-C22-C23-C24 |
| 31  | c     | 515 | BCR  | C7-C8-C9-C34    |
| 31  | d     | 405 | BCR  | C1-C6-C7-C8     |
| 31  | d     | 405 | BCR  | C6-C7-C8-C9     |
| 31  | h     | 101 | BCR  | C6-C7-C8-C9     |
| 31  | h     | 101 | BCR  | C7-C8-C9-C10    |
| 31  | h     | 101 | BCR  | C7-C8-C9-C34    |
| 31  | k     | 101 | BCR  | C18-C19-C20-C21 |
| 31  | k     | 101 | BCR  | C37-C22-C23-C24 |
| 31  | k     | 101 | BCR  | C22-C23-C24-C25 |
| 31  | k     | 102 | BCR  | C1-C6-C7-C8     |
| 31  | B     | 602 | BCR  | C1-C6-C7-C8     |
| 31  | B     | 602 | BCR  | C7-C8-C9-C10    |
| 31  | B     | 602 | BCR  | C7-C8-C9-C34    |
| 31  | B     | 602 | BCR  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 602 | BCR  | C11-C12-C13-C14 |
| 31  | B     | 602 | BCR  | C11-C12-C13-C35 |
| 31  | B     | 602 | BCR  | C16-C17-C18-C36 |
| 31  | B     | 602 | BCR  | C36-C18-C19-C20 |
| 31  | B     | 602 | BCR  | C21-C22-C23-C24 |
| 31  | B     | 602 | BCR  | C37-C22-C23-C24 |
| 31  | B     | 620 | BCR  | C7-C8-C9-C10    |
| 31  | B     | 620 | BCR  | C7-C8-C9-C34    |
| 31  | B     | 620 | BCR  | C37-C22-C23-C24 |
| 31  | C     | 516 | BCR  | C7-C8-C9-C34    |
| 31  | D     | 406 | BCR  | C1-C6-C7-C8     |
| 31  | D     | 406 | BCR  | C6-C7-C8-C9     |
| 31  | H     | 101 | BCR  | C6-C7-C8-C9     |
| 31  | H     | 101 | BCR  | C7-C8-C9-C10    |
| 31  | H     | 101 | BCR  | C7-C8-C9-C34    |
| 31  | K     | 101 | BCR  | C18-C19-C20-C21 |
| 31  | K     | 101 | BCR  | C37-C22-C23-C24 |
| 31  | K     | 101 | BCR  | C22-C23-C24-C25 |
| 31  | K     | 102 | BCR  | C1-C6-C7-C8     |
| 31  | T     | 102 | BCR  | C1-C6-C7-C8     |
| 31  | T     | 102 | BCR  | C7-C8-C9-C10    |
| 31  | T     | 102 | BCR  | C7-C8-C9-C34    |
| 31  | T     | 102 | BCR  | C9-C10-C11-C12  |
| 31  | T     | 102 | BCR  | C11-C12-C13-C14 |
| 31  | T     | 102 | BCR  | C11-C12-C13-C35 |
| 31  | T     | 102 | BCR  | C16-C17-C18-C36 |
| 31  | T     | 102 | BCR  | C36-C18-C19-C20 |
| 31  | T     | 102 | BCR  | C21-C22-C23-C24 |
| 31  | T     | 102 | BCR  | C37-C22-C23-C24 |
| 32  | d     | 406 | PL9  | C12-C13-C14-C15 |
| 32  | d     | 406 | PL9  | C13-C14-C16-C17 |
| 32  | d     | 406 | PL9  | C18-C19-C21-C22 |
| 32  | d     | 406 | PL9  | C24-C26-C27-C28 |
| 32  | d     | 406 | PL9  | C27-C28-C29-C30 |
| 32  | d     | 406 | PL9  | C39-C41-C42-C43 |
| 32  | D     | 407 | PL9  | C12-C13-C14-C15 |
| 32  | D     | 407 | PL9  | C13-C14-C16-C17 |
| 32  | D     | 407 | PL9  | C18-C19-C21-C22 |
| 32  | D     | 407 | PL9  | C24-C26-C27-C28 |
| 32  | D     | 407 | PL9  | C27-C28-C29-C30 |
| 32  | D     | 407 | PL9  | C39-C41-C42-C43 |
| 33  | a     | 411 | SQD  | O5-C1-O6-C44    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | a     | 411 | SQD  | C8-C7-O47-C45   |
| 33  | a     | 411 | SQD  | C5-C6-S-O8      |
| 33  | a     | 411 | SQD  | C5-C6-S-O9      |
| 33  | d     | 402 | SQD  | C5-C6-S-O7      |
| 33  | d     | 402 | SQD  | C5-C6-S-O8      |
| 33  | l     | 101 | SQD  | C2-C1-O6-C44    |
| 33  | l     | 101 | SQD  | O5-C1-O6-C44    |
| 33  | l     | 101 | SQD  | O49-C7-O47-C45  |
| 33  | l     | 101 | SQD  | C8-C7-O47-C45   |
| 33  | l     | 103 | SQD  | C2-C1-O6-C44    |
| 33  | l     | 103 | SQD  | O5-C1-O6-C44    |
| 33  | l     | 103 | SQD  | O49-C7-O47-C45  |
| 33  | A     | 412 | SQD  | O5-C1-O6-C44    |
| 33  | A     | 412 | SQD  | C8-C7-O47-C45   |
| 33  | A     | 412 | SQD  | C5-C6-S-O8      |
| 33  | A     | 412 | SQD  | C5-C6-S-O9      |
| 33  | D     | 402 | SQD  | C5-C6-S-O7      |
| 33  | D     | 402 | SQD  | C5-C6-S-O8      |
| 33  | L     | 101 | SQD  | C2-C1-O6-C44    |
| 33  | L     | 101 | SQD  | O5-C1-O6-C44    |
| 33  | L     | 101 | SQD  | O49-C7-O47-C45  |
| 33  | L     | 102 | SQD  | C2-C1-O6-C44    |
| 33  | L     | 102 | SQD  | O5-C1-O6-C44    |
| 33  | L     | 102 | SQD  | O49-C7-O47-C45  |
| 33  | L     | 102 | SQD  | C8-C7-O47-C45   |
| 35  | a     | 413 | DGD  | C2D-C1D-O3G-C3G |
| 35  | a     | 413 | DGD  | O6D-C1D-O3G-C3G |
| 35  | c     | 518 | DGD  | O1G-C1G-C2G-O2G |
| 35  | c     | 518 | DGD  | C2E-C1E-O5D-C6D |
| 35  | c     | 518 | DGD  | O6E-C1E-O5D-C6D |
| 35  | c     | 519 | DGD  | C2D-C1D-O3G-C3G |
| 35  | c     | 519 | DGD  | O6D-C1D-O3G-C3G |
| 35  | A     | 401 | DGD  | C2D-C1D-O3G-C3G |
| 35  | A     | 401 | DGD  | O6D-C1D-O3G-C3G |
| 35  | C     | 519 | DGD  | O1G-C1G-C2G-O2G |
| 35  | C     | 519 | DGD  | C2E-C1E-O5D-C6D |
| 35  | C     | 519 | DGD  | O6E-C1E-O5D-C6D |
| 35  | J     | 101 | DGD  | C2D-C1D-O3G-C3G |
| 35  | J     | 101 | DGD  | O6D-C1D-O3G-C3G |
| 36  | c     | 523 | LMG  | C2-C1-O1-C7     |
| 36  | c     | 523 | LMG  | O6-C1-O1-C7     |
| 36  | c     | 523 | LMG  | O7-C8-C9-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | c     | 523 | LMG  | O9-C10-O7-C8    |
| 36  | c     | 523 | LMG  | C11-C10-O7-C8   |
| 36  | w     | 102 | LMG  | C2-C1-O1-C7     |
| 36  | w     | 102 | LMG  | O6-C1-O1-C7     |
| 36  | B     | 601 | LMG  | O6-C1-O1-C7     |
| 36  | C     | 502 | LMG  | C2-C1-O1-C7     |
| 36  | C     | 502 | LMG  | O6-C1-O1-C7     |
| 36  | C     | 523 | LMG  | C2-C1-O1-C7     |
| 36  | C     | 523 | LMG  | O6-C1-O1-C7     |
| 36  | C     | 523 | LMG  | O7-C8-C9-O8     |
| 36  | C     | 523 | LMG  | O9-C10-O7-C8    |
| 36  | C     | 523 | LMG  | C11-C10-O7-C8   |
| 36  | I     | 101 | LMG  | O6-C1-O1-C7     |
| 37  | f     | 101 | HEM  | C1A-C2A-CAA-CBA |
| 37  | f     | 101 | HEM  | C3A-C2A-CAA-CBA |
| 37  | F     | 101 | HEM  | C1A-C2A-CAA-CBA |
| 37  | F     | 101 | HEM  | C3A-C2A-CAA-CBA |
| 21  | g     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | n     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | y     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | G     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | N     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | Y     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | n     | 606 | CHL  | O1D-CGD-O2D-CED |
| 22  | b     | 608 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 615 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 505 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 513 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 614 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 618 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 506 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 514 | CLA  | O1D-CGD-O2D-CED |
| 22  | r     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | R     | 308 | CLA  | O1D-CGD-O2D-CED |
| 21  | g     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 21  | n     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 21  | y     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 21  | G     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 21  | N     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 21  | Y     | 601 | CHL  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | g     | 609 | CHL  | O1D-CGD-O2D-CED |
| 21  | n     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | y     | 609 | CHL  | O1D-CGD-O2D-CED |
| 21  | G     | 609 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | Y     | 608 | CHL  | O1D-CGD-O2D-CED |
| 22  | g     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | Y     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 503 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 504 | CLA  | O1D-CGD-O2D-CED |
| 22  | r     | 303 | CLA  | O1D-CGD-O2D-CED |
| 22  | s     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | R     | 302 | CLA  | O1D-CGD-O2D-CED |
| 21  | g     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | g     | 609 | CHL  | CBD-CGD-O2D-CED |
| 21  | n     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | n     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | y     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | y     | 609 | CHL  | CBD-CGD-O2D-CED |
| 21  | G     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | G     | 609 | CHL  | CBD-CGD-O2D-CED |
| 21  | N     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | N     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | Y     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | Y     | 608 | CHL  | CBD-CGD-O2D-CED |
| 21  | s     | 307 | CHL  | CBD-CGD-O2D-CED |
| 21  | S     | 307 | CHL  | CBD-CGD-O2D-CED |
| 22  | g     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | g     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | g     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | g     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | g     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 612 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | y     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | y     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | y     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | y     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 601 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 608 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 510 | CLA  | CBD-CGD-O2D-CED |
| 22  | w     | 101 | CLA  | CBD-CGD-O2D-CED |
| 22  | x     | 101 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 616 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 618 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 511 | CLA  | CBD-CGD-O2D-CED |
| 22  | W     | 101 | CLA  | CBD-CGD-O2D-CED |
| 22  | r     | 303 | CLA  | CBD-CGD-O2D-CED |
| 22  | r     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 303 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 305 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 303 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | R     | 302 | CLA  | CBD-CGD-O2D-CED |
| 22  | R     | 304 | CLA  | CBD-CGD-O2D-CED |
| 30  | a     | 407 | PHO  | CBD-CGD-O2D-CED |
| 30  | A     | 408 | PHO  | CBD-CGD-O2D-CED |
| 22  | g     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 514 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 515 | CLA  | O1A-CGA-O2A-C1  |
| 22  | r     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 22  | r     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 21  | n     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 21  | y     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 21  | G     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 21  | N     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 21  | Y     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 21  | y     | 605 | CHL  | O1D-CGD-O2D-CED |
| 21  | r     | 301 | CHL  | O1D-CGD-O2D-CED |
| 21  | S     | 301 | CHL  | O1D-CGD-O2D-CED |
| 22  | b     | 601 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | r     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | R     | 304 | CLA  | O1D-CGD-O2D-CED |
| 21  | r     | 308 | CHL  | C8-C10-C11-C12  |
| 21  | R     | 307 | CHL  | C8-C10-C11-C12  |
| 21  | g     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 21  | n     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 21  | y     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 21  | G     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 21  | N     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 21  | Y     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 22  | g     | 612 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | n     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | w     | 101 | CLA  | O1D-CGD-O2D-CED |
| 22  | x     | 101 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 603 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 607 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 508 | CLA  | O1D-CGD-O2D-CED |
| 22  | W     | 101 | CLA  | O1D-CGD-O2D-CED |
| 22  | s     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 514 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 515 | CLA  | CBA-CGA-O2A-C1  |
| 22  | r     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 33  | l     | 101 | SQD  | C24-C23-O48-C46 |
| 33  | L     | 102 | SQD  | C24-C23-O48-C46 |
| 22  | a     | 405 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 502 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 509 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 406 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 503 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 510 | CLA  | CBD-CGD-O2D-CED |
| 22  | r     | 312 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | R     | 311 | CLA  | CBD-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 21  | n     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 21  | y     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 21  | G     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 21  | N     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 21  | Y     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 21  | r     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 21  | R     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 22  | g     | 604 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | g     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | g     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | a     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 505 | CLA  | O1A-CGA-O2A-C1  |
| 22  | x     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 407 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 506 | CLA  | O1A-CGA-O2A-C1  |
| 26  | c     | 522 | LHG  | O10-C23-O8-C6   |
| 26  | C     | 522 | LHG  | O10-C23-O8-C6   |
| 33  | l     | 101 | SQD  | O10-C23-O48-C46 |
| 33  | L     | 102 | SQD  | O10-C23-O48-C46 |
| 35  | a     | 413 | DGD  | O1A-C1A-O1G-C1G |
| 35  | A     | 401 | DGD  | O1A-C1A-O1G-C1G |
| 21  | g     | 606 | CHL  | O1D-CGD-O2D-CED |
| 21  | n     | 605 | CHL  | O1D-CGD-O2D-CED |
| 21  | y     | 606 | CHL  | O1D-CGD-O2D-CED |
| 21  | G     | 606 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 605 | CHL  | O1D-CGD-O2D-CED |
| 21  | Y     | 605 | CHL  | O1D-CGD-O2D-CED |
| 22  | b     | 603 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 504 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 606 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 505 | CLA  | O1D-CGD-O2D-CED |
| 22  | s     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 310 | CLA  | O1D-CGD-O2D-CED |
| 30  | d     | 401 | PHO  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | D     | 401 | PHO  | O1D-CGD-O2D-CED |
| 22  | r     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | R     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 406 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 407 | CLA  | CBD-CGD-O2D-CED |
| 22  | g     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | Y     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 510 | CLA  | O1D-CGD-O2D-CED |
| 22  | s     | 303 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 303 | CLA  | O1D-CGD-O2D-CED |
| 26  | c     | 520 | LHG  | O9-C7-O7-C5     |
| 26  | C     | 520 | LHG  | O9-C7-O7-C5     |
| 30  | a     | 407 | PHO  | O1A-CGA-O2A-C1  |
| 30  | A     | 408 | PHO  | O1A-CGA-O2A-C1  |
| 21  | g     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 21  | n     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 33  | l     | 103 | SQD  | C45-C46-O48-C23 |
| 33  | L     | 101 | SQD  | C45-C46-O48-C23 |
| 22  | C     | 511 | CLA  | O1D-CGD-O2D-CED |
| 21  | g     | 608 | CHL  | C3-C5-C6-C7     |
| 21  | n     | 607 | CHL  | C3-C5-C6-C7     |
| 21  | y     | 608 | CHL  | C3-C5-C6-C7     |
| 21  | G     | 608 | CHL  | C3-C5-C6-C7     |
| 21  | N     | 607 | CHL  | C3-C5-C6-C7     |
| 21  | Y     | 607 | CHL  | C3-C5-C6-C7     |
| 22  | g     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | g     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | n     | 610 | CLA  | C3-C5-C6-C7     |
| 22  | n     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | y     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | G     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | G     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | N     | 610 | CLA  | C3-C5-C6-C7     |
| 22  | N     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | Y     | 610 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 601 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 613 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 22  | c     | 502 | CLA  | C3-C5-C6-C7    |
| 22  | c     | 508 | CLA  | C3-C5-C6-C7    |
| 22  | w     | 101 | CLA  | C3-C5-C6-C7    |
| 22  | x     | 101 | CLA  | C3-C5-C6-C7    |
| 22  | B     | 603 | CLA  | C3-C5-C6-C7    |
| 22  | B     | 604 | CLA  | C3-C5-C6-C7    |
| 22  | B     | 615 | CLA  | C3-C5-C6-C7    |
| 22  | B     | 616 | CLA  | C3-C5-C6-C7    |
| 22  | C     | 503 | CLA  | C3-C5-C6-C7    |
| 22  | C     | 509 | CLA  | C3-C5-C6-C7    |
| 22  | W     | 101 | CLA  | C3-C5-C6-C7    |
| 22  | r     | 304 | CLA  | C3-C5-C6-C7    |
| 22  | R     | 303 | CLA  | C3-C5-C6-C7    |
| 30  | a     | 407 | PHO  | C3-C5-C6-C7    |
| 30  | d     | 401 | PHO  | C3-C5-C6-C7    |
| 30  | A     | 408 | PHO  | C3-C5-C6-C7    |
| 30  | D     | 401 | PHO  | C3-C5-C6-C7    |
| 21  | g     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | n     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | y     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | G     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | N     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | Y     | 601 | CHL  | CBA-CGA-O2A-C1 |
| 21  | r     | 306 | CHL  | CBA-CGA-O2A-C1 |
| 21  | R     | 305 | CHL  | CBA-CGA-O2A-C1 |
| 22  | g     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | g     | 604 | CLA  | CBA-CGA-O2A-C1 |
| 22  | g     | 610 | CLA  | CBA-CGA-O2A-C1 |
| 22  | n     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | n     | 609 | CLA  | CBA-CGA-O2A-C1 |
| 22  | y     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | y     | 610 | CLA  | CBA-CGA-O2A-C1 |
| 22  | G     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | G     | 604 | CLA  | CBA-CGA-O2A-C1 |
| 22  | G     | 610 | CLA  | CBA-CGA-O2A-C1 |
| 22  | N     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | N     | 604 | CLA  | CBA-CGA-O2A-C1 |
| 22  | Y     | 602 | CLA  | CBA-CGA-O2A-C1 |
| 22  | Y     | 604 | CLA  | CBA-CGA-O2A-C1 |
| 22  | Y     | 609 | CLA  | CBA-CGA-O2A-C1 |
| 22  | a     | 406 | CLA  | CBA-CGA-O2A-C1 |
| 22  | b     | 603 | CLA  | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 507 | CLA  | CBA-CGA-O2A-C1  |
| 22  | x     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 407 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 606 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 508 | CLA  | CBA-CGA-O2A-C1  |
| 26  | c     | 522 | LHG  | C24-C23-O8-C6   |
| 26  | C     | 522 | LHG  | C24-C23-O8-C6   |
| 35  | a     | 413 | DGD  | C2A-C1A-O1G-C1G |
| 35  | A     | 401 | DGD  | C2A-C1A-O1G-C1G |
| 36  | M     | 101 | LMG  | C29-C28-O8-C9   |
| 36  | T     | 101 | LMG  | C29-C28-O8-C9   |
| 21  | N     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 21  | Y     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 33  | l     | 103 | SQD  | C8-C7-O47-C45   |
| 33  | L     | 101 | SQD  | C8-C7-O47-C45   |
| 36  | b     | 620 | LMG  | C11-C10-O7-C8   |
| 36  | B     | 623 | LMG  | C11-C10-O7-C8   |
| 22  | g     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 609 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 609 | CLA  | O1D-CGD-O2D-CED |
| 22  | Y     | 609 | CLA  | O1D-CGD-O2D-CED |
| 30  | a     | 407 | PHO  | O1D-CGD-O2D-CED |
| 30  | A     | 408 | PHO  | O1D-CGD-O2D-CED |
| 22  | b     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 612 | CLA  | CBD-CGD-O2D-CED |
| 21  | y     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 21  | G     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 21  | r     | 308 | CHL  | C2C-C3C-CAC-CBC |
| 21  | s     | 301 | CHL  | C2-C1-O2A-CGA   |
| 21  | R     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 36  | k     | 103 | LMG  | O6-C5-C6-O5     |
| 36  | K     | 103 | LMG  | O6-C5-C6-O5     |
| 35  | c     | 518 | DGD  | C4D-C5D-C6D-O5D |
| 35  | C     | 519 | DGD  | C4D-C5D-C6D-O5D |
| 22  | c     | 512 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 513 | CLA  | C4-C3-C5-C6     |
| 22  | r     | 310 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 310 | CLA  | C4-C3-C5-C6     |
| 22  | S     | 310 | CLA  | C4-C3-C5-C6     |
| 22  | R     | 309 | CLA  | C4-C3-C5-C6     |
| 21  | s     | 302 | CHL  | CBD-CGD-O2D-CED |
| 21  | S     | 302 | CHL  | CBD-CGD-O2D-CED |
| 22  | g     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | y     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 511 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 512 | CLA  | CBD-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 21  | n     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 21  | y     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 21  | G     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 21  | N     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 21  | Y     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 21  | s     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 21  | S     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 22  | g     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | n     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | y     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | G     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | N     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Y     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 617 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 509 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | n     | 607 | CHL  | O1D-CGD-O2D-CED |
| 21  | y     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | G     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 607 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | Y     | 607 | CHL  | O1D-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 21  | g     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | n     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 21  | n     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 21  | y     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 21  | G     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 21  | N     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 21  | Y     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 22  | g     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | g     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | y     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 22  | y     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | y     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 609 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Y     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Y     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 606 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 615 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 609 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 618 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 506 | CLA  | CBA-CGA-O2A-C1  |
| 22  | r     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 22  | s     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 22  | s     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | S     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 30  | a     | 407 | PHO  | CBA-CGA-O2A-C1  |
| 30  | A     | 408 | PHO  | CBA-CGA-O2A-C1  |
| 22  | C     | 513 | CLA  | CBD-CGD-O2D-CED |
| 21  | g     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | n     | 606 | CHL  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | y     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | G     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | N     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 21  | Y     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 21  | s     | 307 | CHL  | O1D-CGD-O2D-CED |
| 21  | S     | 307 | CHL  | O1D-CGD-O2D-CED |
| 22  | b     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 615 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 616 | CLA  | O1D-CGD-O2D-CED |
| 22  | s     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 305 | CLA  | O1D-CGD-O2D-CED |
| 33  | a     | 411 | SQD  | O49-C7-O47-C45  |
| 33  | A     | 412 | SQD  | O49-C7-O47-C45  |
| 32  | d     | 406 | PL9  | C12-C13-C14-C16 |
| 32  | d     | 406 | PL9  | C27-C28-C29-C31 |
| 32  | d     | 406 | PL9  | C42-C43-C44-C46 |
| 32  | D     | 407 | PL9  | C12-C13-C14-C16 |
| 32  | D     | 407 | PL9  | C27-C28-C29-C31 |
| 32  | D     | 407 | PL9  | C42-C43-C44-C46 |
| 21  | r     | 308 | CHL  | O1A-CGA-O2A-C1  |
| 21  | R     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 22  | b     | 606 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 615 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 618 | CLA  | O1A-CGA-O2A-C1  |
| 22  | r     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 22  | r     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 33  | l     | 103 | SQD  | O10-C23-O48-C46 |
| 33  | L     | 101 | SQD  | O10-C23-O48-C46 |
| 21  | g     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 21  | n     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 21  | y     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 21  | G     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 21  | N     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 21  | Y     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 23  | r     | 313 | LUT  | C9-C10-C11-C12  |
| 23  | R     | 312 | LUT  | C9-C10-C11-C12  |
| 24  | n     | 615 | XAT  | C9-C10-C11-C12  |
| 24  | N     | 616 | XAT  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 602 | BCR  | C19-C20-C21-C22 |
| 31  | T     | 102 | BCR  | C19-C20-C21-C22 |
| 36  | k     | 103 | LMG  | C4-C5-C6-O5     |
| 36  | K     | 103 | LMG  | C4-C5-C6-O5     |
| 22  | c     | 512 | CLA  | CBD-CGD-O2D-CED |
| 26  | G     | 618 | LHG  | O2-C2-C3-O3     |
| 26  | Y     | 617 | LHG  | O2-C2-C3-O3     |
| 21  | y     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | G     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 21  | N     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 21  | Y     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 22  | a     | 405 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 509 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 406 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 22  | r     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 22  | s     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 22  | S     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 22  | S     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 21  | g     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 21  | n     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 21  | y     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 21  | G     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 21  | N     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 21  | Y     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 22  | g     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 606 | CLA  | O1A-CGA-O2A-C1  |
| 22  | s     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 22  | S     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 608 | CHL  | C5-C6-C7-C8     |
| 21  | n     | 607 | CHL  | C5-C6-C7-C8     |
| 21  | y     | 608 | CHL  | C5-C6-C7-C8     |
| 21  | G     | 608 | CHL  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | N     | 607 | CHL  | C5-C6-C7-C8     |
| 21  | Y     | 607 | CHL  | C5-C6-C7-C8     |
| 21  | S     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 22  | g     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | n     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | y     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 612 | CLA  | CBD-CGD-O2D-CED |
| 26  | d     | 407 | LHG  | C28-C29-C30-C31 |
| 26  | D     | 408 | LHG  | C28-C29-C30-C31 |
| 21  | y     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | G     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | N     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 21  | Y     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 35  | c     | 518 | DGD  | O6D-C5D-C6D-O5D |
| 35  | C     | 519 | DGD  | O6D-C5D-C6D-O5D |
| 22  | c     | 511 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 512 | CLA  | C3-C5-C6-C7     |
| 21  | r     | 308 | CHL  | CBA-CGA-O2A-C1  |
| 21  | R     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 22  | r     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 26  | c     | 520 | LHG  | C24-C23-O8-C6   |
| 21  | g     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 21  | n     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 22  | b     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 509 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 22  | r     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | s     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | s     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 22  | S     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | S     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 21  | s     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 21  | S     | 302 | CHL  | C2C-C3C-CAC-CBC |
| 32  | d     | 406 | PL9  | C47-C48-C49-C51 |
| 32  | D     | 407 | PL9  | C47-C48-C49-C51 |
| 36  | C     | 523 | LMG  | O6-C5-C6-O5     |
| 21  | g     | 601 | CHL  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | n     | 601 | CHL  | C4-C3-C5-C6     |
| 21  | y     | 601 | CHL  | C4-C3-C5-C6     |
| 21  | G     | 601 | CHL  | C4-C3-C5-C6     |
| 21  | N     | 601 | CHL  | C4-C3-C5-C6     |
| 21  | Y     | 601 | CHL  | C4-C3-C5-C6     |
| 22  | s     | 309 | CLA  | C4-C3-C5-C6     |
| 22  | S     | 309 | CLA  | C4-C3-C5-C6     |
| 21  | g     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | n     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | y     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | G     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | N     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | Y     | 601 | CHL  | C2-C3-C5-C6     |
| 21  | g     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 21  | G     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 21  | Y     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 21  | r     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 21  | r     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 21  | R     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 22  | g     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | Y     | 610 | CLA  | O1D-CGD-O2D-CED |
| 26  | b     | 619 | LHG  | C28-C29-C30-C31 |
| 26  | B     | 622 | LHG  | C28-C29-C30-C31 |
| 36  | c     | 523 | LMG  | O6-C5-C6-O5     |
| 22  | a     | 405 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 36  | M     | 101 | LMG  | O10-C28-O8-C9   |
| 36  | T     | 101 | LMG  | O10-C28-O8-C9   |
| 35  | c     | 518 | DGD  | O6D-C1D-O3G-C3G |
| 35  | C     | 519 | DGD  | O6D-C1D-O3G-C3G |
| 32  | d     | 406 | PL9  | C9-C11-C12-C13  |
| 32  | d     | 406 | PL9  | C14-C16-C17-C18 |
| 32  | D     | 407 | PL9  | C9-C11-C12-C13  |
| 32  | D     | 407 | PL9  | C14-C16-C17-C18 |
| 21  | r     | 308 | CHL  | C4C-C3C-CAC-CBC |
| 21  | R     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 26  | c     | 520 | LHG  | C28-C29-C30-C31 |
| 26  | C     | 520 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 22  | S     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 26  | C     | 520 | LHG  | C24-C23-O8-C6   |
| 21  | s     | 302 | CHL  | C2C-C3C-CAC-CBC |
| 36  | M     | 101 | LMG  | O6-C5-C6-O5     |
| 36  | T     | 101 | LMG  | O6-C5-C6-O5     |
| 22  | s     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | S     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 405 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 502 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 406 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 503 | CLA  | O1D-CGD-O2D-CED |
| 22  | r     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | R     | 311 | CLA  | O1D-CGD-O2D-CED |
| 26  | N     | 618 | LHG  | C1-C2-C3-O3     |
| 26  | Y     | 617 | LHG  | C1-C2-C3-O3     |
| 22  | s     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 22  | S     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 21  | s     | 301 | CHL  | CBA-CGA-O2A-C1  |
| 22  | b     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 617 | CLA  | CBA-CGA-O2A-C1  |
| 22  | r     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | R     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 26  | r     | 302 | LHG  | C24-C23-O8-C6   |
| 26  | R     | 301 | LHG  | C24-C23-O8-C6   |
| 33  | a     | 411 | SQD  | C24-C23-O48-C46 |
| 33  | l     | 103 | SQD  | C24-C23-O48-C46 |
| 33  | A     | 412 | SQD  | C24-C23-O48-C46 |
| 33  | L     | 101 | SQD  | C24-C23-O48-C46 |
| 22  | b     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 605 | CLA  | O1D-CGD-O2D-CED |
| 21  | G     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | N     | 606 | CHL  | C8-C10-C11-C12  |
| 22  | g     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | y     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | G     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | Y     | 610 | CLA  | C5-C6-C7-C8     |
| 26  | G     | 618 | LHG  | O6-C4-C5-O7     |
| 26  | c     | 522 | LHG  | C29-C30-C31-C32 |
| 26  | C     | 522 | LHG  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | g     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | n     | 606 | CHL  | C8-C10-C11-C12  |
| 21  | y     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | y     | 609 | CHL  | C8-C10-C11-C12  |
| 21  | Y     | 606 | CHL  | C8-C10-C11-C12  |
| 22  | g     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | g     | 613 | CLA  | C8-C10-C11-C12  |
| 22  | n     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | n     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | n     | 612 | CLA  | C8-C10-C11-C12  |
| 22  | y     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | y     | 612 | CLA  | C8-C10-C11-C12  |
| 22  | G     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | G     | 613 | CLA  | C8-C10-C11-C12  |
| 22  | N     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | N     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | N     | 612 | CLA  | C8-C10-C11-C12  |
| 22  | Y     | 603 | CLA  | C10-C11-C12-C13 |
| 22  | Y     | 611 | CLA  | C8-C10-C11-C12  |
| 22  | r     | 309 | CLA  | C5-C6-C7-C8     |
| 22  | R     | 308 | CLA  | C5-C6-C7-C8     |
| 26  | c     | 521 | LHG  | C23-C24-C25-C26 |
| 26  | d     | 407 | LHG  | C23-C24-C25-C26 |
| 26  | C     | 521 | LHG  | C23-C24-C25-C26 |
| 26  | D     | 408 | LHG  | C23-C24-C25-C26 |
| 22  | g     | 614 | CLA  | O2A-C1-C2-C3    |
| 22  | n     | 613 | CLA  | O2A-C1-C2-C3    |
| 22  | y     | 613 | CLA  | O2A-C1-C2-C3    |
| 22  | G     | 614 | CLA  | O2A-C1-C2-C3    |
| 22  | N     | 613 | CLA  | O2A-C1-C2-C3    |
| 22  | Y     | 612 | CLA  | O2A-C1-C2-C3    |
| 26  | s     | 314 | LHG  | O7-C5-C6-O8     |
| 26  | S     | 314 | LHG  | O7-C5-C6-O8     |
| 22  | r     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 22  | R     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 512 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 513 | CLA  | C2-C3-C5-C6     |
| 22  | r     | 310 | CLA  | C2-C3-C5-C6     |
| 21  | g     | 601 | CHL  | C14-C13-C15-C16 |
| 21  | n     | 601 | CHL  | C14-C13-C15-C16 |
| 21  | n     | 608 | CHL  | C14-C13-C15-C16 |
| 21  | y     | 601 | CHL  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | y     | 609 | CHL  | C14-C13-C15-C16 |
| 21  | G     | 601 | CHL  | C14-C13-C15-C16 |
| 21  | N     | 601 | CHL  | C14-C13-C15-C16 |
| 21  | N     | 608 | CHL  | C14-C13-C15-C16 |
| 21  | Y     | 601 | CHL  | C14-C13-C15-C16 |
| 21  | Y     | 608 | CHL  | C14-C13-C15-C16 |
| 22  | g     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | n     | 611 | CLA  | C6-C7-C8-C9     |
| 22  | G     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | N     | 611 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 405 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 601 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 514 | CLA  | C11-C10-C8-C9   |
| 22  | w     | 101 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 406 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 604 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 515 | CLA  | C11-C10-C8-C9   |
| 22  | W     | 101 | CLA  | C6-C7-C8-C9     |
| 21  | g     | 609 | CHL  | C2A-CAA-CBA-CGA |
| 21  | n     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 21  | y     | 609 | CHL  | C2A-CAA-CBA-CGA |
| 21  | G     | 609 | CHL  | C2A-CAA-CBA-CGA |
| 21  | N     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 22  | S     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 23  | g     | 615 | LUT  | C7-C8-C9-C19    |
| 23  | g     | 616 | LUT  | C11-C12-C13-C20 |
| 23  | n     | 614 | LUT  | C7-C8-C9-C19    |
| 23  | y     | 614 | LUT  | C7-C8-C9-C19    |
| 23  | G     | 615 | LUT  | C7-C8-C9-C19    |
| 23  | G     | 616 | LUT  | C11-C12-C13-C20 |
| 23  | N     | 614 | LUT  | C7-C8-C9-C19    |
| 23  | N     | 615 | LUT  | C7-C8-C9-C19    |
| 23  | Y     | 613 | LUT  | C7-C8-C9-C19    |
| 23  | Y     | 614 | LUT  | C27-C28-C29-C39 |
| 23  | r     | 313 | LUT  | C31-C32-C33-C40 |
| 23  | R     | 312 | LUT  | C31-C32-C33-C40 |
| 24  | y     | 615 | XAT  | C7-C8-C9-C19    |
| 24  | y     | 615 | XAT  | C31-C32-C33-C40 |
| 24  | G     | 617 | XAT  | C31-C32-C33-C40 |
| 24  | Y     | 615 | XAT  | C7-C8-C9-C19    |
| 24  | Y     | 615 | XAT  | C31-C32-C33-C40 |
| 24  | r     | 314 | XAT  | C31-C32-C33-C40 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | R     | 313 | XAT  | C27-C28-C29-C39 |
| 24  | R     | 313 | XAT  | C31-C32-C33-C40 |
| 25  | g     | 618 | NEX  | C27-C28-C29-C39 |
| 25  | n     | 616 | NEX  | C31-C32-C33-C40 |
| 25  | y     | 618 | NEX  | C11-C12-C13-C20 |
| 25  | y     | 618 | NEX  | C31-C32-C33-C40 |
| 25  | N     | 617 | NEX  | C27-C28-C29-C39 |
| 25  | r     | 315 | NEX  | C11-C12-C13-C20 |
| 25  | r     | 315 | NEX  | C31-C32-C33-C40 |
| 31  | d     | 405 | BCR  | C7-C8-C9-C34    |
| 31  | k     | 101 | BCR  | C11-C12-C13-C35 |
| 31  | D     | 406 | BCR  | C7-C8-C9-C34    |
| 31  | K     | 101 | BCR  | C11-C12-C13-C35 |
| 23  | g     | 615 | LUT  | C11-C12-C13-C14 |
| 23  | g     | 615 | LUT  | C27-C28-C29-C30 |
| 23  | g     | 616 | LUT  | C7-C8-C9-C10    |
| 23  | n     | 614 | LUT  | C11-C12-C13-C14 |
| 23  | n     | 614 | LUT  | C27-C28-C29-C30 |
| 23  | y     | 614 | LUT  | C11-C12-C13-C14 |
| 23  | y     | 614 | LUT  | C27-C28-C29-C30 |
| 23  | G     | 615 | LUT  | C11-C12-C13-C14 |
| 23  | G     | 615 | LUT  | C27-C28-C29-C30 |
| 23  | G     | 616 | LUT  | C7-C8-C9-C10    |
| 23  | N     | 614 | LUT  | C11-C12-C13-C14 |
| 23  | N     | 614 | LUT  | C27-C28-C29-C30 |
| 23  | Y     | 613 | LUT  | C11-C12-C13-C14 |
| 23  | Y     | 613 | LUT  | C27-C28-C29-C30 |
| 23  | Y     | 614 | LUT  | C7-C8-C9-C10    |
| 23  | r     | 313 | LUT  | C27-C28-C29-C30 |
| 23  | R     | 312 | LUT  | C27-C28-C29-C30 |
| 31  | d     | 405 | BCR  | C7-C8-C9-C10    |
| 31  | k     | 101 | BCR  | C21-C22-C23-C24 |
| 31  | D     | 406 | BCR  | C7-C8-C9-C10    |
| 31  | K     | 101 | BCR  | C21-C22-C23-C24 |
| 35  | h     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 35  | H     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 26  | y     | 617 | LHG  | C7-C8-C9-C10    |
| 21  | s     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 21  | n     | 608 | CHL  | C8-C10-C11-C12  |
| 21  | N     | 608 | CHL  | C8-C10-C11-C12  |
| 22  | g     | 610 | CLA  | C8-C10-C11-C12  |
| 22  | N     | 609 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | Y     | 609 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 615 | CLA  | C15-C16-C17-C18 |
| 22  | d     | 404 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 618 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 514 | CLA  | C15-C16-C17-C18 |
| 22  | D     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | s     | 311 | CLA  | C5-C6-C7-C8     |
| 22  | S     | 311 | CLA  | C5-C6-C7-C8     |
| 36  | B     | 601 | LMG  | O6-C5-C6-O5     |
| 36  | I     | 101 | LMG  | O6-C5-C6-O5     |
| 22  | g     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | y     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Y     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 36  | B     | 601 | LMG  | C29-C28-O8-C9   |
| 36  | I     | 101 | LMG  | C29-C28-O8-C9   |
| 21  | Y     | 608 | CHL  | C8-C10-C11-C12  |
| 21  | r     | 308 | CHL  | C10-C11-C12-C13 |
| 21  | R     | 307 | CHL  | C10-C11-C12-C13 |
| 22  | n     | 609 | CLA  | C8-C10-C11-C12  |
| 22  | y     | 610 | CLA  | C8-C10-C11-C12  |
| 22  | G     | 610 | CLA  | C8-C10-C11-C12  |
| 22  | G     | 610 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 601 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 601 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 502 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 506 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 513 | CLA  | C15-C16-C17-C18 |
| 22  | d     | 404 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 604 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 604 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 503 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 507 | CLA  | C10-C11-C12-C13 |
| 22  | D     | 405 | CLA  | C8-C10-C11-C12  |
| 26  | Y     | 617 | LHG  | C7-C8-C9-C10    |
| 26  | r     | 302 | LHG  | C7-C8-C9-C10    |
| 26  | r     | 302 | LHG  | C23-C24-C25-C26 |
| 26  | R     | 301 | LHG  | C7-C8-C9-C10    |
| 26  | R     | 301 | LHG  | C23-C24-C25-C26 |
| 22  | c     | 509 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 510 | CLA  | O1D-CGD-O2D-CED |
| 21  | n     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 21  | y     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 22  | n     | 609 | CLA  | C15-C16-C17-C18 |
| 22  | G     | 613 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 613 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 505 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 510 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 616 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 506 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 511 | CLA  | C13-C15-C16-C17 |
| 22  | r     | 310 | CLA  | C15-C16-C17-C18 |
| 22  | R     | 309 | CLA  | C15-C16-C17-C18 |
| 21  | g     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 21  | G     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 21  | N     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 21  | Y     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 26  | g     | 619 | LHG  | O1-C1-C2-O2     |
| 26  | d     | 408 | LHG  | O1-C1-C2-O2     |
| 26  | D     | 409 | LHG  | O1-C1-C2-O2     |
| 26  | r     | 302 | LHG  | O1-C1-C2-O2     |
| 26  | R     | 301 | LHG  | O1-C1-C2-O2     |
| 26  | n     | 617 | LHG  | C7-C8-C9-C10    |
| 26  | N     | 618 | LHG  | C7-C8-C9-C10    |
| 26  | b     | 619 | LHG  | C23-C24-C25-C26 |
| 26  | c     | 520 | LHG  | C7-C8-C9-C10    |
| 26  | d     | 409 | LHG  | C23-C24-C25-C26 |
| 26  | B     | 622 | LHG  | C23-C24-C25-C26 |
| 26  | C     | 520 | LHG  | C7-C8-C9-C10    |
| 26  | D     | 410 | LHG  | C23-C24-C25-C26 |
| 26  | s     | 314 | LHG  | C7-C8-C9-C10    |
| 26  | S     | 314 | LHG  | C7-C8-C9-C10    |
| 35  | c     | 517 | DGD  | C1B-C2B-C3B-C4B |
| 35  | h     | 102 | DGD  | C1B-C2B-C3B-C4B |
| 35  | C     | 518 | DGD  | C1B-C2B-C3B-C4B |
| 35  | H     | 102 | DGD  | C1B-C2B-C3B-C4B |
| 36  | M     | 101 | LMG  | C4-C5-C6-O5     |
| 36  | T     | 101 | LMG  | C4-C5-C6-O5     |
| 22  | b     | 614 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 617 | CLA  | C15-C16-C17-C18 |
| 22  | r     | 310 | CLA  | C10-C11-C12-C13 |
| 22  | R     | 309 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | d     | 410 | LMG  | C29-C28-O8-C9   |
| 21  | n     | 605 | CHL  | C2-C1-O2A-CGA   |
| 21  | y     | 606 | CHL  | C2-C1-O2A-CGA   |
| 21  | N     | 605 | CHL  | C2-C1-O2A-CGA   |
| 21  | g     | 601 | CHL  | C13-C15-C16-C17 |
| 21  | n     | 601 | CHL  | C13-C15-C16-C17 |
| 21  | y     | 601 | CHL  | C13-C15-C16-C17 |
| 21  | G     | 601 | CHL  | C13-C15-C16-C17 |
| 21  | N     | 601 | CHL  | C13-C15-C16-C17 |
| 21  | Y     | 601 | CHL  | C13-C15-C16-C17 |
| 22  | b     | 609 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 612 | CLA  | C10-C11-C12-C13 |
| 26  | s     | 314 | LHG  | C23-C24-C25-C26 |
| 26  | S     | 314 | LHG  | C23-C24-C25-C26 |
| 36  | w     | 102 | LMG  | C28-C29-C30-C31 |
| 36  | C     | 502 | LMG  | C28-C29-C30-C31 |
| 37  | f     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 37  | F     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 22  | b     | 604 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 503 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 607 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 504 | CLA  | C13-C15-C16-C17 |
| 22  | g     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 609 | CLA  | C6-C7-C8-C10    |
| 22  | y     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | N     | 609 | CLA  | C6-C7-C8-C10    |
| 22  | Y     | 609 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 610 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 613 | CLA  | C11-C10-C8-C7   |
| 22  | a     | 408 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 409 | CLA  | C3-C5-C6-C7     |
| 24  | g     | 617 | XAT  | C9-C10-C11-C12  |
| 24  | y     | 615 | XAT  | C9-C10-C11-C12  |
| 24  | G     | 617 | XAT  | C9-C10-C11-C12  |
| 24  | Y     | 615 | XAT  | C9-C10-C11-C12  |
| 25  | g     | 618 | NEX  | C13-C14-C15-C35 |
| 22  | C     | 507 | CLA  | CBD-CGD-O2D-CED |
| 22  | S     | 313 | CLA  | CBD-CGD-O2D-CED |
| 36  | D     | 411 | LMG  | C29-C28-O8-C9   |
| 22  | b     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 609 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 22  | s     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 406 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 407 | CLA  | O1D-CGD-O2D-CED |
| 21  | g     | 608 | CHL  | C8-C10-C11-C12  |
| 21  | n     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | y     | 608 | CHL  | C8-C10-C11-C12  |
| 21  | G     | 608 | CHL  | C8-C10-C11-C12  |
| 21  | N     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | Y     | 607 | CHL  | C8-C10-C11-C12  |
| 21  | r     | 306 | CHL  | C10-C11-C12-C13 |
| 21  | R     | 305 | CHL  | C10-C11-C12-C13 |
| 22  | s     | 310 | CLA  | C5-C6-C7-C8     |
| 22  | S     | 310 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 617 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 506 | CLA  | CBD-CGD-O2D-CED |
| 22  | s     | 313 | CLA  | CBD-CGD-O2D-CED |
| 26  | c     | 522 | LHG  | C23-C24-C25-C26 |
| 26  | d     | 407 | LHG  | C7-C8-C9-C10    |
| 26  | C     | 522 | LHG  | C23-C24-C25-C26 |
| 26  | D     | 408 | LHG  | C7-C8-C9-C10    |
| 31  | k     | 102 | BCR  | C10-C11-C12-C13 |
| 31  | B     | 602 | BCR  | C18-C19-C20-C21 |
| 31  | K     | 102 | BCR  | C10-C11-C12-C13 |
| 31  | T     | 102 | BCR  | C18-C19-C20-C21 |
| 26  | s     | 314 | LHG  | O2-C2-C3-O3     |
| 26  | S     | 314 | LHG  | O2-C2-C3-O3     |
| 21  | r     | 307 | CHL  | C3-C5-C6-C7     |
| 21  | R     | 306 | CHL  | C3-C5-C6-C7     |
| 21  | g     | 609 | CHL  | C8-C10-C11-C12  |
| 21  | G     | 609 | CHL  | C8-C10-C11-C12  |
| 22  | d     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 405 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 503 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 506 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 509 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 504 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 507 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 510 | CLA  | C5-C6-C7-C8     |
| 21  | y     | 609 | CHL  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 606 | CLA  | C15-C16-C17-C18 |
| 26  | g     | 619 | LHG  | C3-O3-P-O6      |
| 26  | G     | 618 | LHG  | C3-O3-P-O6      |
| 26  | G     | 618 | LHG  | C4-O6-P-O3      |
| 26  | N     | 618 | LHG  | C3-O3-P-O6      |
| 26  | Y     | 617 | LHG  | C3-O3-P-O6      |
| 26  | Y     | 617 | LHG  | C4-O6-P-O3      |
| 26  | b     | 619 | LHG  | C4-O6-P-O3      |
| 26  | c     | 520 | LHG  | C4-O6-P-O3      |
| 26  | c     | 521 | LHG  | C3-O3-P-O6      |
| 26  | d     | 409 | LHG  | C3-O3-P-O6      |
| 26  | B     | 622 | LHG  | C4-O6-P-O3      |
| 26  | C     | 520 | LHG  | C4-O6-P-O3      |
| 26  | C     | 521 | LHG  | C3-O3-P-O6      |
| 26  | D     | 410 | LHG  | C3-O3-P-O6      |
| 26  | G     | 618 | LHG  | C23-C24-C25-C26 |
| 22  | b     | 607 | CLA  | O1D-CGD-O2D-CED |
| 22  | Y     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | g     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 610 | CLA  | O1D-CGD-O2D-CED |
| 26  | g     | 619 | LHG  | C1-C2-C3-O3     |
| 26  | y     | 617 | LHG  | C1-C2-C3-O3     |
| 26  | G     | 618 | LHG  | C1-C2-C3-O3     |
| 26  | s     | 314 | LHG  | C1-C2-C3-O3     |
| 26  | S     | 314 | LHG  | C1-C2-C3-O3     |
| 35  | c     | 518 | DGD  | O1B-C1B-O2G-C2G |
| 35  | C     | 519 | DGD  | O1B-C1B-O2G-C2G |
| 21  | g     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | n     | 606 | CHL  | C4-C3-C5-C6     |
| 21  | y     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | G     | 607 | CHL  | C4-C3-C5-C6     |
| 21  | N     | 606 | CHL  | C4-C3-C5-C6     |
| 21  | Y     | 606 | CHL  | C4-C3-C5-C6     |
| 22  | d     | 403 | CLA  | C4-C3-C5-C6     |
| 22  | D     | 404 | CLA  | C4-C3-C5-C6     |
| 22  | R     | 309 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 502 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 508 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 503 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 509 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 612 | CLA  | O1D-CGD-O2D-CED |
| 21  | s     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 21  | S     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 21  | r     | 307 | CHL  | C6-C7-C8-C10    |
| 21  | R     | 306 | CHL  | C6-C7-C8-C10    |
| 22  | b     | 611 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 513 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 614 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 514 | CLA  | C16-C17-C18-C20 |
| 36  | b     | 620 | LMG  | O6-C5-C6-O5     |
| 36  | B     | 623 | LMG  | O6-C5-C6-O5     |
| 22  | b     | 609 | CLA  | O1D-CGD-O2D-CED |
| 22  | g     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 22  | w     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 22  | W     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 26  | d     | 407 | LHG  | C24-C23-O8-C6   |
| 26  | D     | 408 | LHG  | C24-C23-O8-C6   |
| 21  | S     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 31  | k     | 101 | BCR  | C14-C15-C16-C17 |
| 31  | K     | 101 | BCR  | C14-C15-C16-C17 |
| 22  | r     | 312 | CLA  | C5-C6-C7-C8     |
| 22  | R     | 311 | CLA  | C5-C6-C7-C8     |
| 24  | g     | 617 | XAT  | C33-C34-C35-C15 |
| 25  | g     | 618 | NEX  | C9-C10-C11-C12  |
| 25  | Y     | 616 | NEX  | C29-C30-C31-C32 |
| 31  | k     | 101 | BCR  | C19-C20-C21-C22 |
| 31  | K     | 101 | BCR  | C19-C20-C21-C22 |
| 26  | l     | 102 | LHG  | C23-C24-C25-C26 |
| 26  | L     | 103 | LHG  | C23-C24-C25-C26 |
| 26  | N     | 618 | LHG  | C29-C30-C31-C32 |
| 26  | Y     | 617 | LHG  | C32-C33-C34-C35 |
| 36  | c     | 523 | LMG  | C11-C12-C13-C14 |
| 36  | B     | 601 | LMG  | C30-C31-C32-C33 |
| 36  | I     | 101 | LMG  | C30-C31-C32-C33 |
| 21  | s     | 302 | CHL  | O1D-CGD-O2D-CED |
| 21  | S     | 302 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | N     | 618 | LHG  | C8-C7-O7-C5     |
| 21  | R     | 306 | CHL  | C5-C6-C7-C8     |
| 23  | N     | 615 | LUT  | C11-C10-C9-C19  |
| 23  | r     | 313 | LUT  | C39-C29-C30-C31 |
| 23  | R     | 312 | LUT  | C39-C29-C30-C31 |
| 24  | g     | 617 | XAT  | C20-C13-C14-C15 |
| 24  | g     | 617 | XAT  | C40-C33-C34-C35 |
| 24  | y     | 615 | XAT  | C40-C33-C34-C35 |
| 24  | G     | 617 | XAT  | C40-C33-C34-C35 |
| 24  | Y     | 615 | XAT  | C20-C13-C14-C15 |
| 24  | Y     | 615 | XAT  | C40-C33-C34-C35 |
| 24  | r     | 314 | XAT  | C11-C10-C9-C19  |
| 24  | r     | 314 | XAT  | C39-C29-C30-C31 |
| 24  | R     | 313 | XAT  | C11-C10-C9-C19  |
| 24  | R     | 313 | XAT  | C39-C29-C30-C31 |
| 25  | y     | 616 | NEX  | C40-C33-C34-C35 |
| 25  | y     | 618 | NEX  | C40-C33-C34-C35 |
| 25  | N     | 617 | NEX  | C11-C10-C9-C19  |
| 25  | r     | 315 | NEX  | C40-C33-C34-C35 |
| 31  | c     | 516 | BCR  | C20-C21-C22-C37 |
| 31  | B     | 602 | BCR  | C11-C10-C9-C34  |
| 31  | C     | 517 | BCR  | C20-C21-C22-C37 |
| 31  | T     | 102 | BCR  | C11-C10-C9-C34  |
| 26  | b     | 619 | LHG  | C32-C33-C34-C35 |
| 26  | c     | 520 | LHG  | C27-C28-C29-C30 |
| 26  | c     | 521 | LHG  | C11-C10-C9-C8   |
| 26  | d     | 408 | LHG  | C27-C28-C29-C30 |
| 26  | d     | 408 | LHG  | C32-C33-C34-C35 |
| 26  | d     | 409 | LHG  | C27-C28-C29-C30 |
| 26  | B     | 622 | LHG  | C32-C33-C34-C35 |
| 26  | C     | 520 | LHG  | C27-C28-C29-C30 |
| 26  | C     | 521 | LHG  | C11-C10-C9-C8   |
| 26  | D     | 409 | LHG  | C27-C28-C29-C30 |
| 26  | D     | 410 | LHG  | C27-C28-C29-C30 |
| 26  | r     | 302 | LHG  | C32-C33-C34-C35 |
| 26  | R     | 301 | LHG  | C12-C13-C14-C15 |
| 26  | R     | 301 | LHG  | C32-C33-C34-C35 |
| 36  | C     | 523 | LMG  | C11-C12-C13-C14 |
| 36  | M     | 101 | LMG  | C17-C18-C19-C20 |
| 36  | T     | 101 | LMG  | C17-C18-C19-C20 |
| 22  | d     | 404 | CLA  | C16-C17-C18-C20 |
| 22  | D     | 405 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | S     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 502 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 503 | CLA  | CBA-CGA-O2A-C1  |
| 26  | n     | 617 | LHG  | C24-C25-C26-C27 |
| 26  | c     | 521 | LHG  | C18-C19-C20-C21 |
| 26  | C     | 521 | LHG  | C18-C19-C20-C21 |
| 26  | D     | 409 | LHG  | C32-C33-C34-C35 |
| 26  | r     | 302 | LHG  | C12-C13-C14-C15 |
| 33  | a     | 411 | SQD  | C26-C27-C28-C29 |
| 33  | A     | 412 | SQD  | C26-C27-C28-C29 |
| 35  | c     | 519 | DGD  | C5B-C6B-C7B-C8B |
| 35  | h     | 102 | DGD  | C5A-C6A-C7A-C8A |
| 35  | H     | 102 | DGD  | C5A-C6A-C7A-C8A |
| 35  | J     | 101 | DGD  | C5B-C6B-C7B-C8B |
| 36  | b     | 620 | LMG  | C22-C23-C24-C25 |
| 36  | B     | 623 | LMG  | C22-C23-C24-C25 |
| 36  | M     | 101 | LMG  | C33-C34-C35-C36 |
| 36  | T     | 101 | LMG  | C33-C34-C35-C36 |
| 33  | a     | 411 | SQD  | C46-C45-O47-C7  |
| 33  | A     | 412 | SQD  | C46-C45-O47-C7  |
| 22  | c     | 511 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 512 | CLA  | O1D-CGD-O2D-CED |
| 21  | r     | 307 | CHL  | C5-C6-C7-C8     |
| 26  | g     | 619 | LHG  | C26-C27-C28-C29 |
| 26  | b     | 619 | LHG  | C29-C30-C31-C32 |
| 26  | d     | 409 | LHG  | C10-C11-C12-C13 |
| 26  | B     | 622 | LHG  | C29-C30-C31-C32 |
| 36  | T     | 101 | LMG  | C30-C31-C32-C33 |
| 22  | g     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | y     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 26  | G     | 618 | LHG  | C29-C30-C31-C32 |
| 26  | N     | 618 | LHG  | C15-C16-C17-C18 |
| 26  | c     | 520 | LHG  | C12-C13-C14-C15 |
| 26  | d     | 408 | LHG  | C30-C31-C32-C33 |
| 26  | C     | 520 | LHG  | C12-C13-C14-C15 |
| 26  | D     | 409 | LHG  | C30-C31-C32-C33 |
| 26  | D     | 410 | LHG  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | c     | 519 | DGD  | C6B-C7B-C8B-C9B |
| 35  | J     | 101 | DGD  | C6B-C7B-C8B-C9B |
| 36  | b     | 620 | LMG  | C19-C20-C21-C22 |
| 36  | B     | 623 | LMG  | C19-C20-C21-C22 |
| 36  | M     | 101 | LMG  | C30-C31-C32-C33 |
| 22  | C     | 512 | CLA  | C5-C6-C7-C8     |
| 26  | C     | 520 | LHG  | O2-C2-C3-O3     |
| 35  | h     | 102 | DGD  | C4A-C5A-C6A-C7A |
| 35  | h     | 102 | DGD  | C3B-C4B-C5B-C6B |
| 35  | H     | 102 | DGD  | C4A-C5A-C6A-C7A |
| 35  | H     | 102 | DGD  | C3B-C4B-C5B-C6B |
| 22  | g     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | n     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | y     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | G     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | N     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | Y     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | s     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | s     | 311 | CLA  | C3-C5-C6-C7     |
| 22  | S     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | S     | 311 | CLA  | C3-C5-C6-C7     |
| 23  | G     | 616 | LUT  | C12-C13-C14-C15 |
| 23  | N     | 615 | LUT  | C11-C10-C9-C8   |
| 23  | N     | 615 | LUT  | C28-C29-C30-C31 |
| 23  | N     | 615 | LUT  | C32-C33-C34-C35 |
| 23  | Y     | 614 | LUT  | C28-C29-C30-C31 |
| 24  | g     | 617 | XAT  | C11-C10-C9-C8   |
| 24  | g     | 617 | XAT  | C12-C13-C14-C15 |
| 24  | g     | 617 | XAT  | C32-C33-C34-C35 |
| 24  | n     | 615 | XAT  | C11-C10-C9-C8   |
| 24  | n     | 615 | XAT  | C12-C13-C14-C15 |
| 24  | y     | 615 | XAT  | C12-C13-C14-C15 |
| 24  | G     | 617 | XAT  | C11-C10-C9-C8   |
| 24  | G     | 617 | XAT  | C12-C13-C14-C15 |
| 24  | N     | 616 | XAT  | C11-C10-C9-C8   |
| 24  | N     | 616 | XAT  | C12-C13-C14-C15 |
| 24  | N     | 616 | XAT  | C32-C33-C34-C35 |
| 24  | Y     | 615 | XAT  | C12-C13-C14-C15 |
| 24  | r     | 314 | XAT  | C28-C29-C30-C31 |
| 24  | R     | 313 | XAT  | C28-C29-C30-C31 |
| 25  | n     | 616 | NEX  | C11-C10-C9-C8   |
| 25  | n     | 616 | NEX  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | y     | 616 | NEX  | C32-C33-C34-C35 |
| 25  | y     | 618 | NEX  | C32-C33-C34-C35 |
| 25  | N     | 617 | NEX  | C11-C10-C9-C8   |
| 25  | r     | 315 | NEX  | C32-C33-C34-C35 |
| 31  | k     | 101 | BCR  | C16-C17-C18-C19 |
| 31  | k     | 101 | BCR  | C20-C21-C22-C23 |
| 31  | B     | 602 | BCR  | C11-C10-C9-C8   |
| 31  | K     | 101 | BCR  | C16-C17-C18-C19 |
| 31  | K     | 101 | BCR  | C20-C21-C22-C23 |
| 31  | T     | 102 | BCR  | C11-C10-C9-C8   |
| 35  | a     | 413 | DGD  | C2E-C1E-O5D-C6D |
| 35  | c     | 518 | DGD  | C2D-C1D-O3G-C3G |
| 35  | A     | 401 | DGD  | C2E-C1E-O5D-C6D |
| 35  | C     | 519 | DGD  | C2D-C1D-O3G-C3G |
| 22  | s     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 22  | S     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 26  | N     | 618 | LHG  | C24-C23-O8-C6   |
| 26  | g     | 619 | LHG  | C28-C29-C30-C31 |
| 26  | d     | 408 | LHG  | C11-C10-C9-C8   |
| 26  | d     | 408 | LHG  | C29-C30-C31-C32 |
| 26  | l     | 102 | LHG  | C25-C26-C27-C28 |
| 26  | D     | 409 | LHG  | C11-C10-C9-C8   |
| 26  | D     | 409 | LHG  | C29-C30-C31-C32 |
| 26  | L     | 103 | LHG  | C25-C26-C27-C28 |
| 26  | r     | 302 | LHG  | C27-C28-C29-C30 |
| 26  | s     | 314 | LHG  | C27-C28-C29-C30 |
| 26  | S     | 314 | LHG  | C27-C28-C29-C30 |
| 26  | R     | 301 | LHG  | C27-C28-C29-C30 |
| 33  | d     | 402 | SQD  | C12-C13-C14-C15 |
| 33  | D     | 402 | SQD  | C12-C13-C14-C15 |
| 36  | c     | 523 | LMG  | C33-C34-C35-C36 |
| 36  | C     | 523 | LMG  | C33-C34-C35-C36 |
| 36  | T     | 101 | LMG  | C29-C30-C31-C32 |
| 22  | c     | 511 | CLA  | C5-C6-C7-C8     |
| 22  | g     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 22  | w     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 22  | W     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 26  | r     | 302 | LHG  | O10-C23-O8-C6   |
| 26  | R     | 301 | LHG  | O10-C23-O8-C6   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | r     | 306 | CHL  | C16-C17-C18-C20 |
| 21  | R     | 305 | CHL  | C16-C17-C18-C20 |
| 22  | a     | 405 | CLA  | C16-C17-C18-C20 |
| 22  | d     | 404 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 406 | CLA  | C16-C17-C18-C20 |
| 22  | D     | 405 | CLA  | C16-C17-C18-C19 |
| 22  | s     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | s     | 313 | CLA  | C6-C7-C8-C10    |
| 22  | S     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | S     | 313 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 512 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 513 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 514 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 515 | CLA  | C4-C3-C5-C6     |
| 26  | n     | 617 | LHG  | C30-C31-C32-C33 |
| 26  | b     | 619 | LHG  | C11-C12-C13-C14 |
| 26  | c     | 521 | LHG  | C29-C30-C31-C32 |
| 26  | B     | 622 | LHG  | C11-C12-C13-C14 |
| 26  | C     | 521 | LHG  | C29-C30-C31-C32 |
| 35  | h     | 102 | DGD  | C5B-C6B-C7B-C8B |
| 35  | H     | 102 | DGD  | C5B-C6B-C7B-C8B |
| 35  | J     | 101 | DGD  | C6A-C7A-C8A-C9A |
| 36  | M     | 101 | LMG  | C29-C30-C31-C32 |
| 21  | g     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | n     | 606 | CHL  | C2-C3-C5-C6     |
| 21  | y     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | G     | 607 | CHL  | C2-C3-C5-C6     |
| 21  | N     | 606 | CHL  | C2-C3-C5-C6     |
| 21  | Y     | 606 | CHL  | C2-C3-C5-C6     |
| 22  | g     | 612 | CLA  | C11-C10-C8-C9   |
| 22  | n     | 611 | CLA  | C11-C10-C8-C9   |
| 22  | G     | 612 | CLA  | C11-C10-C8-C9   |
| 22  | N     | 611 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 505 | CLA  | C11-C10-C8-C9   |
| 22  | d     | 404 | CLA  | C14-C13-C15-C16 |
| 22  | w     | 101 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 506 | CLA  | C11-C10-C8-C9   |
| 22  | D     | 405 | CLA  | C14-C13-C15-C16 |
| 22  | W     | 101 | CLA  | C11-C10-C8-C9   |
| 30  | d     | 401 | PHO  | C11-C10-C8-C9   |
| 30  | d     | 401 | PHO  | C14-C13-C15-C16 |
| 30  | D     | 401 | PHO  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | D     | 401 | PHO  | C14-C13-C15-C16 |
| 35  | a     | 413 | DGD  | O6D-C5D-C6D-O5D |
| 33  | A     | 412 | SQD  | C23-C24-C25-C26 |
| 26  | n     | 617 | LHG  | C28-C29-C30-C31 |
| 26  | y     | 617 | LHG  | C29-C30-C31-C32 |
| 26  | N     | 618 | LHG  | C24-C25-C26-C27 |
| 26  | N     | 618 | LHG  | C27-C28-C29-C30 |
| 26  | b     | 619 | LHG  | C30-C31-C32-C33 |
| 26  | b     | 619 | LHG  | C33-C34-C35-C36 |
| 26  | c     | 521 | LHG  | C27-C28-C29-C30 |
| 26  | c     | 522 | LHG  | C9-C10-C11-C12  |
| 26  | B     | 622 | LHG  | C30-C31-C32-C33 |
| 26  | B     | 622 | LHG  | C33-C34-C35-C36 |
| 26  | C     | 521 | LHG  | C27-C28-C29-C30 |
| 26  | C     | 522 | LHG  | C9-C10-C11-C12  |
| 35  | c     | 518 | DGD  | C7A-C8A-C9A-CAA |
| 35  | c     | 519 | DGD  | C6A-C7A-C8A-C9A |
| 35  | C     | 519 | DGD  | C7A-C8A-C9A-CAA |
| 36  | b     | 620 | LMG  | C20-C21-C22-C23 |
| 36  | B     | 623 | LMG  | C20-C21-C22-C23 |
| 22  | a     | 404 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 405 | CLA  | C15-C16-C17-C18 |
| 21  | Y     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 22  | s     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 22  | S     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 23  | g     | 616 | LUT  | C27-C28-C29-C39 |
| 23  | G     | 616 | LUT  | C27-C28-C29-C39 |
| 23  | r     | 313 | LUT  | C11-C12-C13-C20 |
| 23  | R     | 312 | LUT  | C11-C12-C13-C20 |
| 24  | g     | 617 | XAT  | C11-C12-C13-C20 |
| 24  | n     | 615 | XAT  | C31-C32-C33-C40 |
| 24  | G     | 617 | XAT  | C11-C12-C13-C20 |
| 24  | N     | 616 | XAT  | C31-C32-C33-C40 |
| 24  | r     | 314 | XAT  | C11-C12-C13-C20 |
| 24  | r     | 314 | XAT  | C27-C28-C29-C39 |
| 24  | R     | 313 | XAT  | C11-C12-C13-C20 |
| 25  | n     | 616 | NEX  | C27-C28-C29-C39 |
| 25  | y     | 616 | NEX  | C27-C28-C29-C39 |
| 21  | S     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 26  | Y     | 617 | LHG  | C27-C28-C29-C30 |
| 26  | c     | 520 | LHG  | C32-C33-C34-C35 |
| 26  | C     | 520 | LHG  | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | c     | 519 | DGD  | C2B-C3B-C4B-C5B |
| 35  | J     | 101 | DGD  | C2B-C3B-C4B-C5B |
| 36  | k     | 103 | LMG  | C32-C33-C34-C35 |
| 36  | B     | 623 | LMG  | C16-C17-C18-C19 |
| 36  | K     | 103 | LMG  | C32-C33-C34-C35 |
| 26  | G     | 618 | LHG  | O1-C1-C2-C3     |
| 26  | c     | 520 | LHG  | O1-C1-C2-C3     |
| 26  | d     | 407 | LHG  | O1-C1-C2-C3     |
| 26  | C     | 520 | LHG  | O1-C1-C2-C3     |
| 26  | D     | 408 | LHG  | O1-C1-C2-C3     |
| 26  | s     | 314 | LHG  | O1-C1-C2-C3     |
| 26  | S     | 314 | LHG  | O1-C1-C2-C3     |
| 23  | g     | 615 | LUT  | C31-C32-C33-C34 |
| 23  | n     | 614 | LUT  | C31-C32-C33-C34 |
| 23  | y     | 614 | LUT  | C31-C32-C33-C34 |
| 23  | G     | 615 | LUT  | C31-C32-C33-C34 |
| 23  | N     | 614 | LUT  | C31-C32-C33-C34 |
| 23  | Y     | 613 | LUT  | C31-C32-C33-C34 |
| 24  | y     | 615 | XAT  | C11-C12-C13-C14 |
| 22  | a     | 405 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 512 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 406 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 513 | CLA  | C3-C5-C6-C7     |
| 36  | b     | 620 | LMG  | O9-C10-O7-C8    |
| 36  | B     | 623 | LMG  | O9-C10-O7-C8    |
| 22  | y     | 612 | CLA  | C15-C16-C17-C18 |
| 26  | s     | 314 | LHG  | C8-C7-O7-C5     |
| 26  | S     | 314 | LHG  | C8-C7-O7-C5     |
| 21  | s     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 26  | n     | 617 | LHG  | C12-C13-C14-C15 |
| 26  | s     | 314 | LHG  | C32-C33-C34-C35 |
| 26  | S     | 314 | LHG  | C32-C33-C34-C35 |
| 36  | b     | 620 | LMG  | C16-C17-C18-C19 |
| 33  | a     | 411 | SQD  | C23-C24-C25-C26 |
| 26  | g     | 619 | LHG  | C30-C31-C32-C33 |
| 26  | G     | 618 | LHG  | C25-C26-C27-C28 |
| 26  | N     | 618 | LHG  | C10-C11-C12-C13 |
| 26  | c     | 522 | LHG  | C32-C33-C34-C35 |
| 33  | l     | 103 | SQD  | C9-C10-C11-C12  |
| 33  | L     | 101 | SQD  | C9-C10-C11-C12  |
| 36  | c     | 523 | LMG  | C14-C15-C16-C17 |
| 36  | d     | 410 | LMG  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | k     | 103 | LMG  | C38-C39-C40-C41 |
| 36  | C     | 523 | LMG  | C14-C15-C16-C17 |
| 36  | D     | 411 | LMG  | C15-C16-C17-C18 |
| 36  | K     | 103 | LMG  | C38-C39-C40-C41 |
| 36  | M     | 101 | LMG  | C32-C33-C34-C35 |
| 36  | T     | 101 | LMG  | C32-C33-C34-C35 |
| 35  | A     | 401 | DGD  | O6D-C5D-C6D-O5D |
| 21  | r     | 307 | CHL  | C6-C7-C8-C9     |
| 21  | R     | 306 | CHL  | C6-C7-C8-C9     |
| 22  | b     | 611 | CLA  | C16-C17-C18-C19 |
| 22  | x     | 101 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 603 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 614 | CLA  | C16-C17-C18-C19 |
| 35  | a     | 413 | DGD  | O6E-C1E-O5D-C6D |
| 35  | A     | 401 | DGD  | O6E-C1E-O5D-C6D |
| 26  | b     | 619 | LHG  | C26-C27-C28-C29 |
| 26  | B     | 622 | LHG  | C26-C27-C28-C29 |
| 26  | C     | 522 | LHG  | C32-C33-C34-C35 |
| 33  | l     | 103 | SQD  | C27-C28-C29-C30 |
| 33  | L     | 101 | SQD  | C27-C28-C29-C30 |
| 35  | a     | 413 | DGD  | C8A-C9A-CAA-CBA |
| 35  | A     | 401 | DGD  | C8A-C9A-CAA-CBA |
| 36  | b     | 620 | LMG  | C34-C35-C36-C37 |
| 36  | B     | 623 | LMG  | C34-C35-C36-C37 |
| 35  | a     | 413 | DGD  | C4D-C5D-C6D-O5D |
| 35  | A     | 401 | DGD  | C4D-C5D-C6D-O5D |
| 26  | g     | 619 | LHG  | C11-C12-C13-C14 |
| 26  | c     | 521 | LHG  | C13-C14-C15-C16 |
| 26  | c     | 522 | LHG  | C13-C14-C15-C16 |
| 26  | C     | 521 | LHG  | C13-C14-C15-C16 |
| 26  | C     | 522 | LHG  | C13-C14-C15-C16 |
| 26  | C     | 522 | LHG  | C30-C31-C32-C33 |
| 33  | l     | 101 | SQD  | C12-C13-C14-C15 |
| 33  | L     | 102 | SQD  | C12-C13-C14-C15 |
| 35  | c     | 517 | DGD  | C4A-C5A-C6A-C7A |
| 35  | c     | 519 | DGD  | C7B-C8B-C9B-CAB |
| 35  | A     | 401 | DGD  | C4A-C5A-C6A-C7A |
| 35  | C     | 518 | DGD  | C4A-C5A-C6A-C7A |
| 35  | J     | 101 | DGD  | C7B-C8B-C9B-CAB |
| 36  | k     | 103 | LMG  | C18-C19-C20-C21 |
| 36  | k     | 103 | LMG  | C30-C31-C32-C33 |
| 36  | K     | 103 | LMG  | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | K     | 103 | LMG  | C30-C31-C32-C33 |
| 36  | M     | 101 | LMG  | C16-C17-C18-C19 |
| 36  | T     | 101 | LMG  | C16-C17-C18-C19 |
| 26  | c     | 522 | LHG  | C30-C31-C32-C33 |
| 33  | a     | 411 | SQD  | C14-C15-C16-C17 |
| 33  | A     | 412 | SQD  | C14-C15-C16-C17 |
| 35  | a     | 413 | DGD  | C4A-C5A-C6A-C7A |
| 36  | b     | 620 | LMG  | C31-C32-C33-C34 |
| 36  | B     | 623 | LMG  | C31-C32-C33-C34 |
| 22  | c     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 26  | n     | 617 | LHG  | C24-C23-O8-C6   |
| 26  | G     | 618 | LHG  | C16-C17-C18-C19 |
| 26  | s     | 314 | LHG  | C30-C31-C32-C33 |
| 26  | S     | 314 | LHG  | C30-C31-C32-C33 |
| 35  | a     | 413 | DGD  | C2A-C3A-C4A-C5A |
| 35  | A     | 401 | DGD  | C2A-C3A-C4A-C5A |
| 21  | g     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 21  | y     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 21  | G     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 21  | r     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 21  | r     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 21  | r     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 21  | S     | 301 | CHL  | C3A-C2A-CAA-CBA |
| 21  | R     | 305 | CHL  | C3A-C2A-CAA-CBA |
| 21  | R     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 22  | g     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 22  | g     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | n     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 22  | n     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | y     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 22  | y     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | N     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 22  | N     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Y     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Y     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 511 | CLA  | C3A-C2A-CAA-CBA |
| 22  | x     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 617 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 22  | s     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 22  | S     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 30  | a     | 407 | PHO  | C3A-C2A-CAA-CBA |
| 30  | A     | 408 | PHO  | C3A-C2A-CAA-CBA |
| 22  | g     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | n     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | y     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | G     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | N     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | Y     | 603 | CLA  | C8-C10-C11-C12  |
| 30  | a     | 407 | PHO  | C5-C6-C7-C8     |
| 30  | A     | 408 | PHO  | C5-C6-C7-C8     |
| 24  | g     | 617 | XAT  | C29-C30-C31-C32 |
| 26  | b     | 619 | LHG  | C27-C28-C29-C30 |
| 26  | B     | 622 | LHG  | C27-C28-C29-C30 |
| 35  | c     | 519 | DGD  | C4A-C5A-C6A-C7A |
| 35  | J     | 101 | DGD  | C4A-C5A-C6A-C7A |
| 36  | b     | 620 | LMG  | C15-C16-C17-C18 |
| 36  | k     | 103 | LMG  | C29-C30-C31-C32 |
| 36  | K     | 103 | LMG  | C29-C30-C31-C32 |
| 26  | c     | 520 | LHG  | O10-C23-O8-C6   |
| 26  | C     | 520 | LHG  | O10-C23-O8-C6   |
| 22  | x     | 101 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 603 | CLA  | C16-C17-C18-C20 |
| 21  | s     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 26  | l     | 102 | LHG  | C12-C13-C14-C15 |
| 26  | D     | 410 | LHG  | C29-C30-C31-C32 |
| 26  | L     | 103 | LHG  | C12-C13-C14-C15 |
| 36  | b     | 620 | LMG  | C38-C39-C40-C41 |
| 36  | B     | 623 | LMG  | C15-C16-C17-C18 |
| 36  | B     | 623 | LMG  | C38-C39-C40-C41 |
| 36  | M     | 101 | LMG  | C34-C35-C36-C37 |
| 36  | T     | 101 | LMG  | C34-C35-C36-C37 |
| 26  | d     | 409 | LHG  | C29-C30-C31-C32 |
| 33  | a     | 411 | SQD  | C11-C12-C13-C14 |
| 33  | A     | 412 | SQD  | C11-C12-C13-C14 |
| 36  | c     | 523 | LMG  | C19-C20-C21-C22 |
| 36  | C     | 523 | LMG  | C19-C20-C21-C22 |
| 33  | l     | 103 | SQD  | C25-C26-C27-C28 |
| 33  | L     | 101 | SQD  | C25-C26-C27-C28 |
| 22  | d     | 404 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | D     | 405 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 514 | CLA  | CBA-CGA-O2A-C1  |
| 26  | r     | 302 | LHG  | C5-C6-O8-C23    |
| 26  | R     | 301 | LHG  | C5-C6-O8-C23    |
| 26  | g     | 619 | LHG  | C29-C30-C31-C32 |
| 26  | n     | 617 | LHG  | O1-C1-C2-O2     |
| 26  | N     | 618 | LHG  | O1-C1-C2-O2     |
| 26  | c     | 522 | LHG  | O1-C1-C2-O2     |
| 26  | C     | 522 | LHG  | O1-C1-C2-O2     |
| 36  | c     | 523 | LMG  | C12-C13-C14-C15 |
| 36  | k     | 103 | LMG  | C16-C17-C18-C19 |
| 36  | C     | 523 | LMG  | C12-C13-C14-C15 |
| 36  | K     | 103 | LMG  | C16-C17-C18-C19 |
| 22  | a     | 405 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 406 | CLA  | C16-C17-C18-C19 |
| 26  | d     | 409 | LHG  | C15-C16-C17-C18 |
| 26  | c     | 520 | LHG  | O2-C2-C3-O3     |
| 22  | Y     | 612 | CLA  | O1D-CGD-O2D-CED |
| 26  | D     | 410 | LHG  | C15-C16-C17-C18 |
| 26  | c     | 520 | LHG  | C30-C31-C32-C33 |
| 36  | M     | 101 | LMG  | C28-C29-C30-C31 |
| 36  | T     | 101 | LMG  | C28-C29-C30-C31 |
| 26  | g     | 619 | LHG  | C33-C34-C35-C36 |
| 26  | C     | 520 | LHG  | C30-C31-C32-C33 |
| 26  | N     | 618 | LHG  | O9-C7-O7-C5     |
| 22  | n     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 614 | CLA  | O1D-CGD-O2D-CED |
| 26  | n     | 617 | LHG  | C11-C12-C13-C14 |
| 26  | G     | 618 | LHG  | C17-C18-C19-C20 |
| 35  | c     | 517 | DGD  | C2B-C3B-C4B-C5B |
| 35  | h     | 102 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 518 | DGD  | C2B-C3B-C4B-C5B |
| 35  | H     | 102 | DGD  | C4B-C5B-C6B-C7B |
| 36  | w     | 102 | LMG  | C18-C19-C20-C21 |
| 36  | C     | 502 | LMG  | C18-C19-C20-C21 |
| 22  | d     | 404 | CLA  | C10-C11-C12-C13 |
| 22  | D     | 405 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 502 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 503 | CLA  | O1A-CGA-O2A-C1  |
| 22  | s     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 22  | S     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 26  | n     | 617 | LHG  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | y     | 617 | LHG  | C27-C28-C29-C30 |
| 26  | y     | 617 | LHG  | C33-C34-C35-C36 |
| 22  | c     | 513 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 514 | CLA  | C16-C17-C18-C19 |
| 23  | g     | 615 | LUT  | C5-C6-C7-C8     |
| 23  | n     | 614 | LUT  | C5-C6-C7-C8     |
| 23  | y     | 614 | LUT  | C5-C6-C7-C8     |
| 23  | G     | 615 | LUT  | C5-C6-C7-C8     |
| 23  | N     | 614 | LUT  | C5-C6-C7-C8     |
| 23  | Y     | 613 | LUT  | C5-C6-C7-C8     |
| 31  | a     | 409 | BCR  | C1-C6-C7-C8     |
| 31  | b     | 616 | BCR  | C1-C6-C7-C8     |
| 31  | b     | 616 | BCR  | C5-C6-C7-C8     |
| 31  | c     | 515 | BCR  | C1-C6-C7-C8     |
| 31  | c     | 515 | BCR  | C5-C6-C7-C8     |
| 31  | c     | 515 | BCR  | C23-C24-C25-C30 |
| 31  | c     | 516 | BCR  | C23-C24-C25-C30 |
| 31  | d     | 405 | BCR  | C5-C6-C7-C8     |
| 31  | d     | 405 | BCR  | C23-C24-C25-C30 |
| 31  | h     | 101 | BCR  | C1-C6-C7-C8     |
| 31  | k     | 101 | BCR  | C1-C6-C7-C8     |
| 31  | k     | 102 | BCR  | C5-C6-C7-C8     |
| 31  | A     | 410 | BCR  | C1-C6-C7-C8     |
| 31  | A     | 410 | BCR  | C5-C6-C7-C8     |
| 31  | B     | 602 | BCR  | C5-C6-C7-C8     |
| 31  | B     | 619 | BCR  | C1-C6-C7-C8     |
| 31  | B     | 619 | BCR  | C5-C6-C7-C8     |
| 31  | C     | 516 | BCR  | C1-C6-C7-C8     |
| 31  | C     | 516 | BCR  | C5-C6-C7-C8     |
| 31  | C     | 516 | BCR  | C23-C24-C25-C30 |
| 31  | C     | 517 | BCR  | C23-C24-C25-C30 |
| 31  | D     | 406 | BCR  | C5-C6-C7-C8     |
| 31  | D     | 406 | BCR  | C23-C24-C25-C30 |
| 31  | H     | 101 | BCR  | C1-C6-C7-C8     |
| 31  | K     | 101 | BCR  | C1-C6-C7-C8     |
| 31  | K     | 102 | BCR  | C5-C6-C7-C8     |
| 31  | T     | 102 | BCR  | C5-C6-C7-C8     |
| 26  | s     | 314 | LHG  | C24-C25-C26-C27 |
| 22  | g     | 614 | CLA  | O1D-CGD-O2D-CED |
| 22  | y     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | N     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 503 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 26  | G     | 618 | LHG  | C24-C23-O8-C6   |
| 22  | c     | 508 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 30  | a     | 407 | PHO  | C13-C15-C16-C17 |
| 30  | A     | 408 | PHO  | C13-C15-C16-C17 |
| 33  | d     | 402 | SQD  | C8-C7-O47-C45   |
| 33  | D     | 402 | SQD  | C8-C7-O47-C45   |
| 26  | S     | 314 | LHG  | C24-C25-C26-C27 |
| 36  | k     | 103 | LMG  | C28-C29-C30-C31 |
| 36  | K     | 103 | LMG  | C28-C29-C30-C31 |
| 26  | N     | 618 | LHG  | C28-C29-C30-C31 |
| 35  | c     | 517 | DGD  | C6B-C7B-C8B-C9B |
| 35  | C     | 518 | DGD  | C6B-C7B-C8B-C9B |
| 36  | b     | 620 | LMG  | C37-C38-C39-C40 |
| 36  | B     | 623 | LMG  | C37-C38-C39-C40 |
| 26  | l     | 102 | LHG  | C32-C33-C34-C35 |
| 26  | L     | 103 | LHG  | C32-C33-C34-C35 |
| 22  | b     | 602 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 605 | CLA  | C4-C3-C5-C6     |
| 21  | r     | 308 | CHL  | C6-C7-C8-C10    |
| 21  | R     | 307 | CHL  | C6-C7-C8-C10    |
| 22  | g     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | N     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 614 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 505 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 511 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 511 | CLA  | C11-C12-C13-C15 |
| 22  | d     | 404 | CLA  | C12-C13-C15-C16 |
| 22  | w     | 101 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 617 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 506 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 512 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 512 | CLA  | C11-C12-C13-C15 |
| 22  | D     | 405 | CLA  | C12-C13-C15-C16 |
| 22  | W     | 101 | CLA  | C6-C7-C8-C10    |
| 30  | d     | 401 | PHO  | C11-C10-C8-C7   |
| 30  | d     | 401 | PHO  | C12-C13-C15-C16 |
| 30  | D     | 401 | PHO  | C11-C10-C8-C7   |
| 30  | D     | 401 | PHO  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 514 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 21  | G     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 35  | a     | 413 | DGD  | C7B-C8B-C9B-CAB |
| 35  | A     | 401 | DGD  | C7B-C8B-C9B-CAB |
| 24  | y     | 615 | XAT  | C33-C34-C35-C15 |
| 21  | G     | 608 | CHL  | C16-C17-C18-C20 |
| 21  | N     | 607 | CHL  | C16-C17-C18-C20 |
| 21  | Y     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 36  | k     | 103 | LMG  | C17-C18-C19-C20 |
| 36  | K     | 103 | LMG  | C17-C18-C19-C20 |
| 21  | g     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 21  | n     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 21  | y     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 21  | y     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 21  | G     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 21  | N     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 22  | g     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 22  | n     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | y     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | G     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 22  | N     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Y     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 22  | r     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 22  | s     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 22  | S     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 22  | R     | 309 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 613 | CLA  | C5-C6-C7-C8     |
| 21  | n     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 21  | y     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 21  | N     | 607 | CHL  | C2C-C3C-CAC-CBC |
| 26  | Y     | 617 | LHG  | C30-C31-C32-C33 |
| 22  | B     | 607 | CLA  | C8-C10-C11-C12  |
| 26  | c     | 521 | LHG  | C28-C29-C30-C31 |
| 26  | C     | 521 | LHG  | C28-C29-C30-C31 |
| 33  | a     | 411 | SQD  | C10-C11-C12-C13 |
| 33  | A     | 412 | SQD  | C10-C11-C12-C13 |
| 35  | c     | 518 | DGD  | C6A-C7A-C8A-C9A |
| 35  | C     | 519 | DGD  | C6A-C7A-C8A-C9A |
| 26  | y     | 617 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | a     | 409 | BCR  | C6-C7-C8-C9     |
| 31  | A     | 410 | BCR  | C6-C7-C8-C9     |
| 21  | g     | 608 | CHL  | C16-C17-C18-C20 |
| 21  | n     | 607 | CHL  | C16-C17-C18-C20 |
| 21  | y     | 608 | CHL  | C16-C17-C18-C20 |
| 21  | Y     | 607 | CHL  | C16-C17-C18-C20 |
| 22  | r     | 312 | CLA  | C11-C12-C13-C14 |
| 22  | R     | 311 | CLA  | C11-C12-C13-C14 |
| 21  | N     | 608 | CHL  | C13-C15-C16-C17 |
| 22  | b     | 604 | CLA  | C8-C10-C11-C12  |
| 26  | N     | 618 | LHG  | C11-C10-C9-C8   |
| 26  | Y     | 617 | LHG  | C15-C16-C17-C18 |
| 33  | l     | 103 | SQD  | C14-C15-C16-C17 |
| 33  | L     | 101 | SQD  | C14-C15-C16-C17 |
| 36  | w     | 102 | LMG  | C30-C31-C32-C33 |
| 36  | C     | 502 | LMG  | C30-C31-C32-C33 |
| 26  | d     | 409 | LHG  | C7-C8-C9-C10    |
| 26  | D     | 410 | LHG  | C7-C8-C9-C10    |
| 26  | G     | 618 | LHG  | C8-C7-O7-C5     |
| 35  | c     | 518 | DGD  | C2B-C1B-O2G-C2G |
| 35  | C     | 519 | DGD  | C2B-C1B-O2G-C2G |
| 26  | d     | 409 | LHG  | C24-C25-C26-C27 |
| 26  | r     | 302 | LHG  | C26-C27-C28-C29 |
| 26  | R     | 301 | LHG  | C26-C27-C28-C29 |
| 36  | D     | 411 | LMG  | C18-C19-C20-C21 |
| 26  | D     | 410 | LHG  | C24-C25-C26-C27 |
| 36  | d     | 410 | LMG  | C18-C19-C20-C21 |
| 26  | s     | 314 | LHG  | O9-C7-O7-C5     |
| 26  | S     | 314 | LHG  | O9-C7-O7-C5     |
| 35  | c     | 519 | DGD  | O1B-C1B-O2G-C2G |
| 35  | J     | 101 | DGD  | O1B-C1B-O2G-C2G |
| 33  | a     | 411 | SQD  | C2-C1-O6-C44    |
| 33  | A     | 412 | SQD  | C2-C1-O6-C44    |
| 26  | d     | 408 | LHG  | O7-C5-C6-O8     |
| 26  | D     | 409 | LHG  | O7-C5-C6-O8     |
| 26  | l     | 102 | LHG  | C33-C34-C35-C36 |
| 26  | L     | 103 | LHG  | C33-C34-C35-C36 |
| 26  | s     | 314 | LHG  | C15-C16-C17-C18 |
| 26  | S     | 314 | LHG  | C15-C16-C17-C18 |
| 35  | c     | 519 | DGD  | C5A-C6A-C7A-C8A |
| 35  | J     | 101 | DGD  | C5A-C6A-C7A-C8A |
| 22  | c     | 511 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 512 | CLA  | C4-C3-C5-C6     |
| 26  | n     | 617 | LHG  | C23-C24-C25-C26 |
| 22  | c     | 514 | CLA  | C2-C3-C5-C6     |
| 22  | C     | 515 | CLA  | C2-C3-C5-C6     |
| 22  | s     | 309 | CLA  | C2-C3-C5-C6     |
| 22  | S     | 309 | CLA  | C2-C3-C5-C6     |
| 32  | a     | 410 | PL9  | C4-C3-C7-C8     |
| 32  | A     | 411 | PL9  | C4-C3-C7-C8     |
| 21  | r     | 308 | CHL  | C6-C7-C8-C9     |
| 21  | R     | 307 | CHL  | C6-C7-C8-C9     |
| 22  | g     | 610 | CLA  | C6-C7-C8-C9     |
| 22  | n     | 609 | CLA  | C6-C7-C8-C9     |
| 22  | y     | 610 | CLA  | C6-C7-C8-C9     |
| 22  | G     | 610 | CLA  | C6-C7-C8-C9     |
| 22  | N     | 609 | CLA  | C6-C7-C8-C9     |
| 22  | Y     | 609 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 610 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 611 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 614 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 504 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 511 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 613 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 614 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 617 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 505 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 512 | CLA  | C11-C12-C13-C14 |
| 26  | n     | 617 | LHG  | C11-C10-C9-C8   |
| 26  | d     | 409 | LHG  | C28-C29-C30-C31 |
| 26  | D     | 410 | LHG  | C28-C29-C30-C31 |
| 33  | l     | 101 | SQD  | C10-C11-C12-C13 |
| 33  | L     | 102 | SQD  | C10-C11-C12-C13 |
| 21  | r     | 308 | CHL  | C2A-CAA-CBA-CGA |
| 21  | R     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 22  | g     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | n     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 22  | y     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 22  | G     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | N     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Y     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 21  | r     | 306 | CHL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | R     | 305 | CHL  | C8-C10-C11-C12  |
| 22  | a     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 406 | CLA  | C13-C15-C16-C17 |
| 26  | Y     | 617 | LHG  | C17-C18-C19-C20 |
| 26  | c     | 522 | LHG  | C25-C26-C27-C28 |
| 26  | l     | 102 | LHG  | C29-C30-C31-C32 |
| 26  | C     | 522 | LHG  | C25-C26-C27-C28 |
| 26  | L     | 103 | LHG  | C29-C30-C31-C32 |
| 23  | r     | 313 | LUT  | C7-C8-C9-C10    |
| 23  | R     | 312 | LUT  | C7-C8-C9-C10    |
| 22  | C     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 21  | G     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 21  | r     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 21  | r     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 21  | s     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 21  | S     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 21  | R     | 305 | CHL  | C1A-C2A-CAA-CBA |
| 21  | R     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 22  | a     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 511 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 22  | x     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 406 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 617 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 507 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 513 | CLA  | C1A-C2A-CAA-CBA |
| 22  | r     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 22  | r     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | s     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | s     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | s     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | R     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | R     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 21  | g     | 609 | CHL  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | G     | 609 | CHL  | C11-C12-C13-C15 |
| 21  | r     | 306 | CHL  | C16-C17-C18-C19 |
| 21  | R     | 305 | CHL  | C16-C17-C18-C19 |
| 22  | r     | 312 | CLA  | C11-C12-C13-C15 |
| 22  | R     | 311 | CLA  | C11-C12-C13-C15 |
| 26  | b     | 619 | LHG  | C8-C7-O7-C5     |
| 26  | B     | 622 | LHG  | C8-C7-O7-C5     |
| 26  | d     | 409 | LHG  | C12-C13-C14-C15 |
| 26  | D     | 410 | LHG  | C12-C13-C14-C15 |
| 36  | B     | 601 | LMG  | C32-C33-C34-C35 |
| 36  | I     | 101 | LMG  | C32-C33-C34-C35 |
| 22  | C     | 509 | CLA  | C5-C6-C7-C8     |
| 26  | d     | 407 | LHG  | C4-O6-P-O3      |
| 26  | d     | 408 | LHG  | C4-O6-P-O3      |
| 26  | D     | 408 | LHG  | C4-O6-P-O3      |
| 26  | D     | 409 | LHG  | C4-O6-P-O3      |
| 26  | C     | 520 | LHG  | C33-C34-C35-C36 |
| 36  | B     | 601 | LMG  | C38-C39-C40-C41 |
| 36  | I     | 101 | LMG  | C38-C39-C40-C41 |
| 26  | N     | 618 | LHG  | C23-C24-C25-C26 |
| 26  | c     | 520 | LHG  | C33-C34-C35-C36 |
| 22  | c     | 503 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 33  | a     | 411 | SQD  | C18-C19-C20-C21 |
| 35  | H     | 102 | DGD  | C8A-C9A-CAA-CBA |
| 33  | A     | 412 | SQD  | C18-C19-C20-C21 |
| 35  | h     | 102 | DGD  | C8A-C9A-CAA-CBA |
| 36  | k     | 103 | LMG  | C14-C15-C16-C17 |
| 36  | K     | 103 | LMG  | C14-C15-C16-C17 |
| 22  | c     | 508 | CLA  | C5-C6-C7-C8     |
| 26  | s     | 314 | LHG  | C33-C34-C35-C36 |
| 26  | S     | 314 | LHG  | C33-C34-C35-C36 |
| 26  | n     | 617 | LHG  | C32-C33-C34-C35 |
| 35  | c     | 517 | DGD  | C5A-C6A-C7A-C8A |
| 35  | C     | 518 | DGD  | C5A-C6A-C7A-C8A |
| 36  | k     | 103 | LMG  | C34-C35-C36-C37 |
| 36  | K     | 103 | LMG  | C34-C35-C36-C37 |
| 22  | b     | 608 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 611 | CLA  | C8-C10-C11-C12  |
| 36  | B     | 601 | LMG  | C4-C5-C6-O5     |
| 36  | I     | 101 | LMG  | C4-C5-C6-O5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | G     | 618 | LHG  | C31-C32-C33-C34 |
| 35  | c     | 517 | DGD  | C5B-C6B-C7B-C8B |
| 35  | c     | 518 | DGD  | C5A-C6A-C7A-C8A |
| 35  | C     | 519 | DGD  | C5A-C6A-C7A-C8A |
| 26  | S     | 314 | LHG  | C24-C23-O8-C6   |
| 22  | g     | 612 | CLA  | C4-C3-C5-C6     |
| 22  | n     | 611 | CLA  | C4-C3-C5-C6     |
| 22  | G     | 612 | CLA  | C4-C3-C5-C6     |
| 22  | N     | 611 | CLA  | C4-C3-C5-C6     |
| 22  | w     | 101 | CLA  | C4-C3-C5-C6     |
| 22  | W     | 101 | CLA  | C4-C3-C5-C6     |
| 26  | c     | 522 | LHG  | C27-C28-C29-C30 |
| 26  | C     | 522 | LHG  | C27-C28-C29-C30 |
| 35  | C     | 518 | DGD  | C5B-C6B-C7B-C8B |
| 22  | g     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | n     | 609 | CLA  | C5-C6-C7-C8     |
| 22  | G     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | Y     | 609 | CLA  | C5-C6-C7-C8     |
| 36  | D     | 411 | LMG  | O6-C5-C6-O5     |
| 22  | g     | 610 | CLA  | C15-C16-C17-C18 |
| 26  | y     | 617 | LHG  | C24-C25-C26-C27 |
| 26  | c     | 520 | LHG  | C11-C10-C9-C8   |
| 26  | C     | 520 | LHG  | C11-C10-C9-C8   |
| 35  | a     | 413 | DGD  | C4B-C5B-C6B-C7B |
| 35  | A     | 401 | DGD  | C4B-C5B-C6B-C7B |
| 22  | y     | 610 | CLA  | C5-C6-C7-C8     |
| 22  | N     | 609 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 502 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 503 | CLA  | C15-C16-C17-C18 |
| 21  | g     | 607 | CHL  | C3-C5-C6-C7     |
| 21  | n     | 606 | CHL  | C3-C5-C6-C7     |
| 21  | y     | 607 | CHL  | C3-C5-C6-C7     |
| 21  | G     | 607 | CHL  | C3-C5-C6-C7     |
| 21  | N     | 606 | CHL  | C3-C5-C6-C7     |
| 21  | Y     | 606 | CHL  | C3-C5-C6-C7     |
| 26  | n     | 617 | LHG  | C19-C20-C21-C22 |
| 26  | Y     | 617 | LHG  | C4-C5-C6-O8     |
| 26  | b     | 619 | LHG  | C4-C5-C6-O8     |
| 26  | c     | 520 | LHG  | C16-C17-C18-C19 |
| 26  | c     | 522 | LHG  | C4-C5-C6-O8     |
| 26  | d     | 407 | LHG  | C27-C28-C29-C30 |
| 26  | d     | 408 | LHG  | C4-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | B     | 622 | LHG  | C4-C5-C6-O8     |
| 26  | C     | 520 | LHG  | C16-C17-C18-C19 |
| 26  | C     | 522 | LHG  | C4-C5-C6-O8     |
| 26  | D     | 408 | LHG  | C27-C28-C29-C30 |
| 26  | D     | 409 | LHG  | C4-C5-C6-O8     |
| 33  | l     | 103 | SQD  | O6-C44-C45-C46  |
| 33  | L     | 101 | SQD  | O6-C44-C45-C46  |
| 36  | c     | 523 | LMG  | C7-C8-C9-O8     |
| 36  | B     | 601 | LMG  | C7-C8-C9-O8     |
| 36  | C     | 523 | LMG  | C7-C8-C9-O8     |
| 36  | I     | 101 | LMG  | C7-C8-C9-O8     |
| 26  | s     | 314 | LHG  | C24-C23-O8-C6   |
| 35  | a     | 413 | DGD  | O6E-C5E-C6E-O5E |
| 35  | A     | 401 | DGD  | O6E-C5E-C6E-O5E |
| 36  | d     | 410 | LMG  | O6-C5-C6-O5     |
| 22  | g     | 613 | CLA  | C13-C15-C16-C17 |
| 26  | y     | 617 | LHG  | C12-C13-C14-C15 |
| 26  | c     | 521 | LHG  | C32-C33-C34-C35 |
| 26  | C     | 521 | LHG  | C32-C33-C34-C35 |
| 35  | c     | 518 | DGD  | C2G-C3G-O3G-C1D |
| 35  | C     | 519 | DGD  | C2G-C3G-O3G-C1D |
| 22  | s     | 311 | CLA  | C11-C10-C8-C9   |
| 22  | S     | 311 | CLA  | C11-C10-C8-C9   |
| 26  | G     | 618 | LHG  | C24-C25-C26-C27 |
| 26  | G     | 618 | LHG  | C27-C28-C29-C30 |
| 21  | g     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 21  | n     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 21  | y     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 21  | G     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 21  | N     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 21  | Y     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 22  | b     | 614 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 617 | CLA  | C3-C5-C6-C7     |
| 32  | d     | 406 | PL9  | C44-C46-C47-C48 |
| 26  | c     | 520 | LHG  | O1-C1-C2-O2     |
| 26  | d     | 407 | LHG  | O1-C1-C2-O2     |
| 26  | l     | 102 | LHG  | O1-C1-C2-O2     |
| 26  | C     | 520 | LHG  | O1-C1-C2-O2     |
| 26  | D     | 408 | LHG  | O1-C1-C2-O2     |
| 26  | L     | 103 | LHG  | O1-C1-C2-O2     |
| 26  | b     | 619 | LHG  | C11-C10-C9-C8   |
| 26  | l     | 102 | LHG  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | G     | 613 | CLA  | C15-C16-C17-C18 |
| 26  | B     | 622 | LHG  | C11-C10-C9-C8   |
| 26  | L     | 103 | LHG  | C30-C31-C32-C33 |
| 22  | S     | 313 | CLA  | O1D-CGD-O2D-CED |
| 26  | c     | 522 | LHG  | C8-C7-O7-C5     |
| 26  | C     | 522 | LHG  | C8-C7-O7-C5     |
| 22  | s     | 313 | CLA  | O1D-CGD-O2D-CED |
| 21  | r     | 306 | CHL  | C5-C6-C7-C8     |
| 22  | b     | 614 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 508 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 509 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 515 | CLA  | C8-C10-C11-C12  |
| 22  | r     | 312 | CLA  | C10-C11-C12-C13 |
| 22  | R     | 311 | CLA  | C10-C11-C12-C13 |
| 31  | k     | 101 | BCR  | C16-C17-C18-C36 |
| 31  | B     | 602 | BCR  | C20-C21-C22-C37 |
| 31  | K     | 101 | BCR  | C16-C17-C18-C36 |
| 31  | T     | 102 | BCR  | C20-C21-C22-C37 |
| 22  | b     | 614 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 617 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 35  | a     | 413 | DGD  | C9A-CAA-CBA-CCA |
| 36  | C     | 502 | LMG  | C32-C33-C34-C35 |
| 21  | R     | 305 | CHL  | C5-C6-C7-C8     |
| 22  | Y     | 611 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 514 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 617 | CLA  | C13-C15-C16-C17 |
| 35  | A     | 401 | DGD  | C9A-CAA-CBA-CCA |
| 36  | w     | 102 | LMG  | C32-C33-C34-C35 |
| 22  | c     | 503 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 504 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 608 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 611 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 614 | CLA  | C5-C6-C7-C8     |
| 22  | g     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | n     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | y     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | G     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | N     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | Y     | 604 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 609 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 612 | CLA  | C2-C1-O2A-CGA   |
| 26  | N     | 618 | LHG  | C12-C13-C14-C15 |
| 26  | Y     | 617 | LHG  | C24-C25-C26-C27 |
| 36  | T     | 101 | LMG  | C39-C40-C41-C42 |
| 26  | b     | 619 | LHG  | C24-C23-O8-C6   |
| 26  | B     | 622 | LHG  | C24-C23-O8-C6   |
| 26  | y     | 617 | LHG  | O6-C4-C5-O7     |
| 26  | s     | 314 | LHG  | O6-C4-C5-O7     |
| 26  | S     | 314 | LHG  | O6-C4-C5-O7     |
| 21  | g     | 609 | CHL  | C11-C12-C13-C14 |
| 21  | n     | 608 | CHL  | C16-C17-C18-C20 |
| 21  | G     | 609 | CHL  | C11-C12-C13-C14 |
| 26  | N     | 618 | LHG  | C25-C26-C27-C28 |
| 26  | d     | 407 | LHG  | C32-C33-C34-C35 |
| 26  | D     | 408 | LHG  | C32-C33-C34-C35 |
| 33  | d     | 402 | SQD  | C14-C15-C16-C17 |
| 33  | D     | 402 | SQD  | C14-C15-C16-C17 |
| 36  | M     | 101 | LMG  | C39-C40-C41-C42 |
| 26  | n     | 617 | LHG  | C27-C28-C29-C30 |
| 26  | d     | 408 | LHG  | C19-C20-C21-C22 |
| 26  | D     | 409 | LHG  | C19-C20-C21-C22 |
| 33  | a     | 411 | SQD  | O10-C23-O48-C46 |
| 33  | A     | 412 | SQD  | O10-C23-O48-C46 |
| 35  | h     | 102 | DGD  | CCA-CDA-CEA-CFA |
| 22  | b     | 615 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 618 | CLA  | C13-C15-C16-C17 |
| 24  | y     | 615 | XAT  | C11-C10-C9-C8   |
| 25  | g     | 618 | NEX  | C32-C33-C34-C35 |
| 31  | d     | 405 | BCR  | C12-C13-C14-C15 |
| 31  | D     | 406 | BCR  | C12-C13-C14-C15 |
| 35  | H     | 102 | DGD  | CCA-CDA-CEA-CFA |
| 36  | c     | 523 | LMG  | C31-C32-C33-C34 |
| 36  | C     | 523 | LMG  | C31-C32-C33-C34 |
| 26  | r     | 302 | LHG  | O7-C5-C6-O8     |
| 26  | R     | 301 | LHG  | O7-C5-C6-O8     |
| 33  | d     | 402 | SQD  | O6-C44-C45-O47  |
| 33  | l     | 101 | SQD  | O47-C45-C46-O48 |
| 33  | D     | 402 | SQD  | O6-C44-C45-O47  |
| 33  | L     | 102 | SQD  | O47-C45-C46-O48 |
| 35  | c     | 518 | DGD  | O2G-C2G-C3G-O3G |
| 35  | C     | 519 | DGD  | O2G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | y     | 617 | LHG  | C14-C15-C16-C17 |
| 36  | w     | 102 | LMG  | C33-C34-C35-C36 |
| 22  | g     | 613 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 608 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 502 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 36  | I     | 101 | LMG  | O10-C28-O8-C9   |
| 26  | G     | 618 | LHG  | C28-C29-C30-C31 |
| 26  | N     | 618 | LHG  | C9-C10-C11-C12  |
| 26  | c     | 520 | LHG  | C9-C10-C11-C12  |
| 26  | C     | 520 | LHG  | C9-C10-C11-C12  |
| 36  | C     | 502 | LMG  | C33-C34-C35-C36 |
| 32  | d     | 406 | PL9  | C20-C19-C21-C22 |
| 32  | D     | 407 | PL9  | C20-C19-C21-C22 |
| 22  | N     | 609 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 503 | CLA  | C10-C11-C12-C13 |
| 36  | D     | 411 | LMG  | C4-C5-C6-O5     |
| 21  | g     | 608 | CHL  | C6-C7-C8-C10    |
| 21  | n     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | y     | 608 | CHL  | C6-C7-C8-C10    |
| 21  | y     | 609 | CHL  | C12-C13-C15-C16 |
| 21  | G     | 608 | CHL  | C6-C7-C8-C10    |
| 21  | N     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | Y     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | r     | 306 | CHL  | C12-C13-C15-C16 |
| 21  | R     | 305 | CHL  | C12-C13-C15-C16 |
| 22  | g     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | n     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | y     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | y     | 612 | CLA  | C12-C13-C15-C16 |
| 22  | G     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | G     | 610 | CLA  | C12-C13-C15-C16 |
| 22  | N     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | Y     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 602 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 605 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 612 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 504 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 513 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 514 | CLA  | C11-C10-C8-C7   |
| 22  | d     | 403 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 403 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 605 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 608 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 614 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 615 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 505 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 514 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 515 | CLA  | C11-C10-C8-C7   |
| 22  | D     | 404 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 404 | CLA  | C11-C12-C13-C15 |
| 22  | s     | 303 | CLA  | C6-C7-C8-C10    |
| 22  | S     | 303 | CLA  | C6-C7-C8-C10    |
| 33  | a     | 411 | SQD  | C12-C13-C14-C15 |
| 21  | g     | 608 | CHL  | C11-C10-C8-C9   |
| 21  | n     | 607 | CHL  | C11-C10-C8-C9   |
| 21  | y     | 608 | CHL  | C11-C10-C8-C9   |
| 21  | G     | 608 | CHL  | C11-C10-C8-C9   |
| 21  | N     | 607 | CHL  | C11-C10-C8-C9   |
| 21  | Y     | 607 | CHL  | C11-C10-C8-C9   |
| 22  | g     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | n     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | n     | 609 | CLA  | C14-C13-C15-C16 |
| 22  | y     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | G     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | G     | 610 | CLA  | C14-C13-C15-C16 |
| 22  | N     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | Y     | 602 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 602 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 604 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 606 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 609 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 612 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 614 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 615 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 605 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 607 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 609 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 615 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 617 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 618 | CLA  | C6-C7-C8-C9     |
| 36  | K     | 103 | LMG  | C10-C11-C12-C13 |
| 26  | Y     | 617 | LHG  | C25-C26-C27-C28 |
| 33  | A     | 412 | SQD  | C12-C13-C14-C15 |
| 22  | d     | 403 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 22  | g     | 611 | CLA  | C8-C10-C11-C12  |
| 22  | n     | 610 | CLA  | C8-C10-C11-C12  |
| 22  | y     | 611 | CLA  | C8-C10-C11-C12  |
| 22  | N     | 610 | CLA  | C8-C10-C11-C12  |
| 22  | Y     | 610 | CLA  | C8-C10-C11-C12  |
| 21  | S     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 26  | N     | 618 | LHG  | C13-C14-C15-C16 |
| 36  | d     | 410 | LMG  | C4-C5-C6-O5     |
| 22  | c     | 506 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 36  | B     | 601 | LMG  | O10-C28-O8-C9   |
| 23  | Y     | 614 | LUT  | C31-C32-C33-C40 |
| 22  | G     | 611 | CLA  | C8-C10-C11-C12  |
| 22  | a     | 404 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 405 | CLA  | C16-C17-C18-C20 |
| 25  | g     | 618 | NEX  | C31-C32-C33-C34 |
| 31  | b     | 616 | BCR  | C21-C22-C23-C24 |
| 31  | B     | 619 | BCR  | C21-C22-C23-C24 |
| 26  | n     | 617 | LHG  | C29-C30-C31-C32 |
| 36  | b     | 620 | LMG  | C18-C19-C20-C21 |
| 26  | g     | 619 | LHG  | C9-C10-C11-C12  |
| 35  | c     | 518 | DGD  | CAA-CBA-CCA-CDA |
| 35  | C     | 519 | DGD  | CAA-CBA-CCA-CDA |
| 36  | B     | 623 | LMG  | C18-C19-C20-C21 |
| 22  | C     | 505 | CLA  | O1A-CGA-O2A-C1  |
| 21  | g     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 21  | Y     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 21  | s     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 35  | c     | 519 | DGD  | CCA-CDA-CEA-CFA |
| 35  | J     | 101 | DGD  | CCA-CDA-CEA-CFA |
| 36  | k     | 103 | LMG  | C10-C11-C12-C13 |
| 21  | n     | 608 | CHL  | C15-C16-C17-C18 |
| 21  | Y     | 608 | CHL  | C15-C16-C17-C18 |
| 35  | c     | 518 | DGD  | C4A-C5A-C6A-C7A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | C     | 519 | DGD  | C4A-C5A-C6A-C7A |
| 26  | G     | 618 | LHG  | O6-C4-C5-C6     |
| 26  | Y     | 617 | LHG  | O6-C4-C5-C6     |
| 26  | c     | 521 | LHG  | O6-C4-C5-C6     |
| 26  | c     | 522 | LHG  | O6-C4-C5-C6     |
| 26  | C     | 521 | LHG  | O6-C4-C5-C6     |
| 26  | C     | 522 | LHG  | O6-C4-C5-C6     |
| 26  | r     | 302 | LHG  | O6-C4-C5-C6     |
| 26  | R     | 301 | LHG  | O6-C4-C5-C6     |
| 32  | D     | 407 | PL9  | C44-C46-C47-C48 |
| 33  | a     | 411 | SQD  | C9-C10-C11-C12  |
| 21  | G     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 21  | N     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 33  | A     | 412 | SQD  | C9-C10-C11-C12  |
| 22  | s     | 303 | CLA  | C4-C3-C5-C6     |
| 22  | S     | 303 | CLA  | C4-C3-C5-C6     |
| 22  | s     | 303 | CLA  | C2-C3-C5-C6     |
| 22  | S     | 303 | CLA  | C2-C3-C5-C6     |
| 21  | S     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 26  | n     | 617 | LHG  | C35-C36-C37-C38 |
| 26  | d     | 407 | LHG  | C30-C31-C32-C33 |
| 26  | l     | 102 | LHG  | C27-C28-C29-C30 |
| 26  | D     | 408 | LHG  | C30-C31-C32-C33 |
| 26  | L     | 103 | LHG  | C27-C28-C29-C30 |
| 22  | b     | 605 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 608 | CLA  | C16-C17-C18-C20 |
| 26  | G     | 618 | LHG  | C14-C15-C16-C17 |
| 26  | Y     | 617 | LHG  | C14-C15-C16-C17 |
| 22  | x     | 101 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 603 | CLA  | C8-C10-C11-C12  |
| 21  | n     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 35  | c     | 518 | DGD  | C9B-CAB-CBB-CCB |
| 35  | C     | 519 | DGD  | C9B-CAB-CBB-CCB |
| 21  | g     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | n     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | y     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | G     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | N     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | Y     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 21  | s     | 302 | CHL  | C3A-C2A-CAA-CBA |
| 21  | S     | 302 | CHL  | C3A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 506 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 505 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 507 | CLA  | C3A-C2A-CAA-CBA |
| 24  | G     | 617 | XAT  | C33-C34-C35-C15 |
| 25  | N     | 617 | NEX  | C29-C30-C31-C32 |
| 26  | g     | 619 | LHG  | C23-C24-C25-C26 |
| 26  | g     | 619 | LHG  | C32-C33-C34-C35 |
| 26  | s     | 314 | LHG  | C29-C30-C31-C32 |
| 26  | S     | 314 | LHG  | C29-C30-C31-C32 |
| 33  | l     | 103 | SQD  | C17-C18-C19-C20 |
| 33  | L     | 101 | SQD  | C17-C18-C19-C20 |
| 22  | c     | 506 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 507 | CLA  | C16-C17-C18-C19 |
| 21  | y     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 26  | s     | 314 | LHG  | C10-C11-C12-C13 |
| 26  | S     | 314 | LHG  | C10-C11-C12-C13 |
| 36  | b     | 620 | LMG  | C40-C41-C42-C43 |
| 36  | B     | 623 | LMG  | C40-C41-C42-C43 |
| 22  | b     | 610 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 613 | CLA  | C15-C16-C17-C18 |
| 26  | s     | 314 | LHG  | C4-C5-C6-O8     |
| 26  | S     | 314 | LHG  | C4-C5-C6-O8     |
| 33  | d     | 402 | SQD  | O6-C44-C45-C46  |
| 33  | D     | 402 | SQD  | O6-C44-C45-C46  |
| 35  | c     | 518 | DGD  | O1G-C1G-C2G-C3G |
| 35  | c     | 518 | DGD  | C1G-C2G-C3G-O3G |
| 35  | C     | 519 | DGD  | O1G-C1G-C2G-C3G |
| 35  | C     | 519 | DGD  | C1G-C2G-C3G-O3G |
| 36  | b     | 620 | LMG  | O1-C7-C8-C9     |
| 36  | k     | 103 | LMG  | O1-C7-C8-C9     |
| 36  | B     | 623 | LMG  | O1-C7-C8-C9     |
| 36  | K     | 103 | LMG  | O1-C7-C8-C9     |
| 36  | M     | 101 | LMG  | O1-C7-C8-C9     |
| 36  | T     | 101 | LMG  | O1-C7-C8-C9     |
| 36  | c     | 523 | LMG  | C38-C39-C40-C41 |
| 36  | C     | 523 | LMG  | C38-C39-C40-C41 |
| 22  | c     | 513 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 602 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 605 | CLA  | C2-C3-C5-C6     |
| 26  | b     | 619 | LHG  | C9-C10-C11-C12  |
| 26  | B     | 622 | LHG  | C9-C10-C11-C12  |
| 26  | r     | 302 | LHG  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | r     | 302 | LHG  | C3-O3-P-O6      |
| 26  | R     | 301 | LHG  | C3-O3-P-O6      |
| 26  | R     | 301 | LHG  | C24-C25-C26-C27 |
| 22  | C     | 514 | CLA  | C3-C5-C6-C7     |
| 26  | G     | 618 | LHG  | C30-C31-C32-C33 |
| 26  | d     | 407 | LHG  | C34-C35-C36-C37 |
| 26  | D     | 408 | LHG  | C34-C35-C36-C37 |
| 26  | r     | 302 | LHG  | C30-C31-C32-C33 |
| 26  | R     | 301 | LHG  | C30-C31-C32-C33 |
| 36  | M     | 101 | LMG  | C12-C13-C14-C15 |
| 26  | n     | 617 | LHG  | O6-C4-C5-O7     |
| 26  | N     | 618 | LHG  | O6-C4-C5-O7     |
| 26  | c     | 522 | LHG  | O6-C4-C5-O7     |
| 26  | C     | 522 | LHG  | O6-C4-C5-O7     |
| 22  | c     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 36  | T     | 101 | LMG  | C12-C13-C14-C15 |
| 21  | n     | 608 | CHL  | C16-C17-C18-C19 |
| 21  | N     | 608 | CHL  | C16-C17-C18-C19 |
| 22  | a     | 404 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 405 | CLA  | C16-C17-C18-C19 |
| 26  | g     | 619 | LHG  | C24-C25-C26-C27 |
| 26  | d     | 408 | LHG  | C11-C12-C13-C14 |
| 26  | D     | 409 | LHG  | C11-C12-C13-C14 |
| 22  | d     | 403 | CLA  | O1A-CGA-O2A-C1  |
| 22  | D     | 404 | CLA  | O1A-CGA-O2A-C1  |
| 26  | d     | 409 | LHG  | C32-C33-C34-C35 |
| 26  | D     | 410 | LHG  | C32-C33-C34-C35 |
| 26  | Y     | 617 | LHG  | C16-C17-C18-C19 |
| 33  | d     | 402 | SQD  | O47-C45-C46-O48 |
| 33  | D     | 402 | SQD  | O47-C45-C46-O48 |
| 36  | b     | 620 | LMG  | O1-C7-C8-O7     |
| 36  | w     | 102 | LMG  | O1-C7-C8-O7     |
| 36  | B     | 623 | LMG  | O1-C7-C8-O7     |
| 36  | C     | 502 | LMG  | O1-C7-C8-O7     |
| 36  | M     | 101 | LMG  | O1-C7-C8-O7     |
| 36  | T     | 101 | LMG  | O1-C7-C8-O7     |
| 35  | h     | 102 | DGD  | O2G-C1B-C2B-C3B |
| 35  | H     | 102 | DGD  | O2G-C1B-C2B-C3B |
| 26  | S     | 314 | LHG  | C11-C12-C13-C14 |
| 35  | C     | 519 | DGD  | C5B-C6B-C7B-C8B |
| 21  | g     | 608 | CHL  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | n     | 607 | CHL  | C16-C17-C18-C19 |
| 21  | y     | 608 | CHL  | C16-C17-C18-C19 |
| 21  | G     | 608 | CHL  | C16-C17-C18-C19 |
| 21  | N     | 607 | CHL  | C16-C17-C18-C19 |
| 21  | Y     | 607 | CHL  | C16-C17-C18-C19 |
| 22  | c     | 506 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 507 | CLA  | C16-C17-C18-C20 |
| 22  | s     | 313 | CLA  | C6-C7-C8-C9     |
| 22  | S     | 313 | CLA  | C6-C7-C8-C9     |
| 26  | s     | 314 | LHG  | C11-C12-C13-C14 |
| 35  | c     | 518 | DGD  | C5B-C6B-C7B-C8B |
| 26  | c     | 520 | LHG  | C1-C2-C3-O3     |
| 26  | C     | 520 | LHG  | C1-C2-C3-O3     |
| 35  | a     | 413 | DGD  | C9B-CAB-CBB-CCB |
| 35  | A     | 401 | DGD  | C9B-CAB-CBB-CCB |
| 22  | s     | 312 | CLA  | C2-C1-O2A-CGA   |
| 22  | S     | 312 | CLA  | C2-C1-O2A-CGA   |
| 26  | Y     | 617 | LHG  | C11-C10-C9-C8   |
| 35  | c     | 517 | DGD  | C7B-C8B-C9B-CAB |
| 35  | C     | 518 | DGD  | C7B-C8B-C9B-CAB |
| 21  | r     | 306 | CHL  | C11-C12-C13-C14 |
| 21  | R     | 305 | CHL  | C11-C12-C13-C14 |
| 22  | g     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | n     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | y     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | G     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | N     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | Y     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 607 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 503 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 507 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 510 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 512 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 504 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 508 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 511 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 513 | CLA  | C11-C10-C8-C9   |
| 22  | s     | 311 | CLA  | C6-C7-C8-C9     |
| 22  | S     | 311 | CLA  | C6-C7-C8-C9     |
| 30  | a     | 407 | PHO  | C11-C10-C8-C9   |
| 30  | d     | 401 | PHO  | C6-C7-C8-C9     |
| 30  | A     | 408 | PHO  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | D     | 401 | PHO  | C6-C7-C8-C9     |
| 26  | C     | 520 | LHG  | C14-C15-C16-C17 |
| 26  | c     | 520 | LHG  | C14-C15-C16-C17 |
| 26  | r     | 302 | LHG  | C11-C12-C13-C14 |
| 26  | R     | 301 | LHG  | C11-C12-C13-C14 |
| 22  | c     | 513 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 514 | CLA  | C5-C6-C7-C8     |
| 26  | c     | 521 | LHG  | C5-C4-O6-P      |
| 26  | d     | 407 | LHG  | C2-C3-O3-P      |
| 26  | d     | 409 | LHG  | C2-C3-O3-P      |
| 26  | C     | 521 | LHG  | C5-C4-O6-P      |
| 26  | D     | 408 | LHG  | C2-C3-O3-P      |
| 26  | D     | 410 | LHG  | C2-C3-O3-P      |
| 30  | a     | 407 | PHO  | C1A-C2A-CAA-CBA |
| 30  | A     | 408 | PHO  | C1A-C2A-CAA-CBA |
| 36  | d     | 410 | LMG  | C16-C17-C18-C19 |
| 36  | D     | 411 | LMG  | C16-C17-C18-C19 |
| 22  | b     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 608 | CLA  | C2A-CAA-CBA-CGA |
| 23  | N     | 615 | LUT  | C1-C6-C7-C8     |
| 31  | a     | 409 | BCR  | C5-C6-C7-C8     |
| 31  | a     | 409 | BCR  | C23-C24-C25-C26 |
| 31  | a     | 409 | BCR  | C23-C24-C25-C30 |
| 31  | b     | 617 | BCR  | C1-C6-C7-C8     |
| 31  | b     | 617 | BCR  | C5-C6-C7-C8     |
| 31  | c     | 515 | BCR  | C23-C24-C25-C26 |
| 31  | c     | 516 | BCR  | C1-C6-C7-C8     |
| 31  | c     | 516 | BCR  | C5-C6-C7-C8     |
| 31  | c     | 516 | BCR  | C23-C24-C25-C26 |
| 31  | d     | 405 | BCR  | C23-C24-C25-C26 |
| 31  | h     | 101 | BCR  | C5-C6-C7-C8     |
| 31  | h     | 101 | BCR  | C23-C24-C25-C26 |
| 31  | h     | 101 | BCR  | C23-C24-C25-C30 |
| 31  | k     | 101 | BCR  | C5-C6-C7-C8     |
| 31  | k     | 101 | BCR  | C23-C24-C25-C26 |
| 31  | k     | 101 | BCR  | C23-C24-C25-C30 |
| 31  | k     | 102 | BCR  | C23-C24-C25-C26 |
| 31  | k     | 102 | BCR  | C23-C24-C25-C30 |
| 31  | A     | 410 | BCR  | C23-C24-C25-C26 |
| 31  | A     | 410 | BCR  | C23-C24-C25-C30 |
| 31  | B     | 620 | BCR  | C1-C6-C7-C8     |
| 31  | B     | 620 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | C     | 516 | BCR  | C23-C24-C25-C26 |
| 31  | C     | 517 | BCR  | C1-C6-C7-C8     |
| 31  | C     | 517 | BCR  | C5-C6-C7-C8     |
| 31  | C     | 517 | BCR  | C23-C24-C25-C26 |
| 31  | D     | 406 | BCR  | C23-C24-C25-C26 |
| 31  | H     | 101 | BCR  | C5-C6-C7-C8     |
| 31  | H     | 101 | BCR  | C23-C24-C25-C26 |
| 31  | H     | 101 | BCR  | C23-C24-C25-C30 |
| 31  | K     | 101 | BCR  | C5-C6-C7-C8     |
| 31  | K     | 101 | BCR  | C23-C24-C25-C26 |
| 31  | K     | 101 | BCR  | C23-C24-C25-C30 |
| 31  | K     | 102 | BCR  | C23-C24-C25-C26 |
| 31  | K     | 102 | BCR  | C23-C24-C25-C30 |
| 26  | C     | 520 | LHG  | C11-C12-C13-C14 |
| 26  | G     | 618 | LHG  | C32-C33-C34-C35 |
| 25  | Y     | 616 | NEX  | C11-C12-C13-C14 |
| 21  | N     | 608 | CHL  | C15-C16-C17-C18 |
| 26  | c     | 520 | LHG  | C11-C12-C13-C14 |
| 33  | l     | 101 | SQD  | C9-C10-C11-C12  |
| 36  | w     | 102 | LMG  | C11-C10-O7-C8   |
| 36  | C     | 502 | LMG  | C11-C10-O7-C8   |
| 33  | D     | 402 | SQD  | C10-C11-C12-C13 |
| 33  | L     | 102 | SQD  | C9-C10-C11-C12  |
| 36  | M     | 101 | LMG  | C22-C23-C24-C25 |
| 36  | T     | 101 | LMG  | C22-C23-C24-C25 |
| 26  | s     | 314 | LHG  | C12-C13-C14-C15 |
| 26  | S     | 314 | LHG  | C12-C13-C14-C15 |
| 33  | d     | 402 | SQD  | C10-C11-C12-C13 |
| 22  | C     | 514 | CLA  | C13-C15-C16-C17 |
| 36  | B     | 601 | LMG  | C36-C37-C38-C39 |
| 36  | I     | 101 | LMG  | C36-C37-C38-C39 |
| 22  | c     | 513 | CLA  | C13-C15-C16-C17 |
| 26  | y     | 617 | LHG  | O6-C4-C5-C6     |
| 26  | d     | 408 | LHG  | O2-C2-C3-O3     |
| 26  | D     | 409 | LHG  | O2-C2-C3-O3     |
| 26  | N     | 618 | LHG  | C18-C19-C20-C21 |
| 21  | g     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | g     | 608 | CHL  | C11-C10-C8-C7   |
| 21  | n     | 606 | CHL  | C6-C7-C8-C10    |
| 21  | n     | 607 | CHL  | C11-C10-C8-C7   |
| 21  | y     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | y     | 608 | CHL  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | G     | 607 | CHL  | C6-C7-C8-C10    |
| 21  | G     | 608 | CHL  | C11-C10-C8-C7   |
| 21  | N     | 606 | CHL  | C6-C7-C8-C10    |
| 21  | N     | 607 | CHL  | C11-C10-C8-C7   |
| 21  | Y     | 606 | CHL  | C6-C7-C8-C10    |
| 21  | Y     | 607 | CHL  | C11-C10-C8-C7   |
| 22  | g     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | n     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | y     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | G     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | N     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | Y     | 602 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 606 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 607 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 609 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 612 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 614 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 615 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 507 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 509 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 510 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 512 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 609 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 615 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 617 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 618 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 508 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 510 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 511 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 513 | CLA  | C11-C10-C8-C7   |
| 22  | r     | 304 | CLA  | C6-C7-C8-C10    |
| 22  | r     | 310 | CLA  | C6-C7-C8-C10    |
| 22  | R     | 303 | CLA  | C6-C7-C8-C10    |
| 22  | R     | 309 | CLA  | C6-C7-C8-C10    |
| 30  | a     | 407 | PHO  | C11-C12-C13-C15 |
| 30  | A     | 408 | PHO  | C11-C12-C13-C15 |
| 21  | n     | 608 | CHL  | C13-C15-C16-C17 |
| 23  | g     | 615 | LUT  | C33-C34-C35-C15 |
| 23  | g     | 616 | LUT  | C9-C10-C11-C12  |
| 23  | n     | 614 | LUT  | C33-C34-C35-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | y     | 614 | LUT  | C33-C34-C35-C15 |
| 23  | G     | 615 | LUT  | C33-C34-C35-C15 |
| 23  | N     | 614 | LUT  | C33-C34-C35-C15 |
| 23  | N     | 615 | LUT  | C29-C30-C31-C32 |
| 23  | Y     | 613 | LUT  | C33-C34-C35-C15 |
| 24  | G     | 617 | XAT  | C29-C30-C31-C32 |
| 25  | y     | 616 | NEX  | C13-C14-C15-C35 |
| 22  | R     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 605 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 608 | CLA  | C16-C17-C18-C19 |
| 21  | g     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 36  | k     | 103 | LMG  | C11-C12-C13-C14 |
| 36  | K     | 103 | LMG  | C11-C12-C13-C14 |
| 31  | k     | 101 | BCR  | C20-C21-C22-C37 |
| 31  | K     | 101 | BCR  | C20-C21-C22-C37 |
| 22  | N     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | Y     | 611 | CLA  | C3-C5-C6-C7     |
| 35  | C     | 519 | DGD  | CAB-CBB-CCB-CDB |
| 21  | Y     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 22  | r     | 310 | CLA  | CBD-CGD-O2D-CED |
| 26  | l     | 102 | LHG  | C24-C23-O8-C6   |
| 26  | L     | 103 | LHG  | C24-C23-O8-C6   |
| 33  | d     | 402 | SQD  | O47-C7-C8-C9    |
| 33  | D     | 402 | SQD  | O47-C7-C8-C9    |
| 35  | c     | 518 | DGD  | CAB-CBB-CCB-CDB |
| 26  | Y     | 617 | LHG  | C29-C30-C31-C32 |
| 35  | h     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 35  | H     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 36  | B     | 601 | LMG  | C31-C32-C33-C34 |
| 36  | I     | 101 | LMG  | C31-C32-C33-C34 |
| 36  | M     | 101 | LMG  | C13-C14-C15-C16 |
| 36  | T     | 101 | LMG  | C13-C14-C15-C16 |
| 21  | s     | 307 | CHL  | CAD-CBD-CGD-O2D |
| 21  | S     | 307 | CHL  | CAD-CBD-CGD-O2D |
| 22  | b     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 605 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 606 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 607 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 510 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 605 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 608 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 617 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 511 | CLA  | CAD-CBD-CGD-O2D |
| 22  | r     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 22  | R     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 25  | y     | 616 | NEX  | C7-C8-C9-C19    |
| 25  | y     | 618 | NEX  | C7-C8-C9-C19    |
| 25  | r     | 315 | NEX  | C7-C8-C9-C19    |
| 22  | g     | 613 | CLA  | C3-C5-C6-C7     |
| 22  | n     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | y     | 612 | CLA  | C3-C5-C6-C7     |
| 22  | G     | 613 | CLA  | C3-C5-C6-C7     |
| 26  | d     | 407 | LHG  | C12-C13-C14-C15 |
| 26  | D     | 408 | LHG  | C12-C13-C14-C15 |
| 36  | k     | 103 | LMG  | C40-C41-C42-C43 |
| 36  | K     | 103 | LMG  | C40-C41-C42-C43 |
| 31  | b     | 616 | BCR  | C6-C7-C8-C9     |
| 31  | b     | 616 | BCR  | C22-C23-C24-C25 |
| 31  | b     | 618 | BCR  | C22-C23-C24-C25 |
| 31  | B     | 619 | BCR  | C6-C7-C8-C9     |
| 31  | B     | 619 | BCR  | C22-C23-C24-C25 |
| 31  | B     | 621 | BCR  | C22-C23-C24-C25 |
| 35  | h     | 102 | DGD  | O6E-C1E-O5D-C6D |
| 35  | H     | 102 | DGD  | O6E-C1E-O5D-C6D |
| 26  | r     | 302 | LHG  | C4-C5-C6-O8     |
| 26  | R     | 301 | LHG  | C4-C5-C6-O8     |
| 33  | d     | 402 | SQD  | C44-C45-C46-O48 |
| 33  | D     | 402 | SQD  | C44-C45-C46-O48 |
| 35  | c     | 517 | DGD  | O1G-C1G-C2G-C3G |
| 35  | C     | 518 | DGD  | O1G-C1G-C2G-C3G |
| 26  | b     | 619 | LHG  | C35-C36-C37-C38 |
| 26  | B     | 622 | LHG  | C35-C36-C37-C38 |
| 26  | S     | 314 | LHG  | C28-C29-C30-C31 |
| 36  | B     | 623 | LMG  | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | g     | 619 | LHG  | O6-C4-C5-O7     |
| 26  | Y     | 617 | LHG  | O6-C4-C5-O7     |
| 26  | c     | 521 | LHG  | O6-C4-C5-O7     |
| 26  | C     | 521 | LHG  | O6-C4-C5-O7     |
| 22  | r     | 311 | CLA  | O2A-C1-C2-C3    |
| 22  | R     | 310 | CLA  | O2A-C1-C2-C3    |
| 26  | Y     | 617 | LHG  | C9-C10-C11-C12  |
| 26  | s     | 314 | LHG  | C28-C29-C30-C31 |
| 36  | b     | 620 | LMG  | C42-C43-C44-C45 |
| 37  | f     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 37  | F     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 22  | d     | 403 | CLA  | CBD-CGD-O2D-CED |
| 22  | D     | 404 | CLA  | CBD-CGD-O2D-CED |
| 21  | Y     | 608 | CHL  | C16-C17-C18-C19 |
| 21  | s     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 21  | s     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 21  | S     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 21  | S     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 22  | g     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | g     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | g     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 22  | n     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | n     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | n     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 22  | y     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | y     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | y     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 22  | G     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | G     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | G     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 22  | N     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | N     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | N     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 22  | Y     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | Y     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | Y     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 613 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 613 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 509 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 509 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 511 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 606 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 606 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 616 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 510 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 510 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 512 | CLA  | CHA-CBD-CGD-O1D |
| 22  | r     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 22  | r     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 22  | R     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 22  | R     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 21  | n     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 21  | y     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 21  | G     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 21  | N     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 23  | g     | 616 | LUT  | C12-C13-C14-C15 |
| 23  | G     | 616 | LUT  | C28-C29-C30-C31 |
| 24  | Y     | 615 | XAT  | C11-C10-C9-C8   |
| 31  | c     | 516 | BCR  | C20-C21-C22-C23 |
| 31  | B     | 602 | BCR  | C16-C17-C18-C19 |
| 31  | C     | 517 | BCR  | C20-C21-C22-C23 |
| 31  | T     | 102 | BCR  | C16-C17-C18-C19 |
| 22  | g     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | y     | 603 | CLA  | C5-C6-C7-C8     |
| 26  | c     | 522 | LHG  | O7-C5-C6-O8     |
| 26  | C     | 522 | LHG  | O7-C5-C6-O8     |
| 22  | n     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | G     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | N     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | Y     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 26  | s     | 314 | LHG  | O1-C1-C2-O2     |
| 26  | S     | 314 | LHG  | O1-C1-C2-O2     |
| 26  | b     | 619 | LHG  | C12-C13-C14-C15 |
| 36  | B     | 601 | LMG  | C11-C10-O7-C8   |
| 36  | I     | 101 | LMG  | C11-C10-O7-C8   |
| 21  | r     | 307 | CHL  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | R     | 306 | CHL  | C4-C3-C5-C6     |
| 22  | a     | 405 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 406 | CLA  | C4-C3-C5-C6     |
| 32  | d     | 406 | PL9  | C15-C14-C16-C17 |
| 26  | Y     | 617 | LHG  | C28-C29-C30-C31 |
| 26  | B     | 622 | LHG  | C12-C13-C14-C15 |
| 36  | d     | 410 | LMG  | O10-C28-O8-C9   |
| 36  | D     | 411 | LMG  | O10-C28-O8-C9   |
| 21  | r     | 307 | CHL  | C2-C3-C5-C6     |
| 21  | R     | 306 | CHL  | C2-C3-C5-C6     |
| 22  | b     | 614 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 617 | CLA  | C2-C3-C5-C6     |
| 26  | y     | 617 | LHG  | C24-C23-O8-C6   |
| 33  | D     | 402 | SQD  | O49-C7-O47-C45  |
| 22  | g     | 613 | CLA  | C6-C7-C8-C9     |
| 22  | n     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | y     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | G     | 613 | CLA  | C6-C7-C8-C9     |
| 22  | N     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | Y     | 611 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 607 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 610 | CLA  | C6-C7-C8-C9     |
| 30  | a     | 407 | PHO  | C11-C12-C13-C14 |
| 30  | A     | 408 | PHO  | C11-C12-C13-C14 |
| 22  | c     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 22  | x     | 101 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | r     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 22  | R     | 302 | CLA  | C2A-CAA-CBA-CGA |
| 35  | C     | 518 | DGD  | C6A-C7A-C8A-C9A |
| 23  | G     | 616 | LUT  | C31-C32-C33-C40 |
| 35  | c     | 517 | DGD  | C6A-C7A-C8A-C9A |
| 36  | k     | 103 | LMG  | C19-C20-C21-C22 |
| 36  | K     | 103 | LMG  | C19-C20-C21-C22 |
| 24  | n     | 615 | XAT  | C7-C8-C9-C10    |
| 25  | N     | 617 | NEX  | C11-C12-C13-C14 |
| 35  | c     | 518 | DGD  | C8A-C9A-CAA-CBA |
| 35  | C     | 519 | DGD  | C8A-C9A-CAA-CBA |
| 21  | y     | 609 | CHL  | C16-C17-C18-C19 |
| 33  | d     | 402 | SQD  | O49-C7-O47-C45  |
| 21  | g     | 601 | CHL  | CBD-CGD-O2D-CED |
| 21  | N     | 601 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | r     | 313 | LUT  | C13-C14-C15-C35 |
| 23  | R     | 312 | LUT  | C13-C14-C15-C35 |
| 22  | s     | 309 | CLA  | C5-C6-C7-C8     |
| 26  | b     | 619 | LHG  | C3-O3-P-O6      |
| 26  | c     | 520 | LHG  | C3-O3-P-O6      |
| 26  | d     | 408 | LHG  | C3-O3-P-O6      |
| 26  | d     | 409 | LHG  | C4-O6-P-O3      |
| 26  | l     | 102 | LHG  | C3-O3-P-O6      |
| 26  | B     | 622 | LHG  | C3-O3-P-O6      |
| 26  | C     | 520 | LHG  | C3-O3-P-O6      |
| 26  | D     | 409 | LHG  | C3-O3-P-O6      |
| 26  | D     | 410 | LHG  | C4-O6-P-O3      |
| 26  | L     | 103 | LHG  | C3-O3-P-O6      |
| 26  | s     | 314 | LHG  | C4-O6-P-O3      |
| 26  | S     | 314 | LHG  | C4-O6-P-O3      |
| 26  | r     | 302 | LHG  | C31-C32-C33-C34 |
| 26  | R     | 301 | LHG  | C31-C32-C33-C34 |
| 32  | D     | 407 | PL9  | C15-C14-C16-C17 |
| 22  | S     | 309 | CLA  | C5-C6-C7-C8     |
| 26  | c     | 522 | LHG  | C2-C3-O3-P      |
| 26  | d     | 407 | LHG  | C5-C4-O6-P      |
| 26  | C     | 522 | LHG  | C2-C3-O3-P      |
| 26  | D     | 408 | LHG  | C5-C4-O6-P      |
| 22  | g     | 612 | CLA  | C2-C3-C5-C6     |
| 22  | n     | 611 | CLA  | C2-C3-C5-C6     |
| 22  | G     | 612 | CLA  | C2-C3-C5-C6     |
| 22  | N     | 611 | CLA  | C2-C3-C5-C6     |
| 22  | w     | 101 | CLA  | C2-C3-C5-C6     |
| 22  | W     | 101 | CLA  | C2-C3-C5-C6     |
| 26  | y     | 617 | LHG  | C13-C14-C15-C16 |
| 26  | G     | 618 | LHG  | C3-O3-P-O5      |
| 26  | Y     | 617 | LHG  | C3-O3-P-O5      |
| 26  | b     | 619 | LHG  | C4-O6-P-O4      |
| 26  | c     | 520 | LHG  | C4-O6-P-O5      |
| 26  | c     | 522 | LHG  | C3-O3-P-O4      |
| 26  | d     | 408 | LHG  | C3-O3-P-O4      |
| 26  | d     | 409 | LHG  | C3-O3-P-O4      |
| 26  | B     | 622 | LHG  | C4-O6-P-O4      |
| 26  | C     | 520 | LHG  | C4-O6-P-O5      |
| 26  | C     | 522 | LHG  | C3-O3-P-O4      |
| 26  | D     | 409 | LHG  | C3-O3-P-O4      |
| 26  | D     | 410 | LHG  | C3-O3-P-O4      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | r     | 302 | LHG  | C3-O3-P-O4      |
| 26  | R     | 301 | LHG  | C3-O3-P-O4      |
| 21  | N     | 608 | CHL  | C16-C17-C18-C20 |
| 22  | G     | 613 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 604 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 607 | CLA  | C16-C17-C18-C20 |
| 36  | k     | 103 | LMG  | O6-C1-O1-C7     |
| 36  | K     | 103 | LMG  | O6-C1-O1-C7     |
| 26  | d     | 407 | LHG  | O6-C4-C5-C6     |
| 26  | D     | 408 | LHG  | O6-C4-C5-C6     |
| 26  | s     | 314 | LHG  | O6-C4-C5-C6     |
| 26  | S     | 314 | LHG  | O6-C4-C5-C6     |
| 32  | d     | 406 | PL9  | C42-C43-C44-C45 |
| 26  | d     | 407 | LHG  | C10-C11-C12-C13 |
| 26  | D     | 408 | LHG  | C10-C11-C12-C13 |
| 36  | D     | 411 | LMG  | C31-C32-C33-C34 |
| 36  | c     | 523 | LMG  | C37-C38-C39-C40 |
| 36  | C     | 523 | LMG  | C37-C38-C39-C40 |
| 22  | c     | 506 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 503 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 22  | r     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 36  | d     | 410 | LMG  | C31-C32-C33-C34 |
| 26  | y     | 617 | LHG  | C11-C12-C13-C14 |
| 26  | L     | 103 | LHG  | C11-C10-C9-C8   |
| 35  | c     | 519 | DGD  | C9B-CAB-CBB-CCB |
| 35  | J     | 101 | DGD  | C9B-CAB-CBB-CCB |
| 22  | Y     | 609 | CLA  | C11-C12-C13-C15 |
| 26  | l     | 102 | LHG  | C11-C10-C9-C8   |
| 35  | c     | 517 | DGD  | C4B-C5B-C6B-C7B |
| 21  | s     | 306 | CHL  | CAD-CBD-CGD-O1D |
| 21  | S     | 306 | CHL  | CAD-CBD-CGD-O1D |
| 22  | g     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 22  | n     | 612 | CLA  | CAD-CBD-CGD-O1D |
| 22  | y     | 612 | CLA  | CAD-CBD-CGD-O1D |
| 22  | G     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 22  | N     | 612 | CLA  | CAD-CBD-CGD-O1D |
| 22  | Y     | 611 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 603 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 606 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 616 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | s     | 304 | CLA  | CAD-CBD-CGD-O1D |
| 22  | S     | 304 | CLA  | CAD-CBD-CGD-O1D |
| 33  | a     | 411 | SQD  | C5-C6-S-O7      |
| 33  | d     | 402 | SQD  | C5-C6-S-O9      |
| 33  | l     | 103 | SQD  | O5-C5-C6-S      |
| 33  | A     | 412 | SQD  | C5-C6-S-O7      |
| 33  | D     | 402 | SQD  | C5-C6-S-O9      |
| 33  | L     | 101 | SQD  | O5-C5-C6-S      |
| 26  | c     | 520 | LHG  | C23-C24-C25-C26 |
| 26  | C     | 520 | LHG  | C23-C24-C25-C26 |
| 22  | c     | 512 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 513 | CLA  | C13-C15-C16-C17 |
| 35  | h     | 102 | DGD  | C3A-C4A-C5A-C6A |
| 35  | C     | 518 | DGD  | C4B-C5B-C6B-C7B |
| 35  | H     | 102 | DGD  | C3A-C4A-C5A-C6A |
| 22  | r     | 310 | CLA  | O1D-CGD-O2D-CED |
| 26  | r     | 302 | LHG  | C15-C16-C17-C18 |
| 30  | d     | 401 | PHO  | CBA-CGA-O2A-C1  |
| 30  | D     | 401 | PHO  | CBA-CGA-O2A-C1  |
| 26  | d     | 408 | LHG  | C1-C2-C3-O3     |
| 26  | D     | 409 | LHG  | C1-C2-C3-O3     |
| 26  | R     | 301 | LHG  | C15-C16-C17-C18 |
| 22  | y     | 610 | CLA  | C11-C12-C13-C15 |
| 21  | g     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | g     | 601 | CHL  | C12-C13-C15-C16 |
| 21  | n     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | n     | 601 | CHL  | C12-C13-C15-C16 |
| 21  | y     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | y     | 601 | CHL  | C12-C13-C15-C16 |
| 21  | G     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | G     | 601 | CHL  | C12-C13-C15-C16 |
| 21  | N     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | N     | 601 | CHL  | C12-C13-C15-C16 |
| 21  | Y     | 601 | CHL  | C6-C7-C8-C10    |
| 21  | Y     | 601 | CHL  | C12-C13-C15-C16 |
| 22  | g     | 613 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | y     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 613 | CLA  | C6-C7-C8-C10    |
| 22  | N     | 612 | CLA  | C6-C7-C8-C10    |
| 22  | Y     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 601 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 604 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 607 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 611 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 502 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 503 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 508 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 604 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 607 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 613 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 614 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 503 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 504 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 509 | CLA  | C11-C12-C13-C15 |
| 22  | r     | 303 | CLA  | C11-C10-C8-C7   |
| 22  | R     | 302 | CLA  | C11-C10-C8-C7   |
| 26  | c     | 520 | LHG  | O6-C4-C5-O7     |
| 26  | d     | 407 | LHG  | O6-C4-C5-O7     |
| 26  | C     | 520 | LHG  | O6-C4-C5-O7     |
| 26  | D     | 408 | LHG  | O6-C4-C5-O7     |
| 26  | r     | 302 | LHG  | O6-C4-C5-O7     |
| 26  | R     | 301 | LHG  | O6-C4-C5-O7     |
| 32  | a     | 410 | PL9  | C2-C3-C7-C8     |
| 32  | A     | 411 | PL9  | C2-C3-C7-C8     |
| 24  | n     | 615 | XAT  | C29-C30-C31-C32 |
| 21  | G     | 601 | CHL  | CBD-CGD-O2D-CED |
| 26  | d     | 407 | LHG  | C8-C7-O7-C5     |
| 26  | d     | 409 | LHG  | C8-C7-O7-C5     |
| 26  | D     | 408 | LHG  | C8-C7-O7-C5     |
| 26  | D     | 410 | LHG  | C8-C7-O7-C5     |
| 22  | r     | 304 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 502 | CLA  | C2A-CAA-CBA-CGA |
| 22  | R     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 32  | D     | 407 | PL9  | C42-C43-C44-C45 |
| 21  | g     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 21  | n     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 21  | y     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 21  | G     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 21  | N     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 21  | Y     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 26  | d     | 409 | LHG  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | l     | 101 | SQD  | C44-C45-C46-O48 |
| 33  | L     | 102 | SQD  | C44-C45-C46-O48 |
| 36  | w     | 102 | LMG  | O1-C7-C8-C9     |
| 36  | C     | 502 | LMG  | O1-C7-C8-C9     |
| 36  | T     | 101 | LMG  | C21-C22-C23-C24 |
| 26  | b     | 619 | LHG  | O7-C5-C6-O8     |
| 26  | B     | 622 | LHG  | O7-C5-C6-O8     |
| 33  | a     | 411 | SQD  | O6-C44-C45-O47  |
| 33  | l     | 103 | SQD  | O6-C44-C45-O47  |
| 33  | A     | 412 | SQD  | O6-C44-C45-O47  |
| 33  | L     | 101 | SQD  | O6-C44-C45-O47  |
| 36  | k     | 103 | LMG  | O1-C7-C8-O7     |
| 36  | K     | 103 | LMG  | O1-C7-C8-O7     |
| 26  | N     | 618 | LHG  | C35-C36-C37-C38 |
| 26  | D     | 410 | LHG  | C14-C15-C16-C17 |
| 36  | M     | 101 | LMG  | C21-C22-C23-C24 |
| 22  | R     | 309 | CLA  | O1D-CGD-O2D-CED |
| 21  | y     | 601 | CHL  | CBD-CGD-O2D-CED |
| 31  | B     | 602 | BCR  | C14-C15-C16-C17 |
| 22  | R     | 303 | CLA  | C5-C6-C7-C8     |
| 21  | r     | 306 | CHL  | C3-C5-C6-C7     |
| 21  | R     | 305 | CHL  | C3-C5-C6-C7     |
| 26  | L     | 103 | LHG  | C10-C11-C12-C13 |
| 26  | N     | 618 | LHG  | O10-C23-O8-C6   |
| 36  | b     | 620 | LMG  | C4-C5-C6-O5     |
| 36  | B     | 623 | LMG  | C4-C5-C6-O5     |
| 26  | l     | 102 | LHG  | C10-C11-C12-C13 |
| 22  | G     | 610 | CLA  | C16-C17-C18-C19 |
| 21  | g     | 607 | CHL  | C6-C7-C8-C9     |
| 21  | n     | 606 | CHL  | C6-C7-C8-C9     |
| 21  | y     | 607 | CHL  | C6-C7-C8-C9     |
| 21  | G     | 607 | CHL  | C6-C7-C8-C9     |
| 21  | N     | 606 | CHL  | C6-C7-C8-C9     |
| 21  | Y     | 606 | CHL  | C6-C7-C8-C9     |
| 21  | r     | 306 | CHL  | C14-C13-C15-C16 |
| 21  | R     | 305 | CHL  | C14-C13-C15-C16 |
| 22  | b     | 605 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 610 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 612 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 509 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 608 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 613 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 615 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 510 | CLA  | C11-C10-C8-C9   |
| 22  | r     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | R     | 309 | CLA  | C6-C7-C8-C9     |
| 26  | L     | 103 | LHG  | O10-C23-O8-C6   |
| 26  | s     | 314 | LHG  | C31-C32-C33-C34 |
| 26  | S     | 314 | LHG  | C31-C32-C33-C34 |
| 36  | k     | 103 | LMG  | C37-C38-C39-C40 |
| 36  | b     | 620 | LMG  | C41-C42-C43-C44 |
| 36  | K     | 103 | LMG  | C37-C38-C39-C40 |
| 26  | y     | 617 | LHG  | C23-C24-C25-C26 |
| 26  | l     | 102 | LHG  | O10-C23-O8-C6   |
| 22  | c     | 510 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 36  | B     | 623 | LMG  | C41-C42-C43-C44 |
| 23  | g     | 615 | LUT  | C10-C11-C12-C13 |
| 23  | n     | 614 | LUT  | C10-C11-C12-C13 |
| 23  | y     | 614 | LUT  | C10-C11-C12-C13 |
| 23  | G     | 615 | LUT  | C10-C11-C12-C13 |
| 23  | N     | 614 | LUT  | C10-C11-C12-C13 |
| 23  | Y     | 613 | LUT  | C10-C11-C12-C13 |
| 23  | r     | 313 | LUT  | C10-C11-C12-C13 |
| 23  | R     | 312 | LUT  | C10-C11-C12-C13 |
| 25  | g     | 618 | NEX  | C30-C31-C32-C33 |
| 25  | n     | 616 | NEX  | C30-C31-C32-C33 |
| 25  | y     | 616 | NEX  | C30-C31-C32-C33 |
| 25  | N     | 617 | NEX  | C30-C31-C32-C33 |
| 25  | Y     | 616 | NEX  | C30-C31-C32-C33 |
| 23  | G     | 616 | LUT  | C9-C10-C11-C12  |
| 25  | y     | 618 | NEX  | C13-C14-C15-C35 |
| 25  | r     | 315 | NEX  | C13-C14-C15-C35 |
| 22  | b     | 605 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 608 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 514 | CLA  | C8-C10-C11-C12  |
| 30  | d     | 401 | PHO  | O1A-CGA-O2A-C1  |
| 30  | D     | 401 | PHO  | O1A-CGA-O2A-C1  |
| 24  | G     | 617 | XAT  | C7-C8-C9-C10    |
| 22  | c     | 513 | CLA  | C8-C10-C11-C12  |
| 36  | c     | 523 | LMG  | C4-C5-C6-O5     |
| 26  | n     | 617 | LHG  | O10-C23-O8-C6   |
| 22  | b     | 605 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 608 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | C     | 523 | LMG  | C4-C5-C6-O5     |
| 21  | n     | 601 | CHL  | CBD-CGD-O2D-CED |
| 22  | G     | 613 | CLA  | C16-C17-C18-C19 |
| 36  | w     | 102 | LMG  | C16-C17-C18-C19 |
| 36  | C     | 502 | LMG  | C16-C17-C18-C19 |
| 21  | g     | 606 | CHL  | C1-C2-C3-C4     |
| 21  | n     | 605 | CHL  | C1-C2-C3-C4     |
| 21  | y     | 606 | CHL  | C1-C2-C3-C4     |
| 21  | G     | 606 | CHL  | C1-C2-C3-C4     |
| 21  | N     | 605 | CHL  | C1-C2-C3-C4     |
| 21  | Y     | 605 | CHL  | C1-C2-C3-C4     |
| 22  | s     | 312 | CLA  | C1-C2-C3-C4     |
| 22  | S     | 312 | CLA  | C1-C2-C3-C4     |
| 26  | y     | 617 | LHG  | C11-C10-C9-C8   |
| 35  | c     | 518 | DGD  | C3G-C2G-O2G-C1B |
| 35  | C     | 519 | DGD  | C3G-C2G-O2G-C1B |
| 26  | g     | 619 | LHG  | O6-C4-C5-C6     |
| 21  | g     | 608 | CHL  | C2-C1-O2A-CGA   |
| 21  | n     | 607 | CHL  | C2-C1-O2A-CGA   |
| 21  | y     | 608 | CHL  | C2-C1-O2A-CGA   |
| 21  | G     | 608 | CHL  | C2-C1-O2A-CGA   |
| 21  | N     | 607 | CHL  | C2-C1-O2A-CGA   |
| 21  | Y     | 607 | CHL  | C2-C1-O2A-CGA   |
| 21  | r     | 308 | CHL  | C2-C1-O2A-CGA   |
| 21  | R     | 307 | CHL  | C2-C1-O2A-CGA   |
| 22  | b     | 601 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 508 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 604 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 509 | CLA  | C2-C1-O2A-CGA   |
| 22  | r     | 312 | CLA  | C2-C1-O2A-CGA   |
| 22  | R     | 311 | CLA  | C2-C1-O2A-CGA   |
| 36  | c     | 523 | LMG  | C35-C36-C37-C38 |
| 36  | C     | 523 | LMG  | C35-C36-C37-C38 |
| 36  | D     | 411 | LMG  | C32-C33-C34-C35 |
| 31  | T     | 102 | BCR  | C14-C15-C16-C17 |
| 36  | d     | 410 | LMG  | C32-C33-C34-C35 |
| 26  | y     | 617 | LHG  | C35-C36-C37-C38 |
| 33  | D     | 402 | SQD  | C11-C10-C9-C8   |
| 33  | d     | 402 | SQD  | C11-C10-C9-C8   |
| 35  | C     | 518 | DGD  | C2A-C3A-C4A-C5A |
| 35  | c     | 517 | DGD  | C2A-C3A-C4A-C5A |
| 22  | D     | 404 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 618 | BCR  | C5-C6-C7-C8     |
| 31  | b     | 618 | BCR  | C23-C24-C25-C26 |
| 31  | B     | 621 | BCR  | C5-C6-C7-C8     |
| 31  | B     | 621 | BCR  | C23-C24-C25-C26 |
| 22  | a     | 405 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 406 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 403 | CLA  | O1D-CGD-O2D-CED |
| 36  | c     | 523 | LMG  | C16-C17-C18-C19 |
| 22  | c     | 510 | CLA  | C4C-C3C-CAC-CBC |
| 26  | c     | 520 | LHG  | C31-C32-C33-C34 |
| 26  | C     | 520 | LHG  | C31-C32-C33-C34 |
| 36  | d     | 410 | LMG  | C14-C15-C16-C17 |
| 36  | C     | 523 | LMG  | C16-C17-C18-C19 |
| 21  | s     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 21  | S     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 22  | C     | 511 | CLA  | C4C-C3C-CAC-CBC |
| 36  | D     | 411 | LMG  | C14-C15-C16-C17 |
| 21  | g     | 601 | CHL  | C16-C17-C18-C20 |
| 21  | n     | 601 | CHL  | C16-C17-C18-C20 |
| 21  | y     | 601 | CHL  | C16-C17-C18-C20 |
| 21  | G     | 601 | CHL  | C16-C17-C18-C20 |
| 21  | N     | 601 | CHL  | C16-C17-C18-C20 |
| 21  | Y     | 601 | CHL  | C16-C17-C18-C20 |
| 22  | c     | 503 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 504 | CLA  | C16-C17-C18-C20 |
| 35  | C     | 518 | DGD  | C4D-C5D-C6D-O5D |
| 21  | G     | 601 | CHL  | C8-C10-C11-C12  |
| 21  | Y     | 601 | CHL  | C8-C10-C11-C12  |
| 30  | d     | 401 | PHO  | C2A-CAA-CBA-CGA |
| 30  | D     | 401 | PHO  | C2A-CAA-CBA-CGA |
| 35  | h     | 102 | DGD  | C2E-C1E-O5D-C6D |
| 35  | H     | 102 | DGD  | C2E-C1E-O5D-C6D |
| 36  | B     | 601 | LMG  | O7-C8-C9-O8     |
| 36  | I     | 101 | LMG  | O7-C8-C9-O8     |
| 21  | Y     | 601 | CHL  | CBD-CGD-O2D-CED |
| 26  | c     | 522 | LHG  | C3-O3-P-O6      |
| 26  | C     | 522 | LHG  | C3-O3-P-O6      |
| 35  | c     | 517 | DGD  | C4D-C5D-C6D-O5D |
| 21  | y     | 601 | CHL  | C8-C10-C11-C12  |
| 30  | d     | 401 | PHO  | CHA-CBD-CGD-O2D |
| 30  | D     | 401 | PHO  | CHA-CBD-CGD-O2D |
| 21  | G     | 601 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | N     | 601 | CHL  | O1D-CGD-O2D-CED |
| 21  | g     | 601 | CHL  | C8-C10-C11-C12  |
| 22  | x     | 101 | CLA  | C13-C15-C16-C17 |
| 33  | D     | 402 | SQD  | C30-C31-C32-C33 |
| 33  | a     | 411 | SQD  | O6-C44-C45-C46  |
| 33  | A     | 412 | SQD  | O6-C44-C45-C46  |
| 26  | C     | 522 | LHG  | C14-C15-C16-C17 |
| 33  | d     | 402 | SQD  | C30-C31-C32-C33 |
| 21  | g     | 601 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 601 | CHL  | C8-C10-C11-C12  |
| 21  | n     | 608 | CHL  | C11-C12-C13-C15 |
| 22  | g     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | g     | 612 | CLA  | C11-C10-C8-C7   |
| 22  | n     | 609 | CLA  | C12-C13-C15-C16 |
| 22  | n     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 611 | CLA  | C11-C10-C8-C7   |
| 22  | y     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 612 | CLA  | C11-C10-C8-C7   |
| 22  | N     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | N     | 611 | CLA  | C11-C10-C8-C7   |
| 22  | Y     | 610 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 503 | CLA  | C12-C13-C15-C16 |
| 22  | w     | 101 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 504 | CLA  | C12-C13-C15-C16 |
| 22  | W     | 101 | CLA  | C11-C10-C8-C7   |
| 22  | s     | 311 | CLA  | C6-C7-C8-C10    |
| 22  | S     | 311 | CLA  | C6-C7-C8-C10    |
| 26  | c     | 522 | LHG  | C14-C15-C16-C17 |
| 21  | Y     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | g     | 608 | CHL  | C6-C7-C8-C9     |
| 21  | n     | 607 | CHL  | C6-C7-C8-C9     |
| 21  | y     | 608 | CHL  | C6-C7-C8-C9     |
| 21  | G     | 608 | CHL  | C6-C7-C8-C9     |
| 21  | N     | 607 | CHL  | C6-C7-C8-C9     |
| 21  | Y     | 607 | CHL  | C6-C7-C8-C9     |
| 22  | g     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | n     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | y     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | y     | 612 | CLA  | C14-C13-C15-C16 |
| 22  | G     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | N     | 602 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | Y     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 604 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 607 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 610 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 502 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 508 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 513 | CLA  | C11-C12-C13-C14 |
| 22  | d     | 403 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 607 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 613 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 503 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 509 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 514 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 404 | CLA  | C11-C12-C13-C14 |
| 22  | s     | 303 | CLA  | C6-C7-C8-C9     |
| 22  | S     | 303 | CLA  | C6-C7-C8-C9     |
| 21  | n     | 601 | CHL  | C8-C10-C11-C12  |
| 21  | n     | 606 | CHL  | C10-C11-C12-C13 |
| 21  | N     | 606 | CHL  | C10-C11-C12-C13 |
| 22  | B     | 603 | CLA  | C13-C15-C16-C17 |
| 24  | N     | 616 | XAT  | C29-C30-C31-C32 |
| 31  | k     | 101 | BCR  | C15-C16-C17-C18 |
| 31  | K     | 101 | BCR  | C15-C16-C17-C18 |
| 22  | b     | 604 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 607 | CLA  | C16-C17-C18-C19 |
| 21  | g     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 26  | N     | 618 | LHG  | C19-C20-C21-C22 |
| 33  | d     | 402 | SQD  | C23-C24-C25-C26 |
| 33  | D     | 402 | SQD  | C23-C24-C25-C26 |
| 21  | n     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | y     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 21  | G     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 26  | c     | 520 | LHG  | C26-C27-C28-C29 |
| 26  | C     | 520 | LHG  | C26-C27-C28-C29 |
| 21  | y     | 601 | CHL  | O1D-CGD-O2D-CED |
| 21  | N     | 607 | CHL  | C4C-C3C-CAC-CBC |
| 21  | g     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 21  | n     | 605 | CHL  | CAA-CBA-CGA-O1A |
| 21  | y     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 21  | G     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 21  | N     | 605 | CHL  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | Y     | 605 | CHL  | CAA-CBA-CGA-O1A |
| 21  | g     | 607 | CHL  | C10-C11-C12-C13 |
| 21  | y     | 607 | CHL  | C10-C11-C12-C13 |
| 21  | G     | 607 | CHL  | C10-C11-C12-C13 |
| 26  | L     | 103 | LHG  | C28-C29-C30-C31 |
| 26  | l     | 102 | LHG  | C28-C29-C30-C31 |
| 26  | D     | 408 | LHG  | O10-C23-O8-C6   |
| 21  | Y     | 606 | CHL  | C10-C11-C12-C13 |
| 26  | c     | 521 | LHG  | O1-C1-C2-C3     |
| 26  | C     | 521 | LHG  | O1-C1-C2-C3     |
| 26  | d     | 407 | LHG  | O10-C23-O8-C6   |
| 22  | B     | 605 | CLA  | C16-C17-C18-C20 |
| 22  | r     | 310 | CLA  | C16-C17-C18-C20 |
| 22  | R     | 309 | CLA  | C16-C17-C18-C20 |
| 22  | g     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | n     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | y     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | N     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Y     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 26  | Y     | 617 | LHG  | C24-C23-O8-C6   |
| 21  | Y     | 601 | CHL  | O1D-CGD-O2D-CED |
| 36  | M     | 101 | LMG  | C19-C20-C21-C22 |
| 36  | T     | 101 | LMG  | C19-C20-C21-C22 |
| 22  | b     | 601 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 604 | CLA  | C5-C6-C7-C8     |
| 21  | n     | 601 | CHL  | O1D-CGD-O2D-CED |
| 22  | B     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 33  | D     | 402 | SQD  | O49-C7-C8-C9    |
| 24  | y     | 615 | XAT  | C29-C30-C31-C32 |
| 24  | N     | 616 | XAT  | C33-C34-C35-C15 |
| 24  | Y     | 615 | XAT  | C33-C34-C35-C15 |
| 24  | r     | 314 | XAT  | C13-C14-C15-C35 |
| 24  | R     | 313 | XAT  | C13-C14-C15-C35 |
| 36  | B     | 601 | LMG  | C37-C38-C39-C40 |
| 36  | I     | 101 | LMG  | C37-C38-C39-C40 |
| 26  | n     | 617 | LHG  | O6-C4-C5-C6     |
| 22  | y     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 22  | N     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 26  | y     | 617 | LHG  | C30-C31-C32-C33 |
| 36  | B     | 601 | LMG  | C33-C34-C35-C36 |
| 36  | I     | 101 | LMG  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 602 | CLA  | C16-C17-C18-C20 |
| 36  | k     | 103 | LMG  | C39-C40-C41-C42 |
| 21  | r     | 306 | CHL  | C4-C3-C5-C6     |
| 21  | R     | 305 | CHL  | C4-C3-C5-C6     |
| 22  | b     | 604 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 607 | CLA  | C4-C3-C5-C6     |
| 36  | K     | 103 | LMG  | C39-C40-C41-C42 |
| 22  | g     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 22  | n     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Y     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 21  | R     | 307 | CHL  | C5-C6-C7-C8     |
| 26  | G     | 618 | LHG  | O9-C7-O7-C5     |
| 33  | d     | 402 | SQD  | O49-C7-C8-C9    |
| 22  | s     | 304 | CLA  | CAA-CBA-CGA-O1A |
| 22  | S     | 304 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 514 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 515 | CLA  | C2-C1-O2A-CGA   |
| 21  | r     | 308 | CHL  | C5-C6-C7-C8     |
| 36  | B     | 623 | LMG  | C29-C30-C31-C32 |
| 36  | C     | 502 | LMG  | O6-C5-C6-O5     |
| 21  | s     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 22  | b     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | s     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 22  | S     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 35  | c     | 517 | DGD  | O1G-C1G-C2G-O2G |
| 35  | C     | 518 | DGD  | O1G-C1G-C2G-O2G |
| 36  | b     | 620 | LMG  | C29-C30-C31-C32 |
| 21  | g     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 21  | n     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 21  | y     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 21  | G     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 21  | N     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 21  | Y     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 22  | b     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 21  | S     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 26  | g     | 619 | LHG  | C27-C28-C29-C30 |
| 36  | w     | 102 | LMG  | O6-C5-C6-O5     |
| 26  | c     | 522 | LHG  | C11-C10-C9-C8   |
| 26  | C     | 522 | LHG  | C11-C10-C9-C8   |
| 22  | b     | 601 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 603 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 503 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 512 | CLA  | C11-C12-C13-C14 |
| 22  | d     | 403 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 604 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 606 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 504 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 513 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 404 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 405 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 406 | CLA  | C15-C16-C17-C18 |
| 26  | Y     | 617 | LHG  | C23-C24-C25-C26 |
| 25  | Y     | 616 | NEX  | C39-C29-C30-C31 |
| 35  | a     | 413 | DGD  | C1G-C2G-C3G-O3G |
| 35  | A     | 401 | DGD  | C1G-C2G-C3G-O3G |
| 36  | c     | 523 | LMG  | O1-C7-C8-C9     |
| 36  | C     | 523 | LMG  | O1-C7-C8-C9     |
| 36  | K     | 103 | LMG  | O9-C10-O7-C8    |
| 35  | c     | 518 | DGD  | O2G-C1B-C2B-C3B |
| 35  | C     | 519 | DGD  | O2G-C1B-C2B-C3B |
| 22  | S     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 21  | S     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 26  | G     | 618 | LHG  | O10-C23-O8-C6   |
| 22  | y     | 610 | CLA  | C11-C12-C13-C14 |
| 22  | Y     | 609 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 614 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 617 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 504 | CLA  | C16-C17-C18-C19 |
| 35  | a     | 413 | DGD  | C6A-C7A-C8A-C9A |
| 35  | A     | 401 | DGD  | C6A-C7A-C8A-C9A |
| 35  | H     | 102 | DGD  | C7B-C8B-C9B-CAB |
| 22  | s     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 35  | h     | 102 | DGD  | C7B-C8B-C9B-CAB |
| 21  | s     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 22  | c     | 509 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 510 | CLA  | C4-C3-C5-C6     |
| 21  | g     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 21  | n     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 21  | y     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 21  | G     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 21  | N     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 21  | Y     | 607 | CHL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 605 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 605 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 503 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 503 | CLA  | C16-C17-C18-C19 |
| 36  | k     | 103 | LMG  | O9-C10-O7-C8    |
| 21  | N     | 608 | CHL  | C11-C12-C13-C15 |
| 22  | a     | 405 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 604 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 406 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 606 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 607 | CLA  | C11-C10-C8-C7   |
| 35  | c     | 518 | DGD  | C3B-C4B-C5B-C6B |
| 35  | C     | 519 | DGD  | C3B-C4B-C5B-C6B |
| 36  | d     | 410 | LMG  | C35-C36-C37-C38 |
| 36  | D     | 411 | LMG  | C35-C36-C37-C38 |
| 21  | s     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 21  | S     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 36  | B     | 623 | LMG  | C39-C40-C41-C42 |
| 36  | b     | 620 | LMG  | C39-C40-C41-C42 |
| 22  | s     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 22  | S     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 508 | CLA  | C5-C6-C7-C8     |
| 26  | r     | 302 | LHG  | C5-C4-O6-P      |
| 26  | R     | 301 | LHG  | C5-C4-O6-P      |
| 36  | C     | 502 | LMG  | C4-C5-C6-O5     |
| 22  | c     | 507 | CLA  | C5-C6-C7-C8     |
| 21  | g     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 22  | c     | 506 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 507 | CLA  | C15-C16-C17-C18 |
| 36  | w     | 102 | LMG  | C4-C5-C6-O5     |
| 22  | b     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 21  | n     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 21  | G     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 21  | N     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 24  | r     | 314 | XAT  | C32-C33-C34-C35 |
| 24  | R     | 313 | XAT  | C32-C33-C34-C35 |
| 35  | a     | 413 | DGD  | O2G-C2G-C3G-O3G |
| 35  | A     | 401 | DGD  | O2G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 607 | CLA  | CBA-CGA-O2A-C1  |
| 21  | y     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 21  | Y     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 22  | A     | 406 | CLA  | C2A-CAA-CBA-CGA |
| 23  | r     | 313 | LUT  | C29-C30-C31-C32 |
| 23  | R     | 312 | LUT  | C29-C30-C31-C32 |
| 36  | C     | 502 | LMG  | C38-C39-C40-C41 |
| 36  | w     | 102 | LMG  | C38-C39-C40-C41 |
| 26  | c     | 521 | LHG  | C1-C2-C3-O3     |
| 26  | C     | 521 | LHG  | C1-C2-C3-O3     |
| 21  | g     | 601 | CHL  | C2-C1-O2A-CGA   |
| 21  | n     | 601 | CHL  | C2-C1-O2A-CGA   |
| 21  | y     | 601 | CHL  | C2-C1-O2A-CGA   |
| 21  | G     | 601 | CHL  | C2-C1-O2A-CGA   |
| 21  | Y     | 601 | CHL  | C2-C1-O2A-CGA   |
| 35  | c     | 519 | DGD  | O6D-C5D-C6D-O5D |
| 35  | J     | 101 | DGD  | O6D-C5D-C6D-O5D |
| 21  | r     | 306 | CHL  | C2-C3-C5-C6     |
| 21  | R     | 305 | CHL  | C2-C3-C5-C6     |
| 22  | a     | 408 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 607 | CLA  | O1A-CGA-O2A-C1  |
| 21  | S     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 22  | x     | 101 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 603 | CLA  | C14-C13-C15-C16 |
| 21  | s     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 26  | C     | 521 | LHG  | C19-C20-C21-C22 |
| 26  | r     | 302 | LHG  | C10-C11-C12-C13 |
| 26  | R     | 301 | LHG  | C10-C11-C12-C13 |
| 26  | c     | 521 | LHG  | C19-C20-C21-C22 |
| 26  | c     | 522 | LHG  | C28-C29-C30-C31 |
| 22  | g     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | n     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | y     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | G     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | N     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Y     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 405 | CLA  | C2A-CAA-CBA-CGA |
| 26  | C     | 522 | LHG  | C28-C29-C30-C31 |
| 26  | s     | 314 | LHG  | O10-C23-O8-C6   |
| 26  | S     | 314 | LHG  | O10-C23-O8-C6   |
| 23  | N     | 615 | LUT  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 616 | BCR  | C23-C24-C25-C30 |
| 31  | b     | 617 | BCR  | C23-C24-C25-C26 |
| 31  | b     | 617 | BCR  | C23-C24-C25-C30 |
| 31  | b     | 618 | BCR  | C1-C6-C7-C8     |
| 31  | b     | 618 | BCR  | C23-C24-C25-C30 |
| 31  | B     | 602 | BCR  | C23-C24-C25-C30 |
| 31  | B     | 619 | BCR  | C23-C24-C25-C30 |
| 31  | B     | 620 | BCR  | C23-C24-C25-C26 |
| 31  | B     | 620 | BCR  | C23-C24-C25-C30 |
| 31  | B     | 621 | BCR  | C1-C6-C7-C8     |
| 31  | B     | 621 | BCR  | C23-C24-C25-C30 |
| 31  | T     | 102 | BCR  | C23-C24-C25-C30 |
| 22  | g     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 22  | N     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Y     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 35  | c     | 517 | DGD  | C1G-C2G-C3G-O3G |
| 35  | C     | 518 | DGD  | C1G-C2G-C3G-O3G |
| 22  | s     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 22  | S     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 26  | g     | 619 | LHG  | C14-C15-C16-C17 |
| 26  | Y     | 617 | LHG  | C10-C11-C12-C13 |
| 24  | Y     | 615 | XAT  | C29-C30-C31-C32 |
| 25  | n     | 616 | NEX  | C29-C30-C31-C32 |
| 25  | n     | 616 | NEX  | C33-C34-C35-C15 |
| 32  | d     | 406 | PL9  | C35-C34-C36-C37 |
| 32  | D     | 407 | PL9  | C35-C34-C36-C37 |
| 22  | r     | 310 | CLA  | C16-C17-C18-C19 |
| 22  | R     | 309 | CLA  | C16-C17-C18-C19 |
| 22  | s     | 303 | CLA  | C5-C6-C7-C8     |
| 22  | S     | 303 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 409 | CLA  | C2-C3-C5-C6     |
| 36  | B     | 601 | LMG  | C8-C7-O1-C1     |
| 36  | D     | 411 | LMG  | C8-C7-O1-C1     |
| 36  | I     | 101 | LMG  | C8-C7-O1-C1     |
| 26  | c     | 521 | LHG  | C24-C23-O8-C6   |
| 26  | C     | 521 | LHG  | C24-C23-O8-C6   |
| 26  | c     | 520 | LHG  | C35-C36-C37-C38 |
| 21  | S     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 22  | G     | 603 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | C     | 520 | LHG  | C35-C36-C37-C38 |
| 26  | b     | 619 | LHG  | C13-C14-C15-C16 |
| 22  | B     | 618 | CLA  | C3-C5-C6-C7     |
| 21  | s     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 22  | b     | 614 | CLA  | O1D-CGD-O2D-CED |
| 26  | B     | 622 | LHG  | C13-C14-C15-C16 |
| 26  | N     | 618 | LHG  | O6-C4-C5-C6     |
| 26  | c     | 520 | LHG  | O6-C4-C5-C6     |
| 26  | C     | 520 | LHG  | O6-C4-C5-C6     |
| 30  | d     | 401 | PHO  | C4-C3-C5-C6     |
| 30  | D     | 401 | PHO  | C4-C3-C5-C6     |
| 35  | h     | 102 | DGD  | C2A-C3A-C4A-C5A |
| 35  | H     | 102 | DGD  | C2A-C3A-C4A-C5A |
| 21  | Y     | 608 | CHL  | C12-C13-C15-C16 |
| 22  | g     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | g     | 610 | CLA  | C11-C12-C13-C15 |
| 22  | n     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | y     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | G     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | N     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | N     | 609 | CLA  | C11-C12-C13-C15 |
| 22  | Y     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 613 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 514 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 616 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 515 | CLA  | C12-C13-C15-C16 |
| 22  | g     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 615 | CLA  | C3-C5-C6-C7     |
| 26  | g     | 619 | LHG  | C35-C36-C37-C38 |
| 26  | b     | 619 | LHG  | O7-C7-C8-C9     |
| 36  | T     | 101 | LMG  | O8-C28-C29-C30  |
| 22  | y     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | N     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | Y     | 603 | CLA  | CBD-CGD-O2D-CED |
| 26  | n     | 617 | LHG  | C34-C35-C36-C37 |
| 22  | b     | 613 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 616 | CLA  | C15-C16-C17-C18 |
| 22  | r     | 303 | CLA  | C10-C11-C12-C13 |
| 22  | R     | 302 | CLA  | C10-C11-C12-C13 |
| 22  | s     | 312 | CLA  | O2A-C1-C2-C3    |
| 22  | S     | 312 | CLA  | O2A-C1-C2-C3    |
| 26  | N     | 618 | LHG  | O8-C23-C24-C25  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | B     | 622 | LHG  | O7-C7-C8-C9     |
| 36  | M     | 101 | LMG  | O8-C28-C29-C30  |
| 21  | g     | 601 | CHL  | C16-C17-C18-C19 |
| 21  | n     | 601 | CHL  | C16-C17-C18-C19 |
| 21  | y     | 601 | CHL  | C16-C17-C18-C19 |
| 21  | G     | 601 | CHL  | C16-C17-C18-C19 |
| 21  | N     | 601 | CHL  | C16-C17-C18-C19 |
| 21  | Y     | 601 | CHL  | C16-C17-C18-C19 |
| 22  | b     | 601 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 604 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 617 | CLA  | O1D-CGD-O2D-CED |
| 22  | n     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 603 | CLA  | CBD-CGD-O2D-CED |
| 26  | D     | 408 | LHG  | C15-C16-C17-C18 |
| 21  | r     | 308 | CHL  | C4-C3-C5-C6     |
| 21  | R     | 307 | CHL  | C4-C3-C5-C6     |
| 22  | c     | 504 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 505 | CLA  | C4-C3-C5-C6     |
| 22  | Y     | 611 | CLA  | C15-C16-C17-C18 |
| 26  | d     | 407 | LHG  | C15-C16-C17-C18 |
| 26  | D     | 408 | LHG  | C3-O3-P-O6      |
| 22  | s     | 310 | CLA  | C2-C3-C5-C6     |
| 22  | S     | 310 | CLA  | C2-C3-C5-C6     |
| 22  | g     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | N     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Y     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 22  | s     | 311 | CLA  | C11-C10-C8-C7   |
| 22  | S     | 311 | CLA  | C11-C10-C8-C7   |
| 21  | g     | 601 | CHL  | C6-C7-C8-C9     |
| 21  | n     | 601 | CHL  | C6-C7-C8-C9     |
| 21  | y     | 601 | CHL  | C6-C7-C8-C9     |
| 21  | G     | 601 | CHL  | C6-C7-C8-C9     |
| 21  | N     | 601 | CHL  | C6-C7-C8-C9     |
| 21  | Y     | 601 | CHL  | C6-C7-C8-C9     |
| 22  | b     | 603 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 611 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 510 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 606 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 614 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 511 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | r     | 303 | CLA  | C11-C10-C8-C9   |
| 22  | R     | 302 | CLA  | C11-C10-C8-C9   |
| 33  | A     | 412 | SQD  | C27-C28-C29-C30 |
| 33  | a     | 411 | SQD  | C27-C28-C29-C30 |
| 22  | c     | 514 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 515 | CLA  | C3A-C2A-CAA-CBA |
| 30  | d     | 401 | PHO  | C3A-C2A-CAA-CBA |
| 30  | D     | 401 | PHO  | C3A-C2A-CAA-CBA |
| 22  | g     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | g     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 22  | n     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | n     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | y     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | y     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 22  | G     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | G     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 22  | N     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | N     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | Y     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 22  | Y     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 612 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 505 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 512 | CLA  | CAD-CBD-CGD-O2D |
| 22  | x     | 101 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 612 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 615 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 506 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 513 | CLA  | CAD-CBD-CGD-O2D |
| 22  | r     | 305 | CLA  | CAD-CBD-CGD-O2D |
| 22  | s     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 22  | S     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 22  | R     | 304 | CLA  | CAD-CBD-CGD-O2D |
| 25  | Y     | 616 | NEX  | C7-C8-C9-C19    |
| 26  | B     | 622 | LHG  | C10-C11-C12-C13 |
| 26  | b     | 619 | LHG  | C10-C11-C12-C13 |
| 26  | g     | 619 | LHG  | C7-C8-C9-C10    |
| 22  | c     | 502 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 503 | CLA  | CAA-CBA-CGA-O2A |
| 22  | r     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 22  | R     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 35  | c     | 517 | DGD  | O2G-C1B-C2B-C3B |
| 35  | C     | 518 | DGD  | O2G-C1B-C2B-C3B |
| 22  | a     | 408 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 409 | CLA  | C4-C3-C5-C6     |
| 21  | g     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 22  | s     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 22  | S     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 514 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 515 | CLA  | C13-C15-C16-C17 |
| 21  | g     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 21  | n     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 21  | y     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 21  | G     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 21  | N     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 21  | Y     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 22  | c     | 506 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 507 | CLA  | CAA-CBA-CGA-O2A |
| 22  | s     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 22  | S     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 26  | Y     | 617 | LHG  | C31-C32-C33-C34 |
| 24  | g     | 617 | XAT  | C7-C8-C9-C10    |
| 26  | d     | 408 | LHG  | C31-C32-C33-C34 |
| 26  | D     | 409 | LHG  | C31-C32-C33-C34 |
| 24  | y     | 615 | XAT  | O4-C6-C7-C8     |
| 24  | Y     | 615 | XAT  | O4-C6-C7-C8     |
| 35  | a     | 413 | DGD  | O1G-C1G-C2G-C3G |
| 35  | A     | 401 | DGD  | O1G-C1G-C2G-C3G |
| 21  | G     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 35  | c     | 517 | DGD  | O6D-C5D-C6D-O5D |
| 35  | c     | 517 | DGD  | C3B-C4B-C5B-C6B |
| 22  | b     | 603 | CLA  | O2A-C1-C2-C3    |
| 22  | B     | 606 | CLA  | O2A-C1-C2-C3    |
| 22  | s     | 305 | CLA  | O2A-C1-C2-C3    |
| 22  | S     | 305 | CLA  | O2A-C1-C2-C3    |
| 35  | J     | 101 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 518 | DGD  | O6D-C5D-C6D-O5D |
| 21  | r     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 22  | C     | 505 | CLA  | C8-C10-C11-C12  |
| 26  | c     | 521 | LHG  | O7-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | L     | 103 | LHG  | C31-C32-C33-C34 |
| 35  | c     | 519 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 518 | DGD  | C3B-C4B-C5B-C6B |
| 22  | b     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 617 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 608 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 608 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 502 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 502 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 504 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 504 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 511 | CLA  | CHA-CBD-CGD-O2D |
| 22  | d     | 403 | CLA  | CHA-CBD-CGD-O1D |
| 22  | d     | 403 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 503 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 503 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 505 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 505 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 512 | CLA  | CHA-CBD-CGD-O2D |
| 22  | D     | 404 | CLA  | CHA-CBD-CGD-O1D |
| 22  | D     | 404 | CLA  | CHA-CBD-CGD-O2D |
| 22  | r     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 22  | r     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 22  | r     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 22  | s     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 22  | S     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 22  | R     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 22  | R     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 22  | R     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 21  | G     | 605 | CHL  | CAA-CBA-CGA-O1A |
| 26  | C     | 521 | LHG  | O7-C7-C8-C9     |
| 26  | B     | 622 | LHG  | C17-C18-C19-C20 |
| 26  | l     | 102 | LHG  | C31-C32-C33-C34 |
| 22  | c     | 504 | CLA  | C8-C10-C11-C12  |
| 31  | T     | 102 | BCR  | C12-C13-C14-C15 |
| 21  | g     | 605 | CHL  | CAA-CBA-CGA-O1A |
| 26  | b     | 619 | LHG  | C17-C18-C19-C20 |
| 22  | s     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 613 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 616 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | g     | 610 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 609 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 610 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Y     | 609 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 513 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 514 | CLA  | CAA-CBA-CGA-O2A |
| 22  | r     | 312 | CLA  | CAA-CBA-CGA-O2A |
| 22  | s     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 22  | S     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 22  | R     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 26  | G     | 618 | LHG  | O7-C7-C8-C9     |
| 35  | c     | 519 | DGD  | O2G-C1B-C2B-C3B |
| 22  | n     | 603 | CLA  | O1D-CGD-O2D-CED |
| 35  | c     | 517 | DGD  | O2G-C2G-C3G-O3G |
| 35  | C     | 518 | DGD  | O2G-C2G-C3G-O3G |
| 33  | d     | 402 | SQD  | C7-C8-C9-C10    |
| 33  | D     | 402 | SQD  | C7-C8-C9-C10    |
| 35  | H     | 102 | DGD  | C9B-CAB-CBB-CCB |
| 36  | M     | 101 | LMG  | C38-C39-C40-C41 |
| 36  | T     | 101 | LMG  | C38-C39-C40-C41 |
| 22  | N     | 603 | CLA  | O1D-CGD-O2D-CED |
| 36  | C     | 523 | LMG  | C30-C31-C32-C33 |
| 21  | y     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 22  | G     | 610 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 607 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 610 | CLA  | CAA-CBA-CGA-O2A |
| 22  | r     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 22  | s     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 22  | S     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 22  | R     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 35  | h     | 102 | DGD  | C9B-CAB-CBB-CCB |
| 36  | c     | 523 | LMG  | C30-C31-C32-C33 |
| 21  | R     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 22  | S     | 310 | CLA  | C6-C7-C8-C9     |
| 21  | s     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 22  | Y     | 603 | CLA  | O1D-CGD-O2D-CED |
| 26  | d     | 409 | LHG  | C24-C23-O8-C6   |
| 26  | D     | 410 | LHG  | C24-C23-O8-C6   |
| 22  | G     | 603 | CLA  | O1D-CGD-O2D-CED |
| 36  | k     | 103 | LMG  | C11-C10-O7-C8   |
| 36  | K     | 103 | LMG  | C11-C10-O7-C8   |
| 22  | N     | 609 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | r     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 22  | R     | 302 | CLA  | CAA-CBA-CGA-O2A |
| 35  | J     | 101 | DGD  | O2G-C1B-C2B-C3B |
| 22  | g     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | n     | 609 | CLA  | C11-C12-C13-C15 |
| 22  | y     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | G     | 610 | CLA  | C11-C12-C13-C15 |
| 22  | N     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | Y     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 602 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 614 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 605 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 617 | CLA  | C6-C7-C8-C10    |
| 26  | d     | 408 | LHG  | C28-C29-C30-C31 |
| 26  | D     | 409 | LHG  | C28-C29-C30-C31 |
| 36  | b     | 620 | LMG  | O6-C1-O1-C7     |
| 21  | S     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 21  | n     | 608 | CHL  | C11-C12-C13-C14 |
| 21  | y     | 609 | CHL  | C11-C12-C13-C14 |
| 21  | N     | 608 | CHL  | C11-C12-C13-C14 |
| 22  | c     | 514 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 509 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 515 | CLA  | C14-C13-C15-C16 |
| 22  | r     | 310 | CLA  | C14-C13-C15-C16 |
| 22  | R     | 309 | CLA  | C14-C13-C15-C16 |
| 26  | C     | 521 | LHG  | C9-C10-C11-C12  |
| 26  | S     | 314 | LHG  | C9-C10-C11-C12  |
| 22  | Y     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 614 | CLA  | C15-C16-C17-C18 |
| 36  | k     | 103 | LMG  | O7-C10-C11-C12  |
| 36  | K     | 103 | LMG  | O7-C10-C11-C12  |
| 33  | a     | 411 | SQD  | C4-C5-C6-S      |
| 33  | A     | 412 | SQD  | C4-C5-C6-S      |
| 21  | r     | 308 | CHL  | C11-C12-C13-C14 |
| 26  | s     | 314 | LHG  | C9-C10-C11-C12  |
| 26  | R     | 301 | LHG  | C29-C30-C31-C32 |
| 22  | g     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | y     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | G     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 611 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 615 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 26  | r     | 302 | LHG  | C29-C30-C31-C32 |
| 32  | a     | 410 | PL9  | C7-C8-C9-C11    |
| 32  | A     | 411 | PL9  | C7-C8-C9-C11    |
| 22  | y     | 603 | CLA  | O1D-CGD-O2D-CED |
| 26  | c     | 521 | LHG  | C9-C10-C11-C12  |
| 21  | g     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 21  | G     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 21  | N     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 22  | n     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 22  | S     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 22  | n     | 603 | CLA  | C15-C16-C17-C18 |
| 22  | N     | 603 | CLA  | C15-C16-C17-C18 |
| 21  | R     | 307 | CHL  | C11-C12-C13-C14 |
| 26  | b     | 619 | LHG  | C31-C32-C33-C34 |
| 26  | B     | 622 | LHG  | C31-C32-C33-C34 |
| 26  | Y     | 617 | LHG  | O1-C1-C2-C3     |
| 30  | d     | 401 | PHO  | C2-C3-C5-C6     |
| 35  | a     | 413 | DGD  | O2G-C1B-C2B-C3B |
| 35  | A     | 401 | DGD  | O2G-C1B-C2B-C3B |
| 22  | g     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 22  | y     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 22  | G     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 22  | N     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Y     | 611 | CLA  | CAA-CBA-CGA-O1A |
| 22  | s     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 618 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 607 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 513 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 514 | CLA  | C1A-C2A-CAA-CBA |
| 22  | s     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | S     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 21  | n     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 21  | y     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 21  | Y     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 22  | c     | 506 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 507 | CLA  | CAA-CBA-CGA-O1A |
| 22  | g     | 603 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | N     | 601 | CHL  | C2-C1-O2A-CGA   |
| 26  | G     | 618 | LHG  | O9-C7-C8-C9     |
| 35  | h     | 102 | DGD  | C1G-C2G-C3G-O3G |
| 35  | H     | 102 | DGD  | C1G-C2G-C3G-O3G |
| 22  | N     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 21  | s     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 22  | b     | 607 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 616 | CLA  | C2A-CAA-CBA-CGA |
| 26  | d     | 407 | LHG  | C3-O3-P-O6      |
| 26  | c     | 521 | LHG  | O2-C2-C3-O3     |
| 26  | C     | 521 | LHG  | O2-C2-C3-O3     |
| 22  | R     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 26  | b     | 619 | LHG  | O9-C7-C8-C9     |
| 22  | x     | 101 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 603 | CLA  | C5-C6-C7-C8     |
| 35  | h     | 102 | DGD  | C6A-C7A-C8A-C9A |
| 22  | g     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Y     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 35  | H     | 102 | DGD  | C6A-C7A-C8A-C9A |
| 22  | r     | 304 | CLA  | CAA-CBA-CGA-O1A |
| 26  | B     | 622 | LHG  | O9-C7-C8-C9     |
| 30  | D     | 401 | PHO  | C2-C3-C5-C6     |
| 35  | C     | 519 | DGD  | C4B-C5B-C6B-C7B |
| 26  | d     | 407 | LHG  | C4-O6-P-O5      |
| 26  | d     | 408 | LHG  | C4-O6-P-O4      |
| 26  | l     | 102 | LHG  | C3-O3-P-O5      |
| 26  | D     | 408 | LHG  | C4-O6-P-O5      |
| 26  | D     | 409 | LHG  | C4-O6-P-O4      |
| 26  | L     | 103 | LHG  | C3-O3-P-O5      |
| 26  | r     | 302 | LHG  | C4-O6-P-O5      |
| 26  | R     | 301 | LHG  | C4-O6-P-O5      |
| 35  | c     | 518 | DGD  | C4B-C5B-C6B-C7B |
| 22  | b     | 607 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 610 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 503 | CLA  | CAA-CBA-CGA-O1A |
| 22  | S     | 313 | CLA  | CAA-CBA-CGA-O1A |
| 22  | R     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 33  | l     | 103 | SQD  | O10-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | L     | 101 | SQD  | O10-C23-C24-C25 |
| 36  | K     | 103 | LMG  | O9-C10-C11-C12  |
| 33  | l     | 101 | SQD  | O47-C7-C8-C9    |
| 33  | L     | 102 | SQD  | O47-C7-C8-C9    |
| 36  | B     | 623 | LMG  | O6-C1-O1-C7     |
| 31  | b     | 616 | BCR  | C23-C24-C25-C26 |
| 31  | B     | 602 | BCR  | C23-C24-C25-C26 |
| 31  | B     | 619 | BCR  | C23-C24-C25-C26 |
| 31  | T     | 102 | BCR  | C23-C24-C25-C26 |
| 22  | b     | 604 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 607 | CLA  | C5-C6-C7-C8     |
| 22  | G     | 610 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 502 | CLA  | CAA-CBA-CGA-O1A |
| 22  | r     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 22  | r     | 312 | CLA  | CAA-CBA-CGA-O1A |
| 22  | s     | 313 | CLA  | CAA-CBA-CGA-O1A |
| 22  | R     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 26  | y     | 617 | LHG  | C15-C16-C17-C18 |
| 36  | w     | 102 | LMG  | C11-C12-C13-C14 |
| 22  | r     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 22  | R     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 22  | g     | 610 | CLA  | CAA-CBA-CGA-O1A |
| 22  | n     | 609 | CLA  | CAA-CBA-CGA-O1A |
| 22  | y     | 610 | CLA  | CAA-CBA-CGA-O1A |
| 22  | N     | 609 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Y     | 609 | CLA  | CAA-CBA-CGA-O1A |
| 22  | s     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 22  | S     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 33  | l     | 101 | SQD  | O49-C7-C8-C9    |
| 33  | L     | 102 | SQD  | O49-C7-C8-C9    |
| 36  | k     | 103 | LMG  | O9-C10-C11-C12  |
| 36  | B     | 601 | LMG  | O10-C28-C29-C30 |
| 36  | I     | 101 | LMG  | O10-C28-C29-C30 |
| 36  | C     | 502 | LMG  | C11-C12-C13-C14 |
| 22  | G     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | N     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 22  | w     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 26  | d     | 407 | LHG  | C26-C27-C28-C29 |
| 26  | D     | 408 | LHG  | C26-C27-C28-C29 |
| 21  | S     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 21  | g     | 606 | CHL  | CAD-CBD-CGD-O1D |
| 21  | n     | 605 | CHL  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | y     | 606 | CHL  | CAD-CBD-CGD-O1D |
| 21  | G     | 606 | CHL  | CAD-CBD-CGD-O1D |
| 21  | N     | 605 | CHL  | CAD-CBD-CGD-O1D |
| 21  | Y     | 605 | CHL  | CAD-CBD-CGD-O1D |
| 21  | s     | 307 | CHL  | CAD-CBD-CGD-O1D |
| 21  | S     | 307 | CHL  | CAD-CBD-CGD-O1D |
| 22  | b     | 615 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 618 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 25  | y     | 616 | NEX  | C7-C8-C9-C10    |
| 25  | y     | 618 | NEX  | C7-C8-C9-C10    |
| 25  | r     | 315 | NEX  | C7-C8-C9-C10    |
| 30  | a     | 407 | PHO  | CAD-CBD-CGD-O1D |
| 30  | A     | 408 | PHO  | CAD-CBD-CGD-O1D |
| 33  | a     | 411 | SQD  | O5-C5-C6-S      |
| 33  | A     | 412 | SQD  | O5-C5-C6-S      |
| 21  | y     | 605 | CHL  | CAA-CBA-CGA-O1A |
| 22  | g     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | n     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Y     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 601 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 507 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 508 | CLA  | CAA-CBA-CGA-O2A |
| 22  | W     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 612 | CLA  | C13-C15-C16-C17 |
| 22  | g     | 610 | CLA  | C11-C12-C13-C14 |
| 22  | n     | 609 | CLA  | C11-C12-C13-C14 |
| 22  | G     | 610 | CLA  | C11-C12-C13-C14 |
| 22  | N     | 609 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 602 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 613 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 614 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 506 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 508 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 605 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 616 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 617 | CLA  | C6-C7-C8-C9     |
| 22  | d     | 404 | CLA  | C15-C16-C17-C18 |
| 22  | D     | 405 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 605 | CLA  | C3-C5-C6-C7     |
| 21  | r     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 21  | r     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 21  | S     | 301 | CHL  | CAA-CBA-CGA-O2A |
| 21  | R     | 305 | CHL  | CAA-CBA-CGA-O2A |
| 21  | R     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 22  | g     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | y     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | N     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 604 | CLA  | CAA-CBA-CGA-O2A |
| 26  | c     | 520 | LHG  | O8-C23-C24-C25  |
| 26  | C     | 520 | LHG  | O8-C23-C24-C25  |
| 36  | M     | 101 | LMG  | C35-C36-C37-C38 |
| 21  | s     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 21  | S     | 301 | CHL  | C2-C1-O2A-CGA   |
| 36  | T     | 101 | LMG  | C35-C36-C37-C38 |
| 36  | w     | 102 | LMG  | C34-C35-C36-C37 |
| 36  | C     | 502 | LMG  | C34-C35-C36-C37 |
| 22  | c     | 512 | CLA  | CAA-CBA-CGA-O2A |
| 22  | d     | 403 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 513 | CLA  | CAA-CBA-CGA-O2A |
| 33  | l     | 103 | SQD  | O47-C7-C8-C9    |
| 33  | L     | 101 | SQD  | O47-C7-C8-C9    |
| 22  | B     | 608 | CLA  | C3-C5-C6-C7     |
| 33  | l     | 103 | SQD  | O49-C7-C8-C9    |
| 33  | L     | 101 | SQD  | O49-C7-C8-C9    |
| 31  | K     | 102 | BCR  | C11-C12-C13-C35 |
| 21  | y     | 609 | CHL  | C11-C12-C13-C15 |
| 22  | G     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 604 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 610 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 610 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 506 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 509 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 513 | CLA  | C3A-C2A-CAA-CBA |
| 22  | x     | 101 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 603 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 607 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 613 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 613 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 510 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 514 | CLA  | C3A-C2A-CAA-CBA |
| 22  | r     | 310 | CLA  | C12-C13-C15-C16 |
| 22  | s     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 22  | s     | 303 | CLA  | C11-C12-C13-C15 |
| 22  | S     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 22  | S     | 303 | CLA  | C11-C12-C13-C15 |
| 22  | R     | 309 | CLA  | C12-C13-C15-C16 |
| 22  | g     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | n     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | y     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | G     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | N     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Y     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 22  | D     | 404 | CLA  | CAA-CBA-CGA-O1A |
| 22  | r     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 22  | R     | 302 | CLA  | CAA-CBA-CGA-O1A |
| 22  | a     | 404 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | D     | 404 | CLA  | CAA-CBA-CGA-O2A |
| 26  | d     | 408 | LHG  | O8-C23-C24-C25  |
| 26  | D     | 409 | LHG  | O8-C23-C24-C25  |
| 21  | r     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 22  | g     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 22  | y     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 22  | N     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 512 | CLA  | CAA-CBA-CGA-O1A |
| 22  | d     | 403 | CLA  | CAA-CBA-CGA-O1A |
| 35  | J     | 101 | DGD  | O1B-C1B-C2B-C3B |
| 22  | b     | 615 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 405 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 616 | CLA  | CAA-CBA-CGA-O2A |
| 36  | B     | 601 | LMG  | O8-C28-C29-C30  |
| 36  | I     | 101 | LMG  | O8-C28-C29-C30  |
| 22  | b     | 613 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 513 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 514 | CLA  | C10-C11-C12-C13 |
| 21  | S     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 21  | r     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 21  | R     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 22  | n     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 22  | G     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Y     | 602 | CLA  | CAA-CBA-CGA-O1A |

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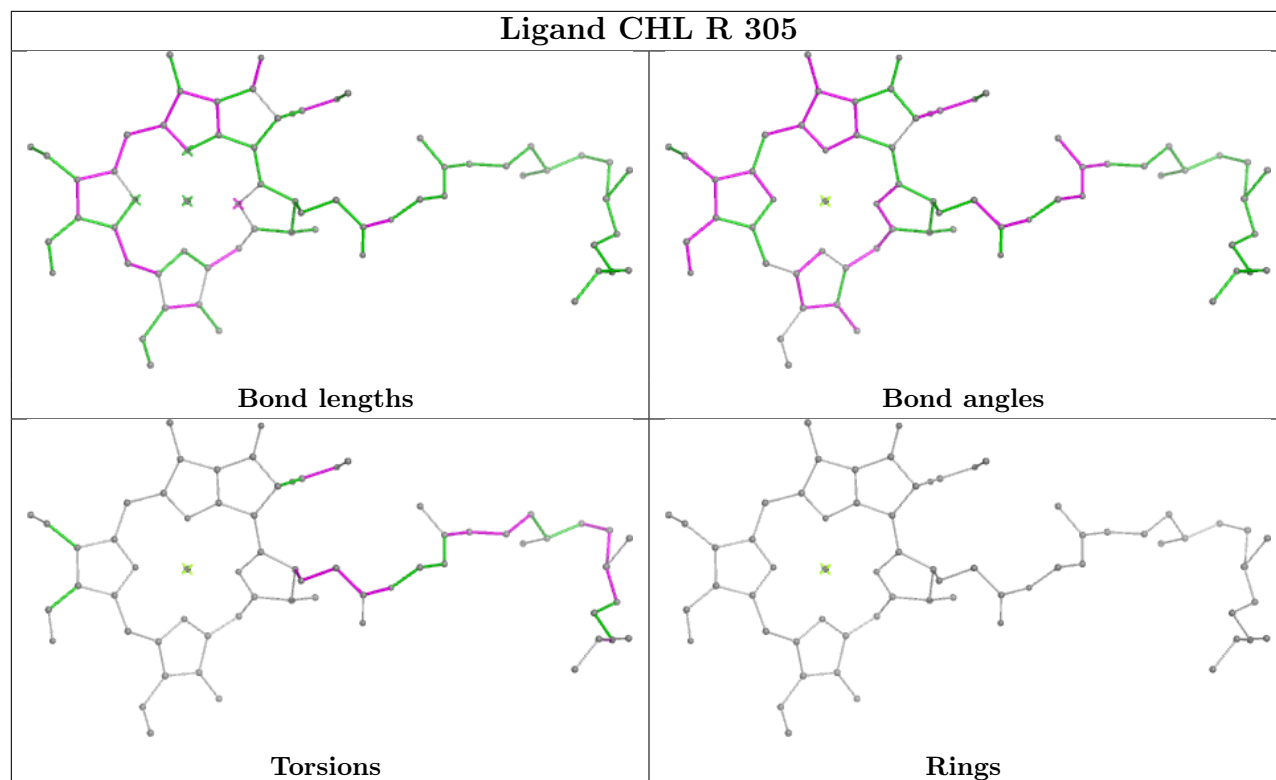
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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 507 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 513 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 508 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 514 | CLA  | CAA-CBA-CGA-O1A |
| 35  | c     | 519 | DGD  | O1B-C1B-C2B-C3B |
| 36  | K     | 103 | LMG  | C15-C16-C17-C18 |
| 36  | k     | 103 | LMG  | C15-C16-C17-C18 |
| 22  | b     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 514 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 618 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 515 | CLA  | CAA-CBA-CGA-O2A |
| 26  | R     | 301 | LHG  | C28-C29-C30-C31 |
| 22  | B     | 616 | CLA  | C10-C11-C12-C13 |
| 21  | R     | 305 | CHL  | CAA-CBA-CGA-O1A |
| 22  | C     | 513 | CLA  | CAA-CBA-CGA-O1A |
| 22  | r     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 22  | R     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 26  | r     | 302 | LHG  | C28-C29-C30-C31 |
| 26  | C     | 522 | LHG  | C15-C16-C17-C18 |
| 21  | r     | 301 | CHL  | CAA-CBA-CGA-O2A |
| 22  | B     | 605 | CLA  | CAA-CBA-CGA-O2A |

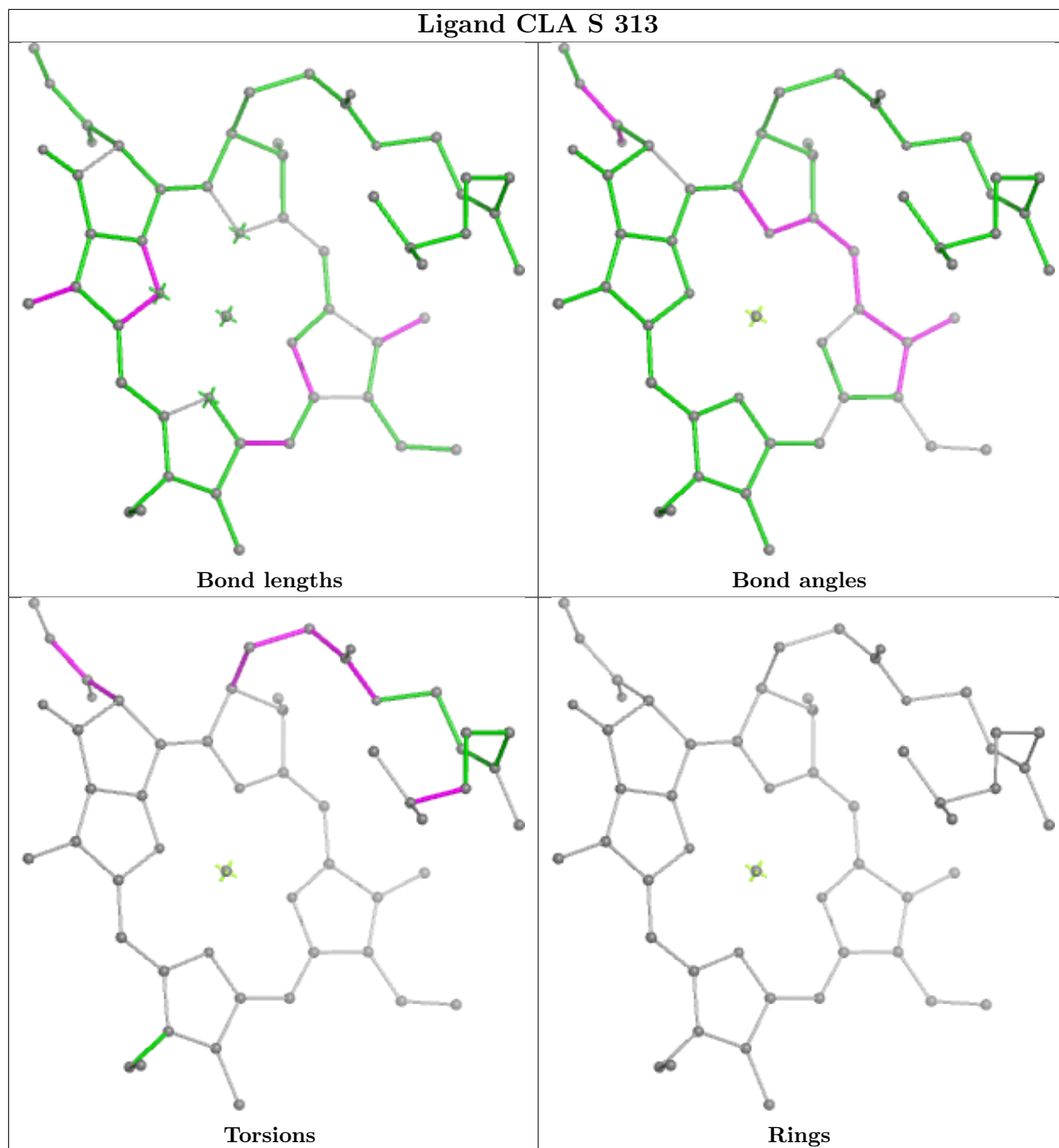
There are no ring outliers.

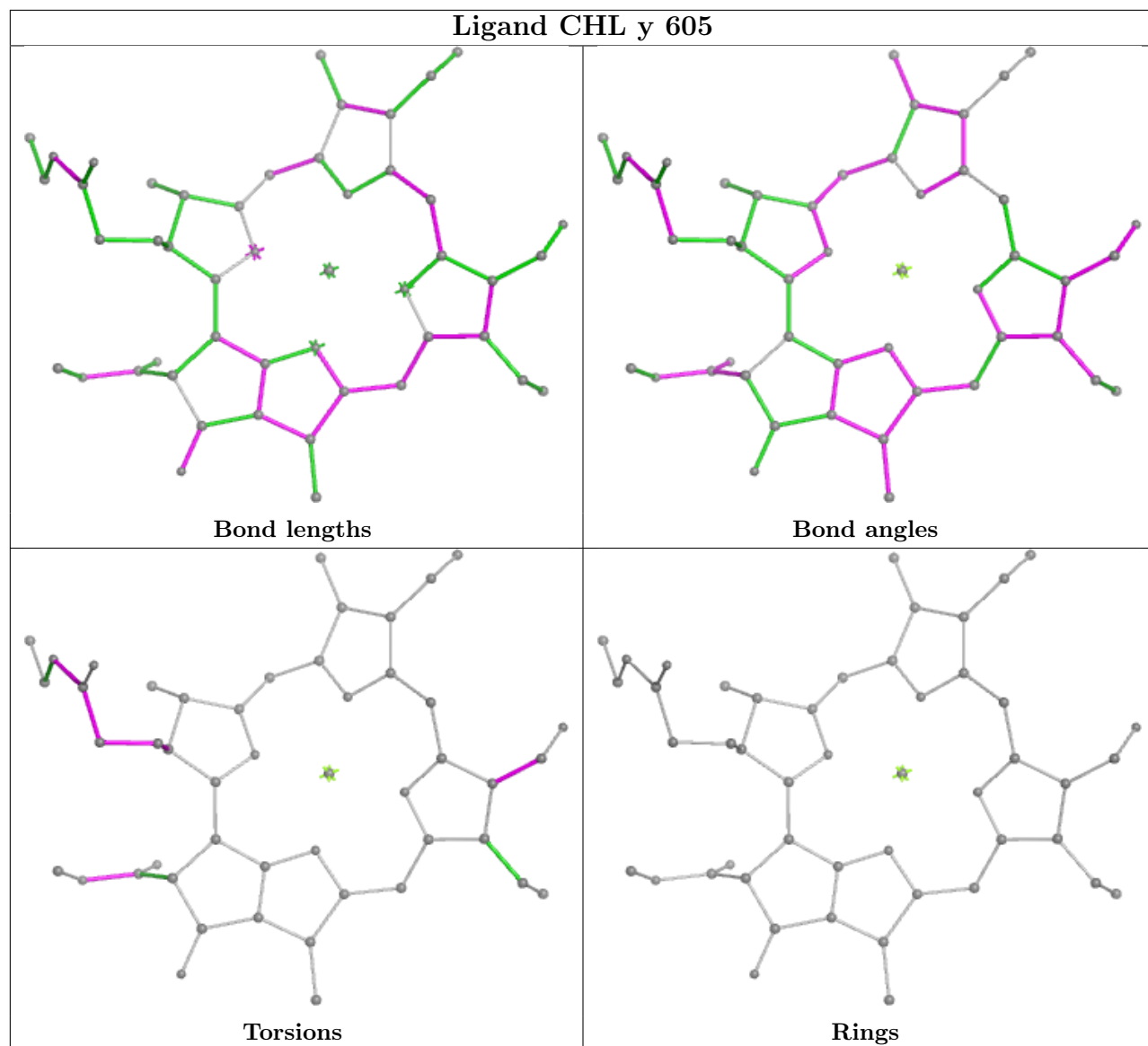
No monomer is involved in short contacts.

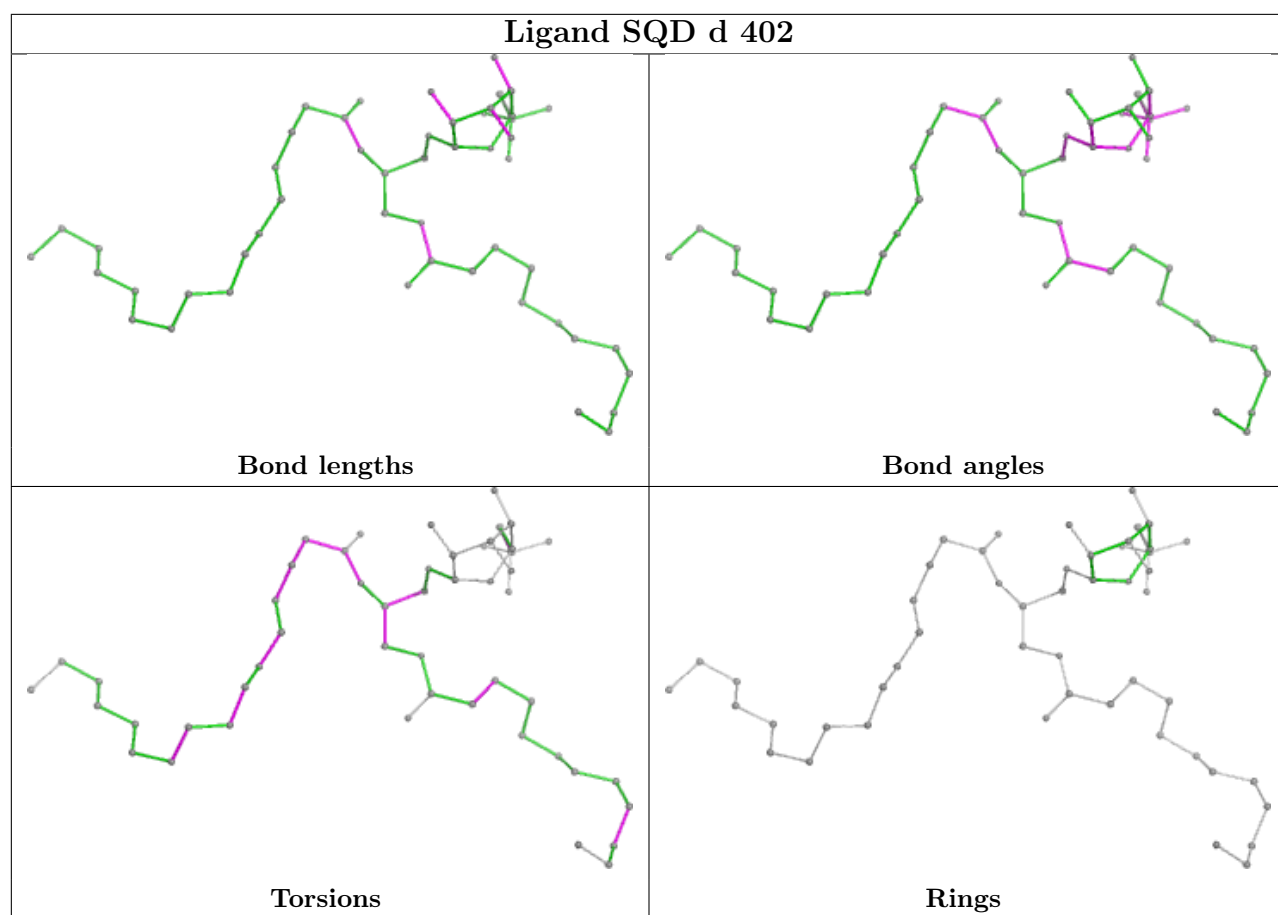
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand CLA S 313

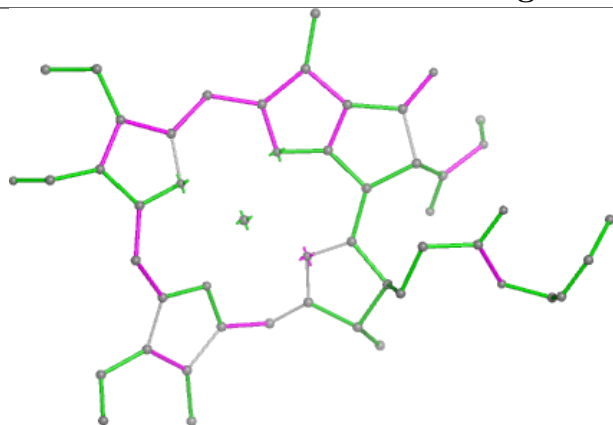




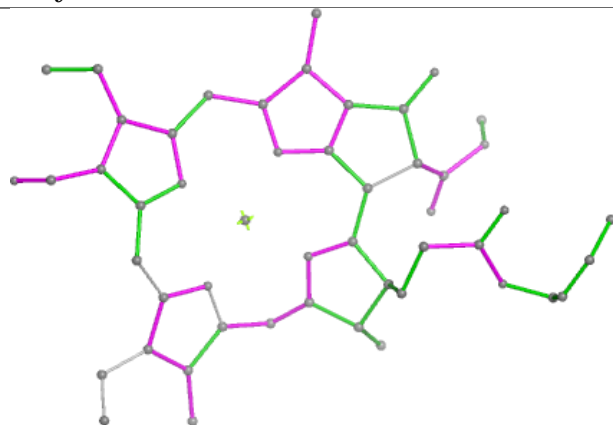




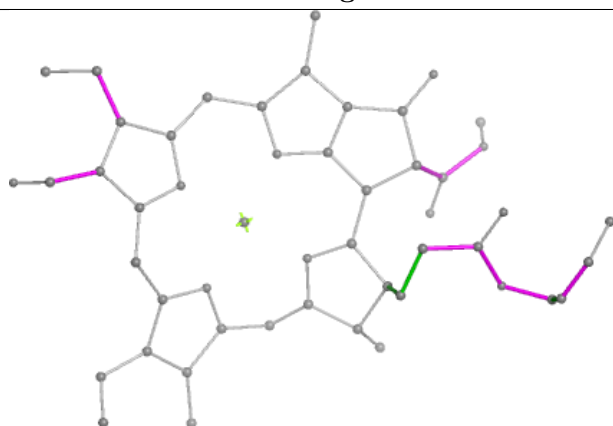
## Ligand CHL y 606



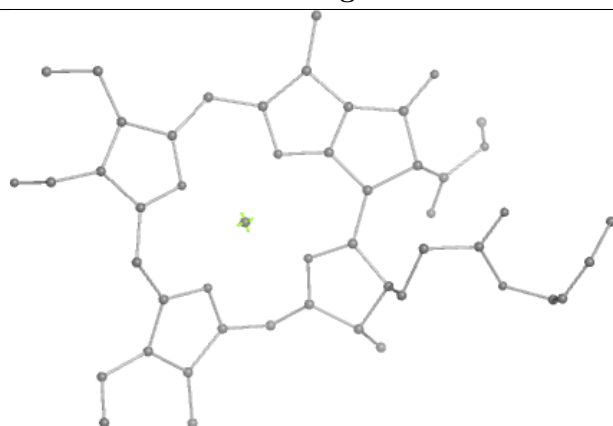
Bond lengths



Bond angles

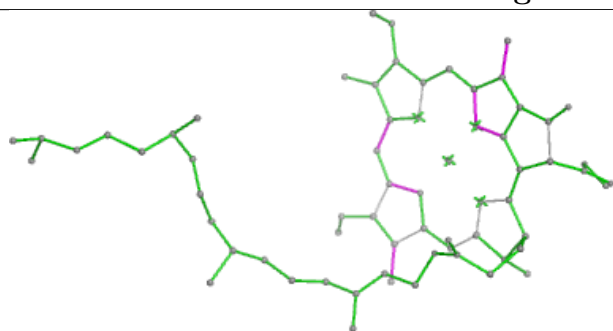


Torsions

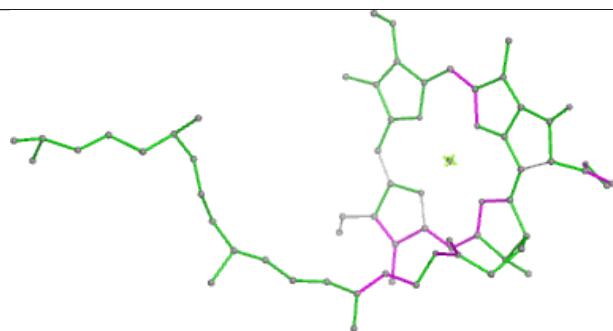


Rings

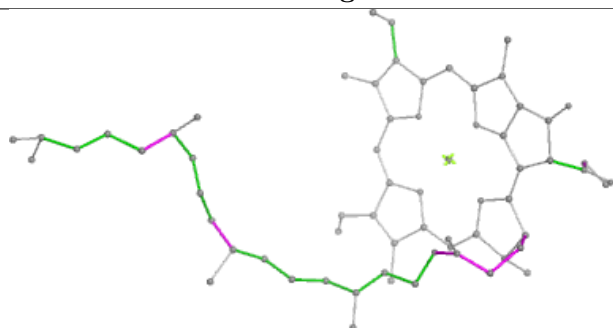
## Ligand CLA Y 602



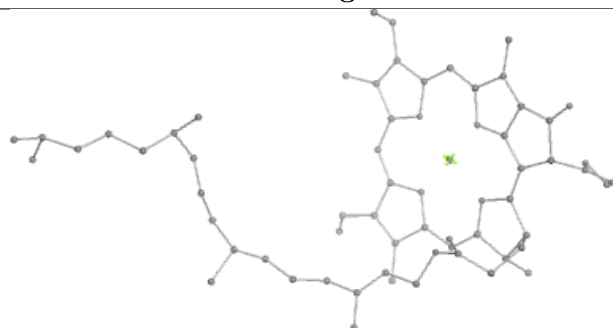
Bond lengths



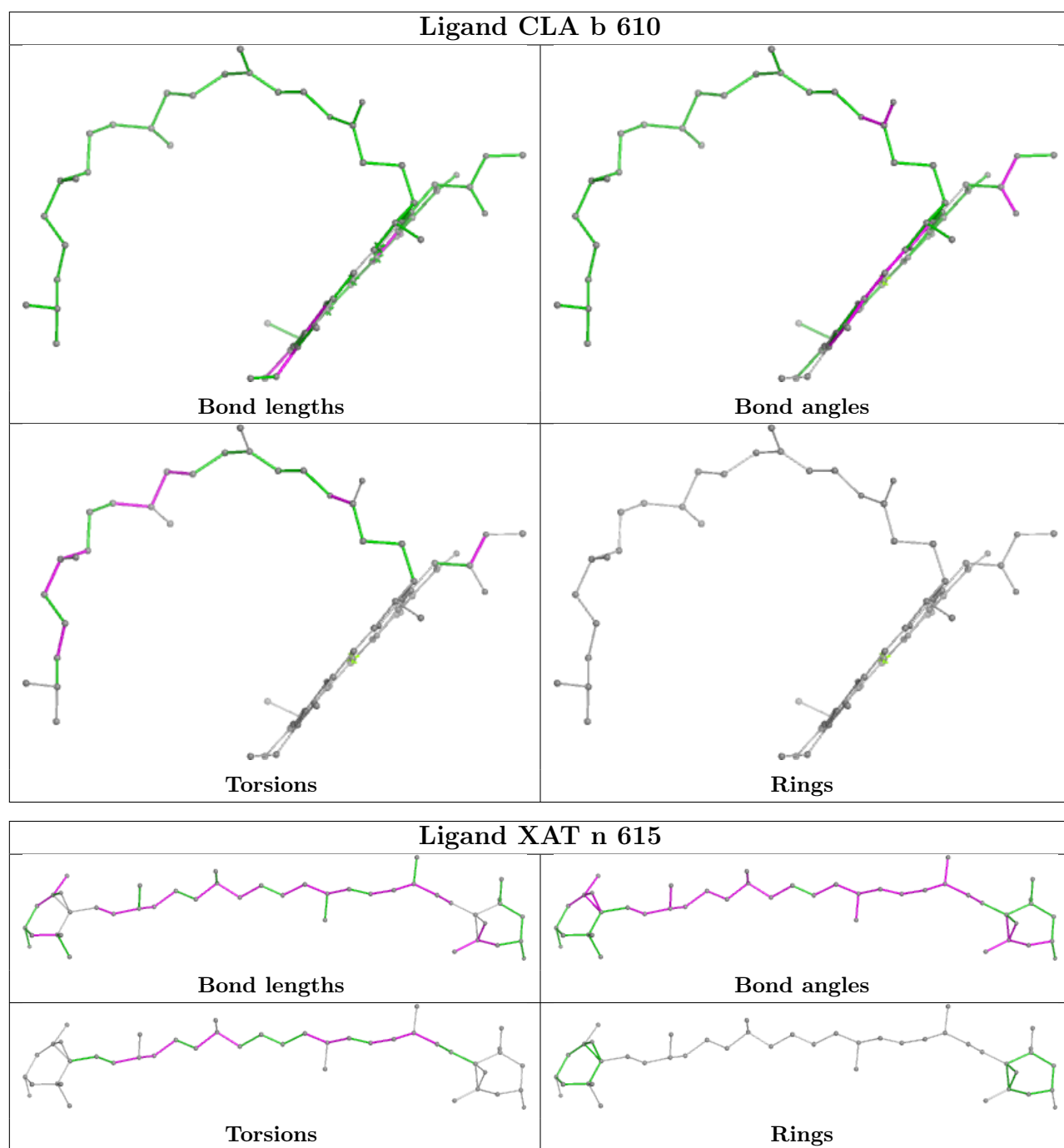
Bond angles

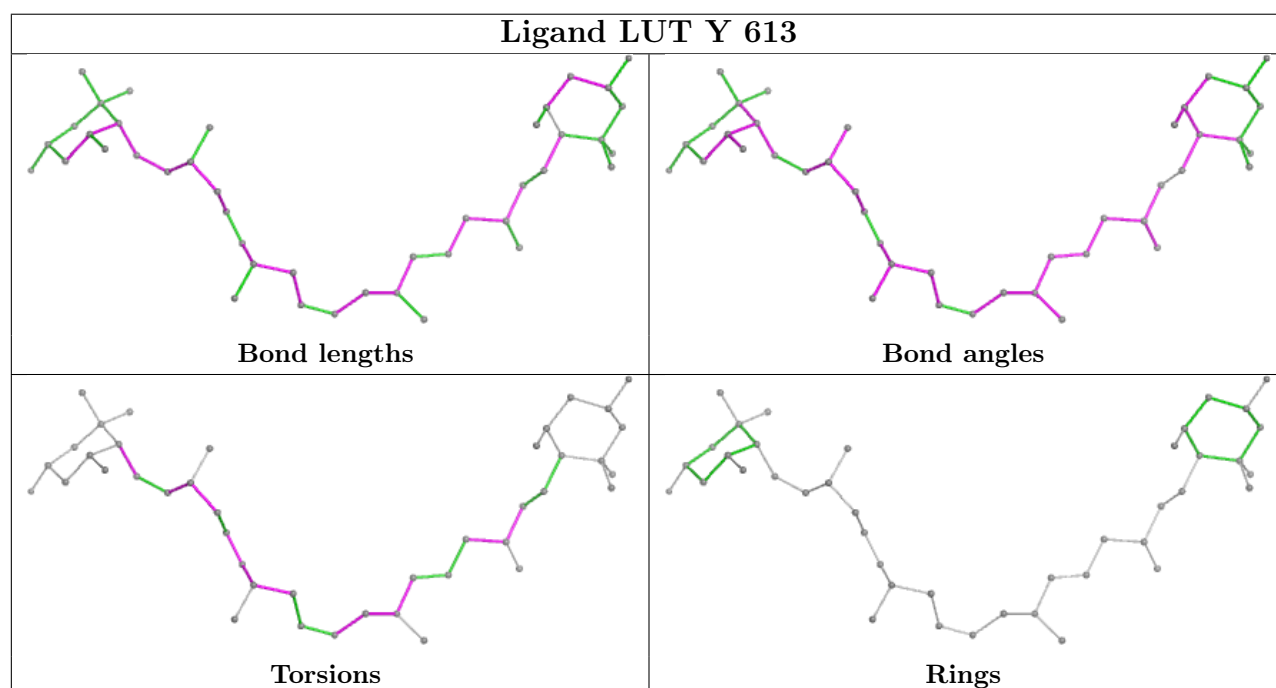
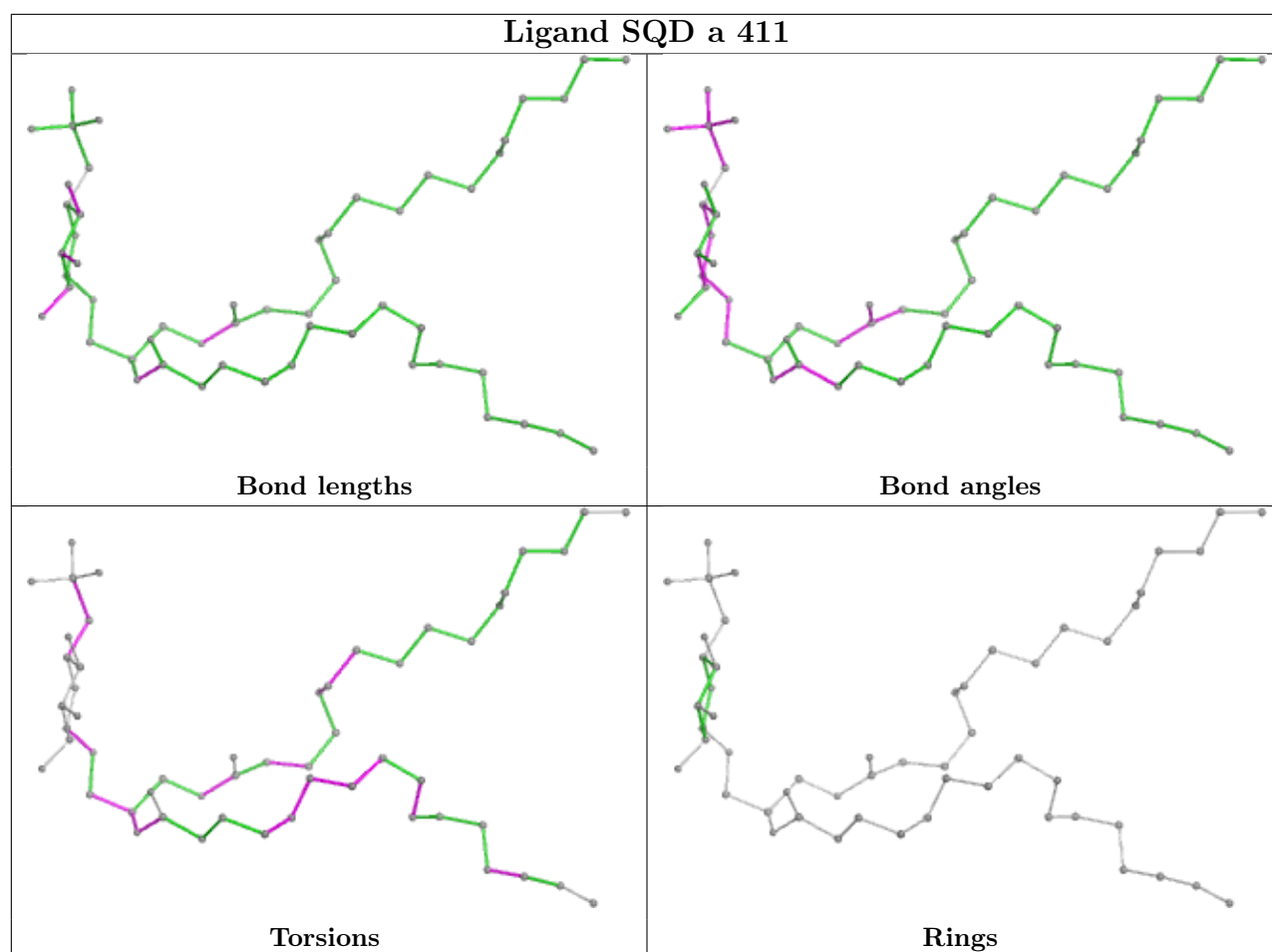


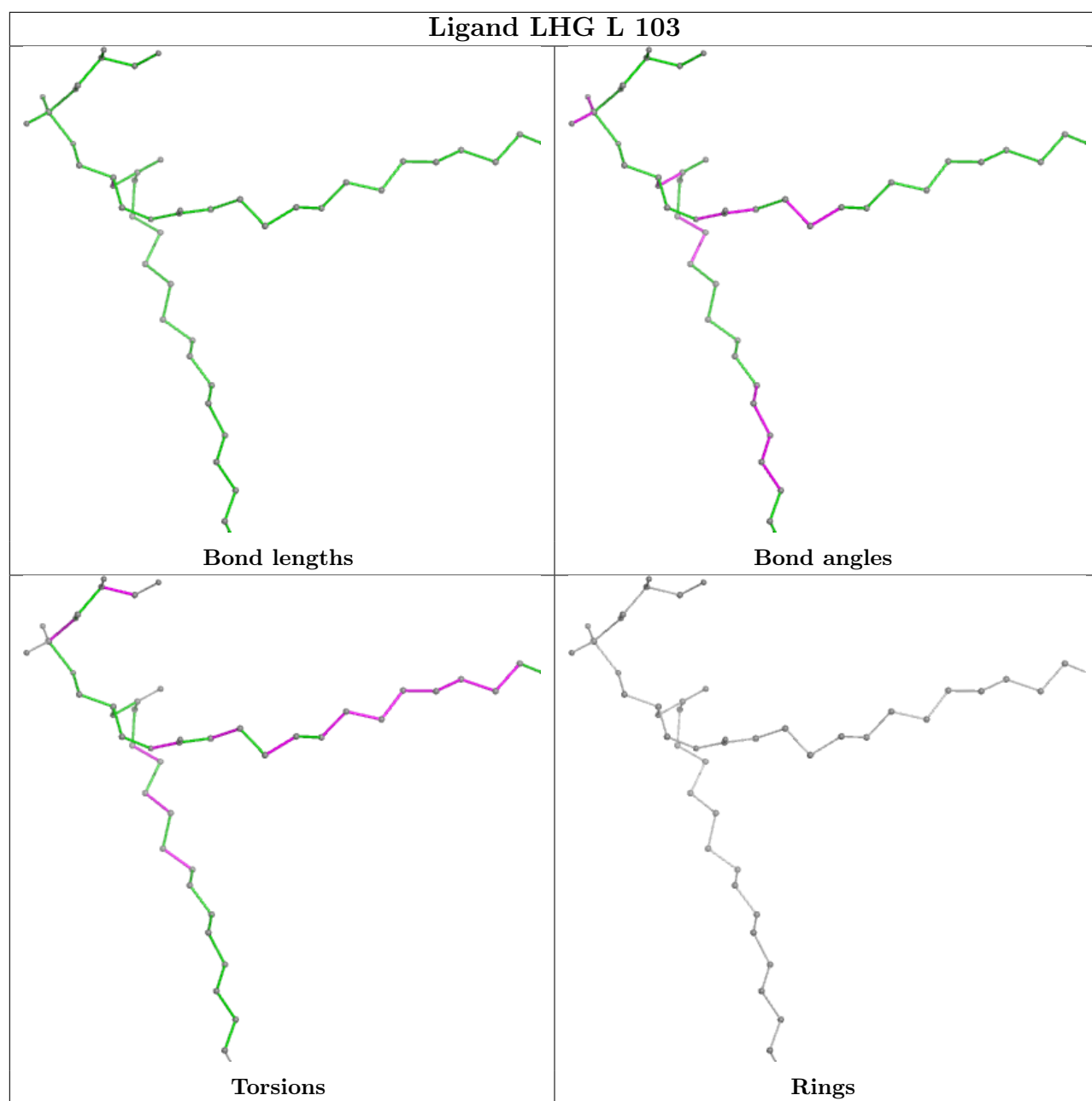
Torsions

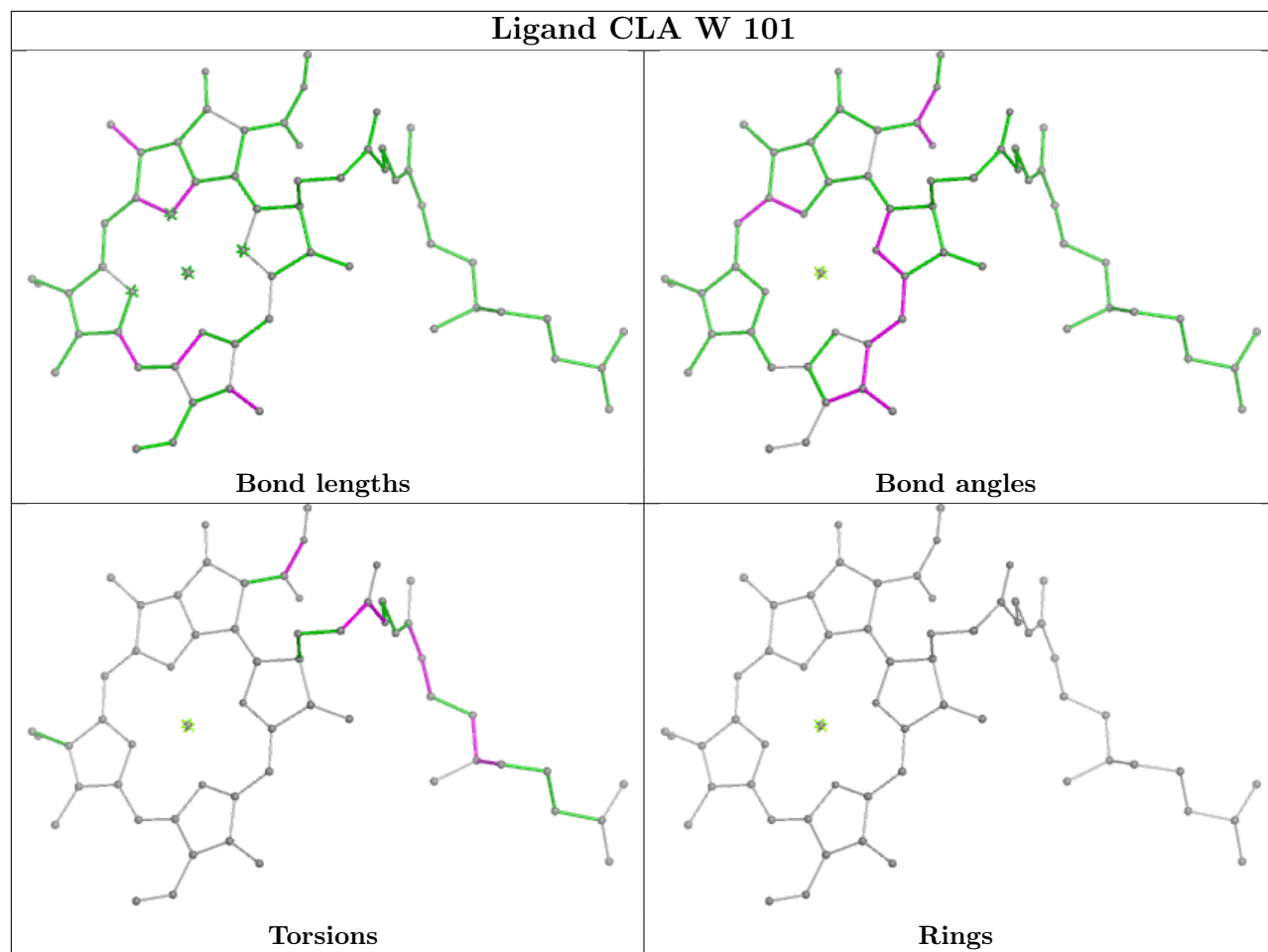


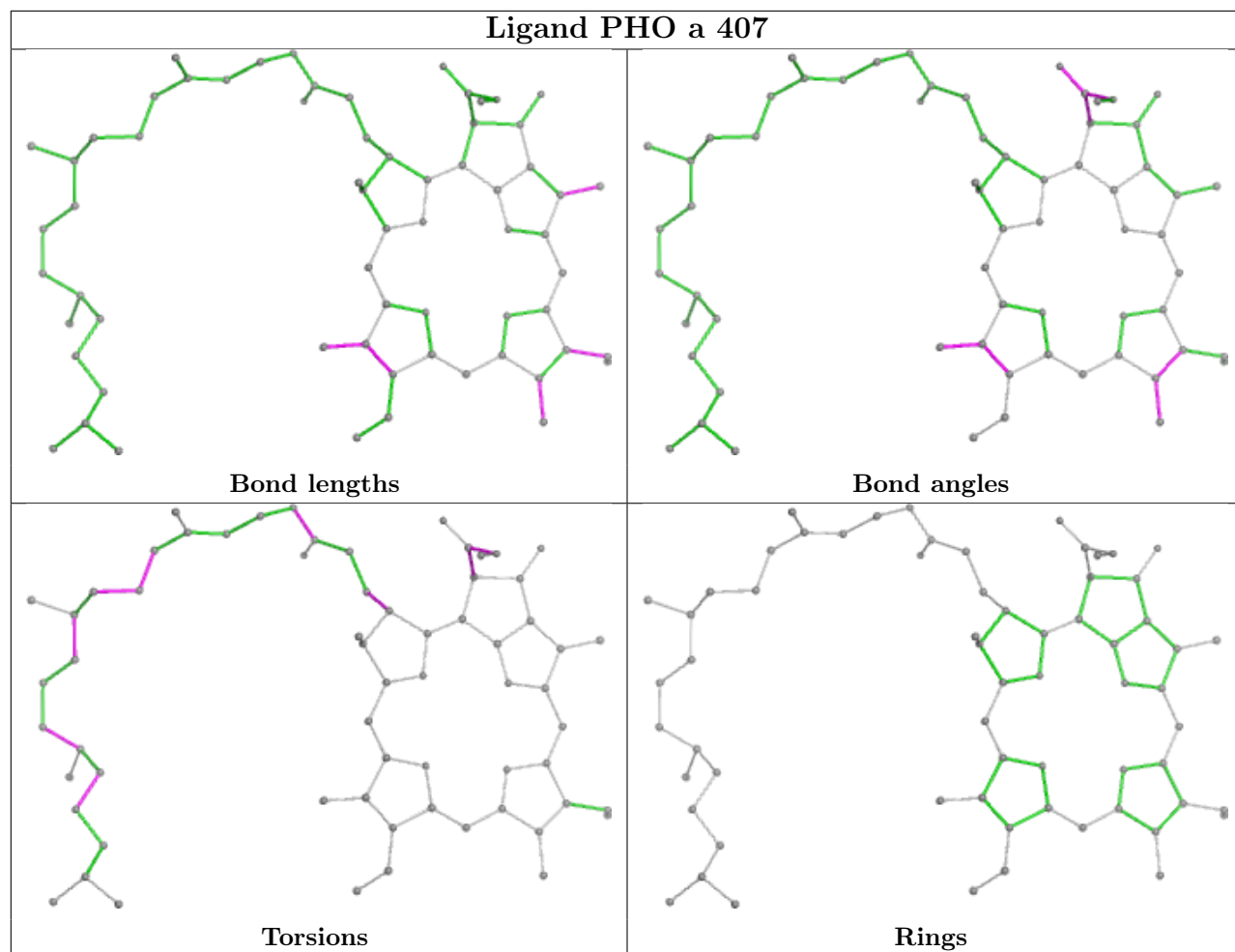
Rings

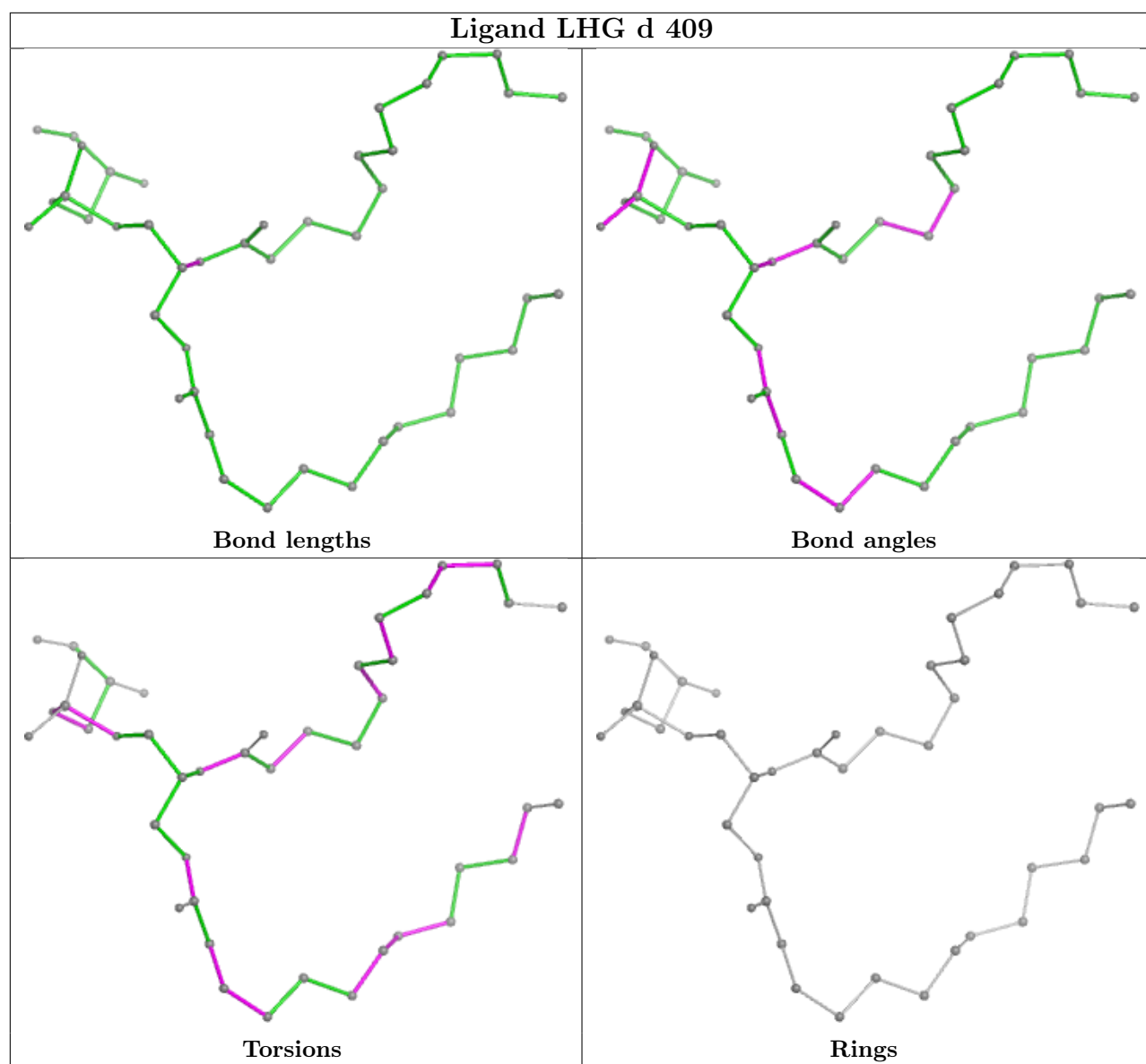




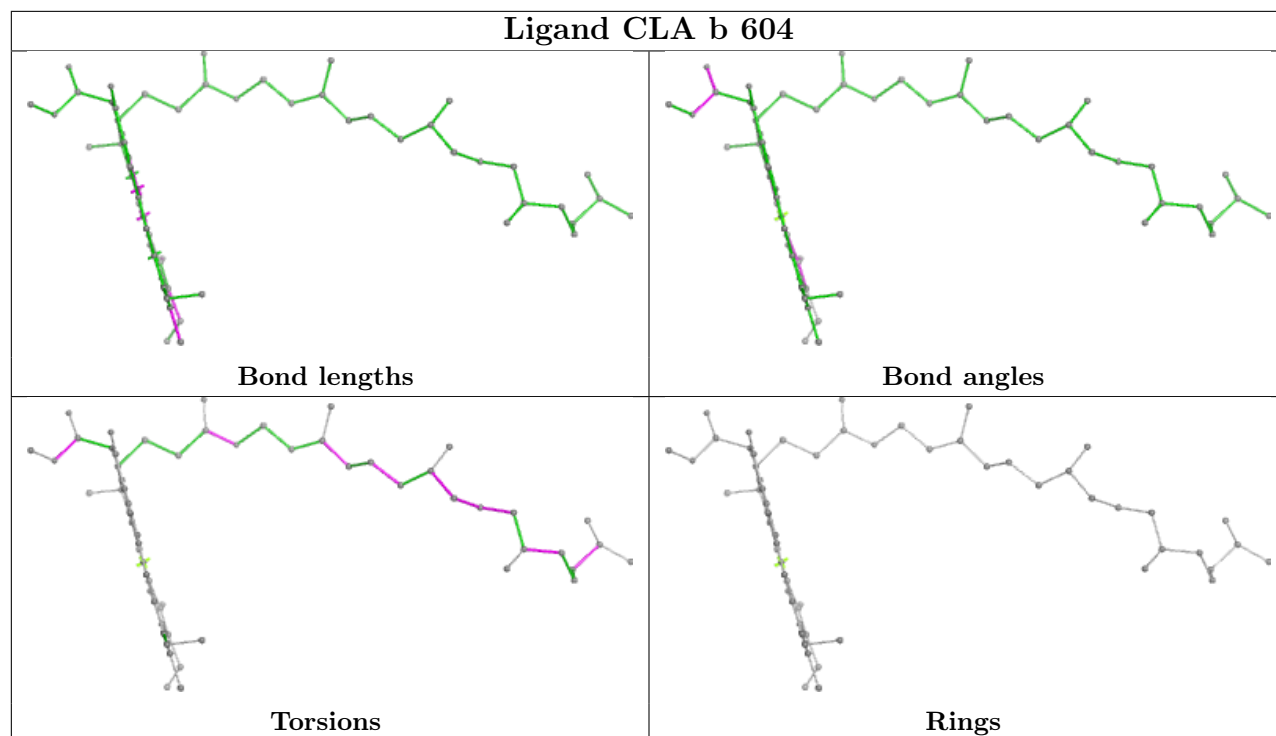




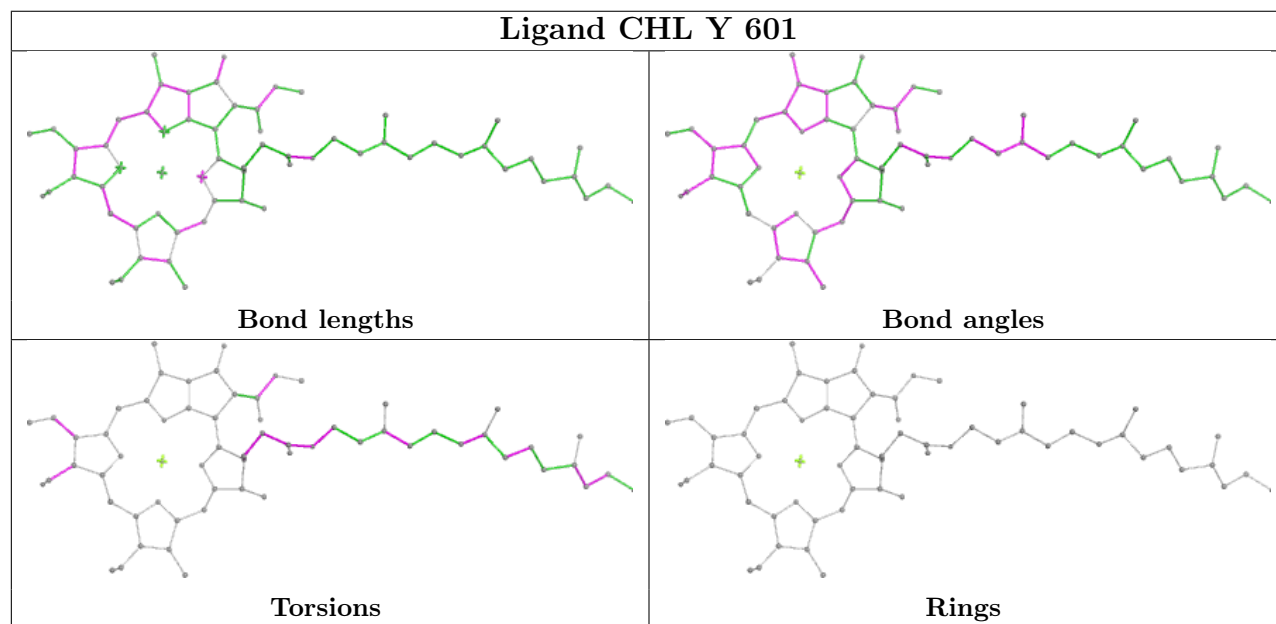




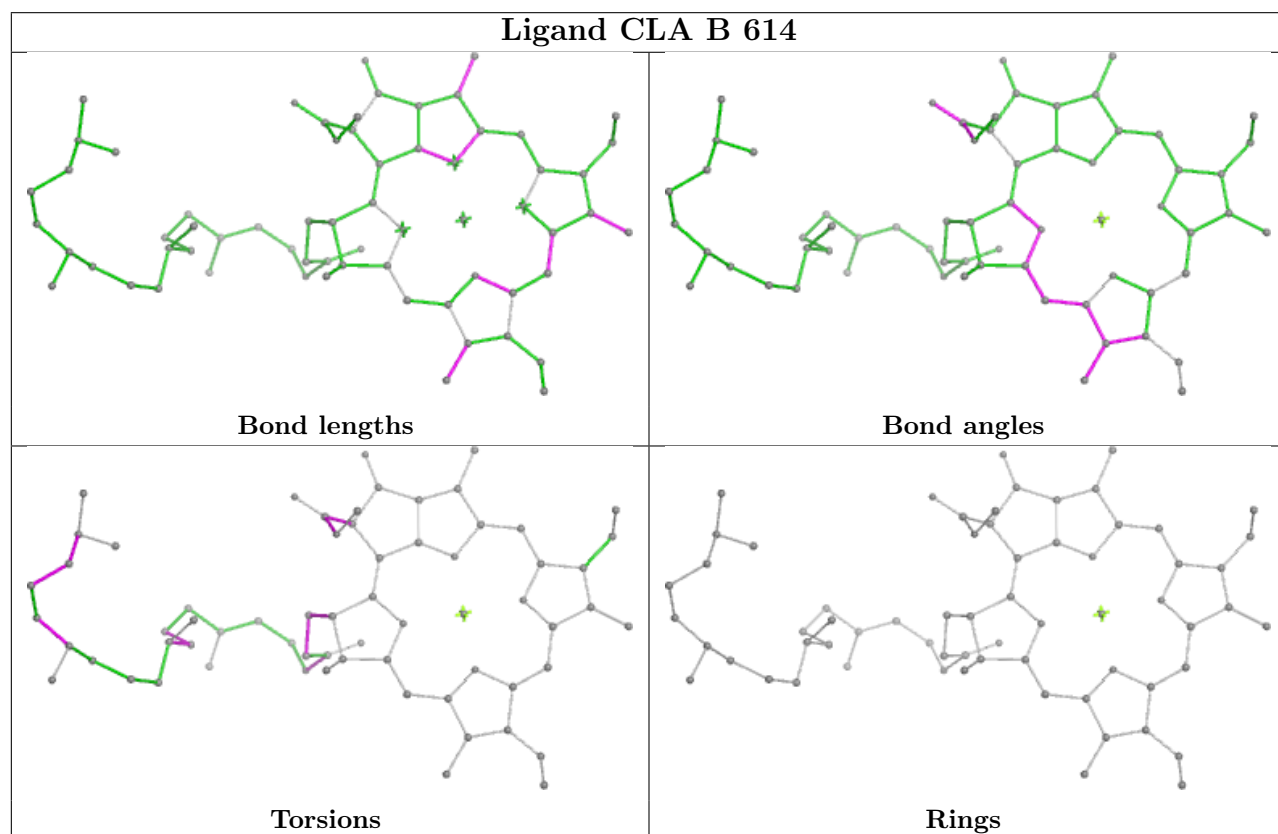
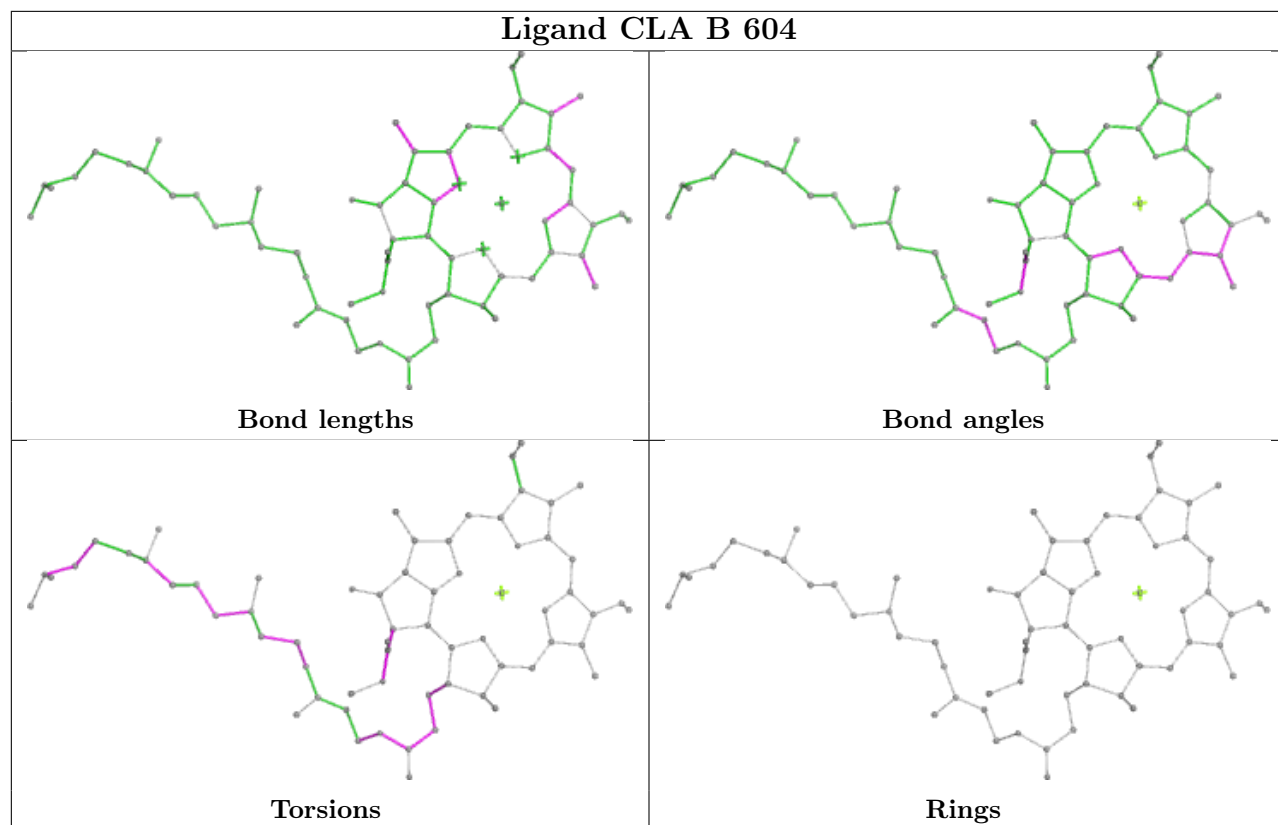
## Ligand CLA b 604

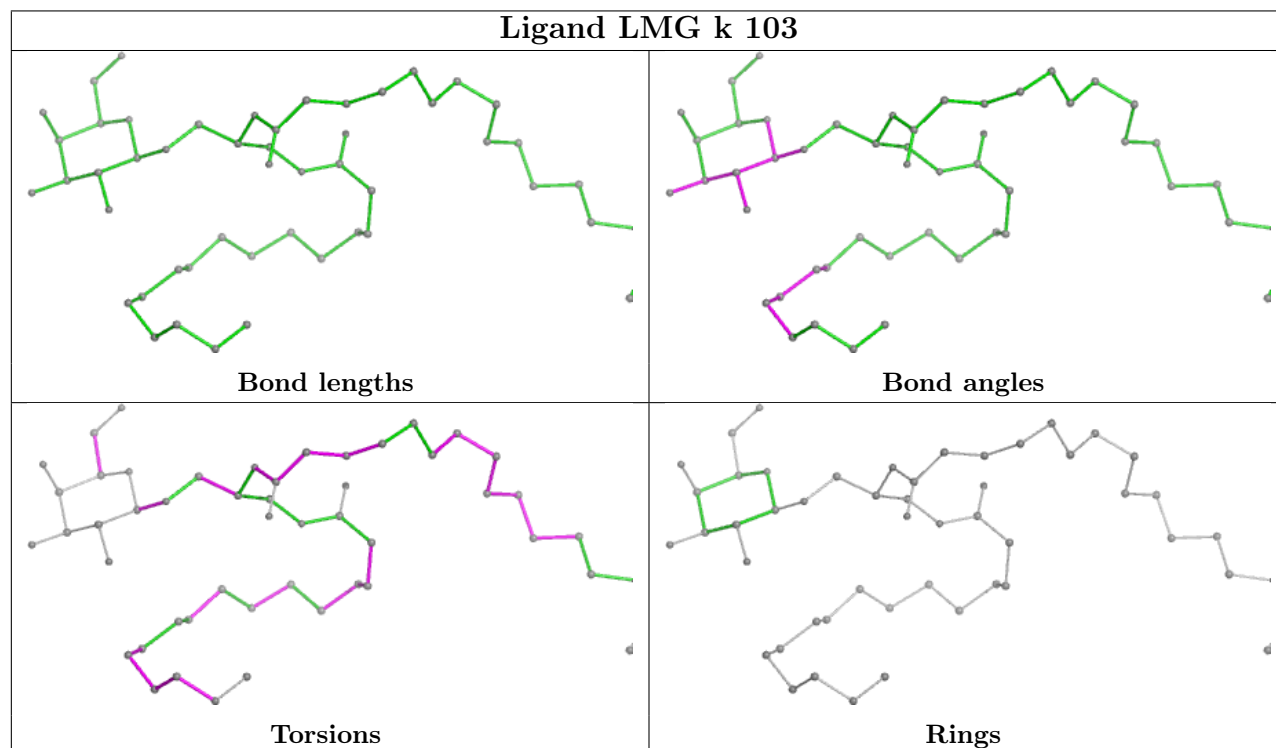
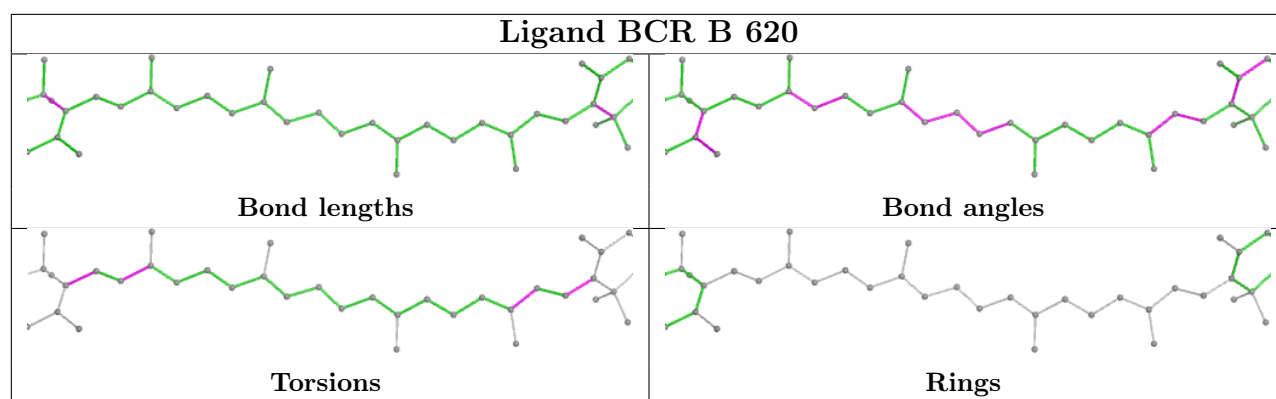


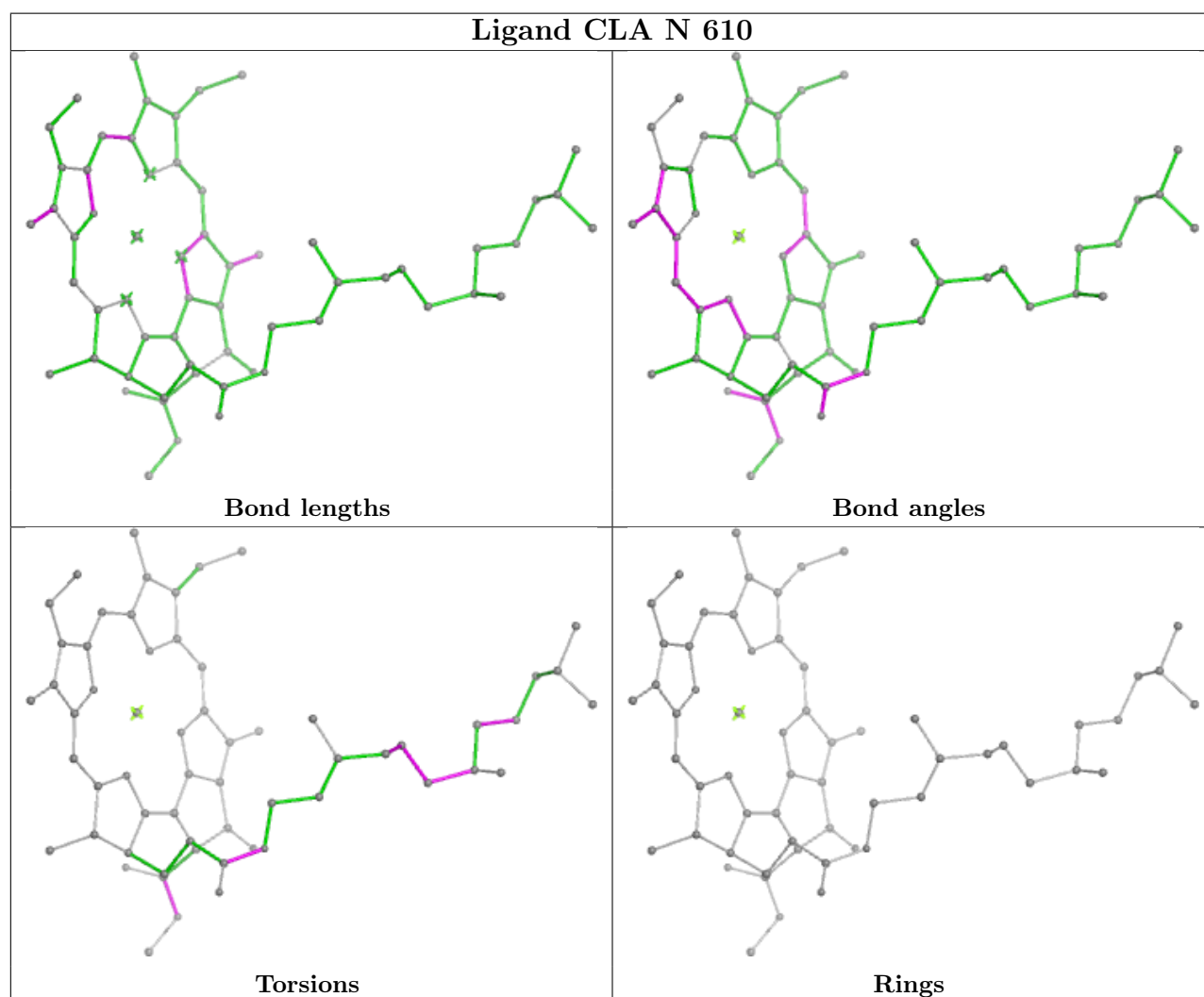
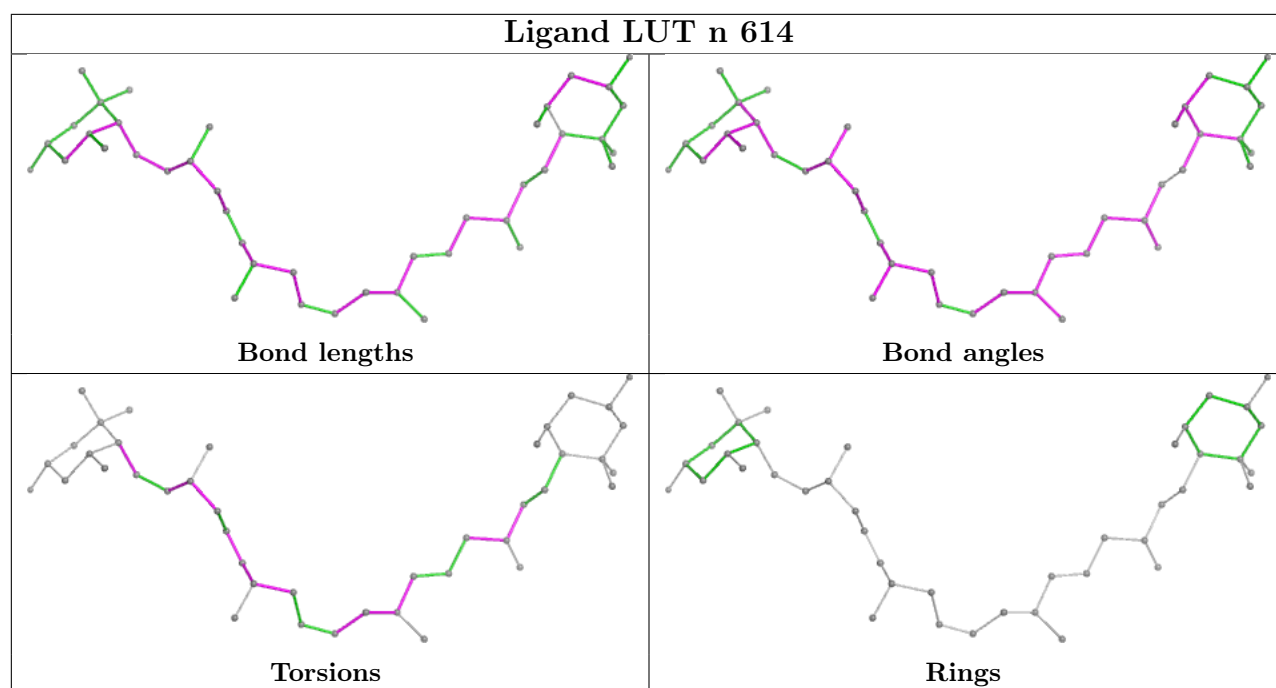
## Ligand CHL Y 601



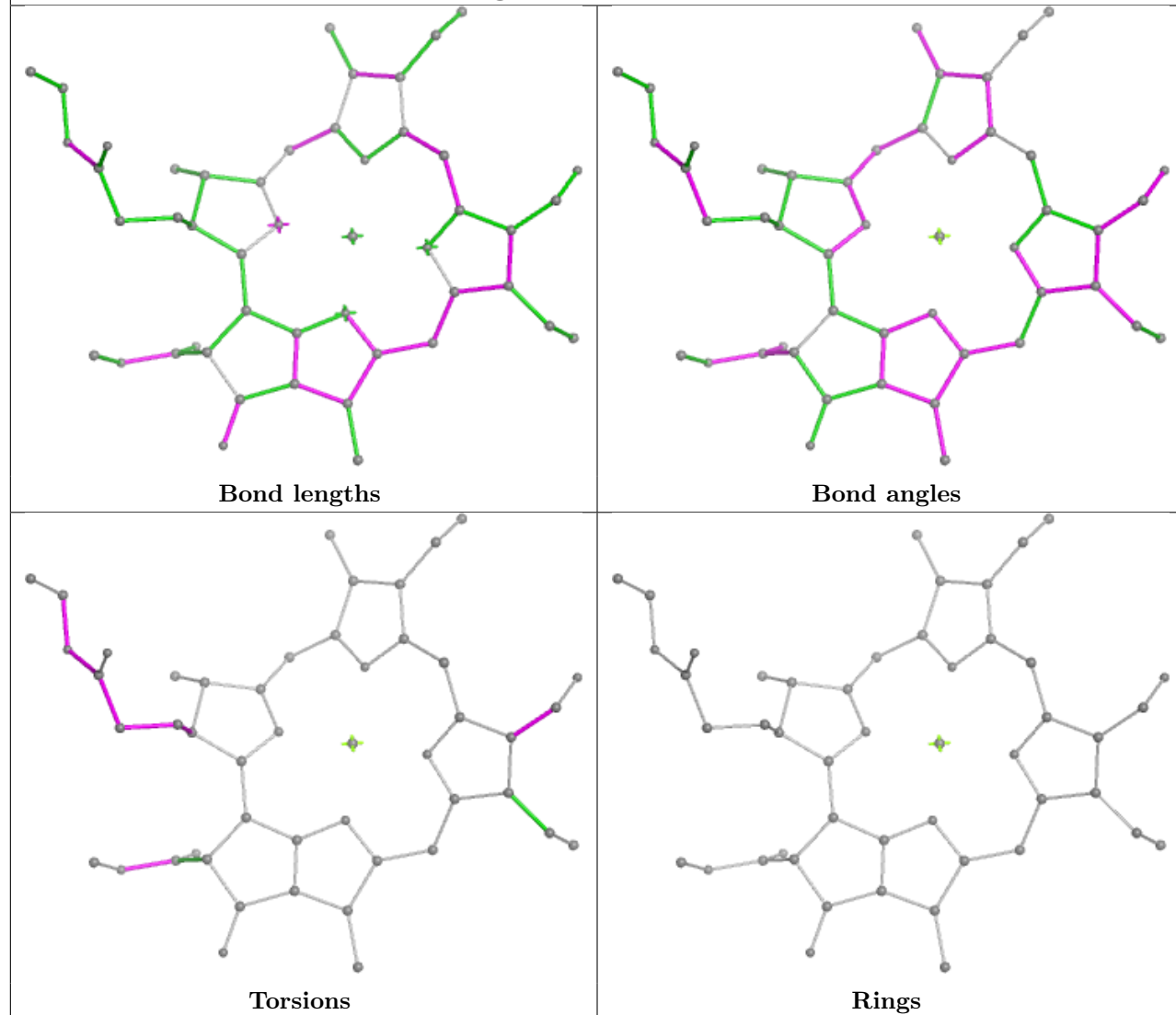


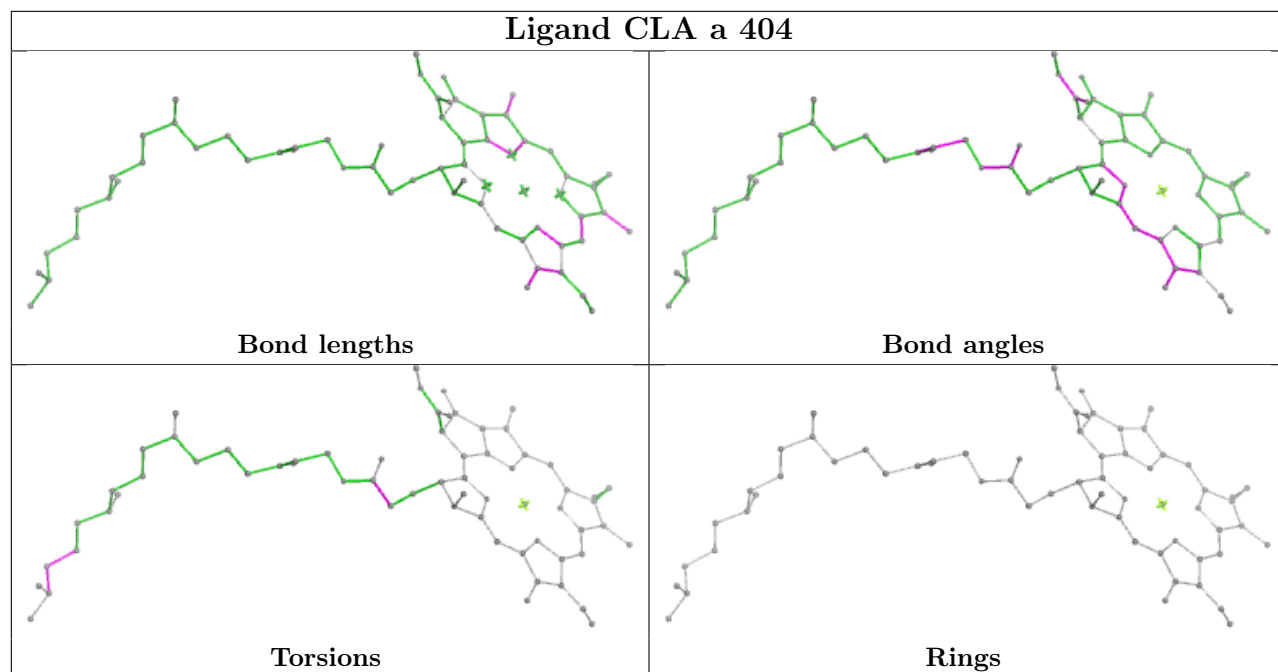
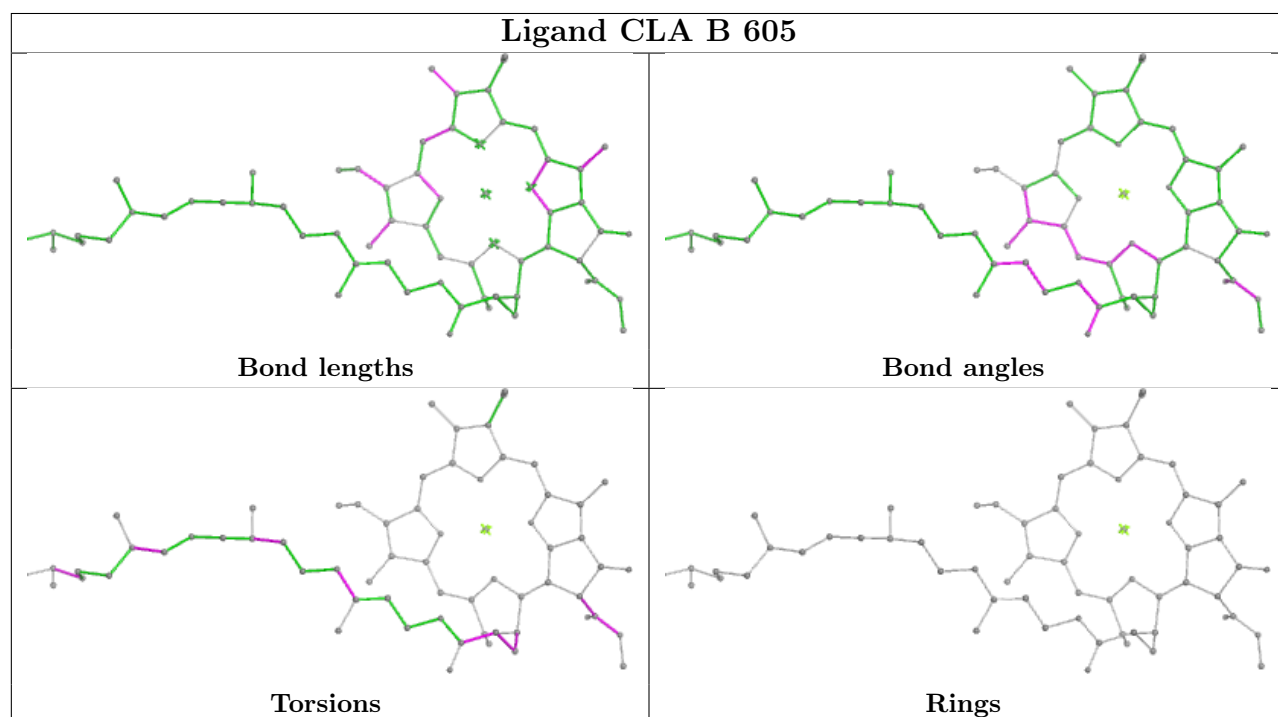


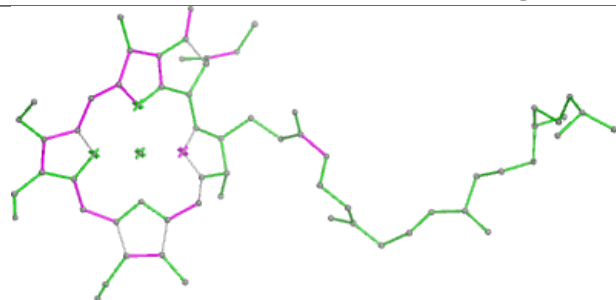
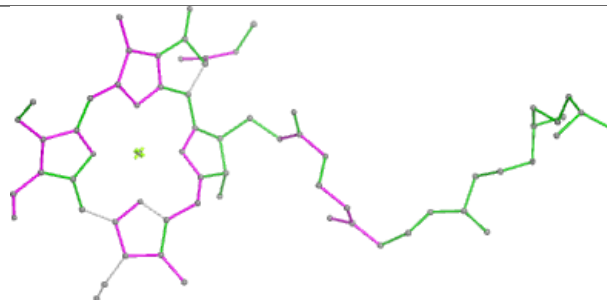
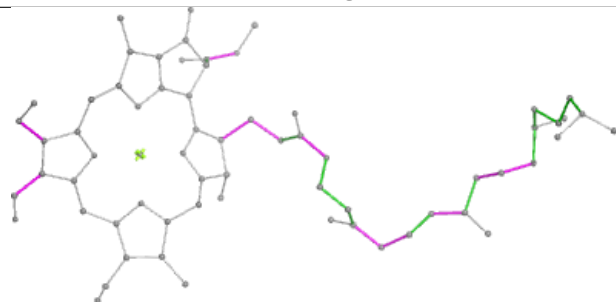
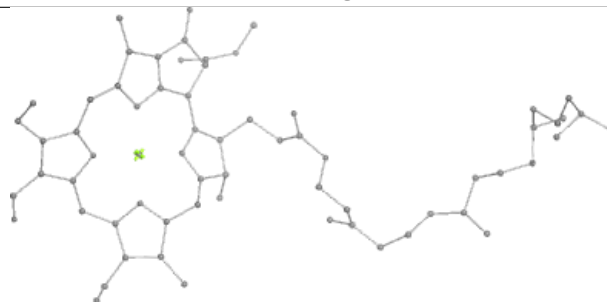
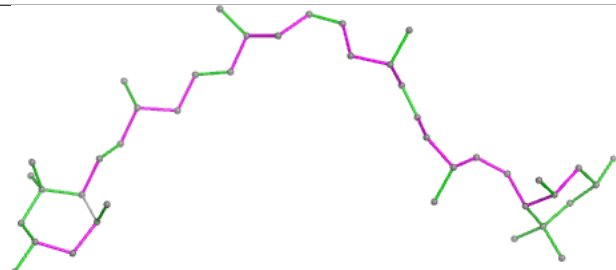
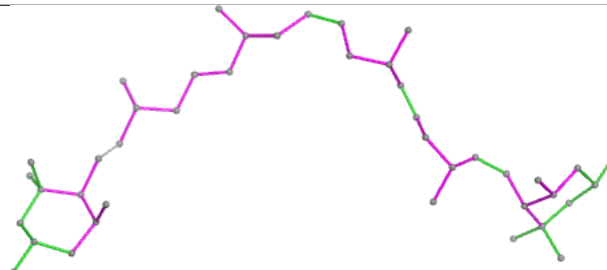
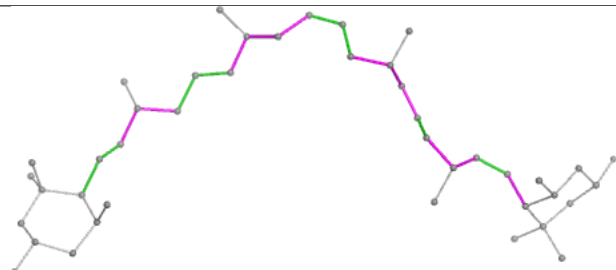
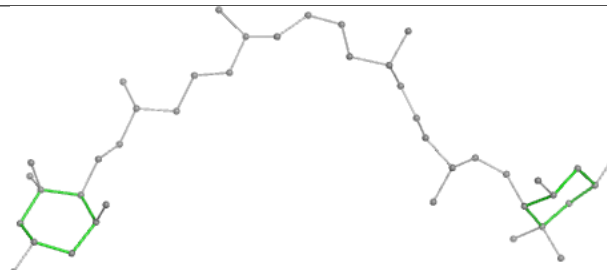


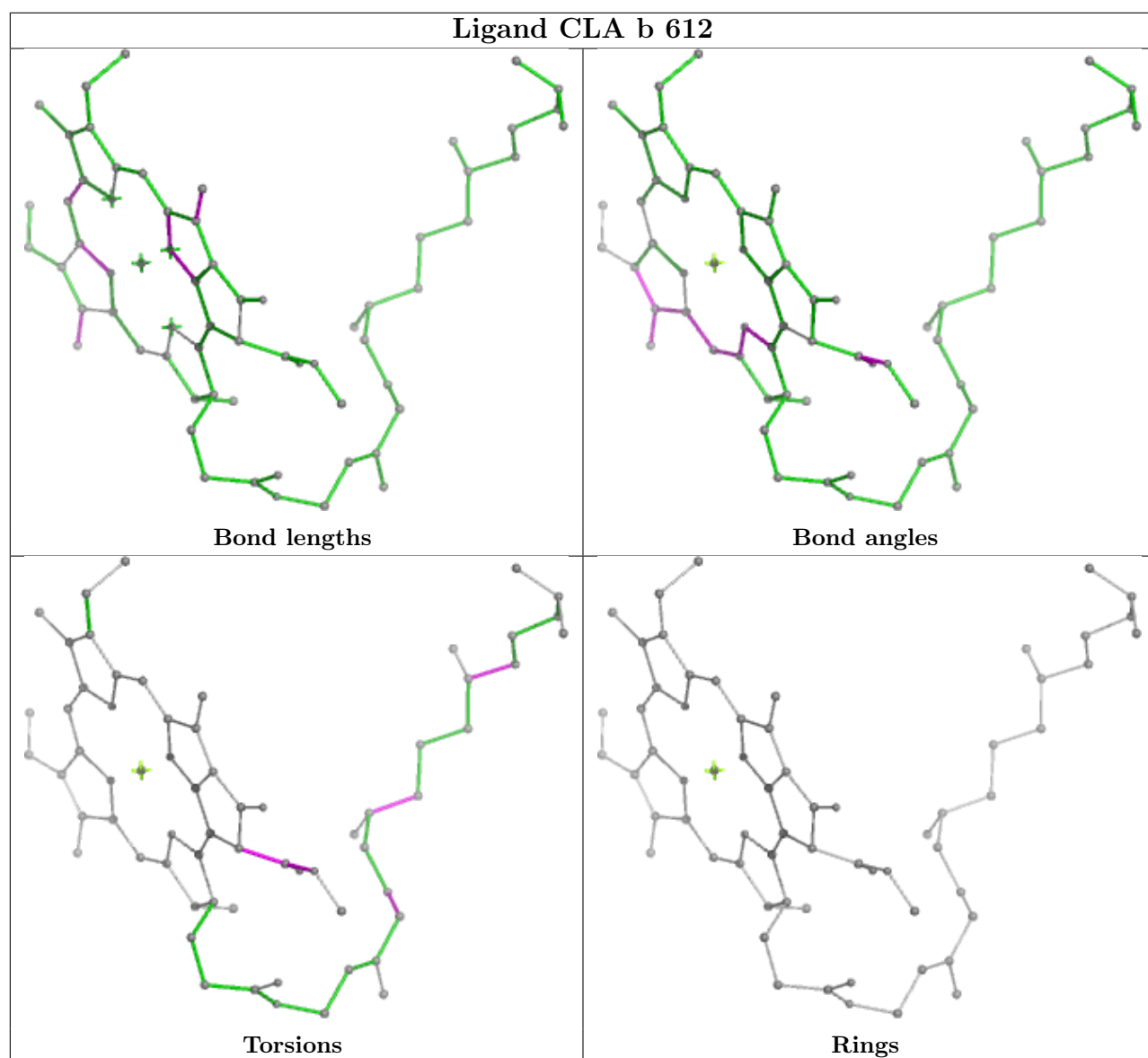


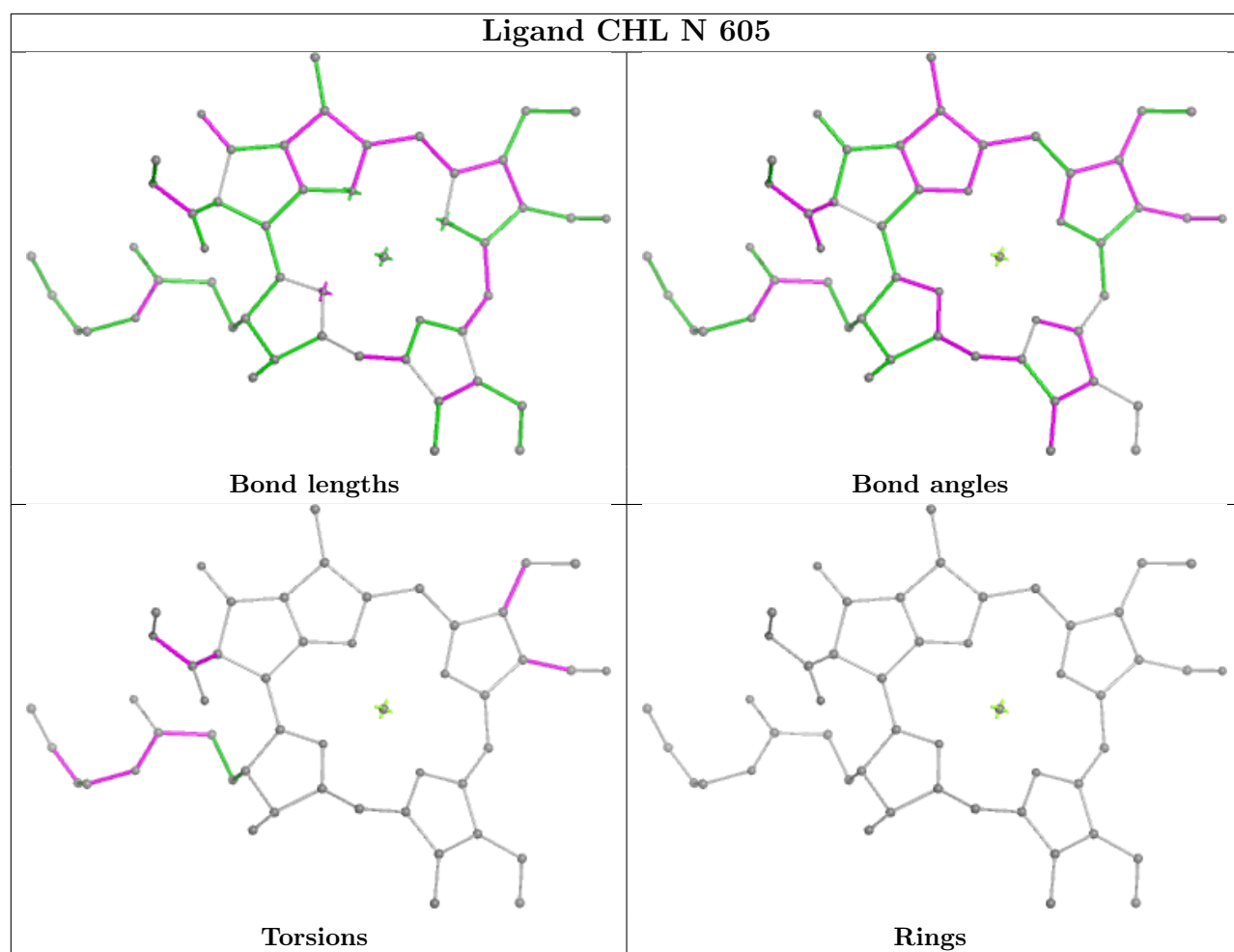
## Ligand CHL S 301



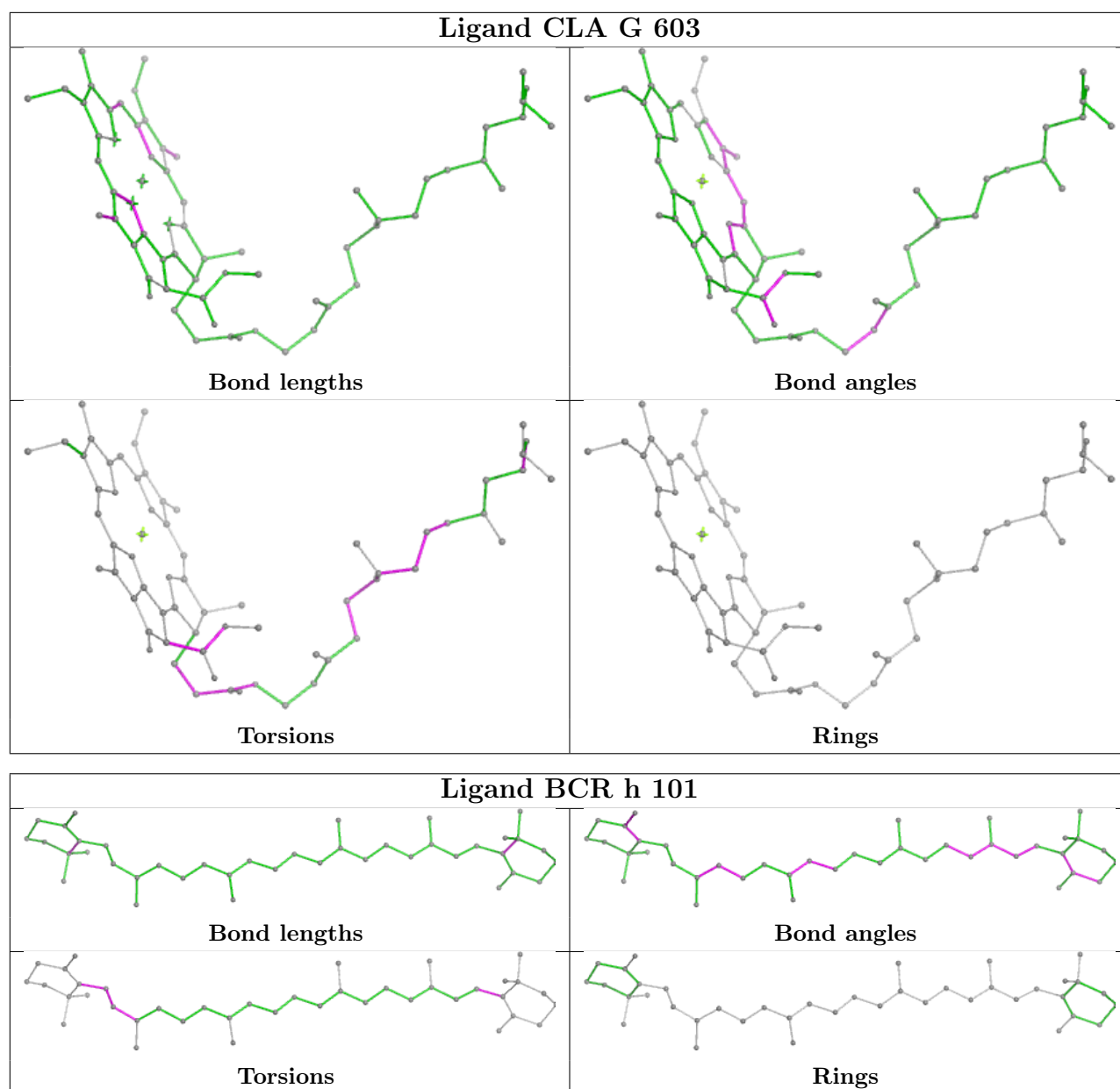
**Ligand CLA a 404****Ligand CLA B 605**

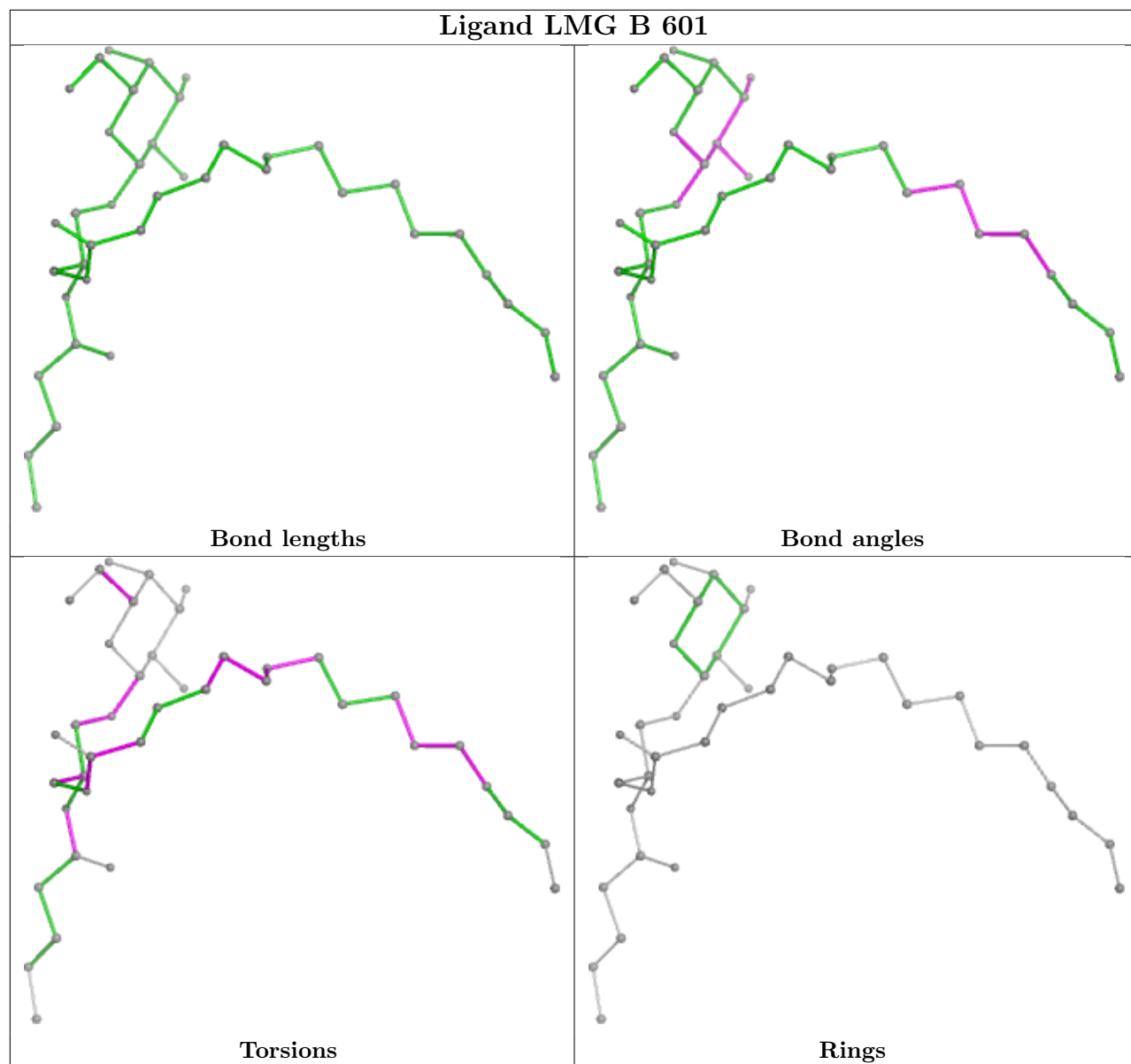
**Ligand CHL N 606****Bond lengths****Bond angles****Torsions****Rings****Ligand LUT N 614****Bond lengths****Bond angles****Torsions****Rings**



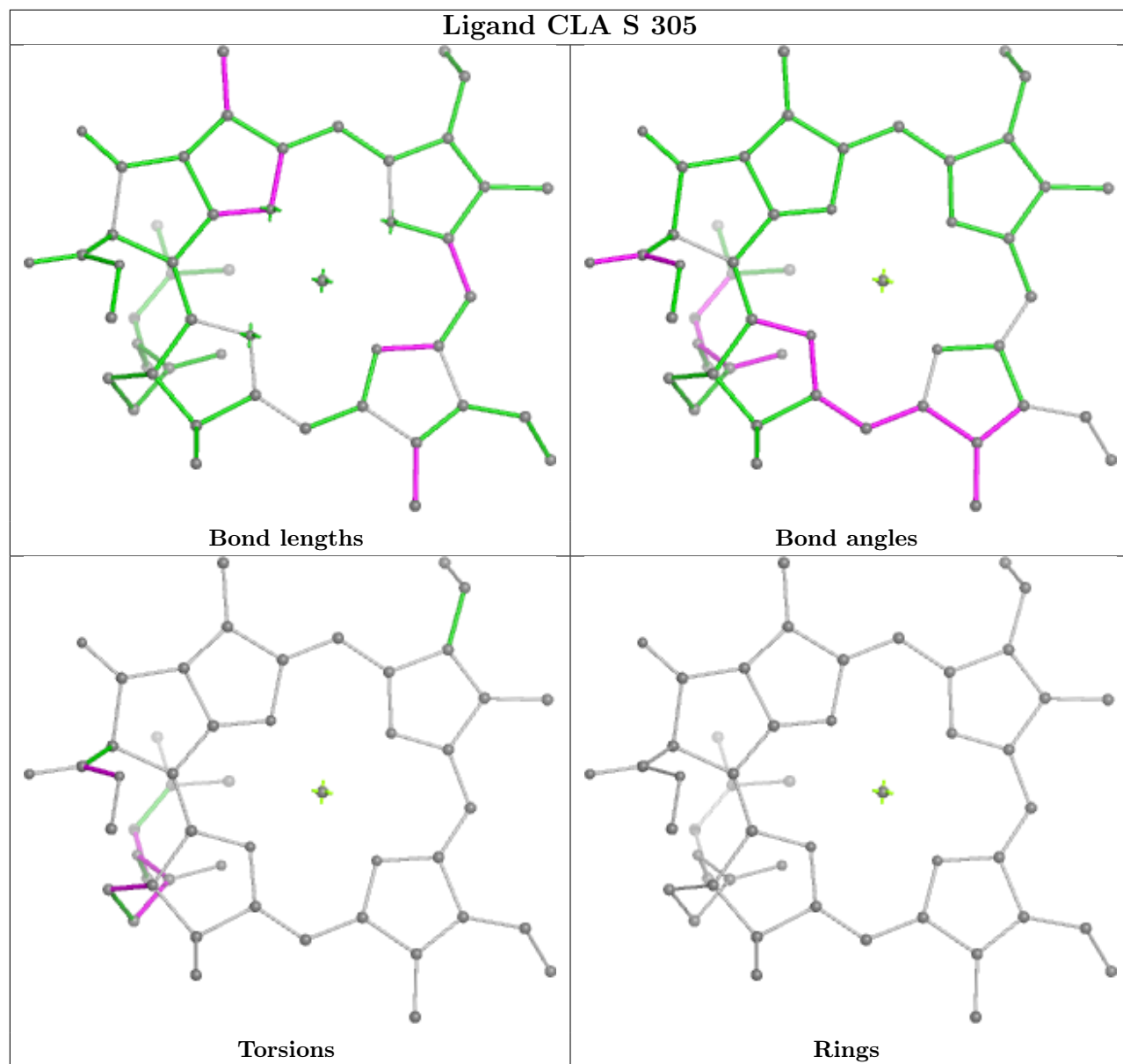


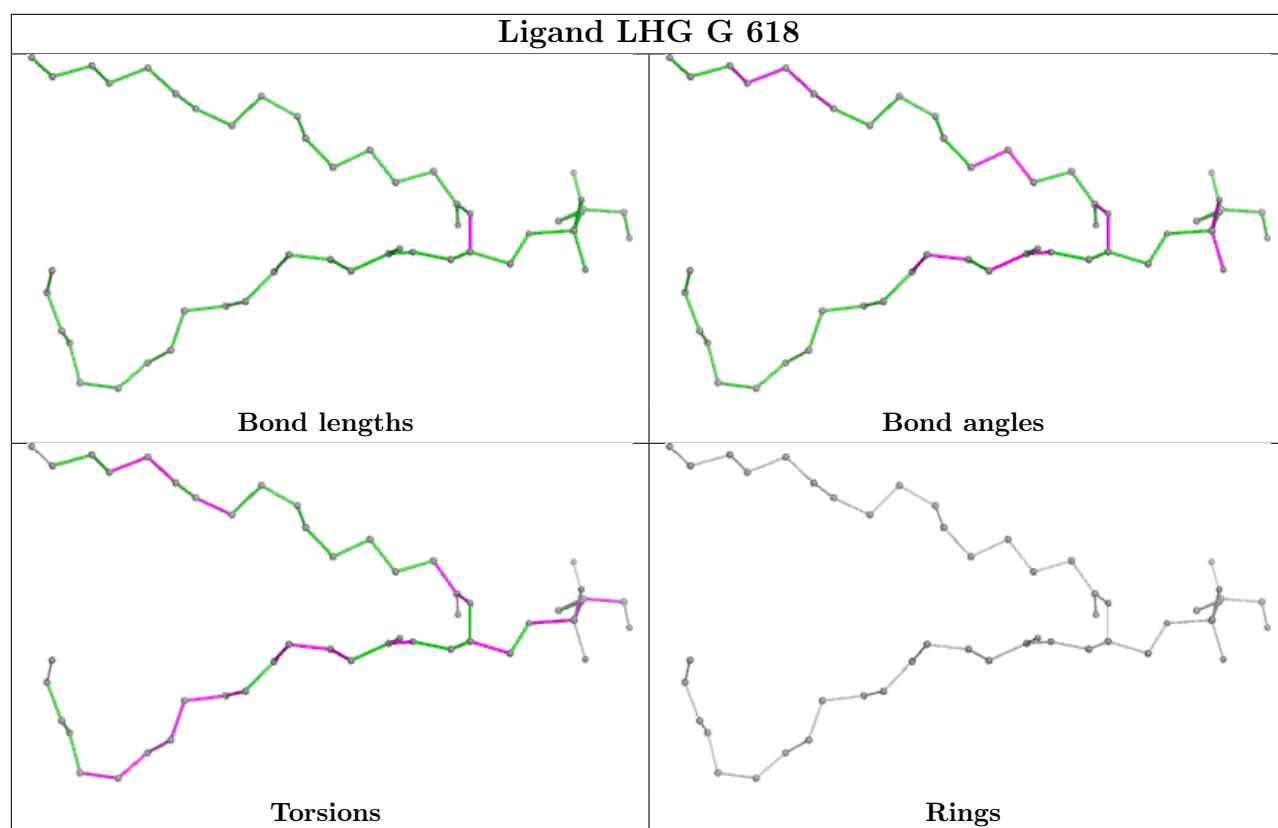




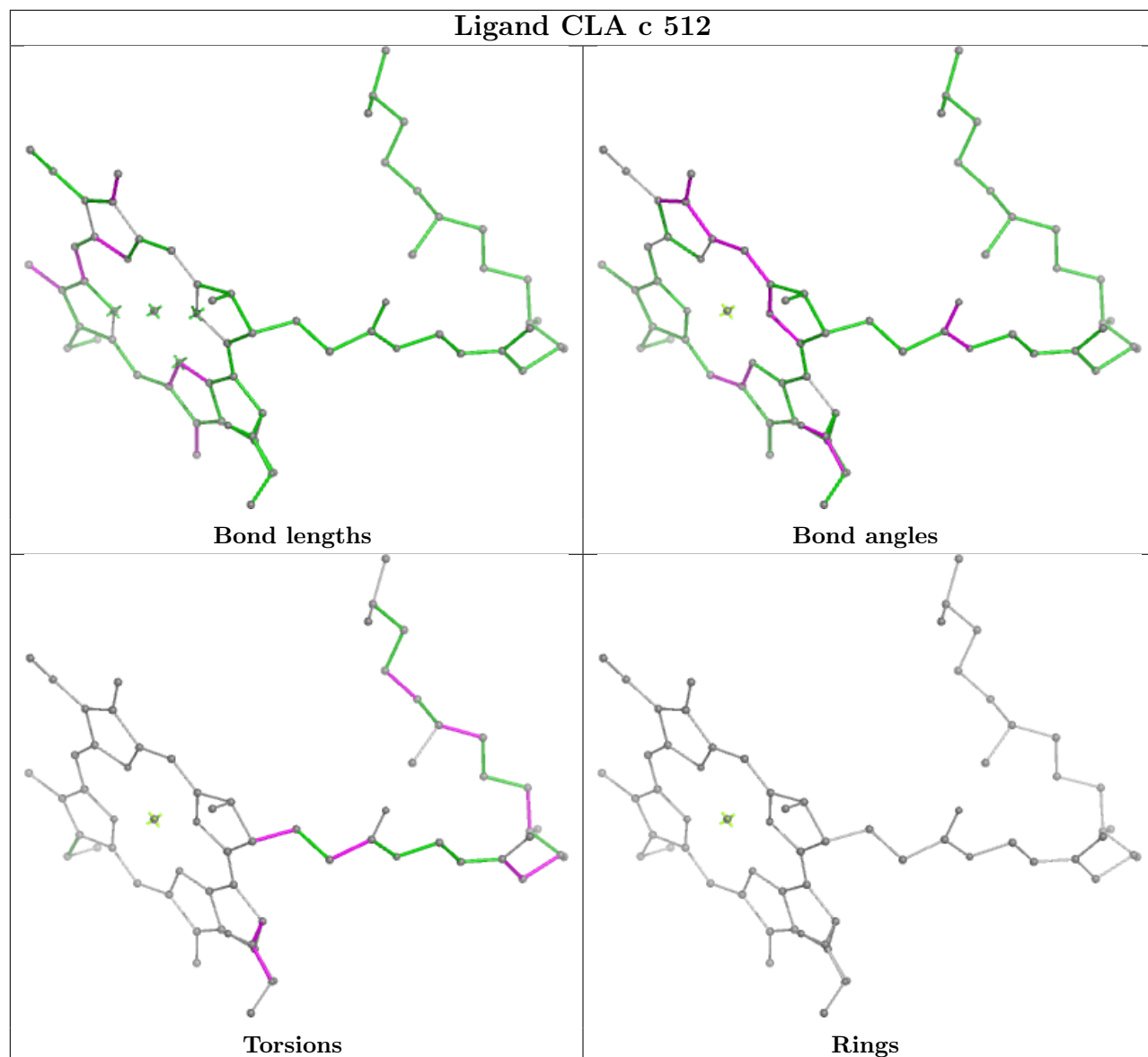


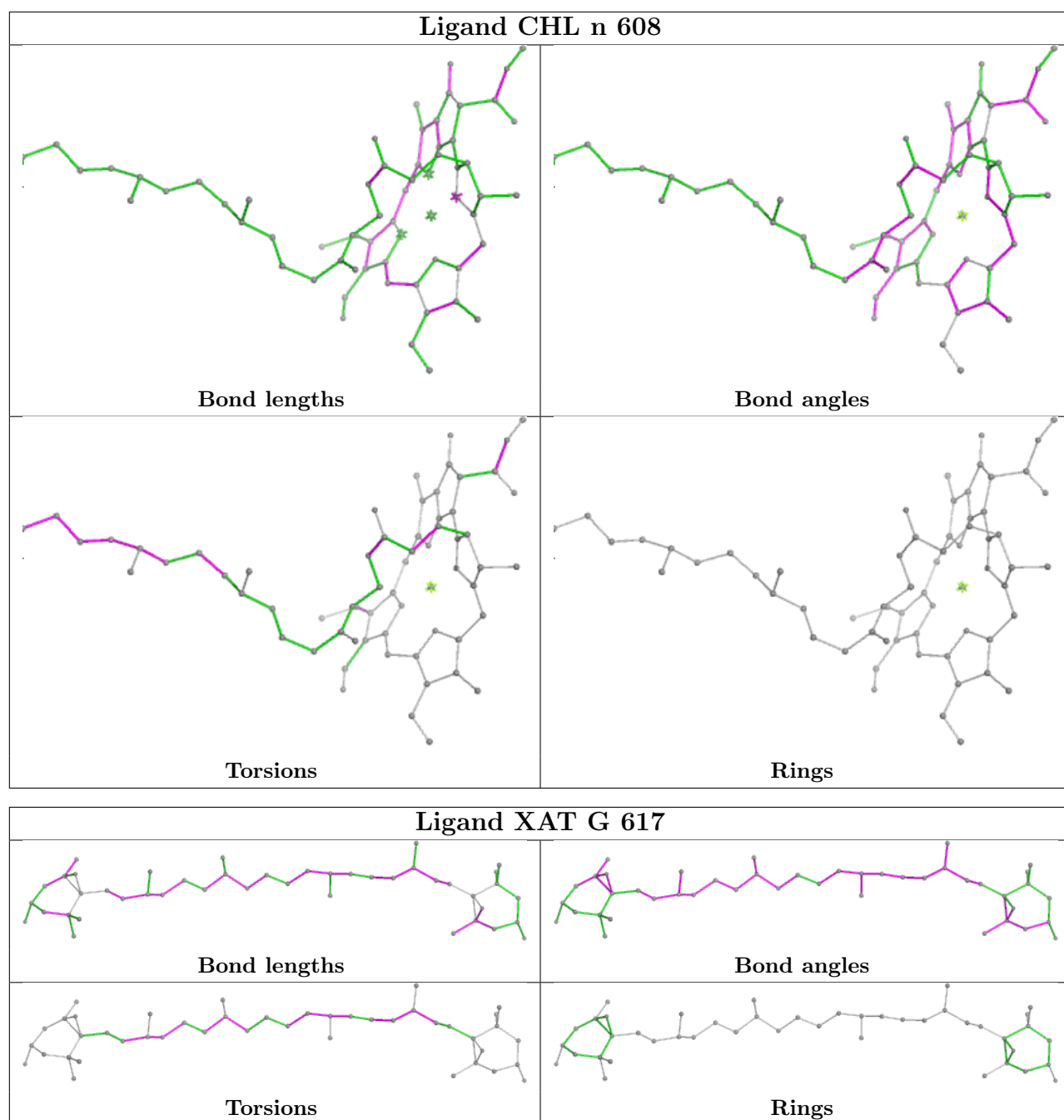
## Ligand CLA S 305



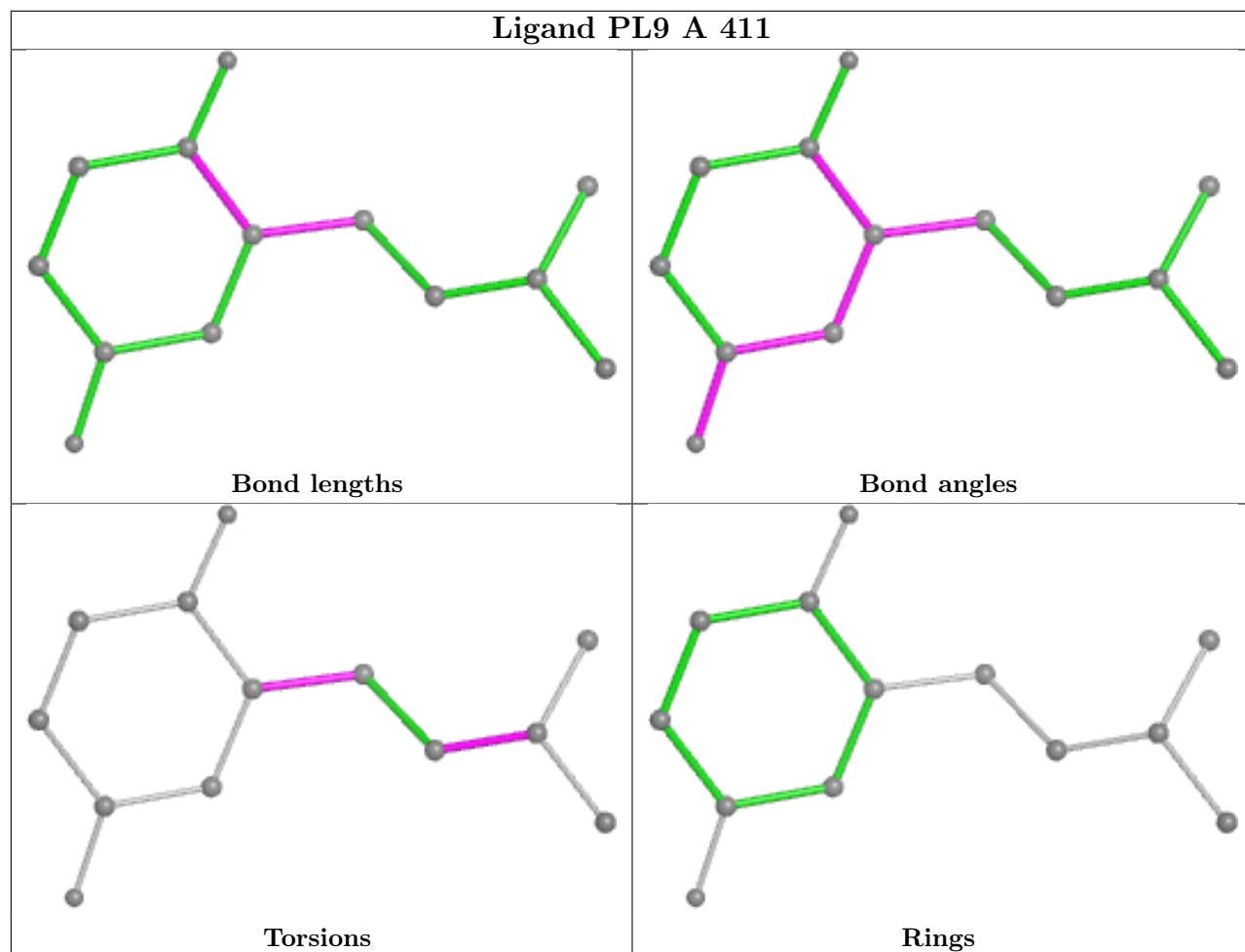


## Ligand CLA c 512

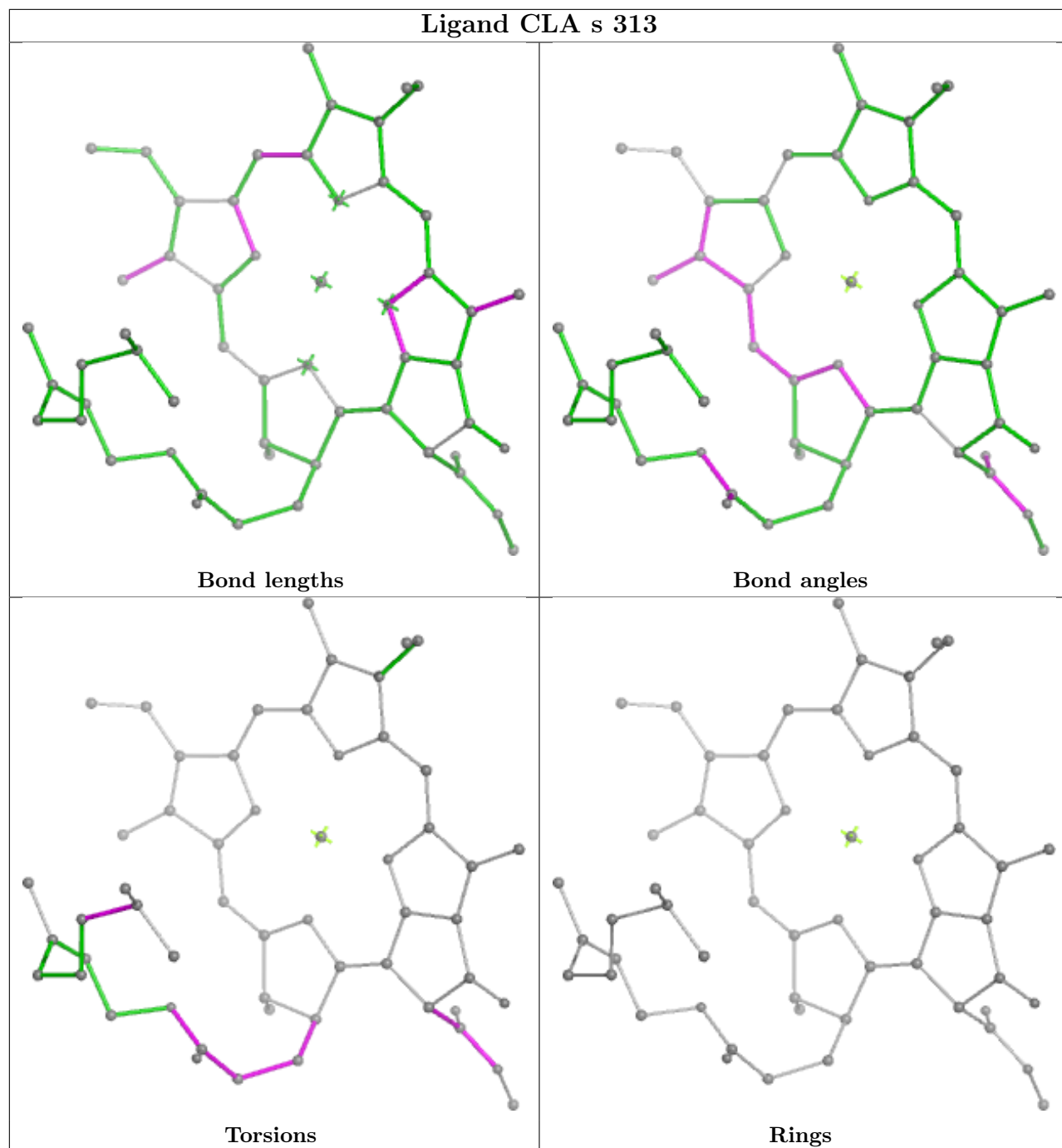




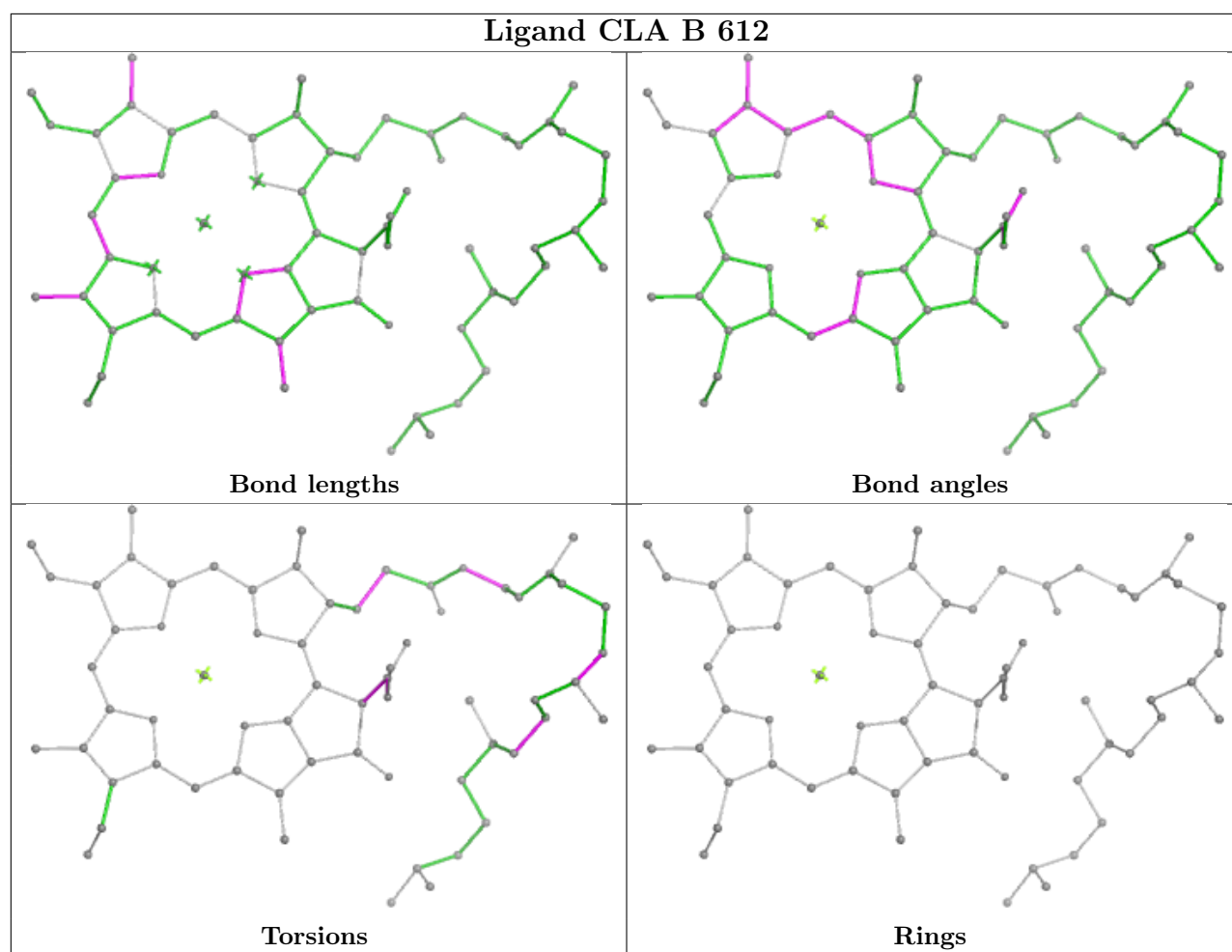
## Ligand PL9 A 411



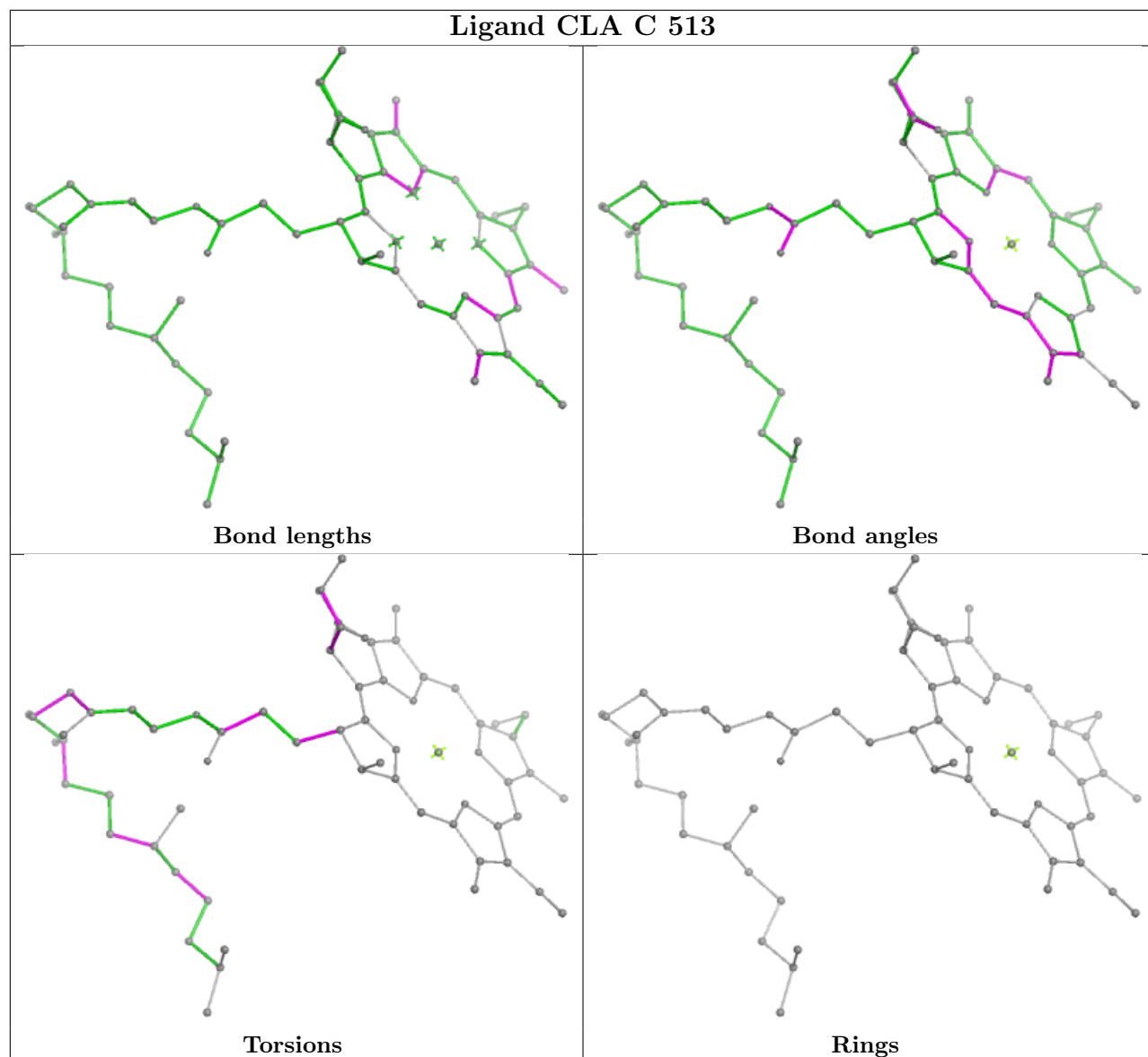
## Ligand CLA s 313



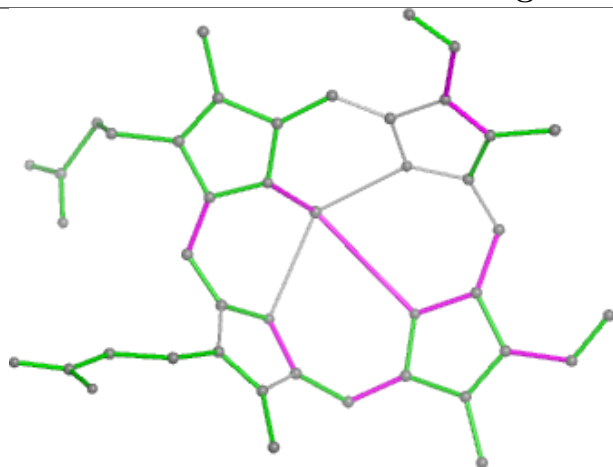




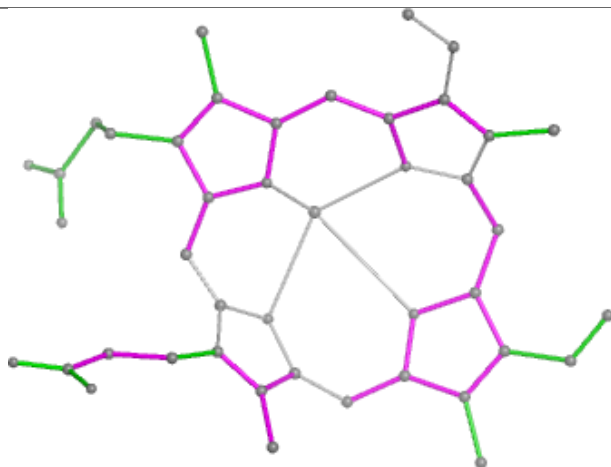
## Ligand CLA C 513



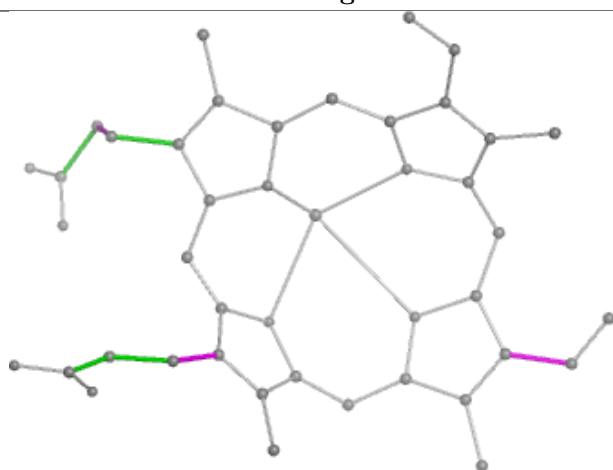
## Ligand HEM f 101



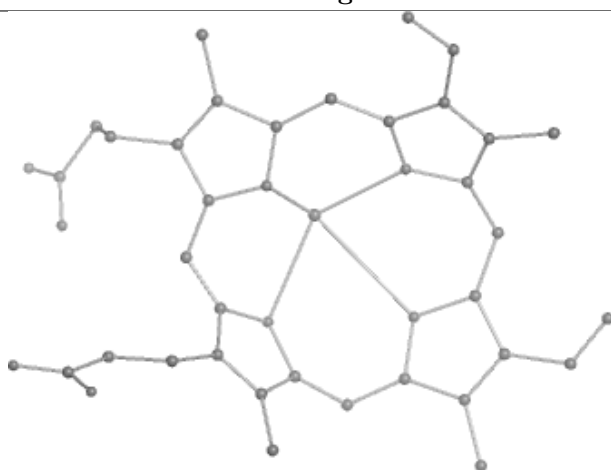
Bond lengths



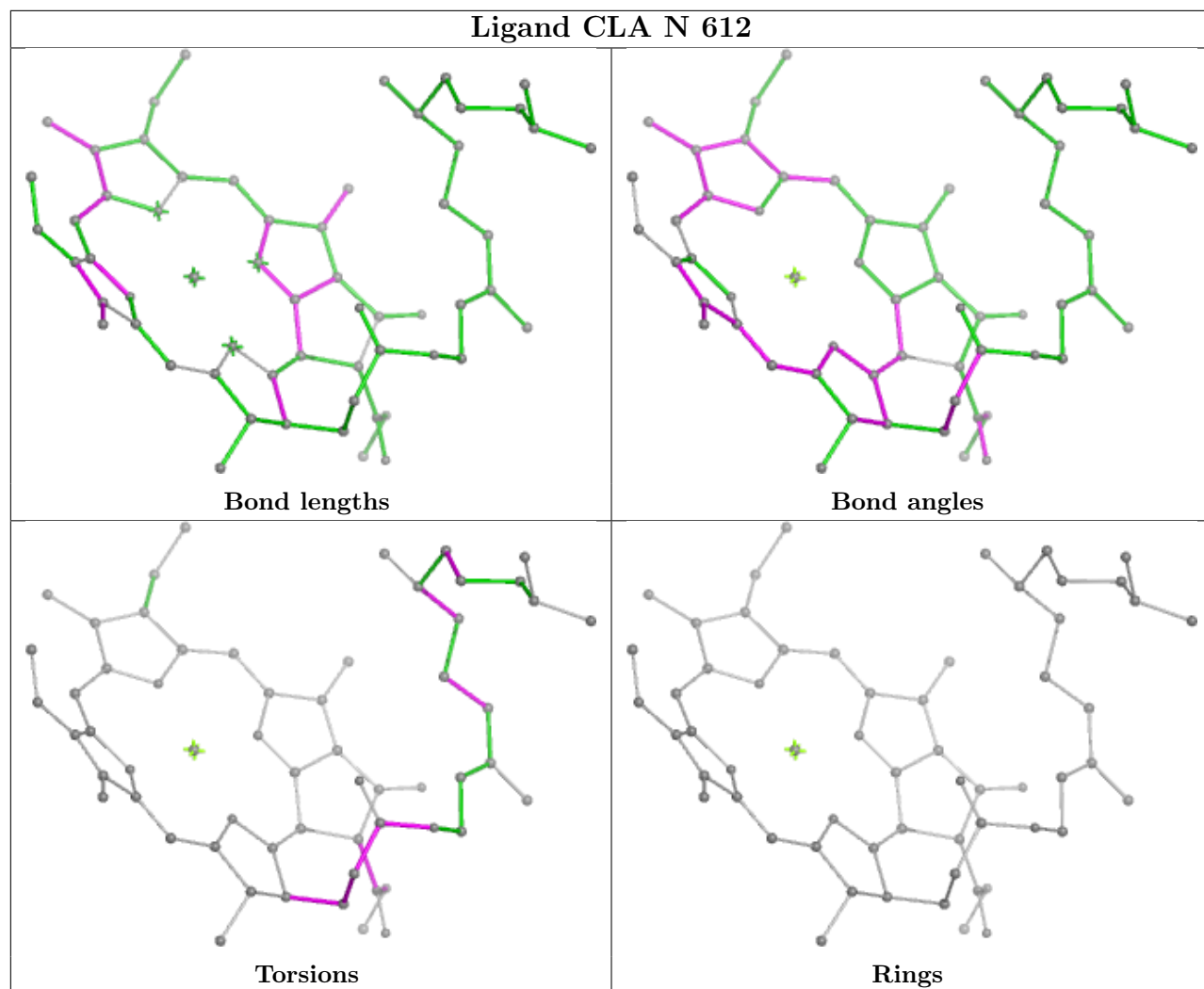
Bond angles

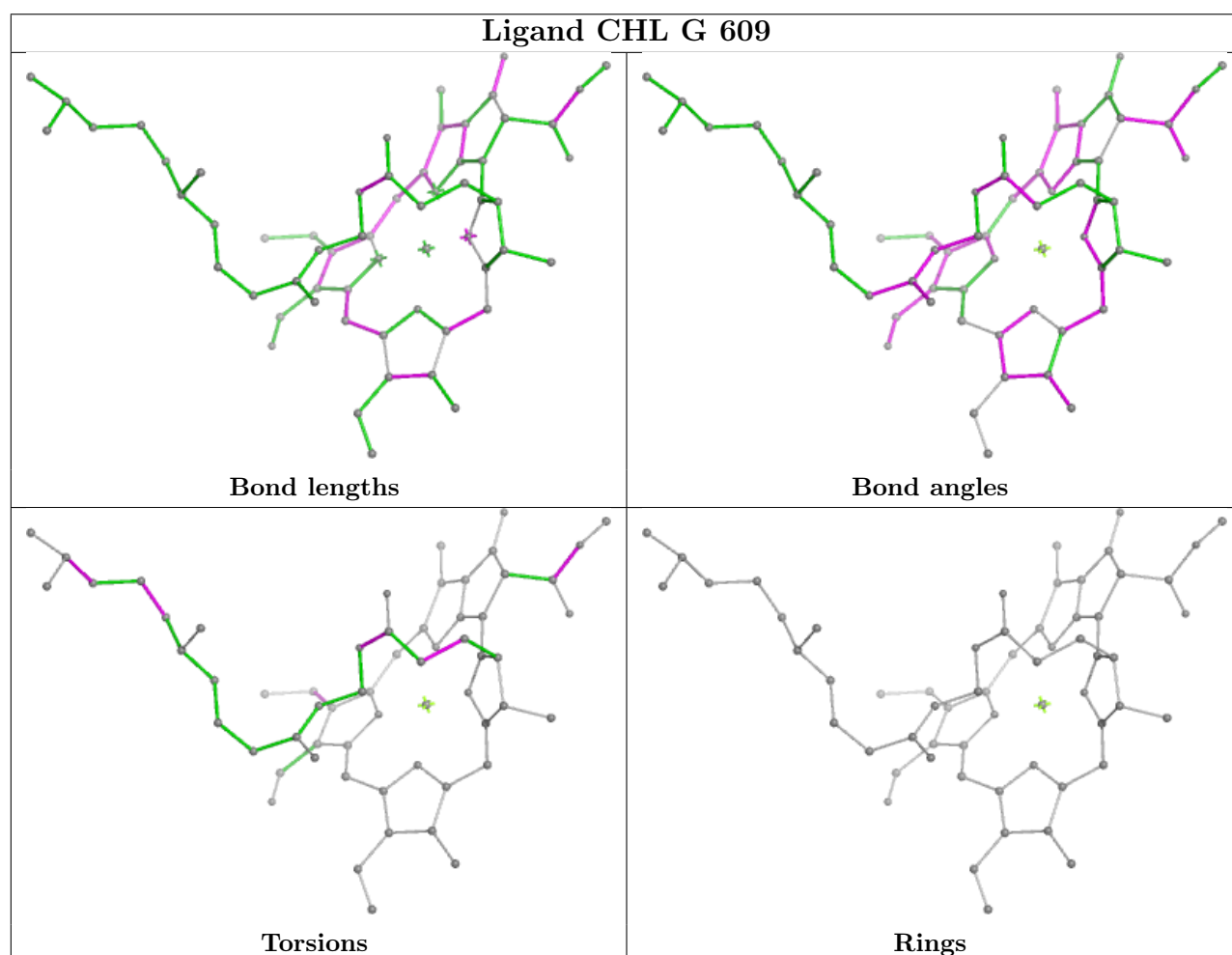
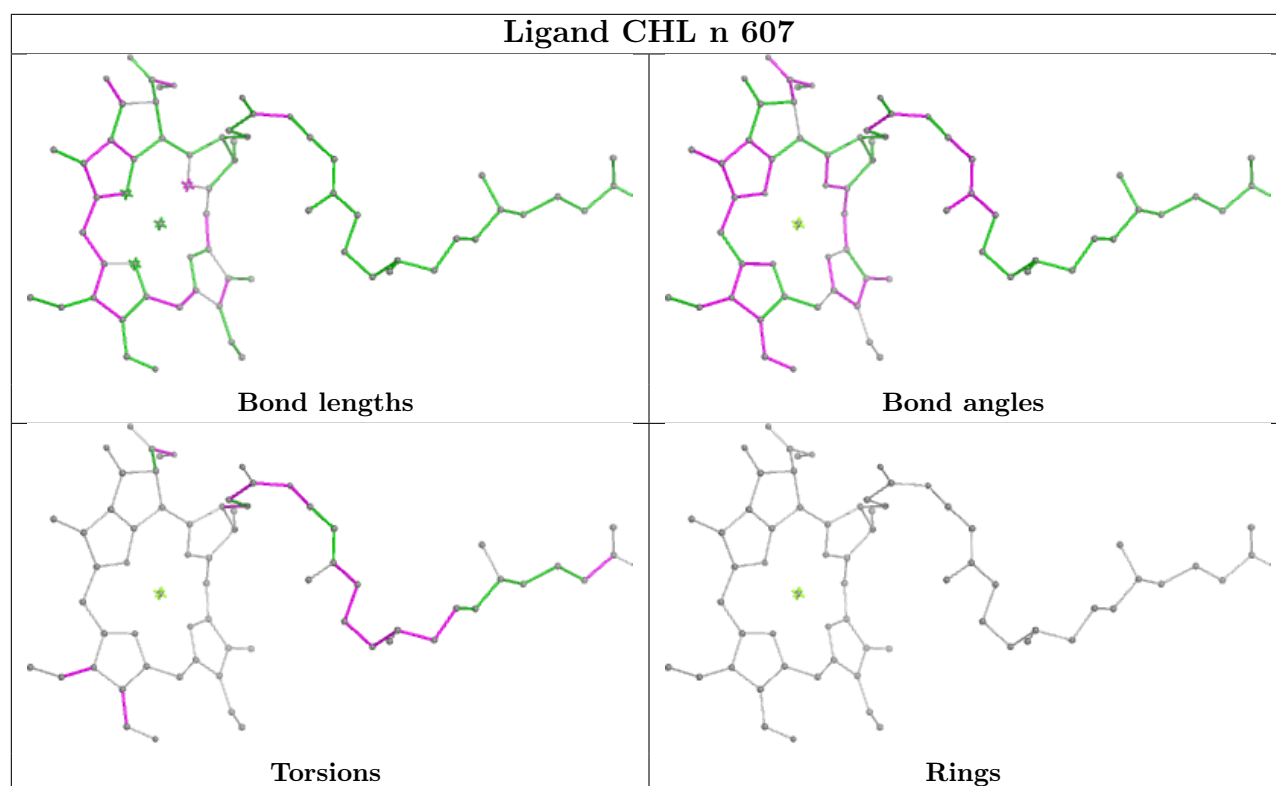


Torsions

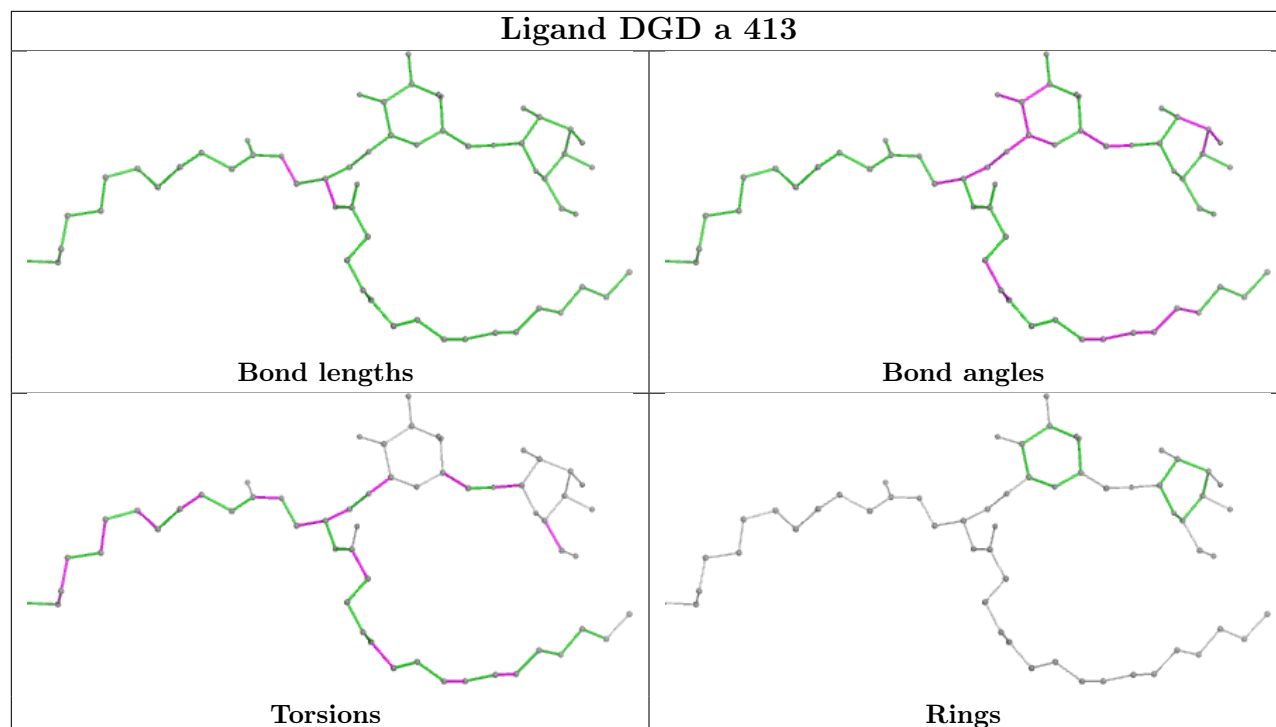


Rings

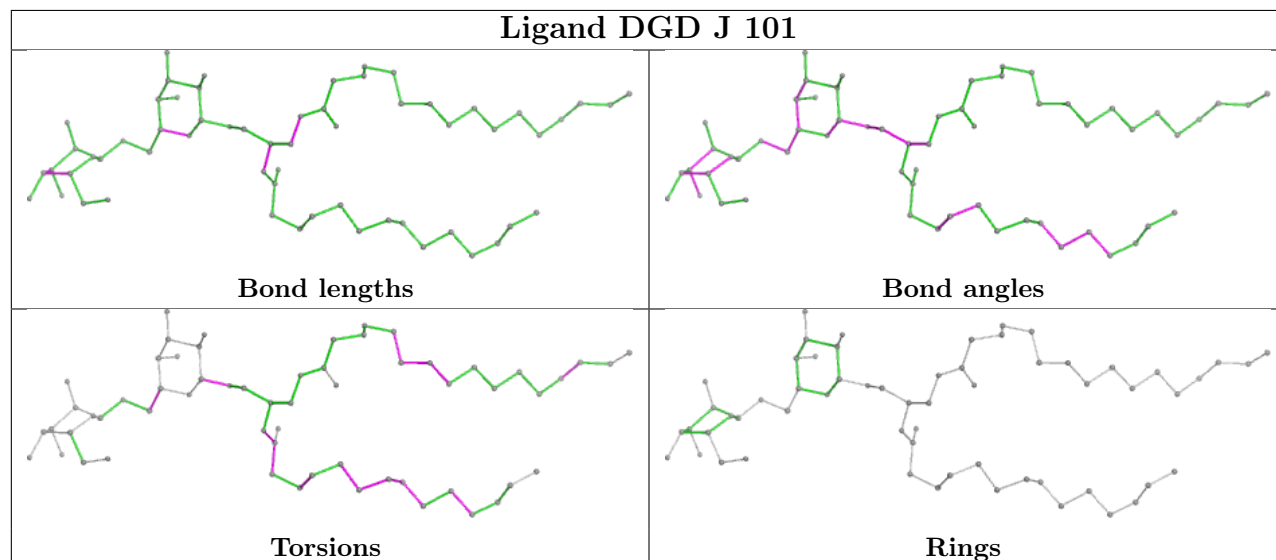


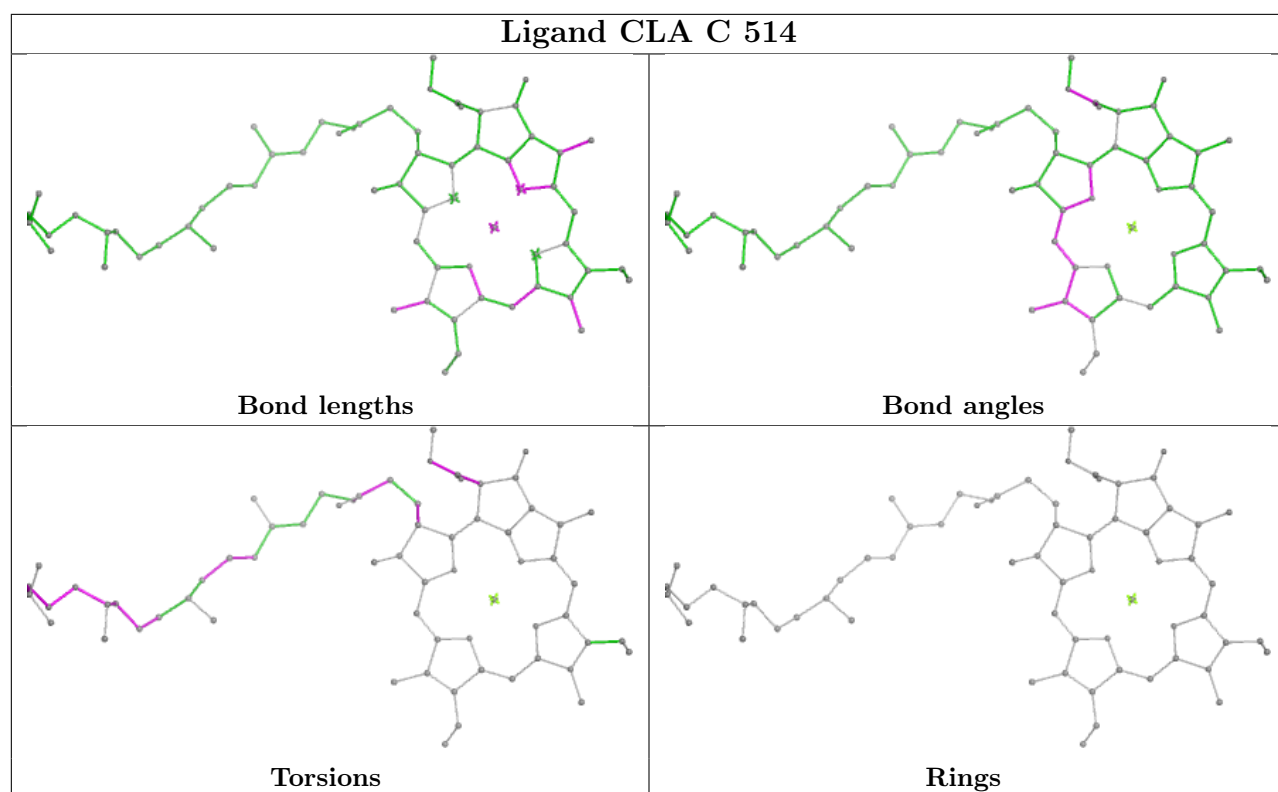


## Ligand DGD a 413

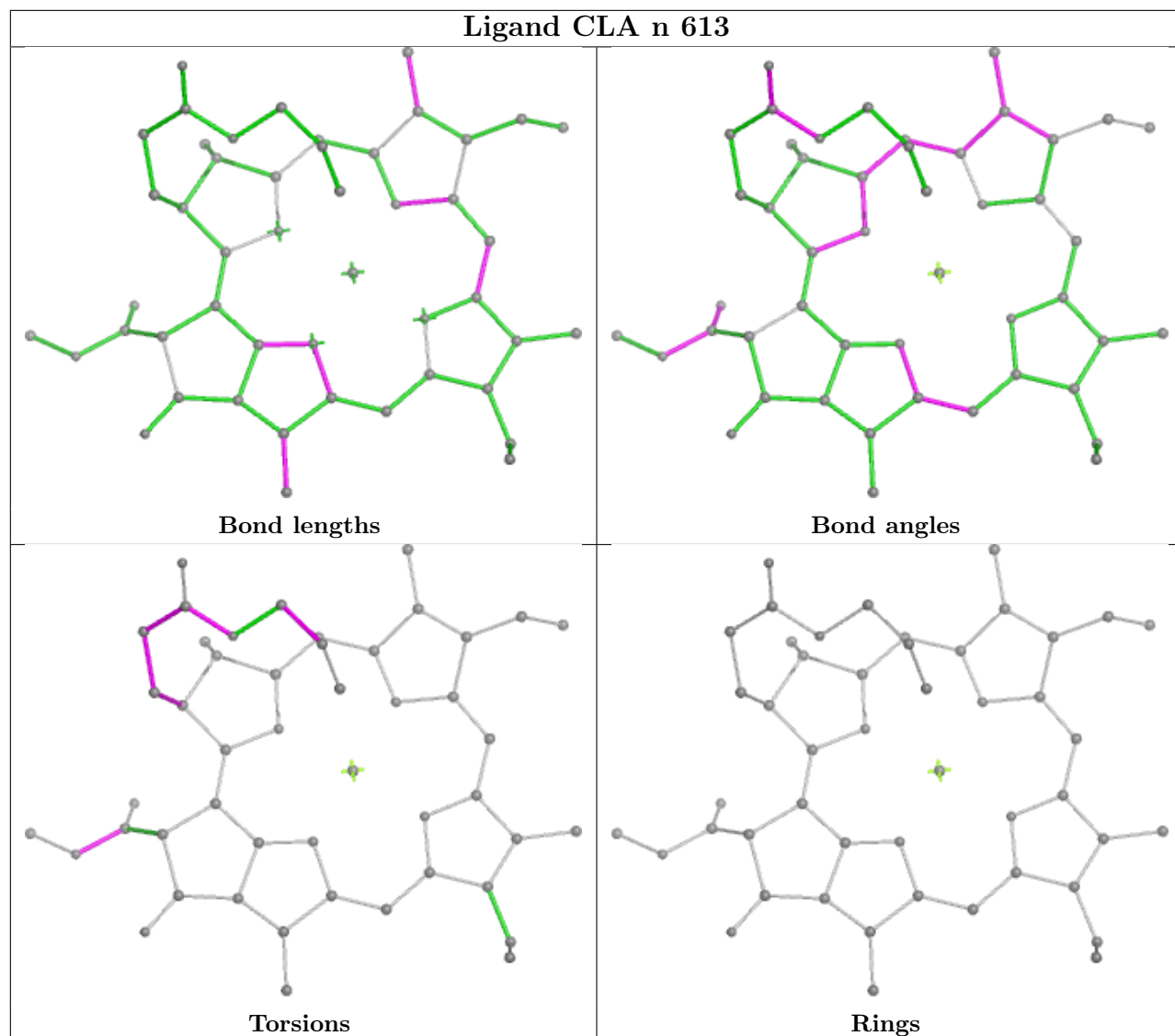


## Ligand DGD J 101



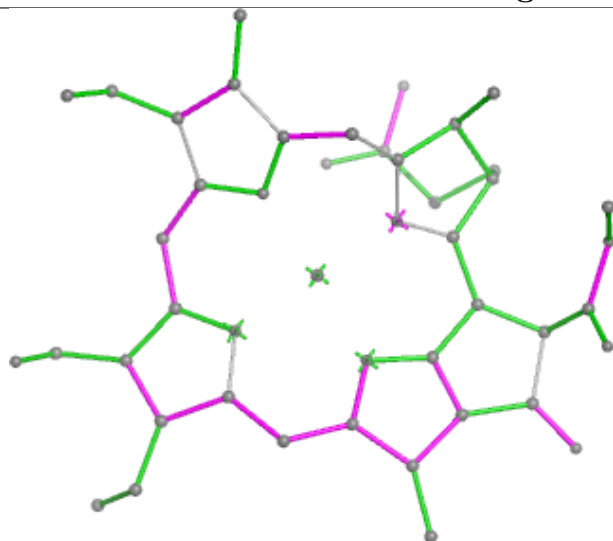


## Ligand CLA n 613

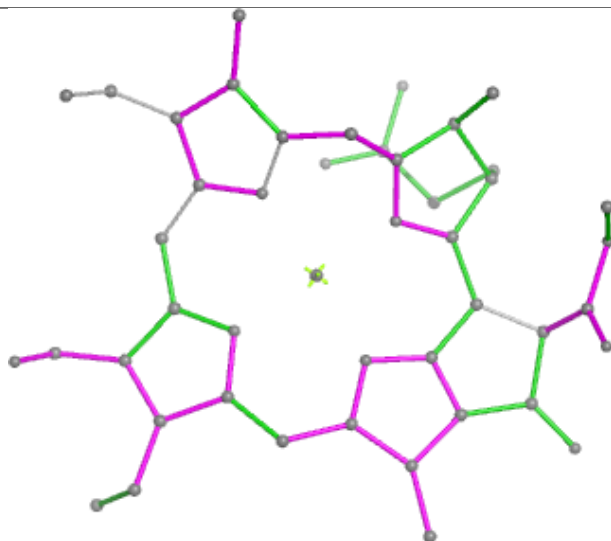




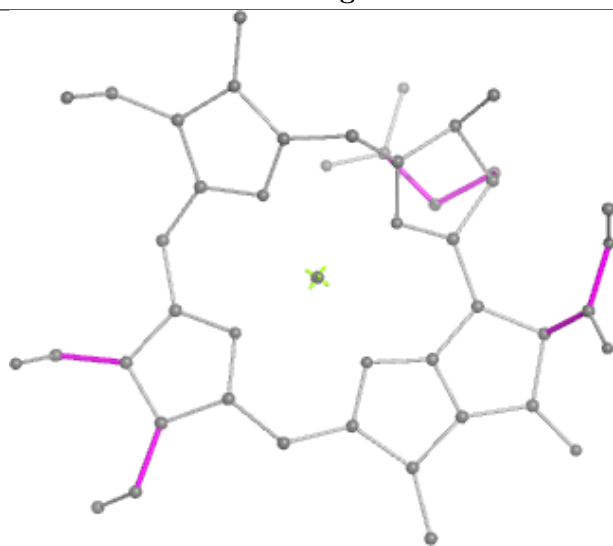
## Ligand CHL S 307



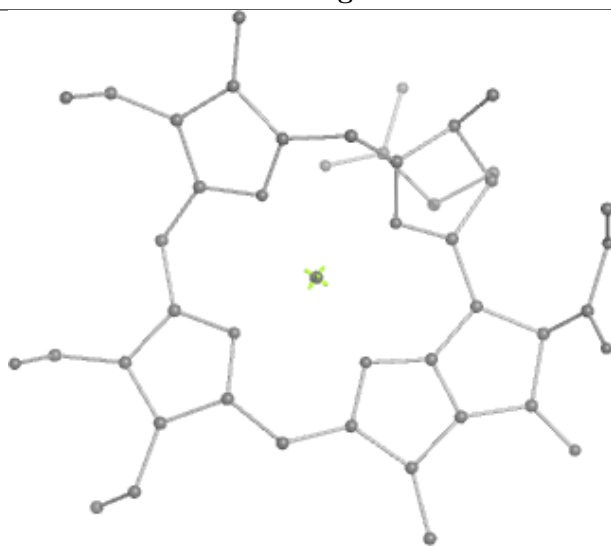
Bond lengths



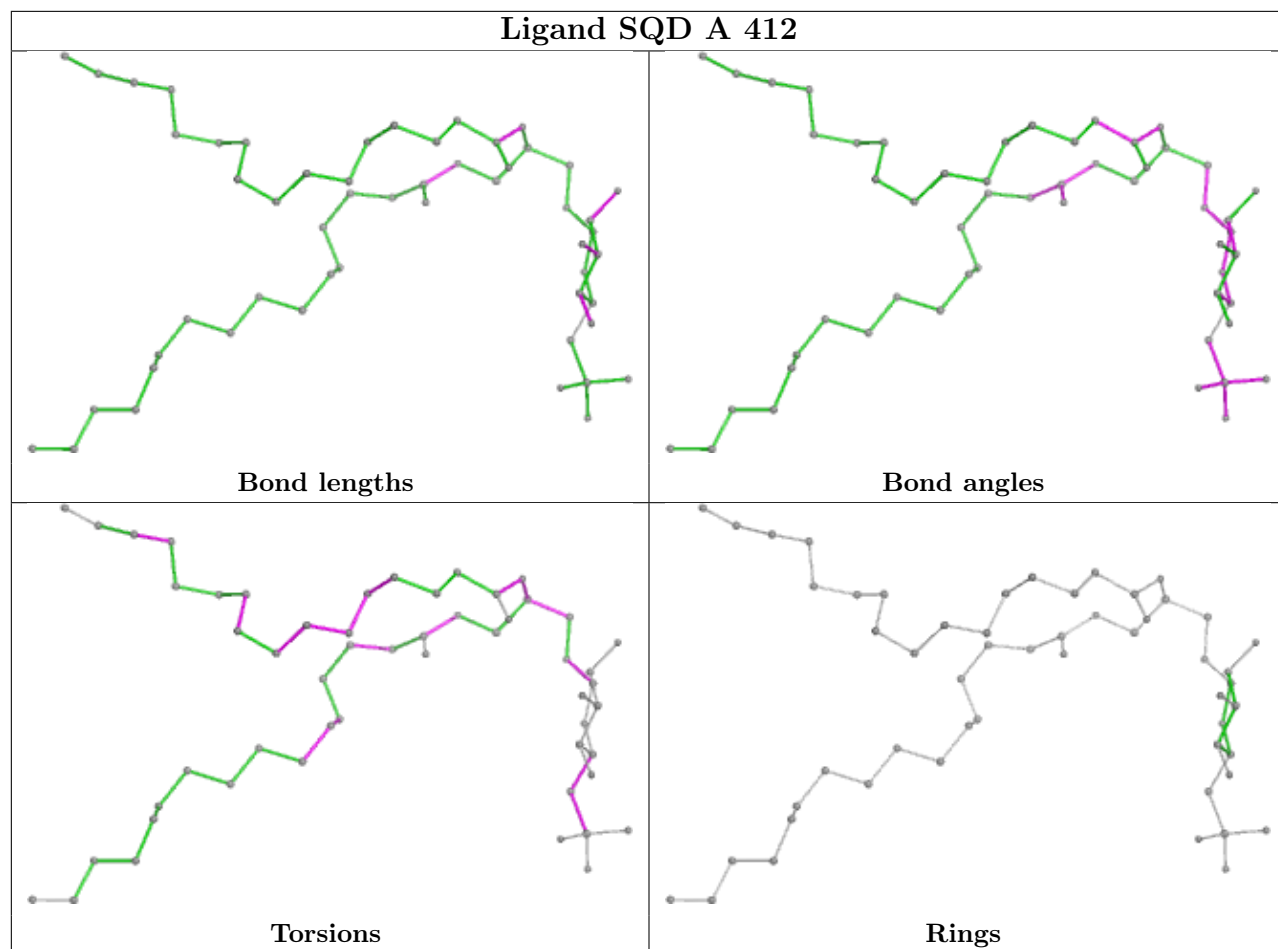
Bond angles



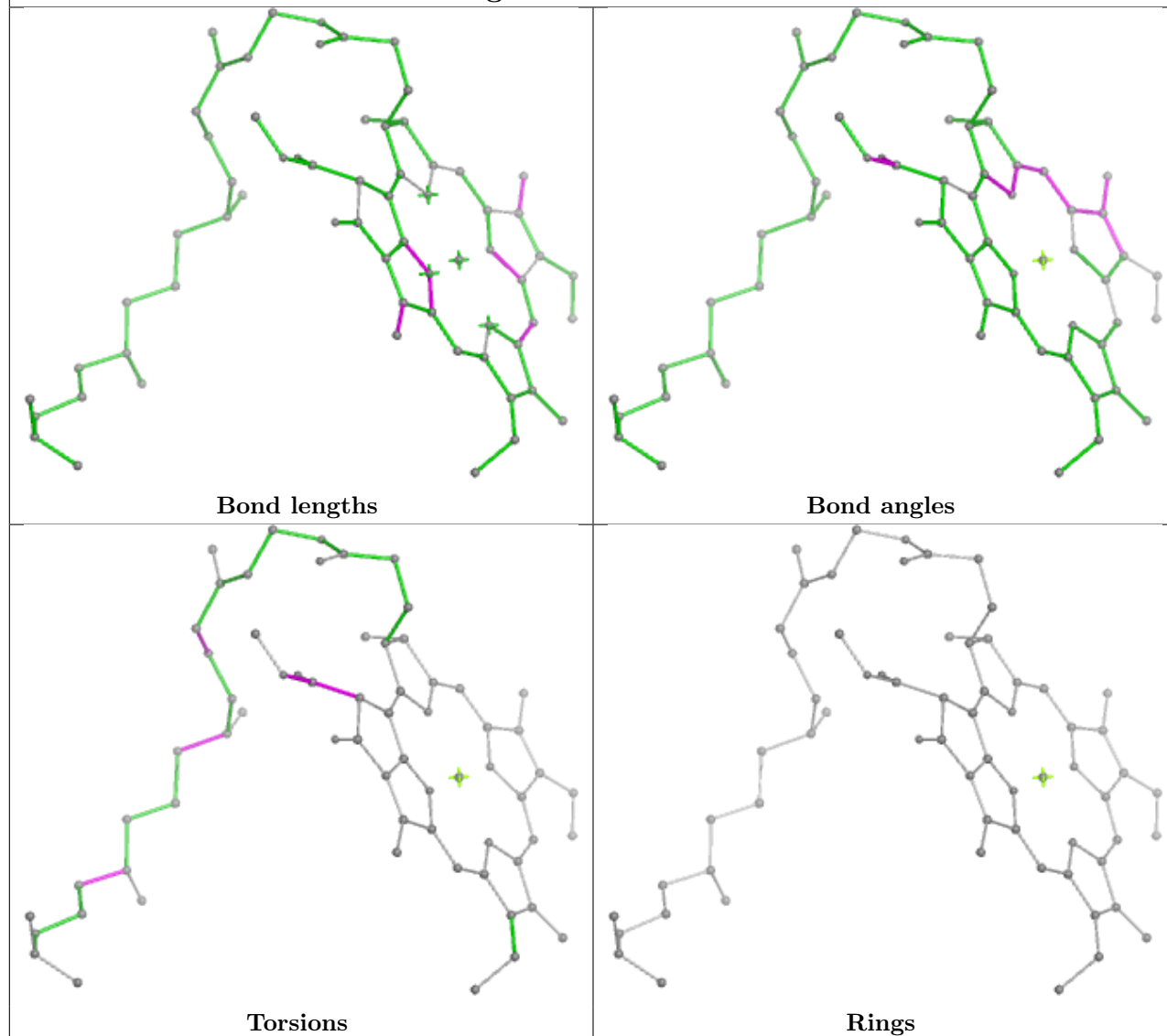
Torsions



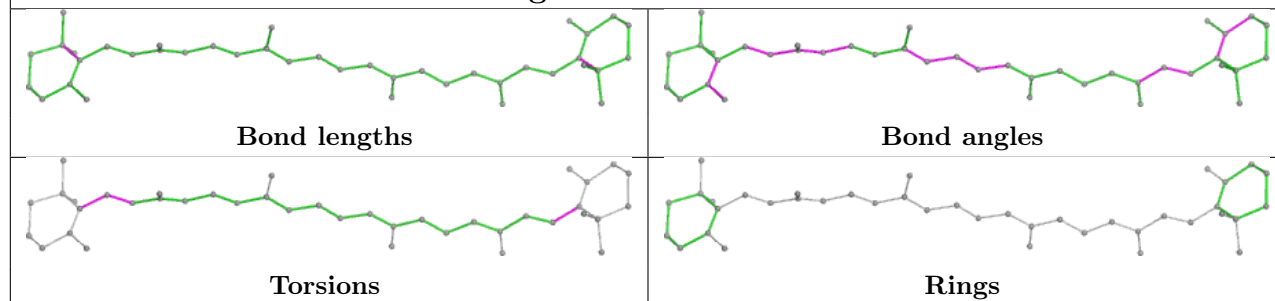
Rings

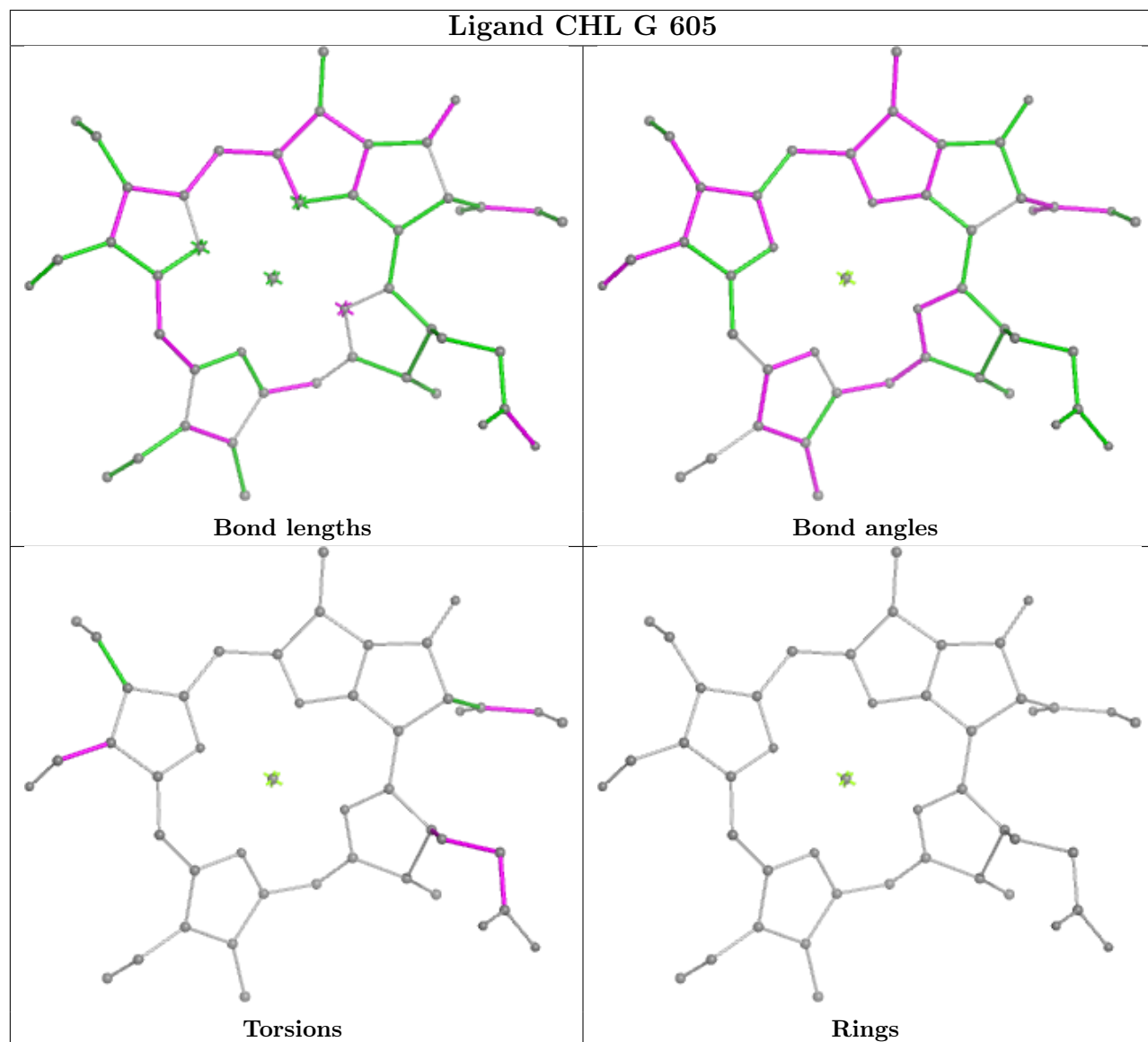


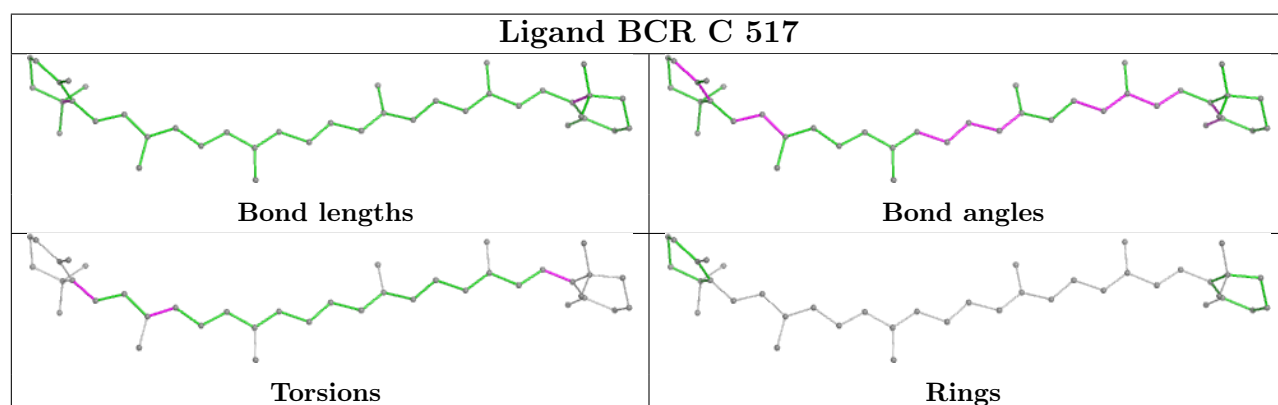
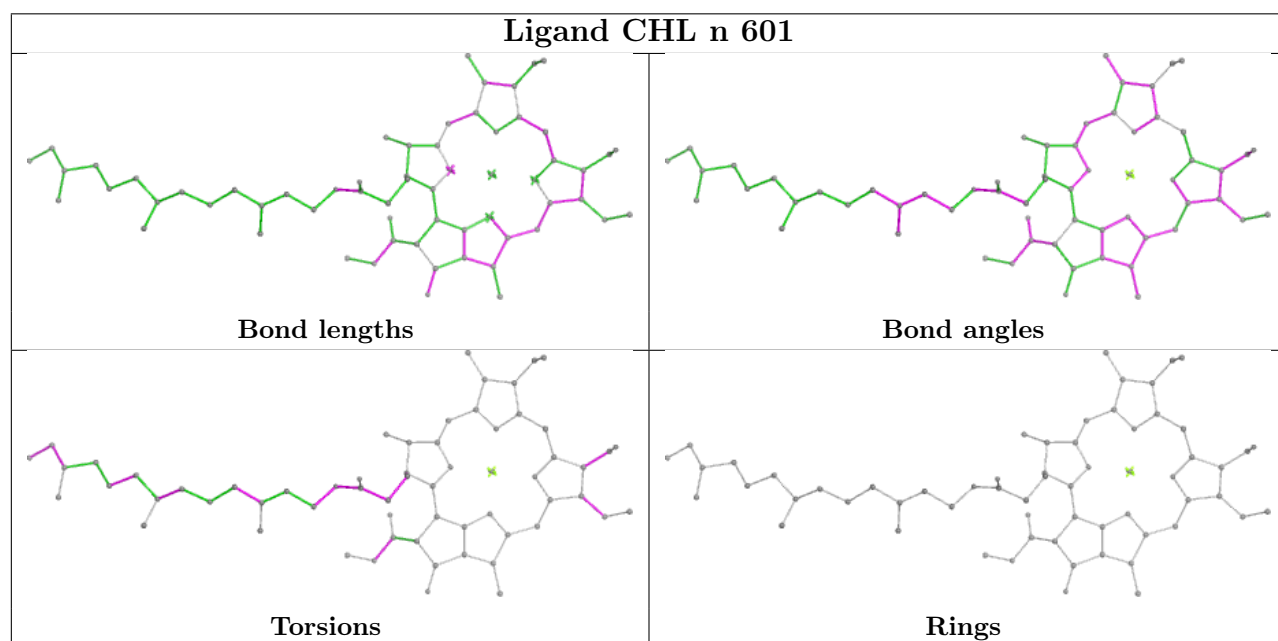
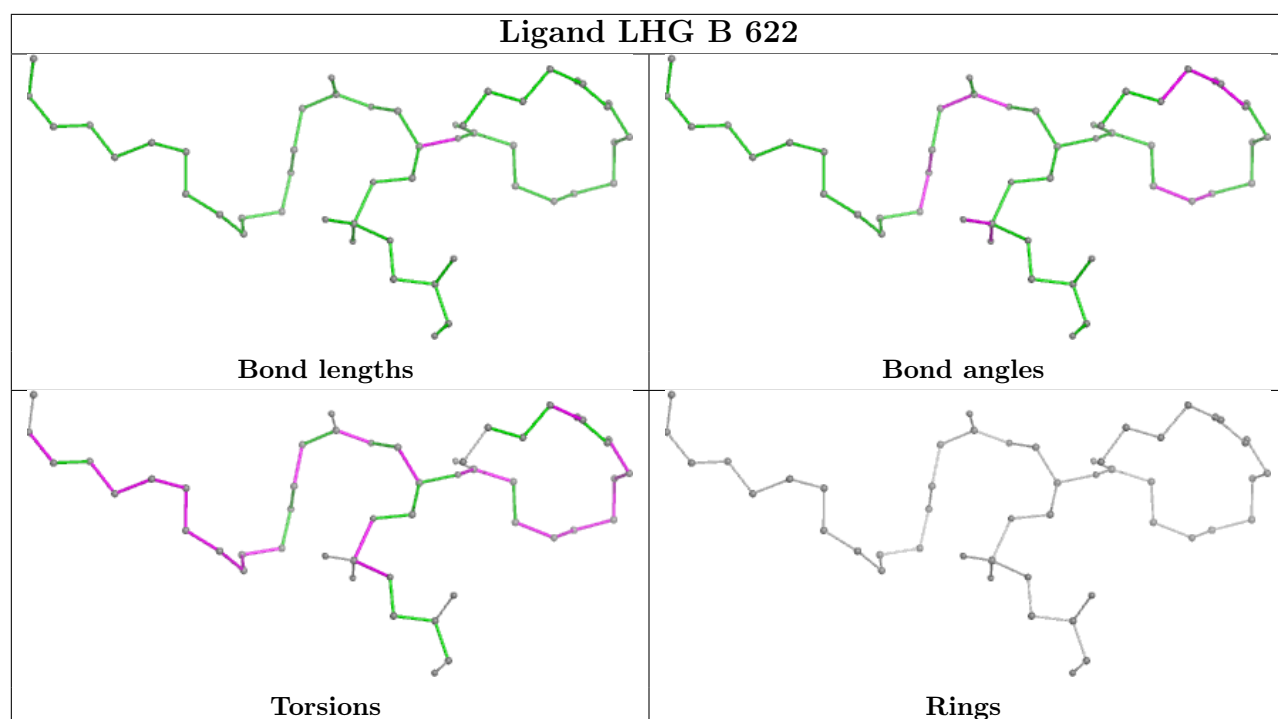
## Ligand CLA B 615



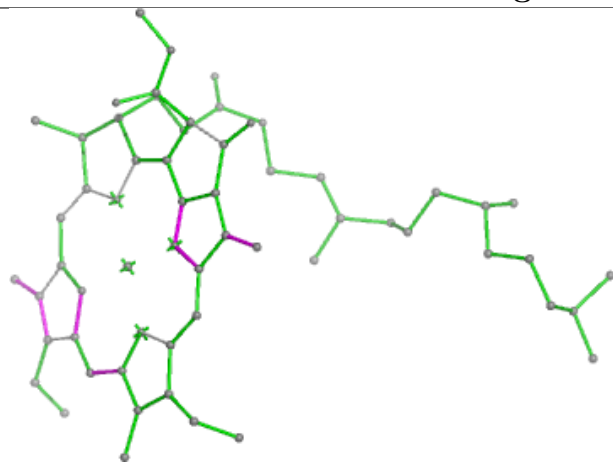
## Ligand BCR A 410



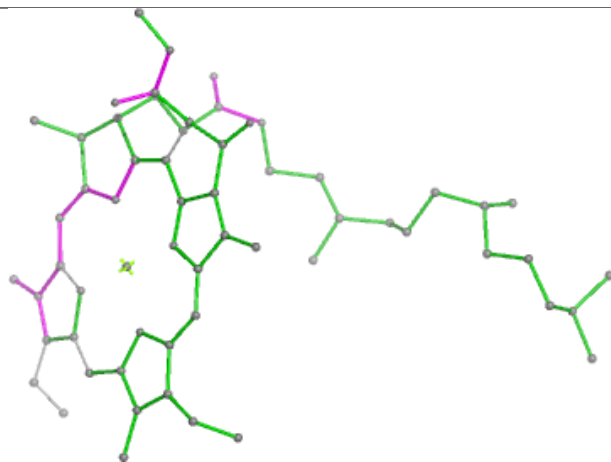




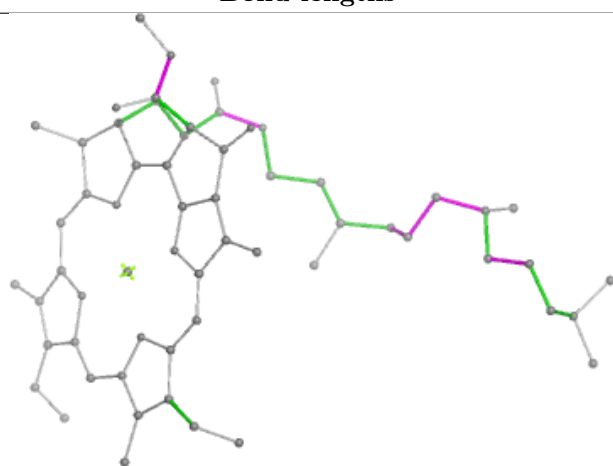
## Ligand CLA Y 610



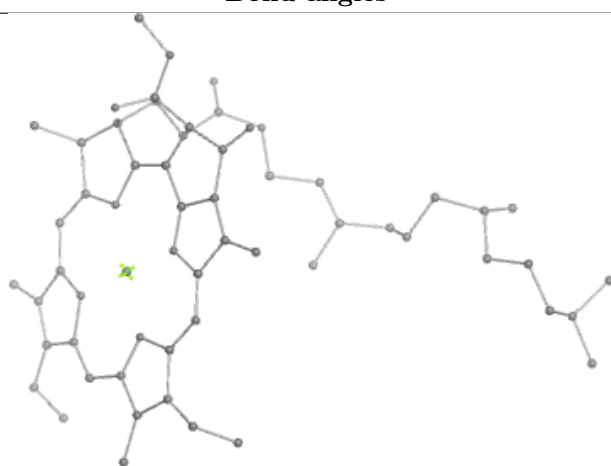
Bond lengths



Bond angles

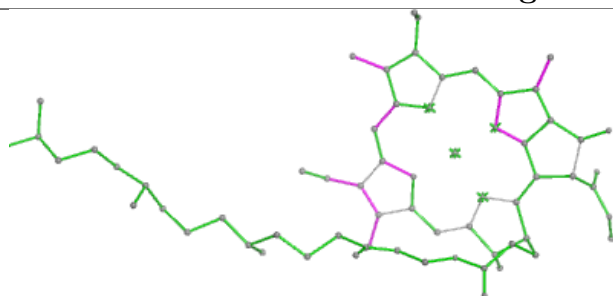


Torsions

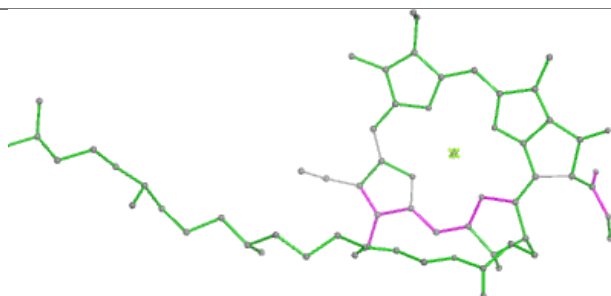


Rings

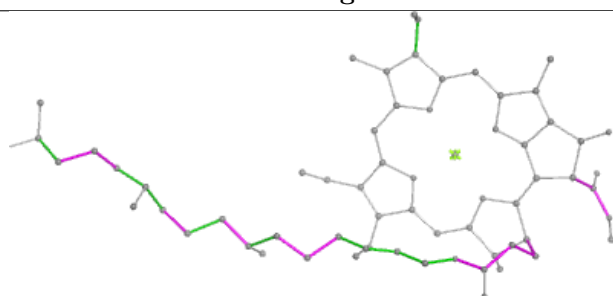
## Ligand CLA c 502



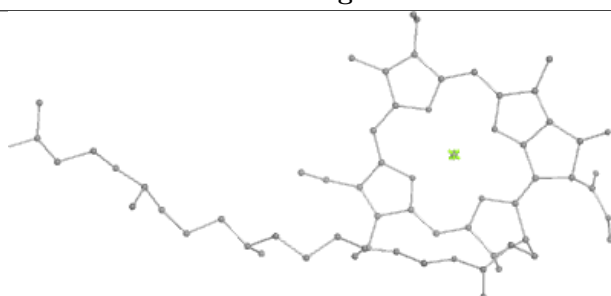
Bond lengths



Bond angles

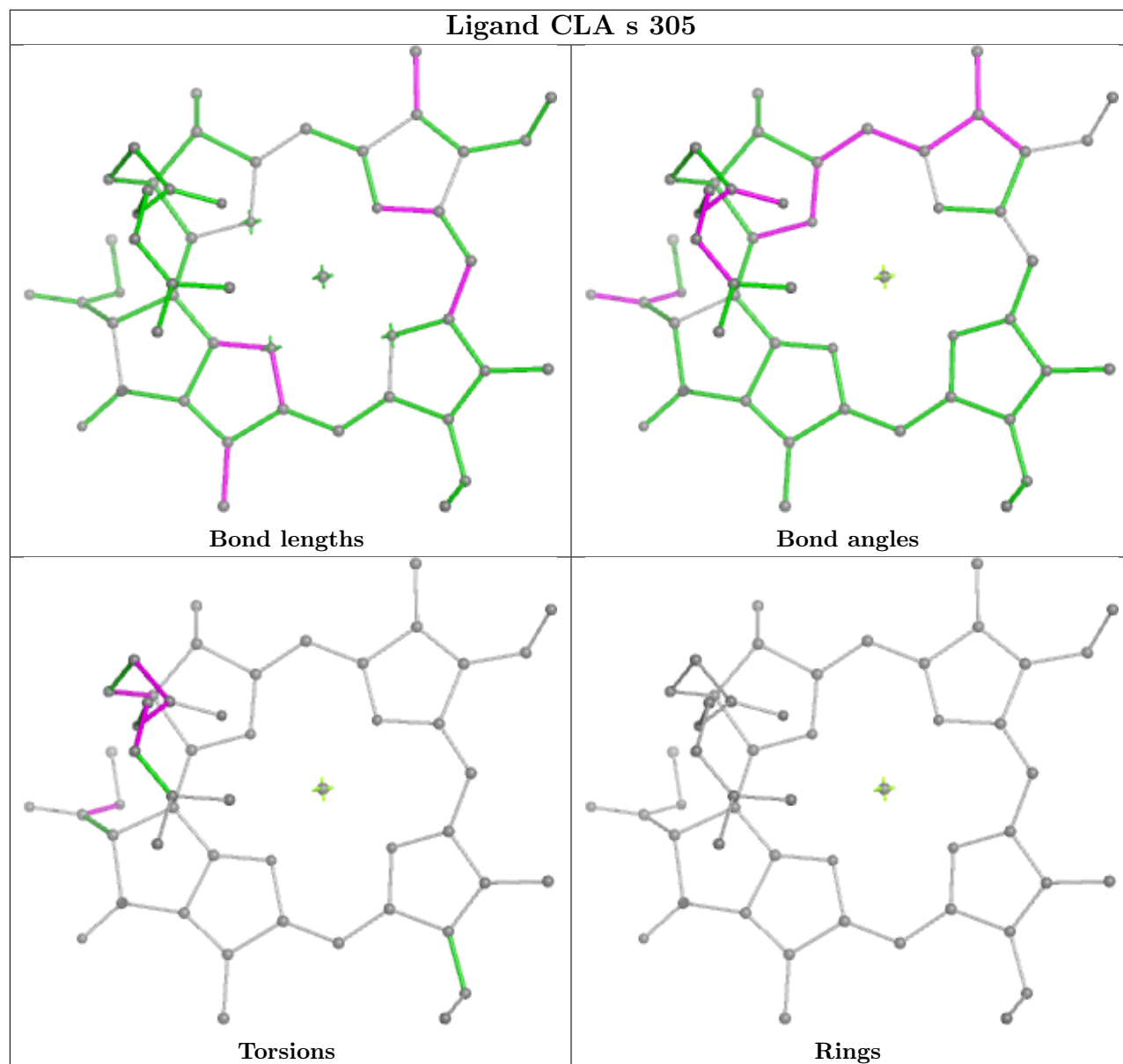


Torsions

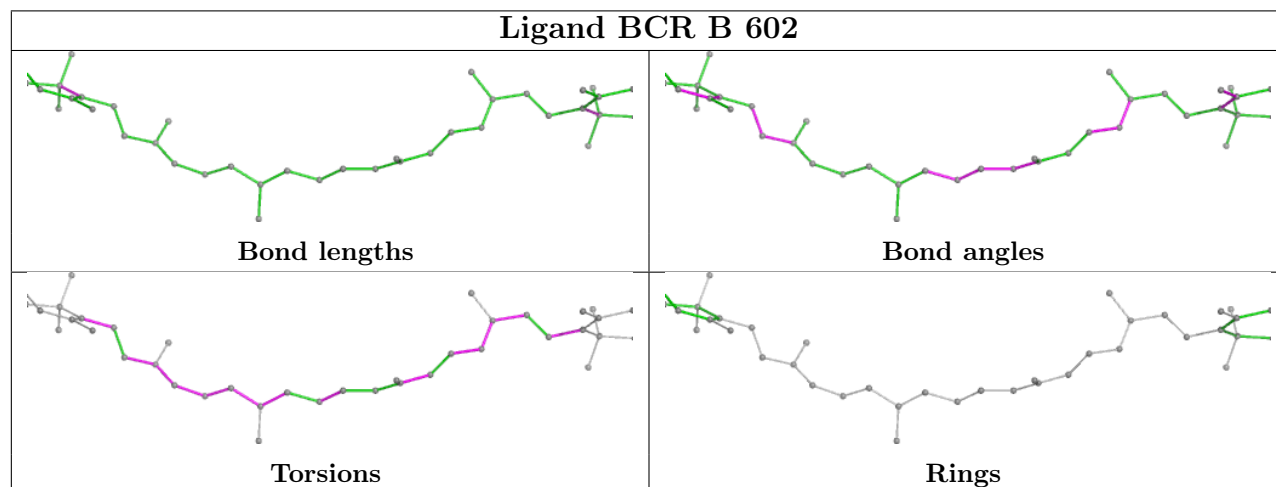


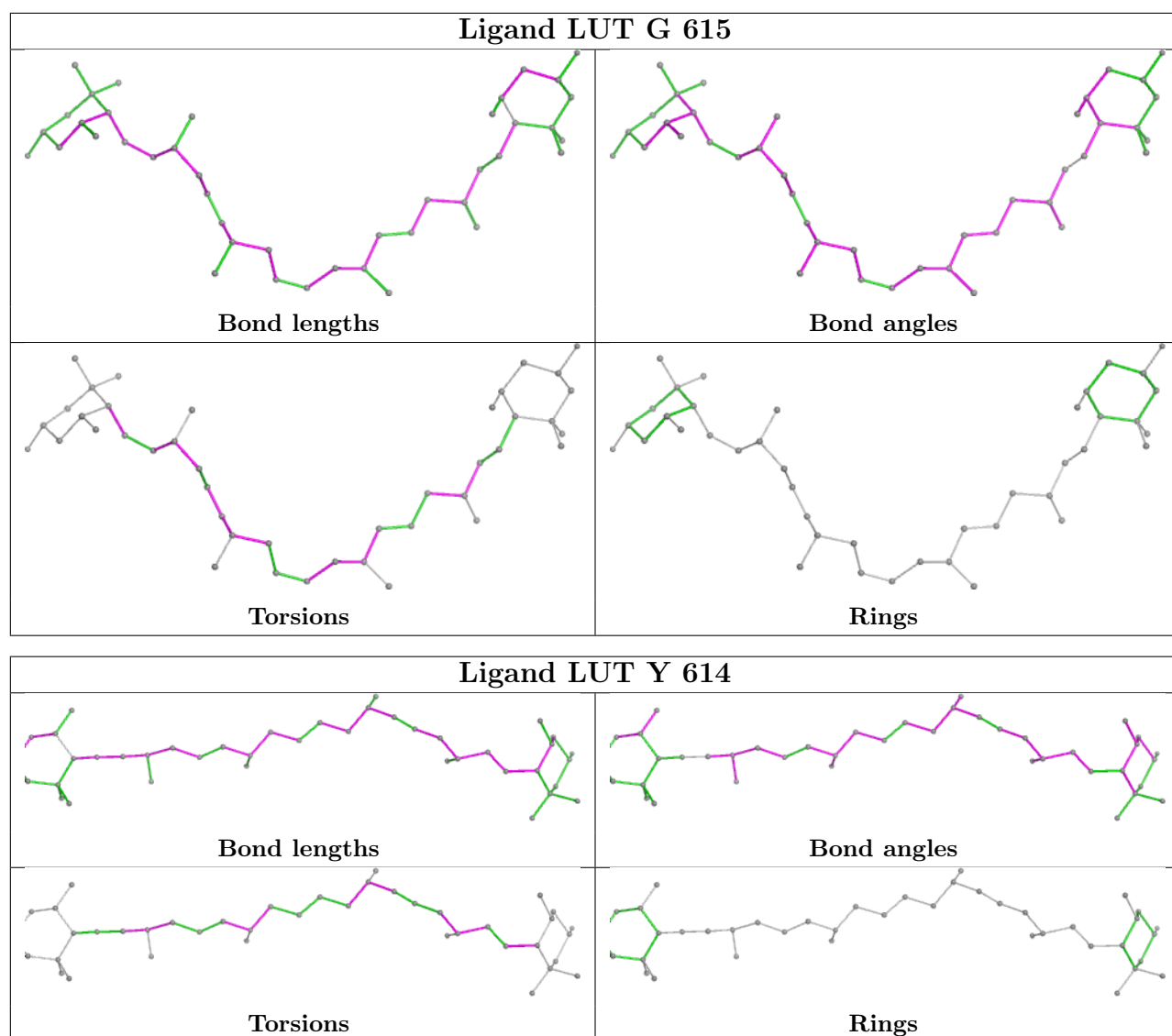
Rings

## Ligand CLA s 305



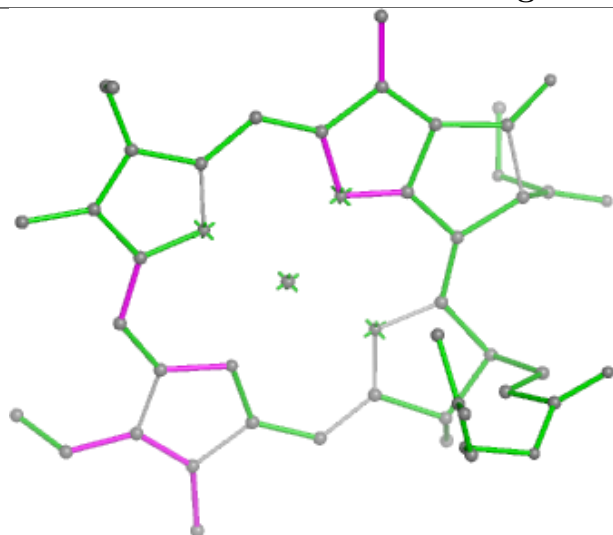
## Ligand BCR B 602



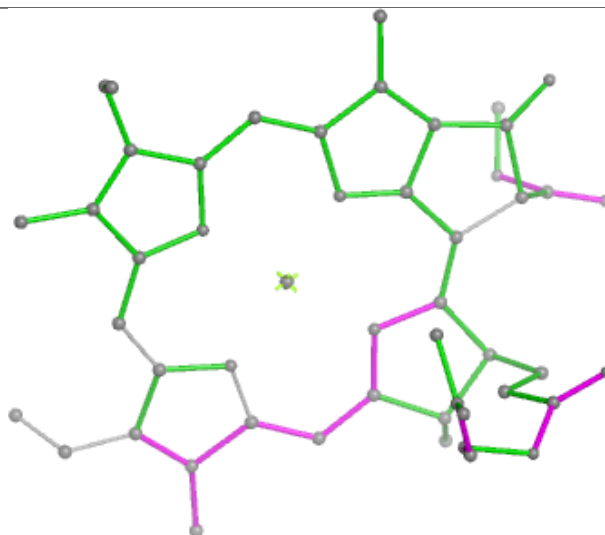




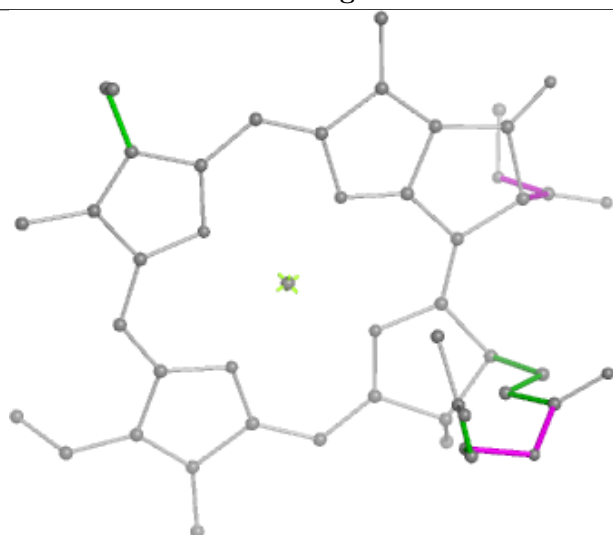
## Ligand CLA n 604



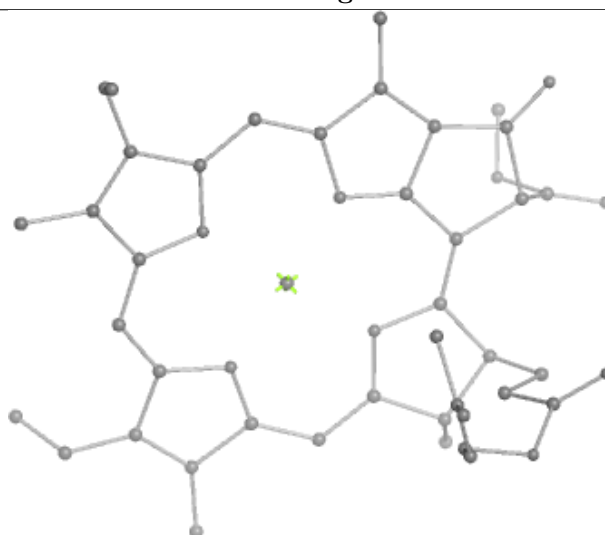
Bond lengths



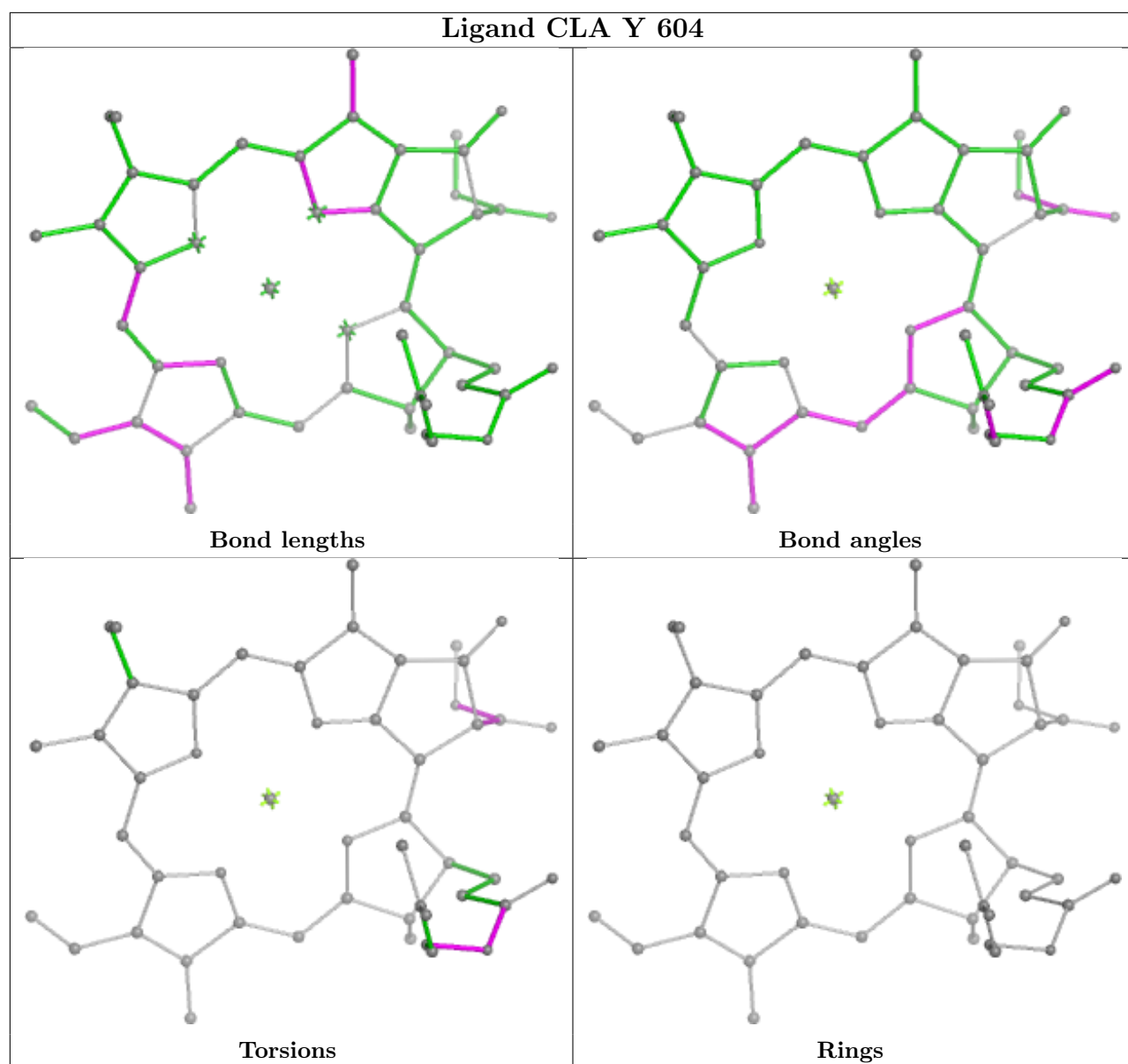
Bond angles

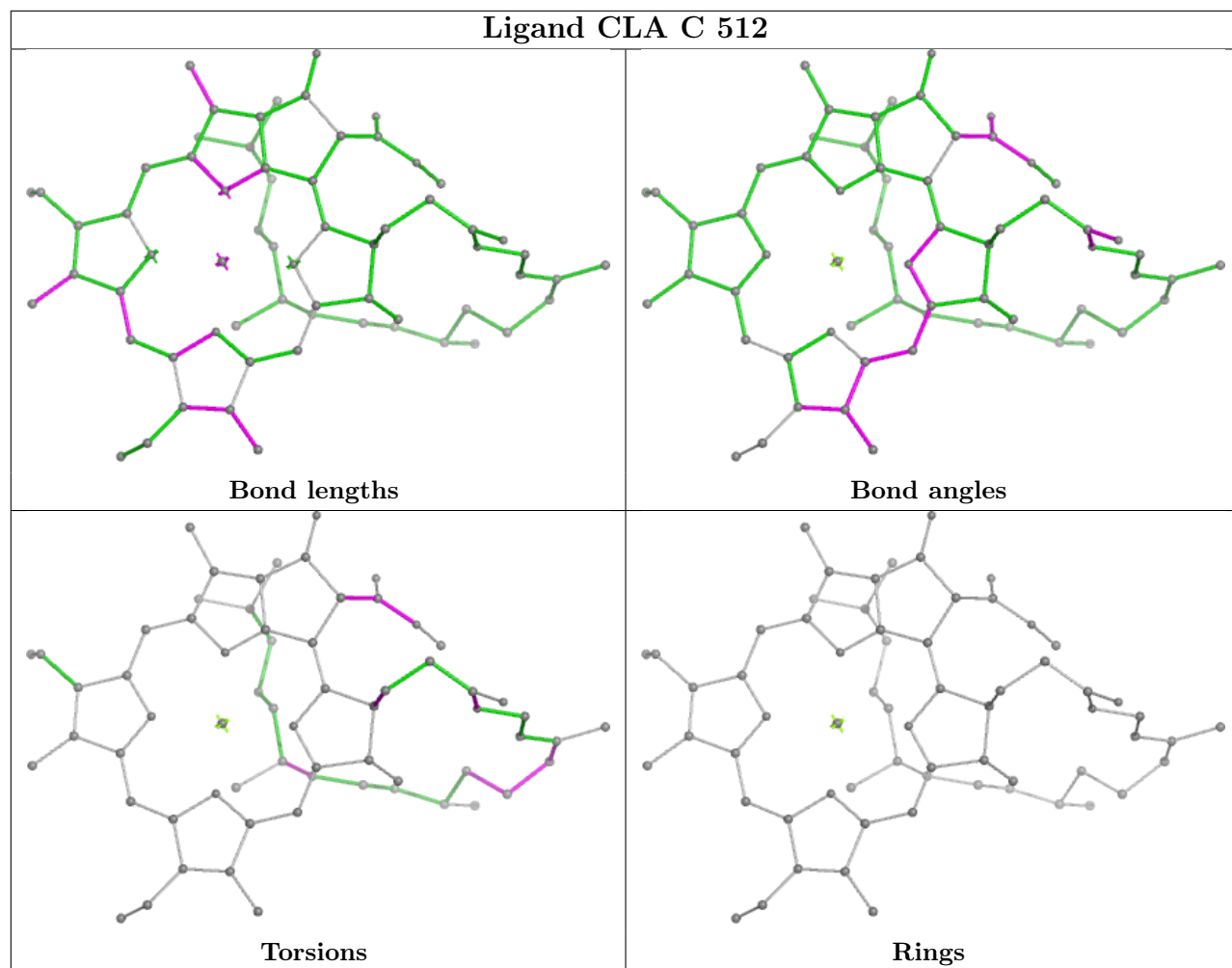


Torsions

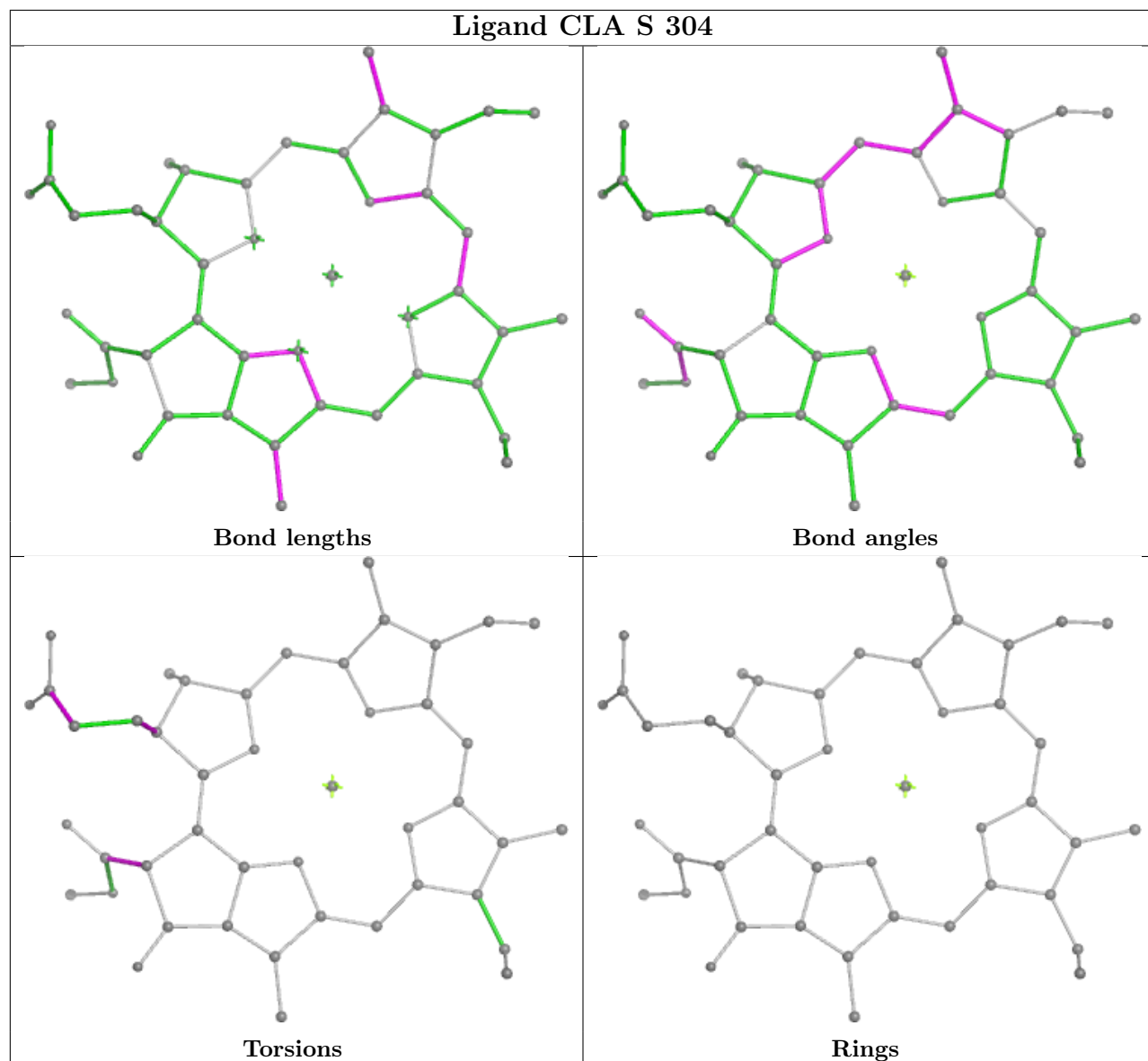


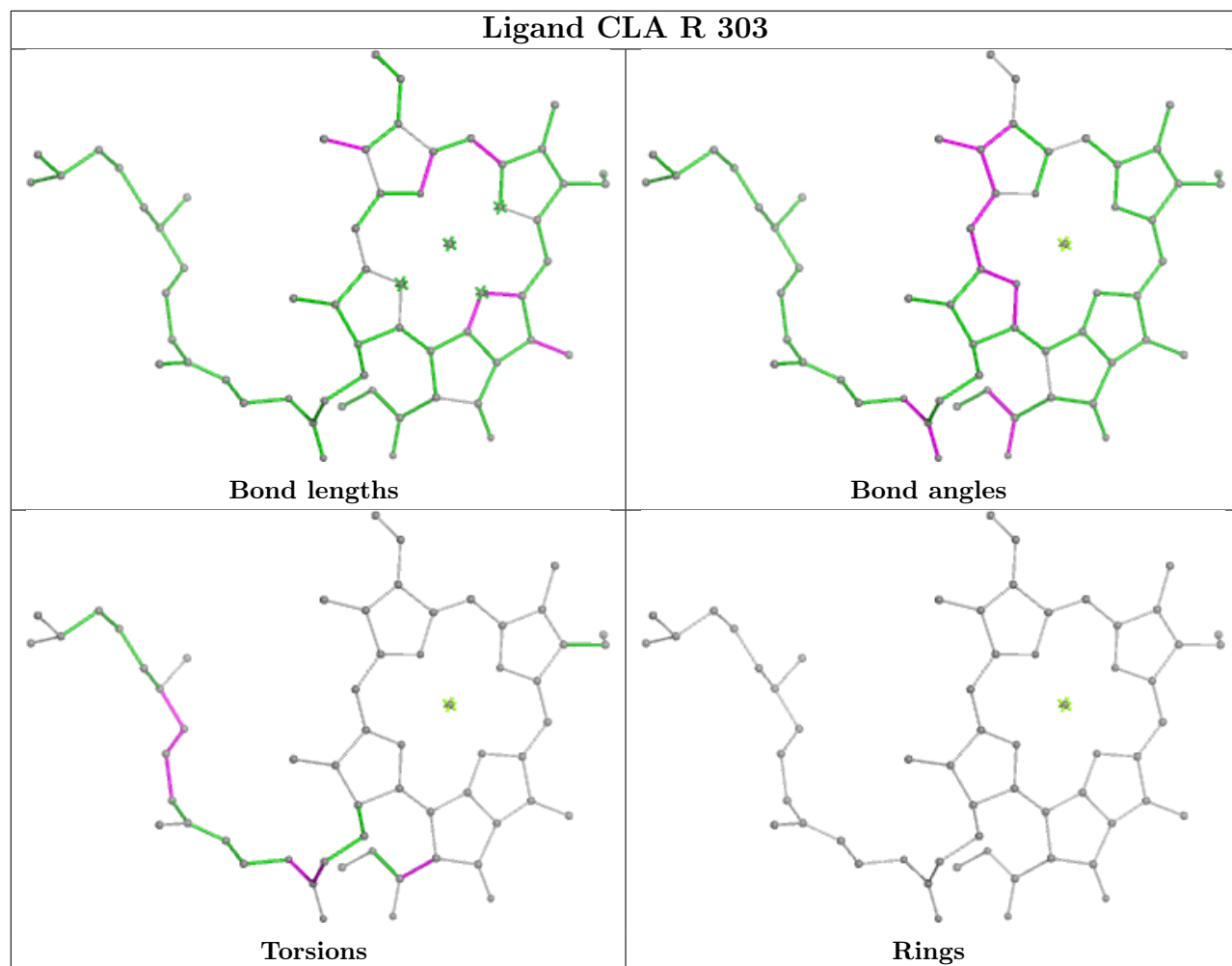
Rings



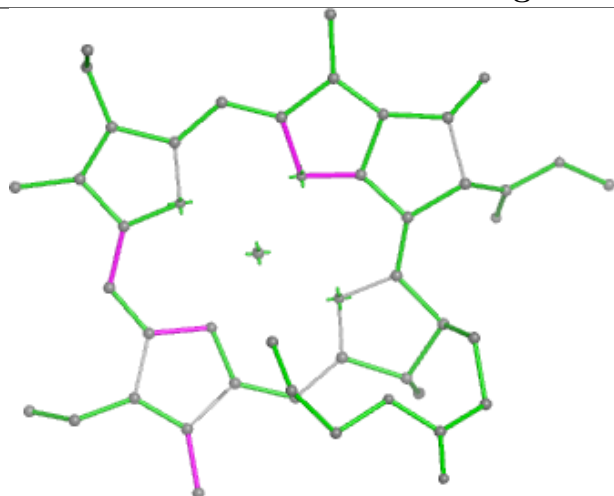


## Ligand CLA S 304

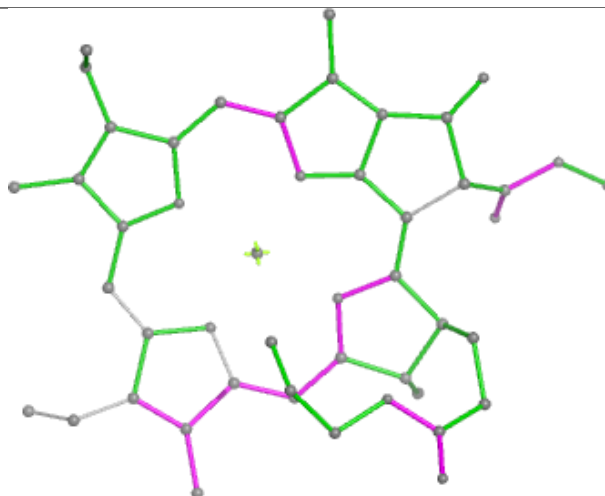




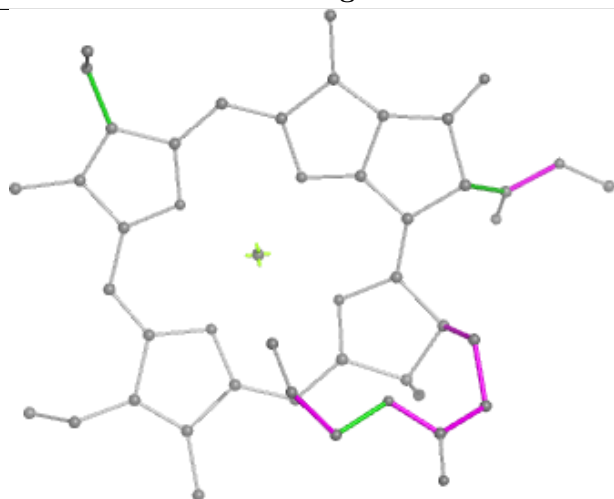
## Ligand CLA N 613



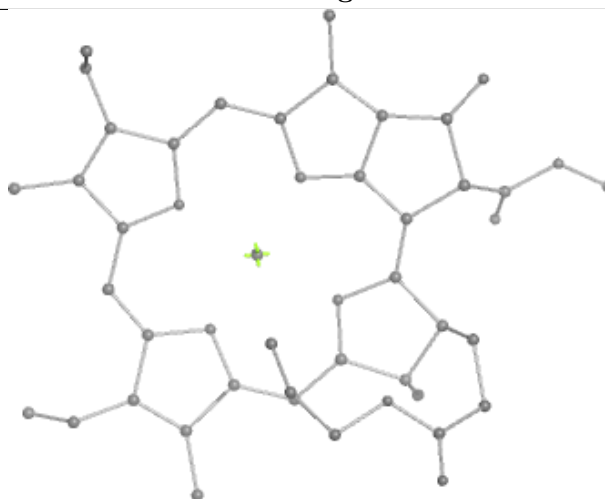
Bond lengths



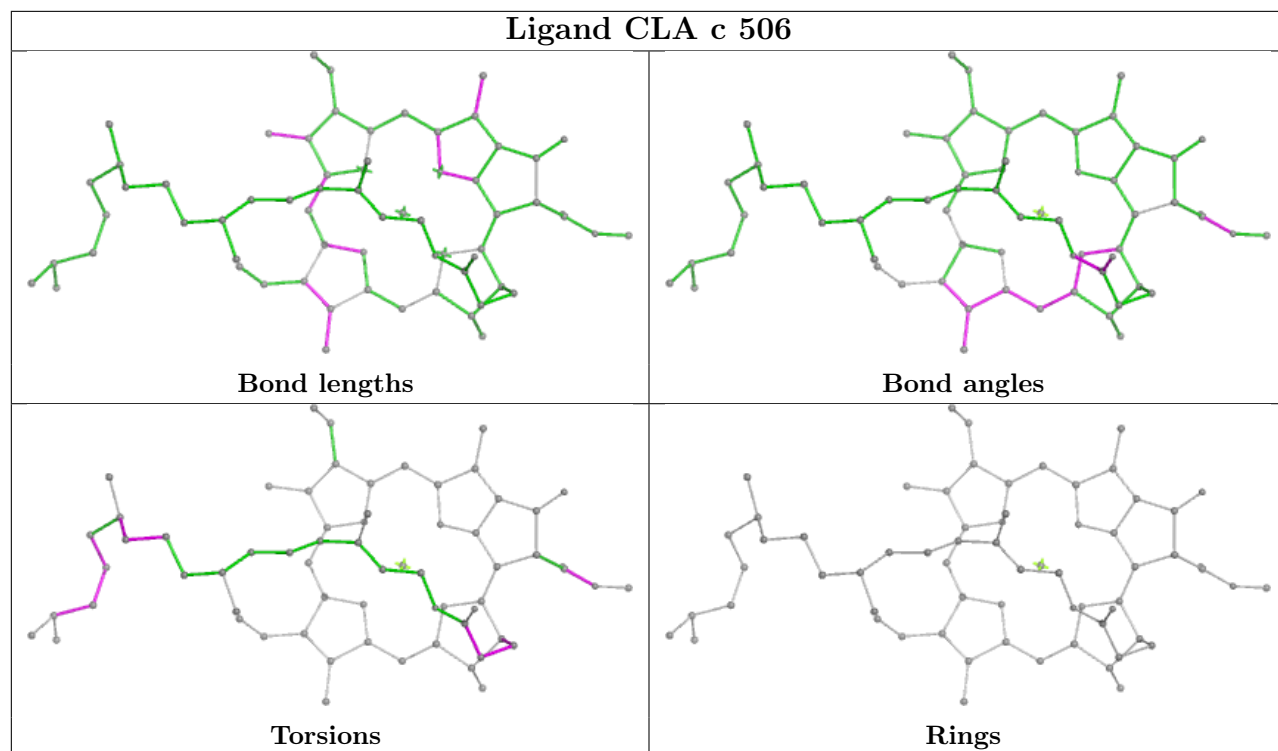
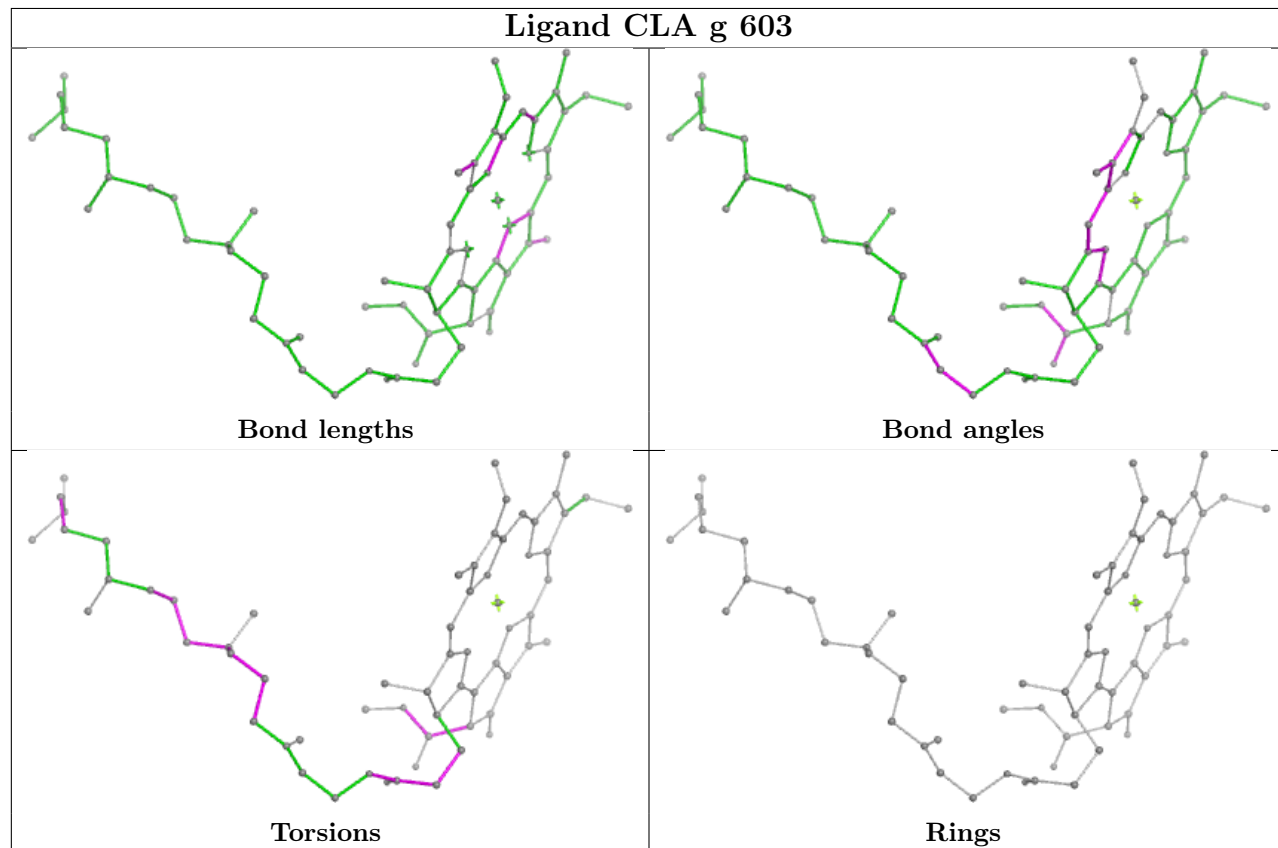
Bond angles

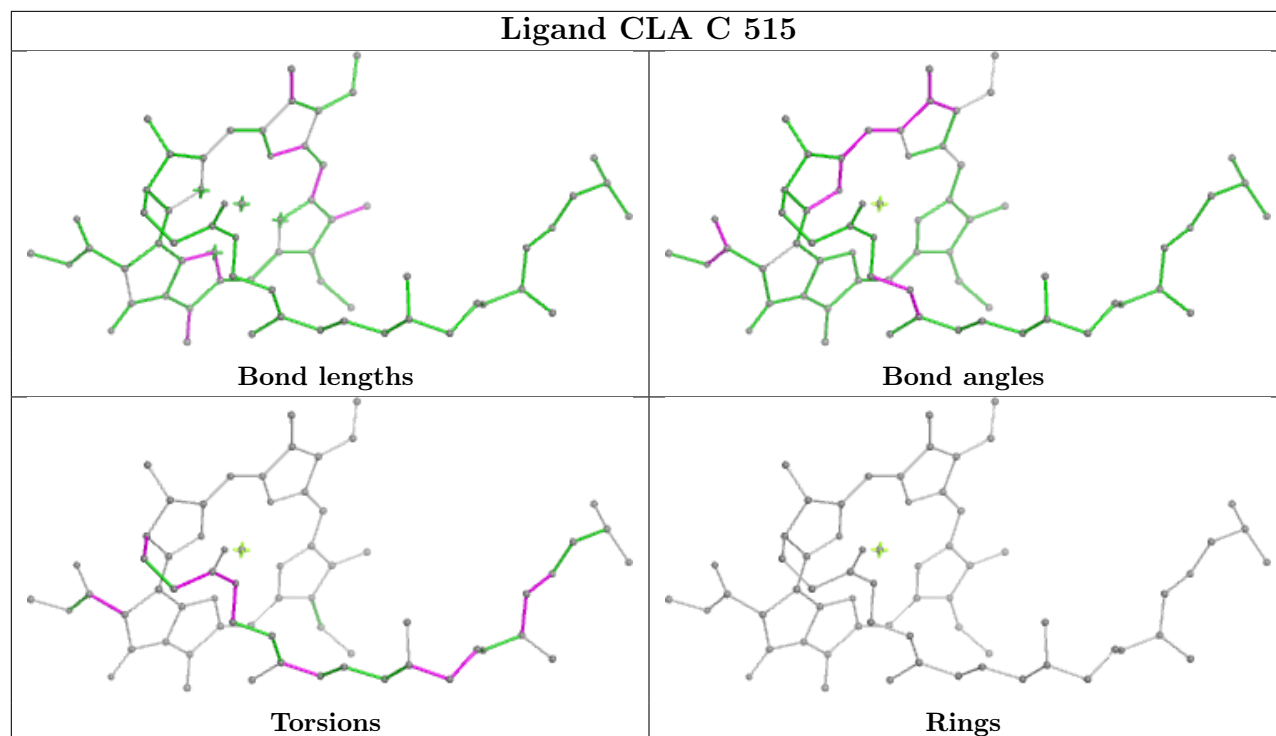
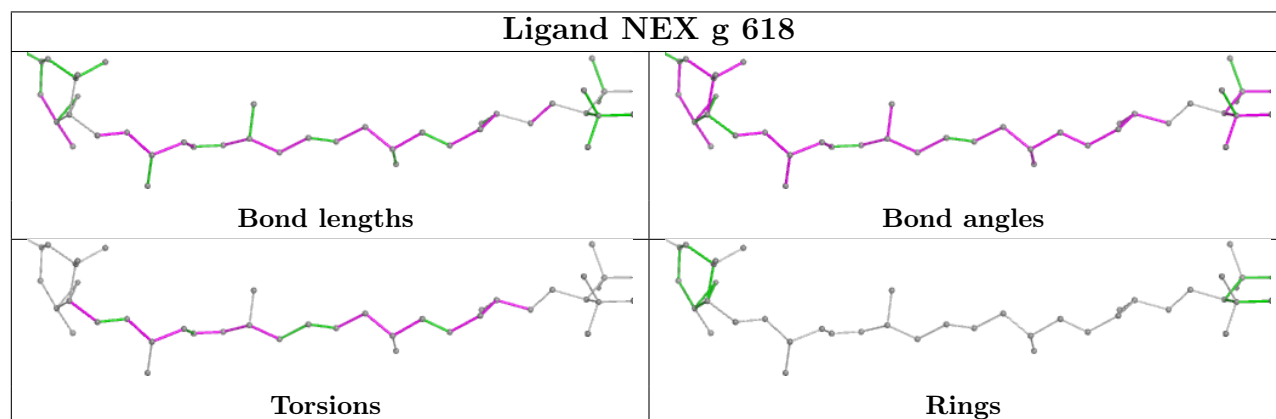


Torsions



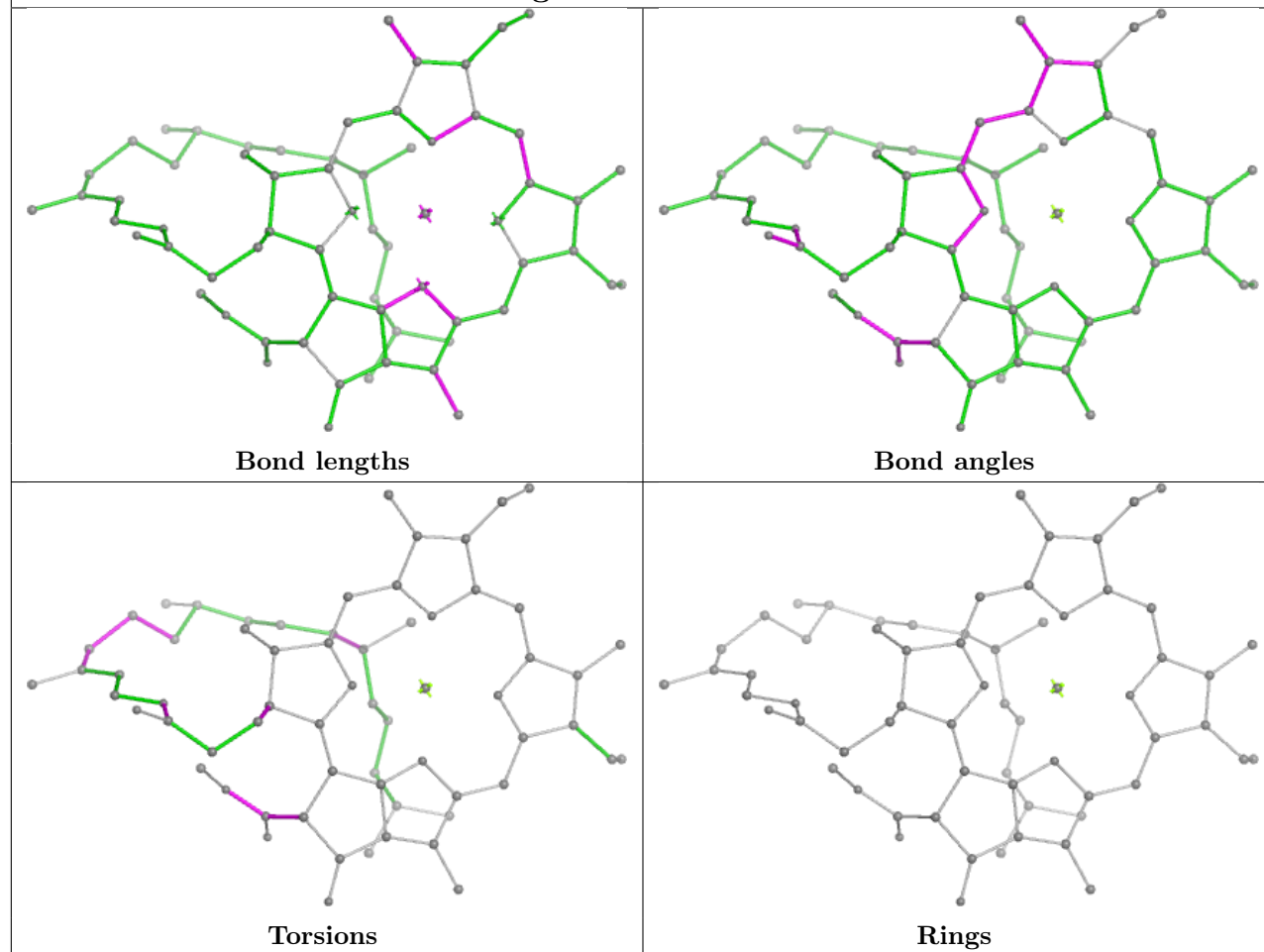
Rings

**Ligand CLA c 506****Ligand CLA g 603**

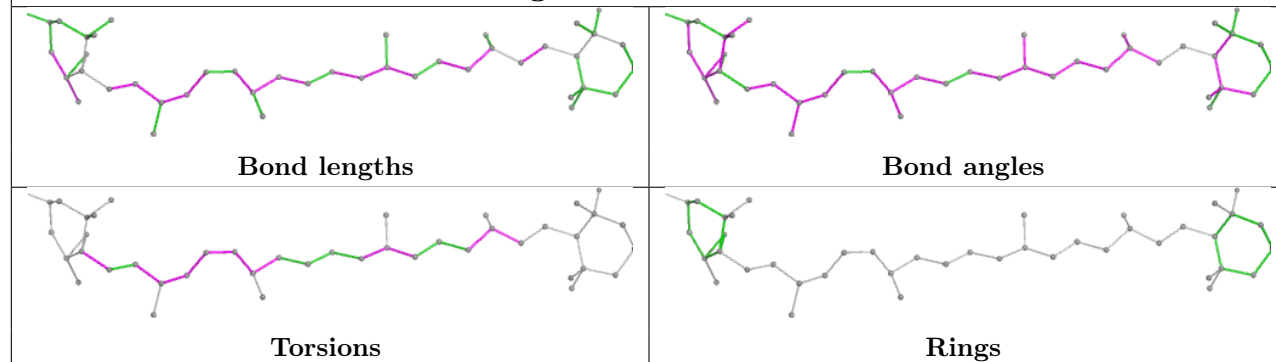
**Ligand CLA C 515****Ligand NEX g 618**

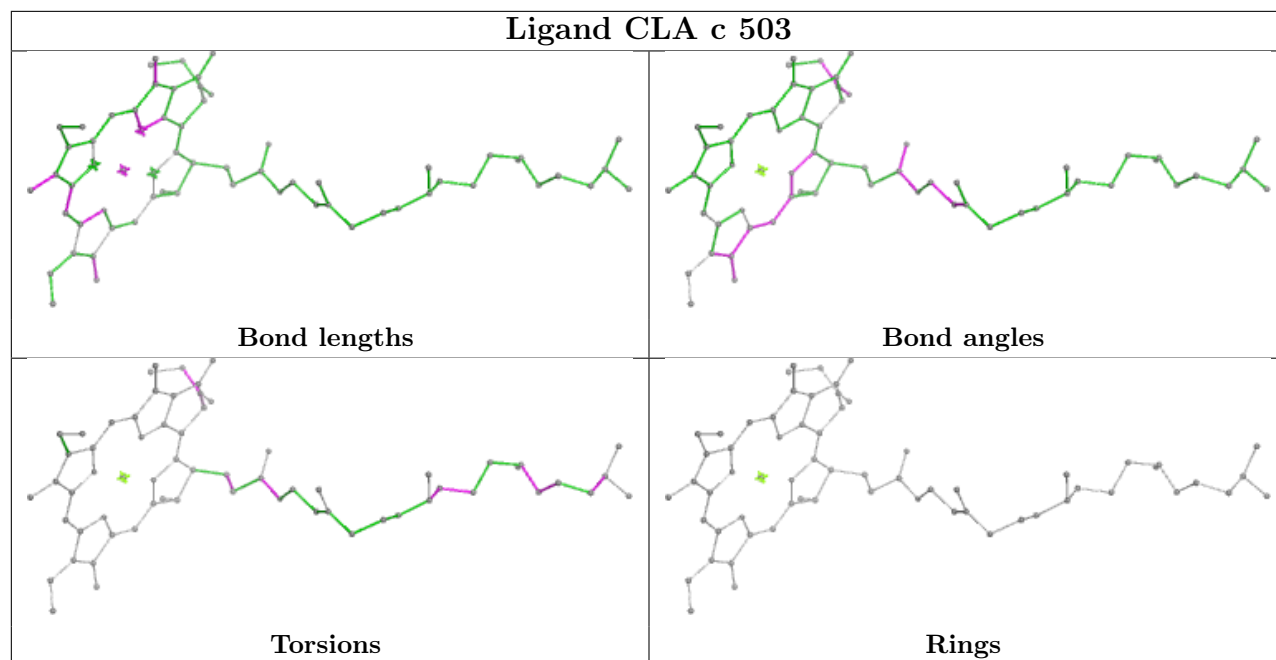
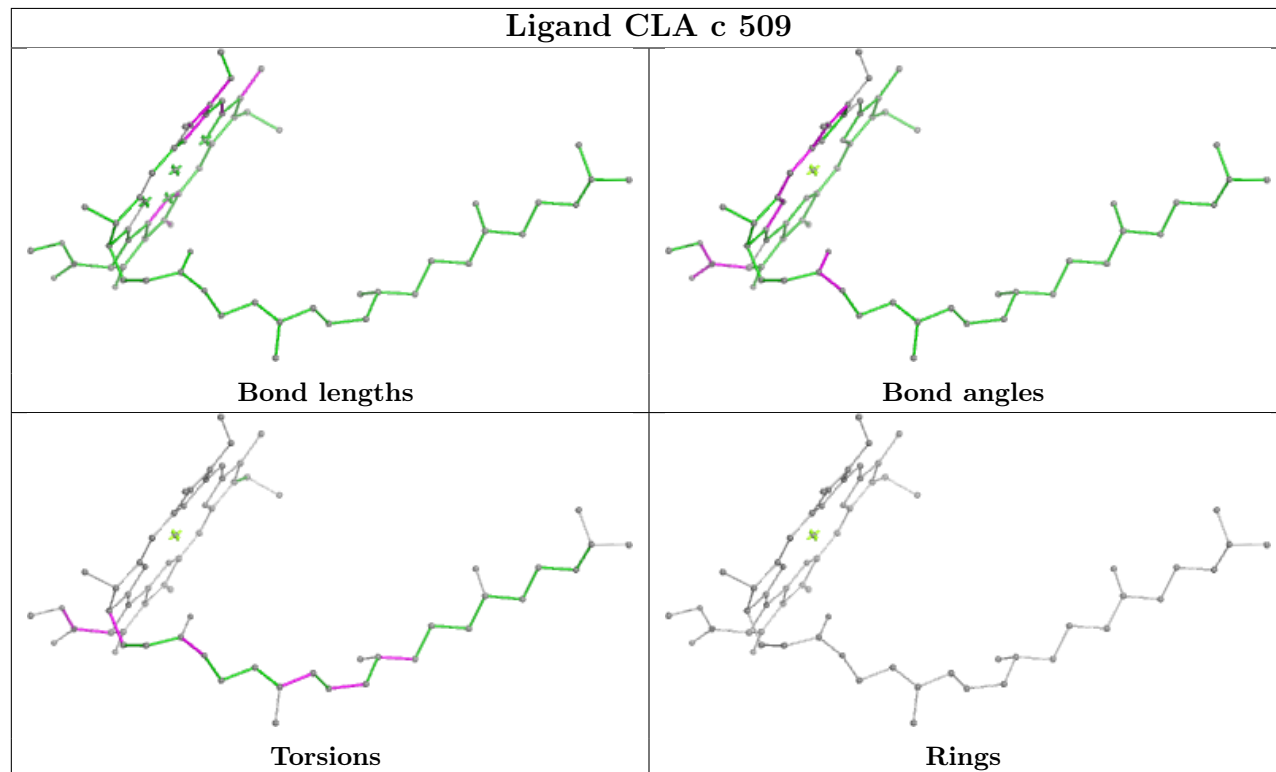


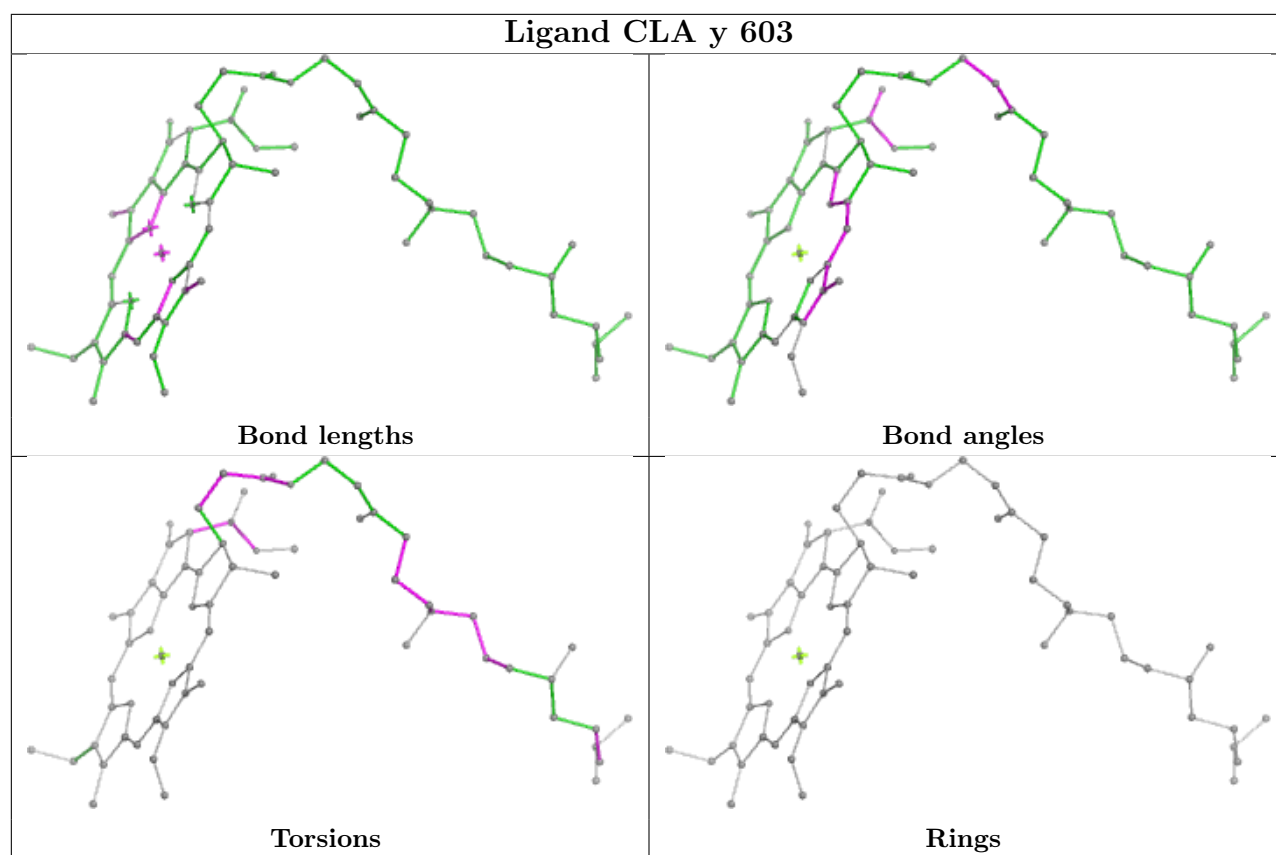
## Ligand CLA c 511

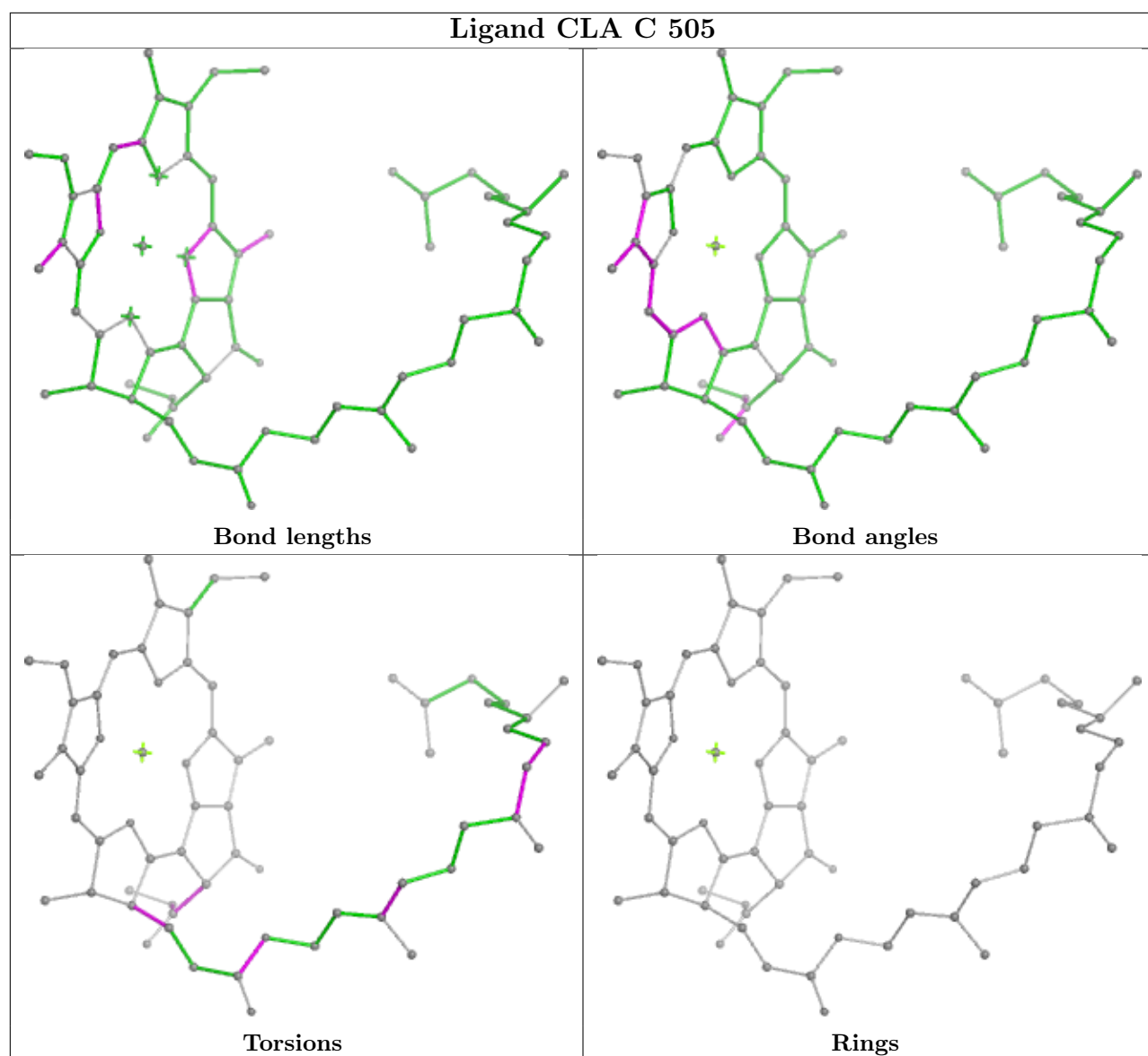


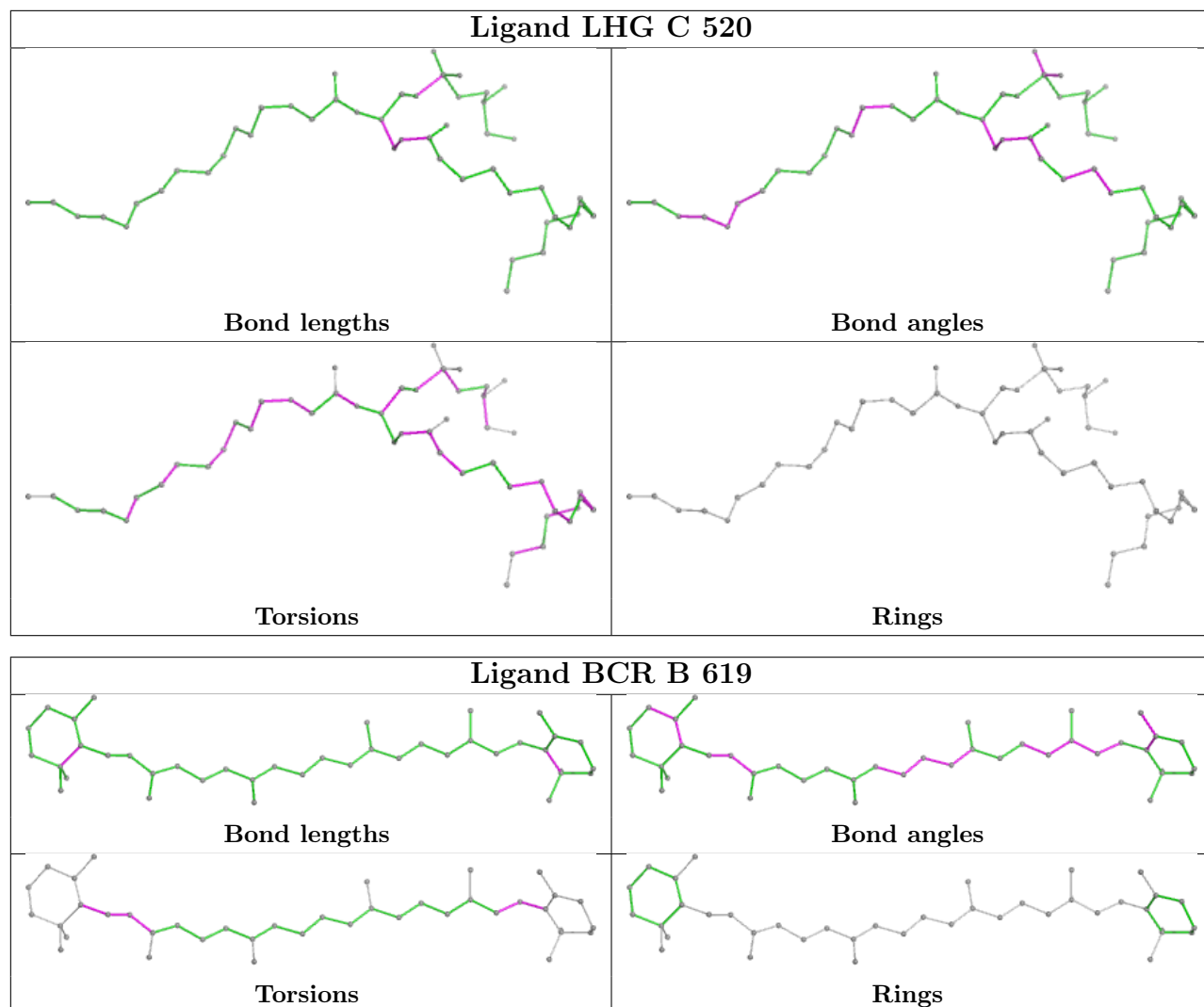
## Ligand NEX N 617



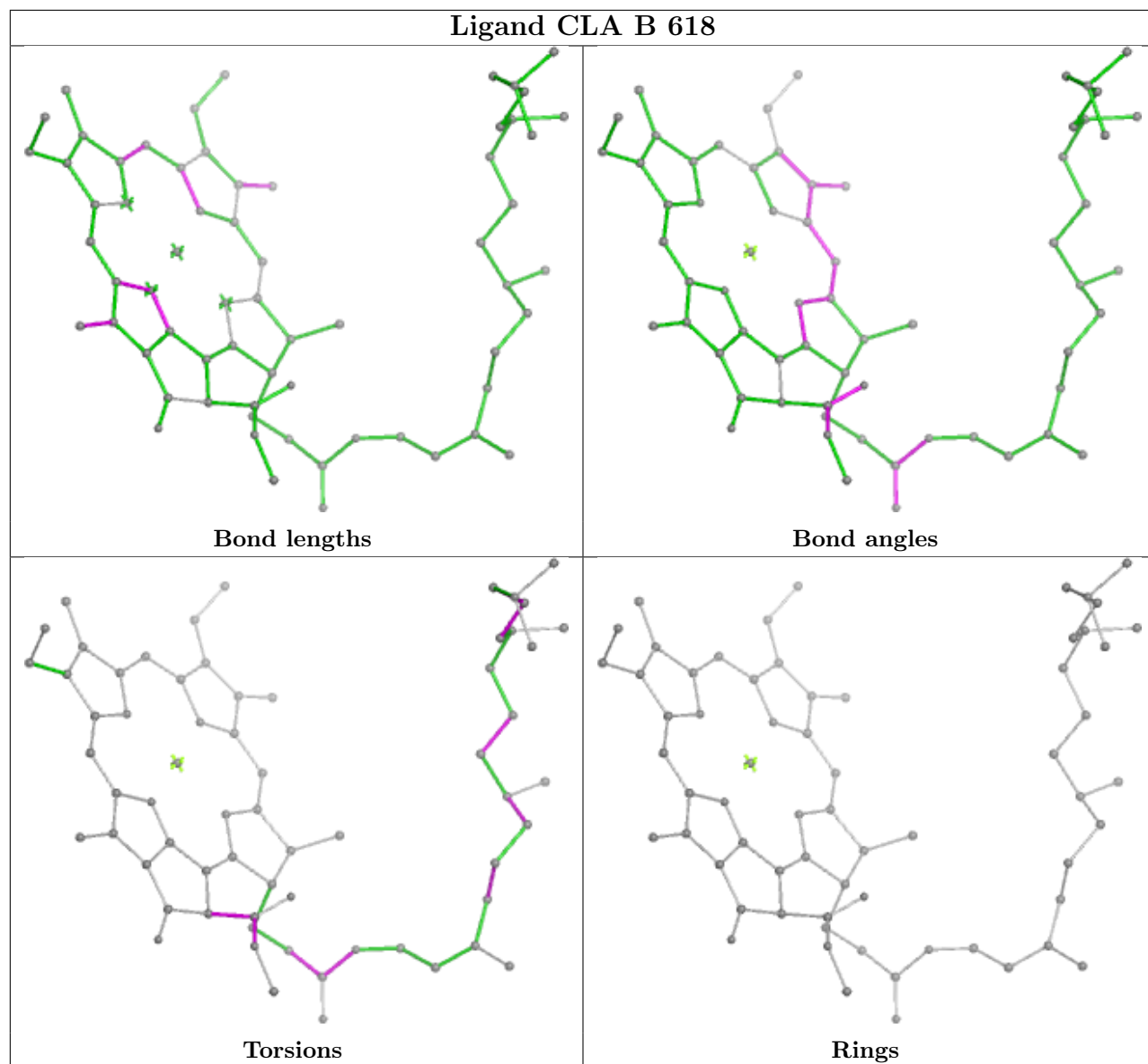
**Ligand CLA c 503****Ligand CLA c 509**

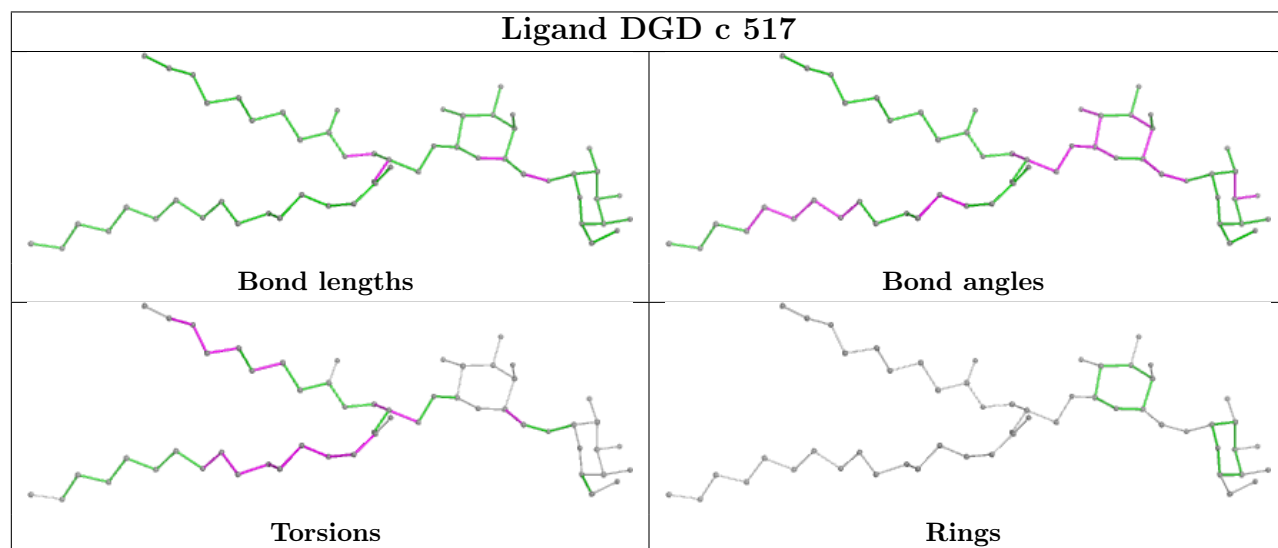
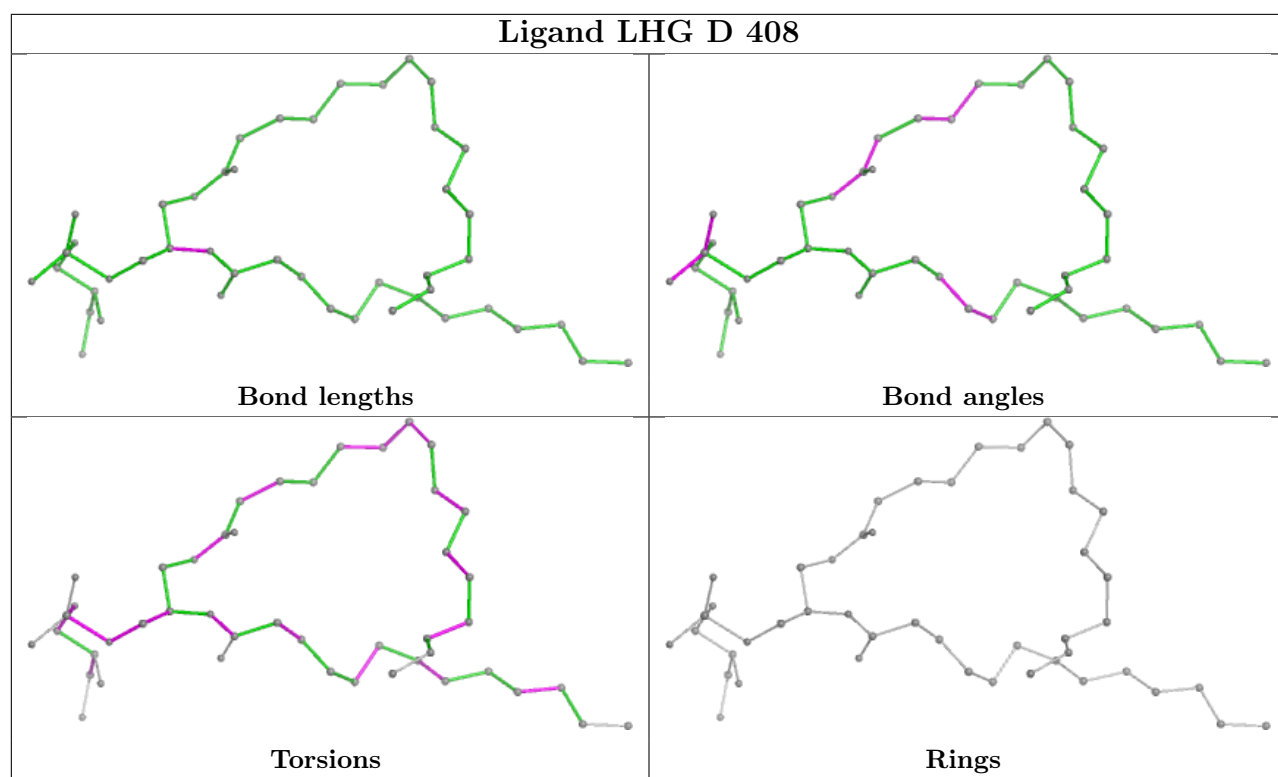




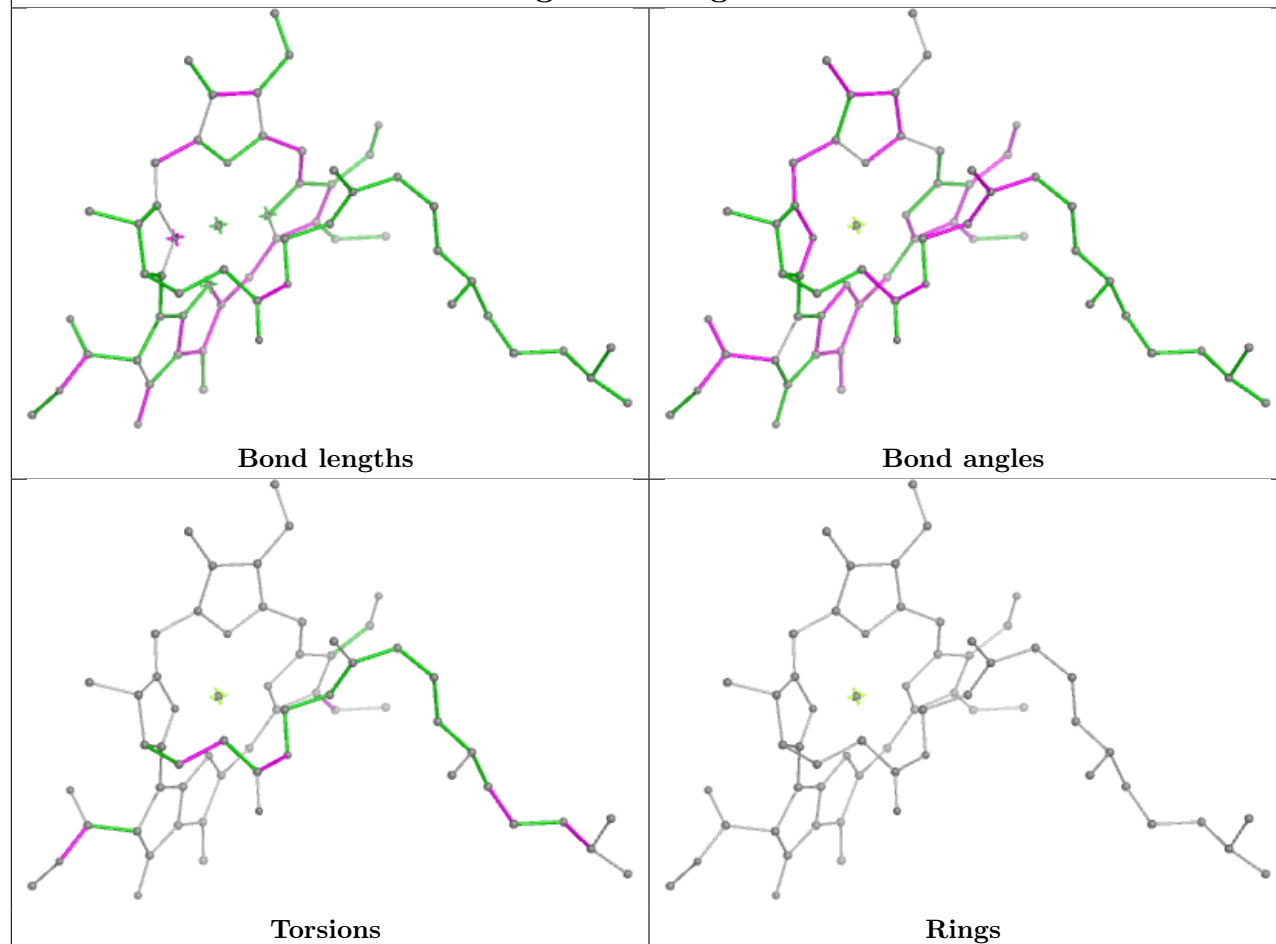


## Ligand CLA B 618

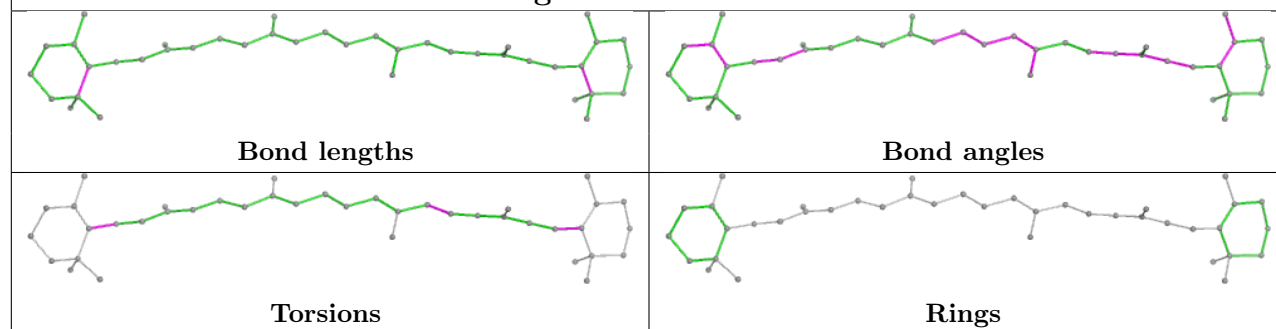




## Ligand CHL g 609

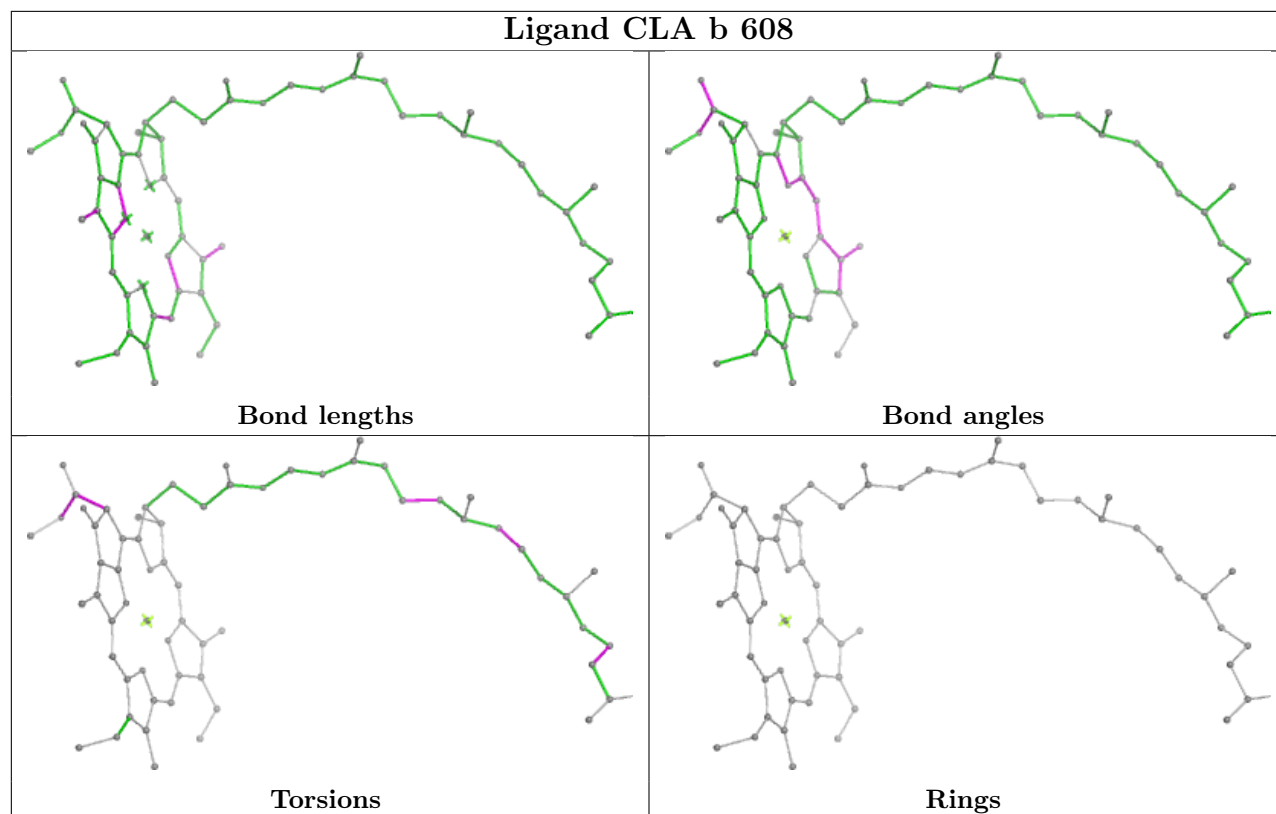


## Ligand BCR k 102

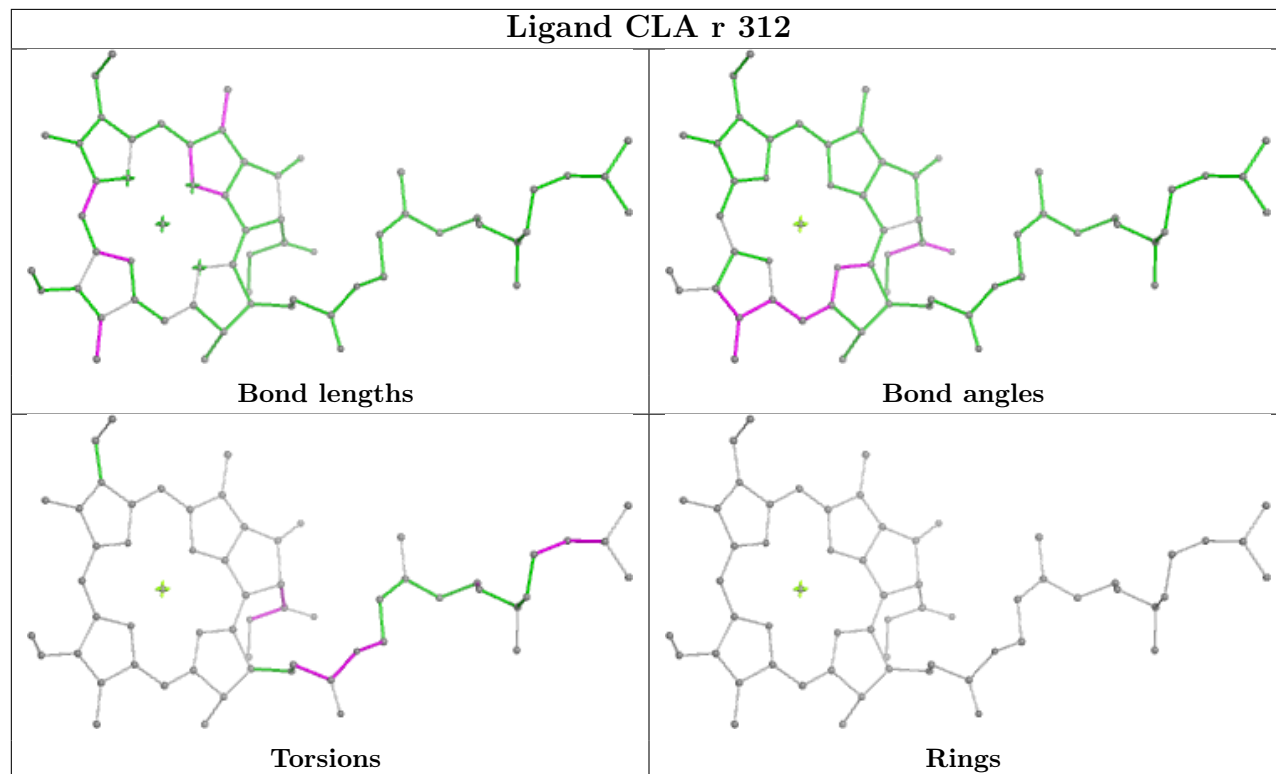


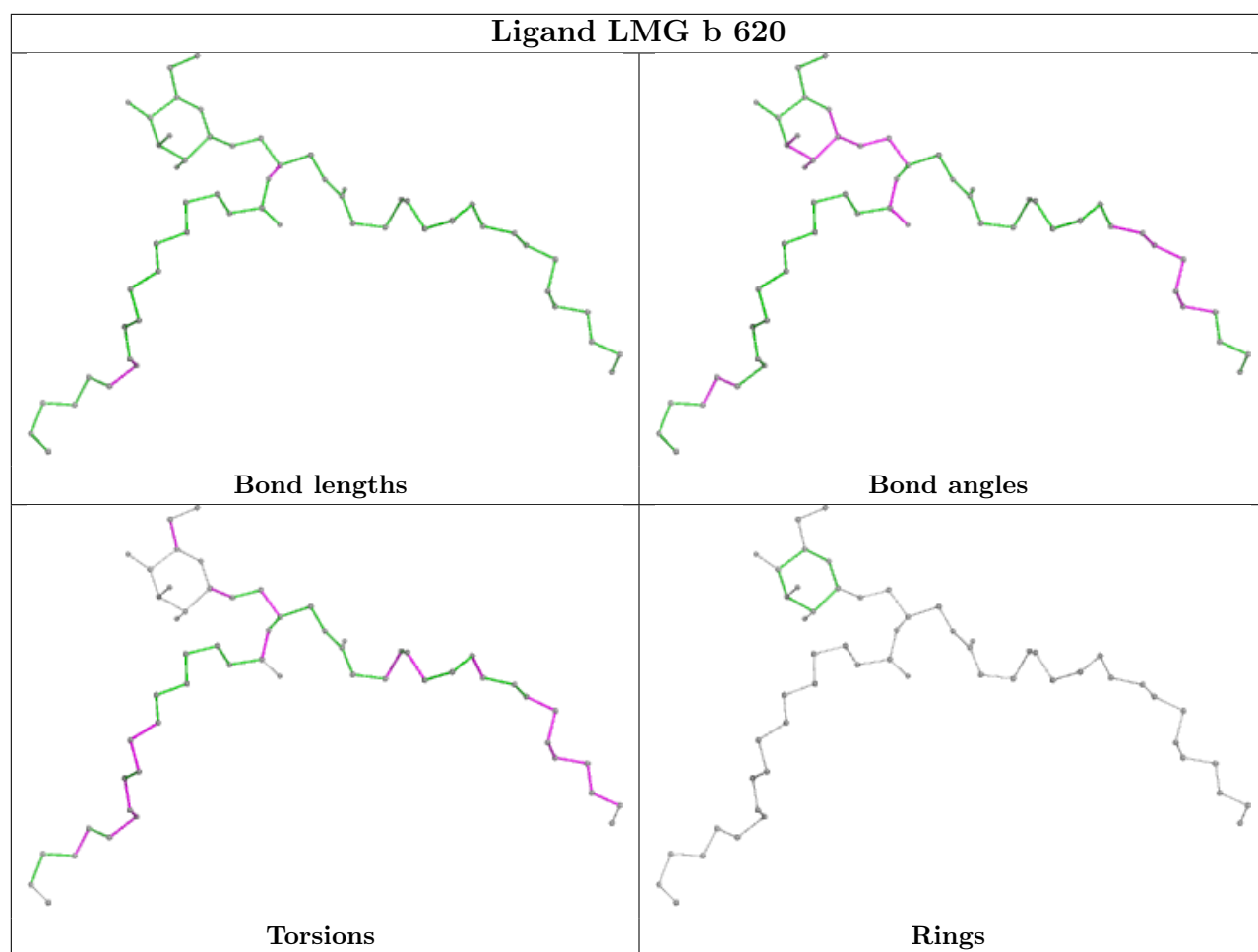


## Ligand CLA b 608

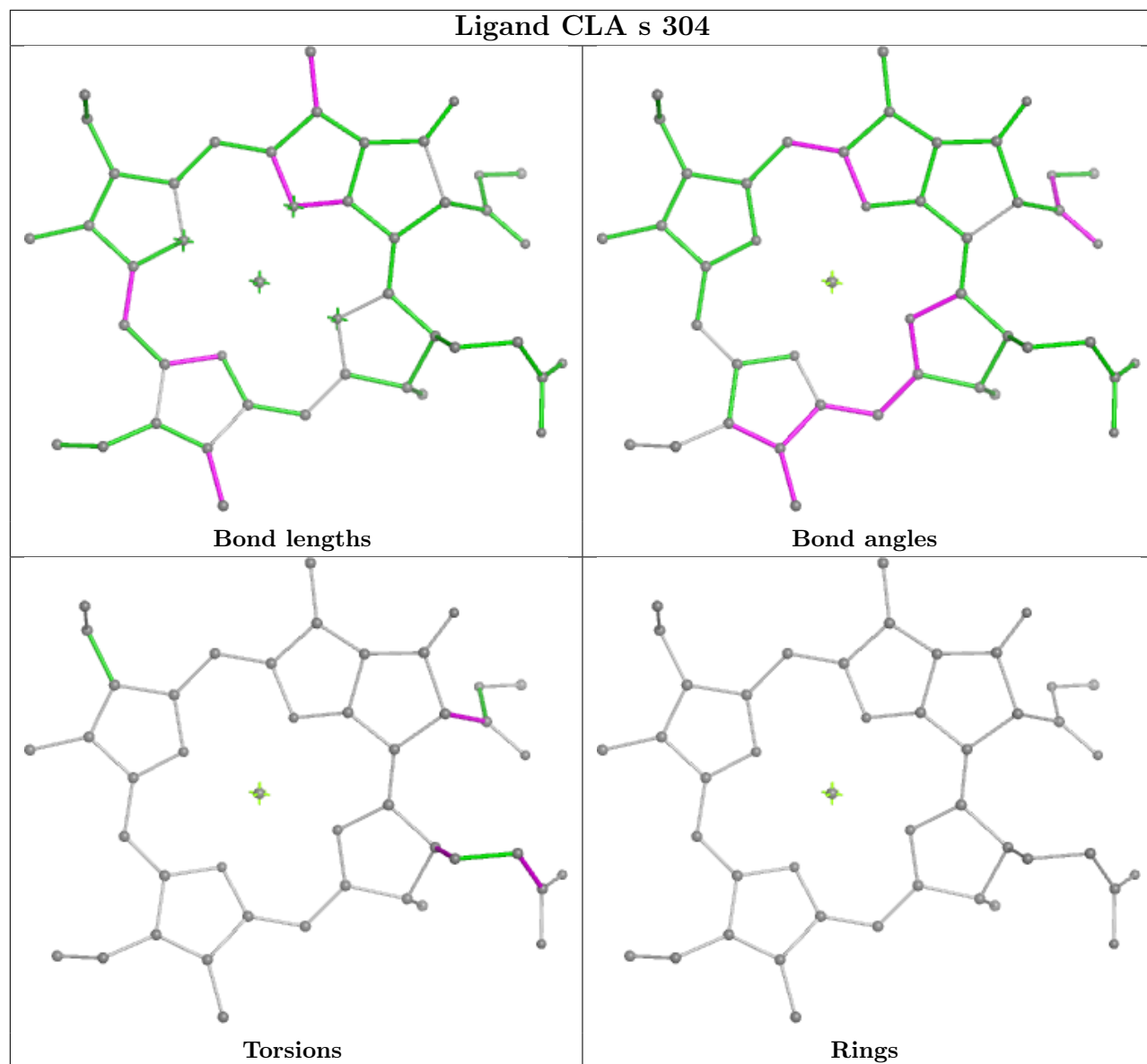


## Ligand CLA r 312

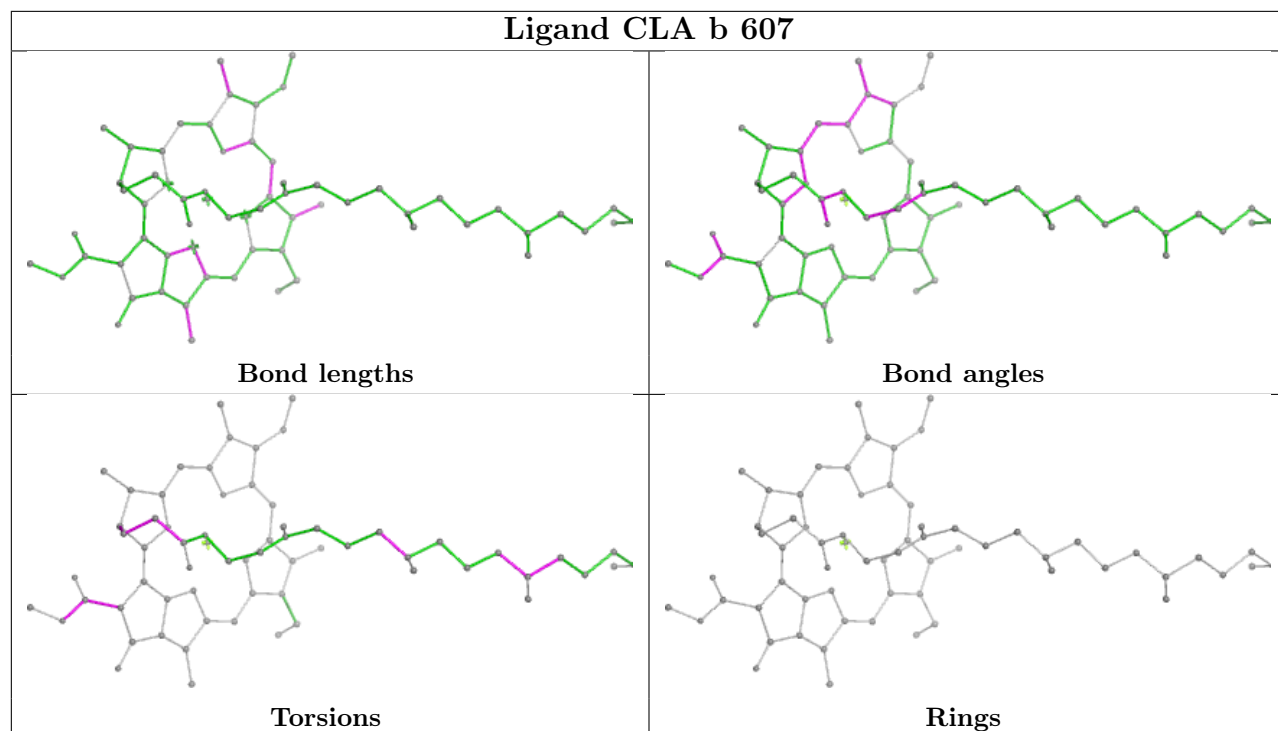




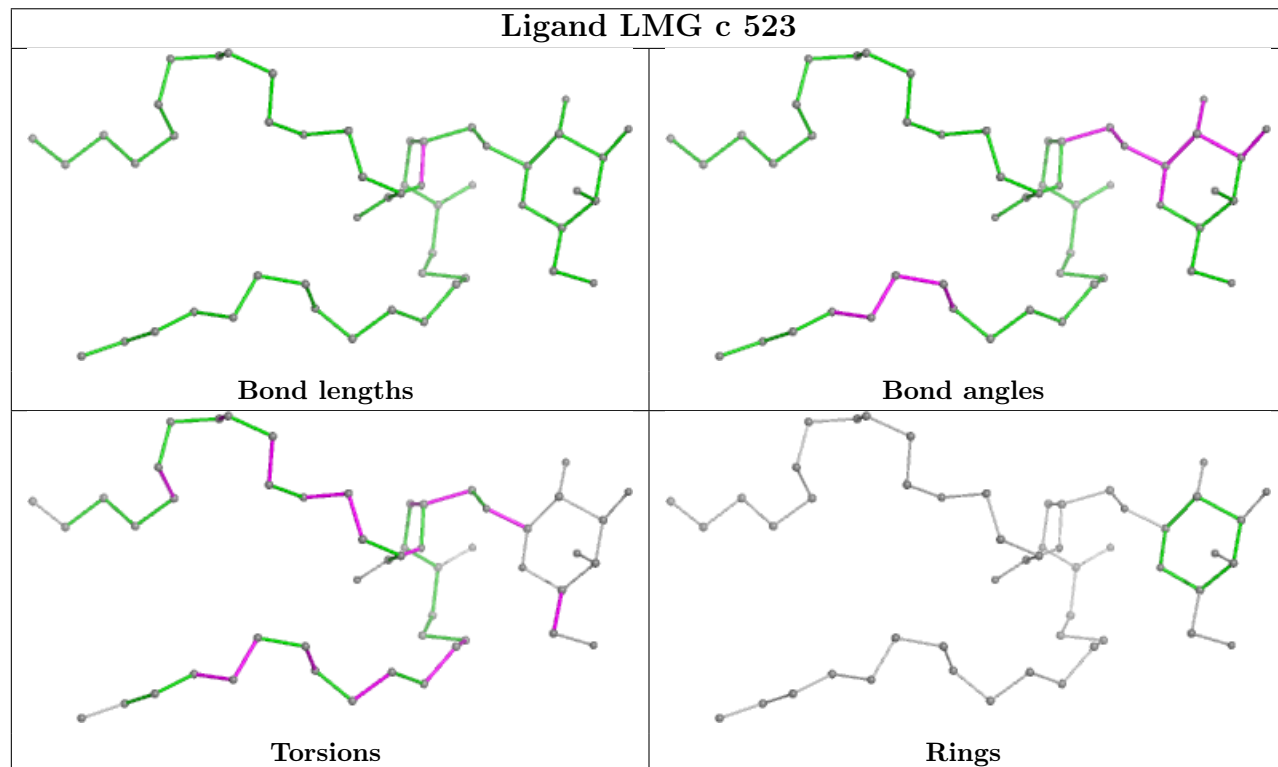
## Ligand CLA s 304



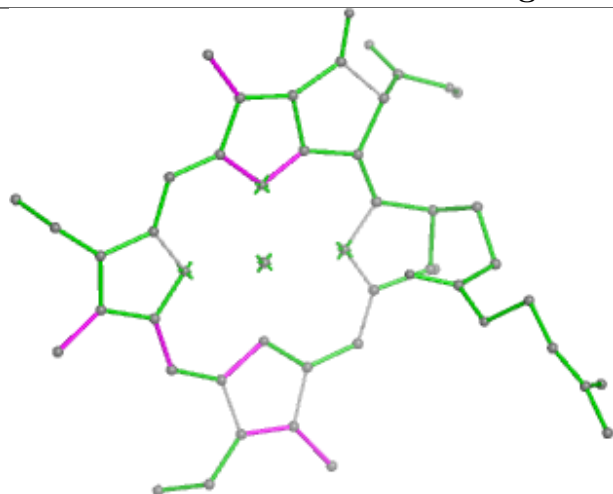
## Ligand CLA b 607



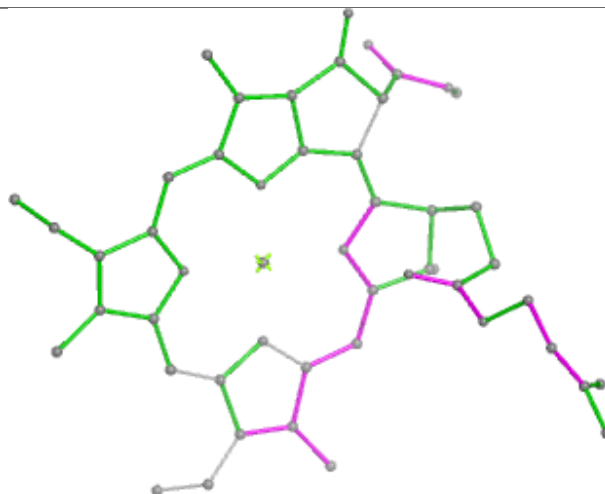
## Ligand LMG c 523



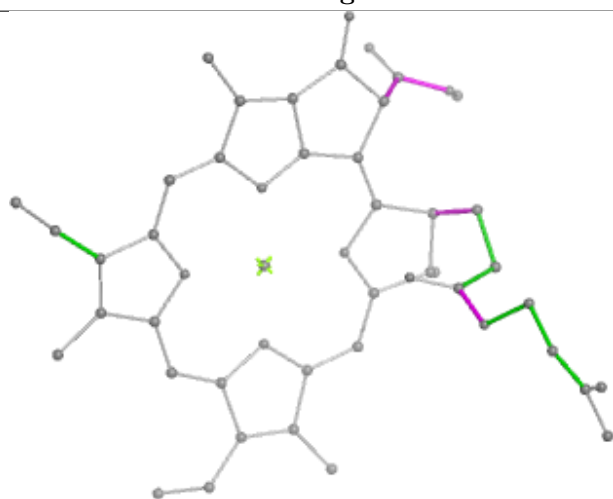
## Ligand CLA a 406



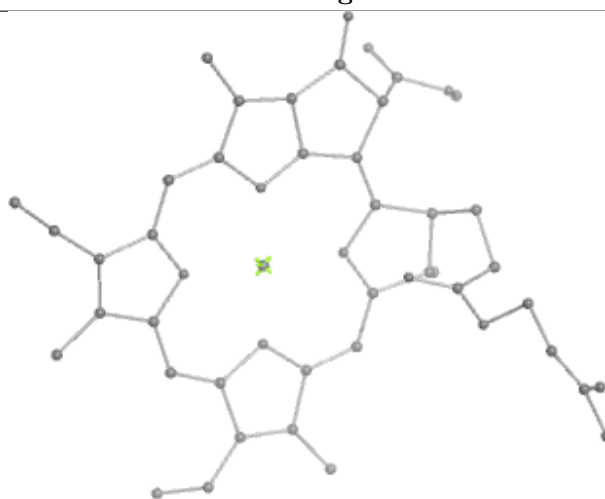
Bond lengths



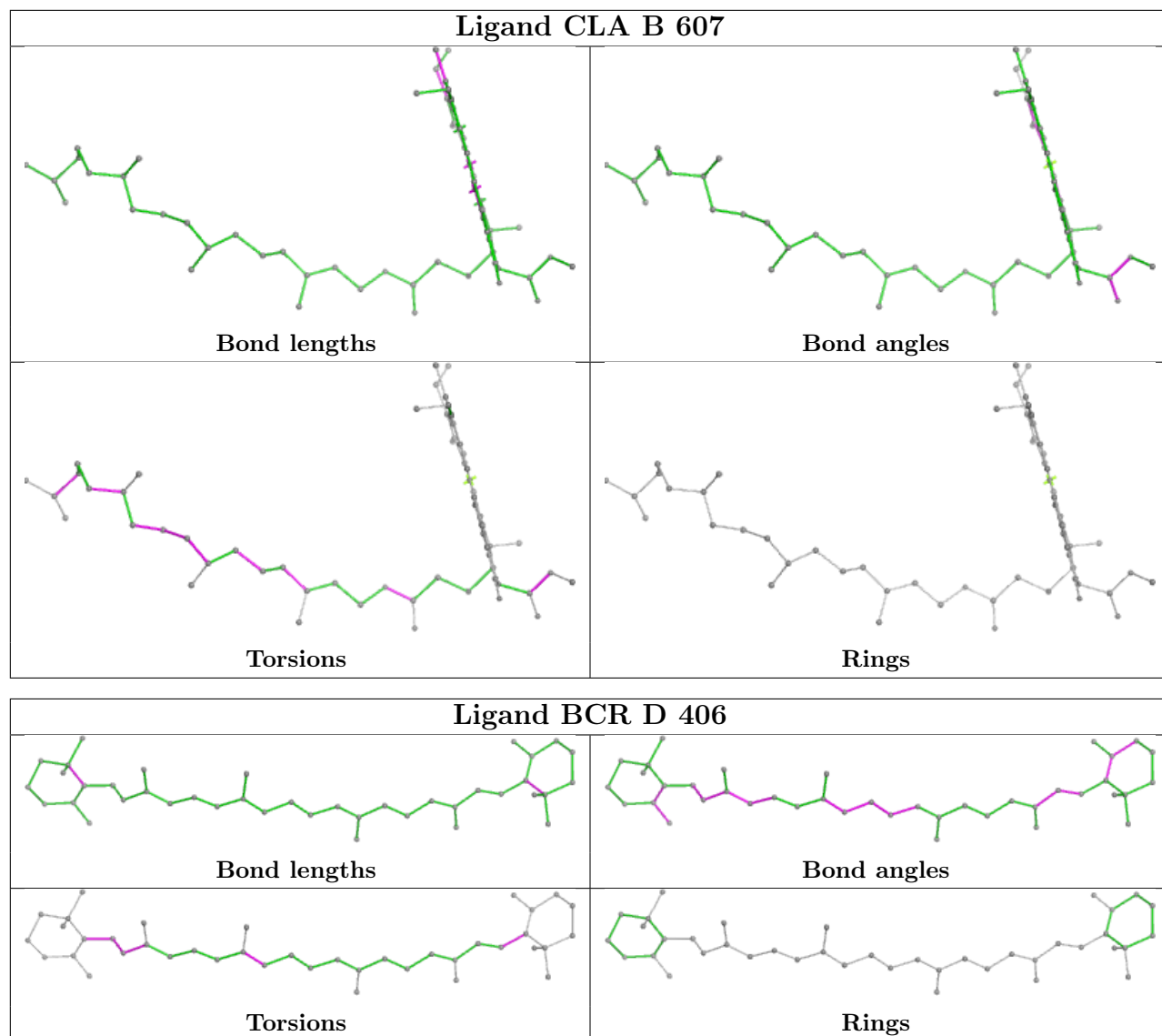
Bond angles

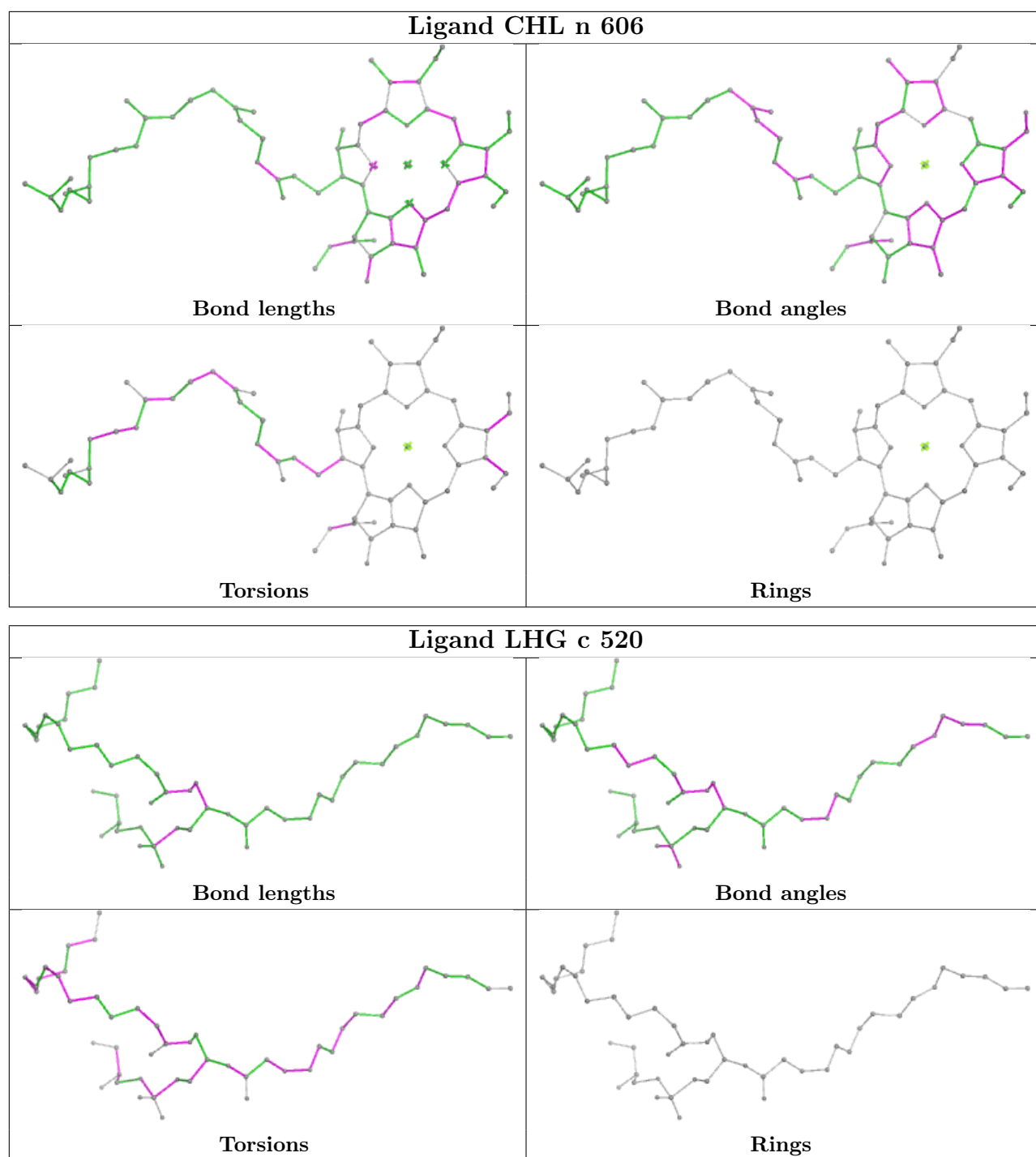


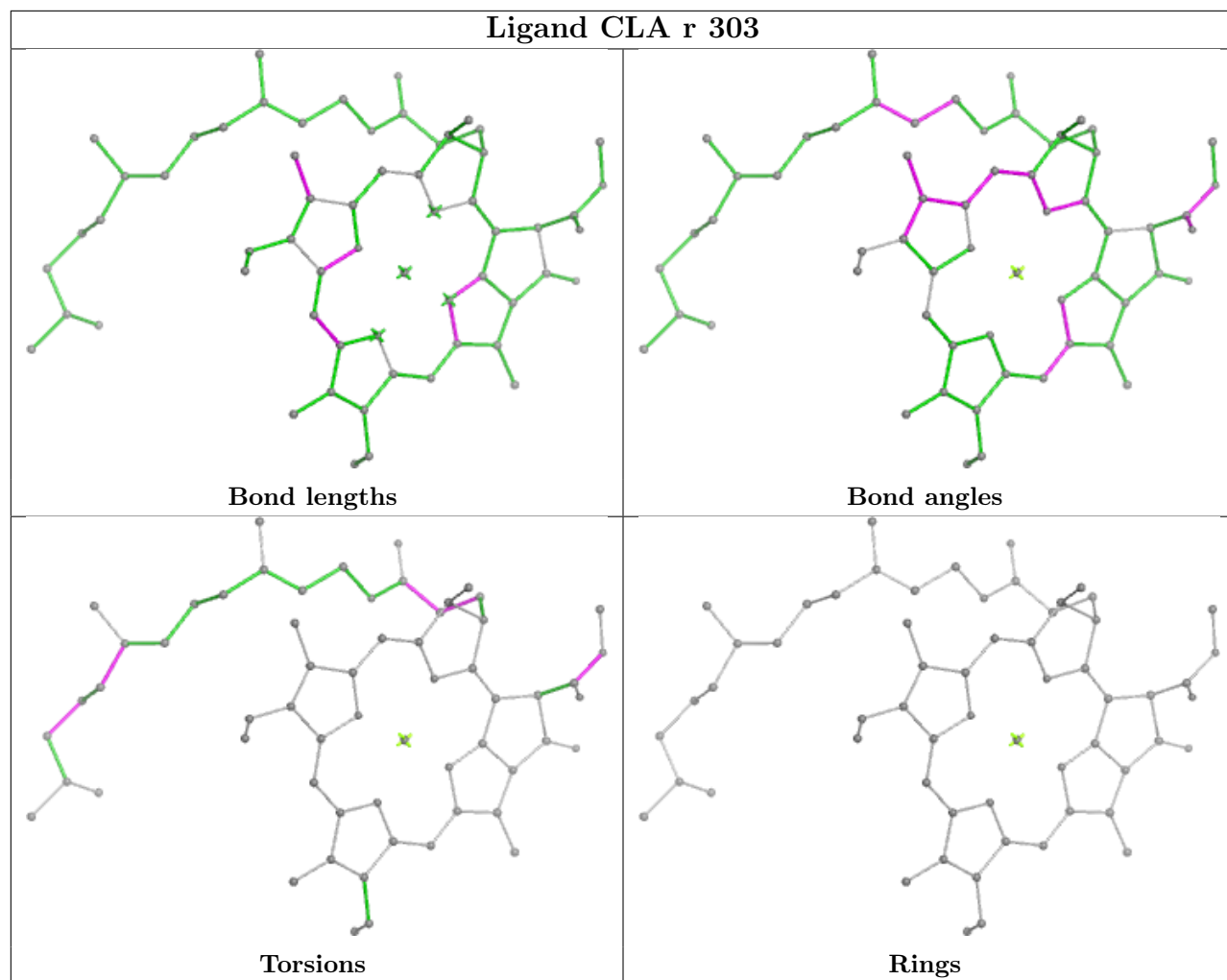
Torsions



Rings

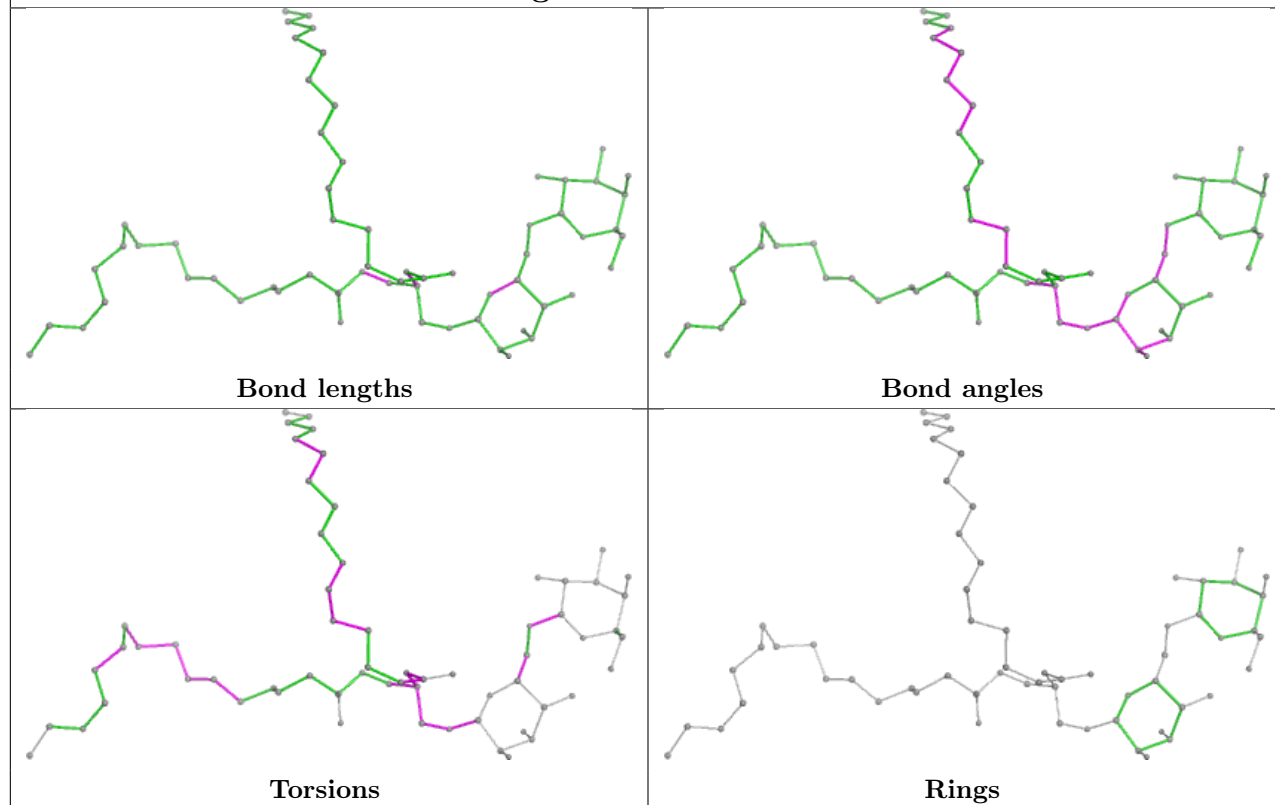




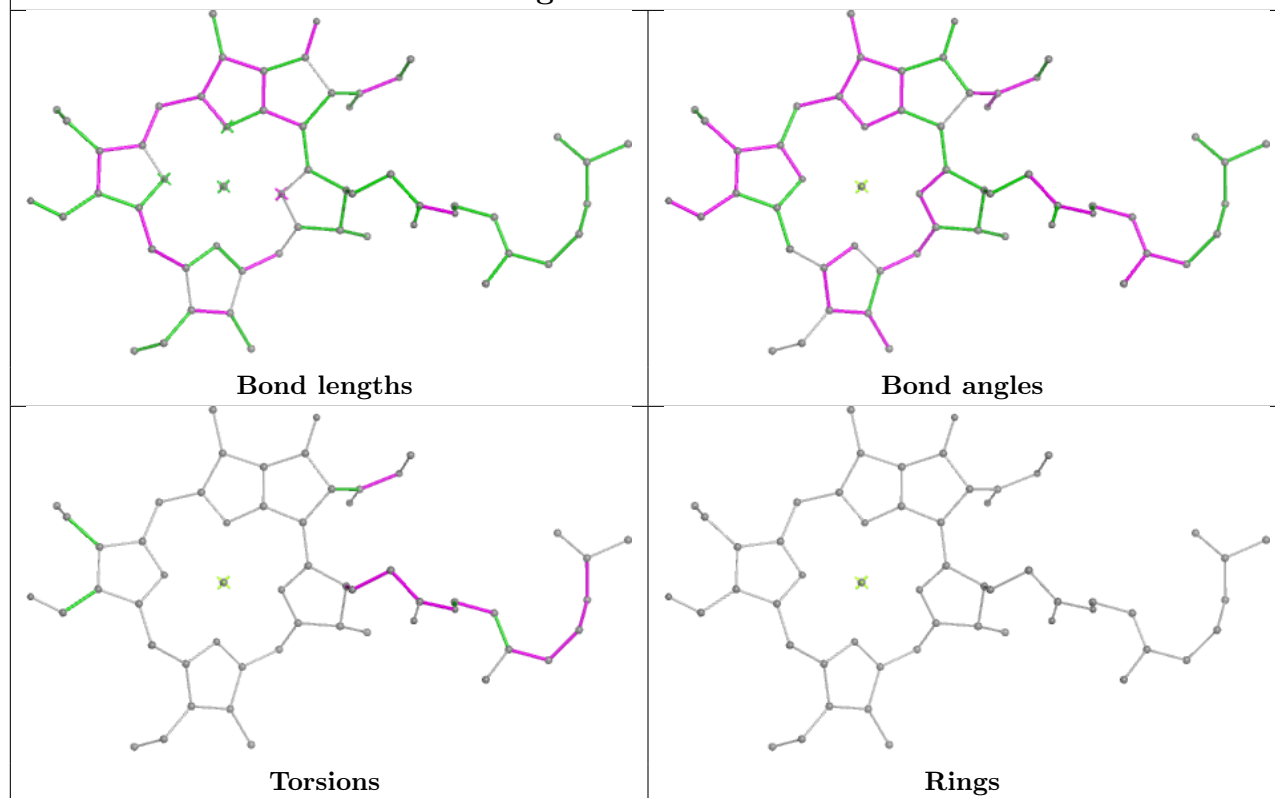


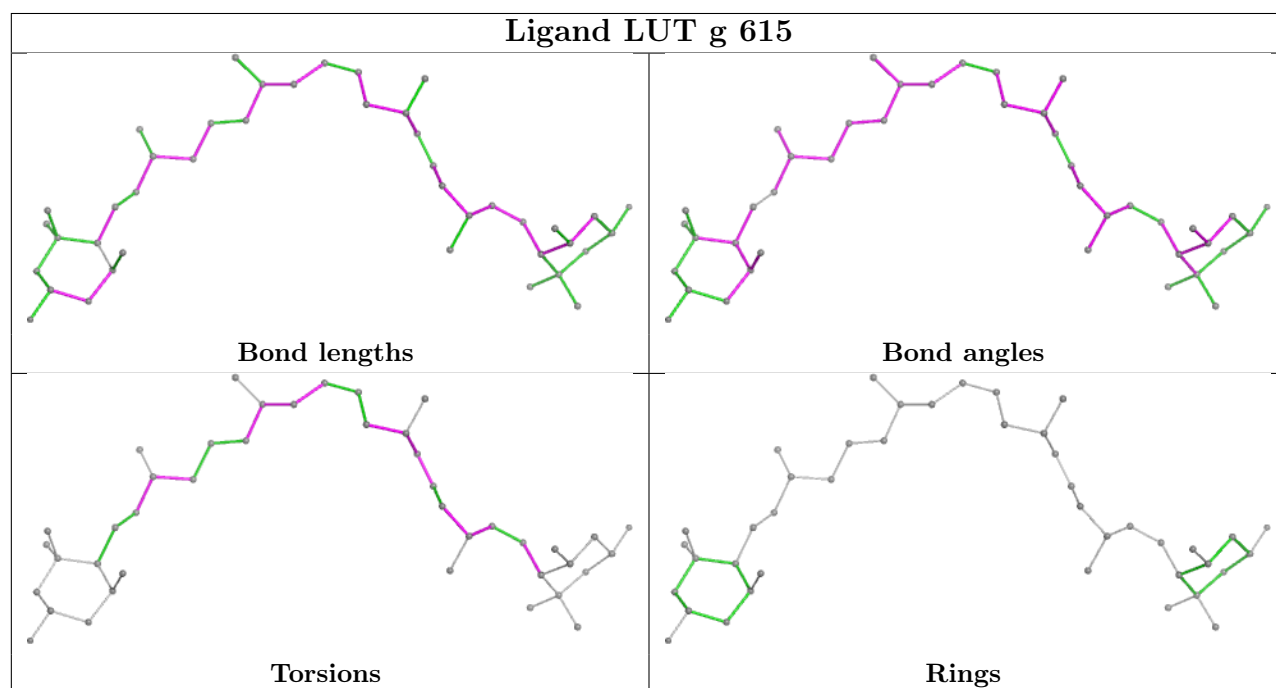
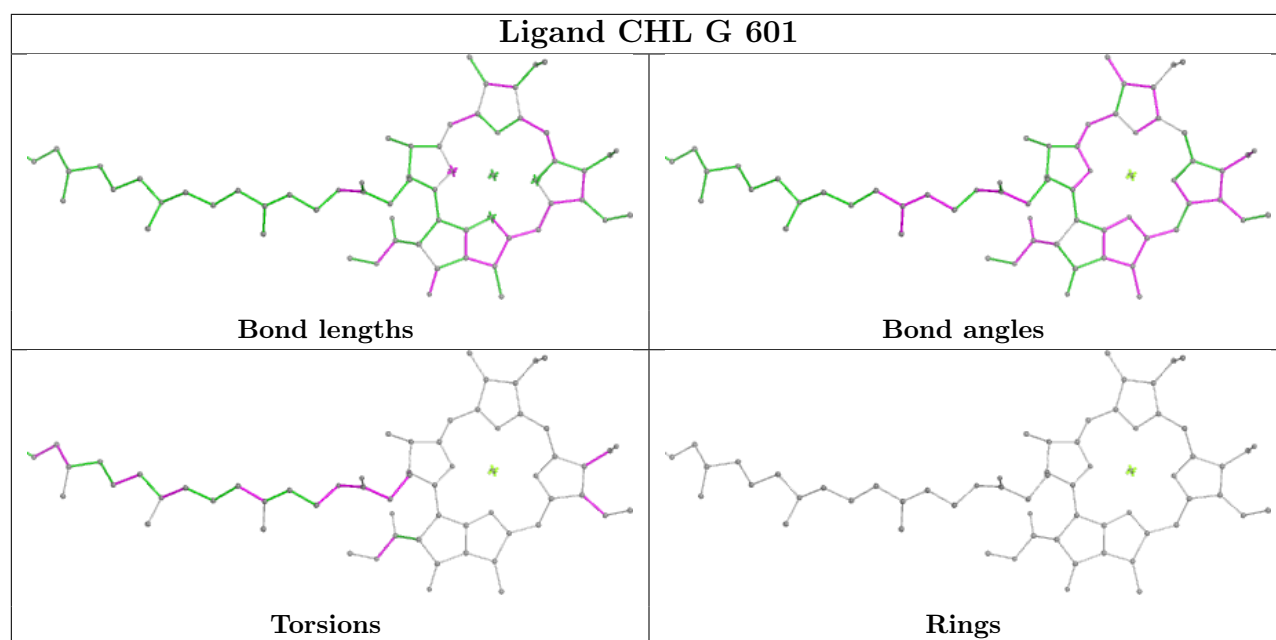


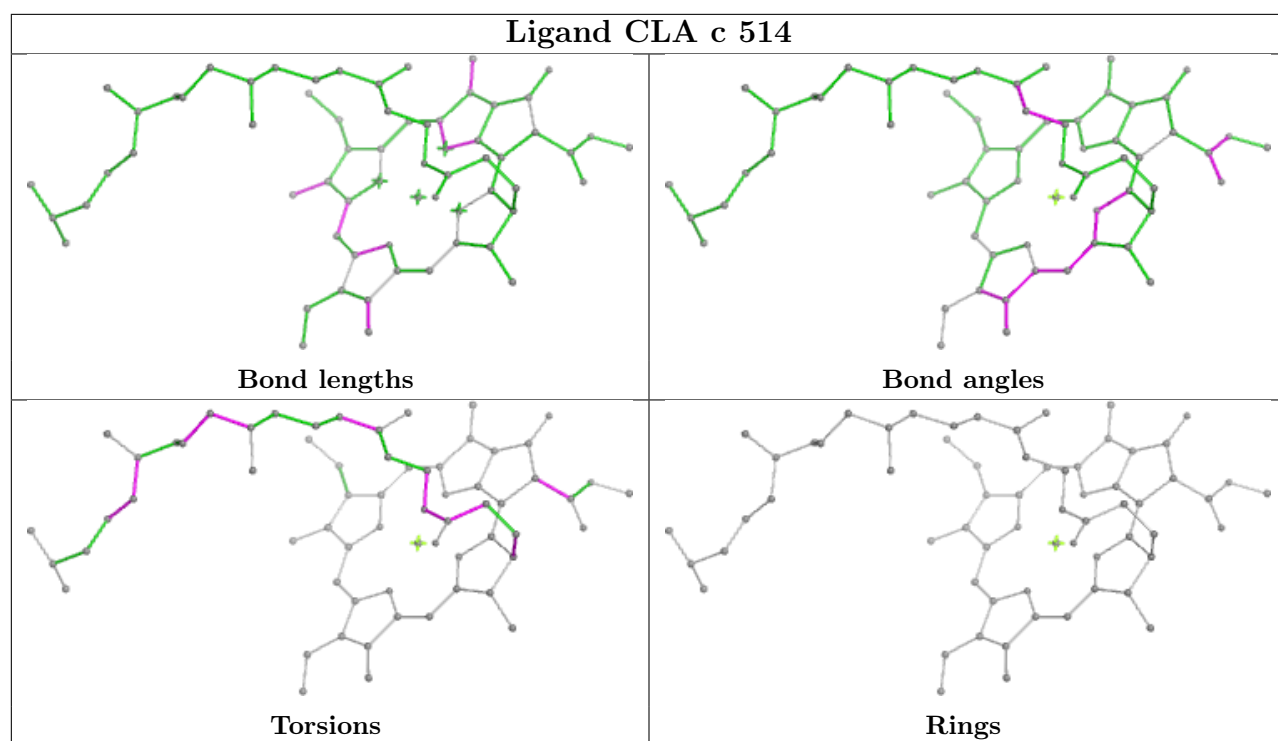
## Ligand DGD c 518

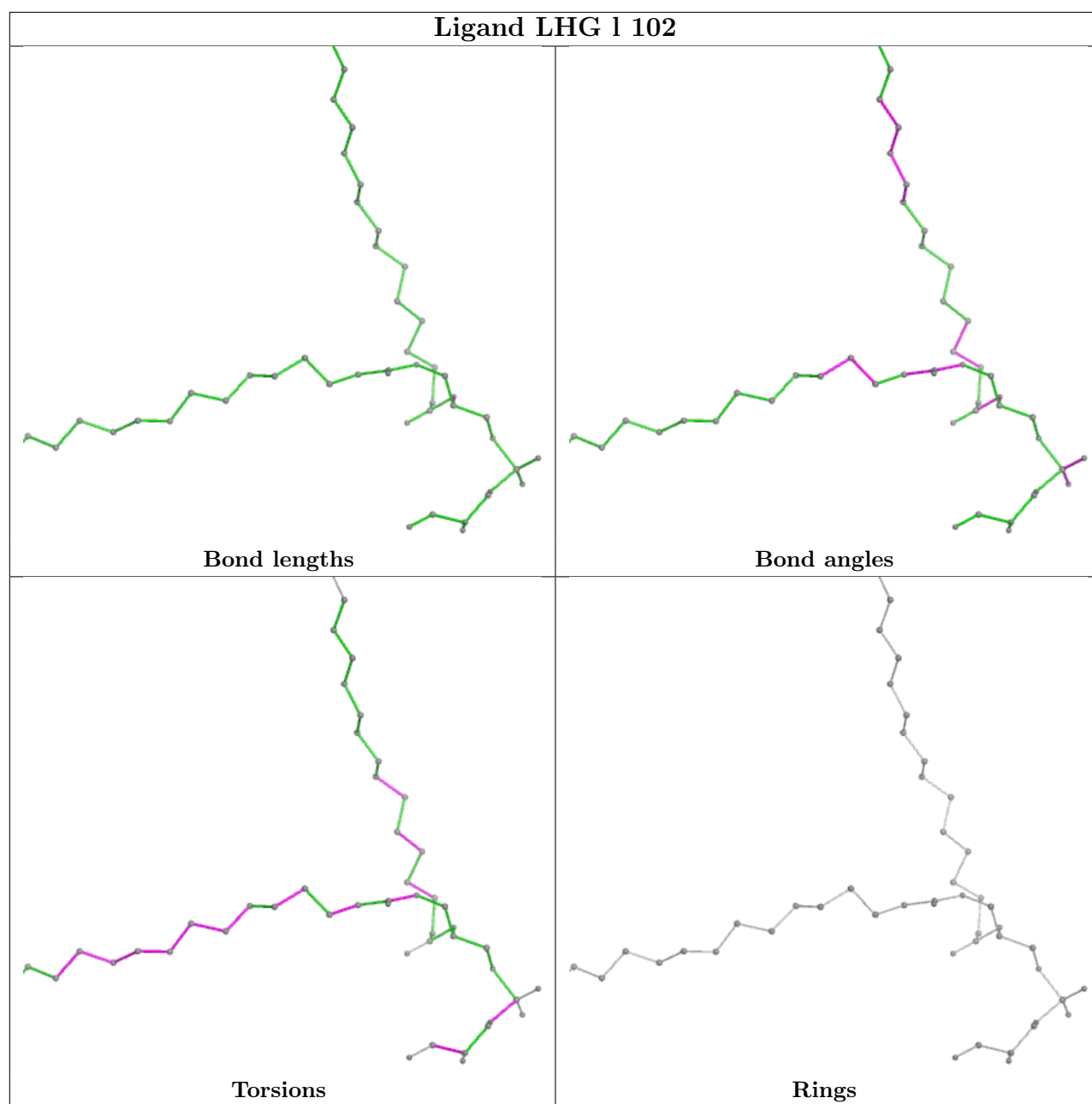


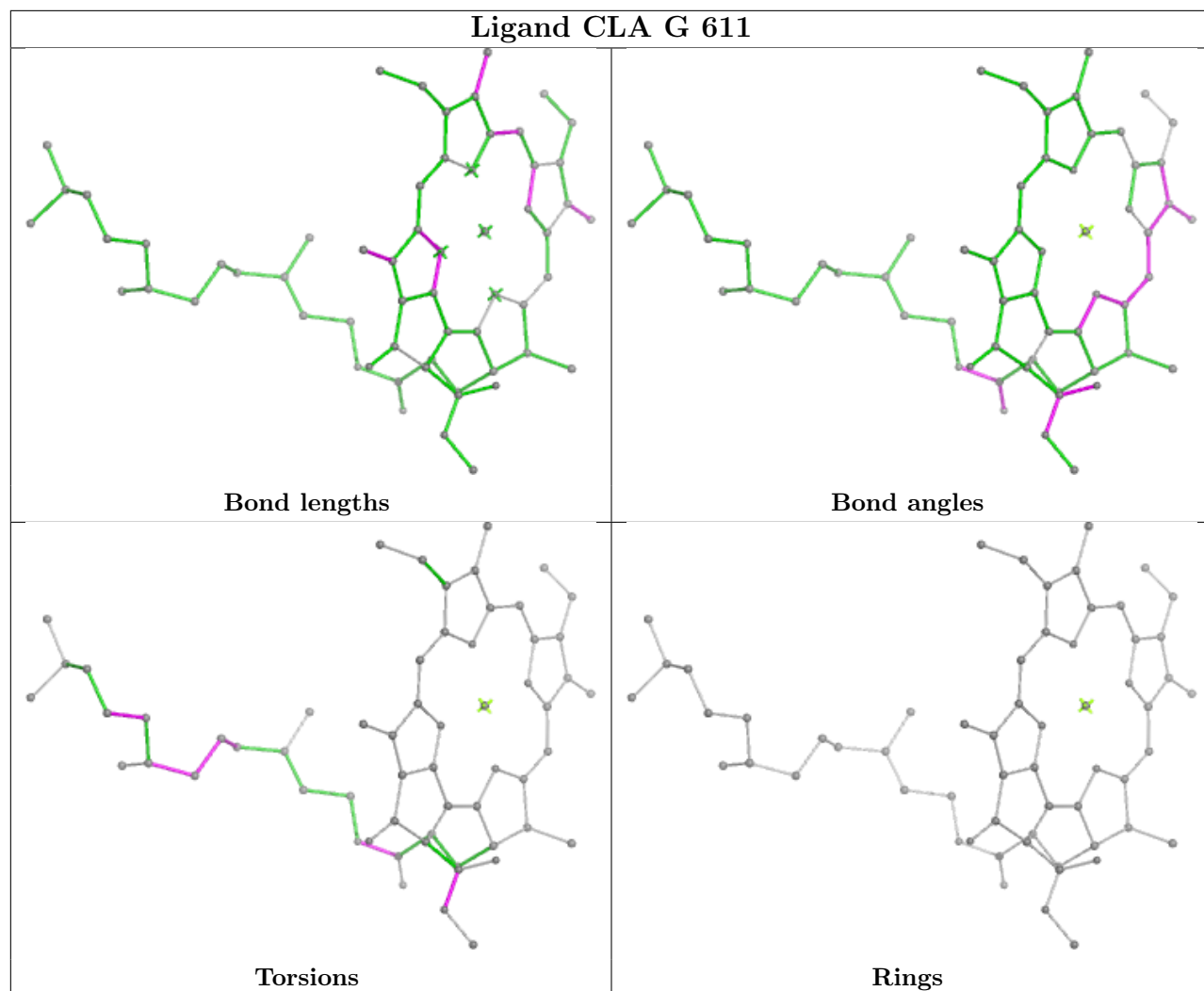
## Ligand CHL r 307



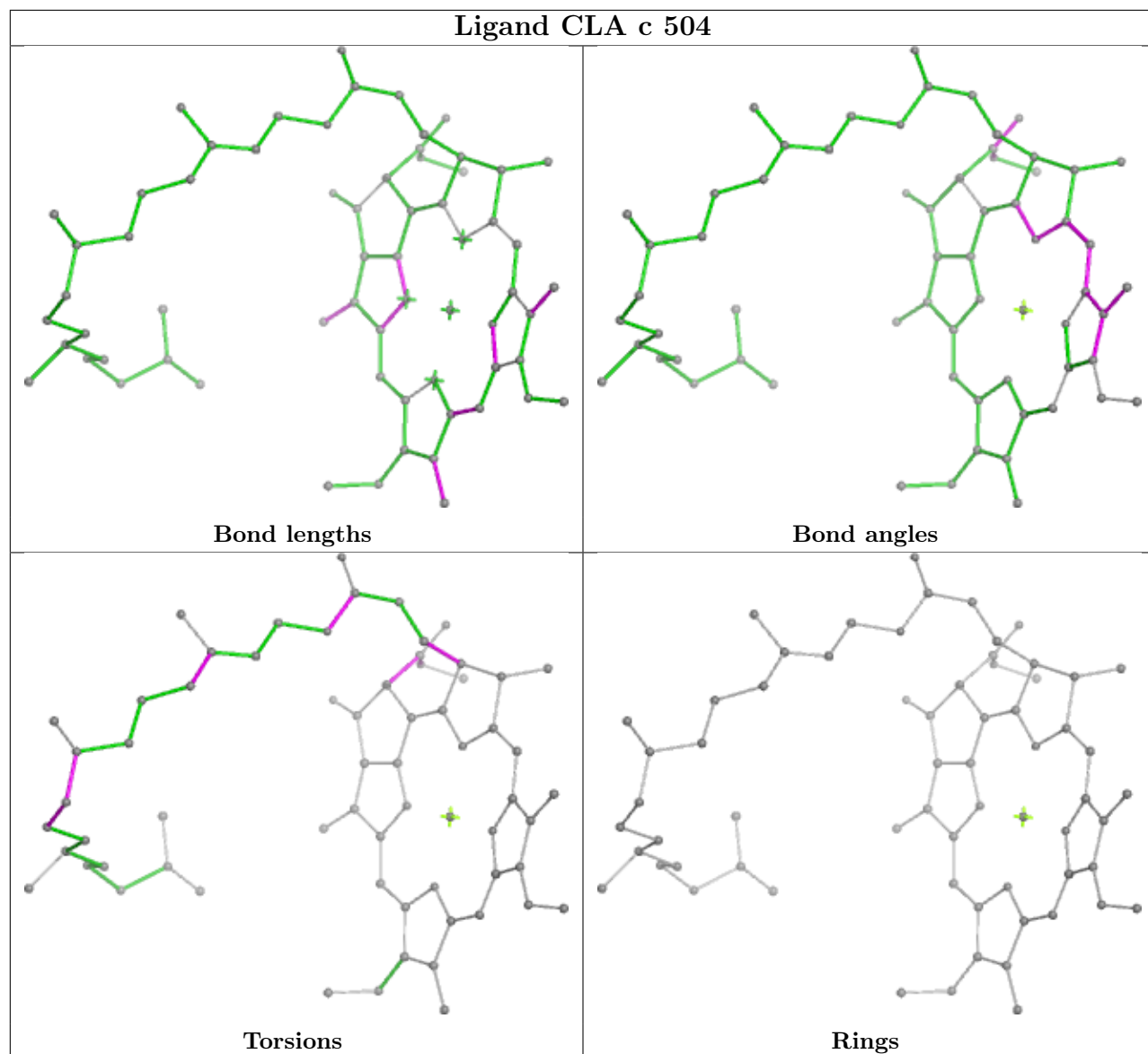




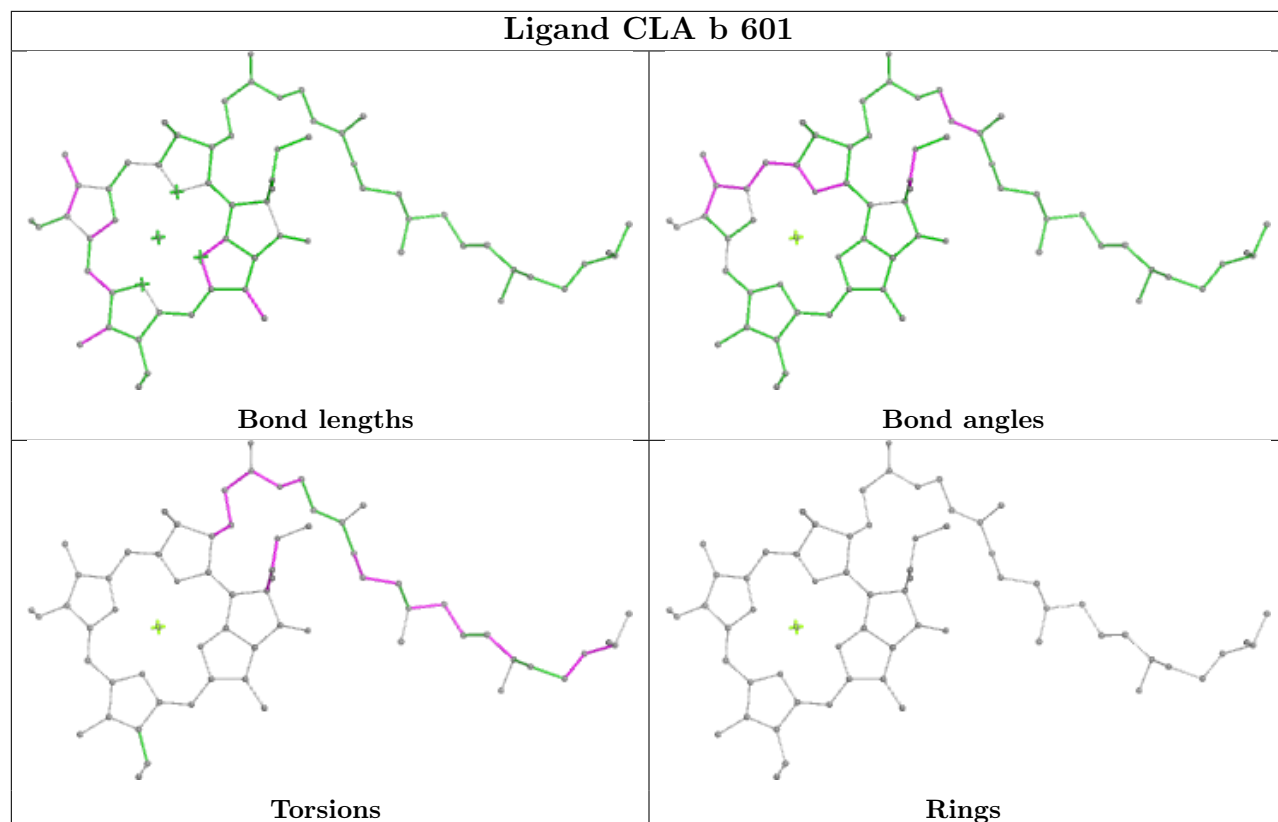




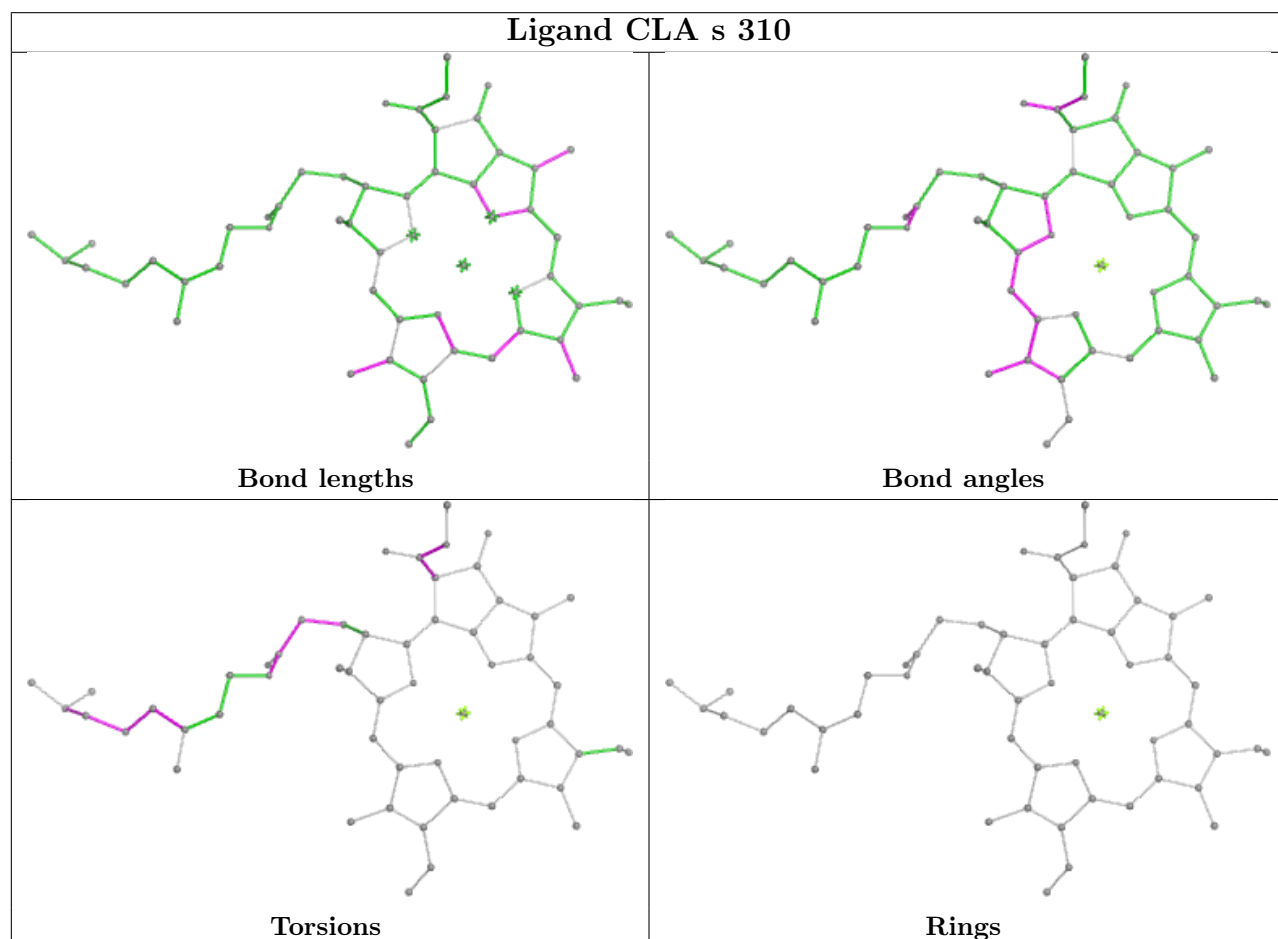
## Ligand CLA c 504

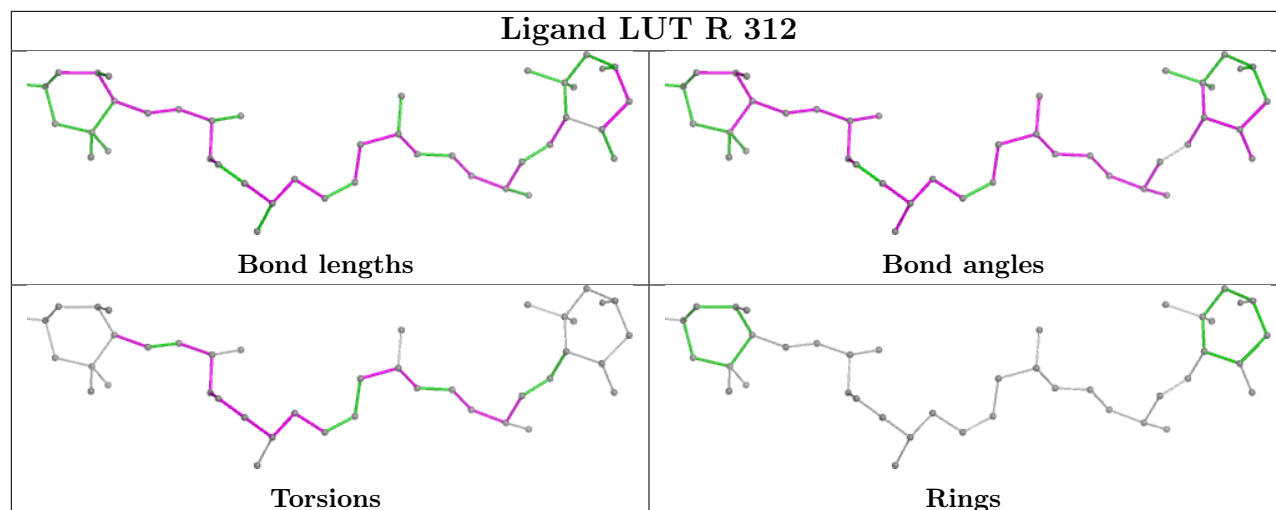
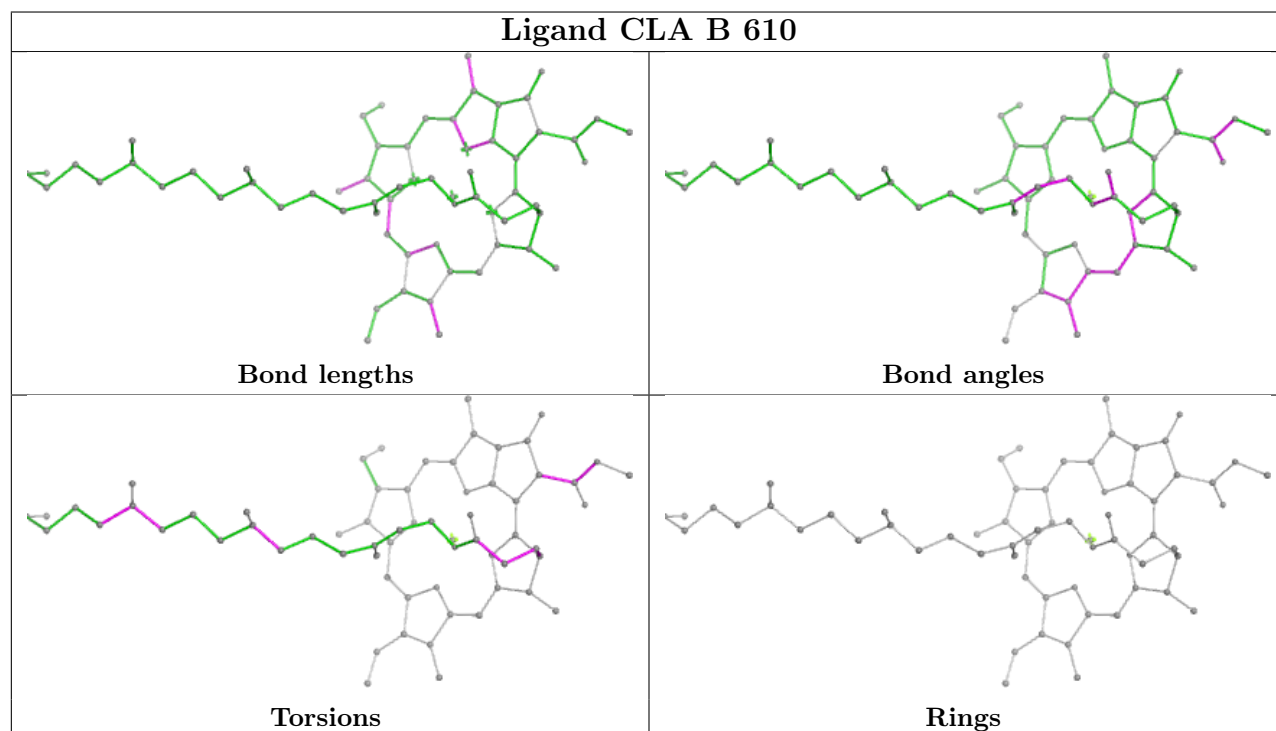
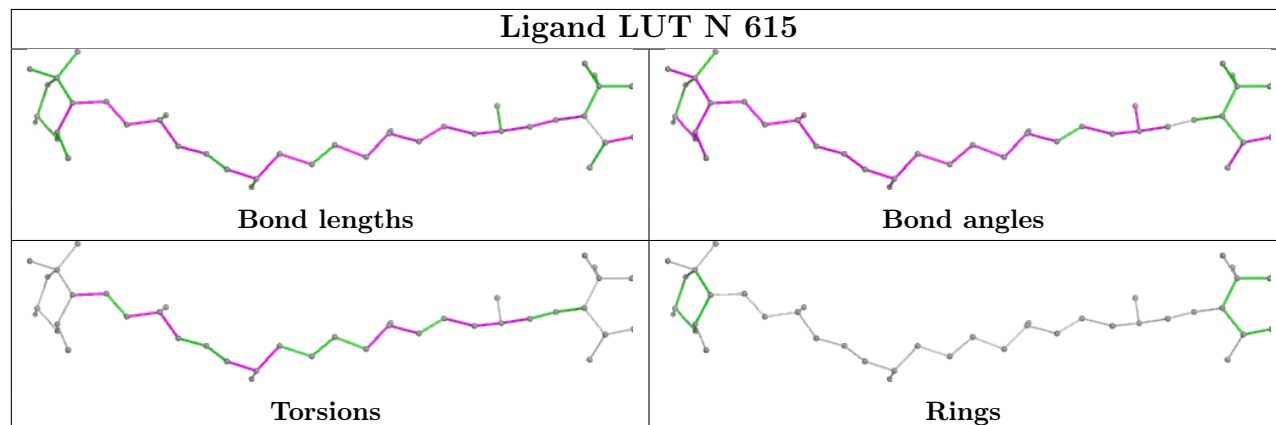


## Ligand CLA b 601

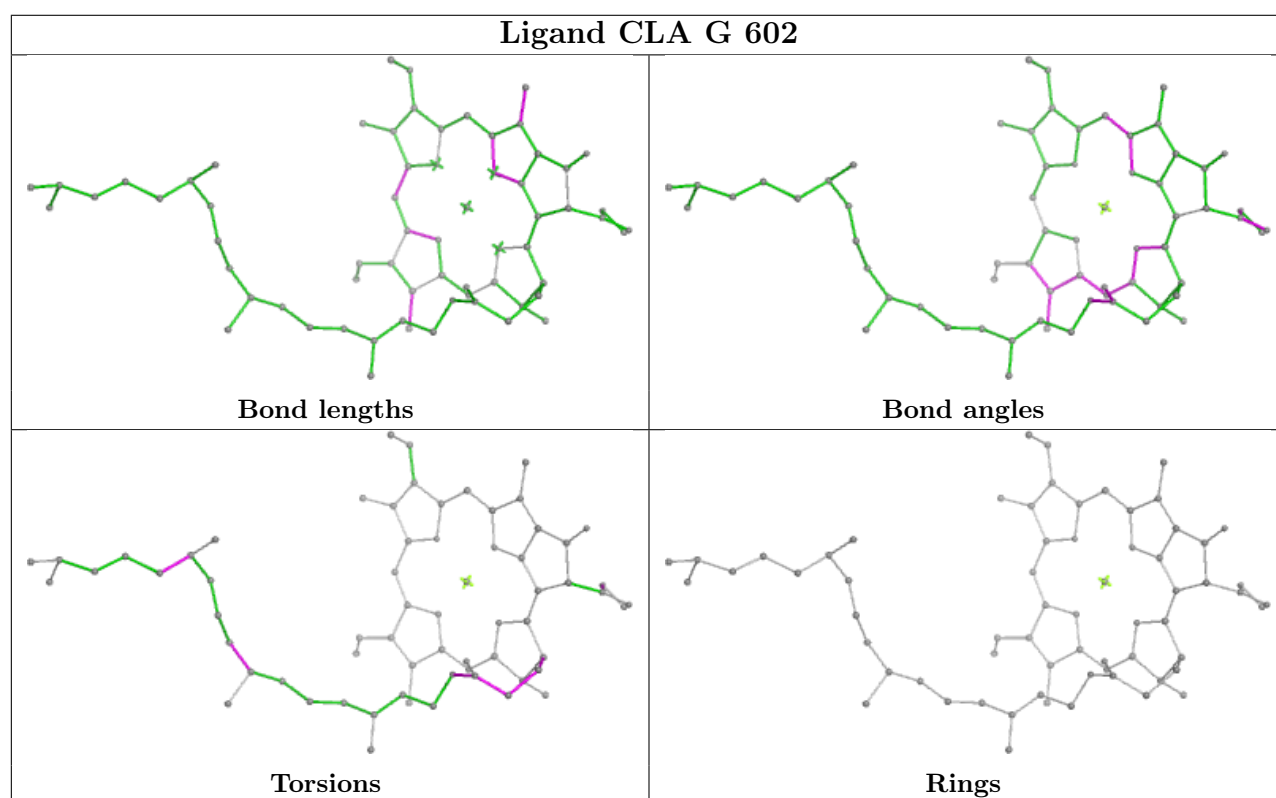
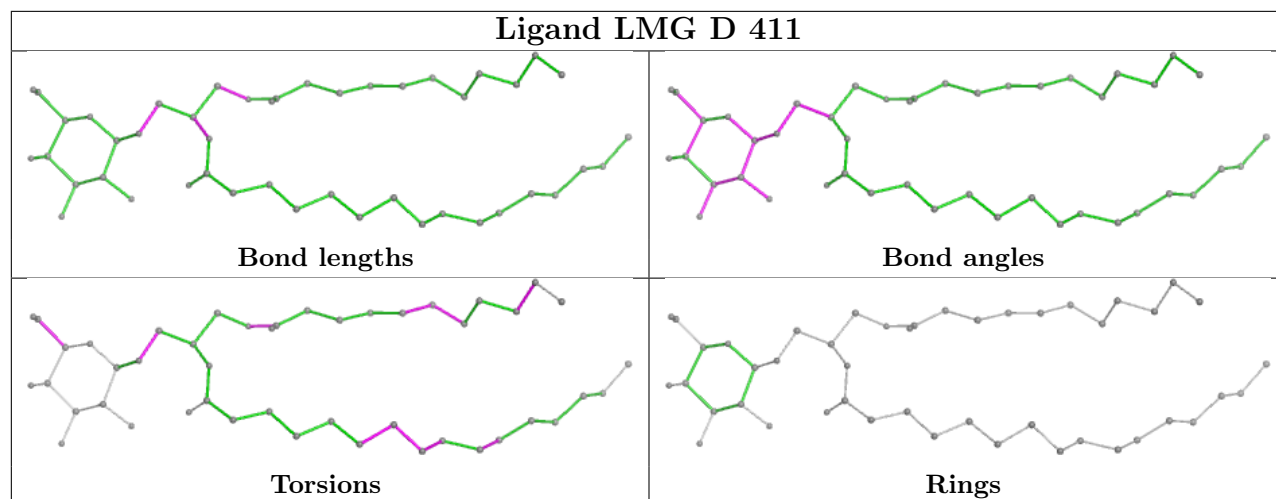


## Ligand CLA s 310

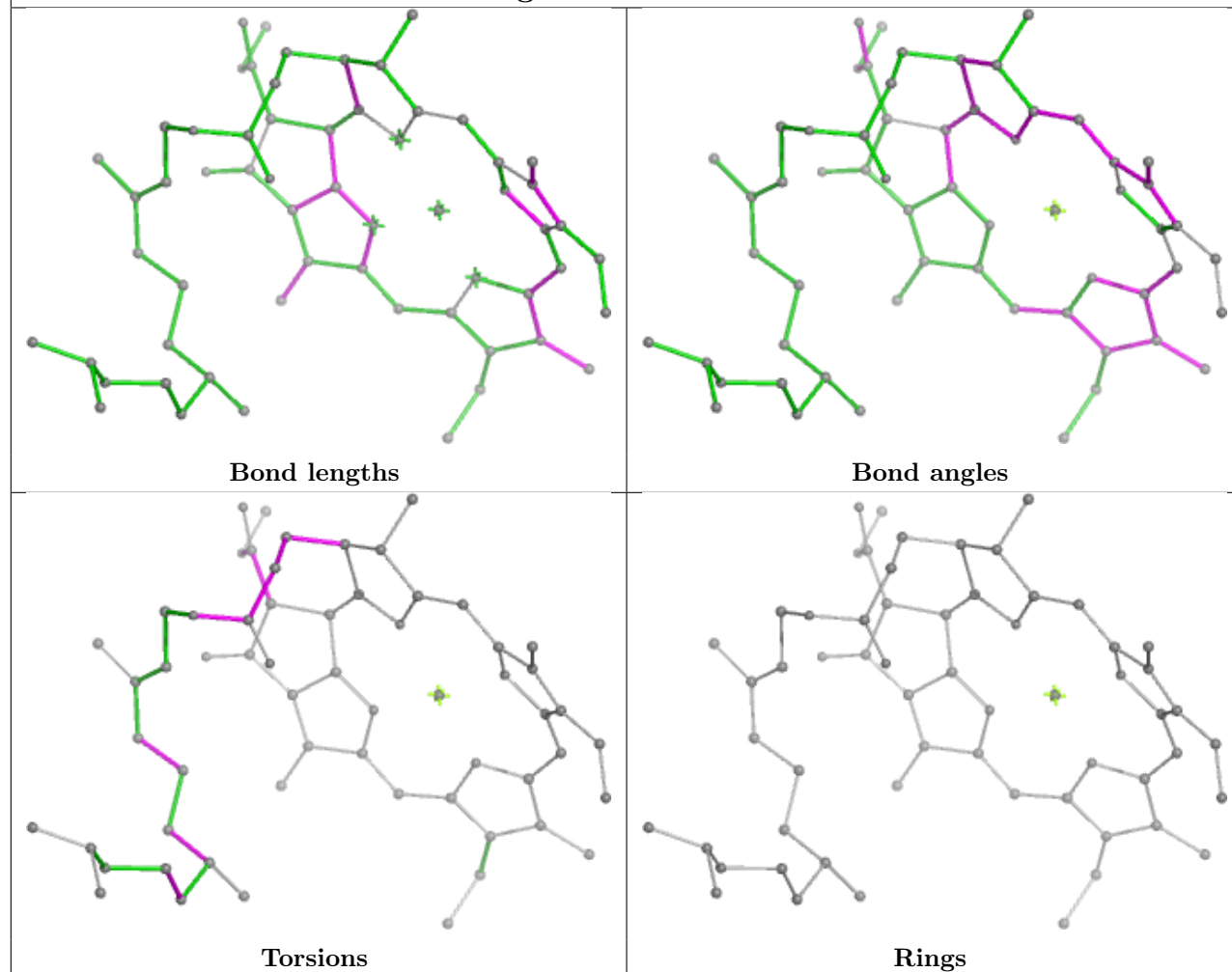


**Ligand LUT R 312****Ligand CLA B 610****Ligand LUT N 615**

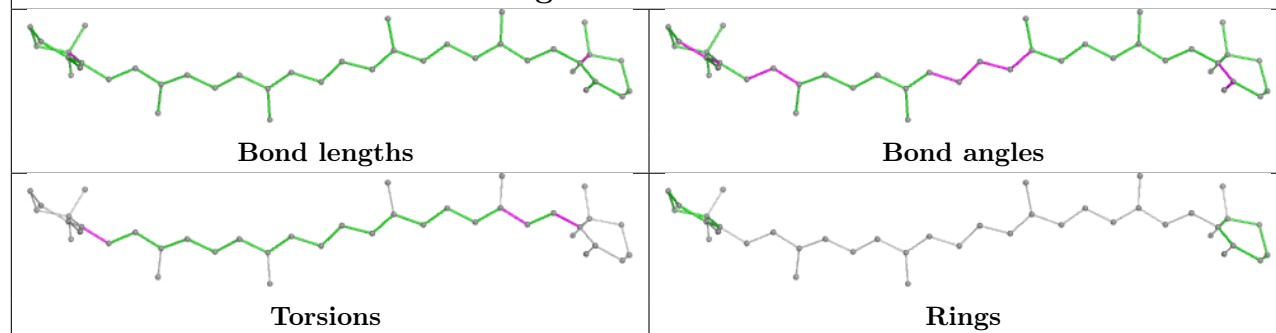


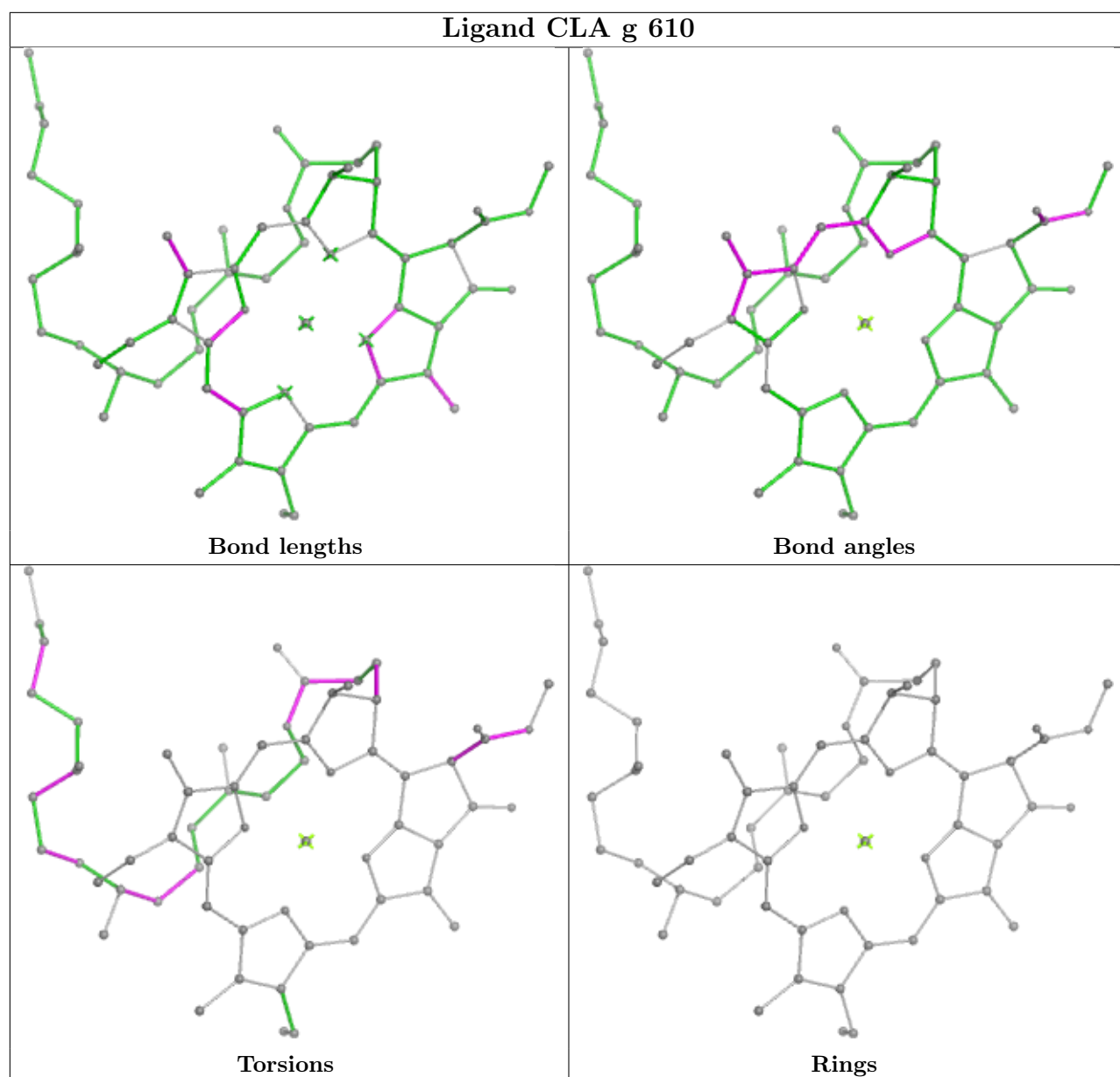


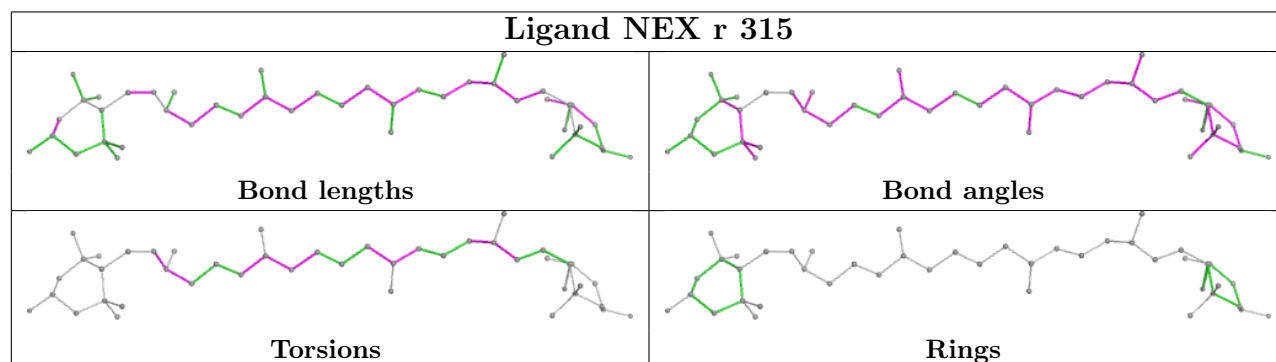
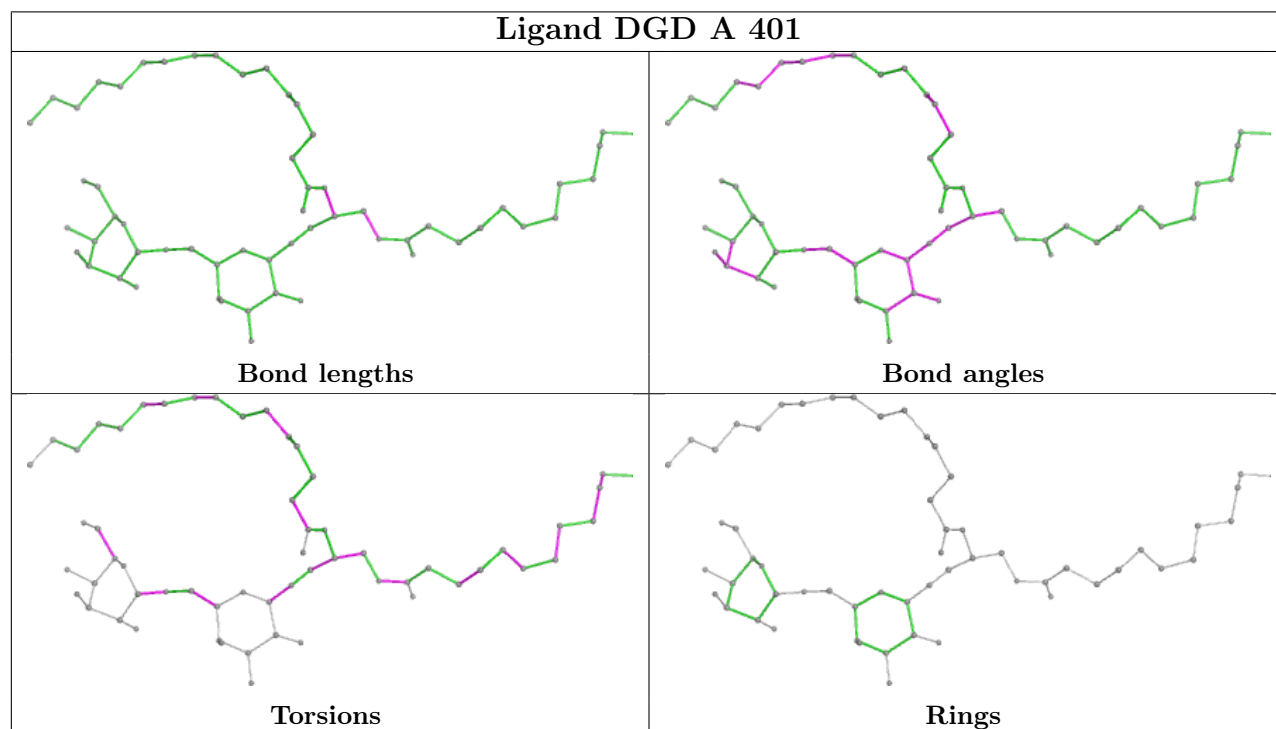
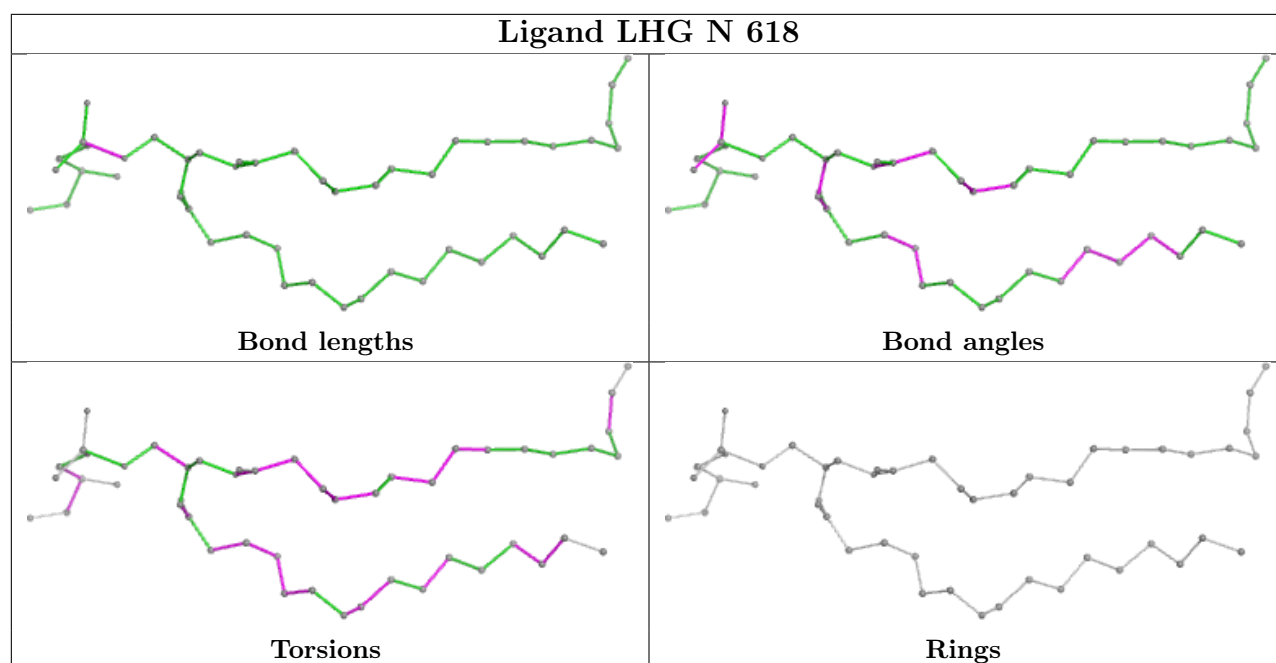
## Ligand CLA n 612

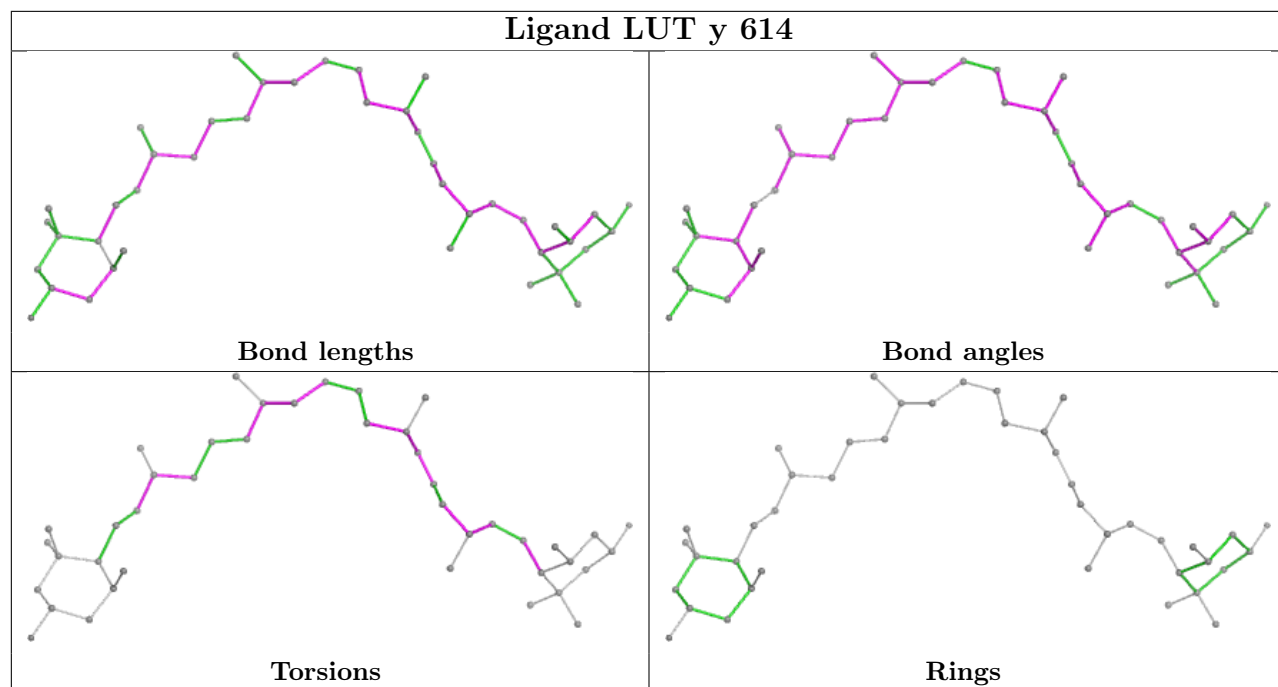
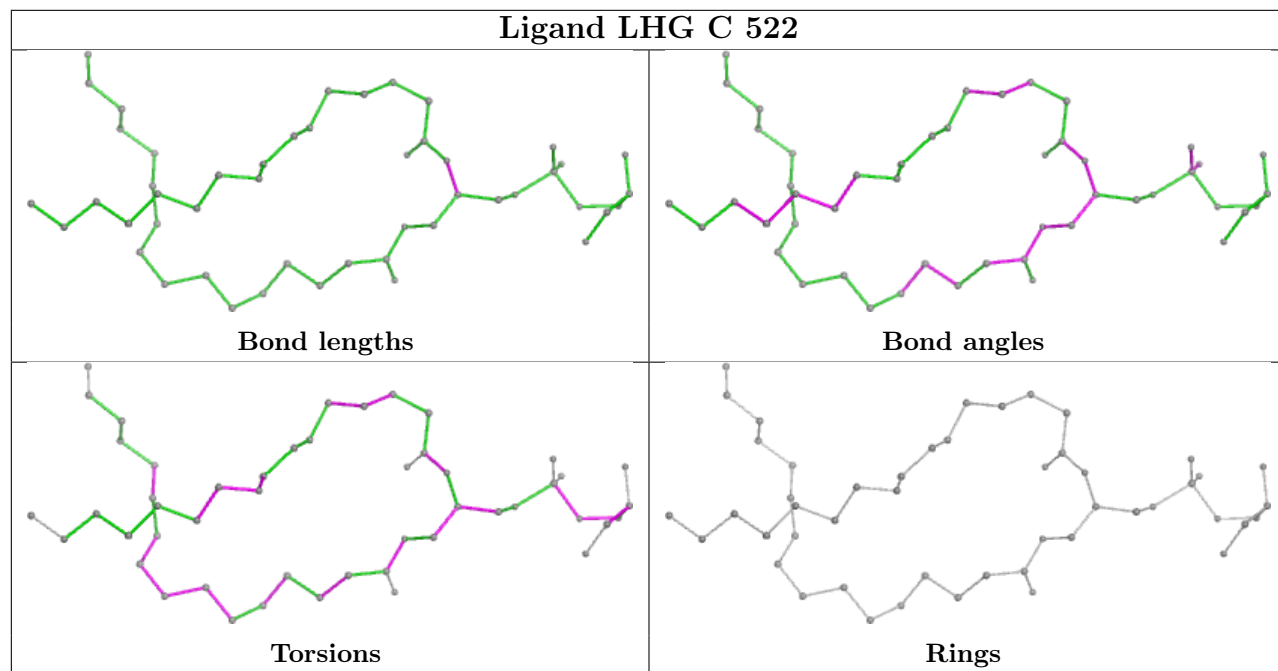


## Ligand BCR c 515

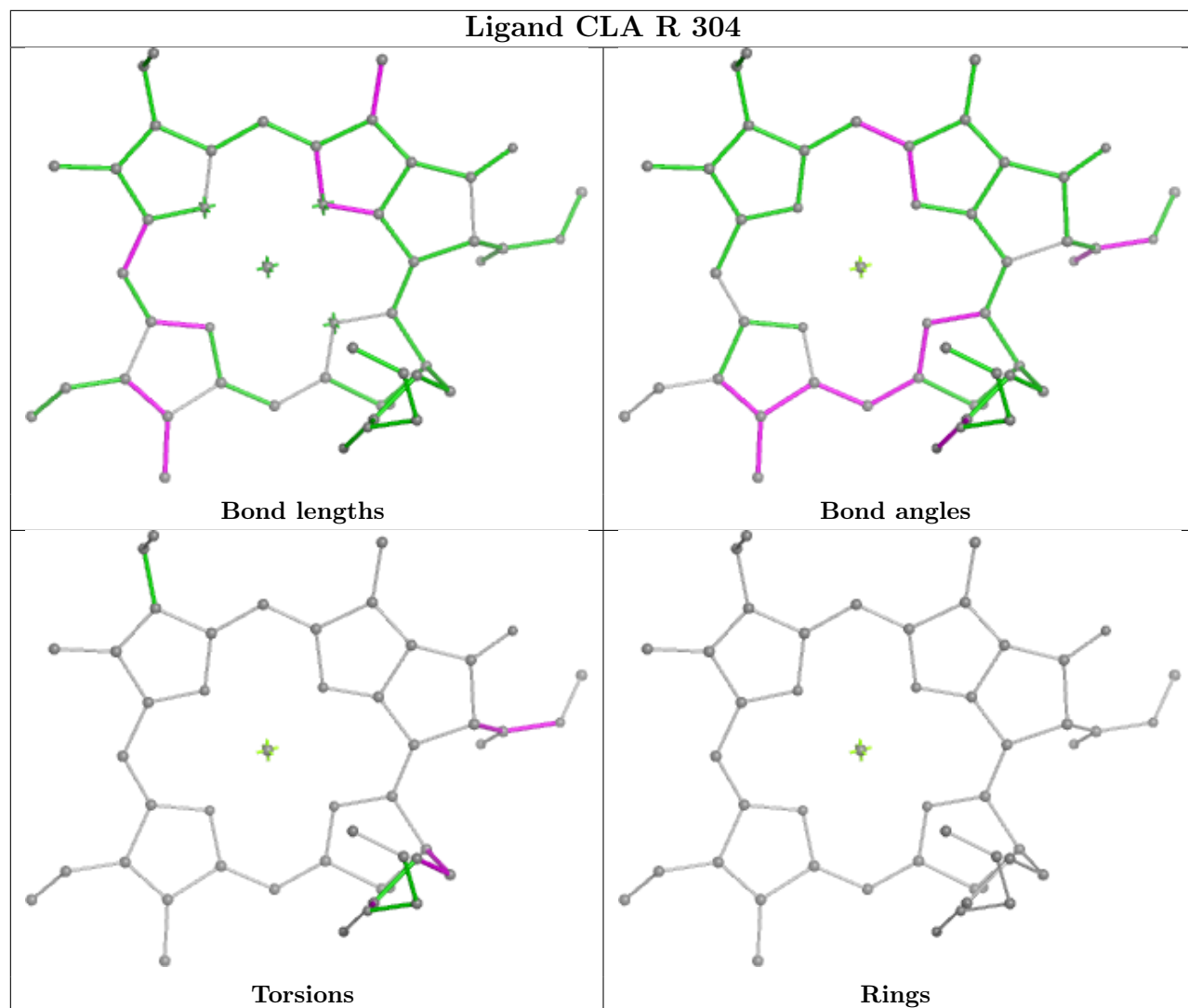


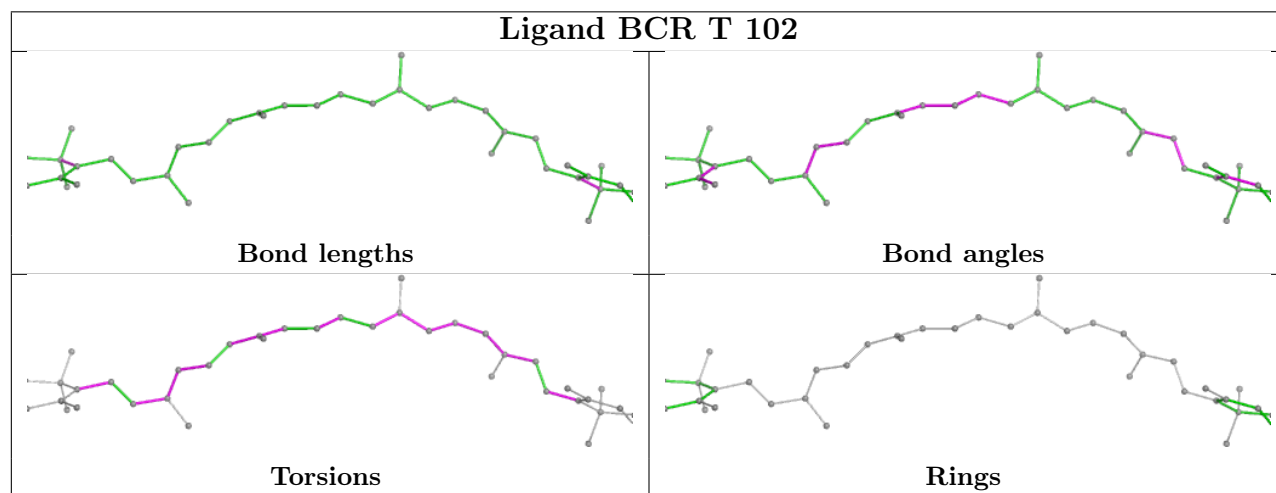
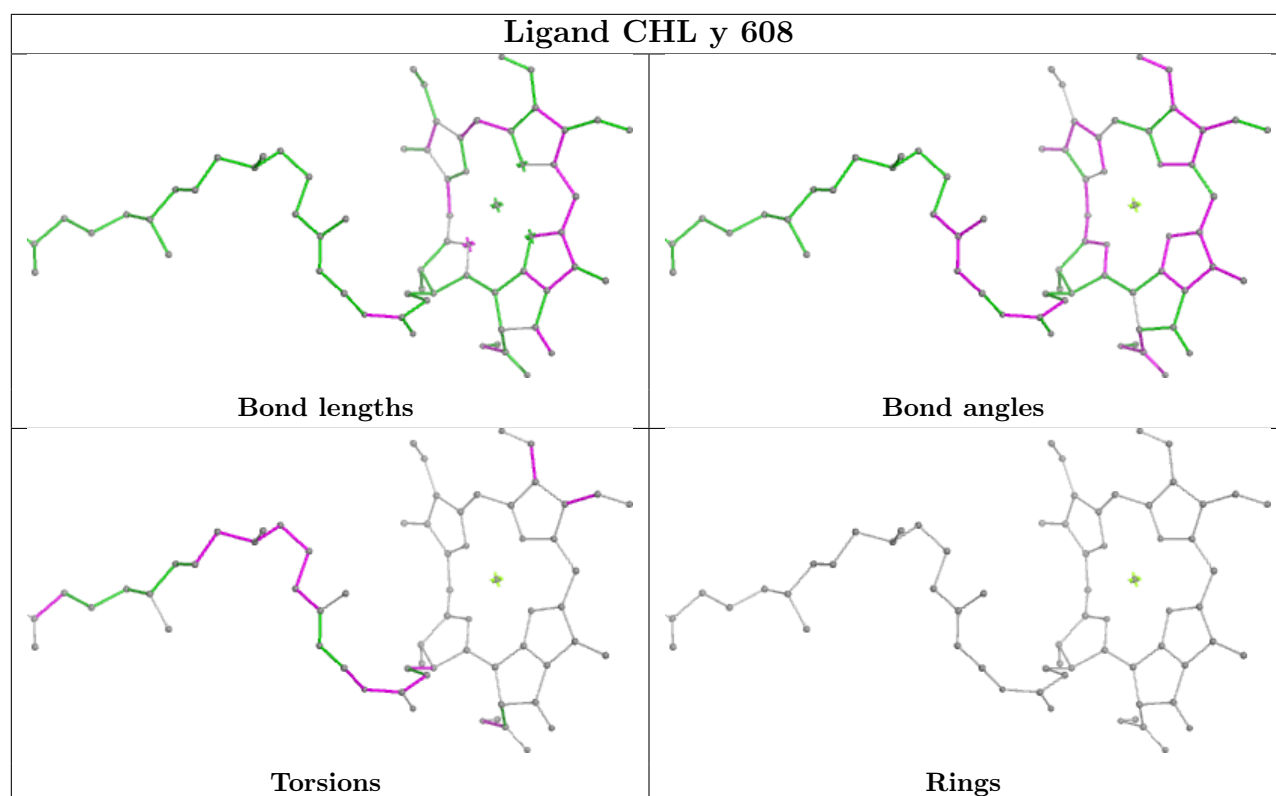


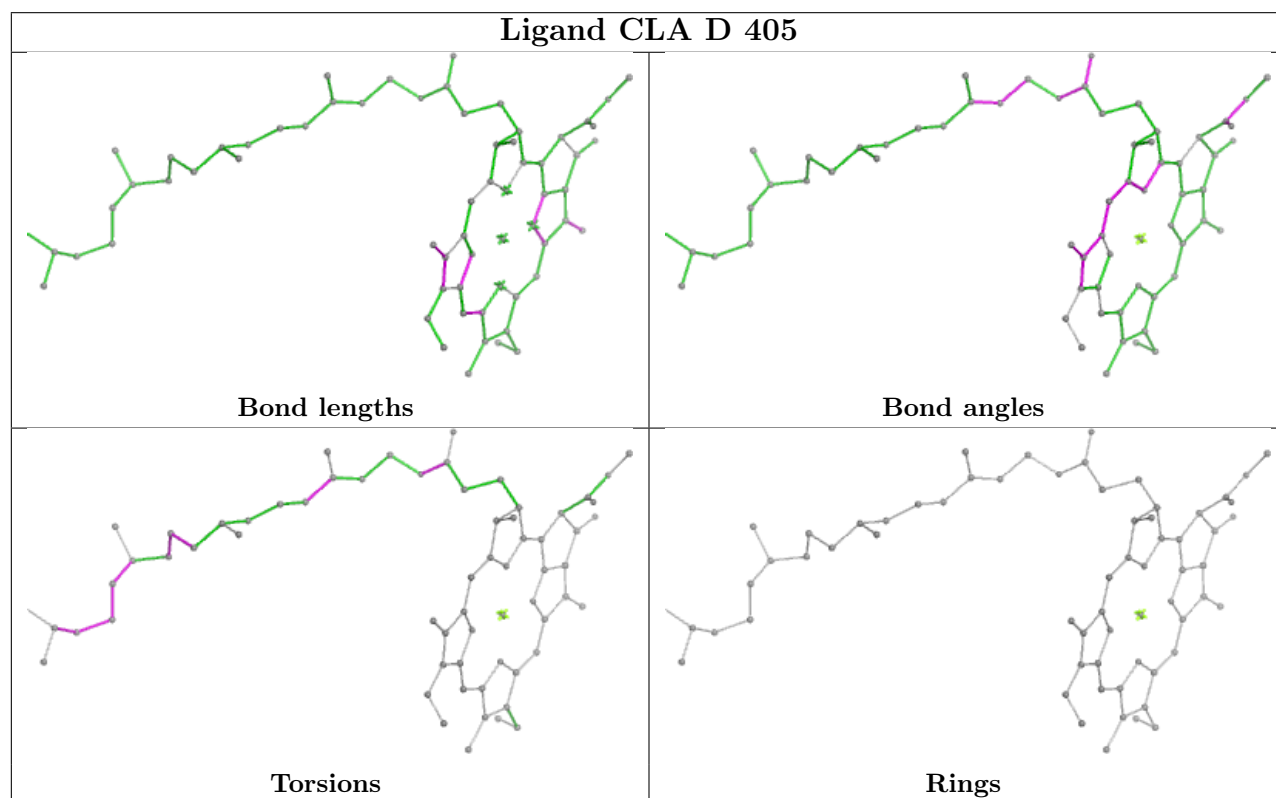
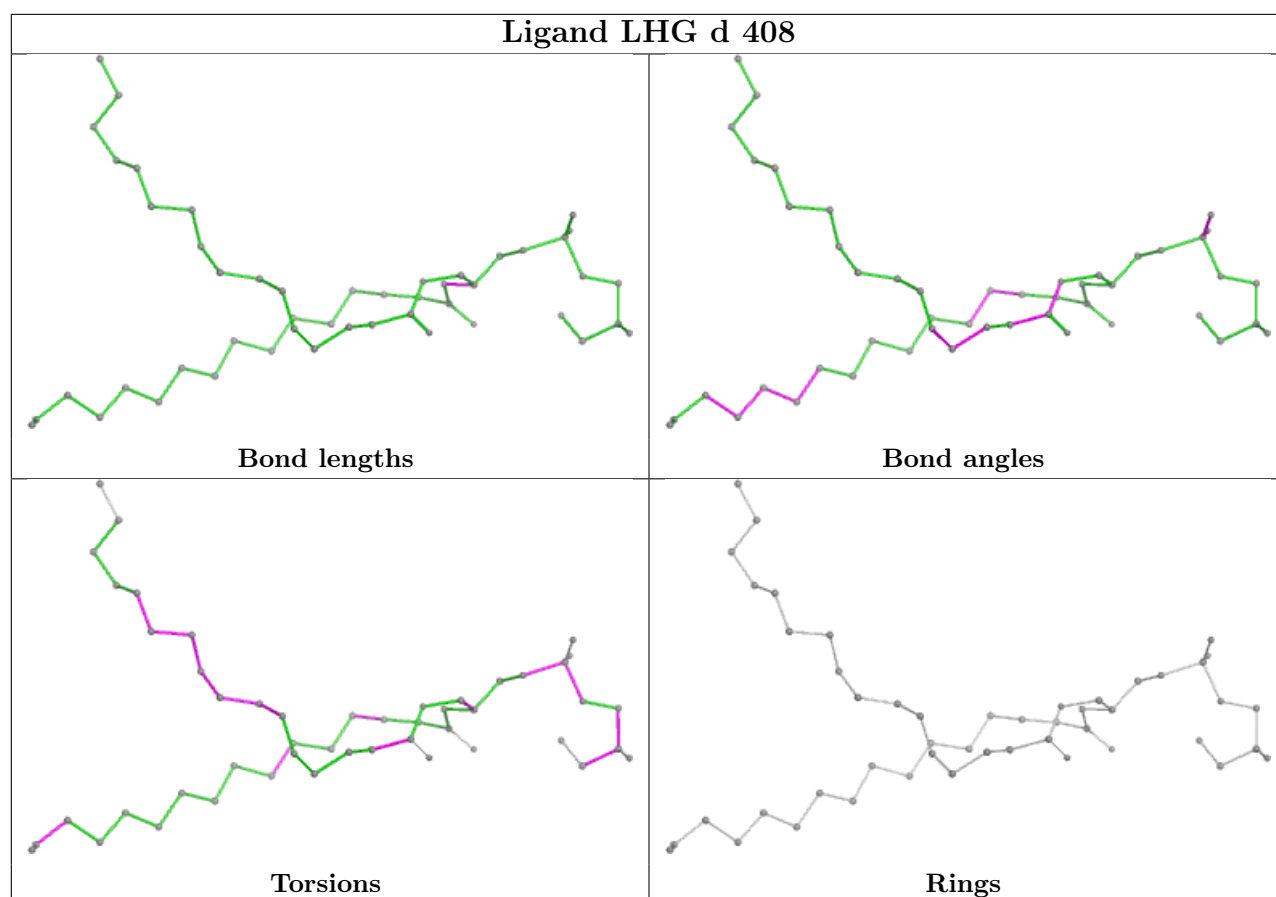


**Ligand LUT y 614****Ligand LHG C 522**

## Ligand CLA R 304

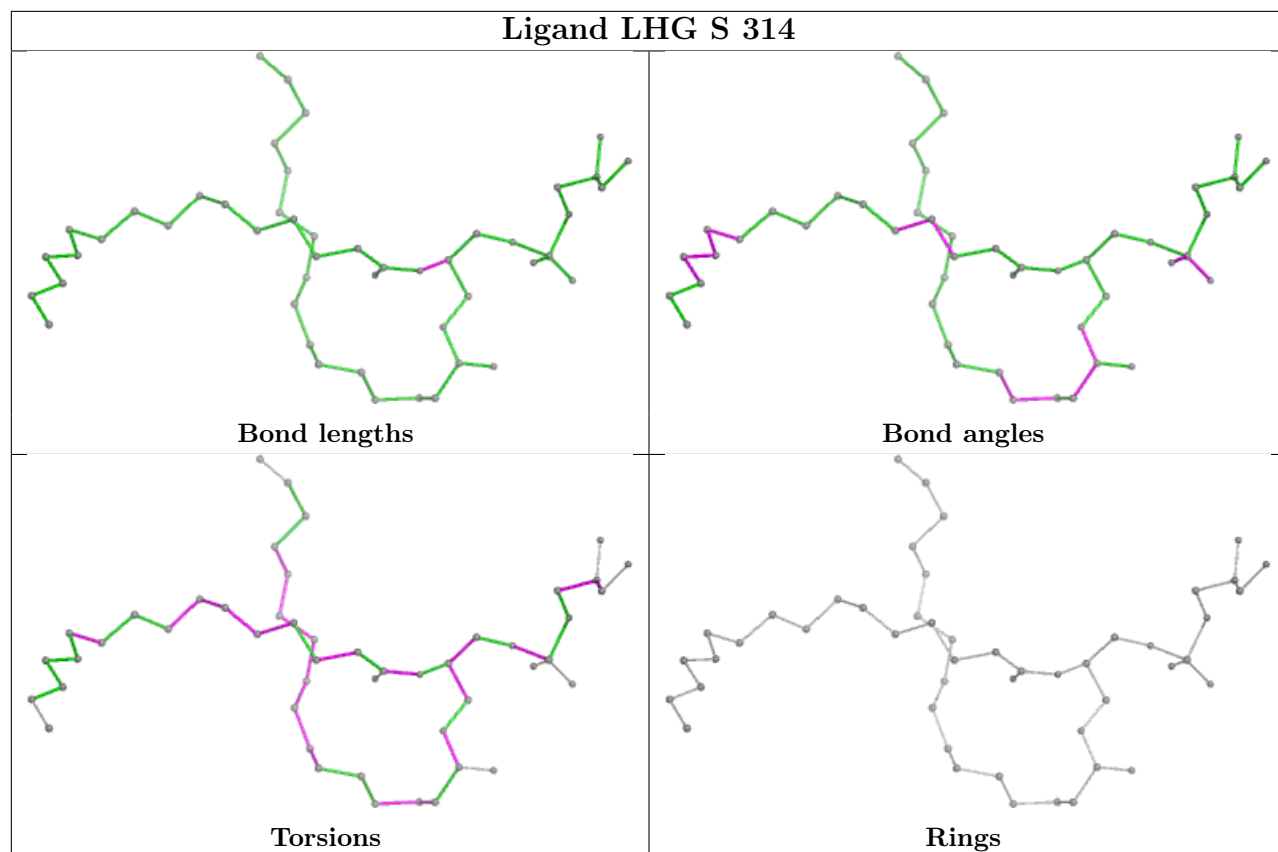




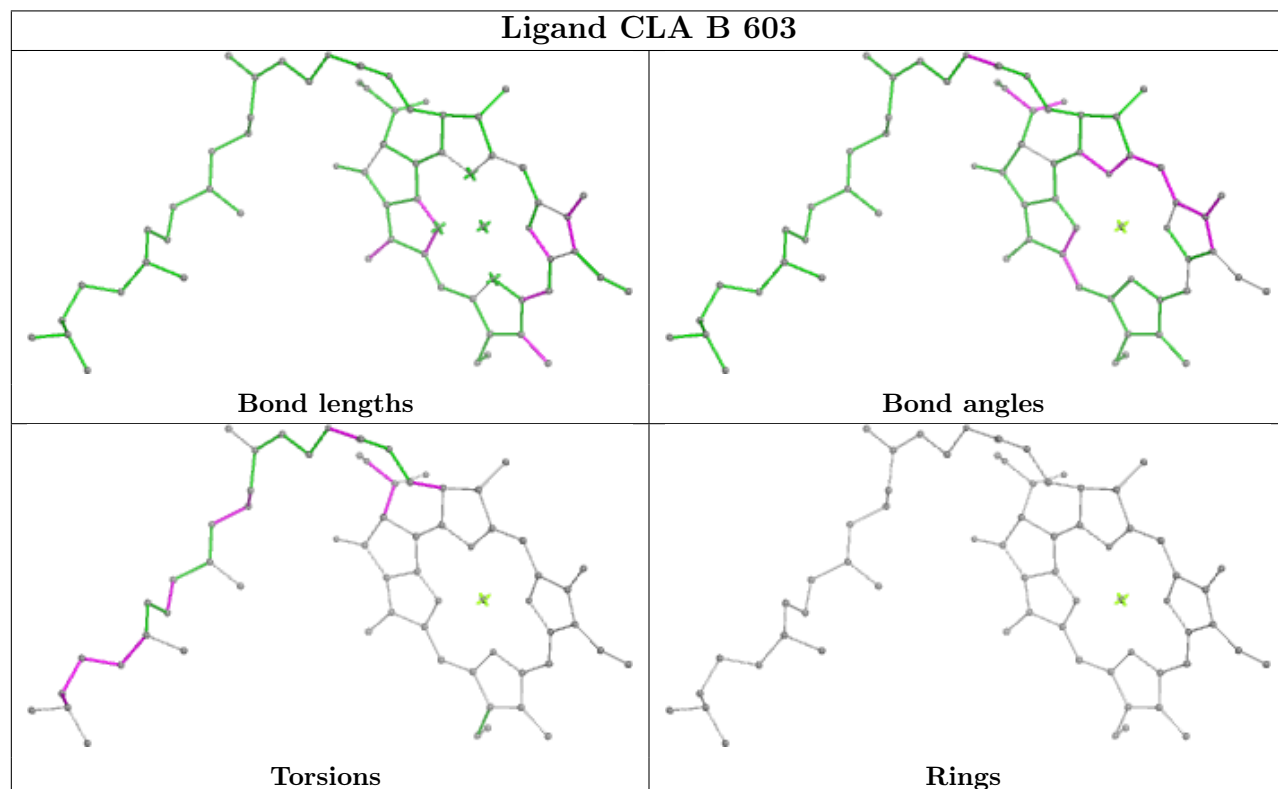


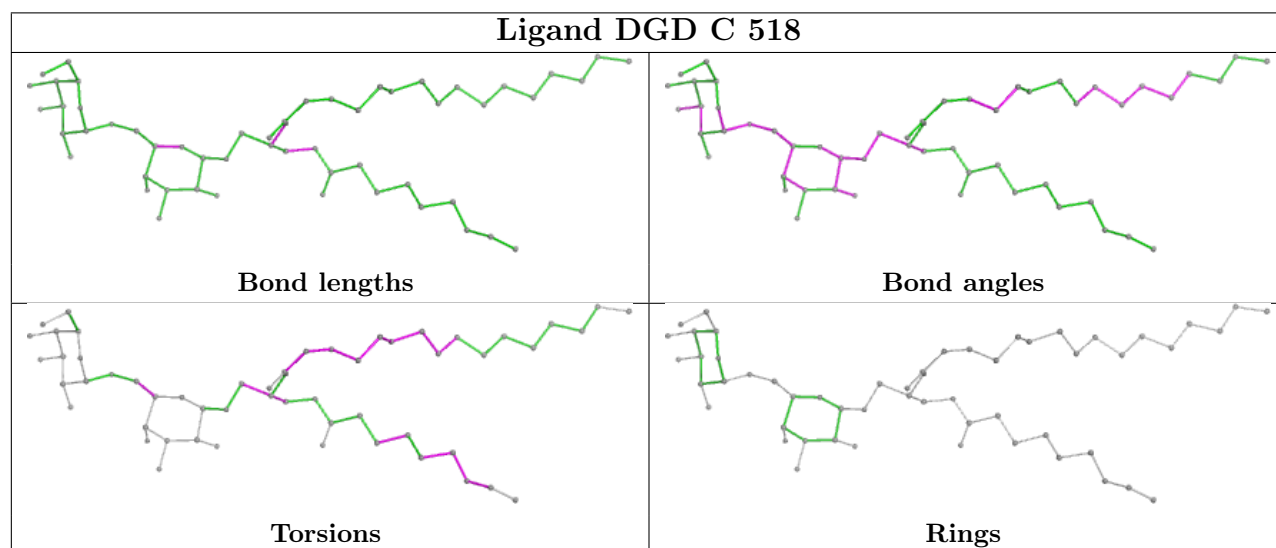
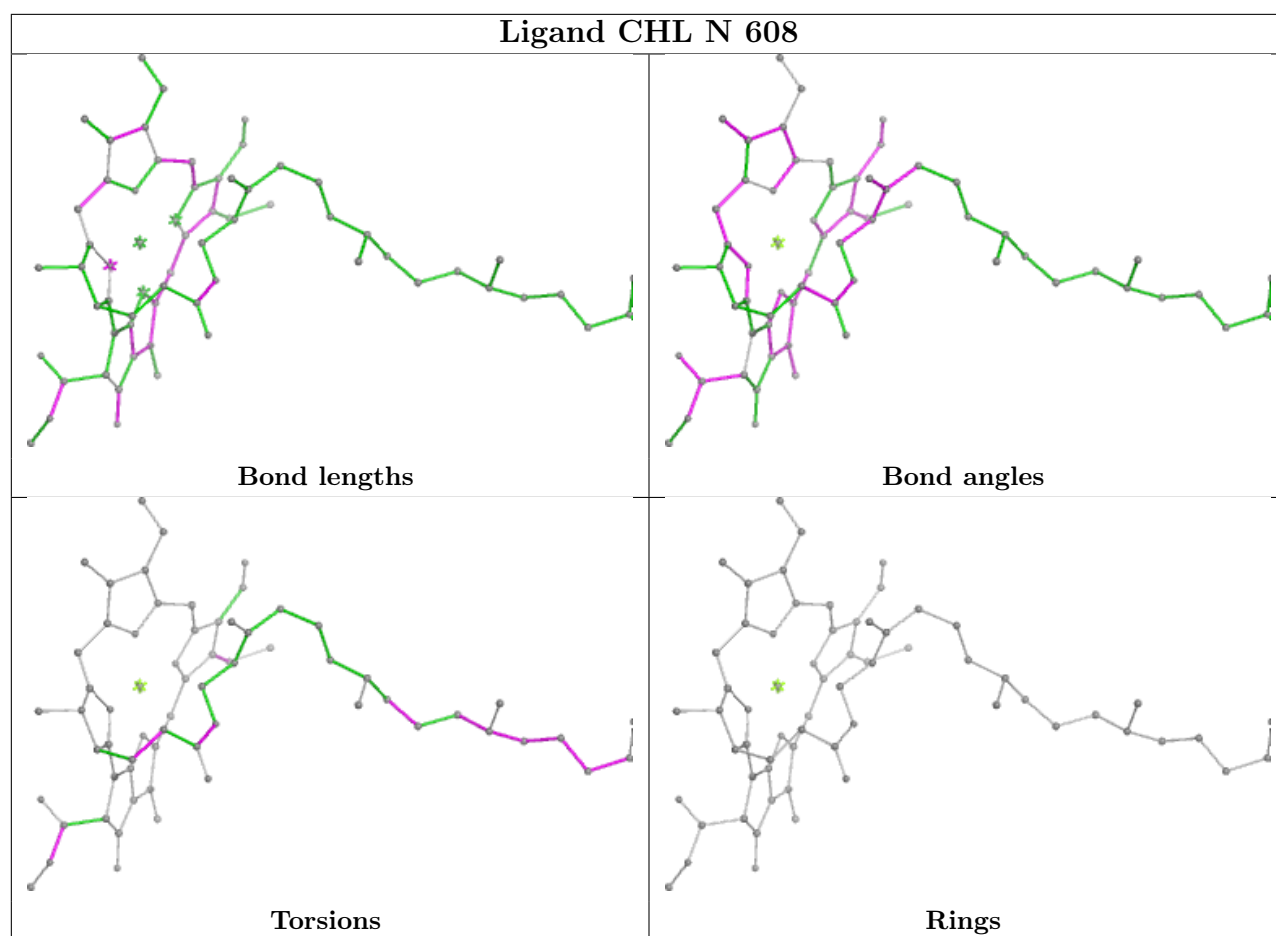


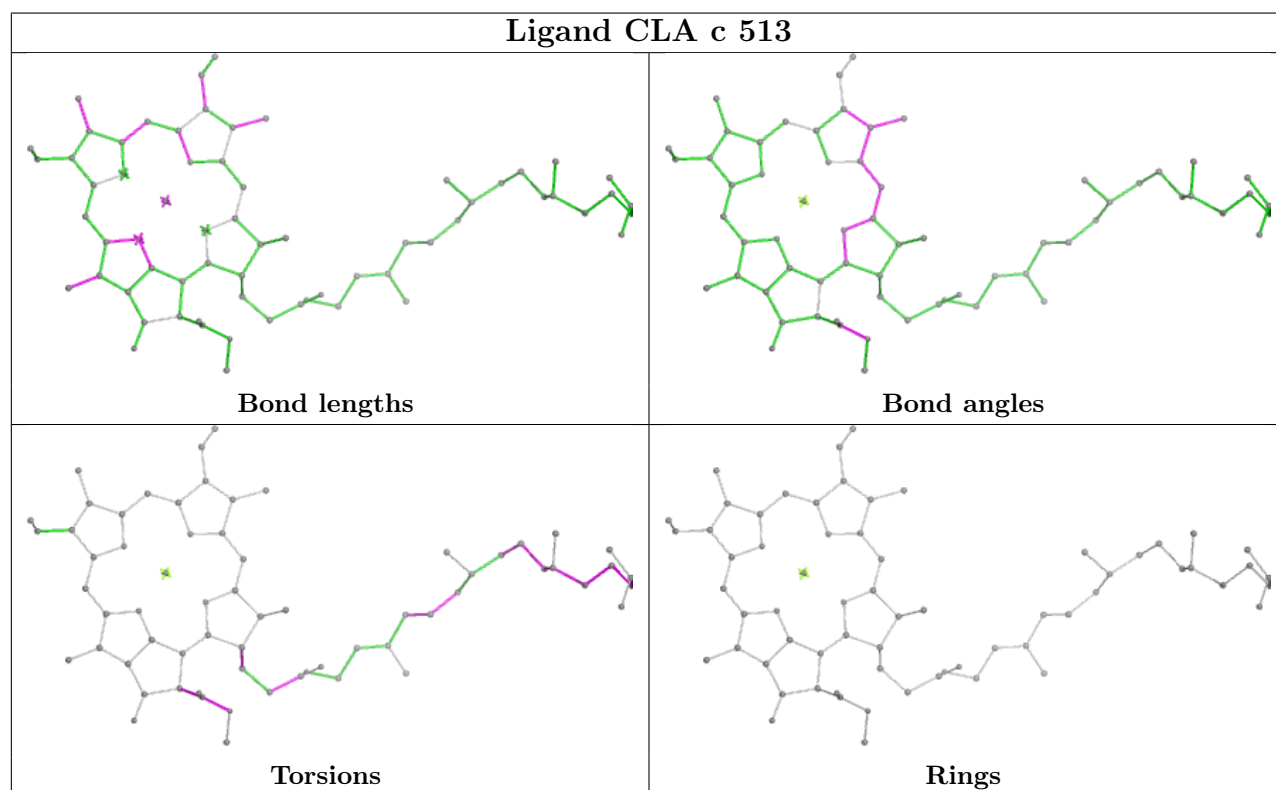
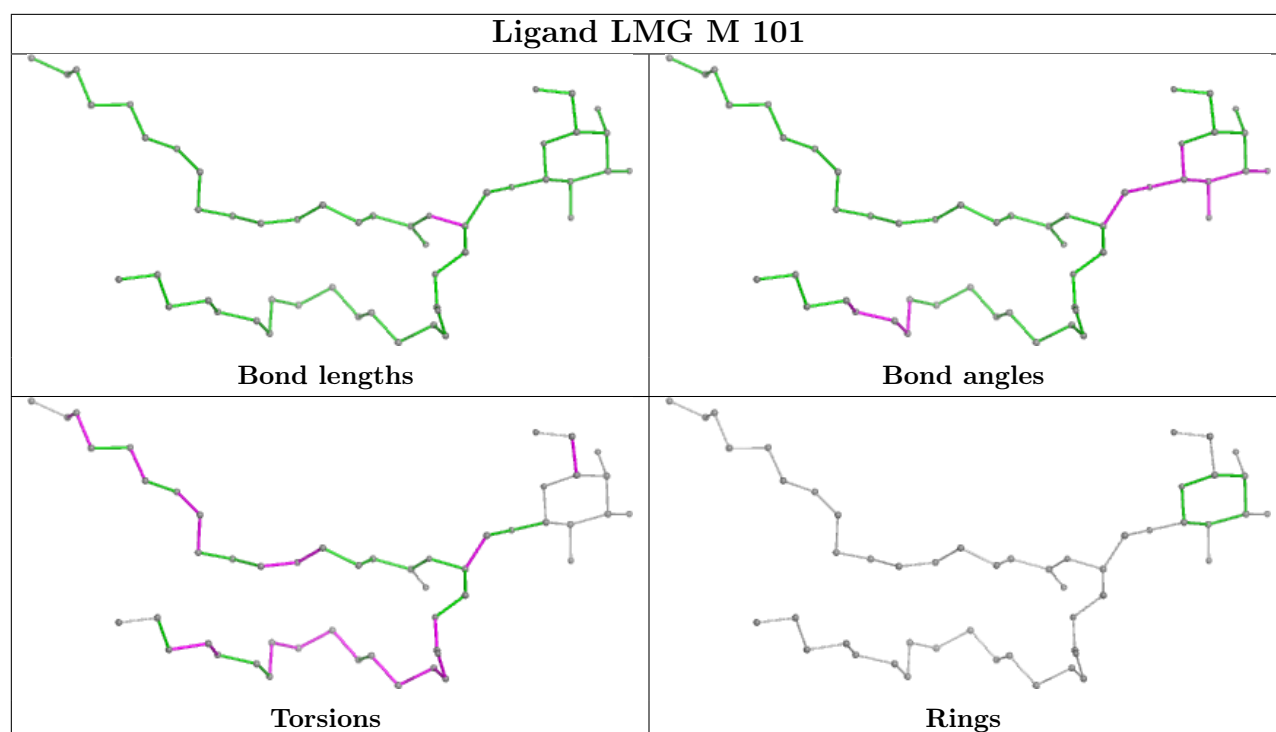
## Ligand LHG S 314

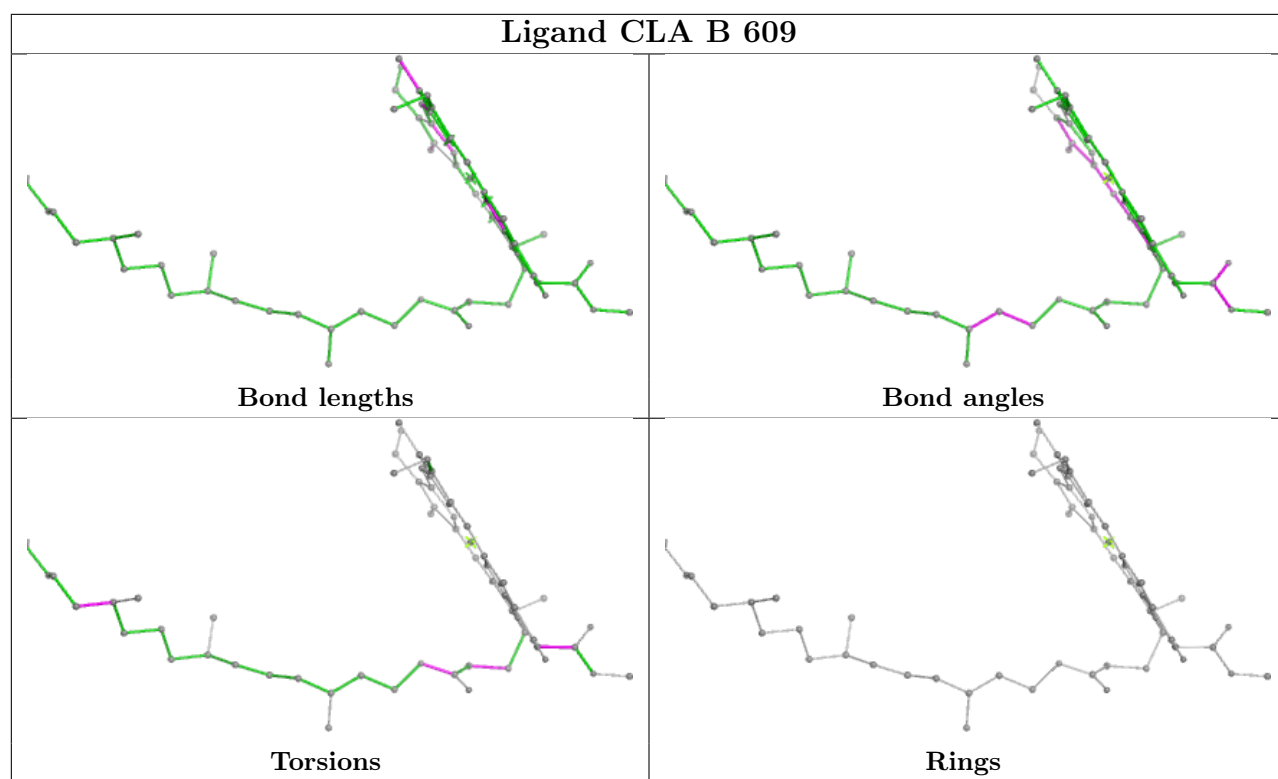


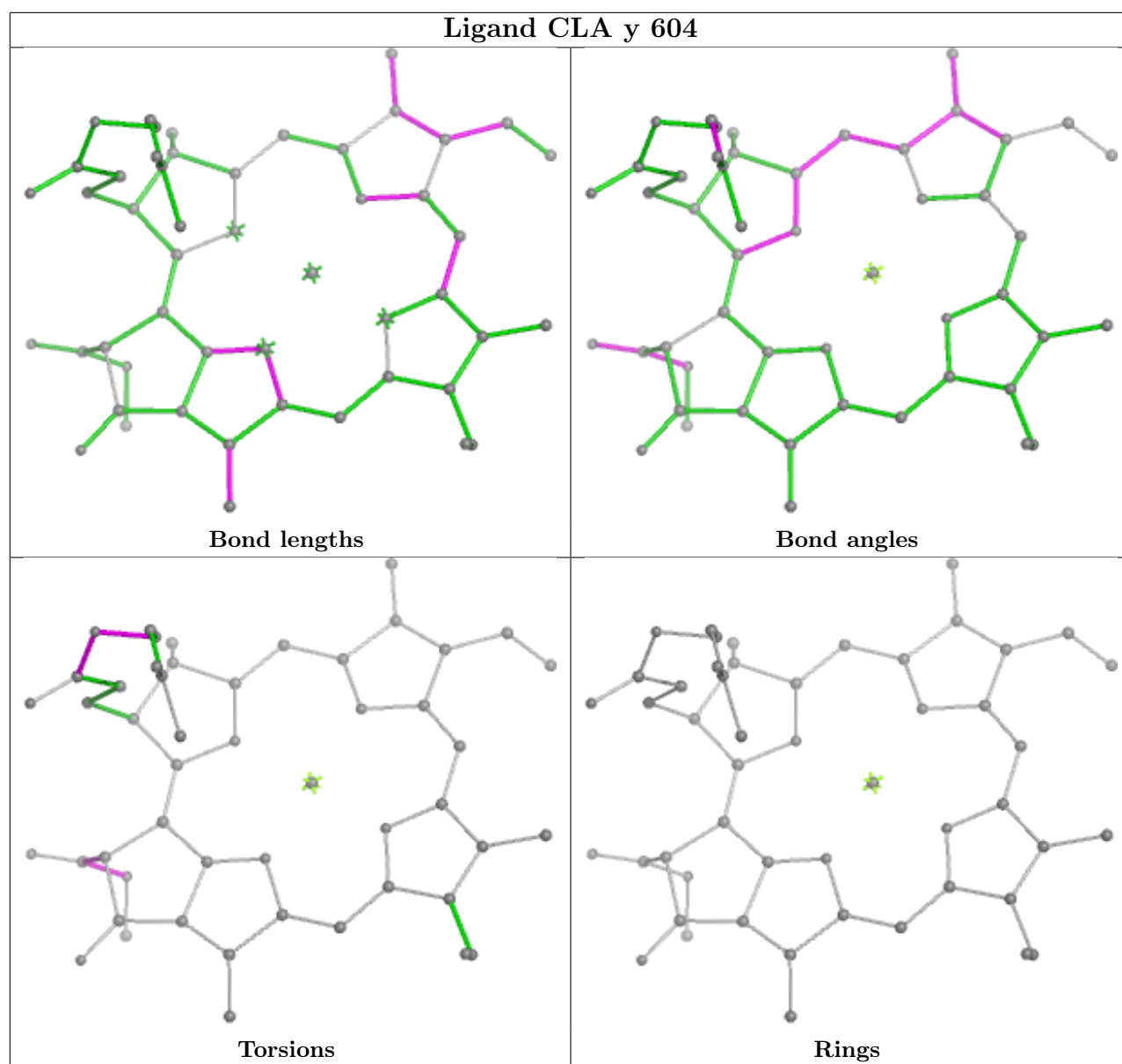
## Ligand CLA B 603

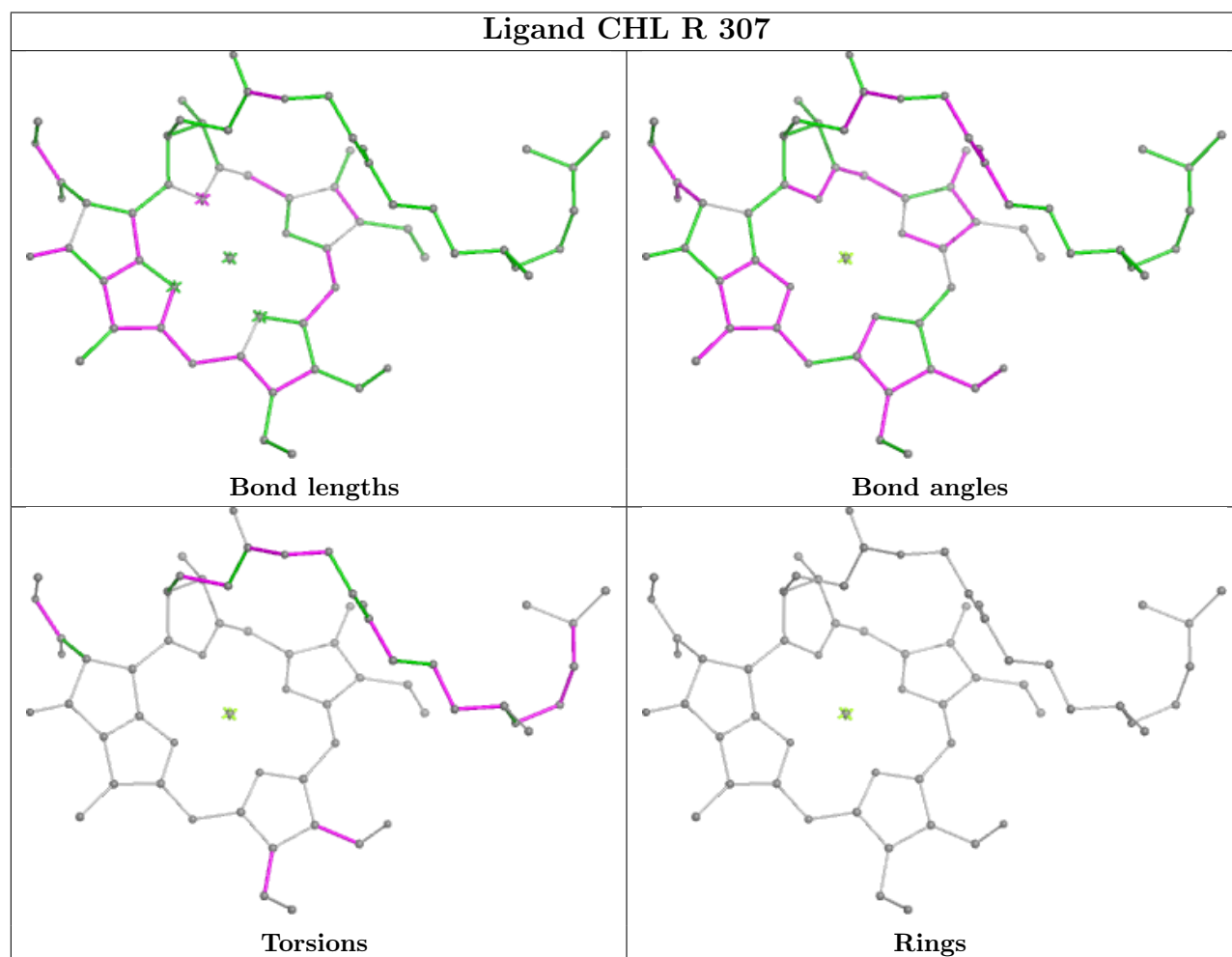
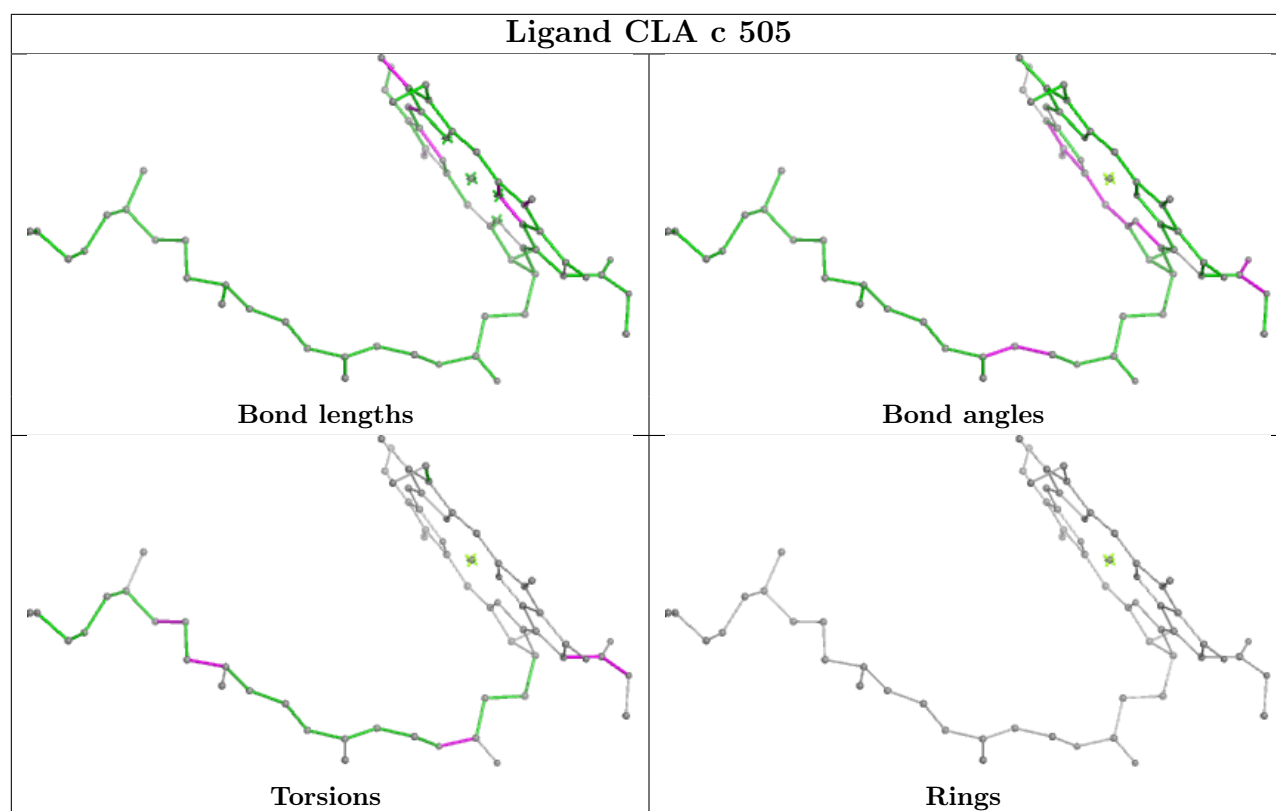


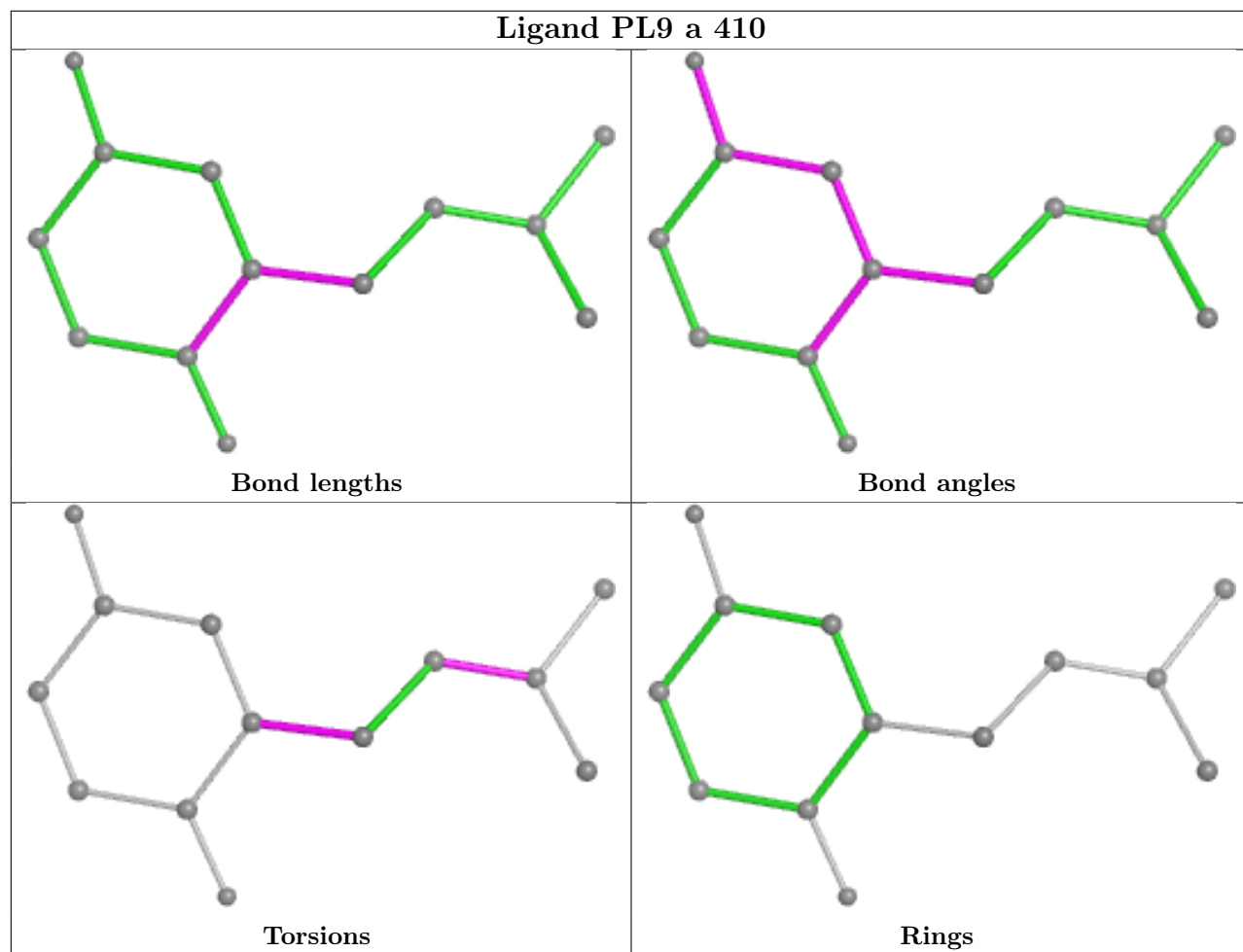


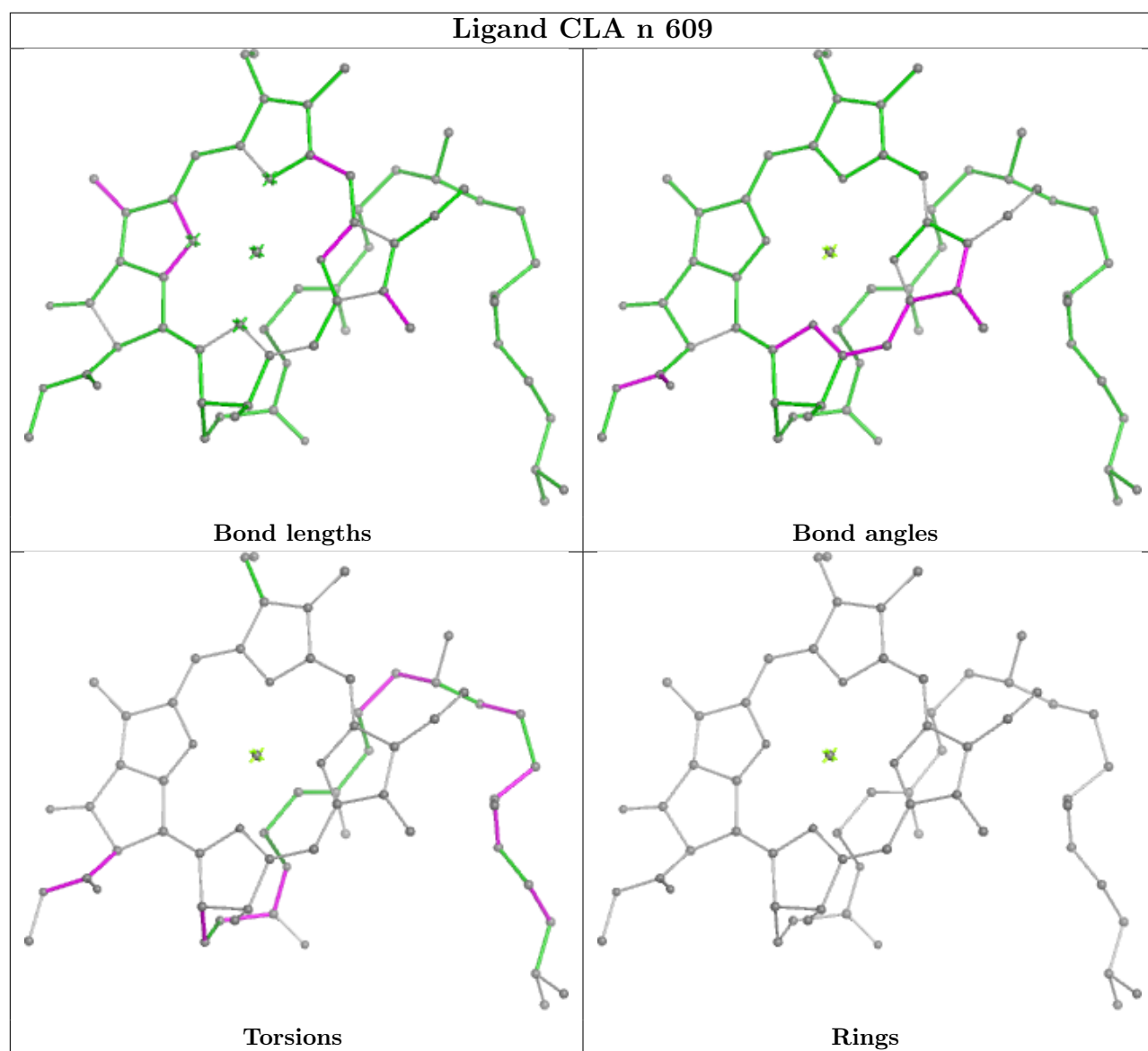




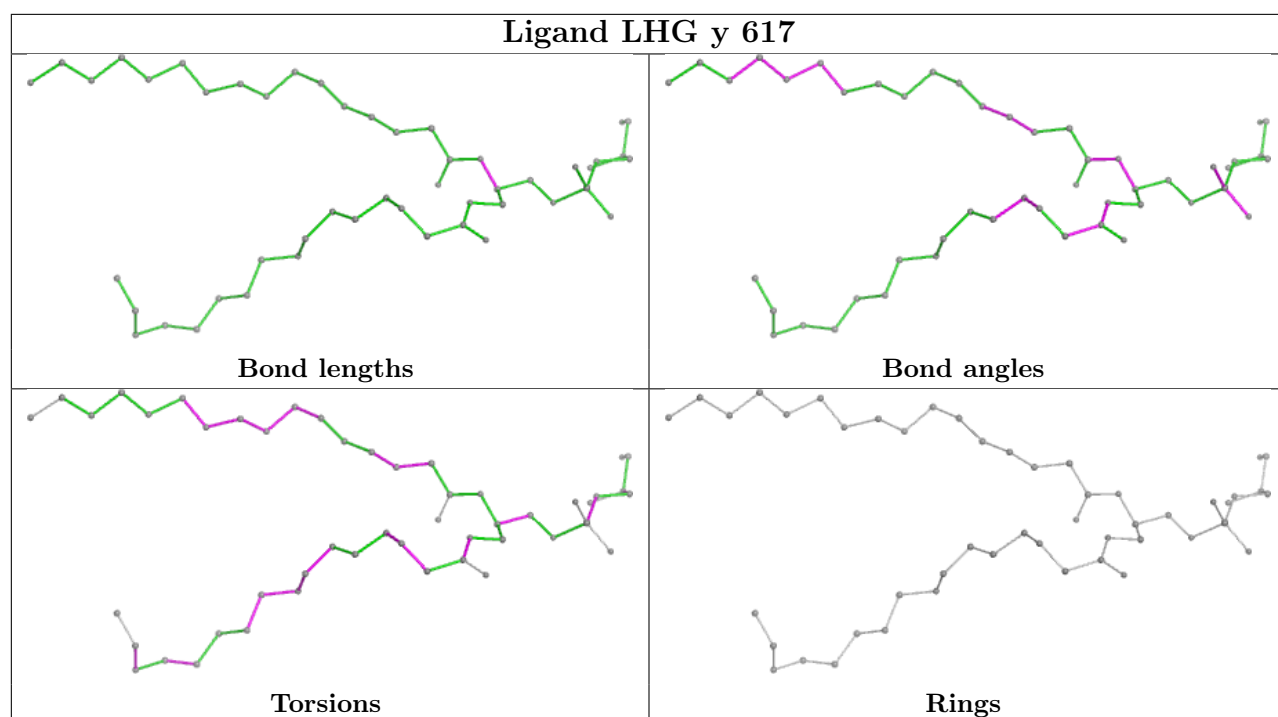




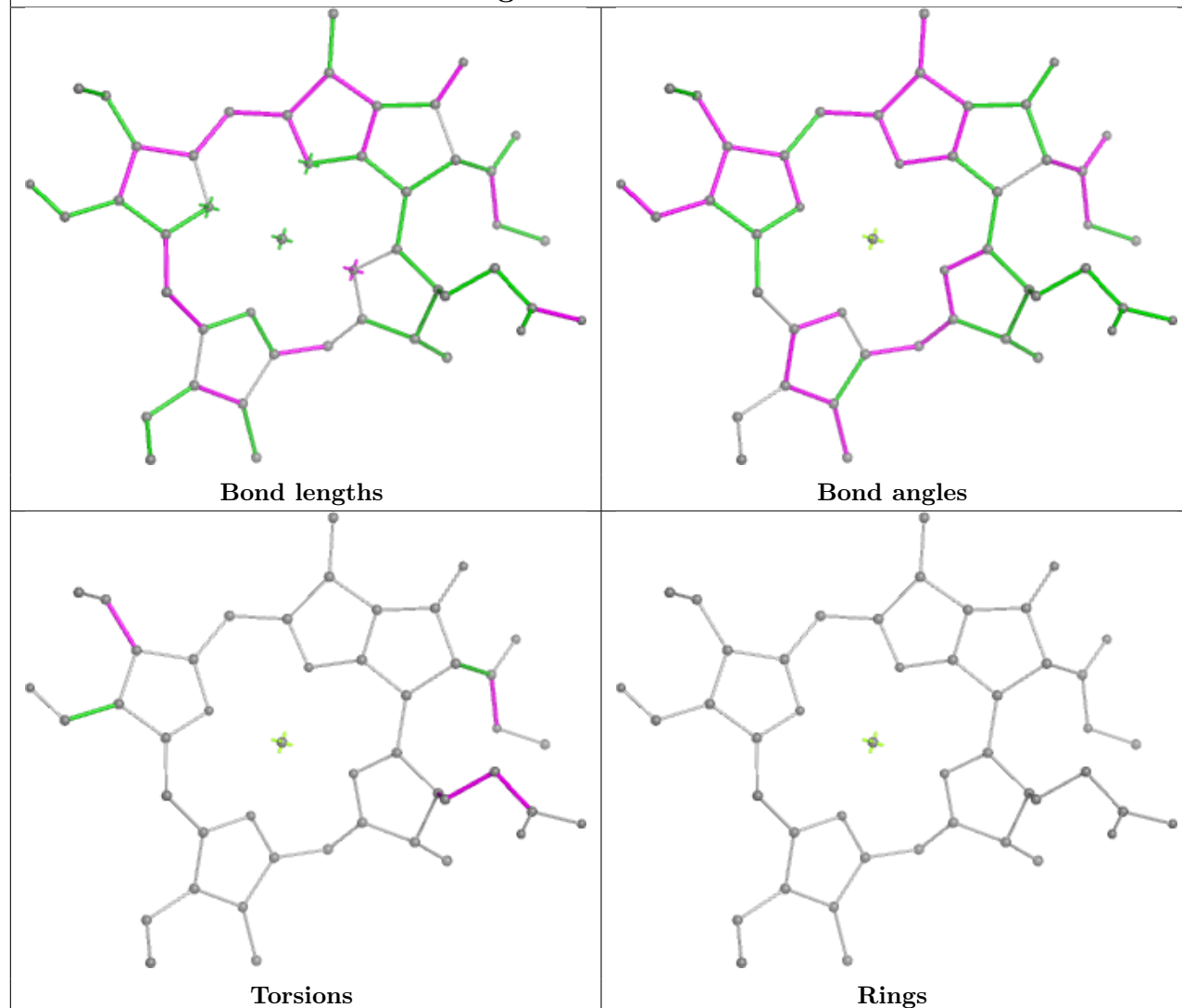




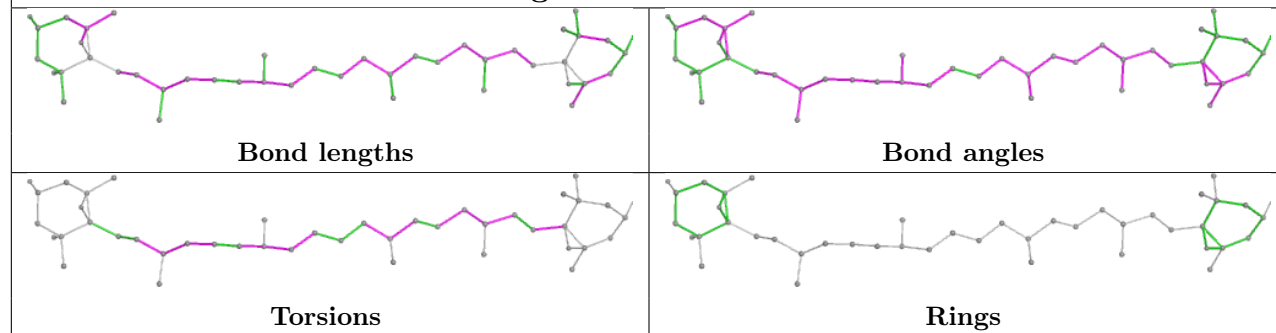


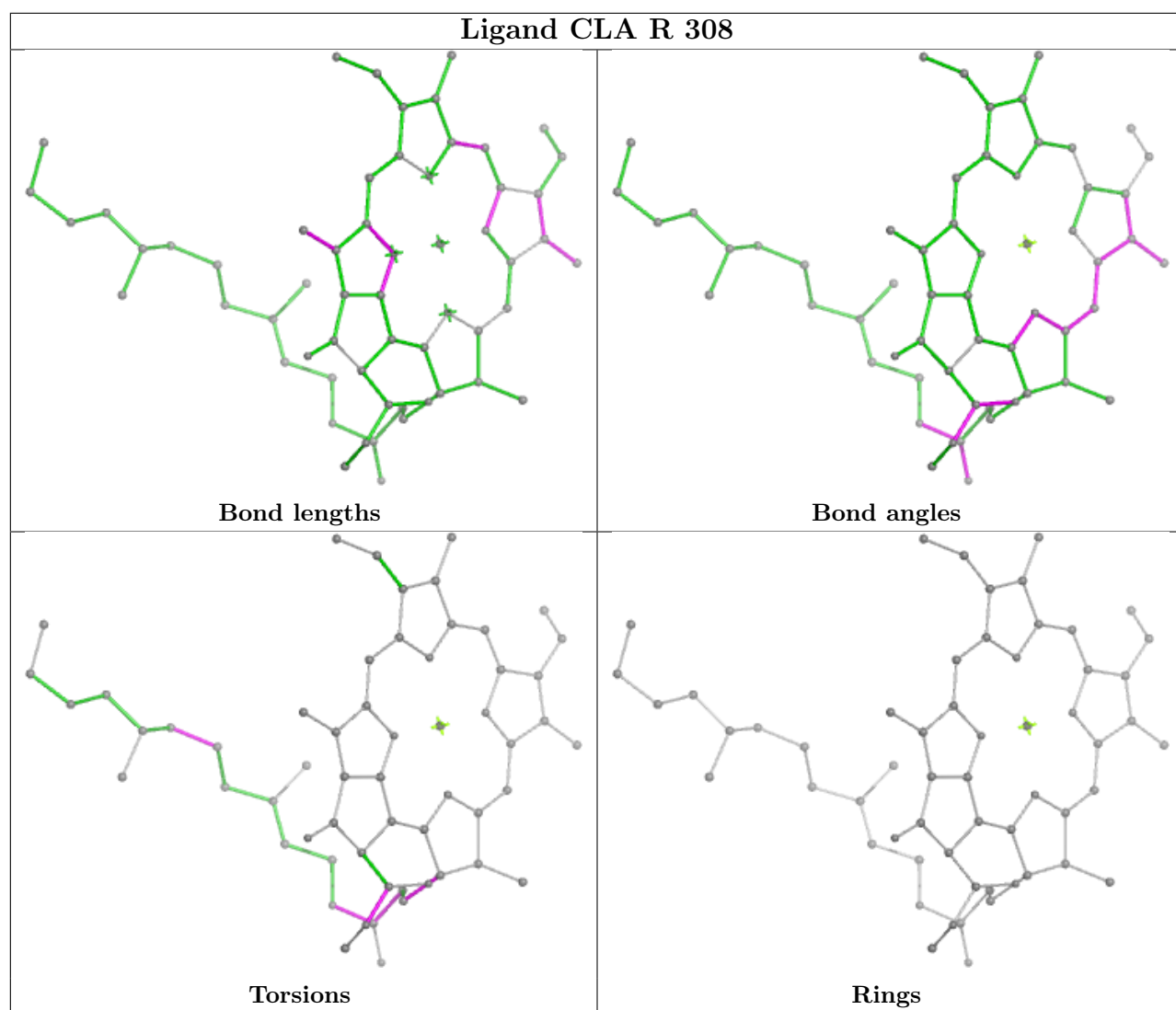


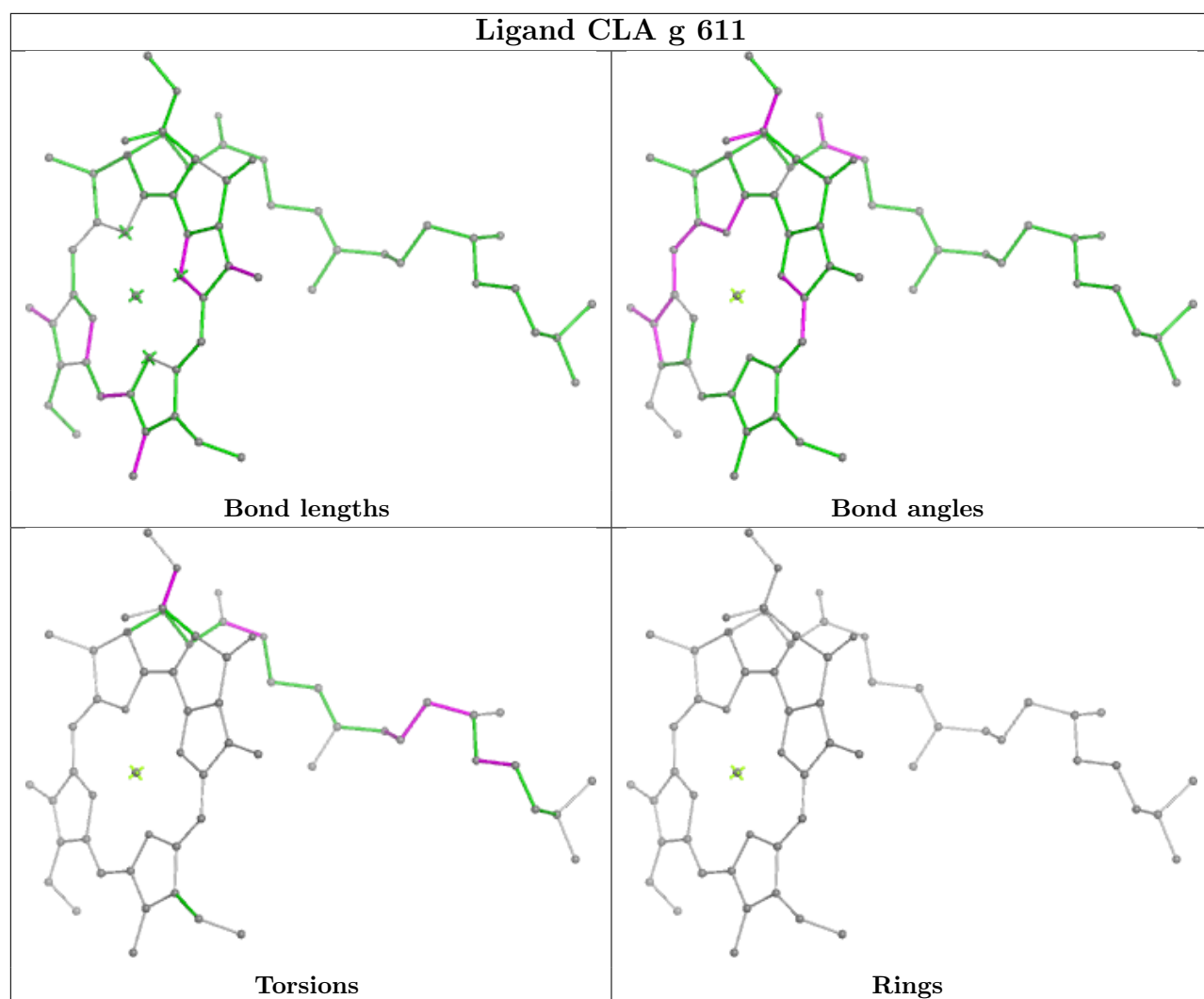
## Ligand CHL s 302



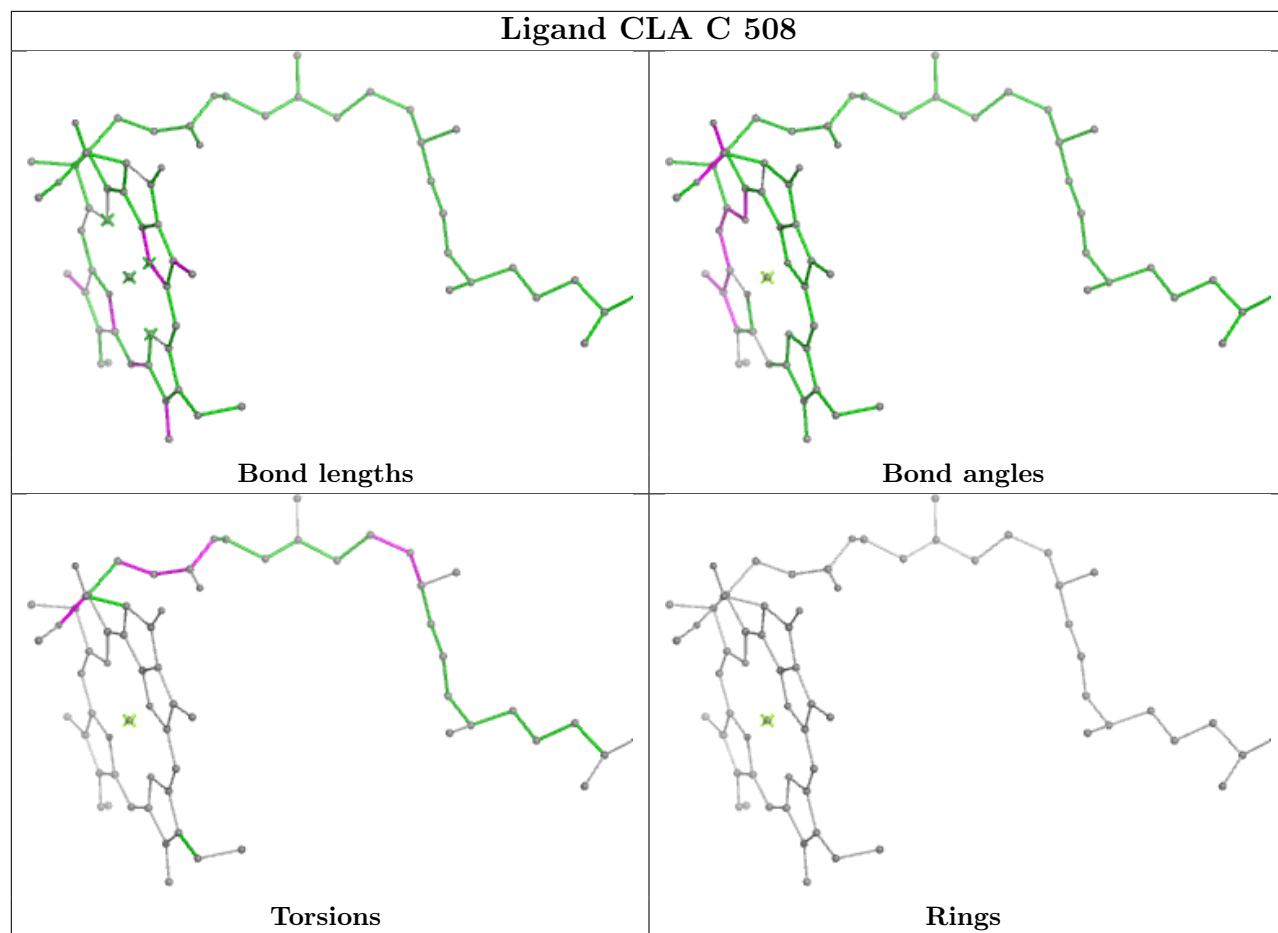
## Ligand XAT Y 615



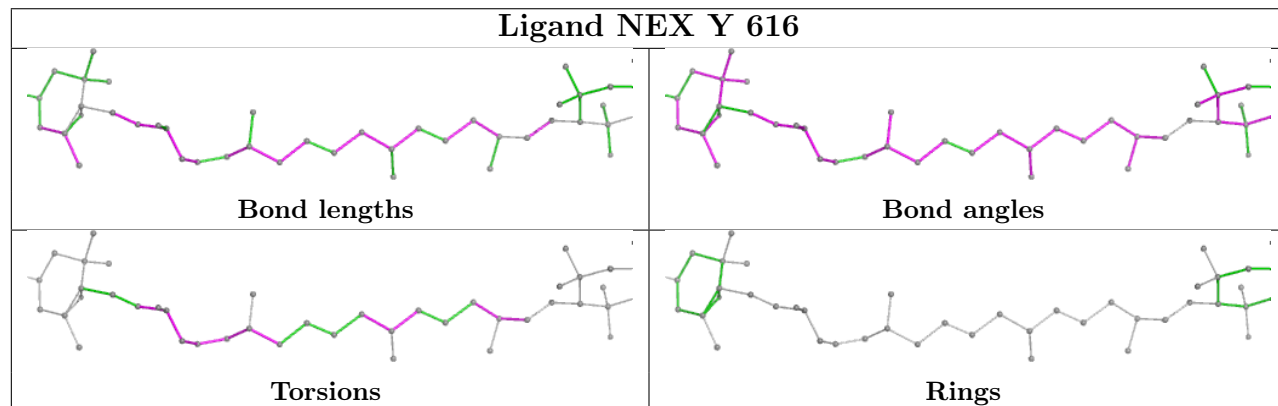


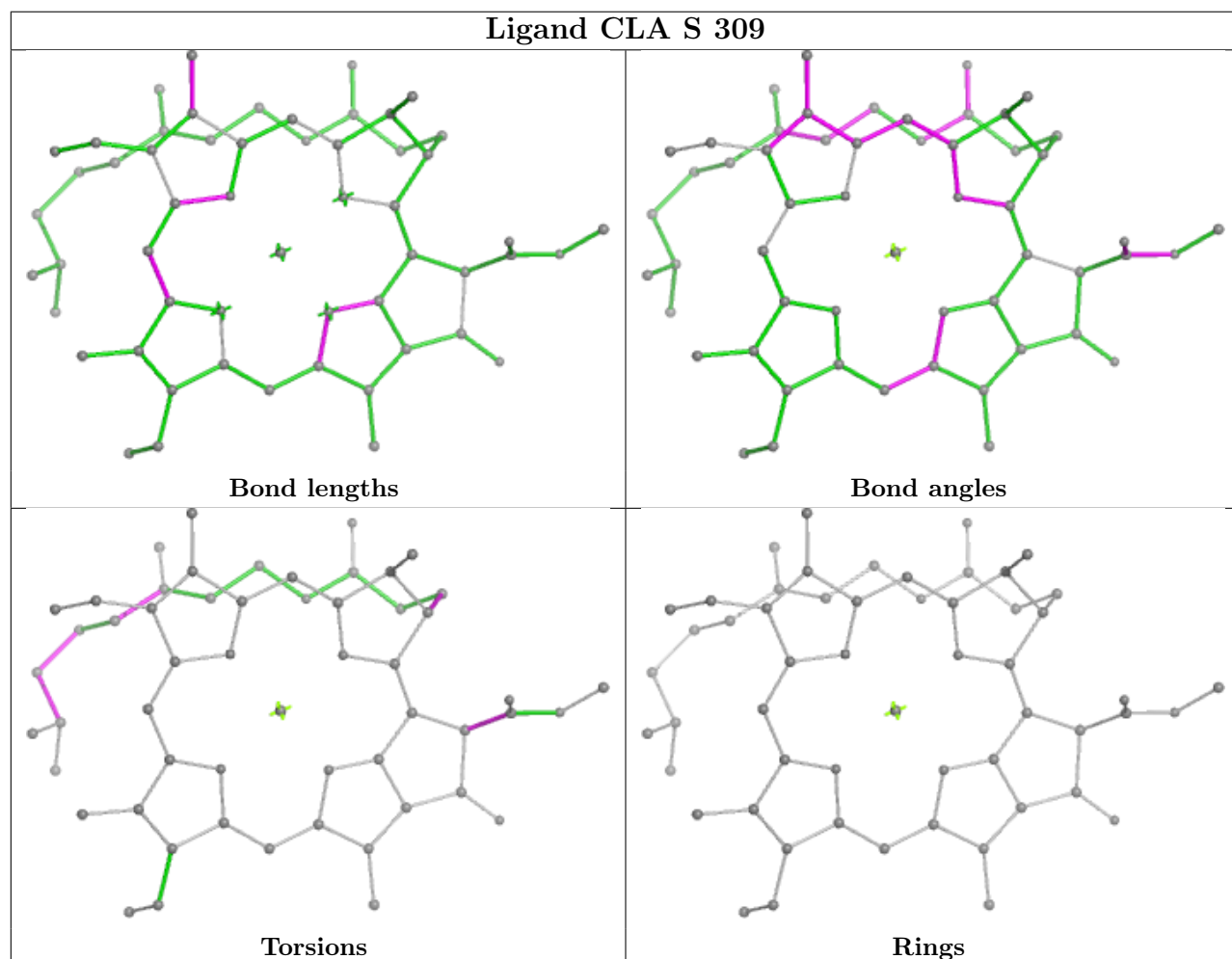
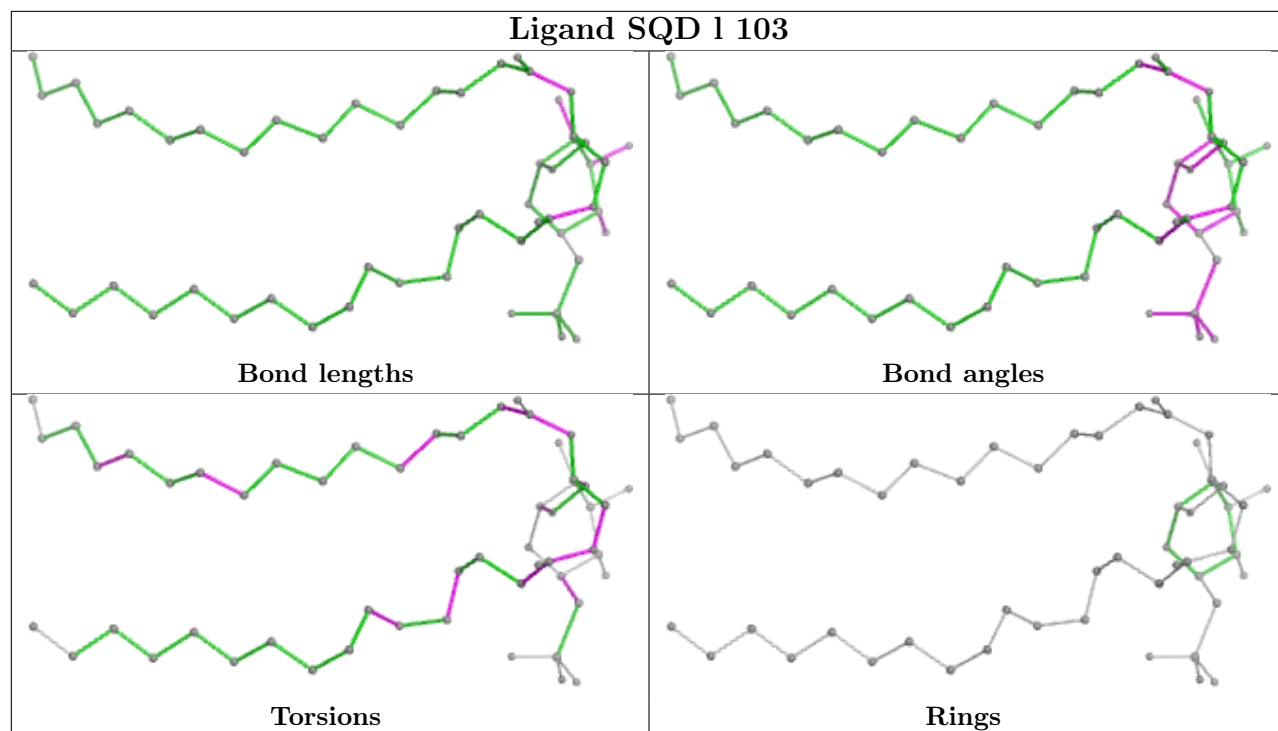


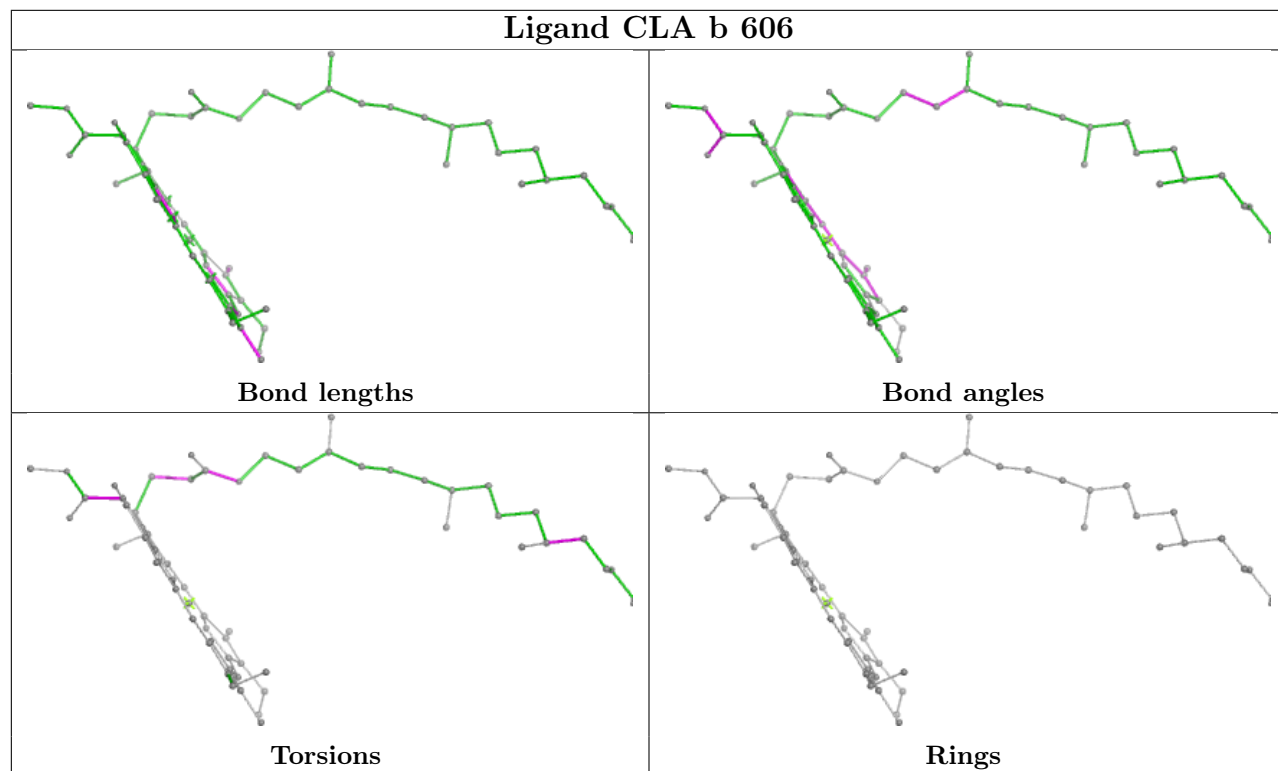
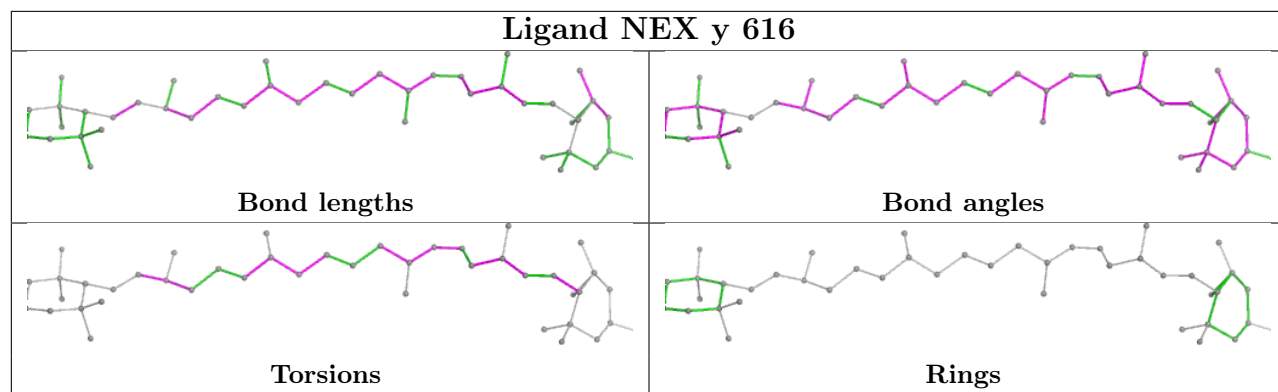
## Ligand CLA C 508

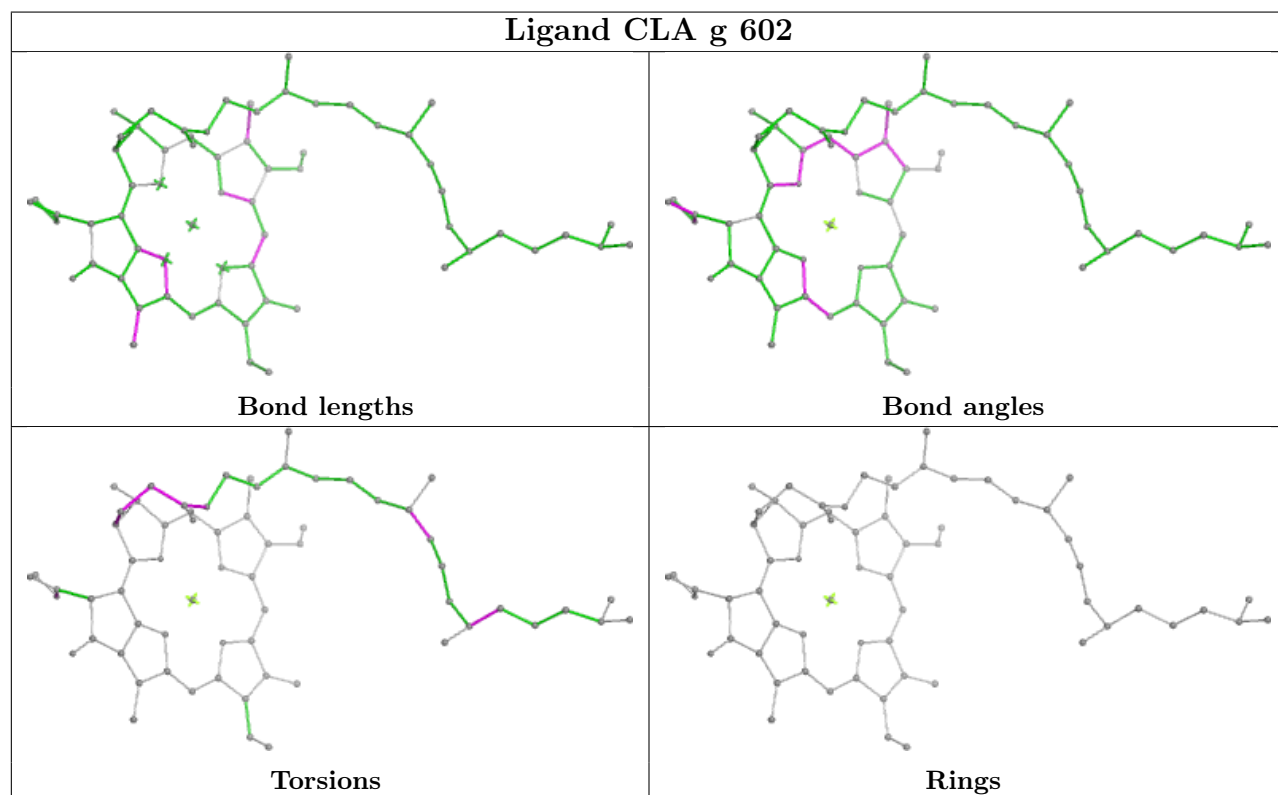
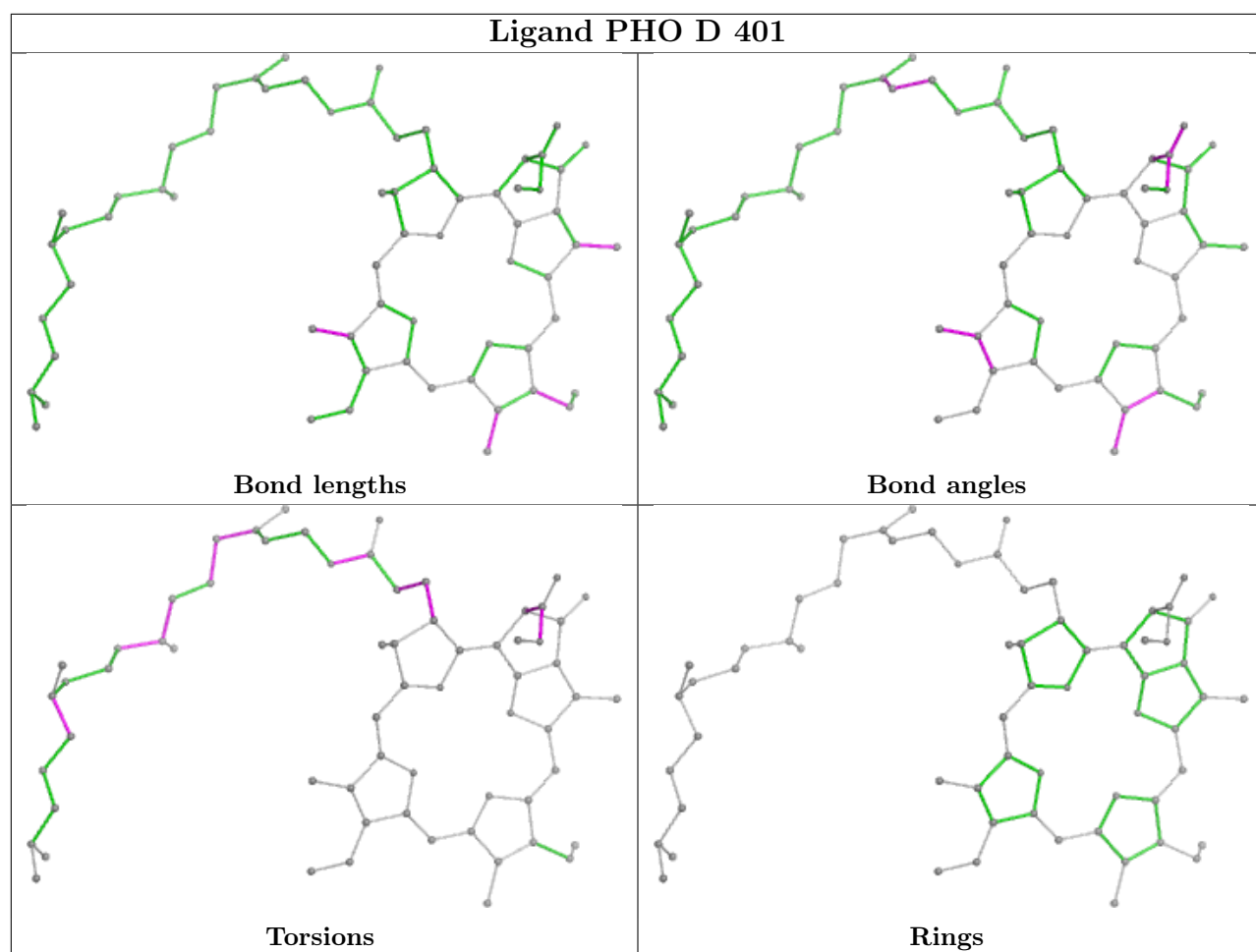


## Ligand NEX Y 616

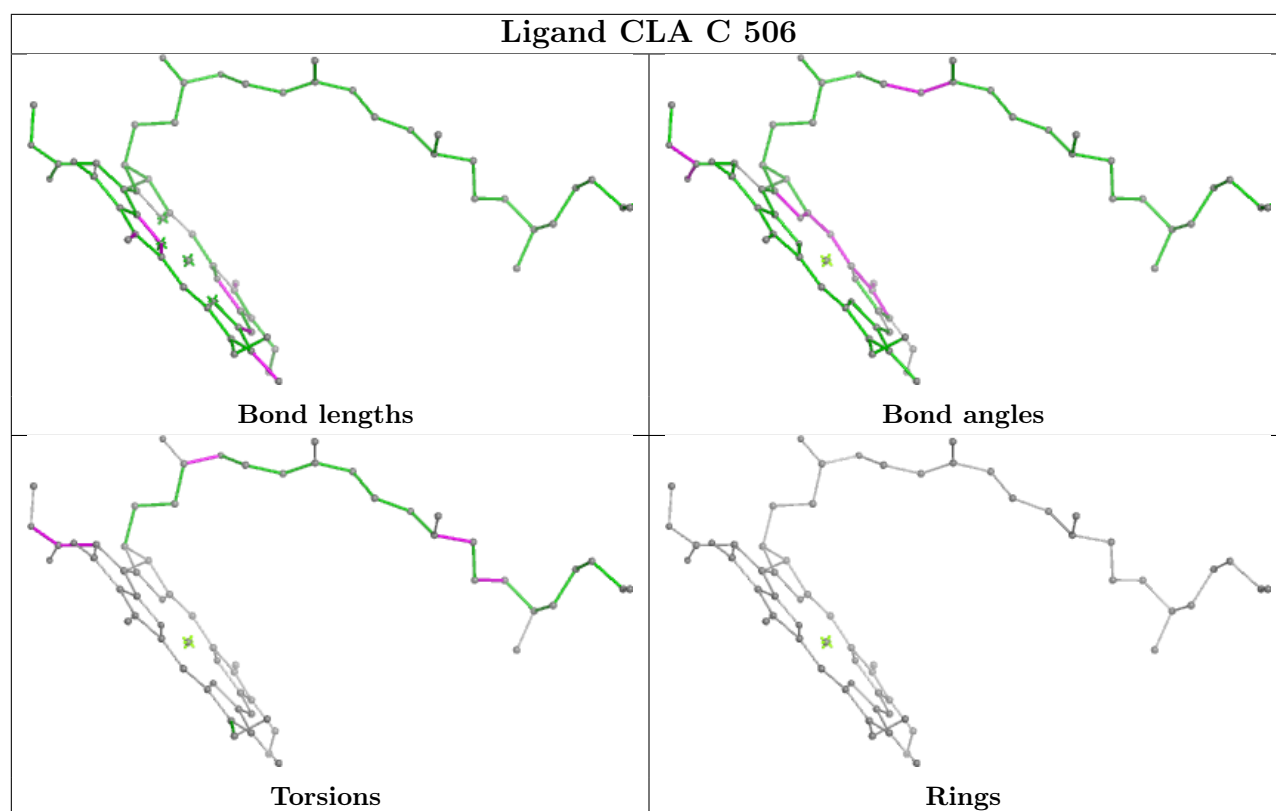




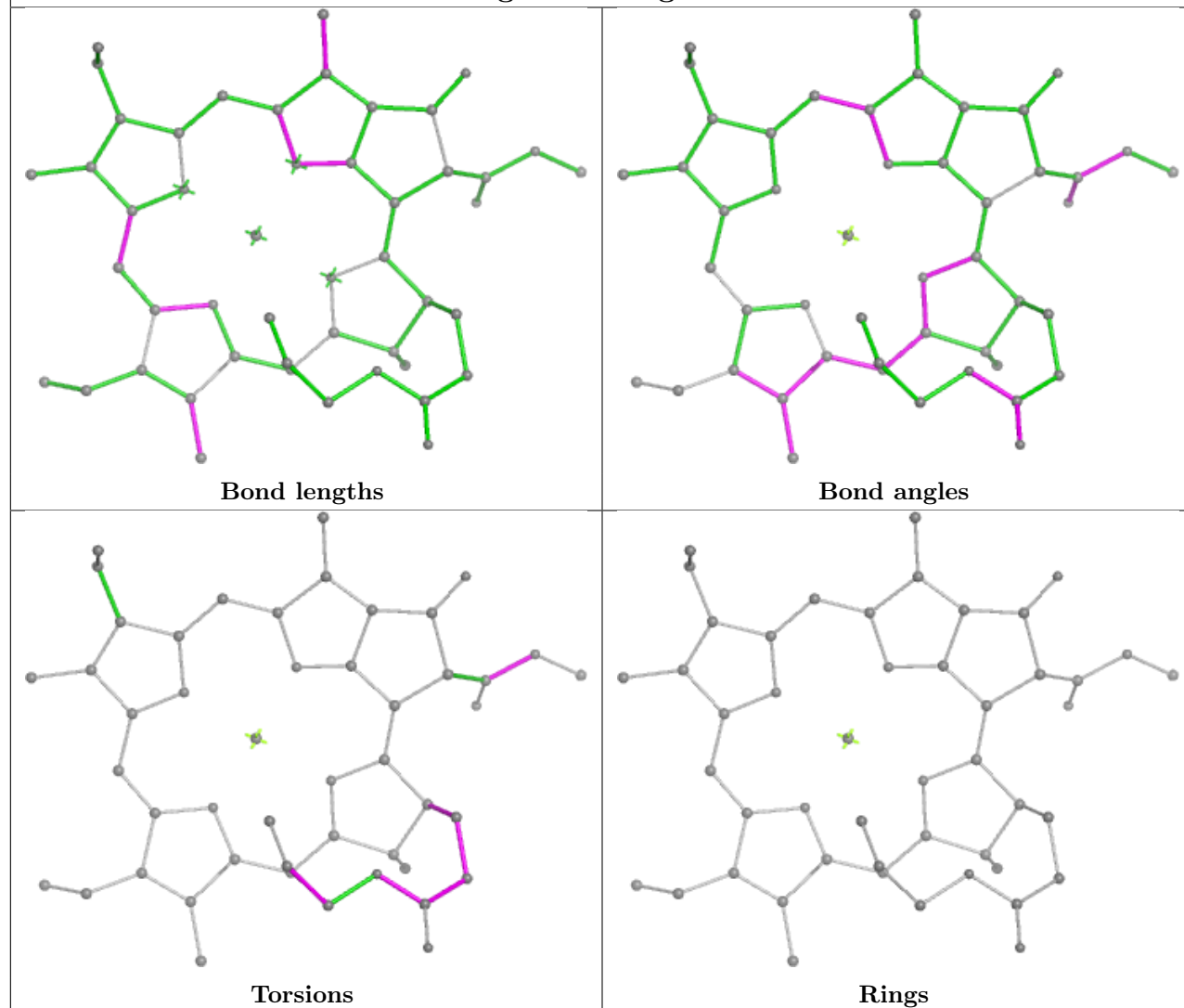


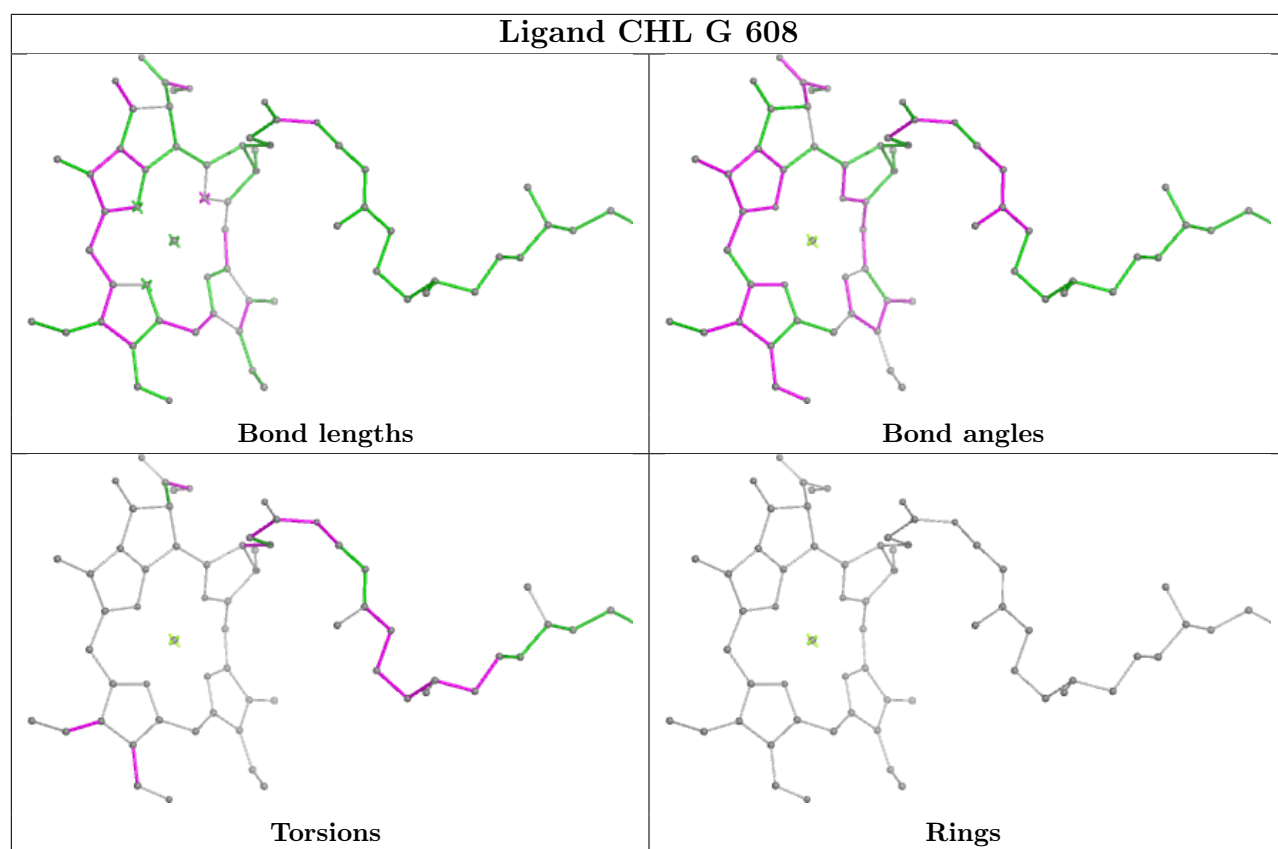


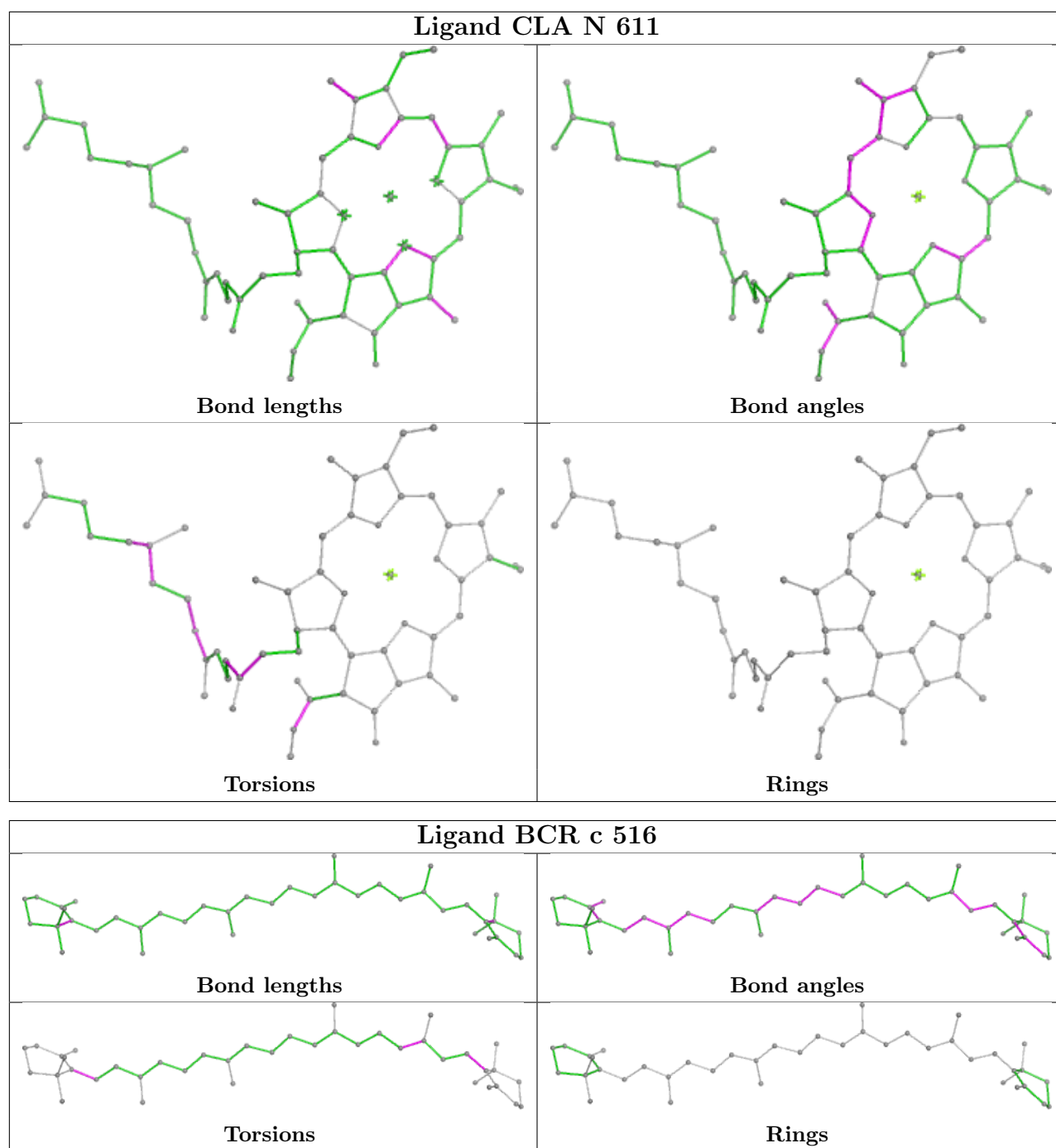


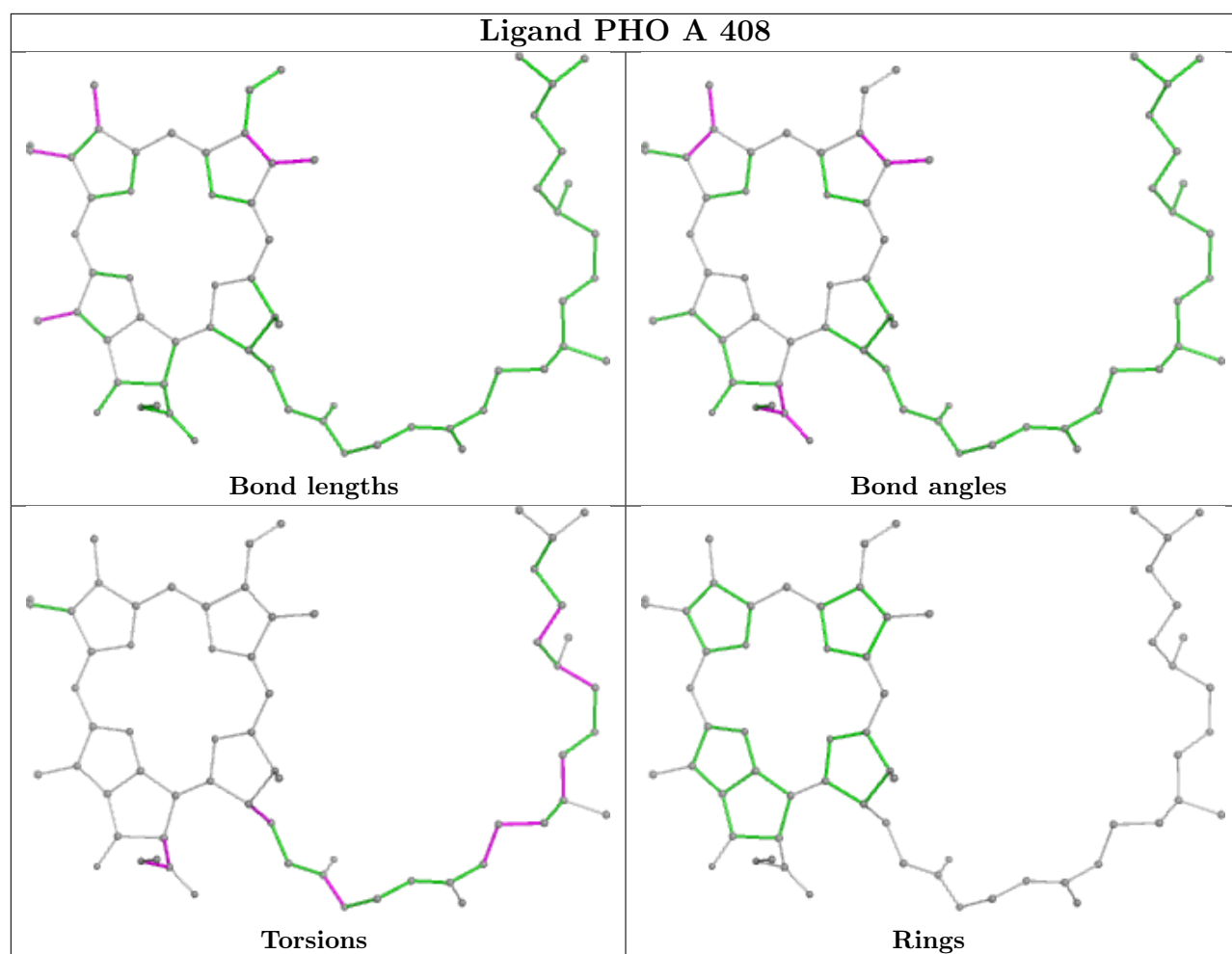


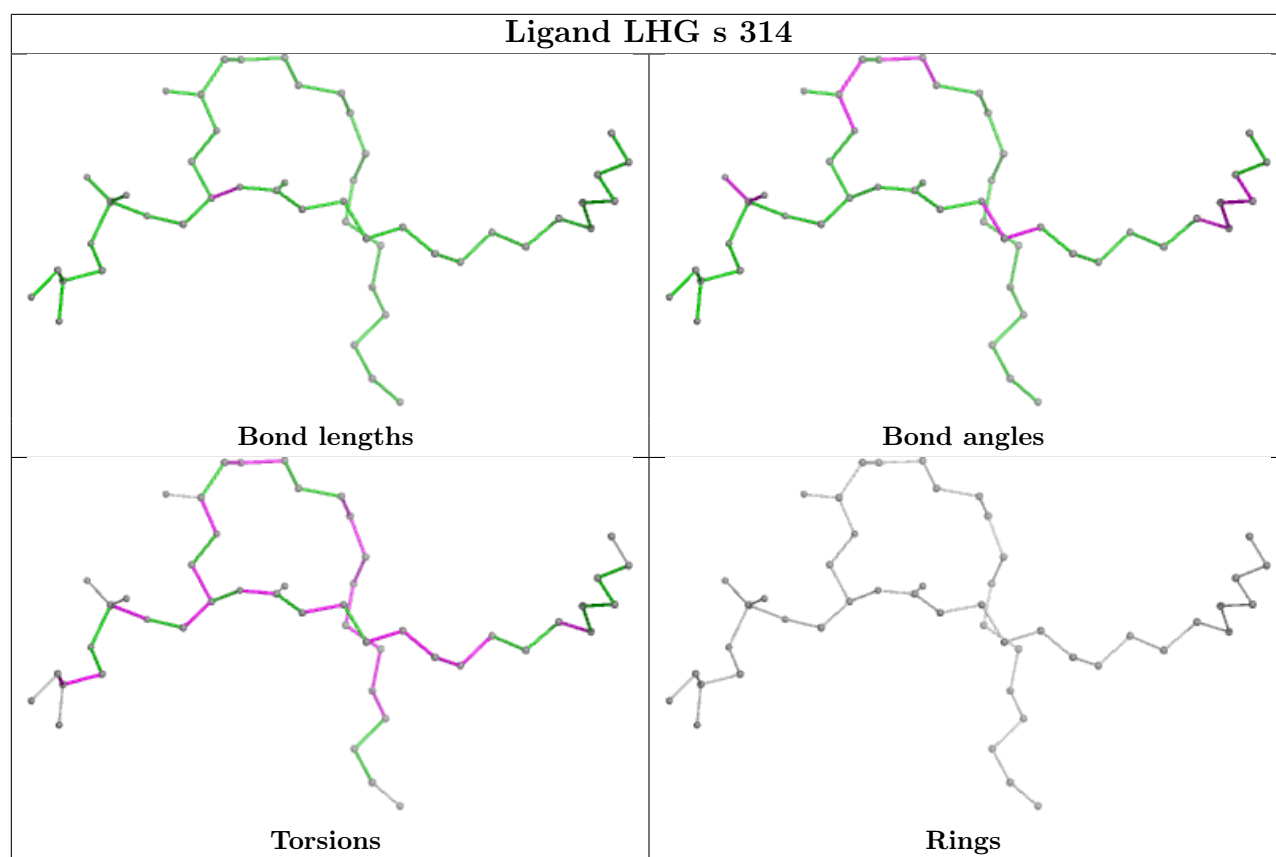
## Ligand CLA g 614

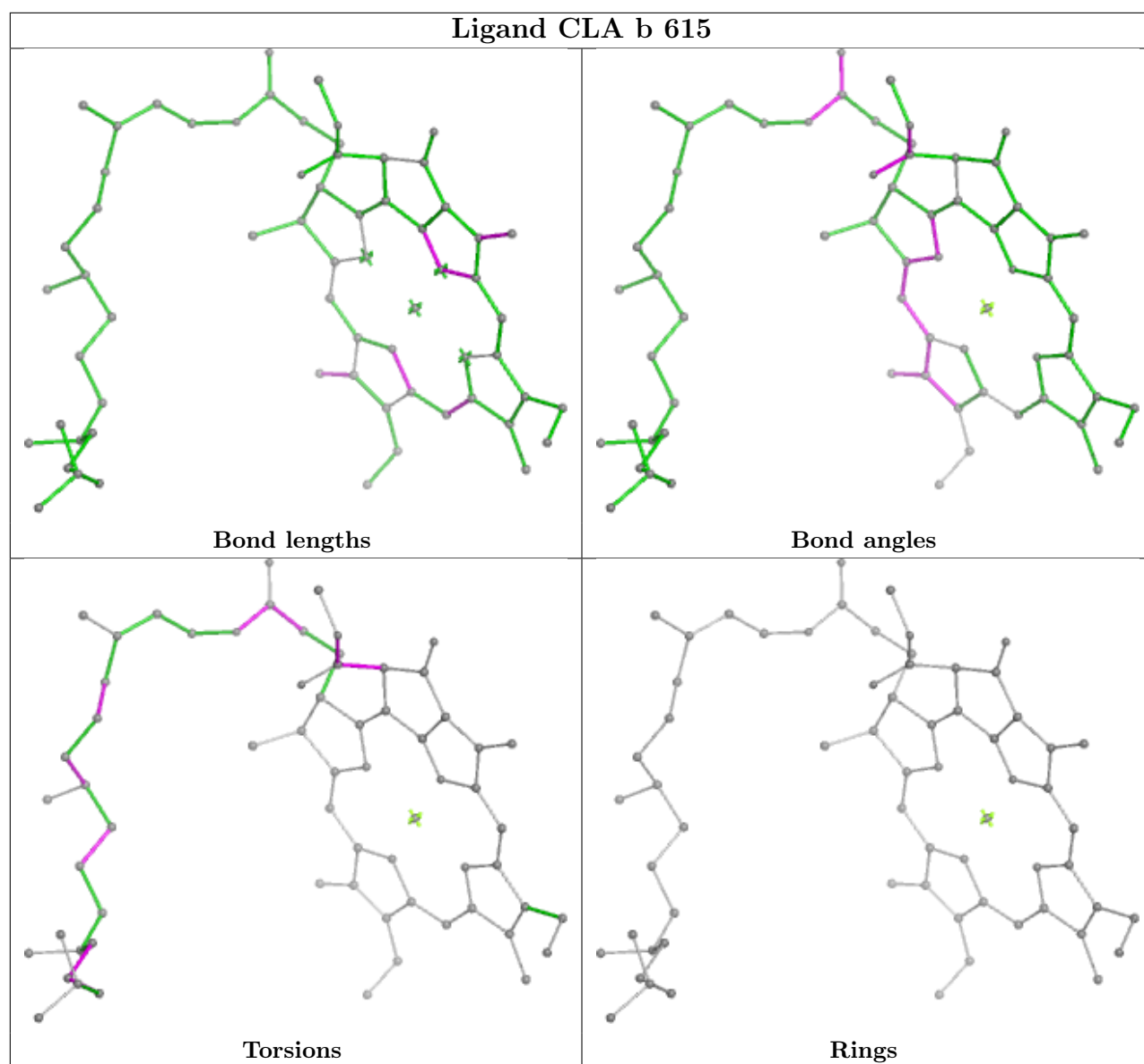


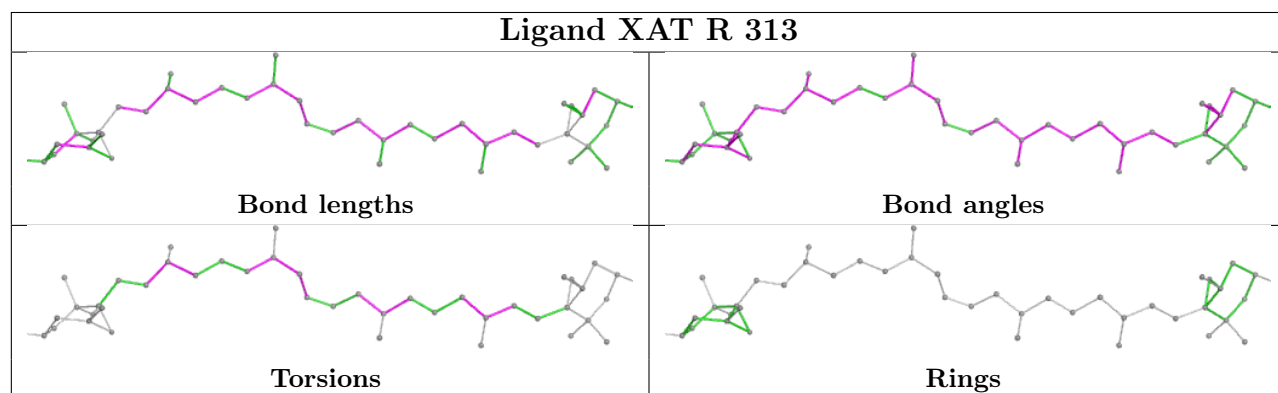
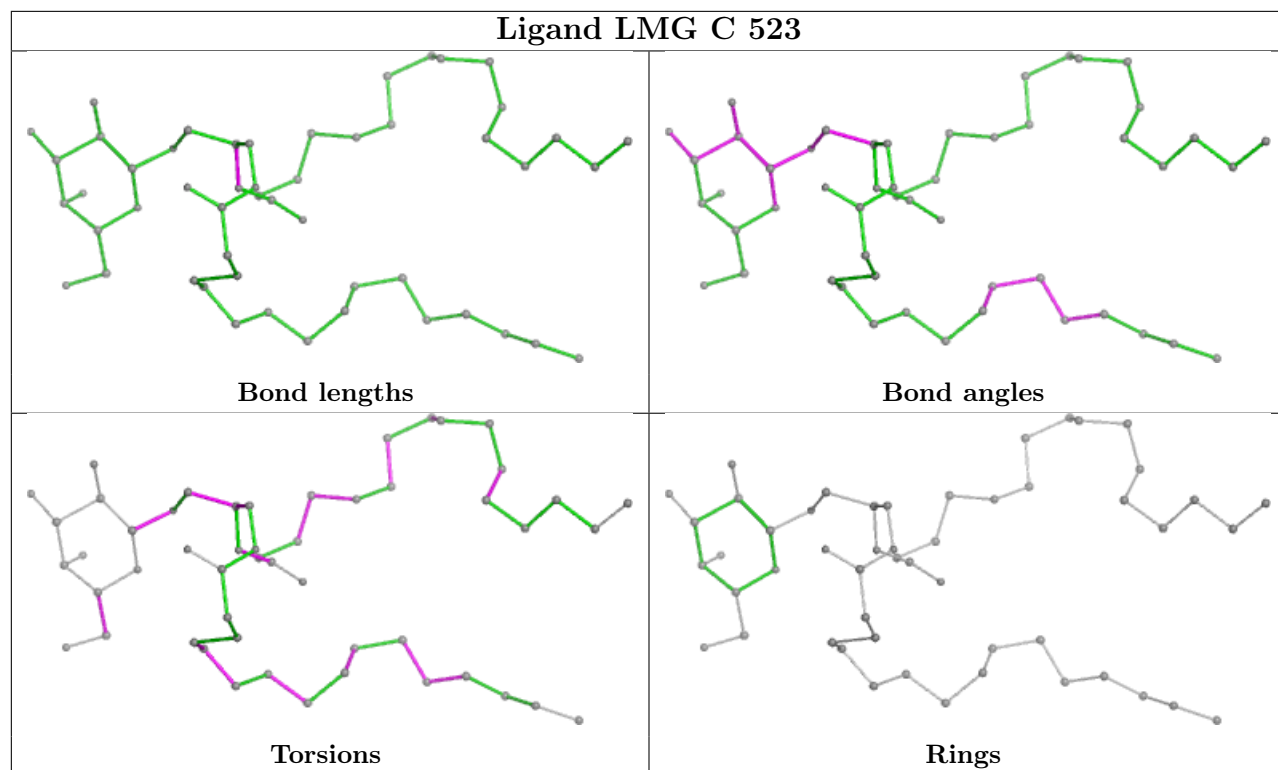




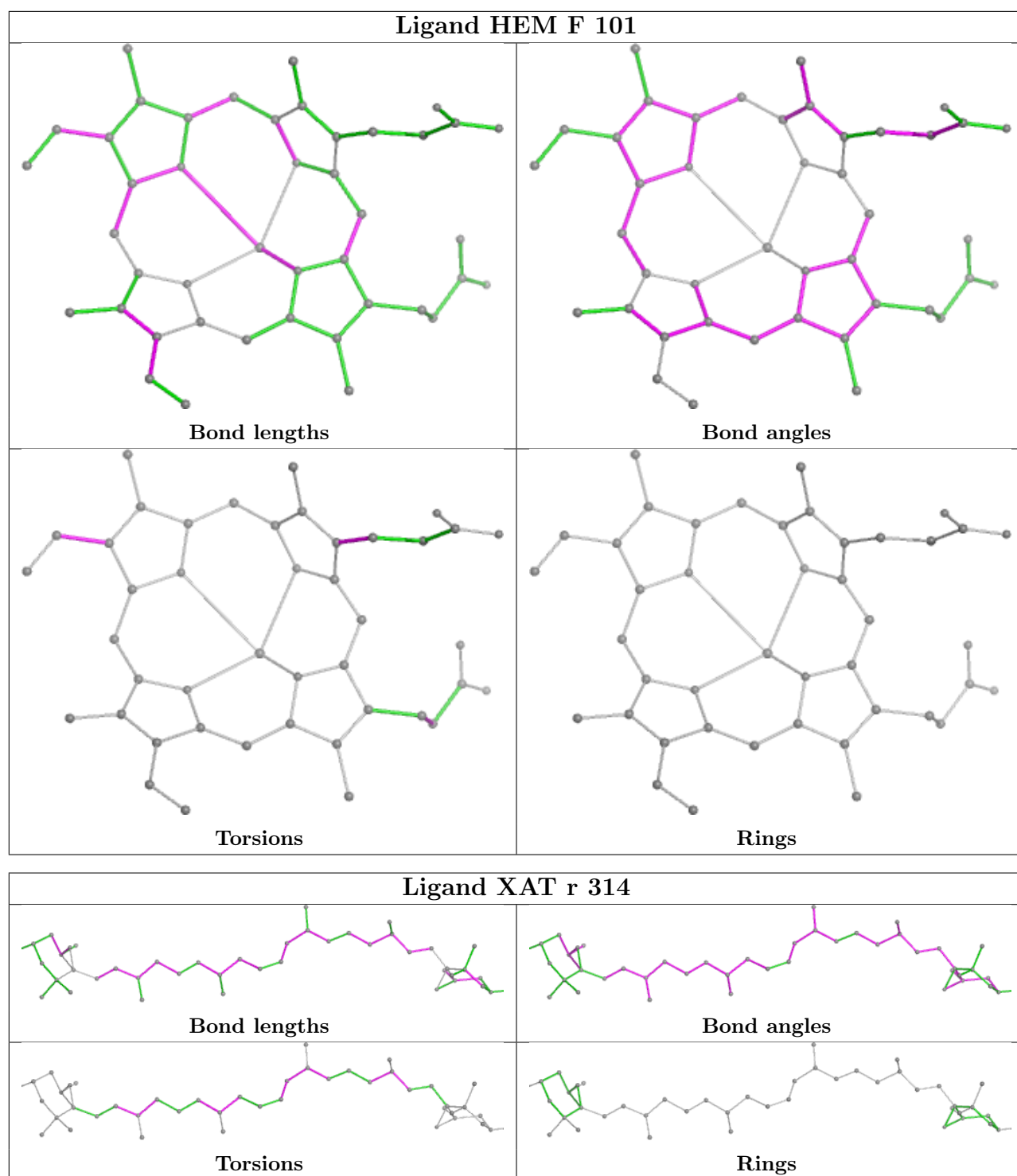


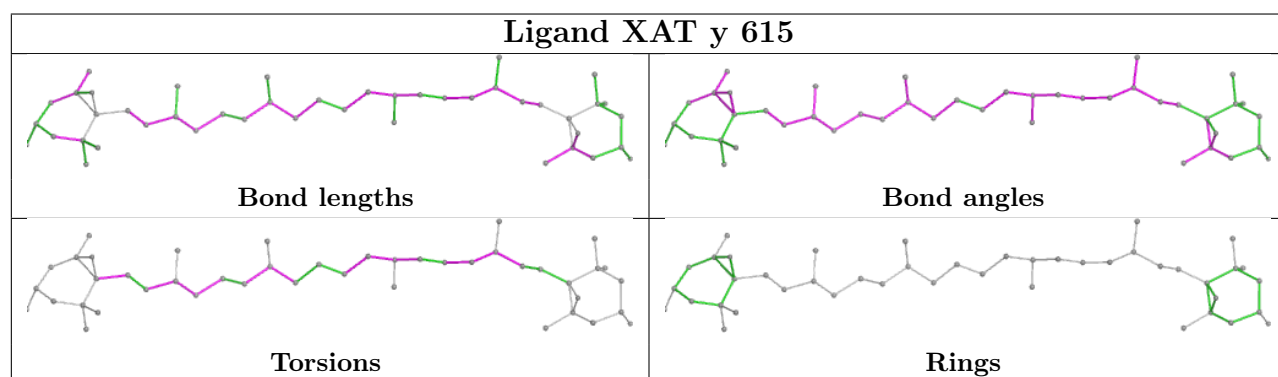
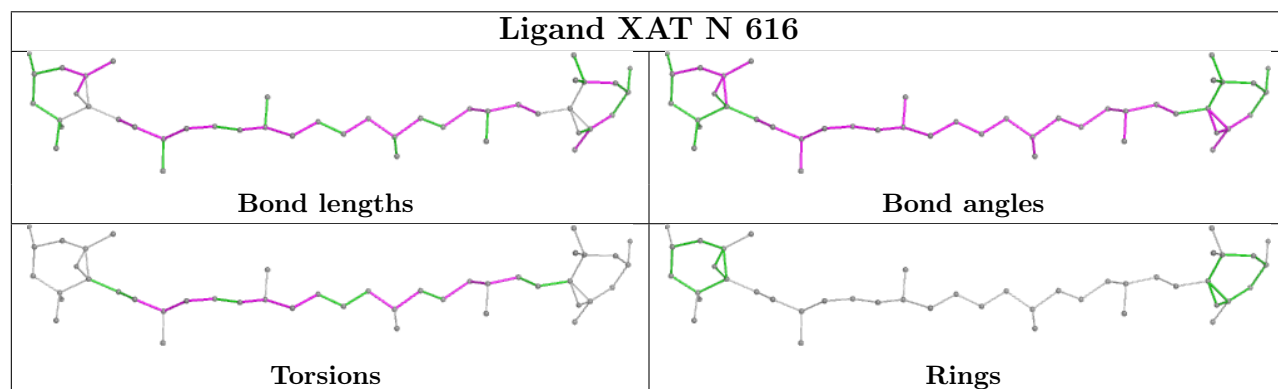
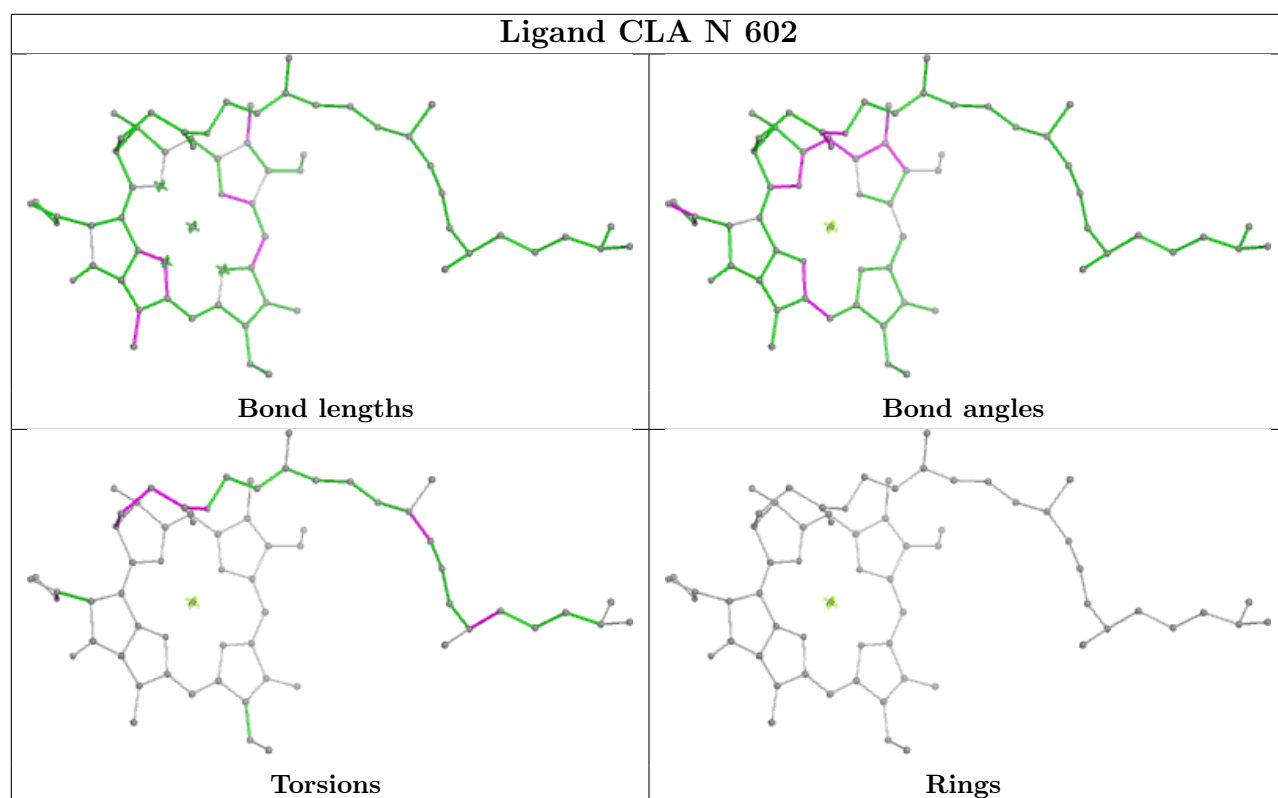


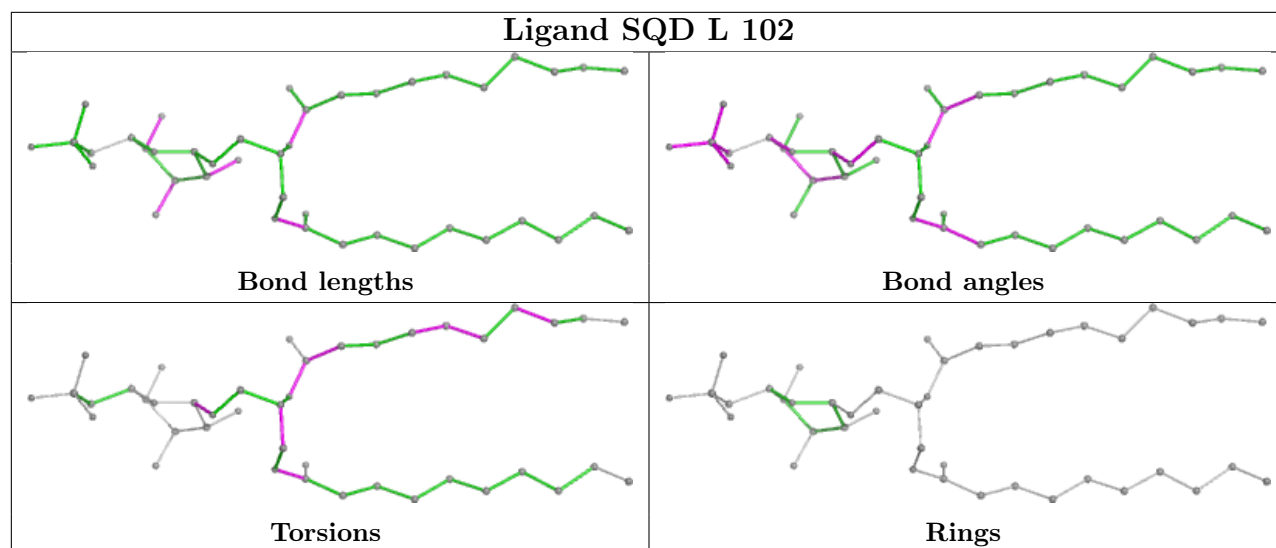
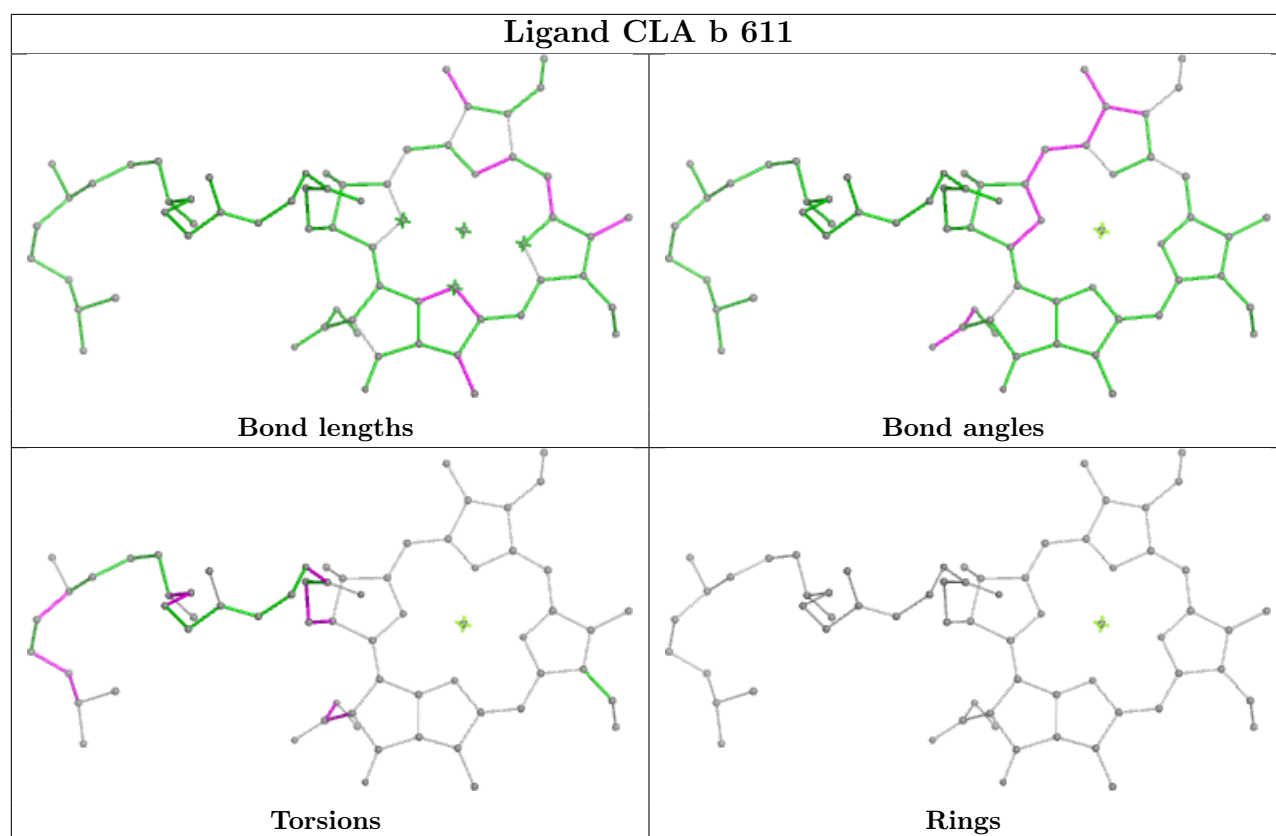


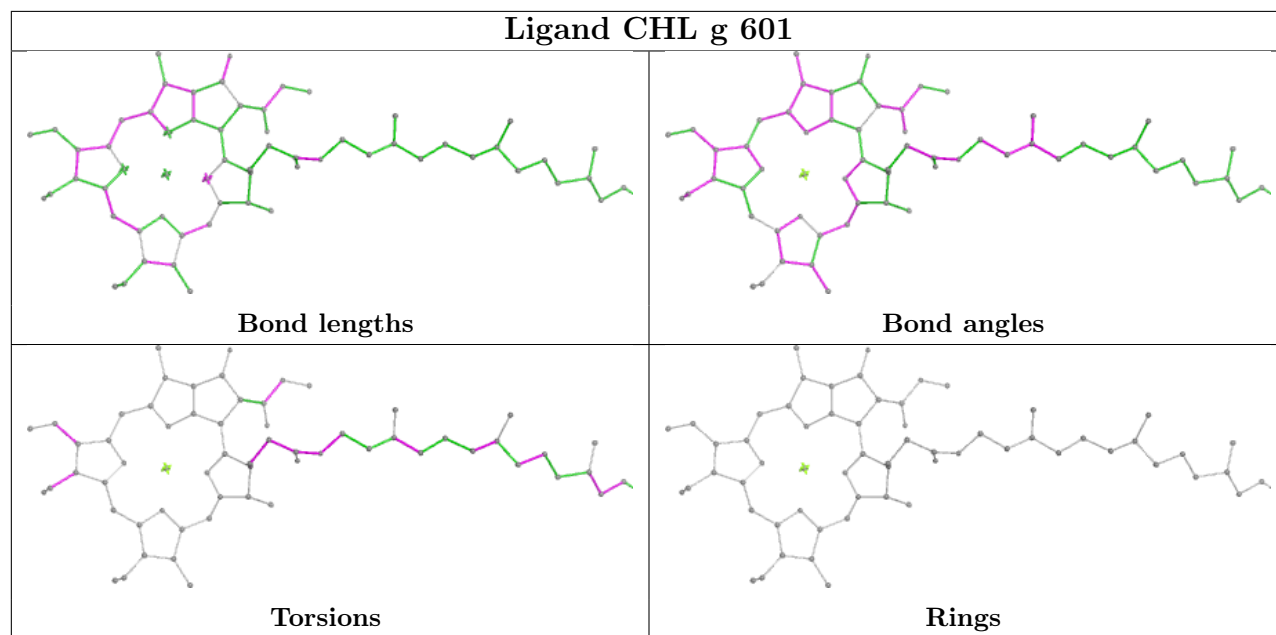
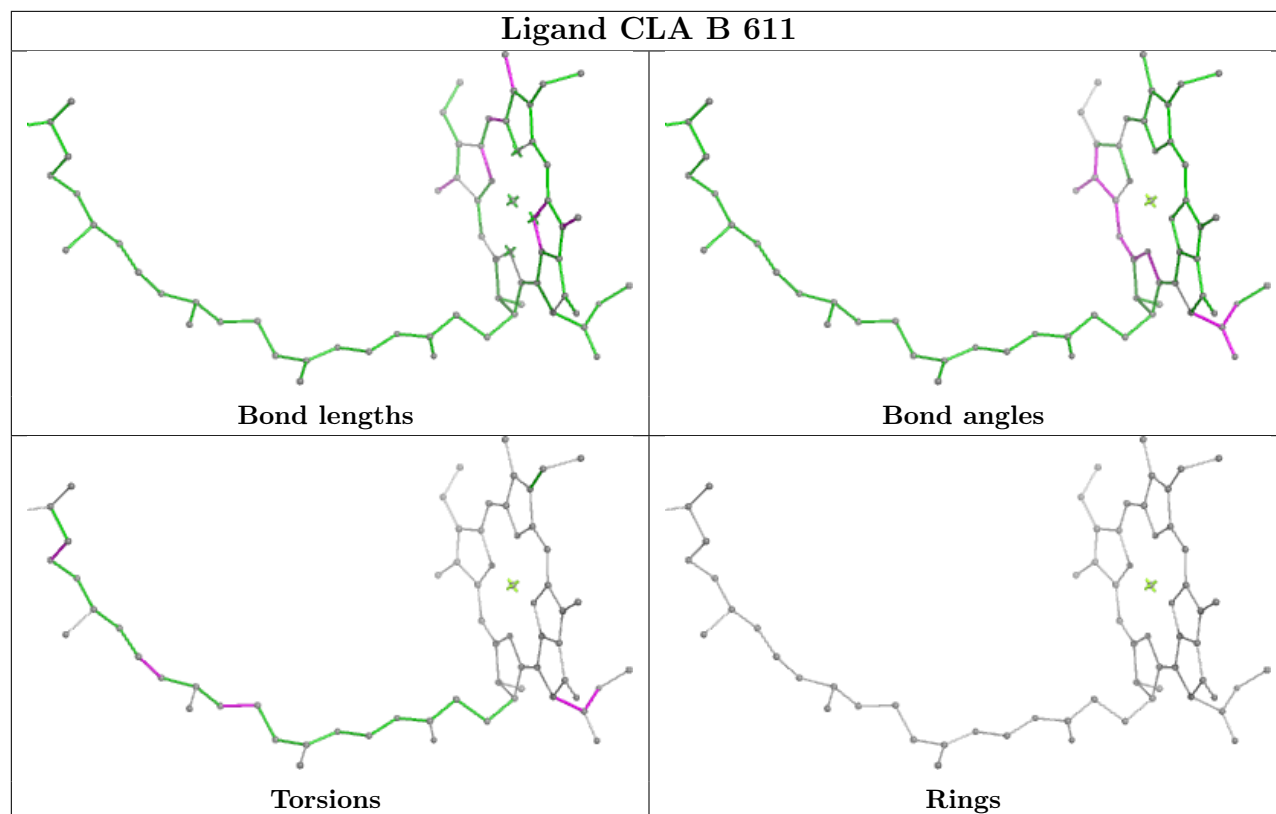




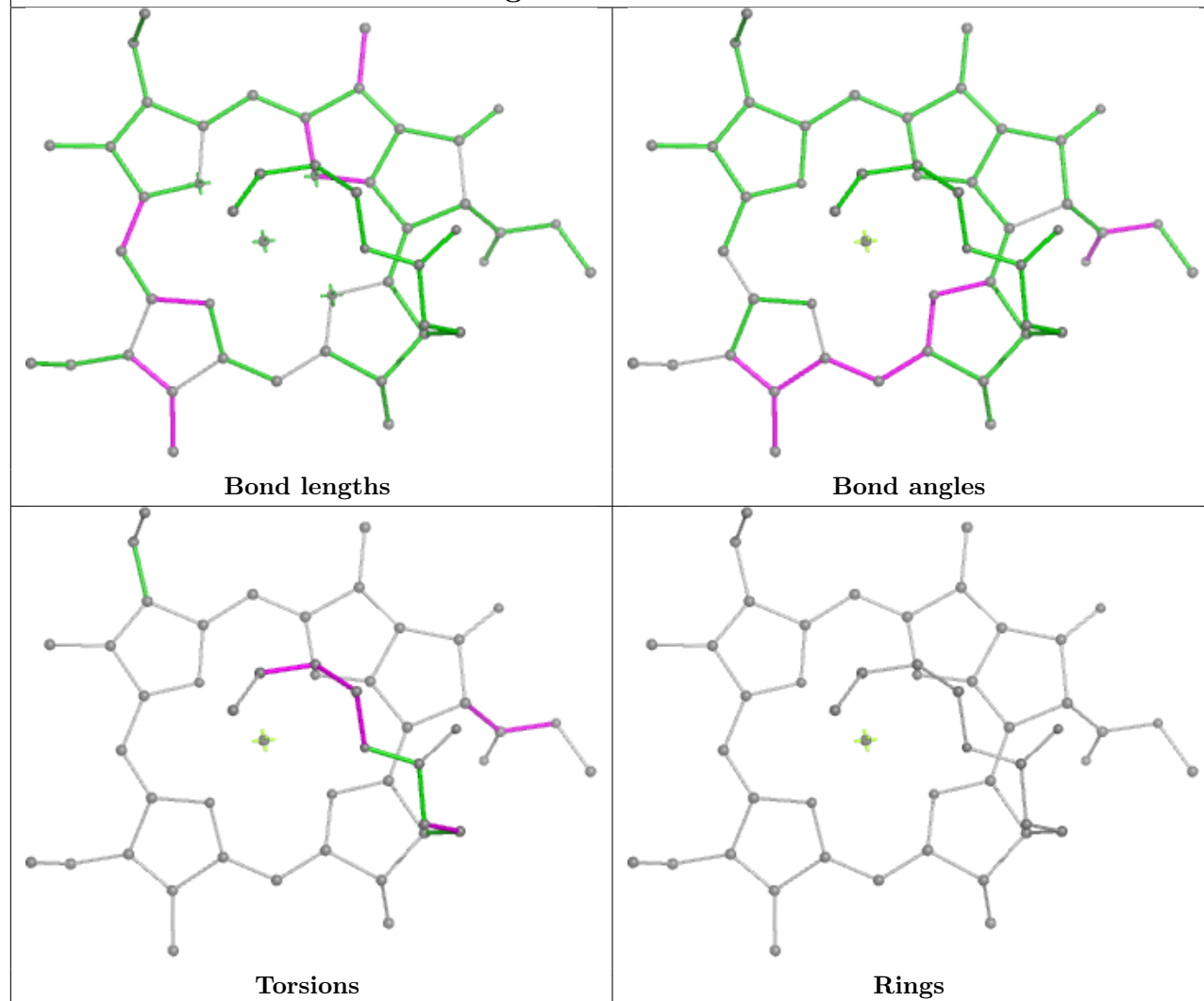




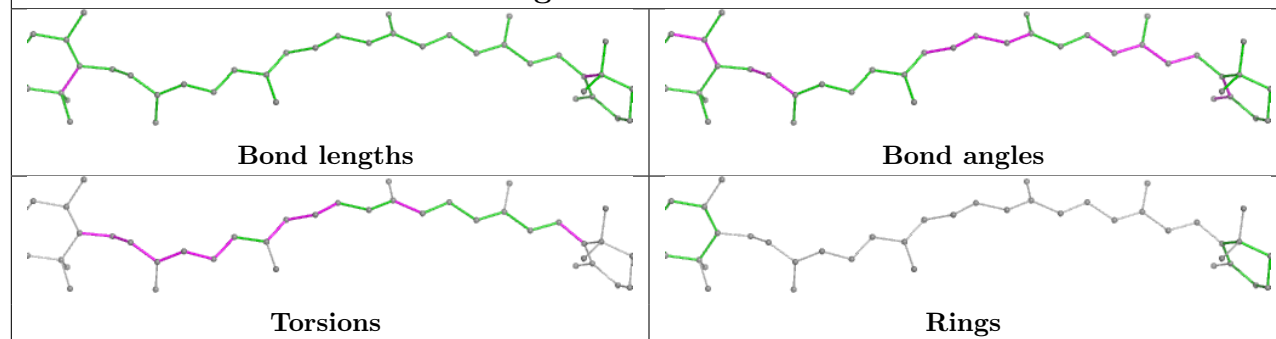


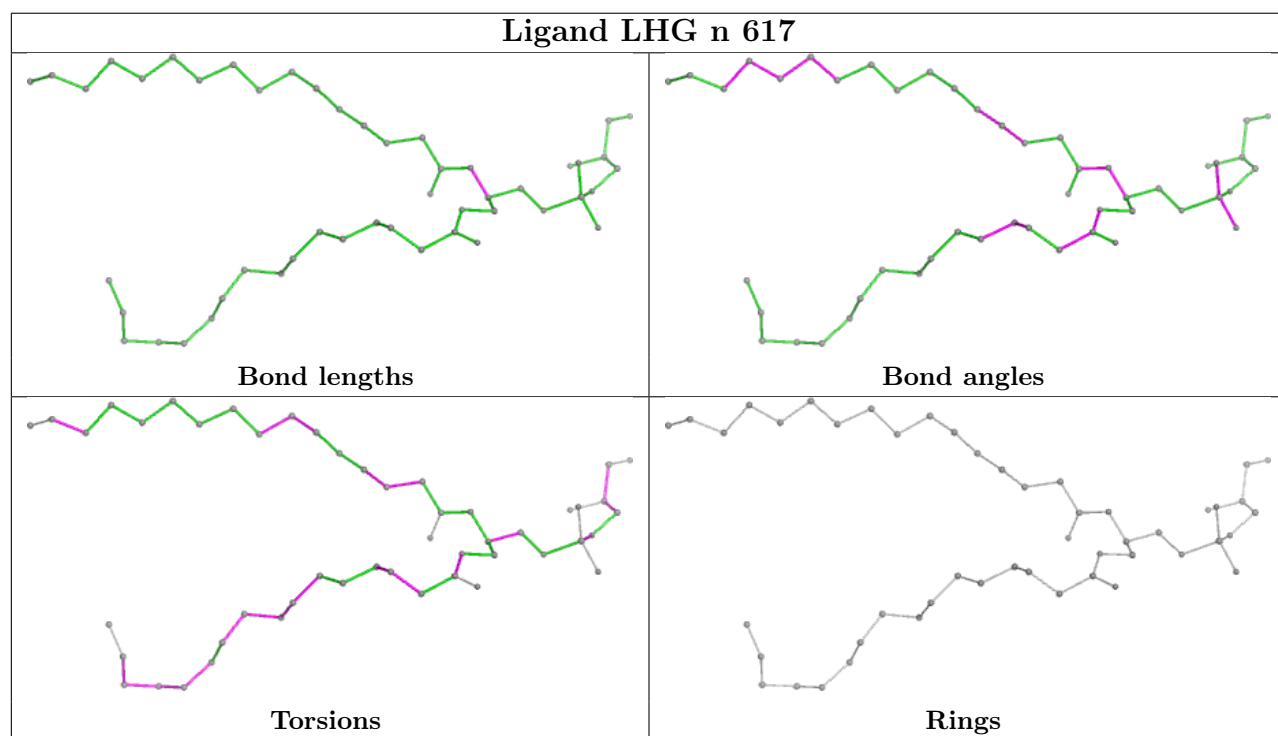
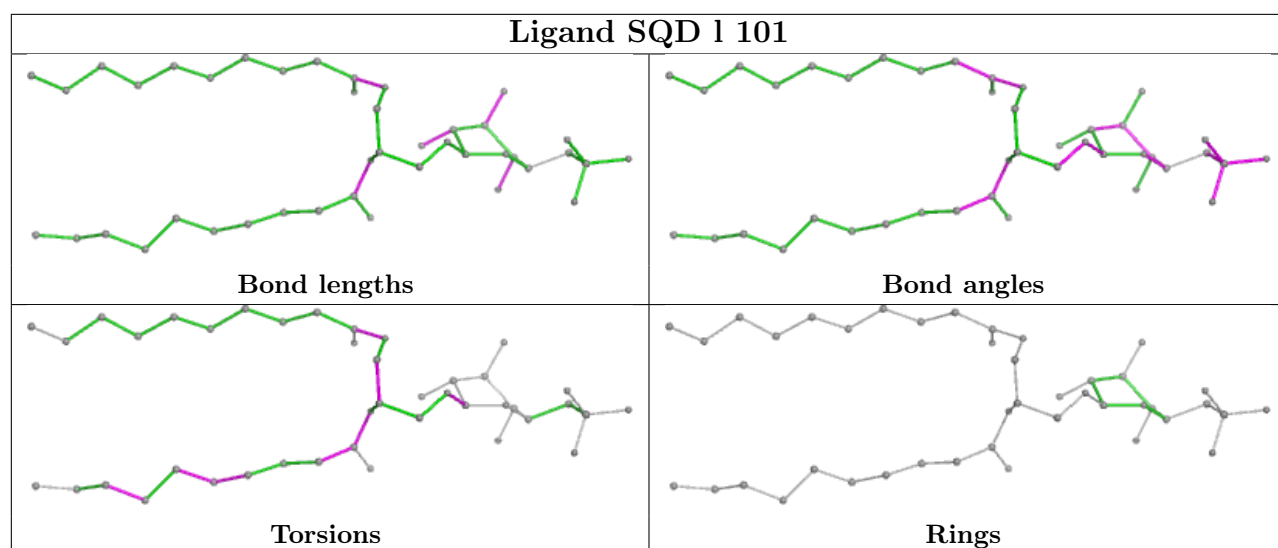


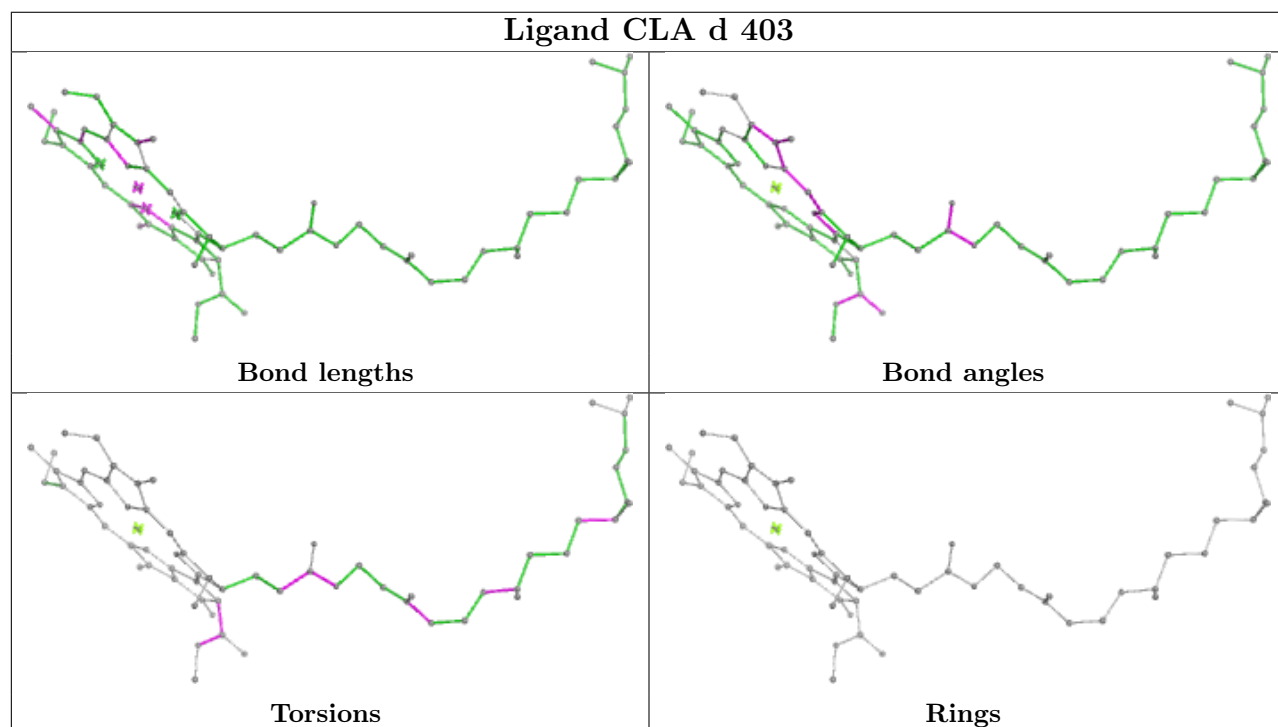
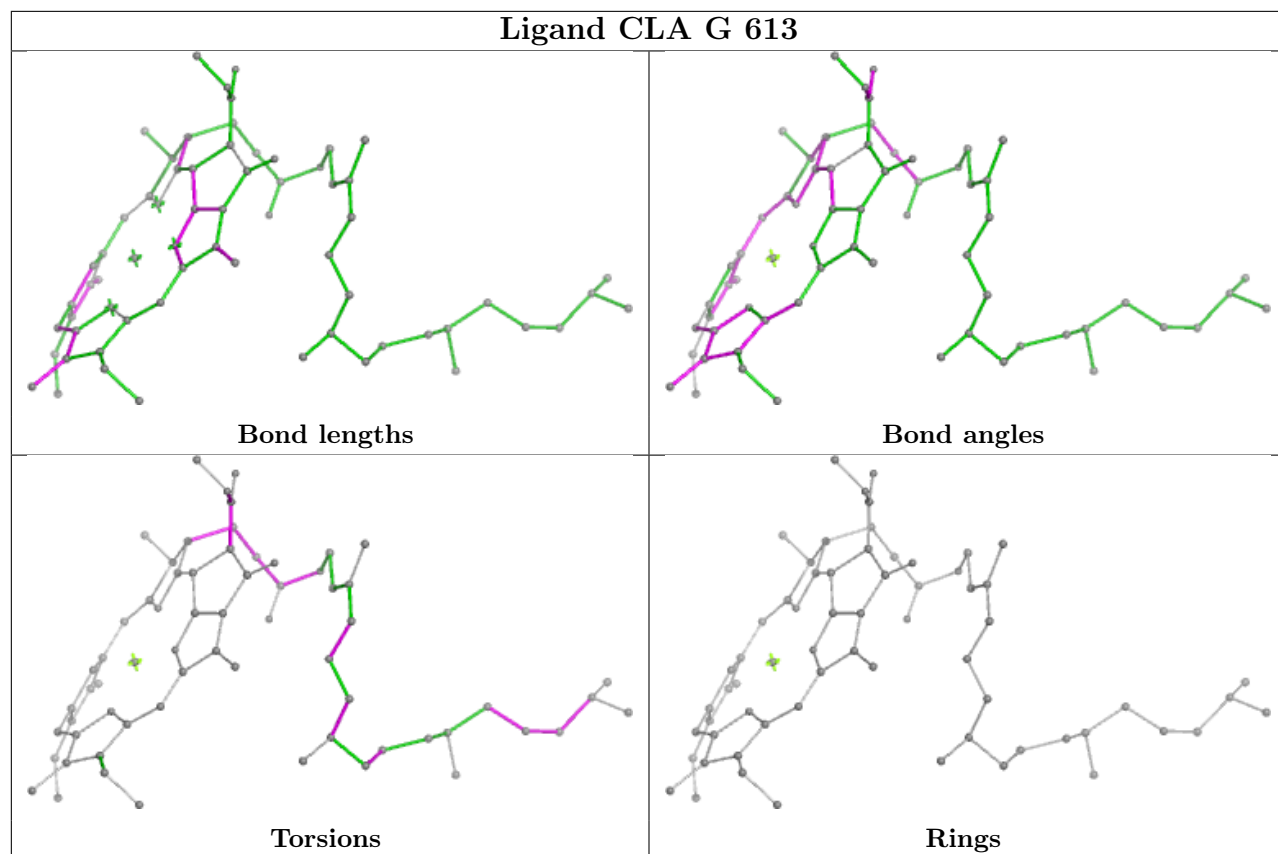
## Ligand CLA S 312



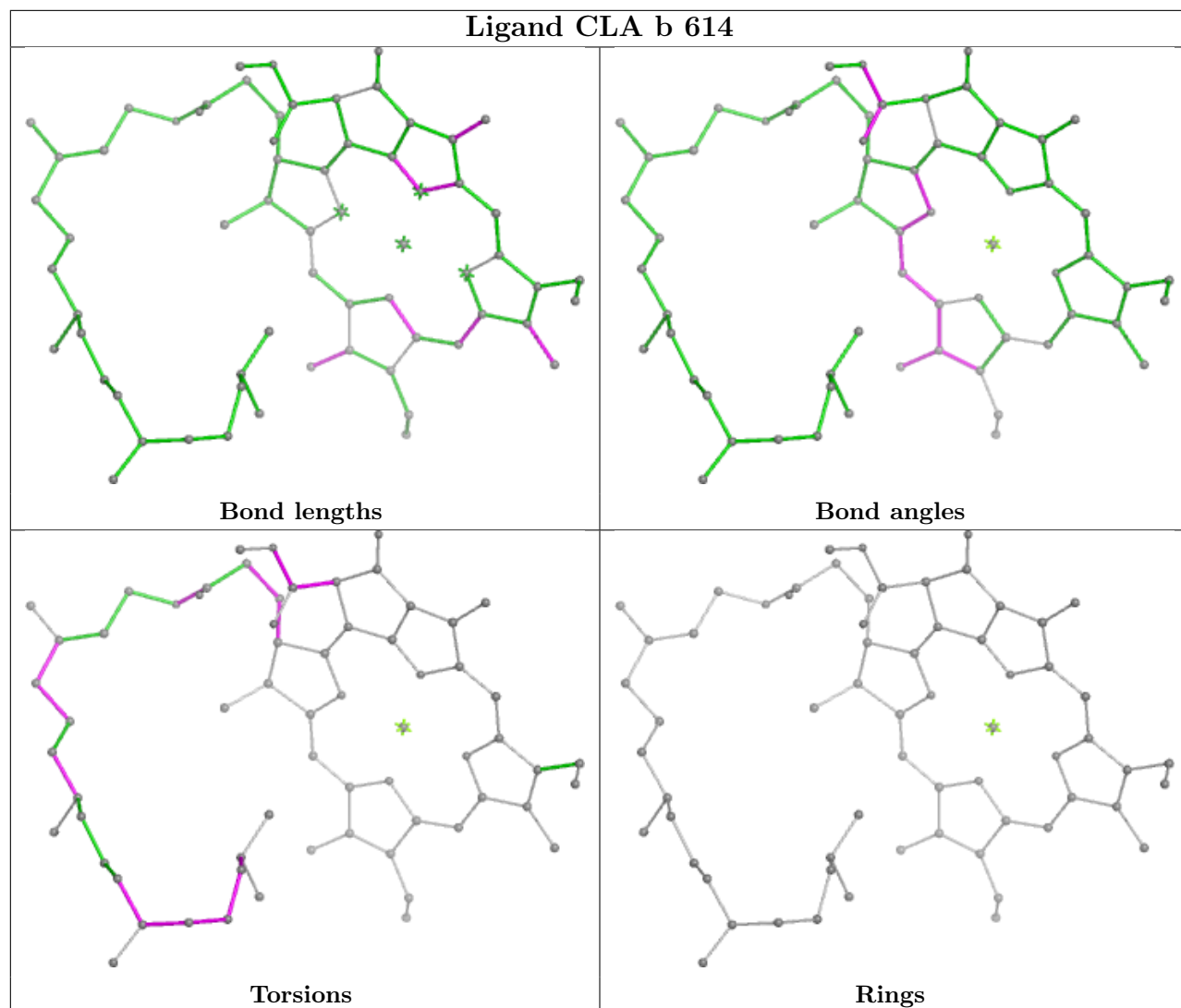
## Ligand BCR k 101



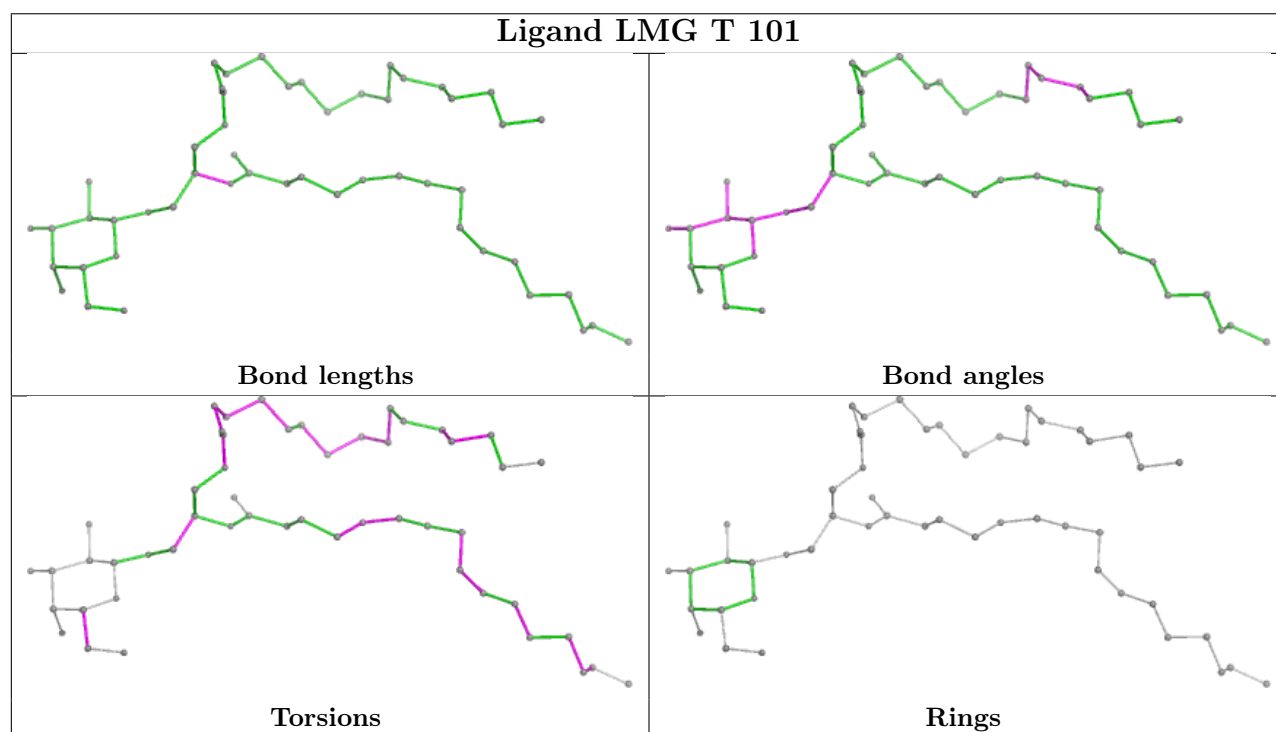
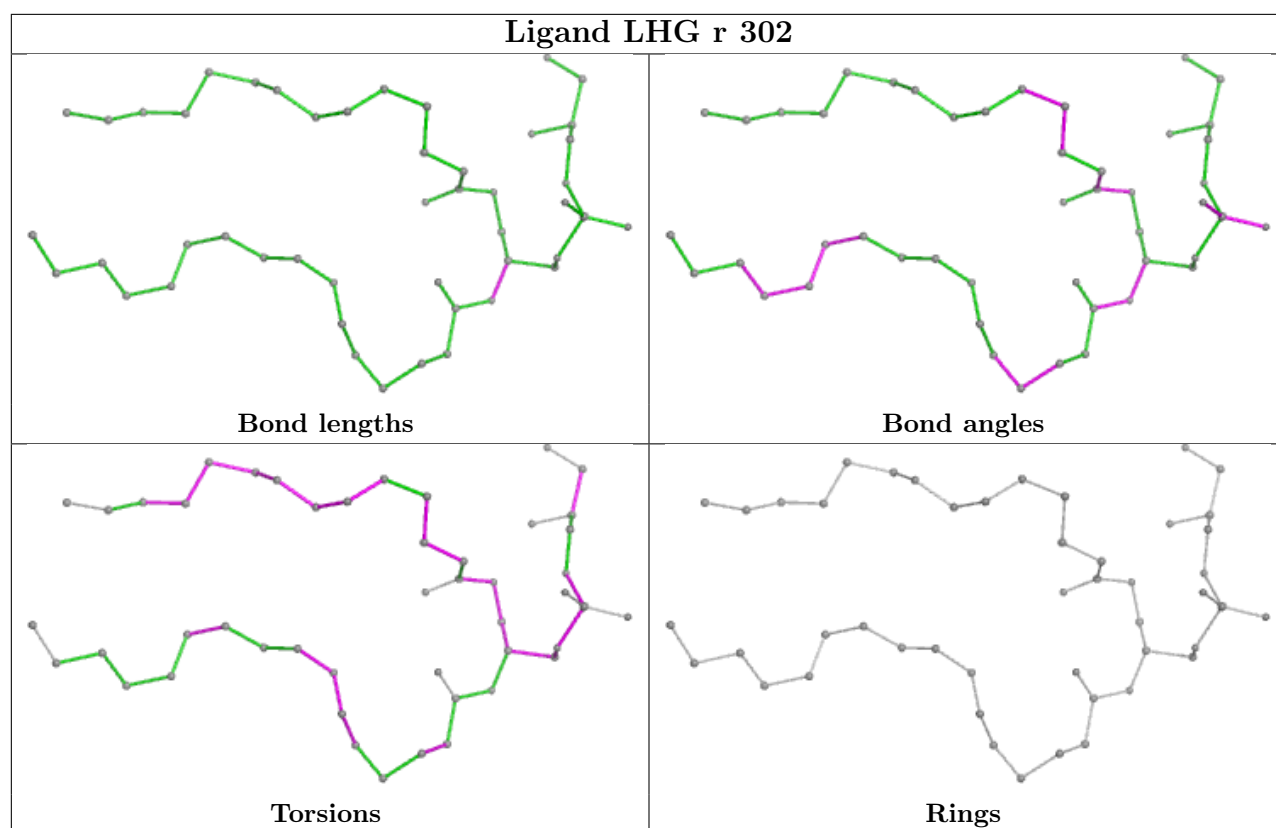


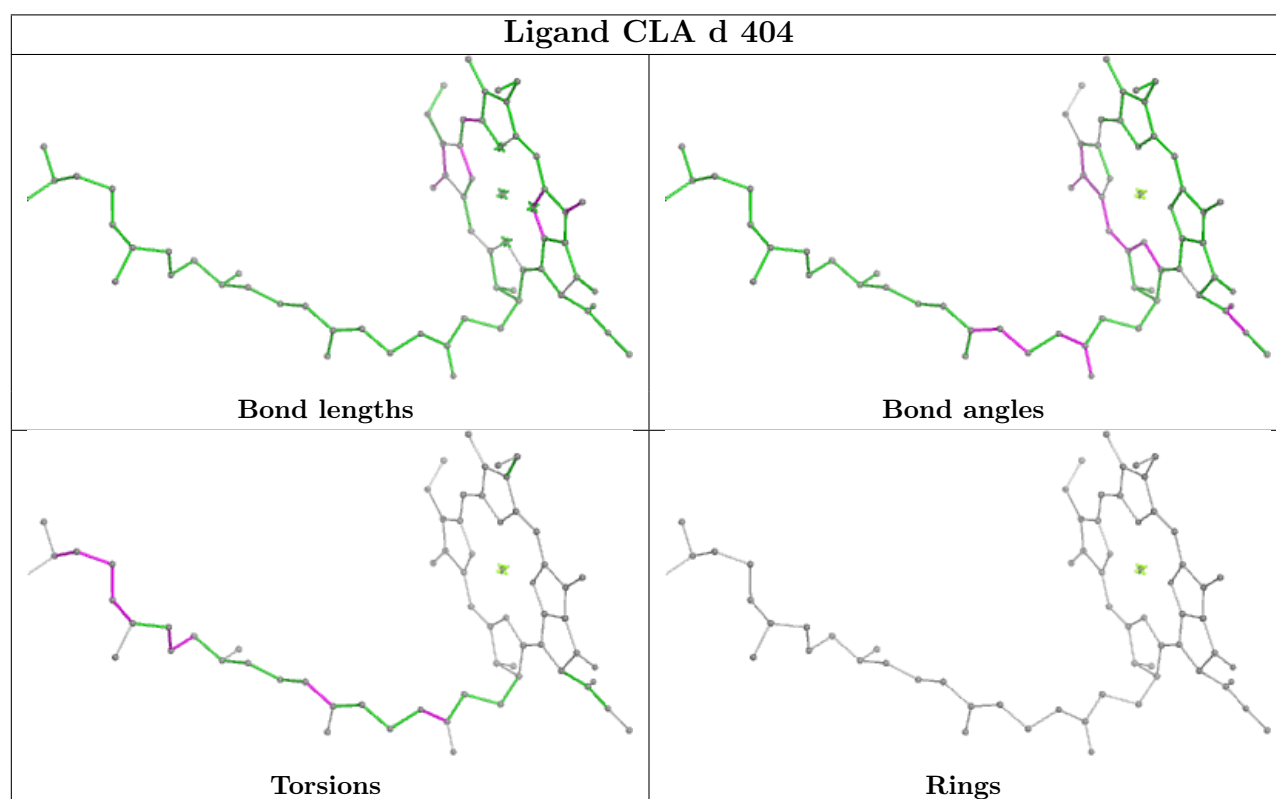
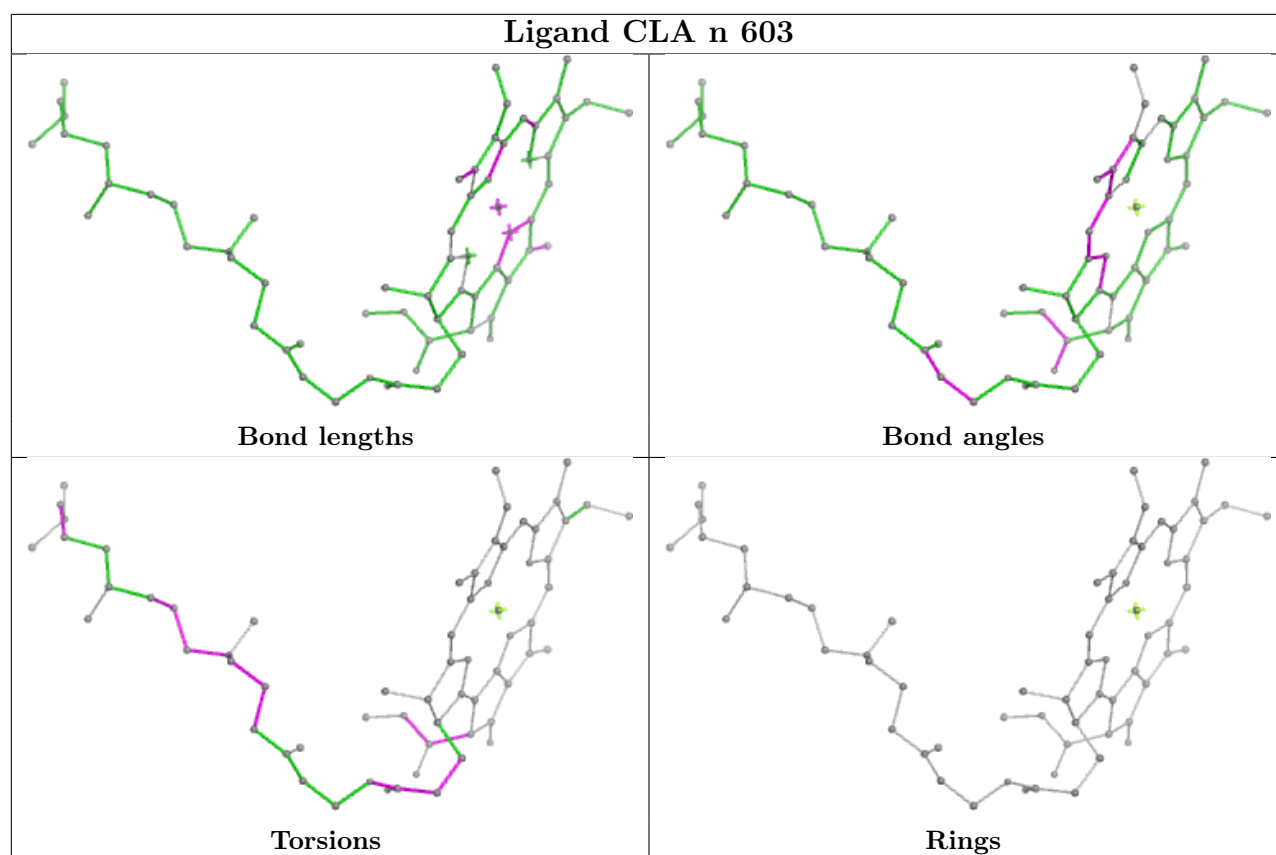


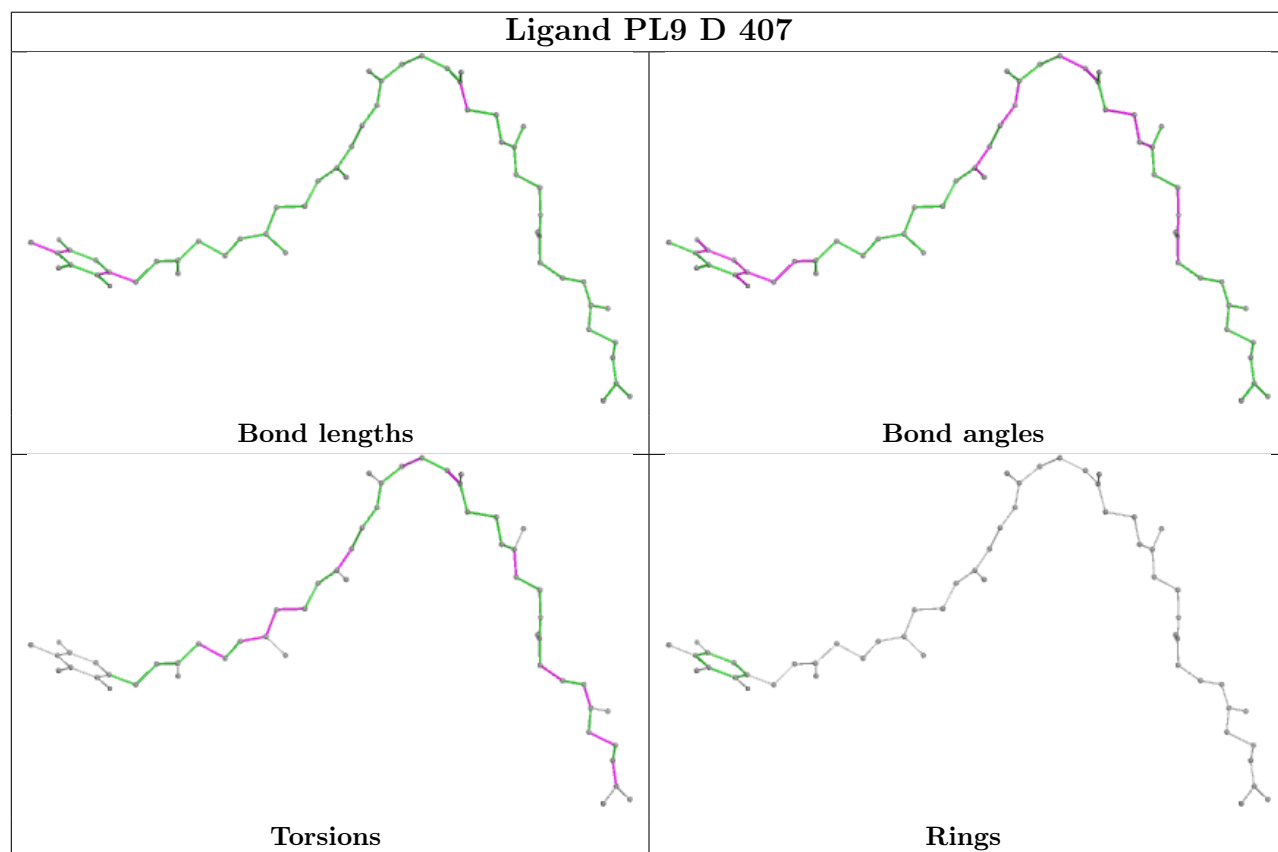
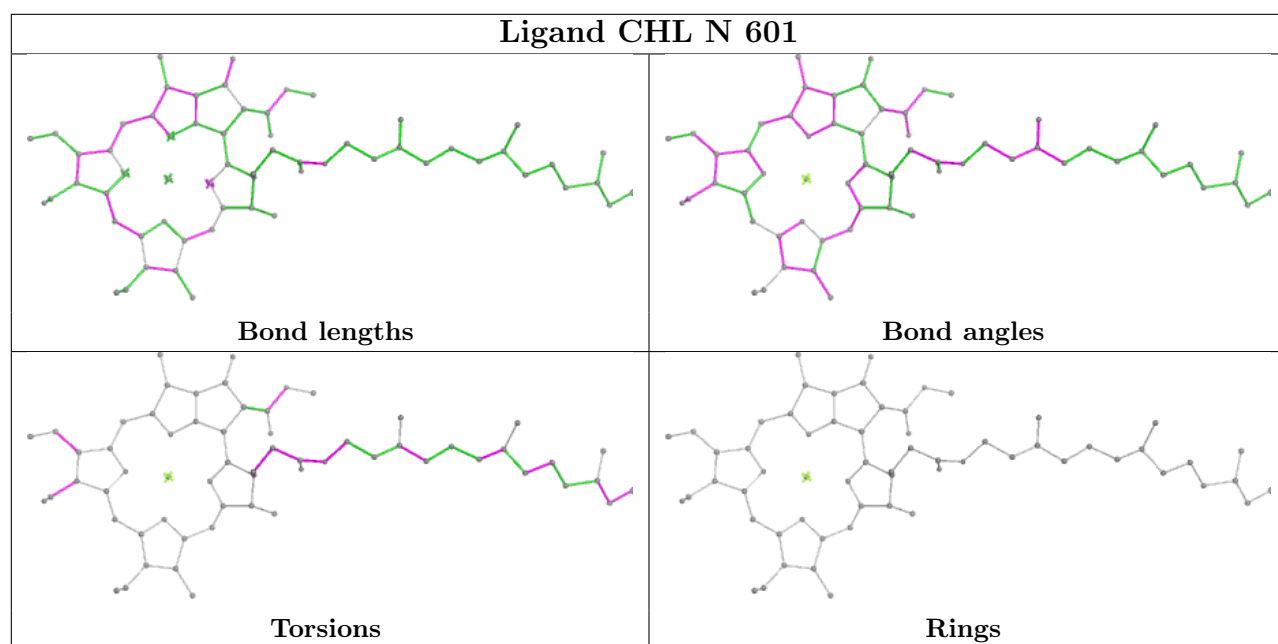
## Ligand CLA b 614

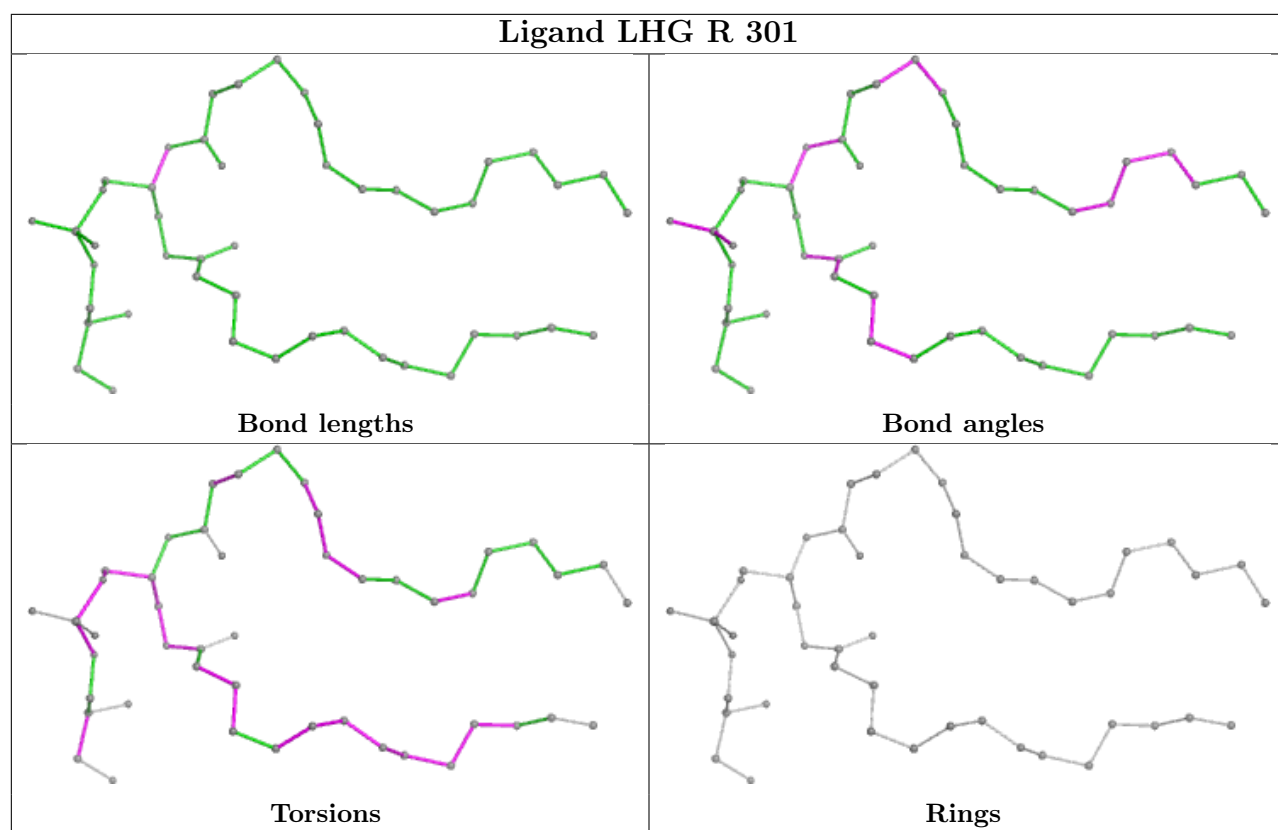




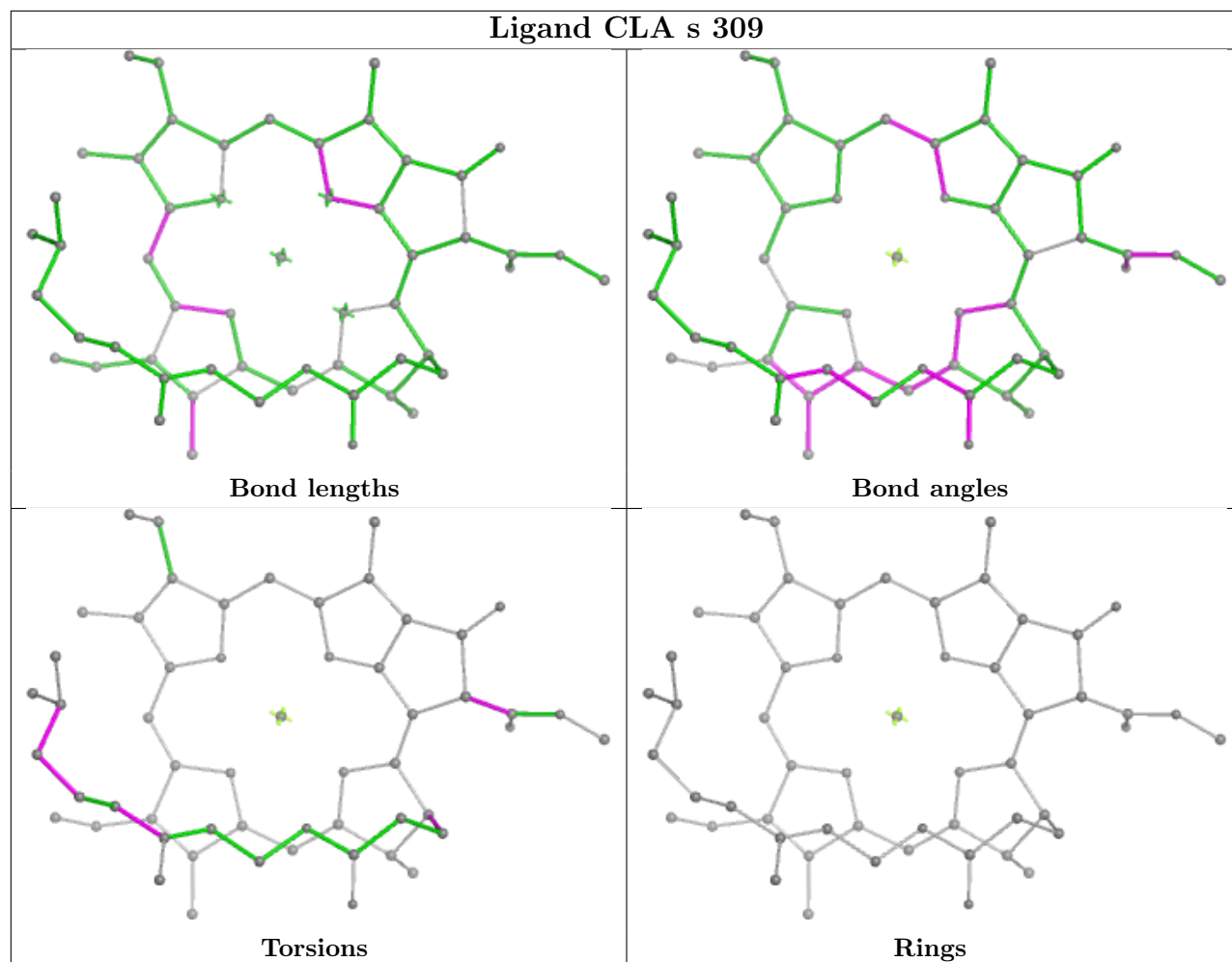




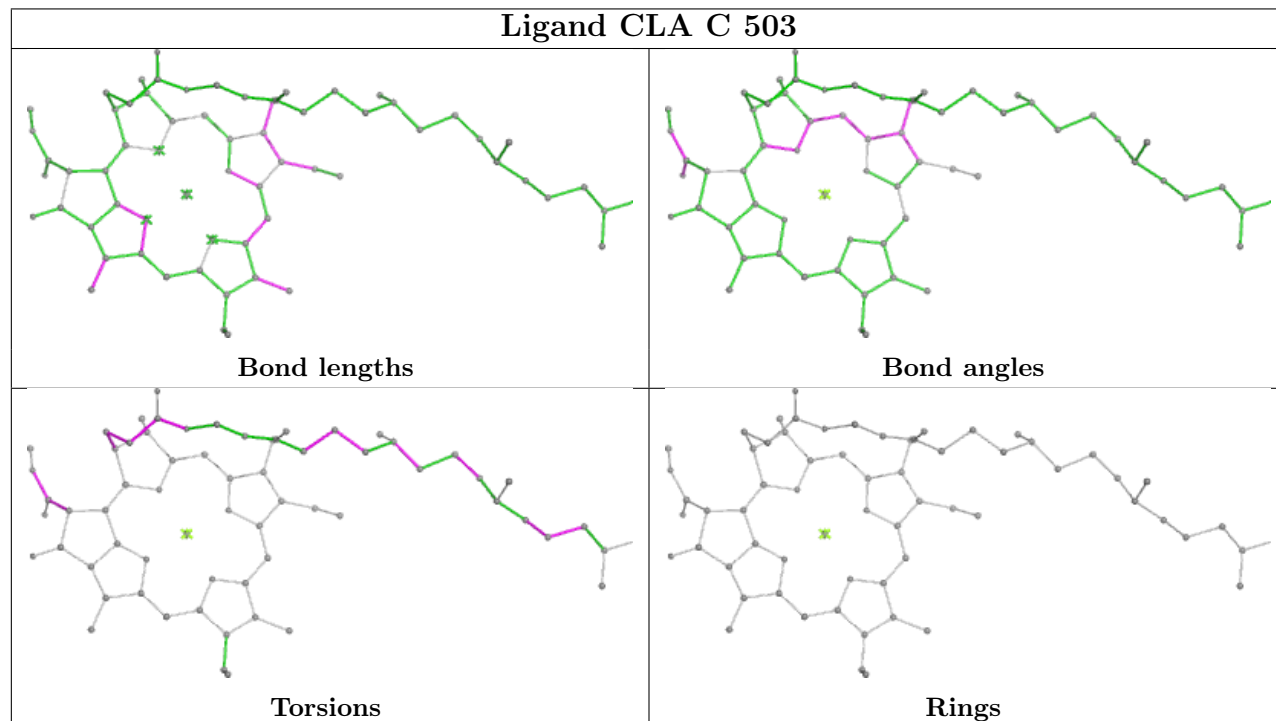




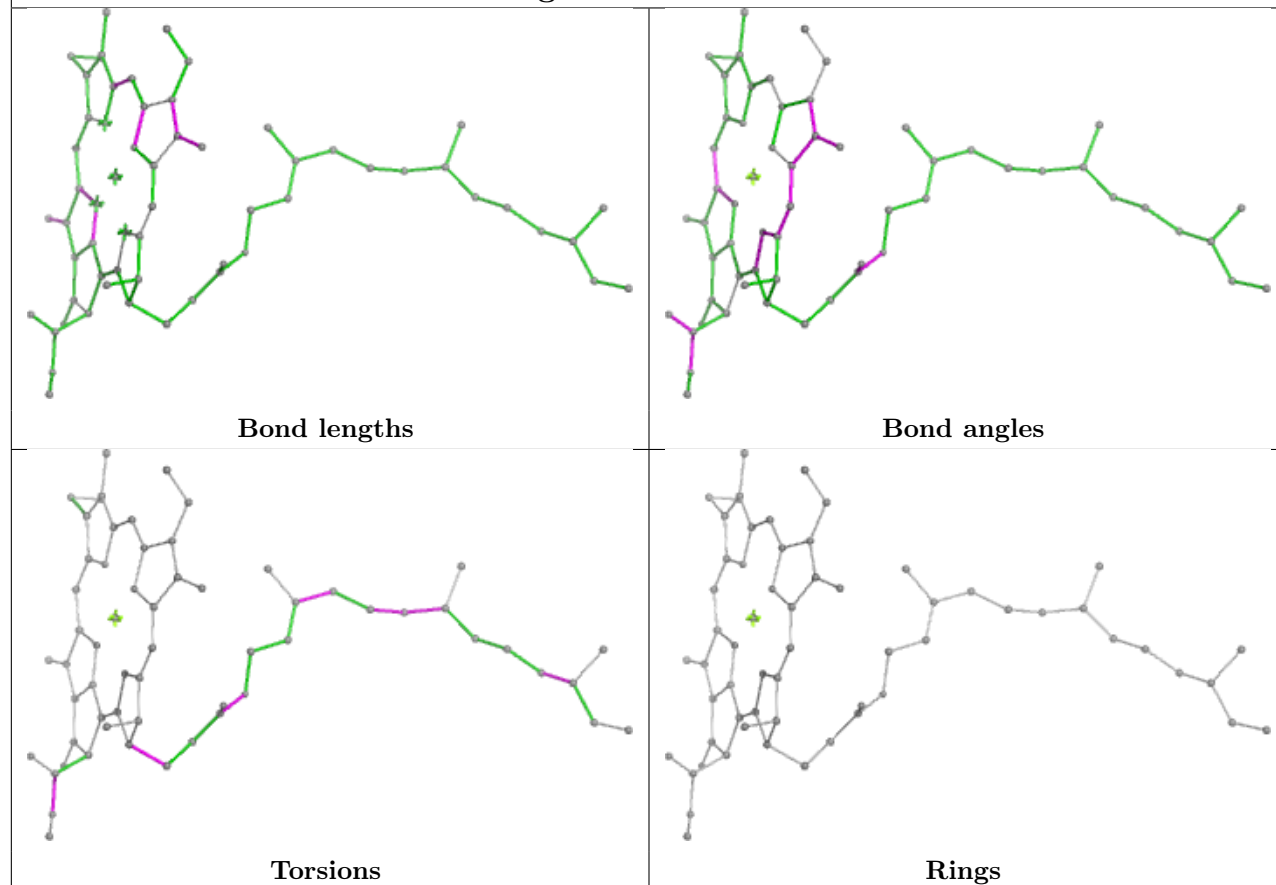
## Ligand CLA s 309



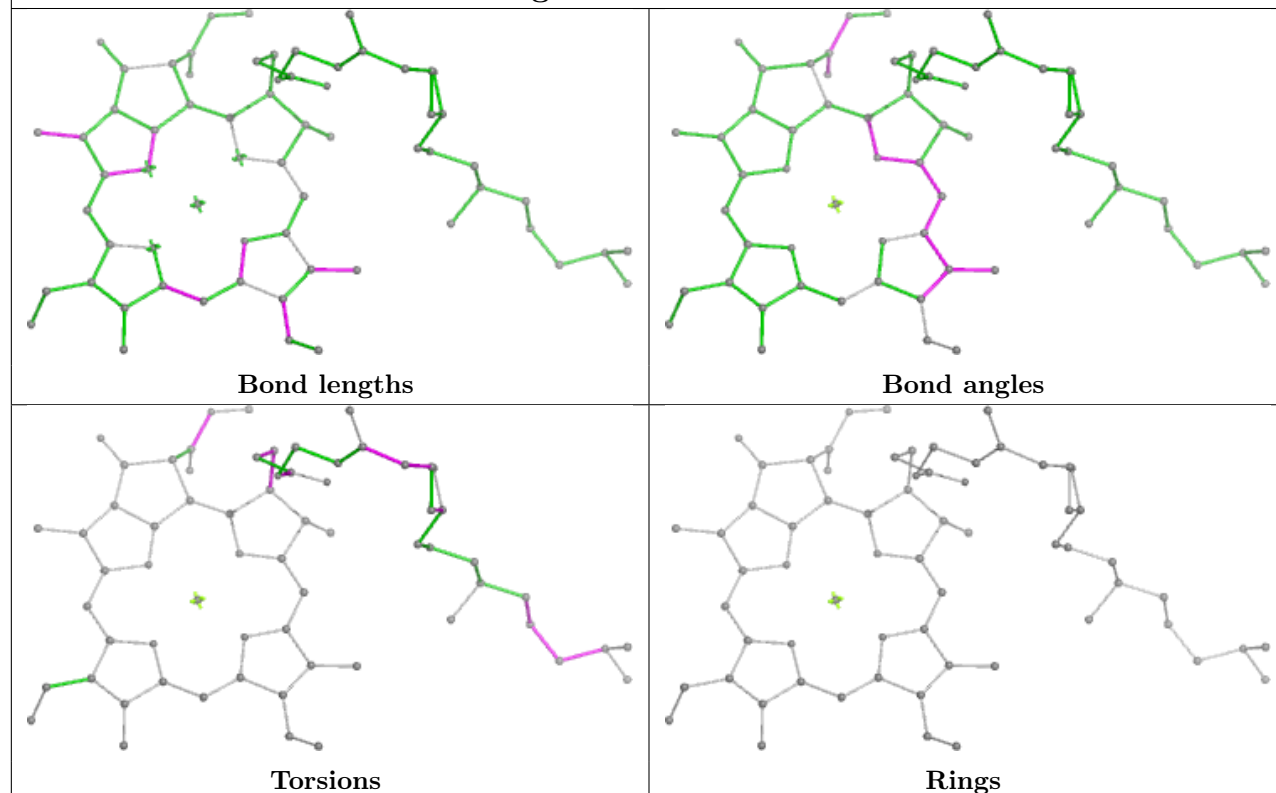
## Ligand CLA C 503

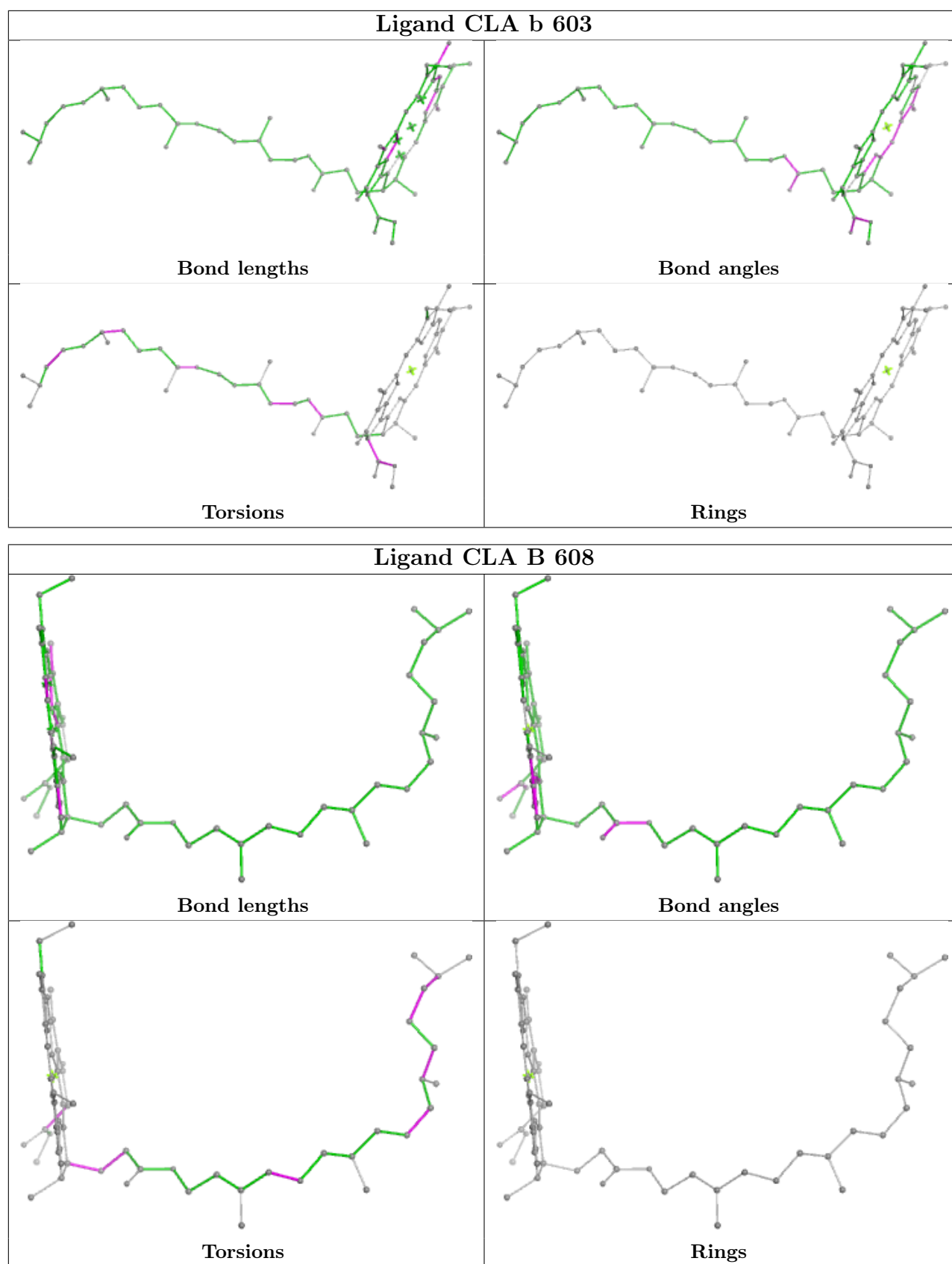


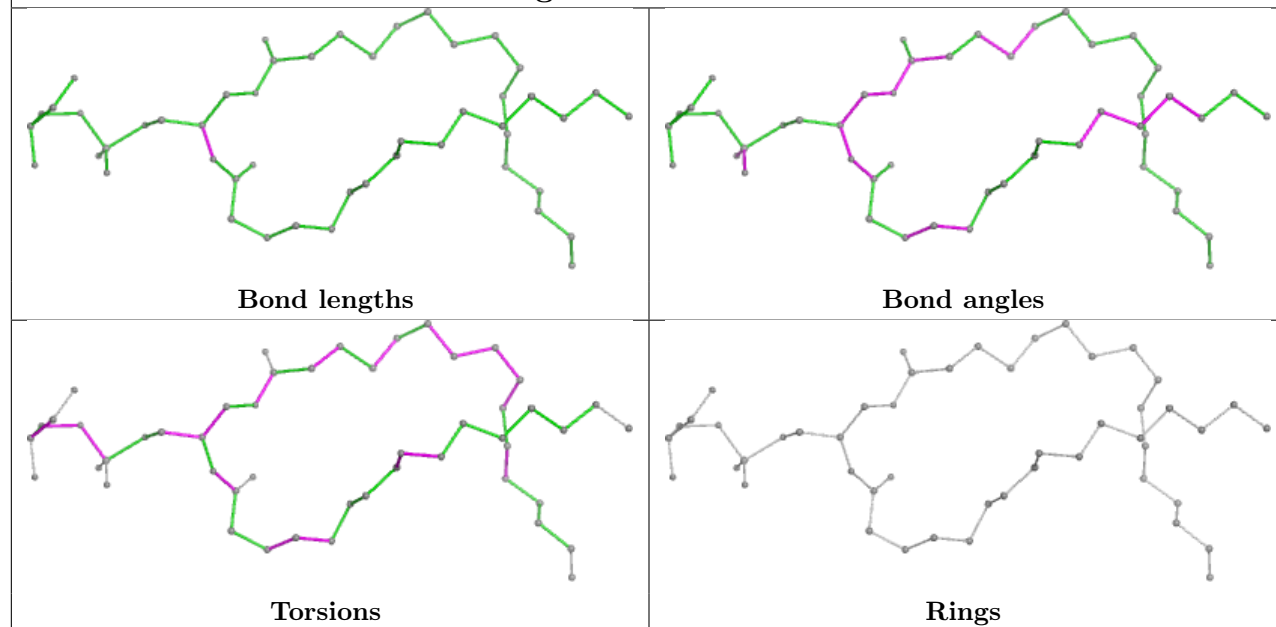
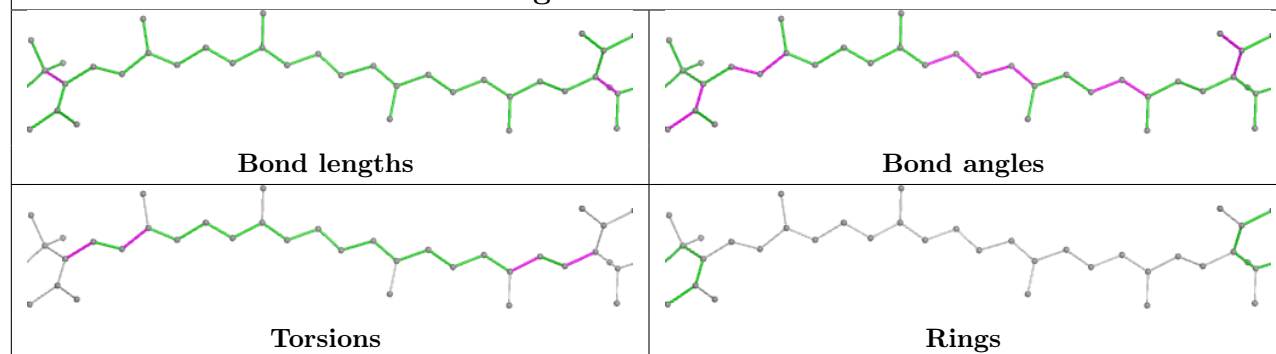
## Ligand CLA s 303



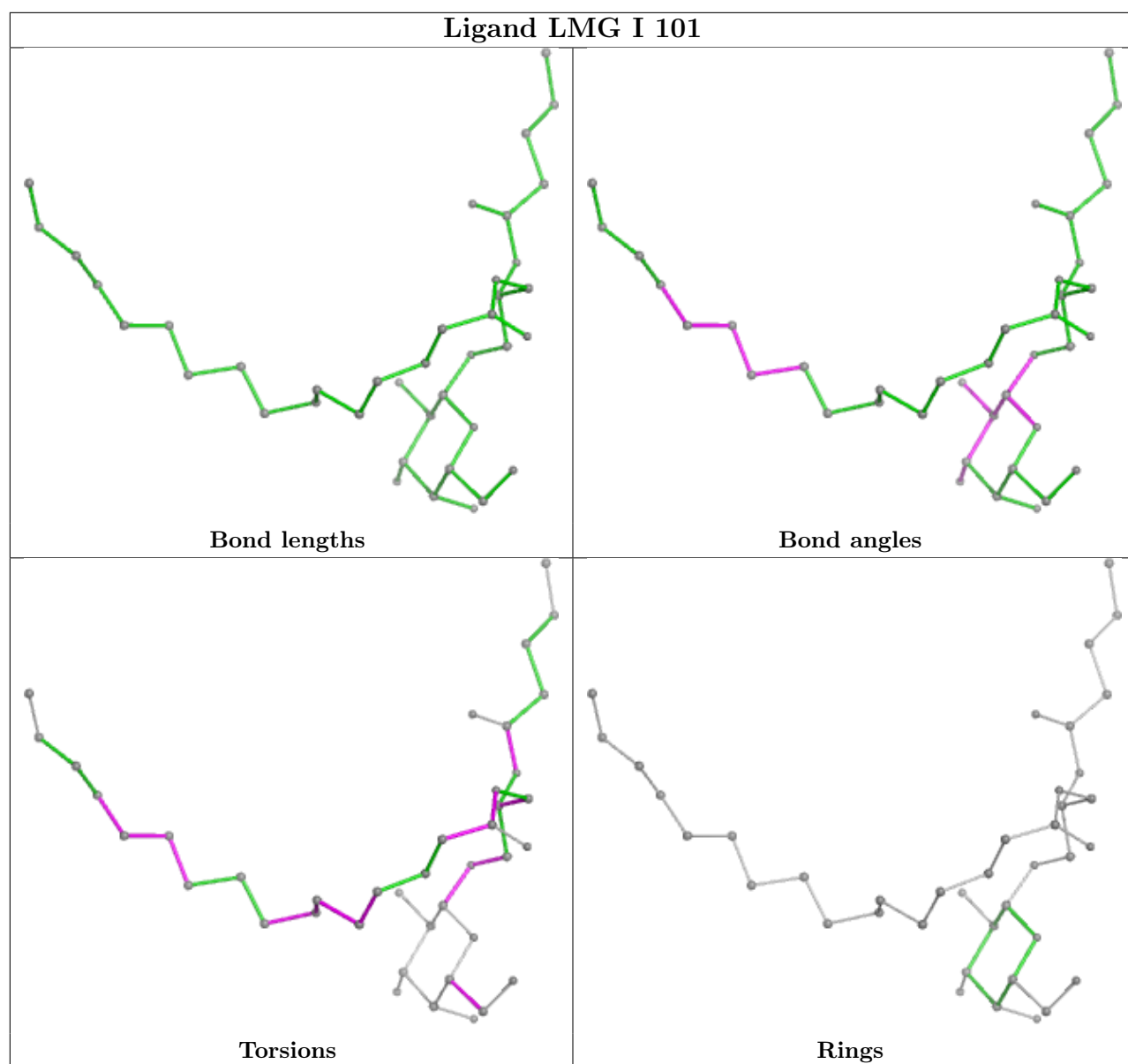
## Ligand CLA A 406

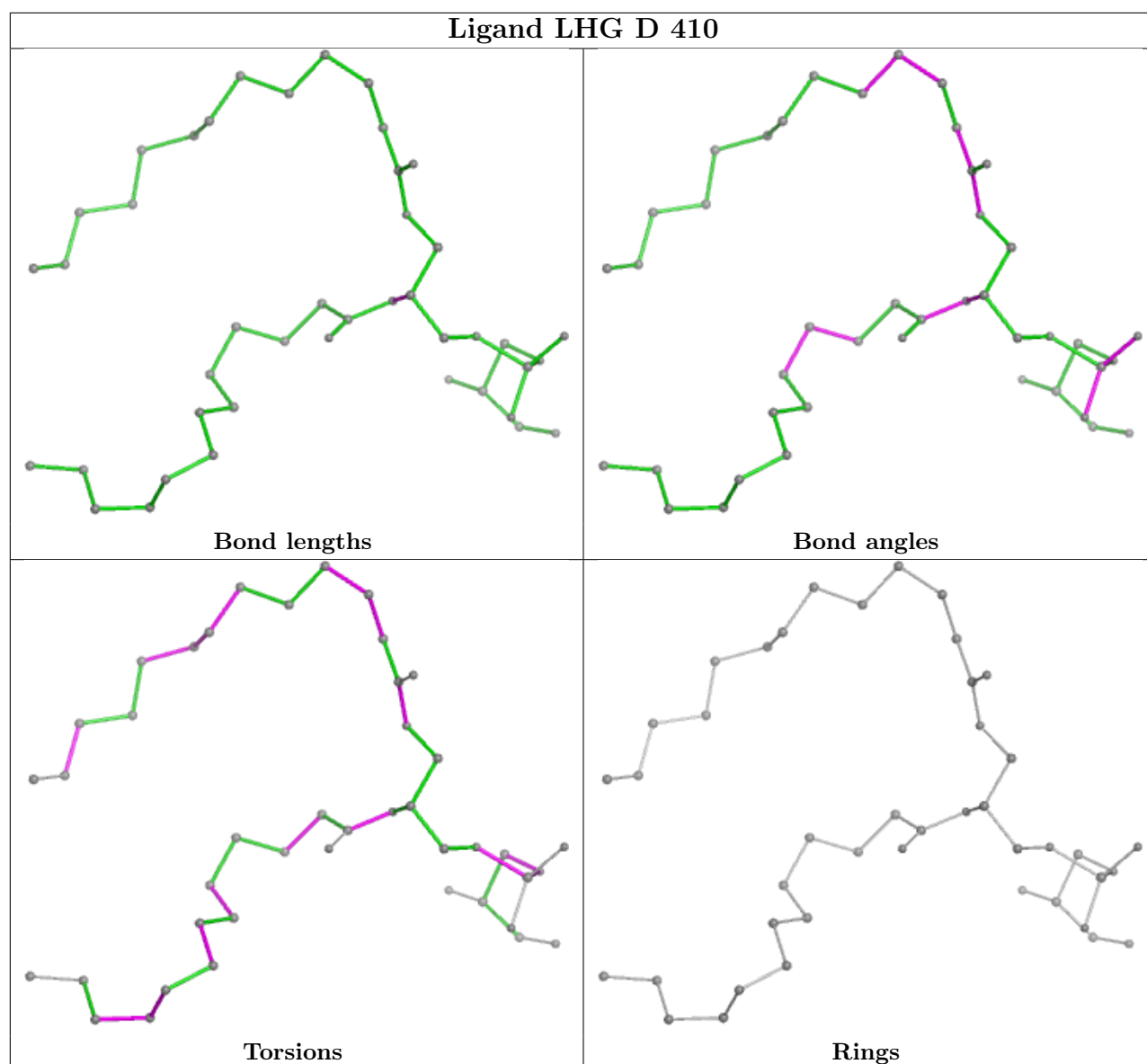


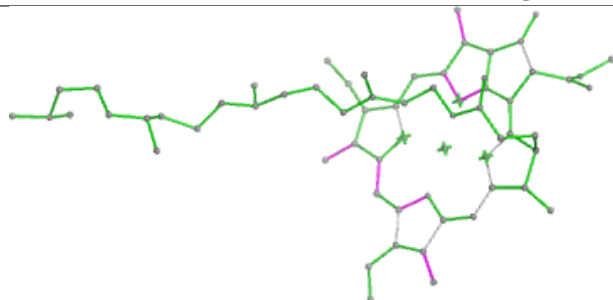
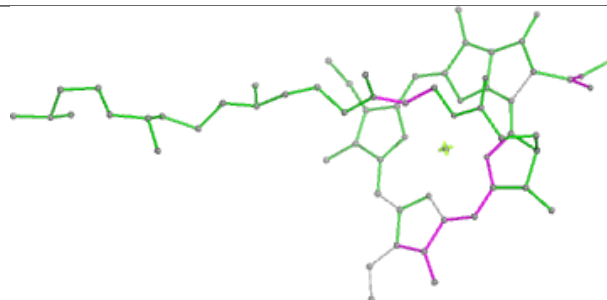
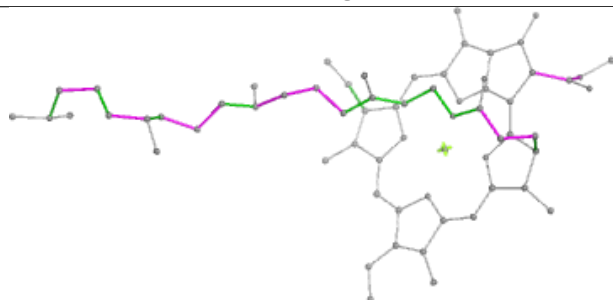
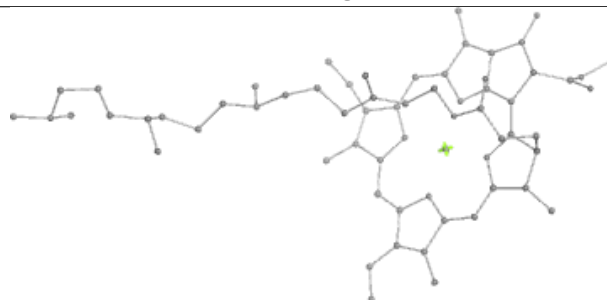
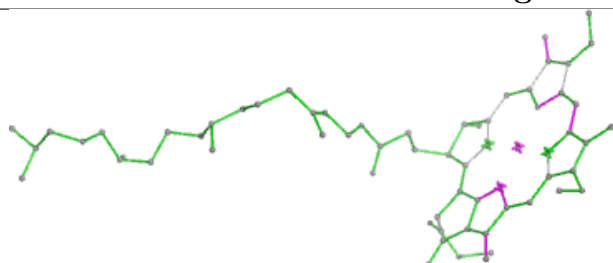
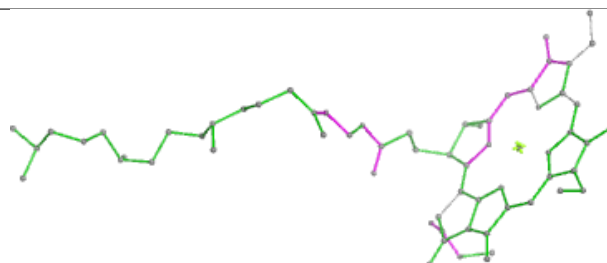
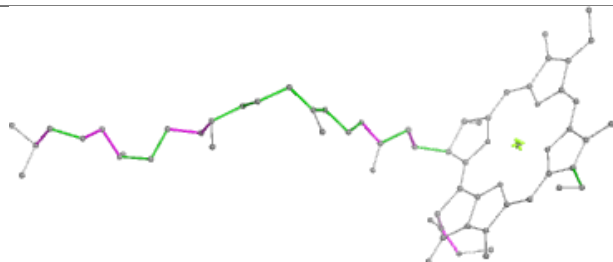
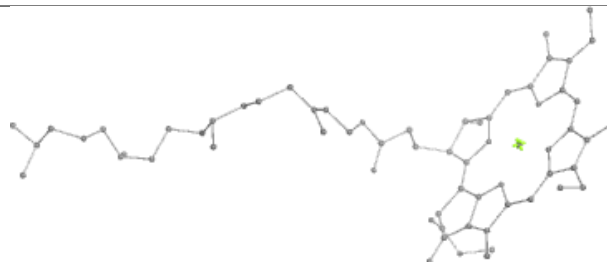


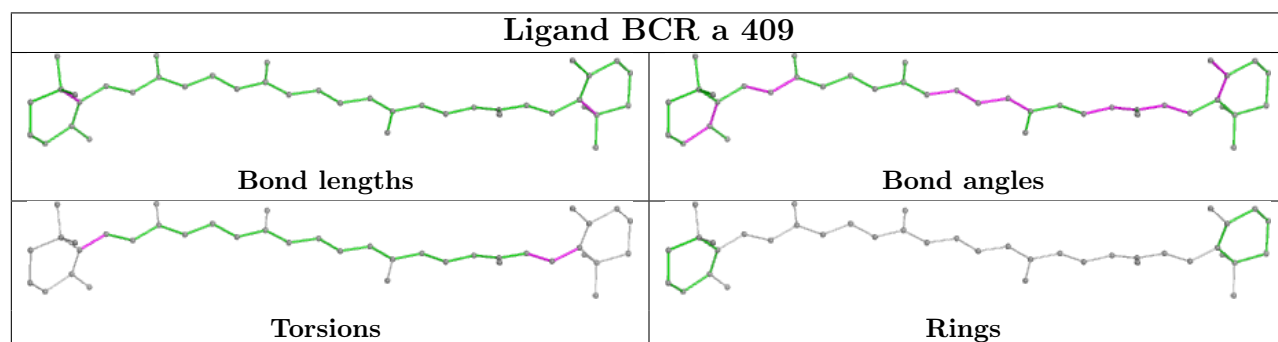
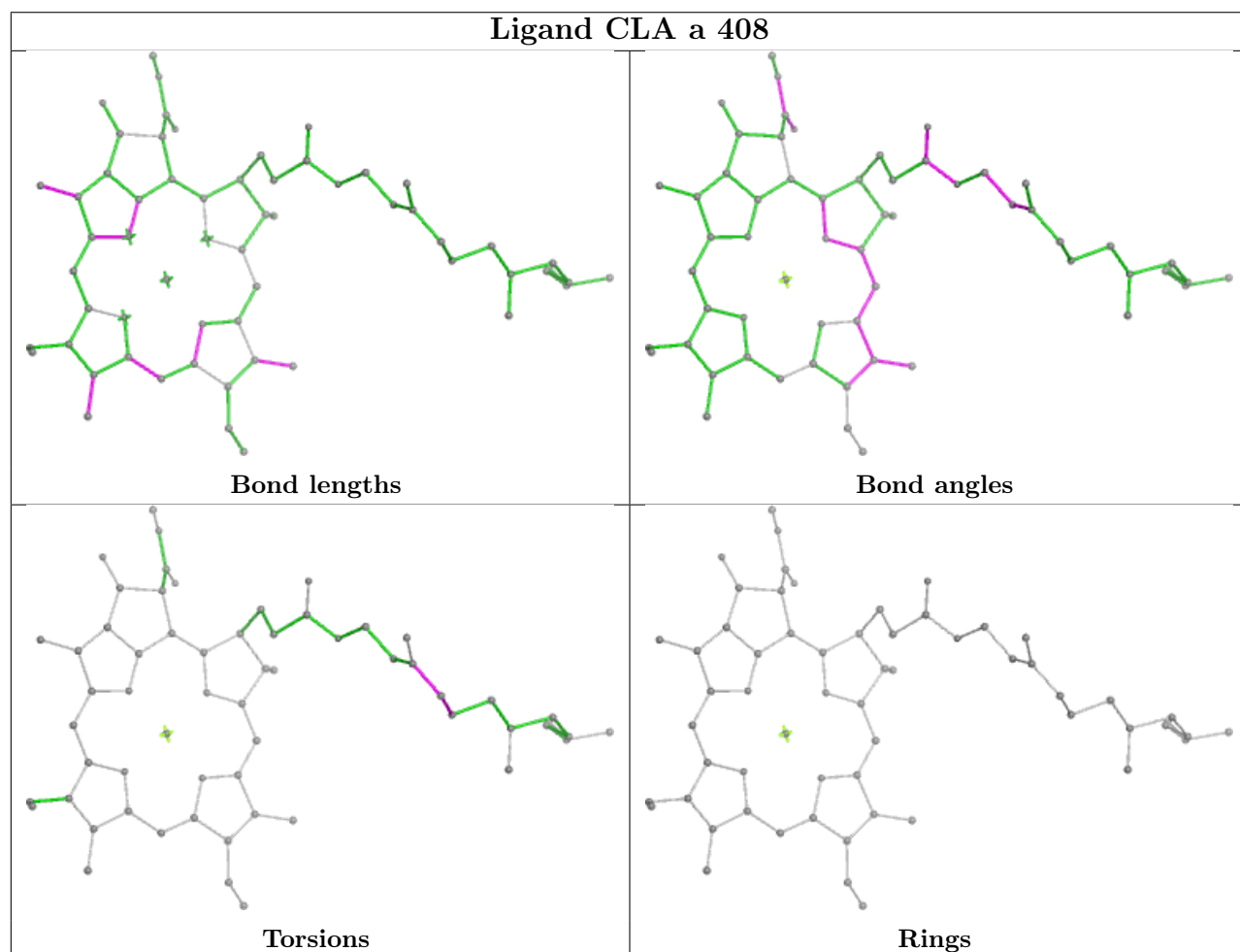
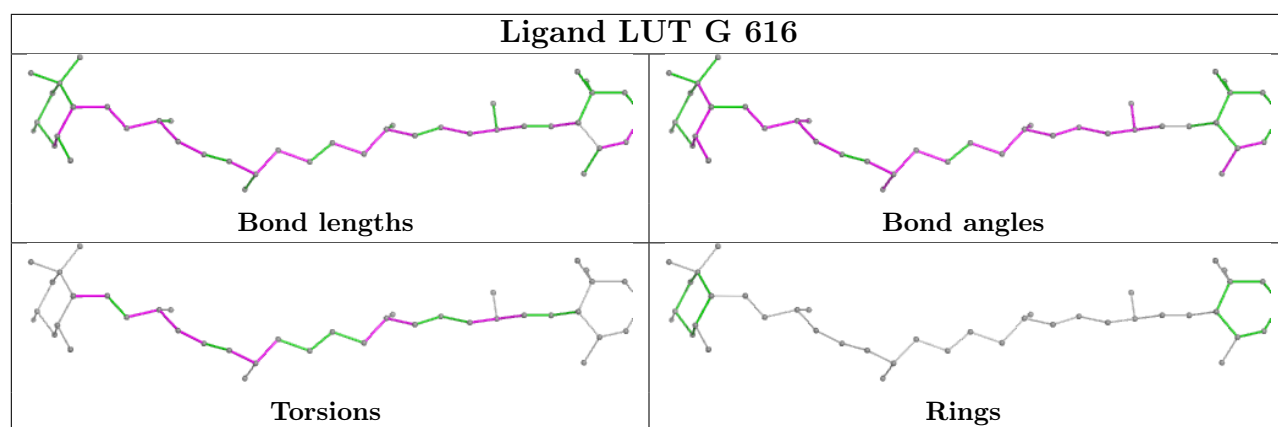
**Ligand LHG c 522****Ligand BCR b 617**



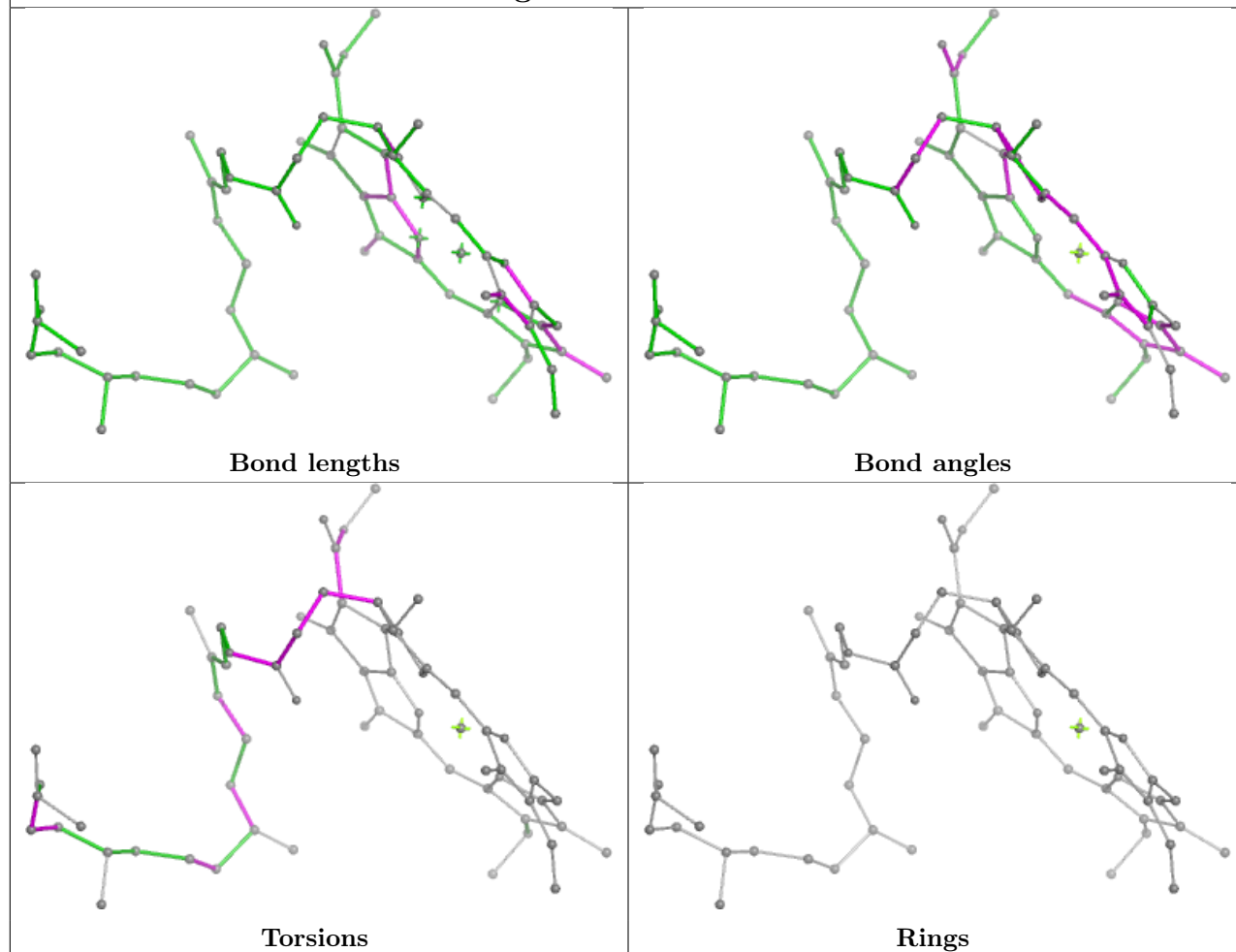




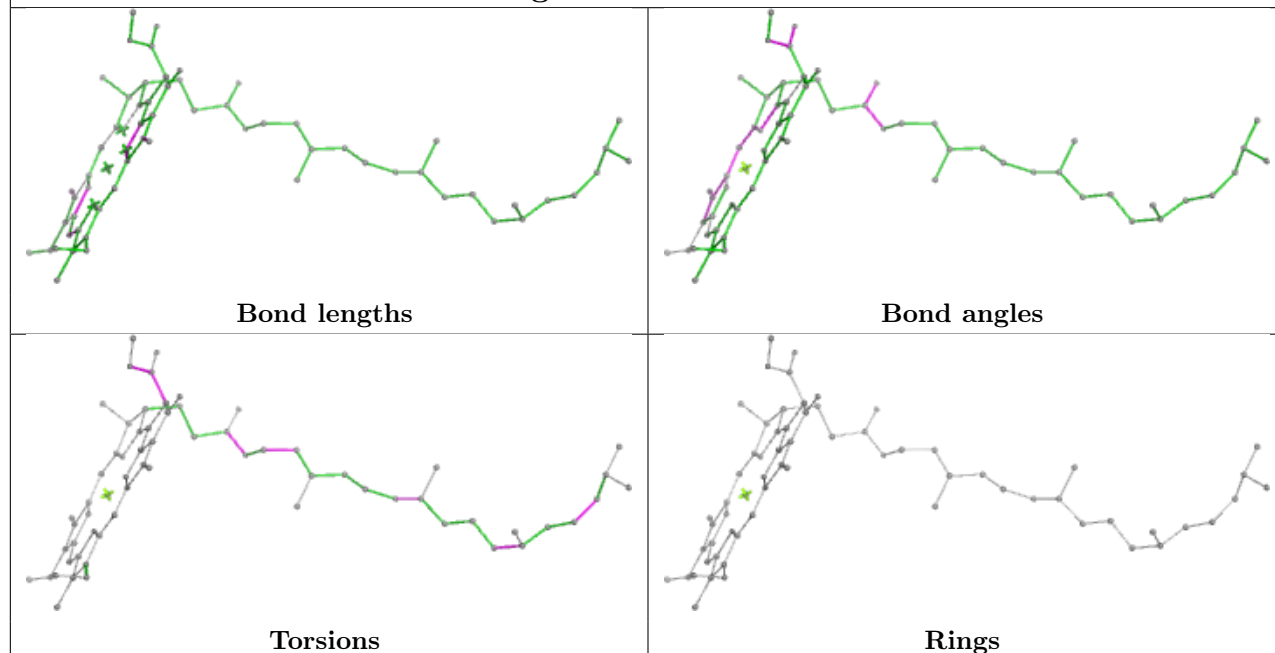
**Ligand CLA b 613****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA C 504****Bond lengths****Bond angles****Torsions****Rings**



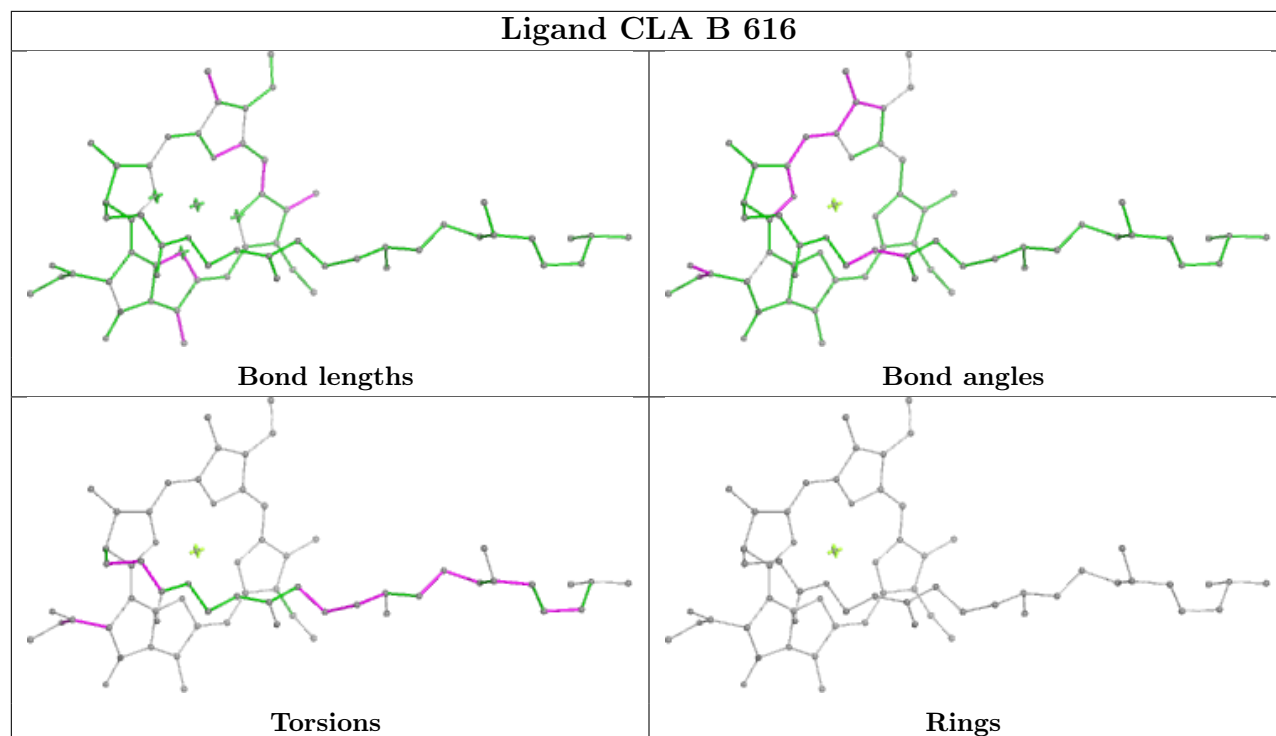
## Ligand CLA Y 611



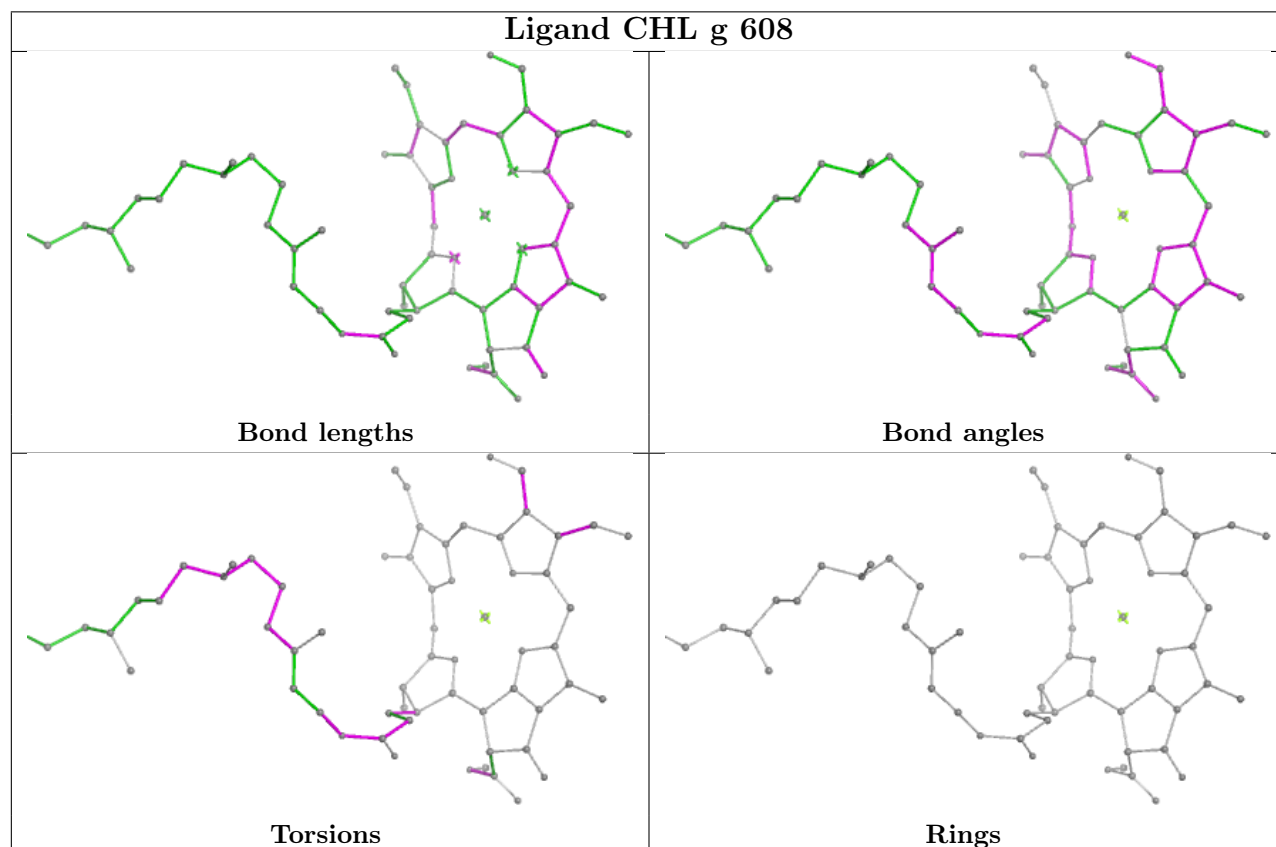
## Ligand CLA B 606

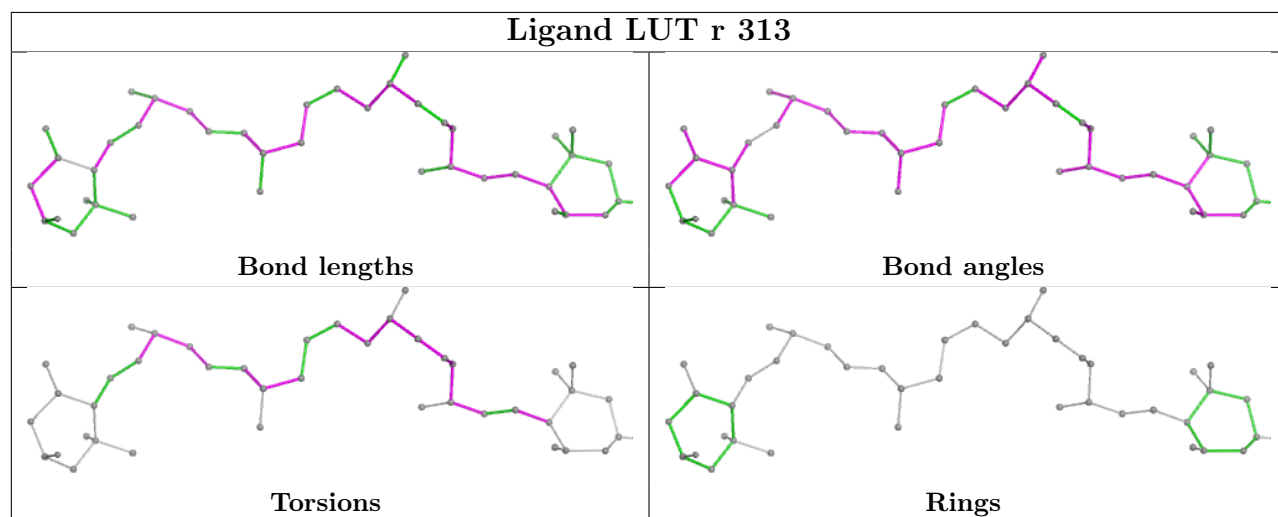
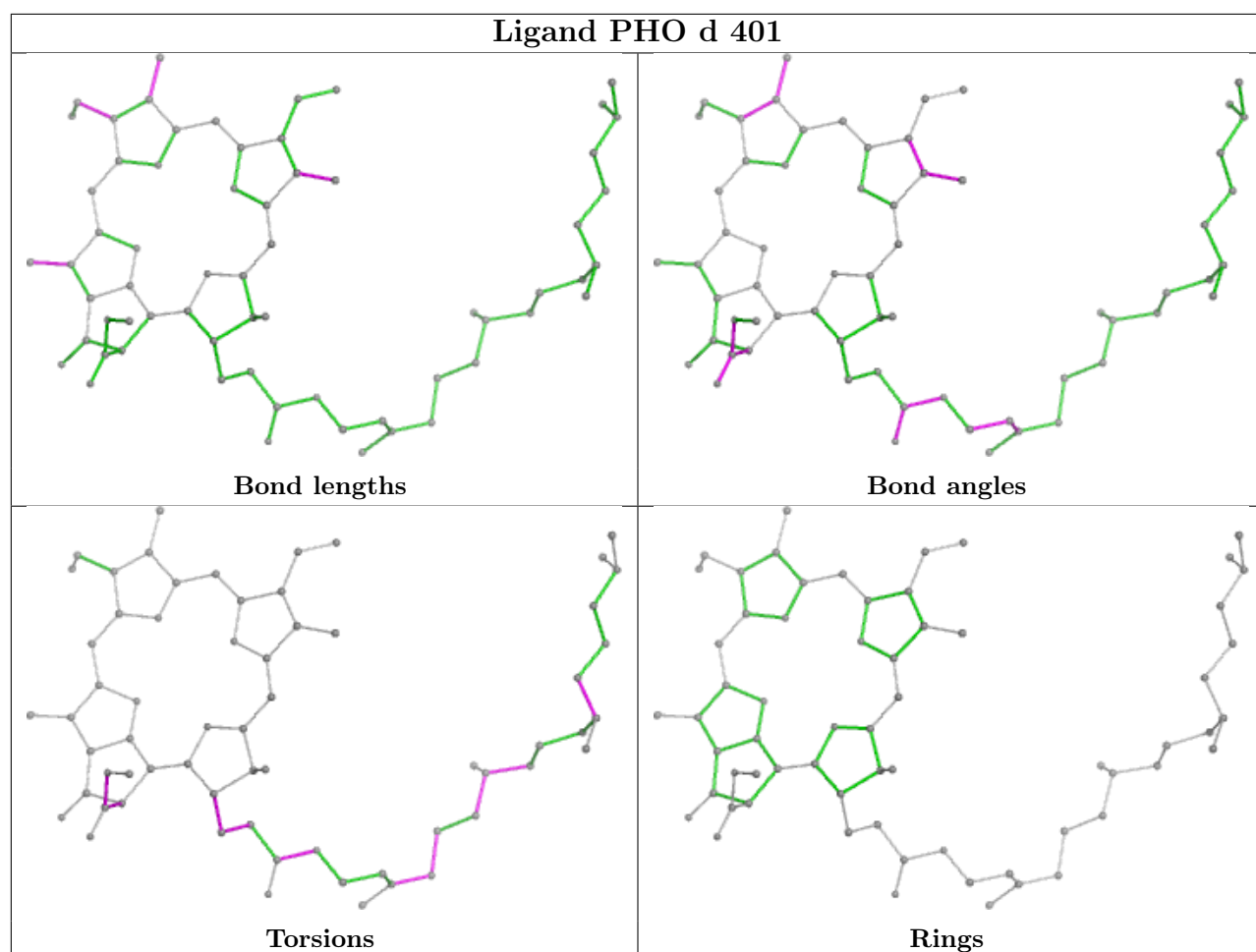


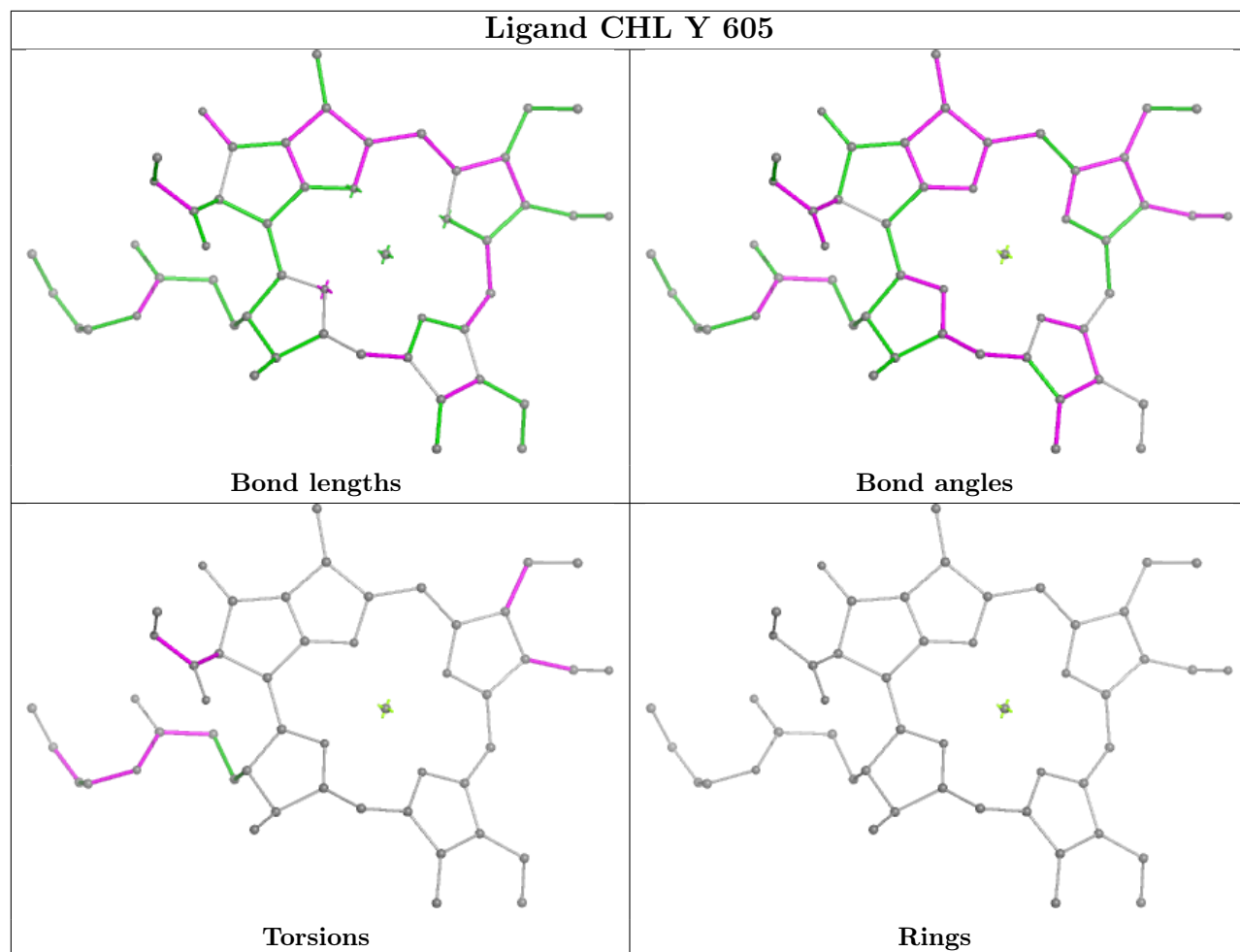
## Ligand CLA B 616



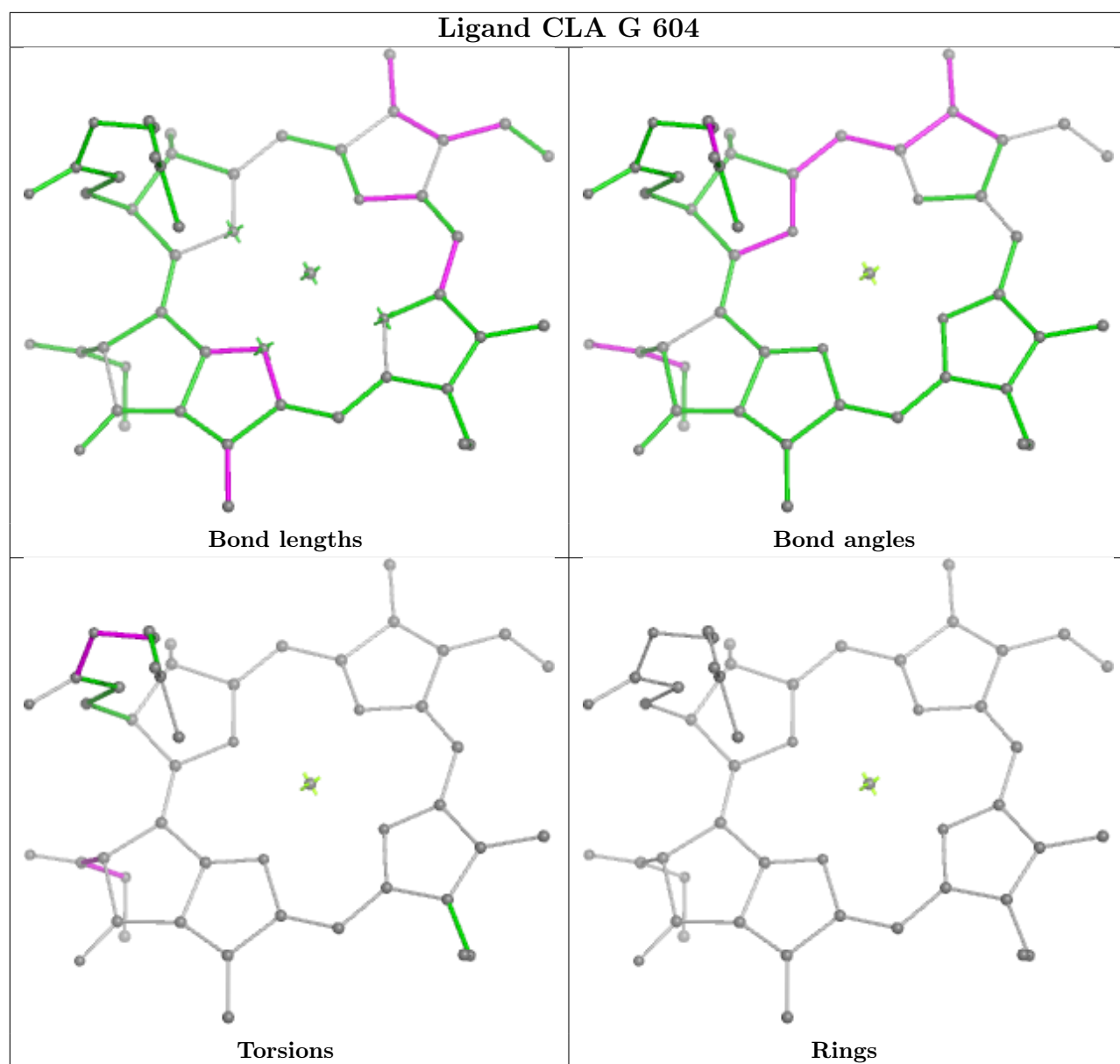
## Ligand CHL g 608

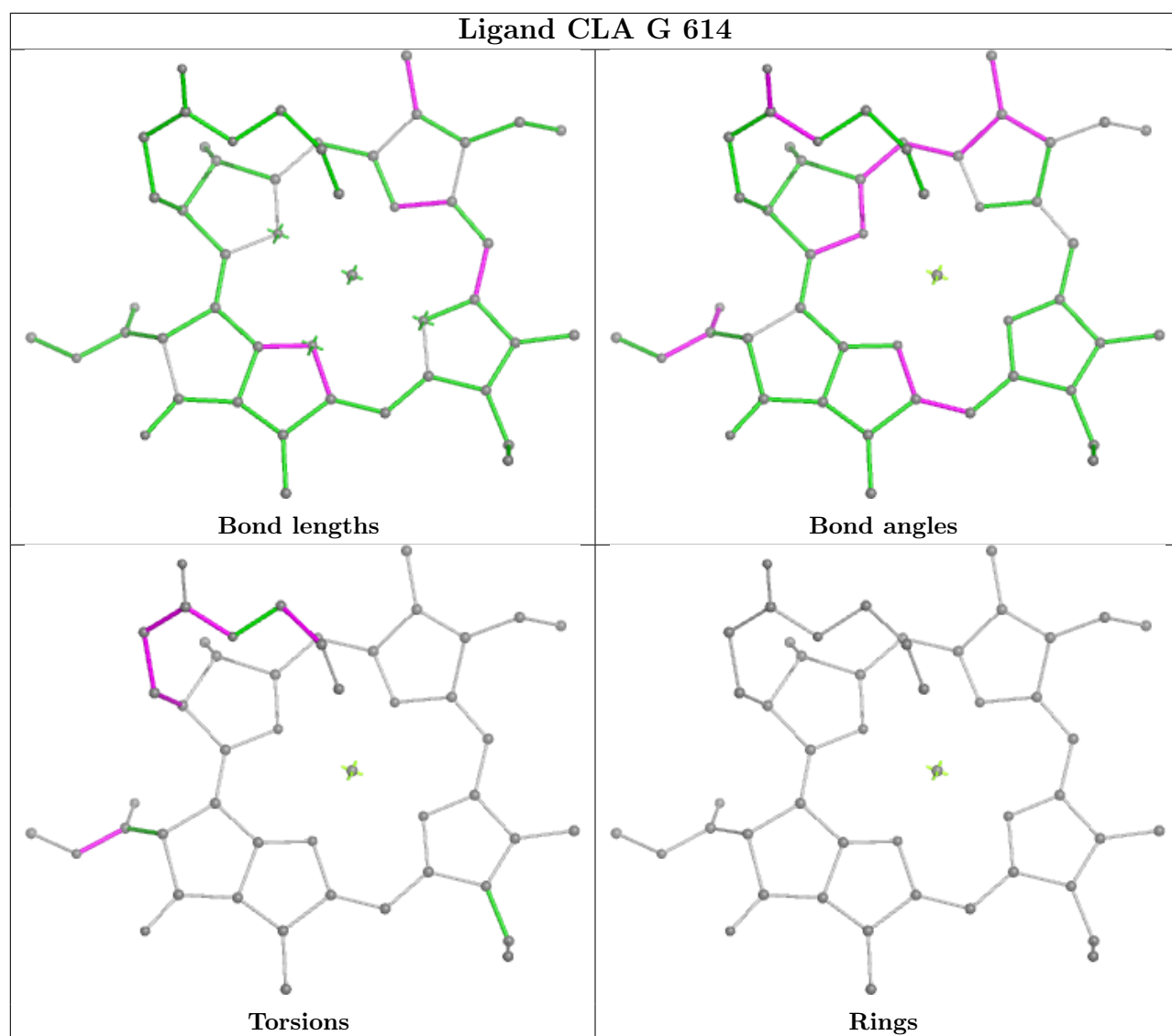


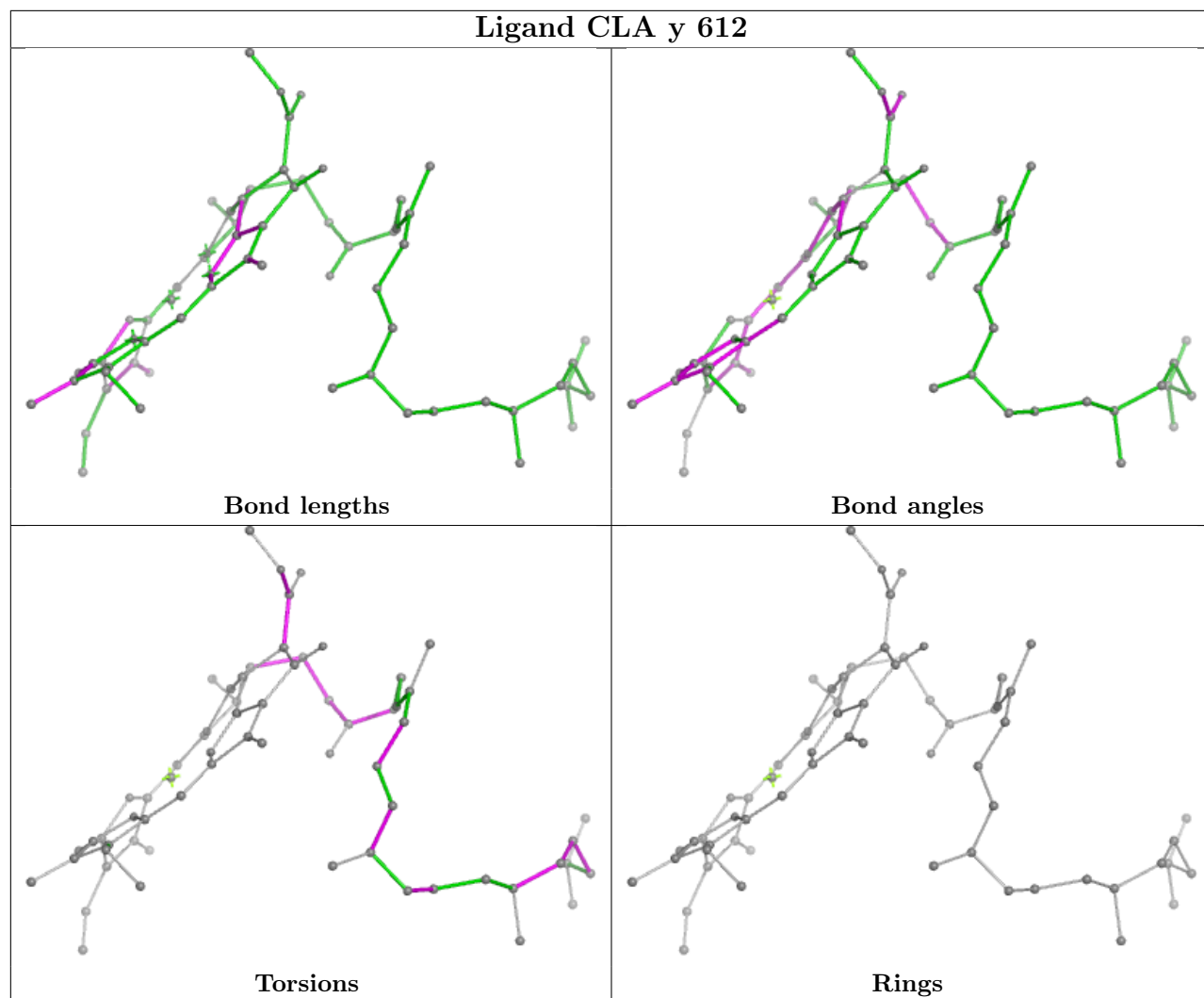


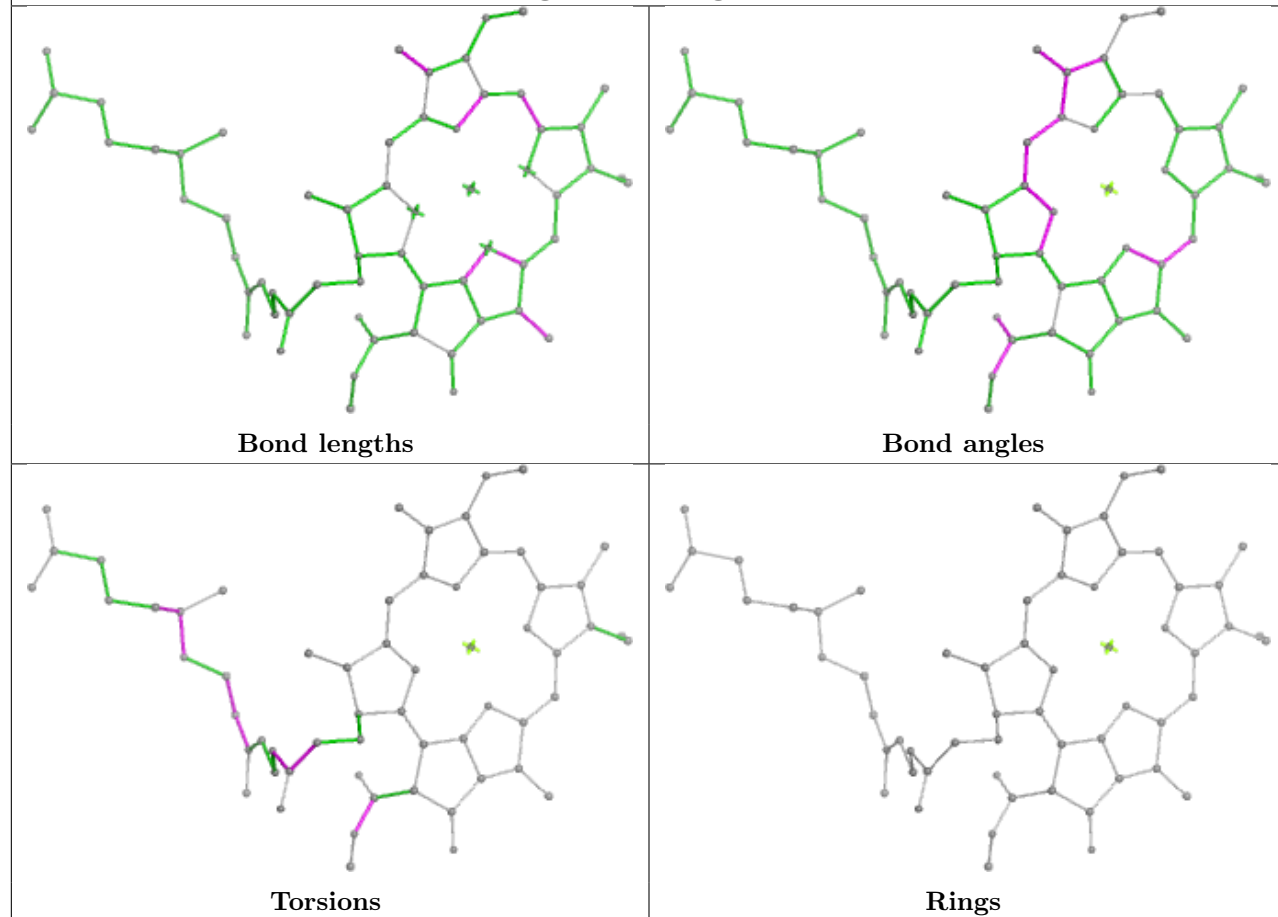
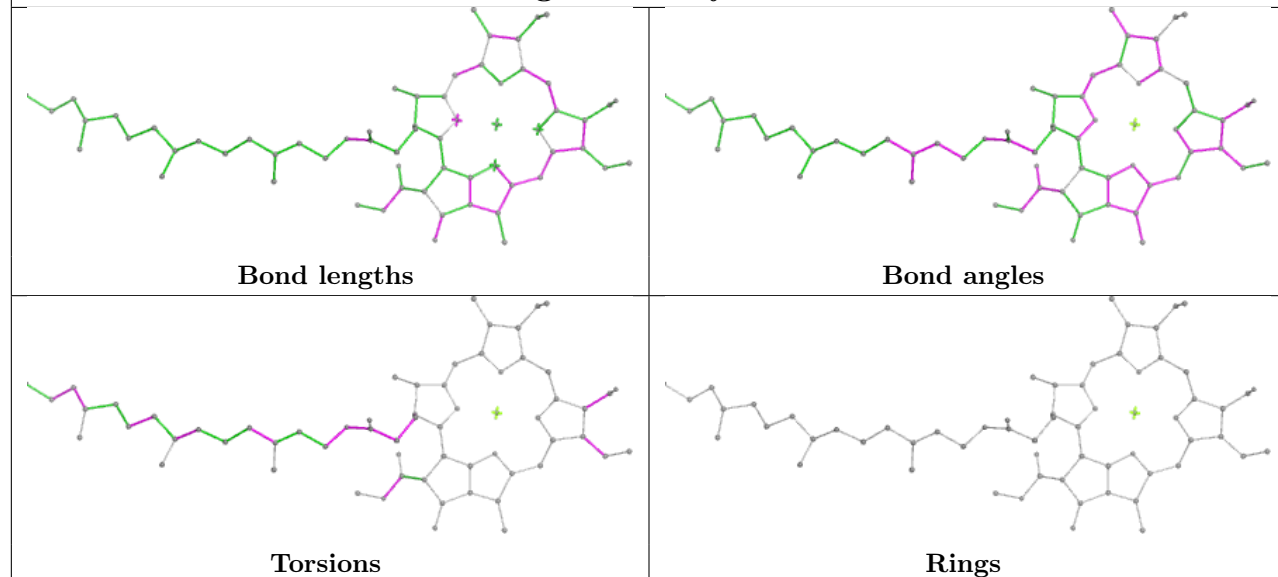




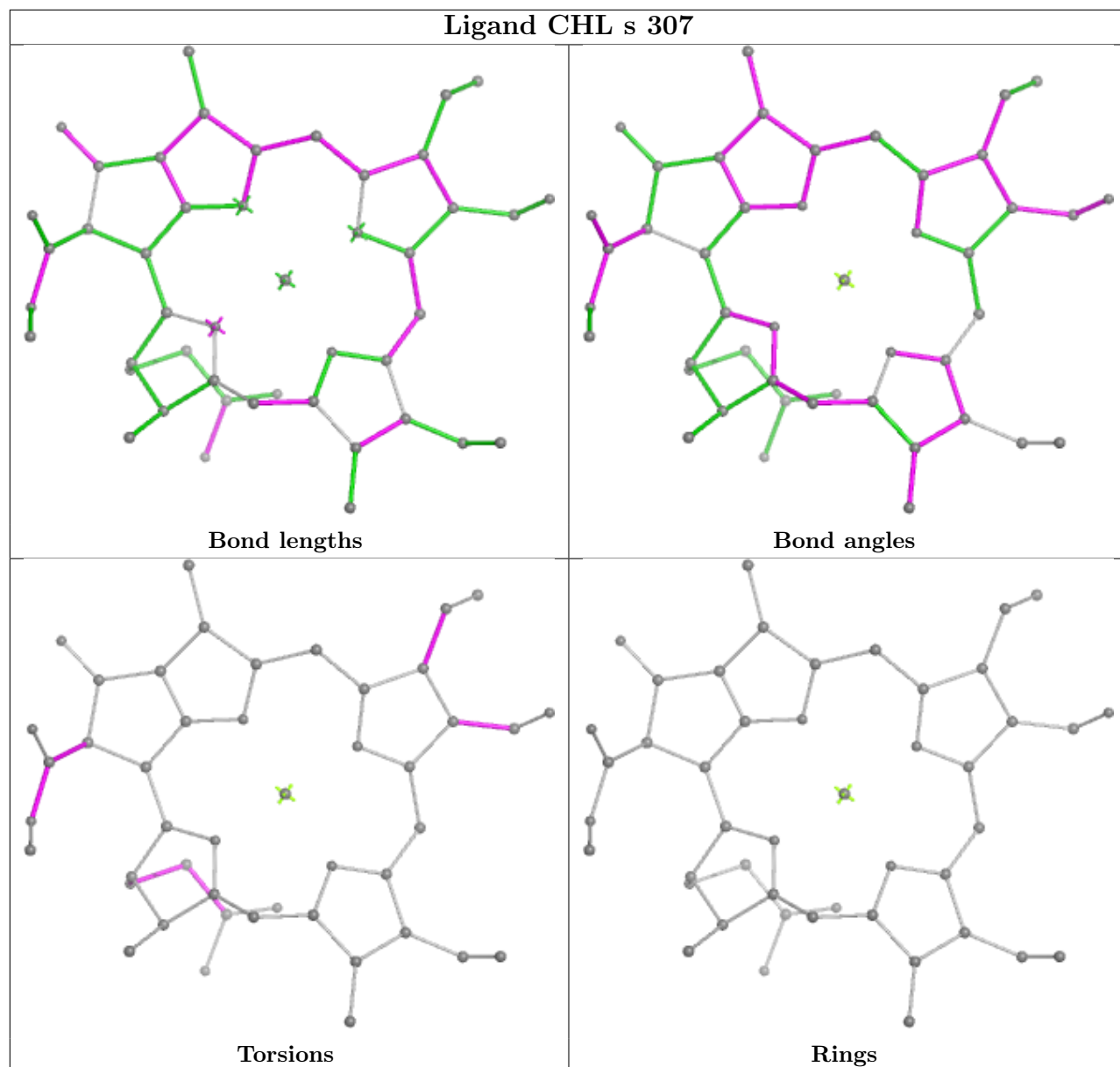


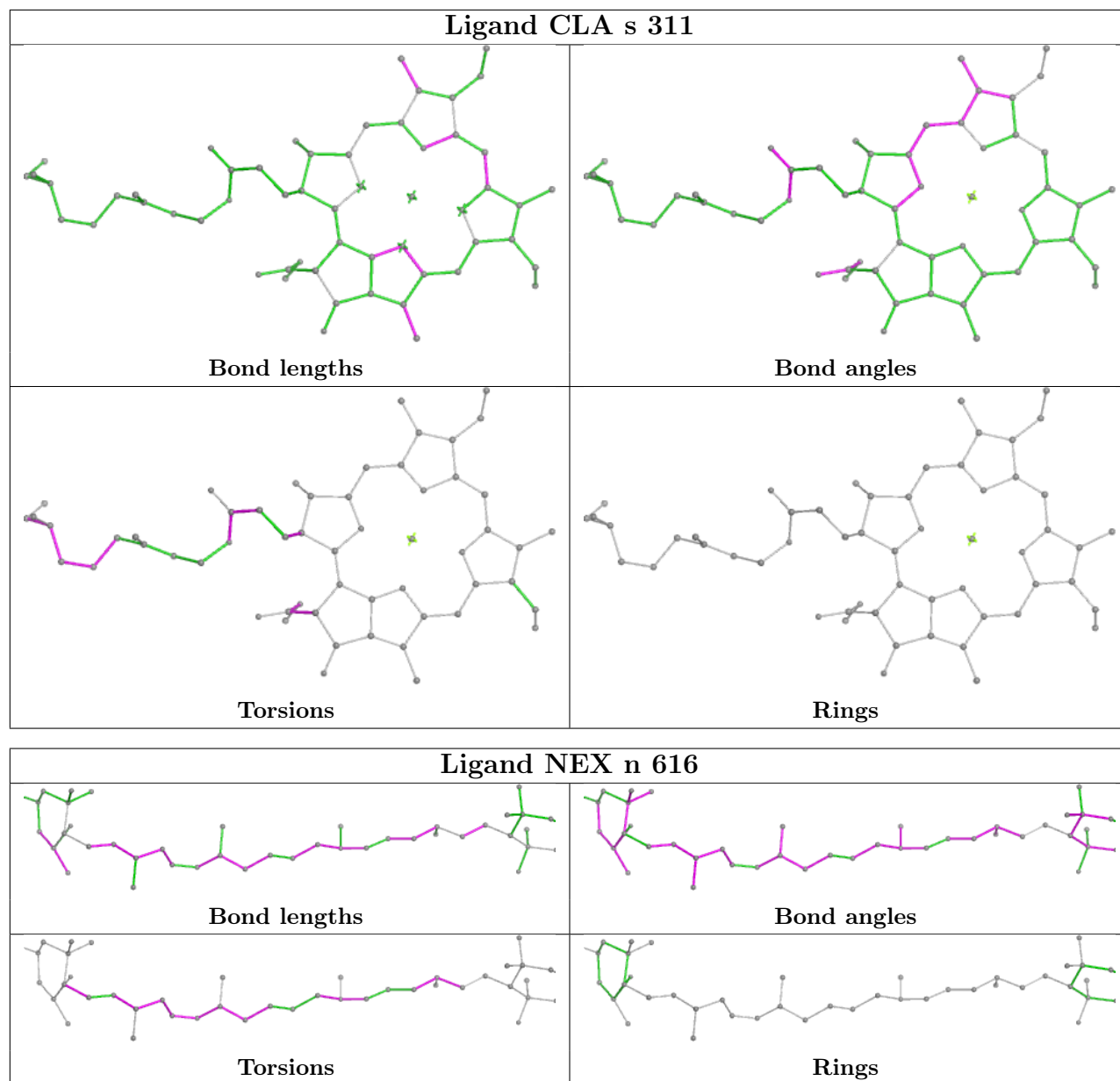




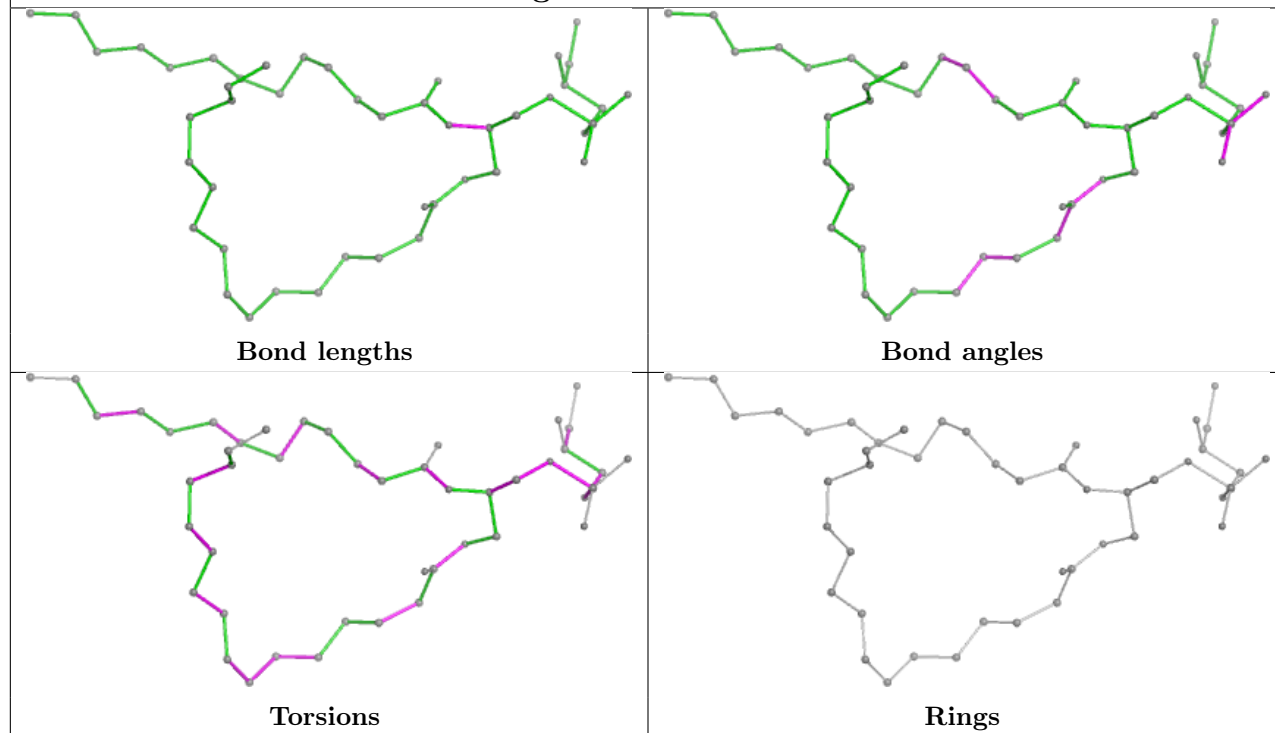
**Ligand CLA g 612****Ligand CHL y 601**

## Ligand CHL s 307

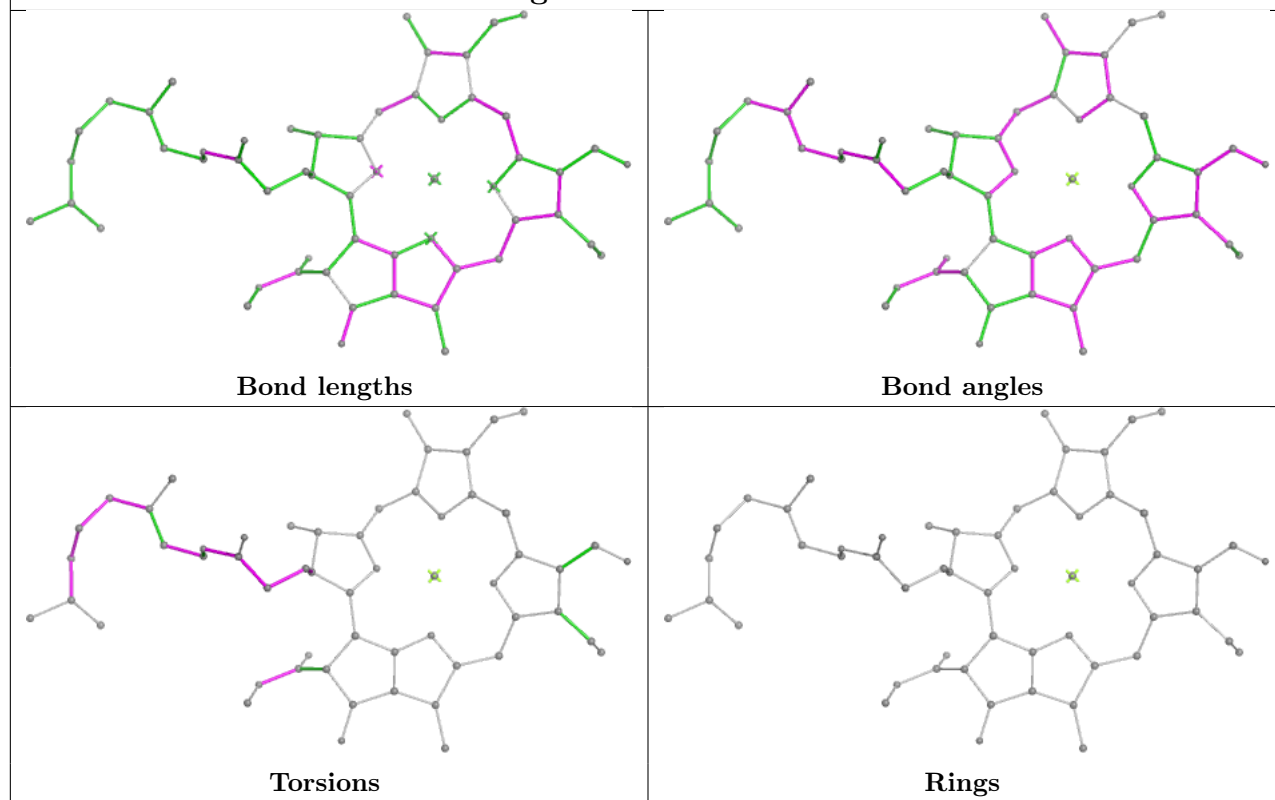




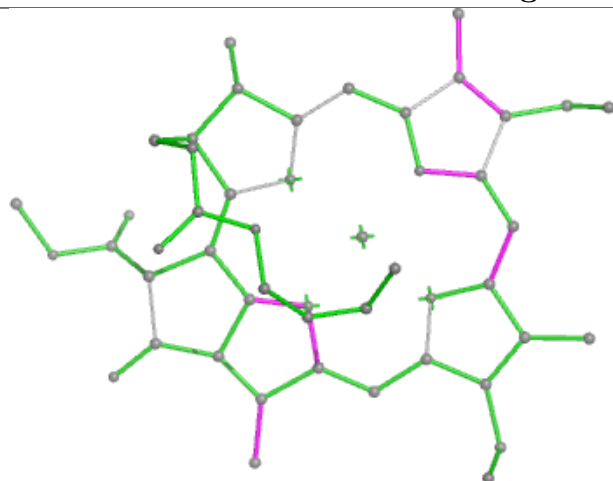
## Ligand LHG d 407



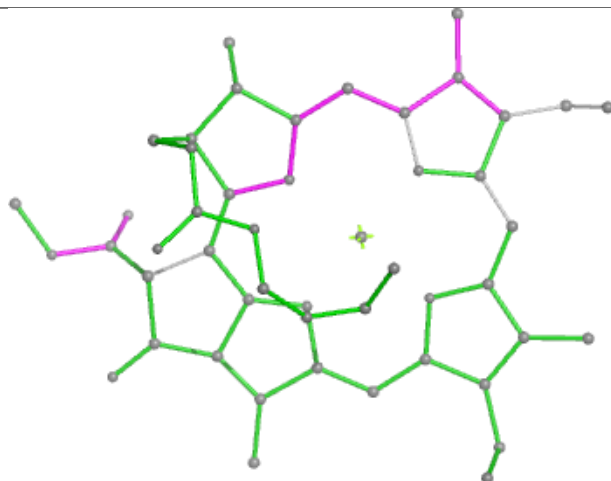
## Ligand CHL R 306



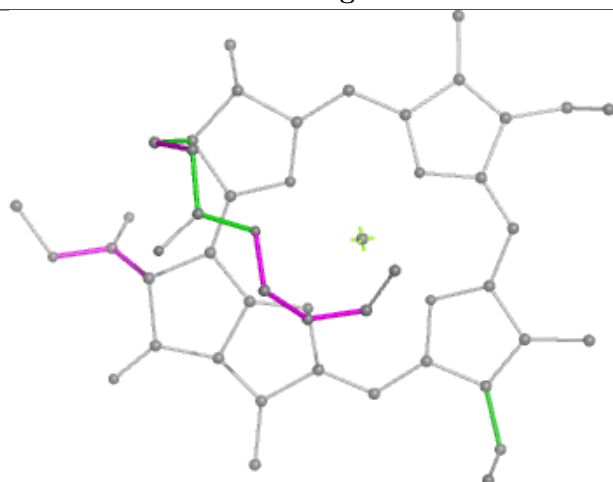
## Ligand CLA s 312



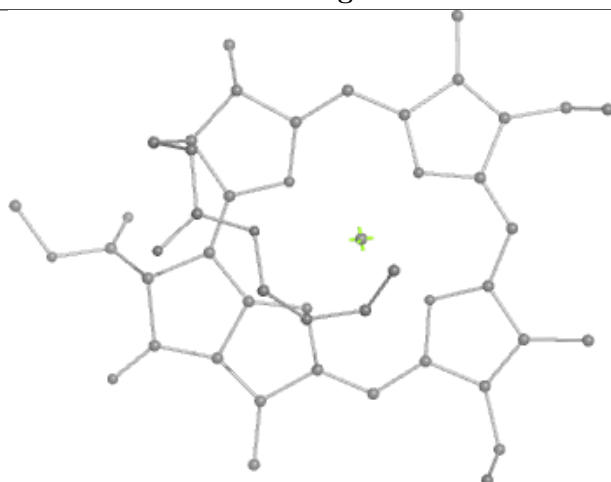
Bond lengths



Bond angles



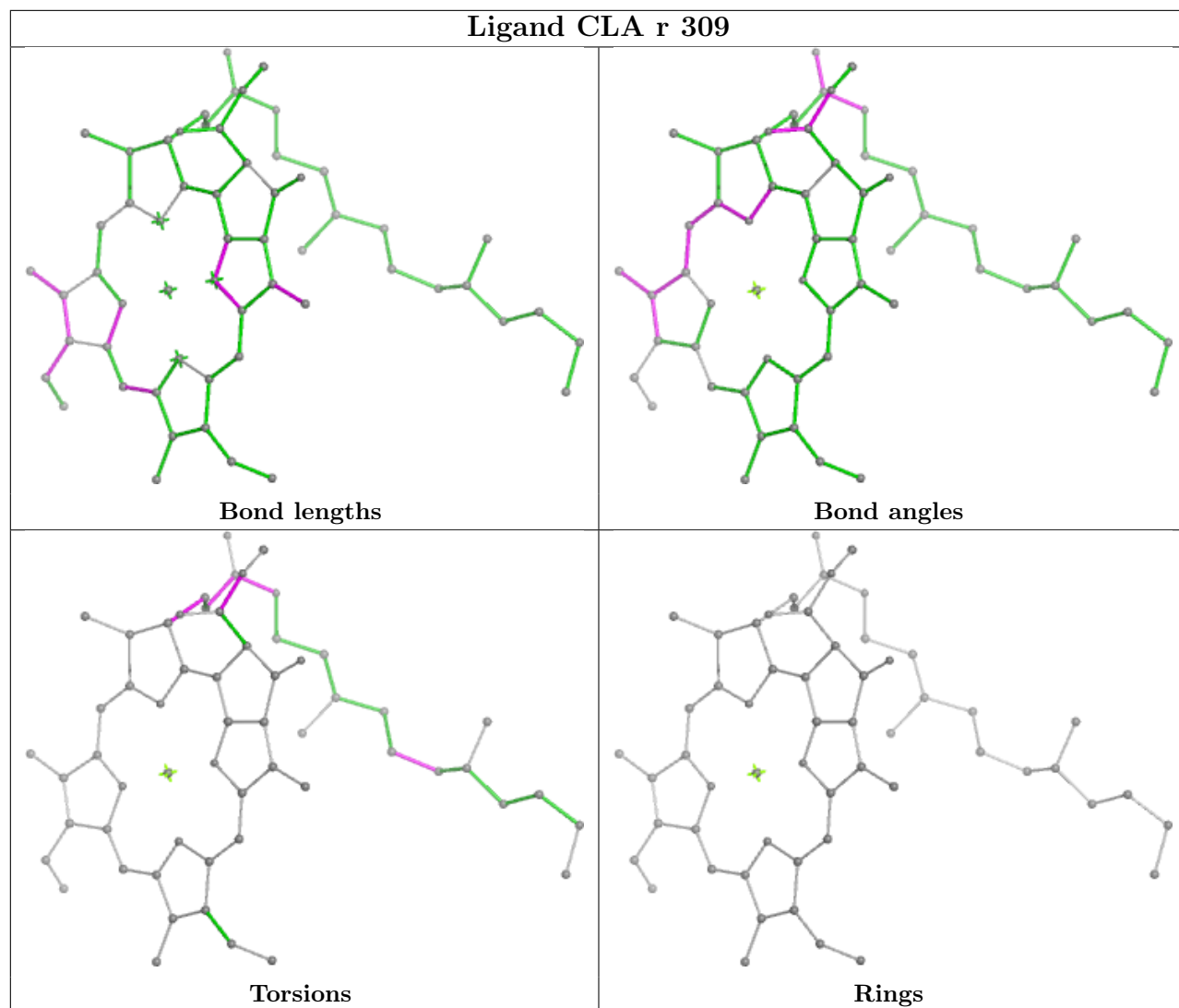
Torsions

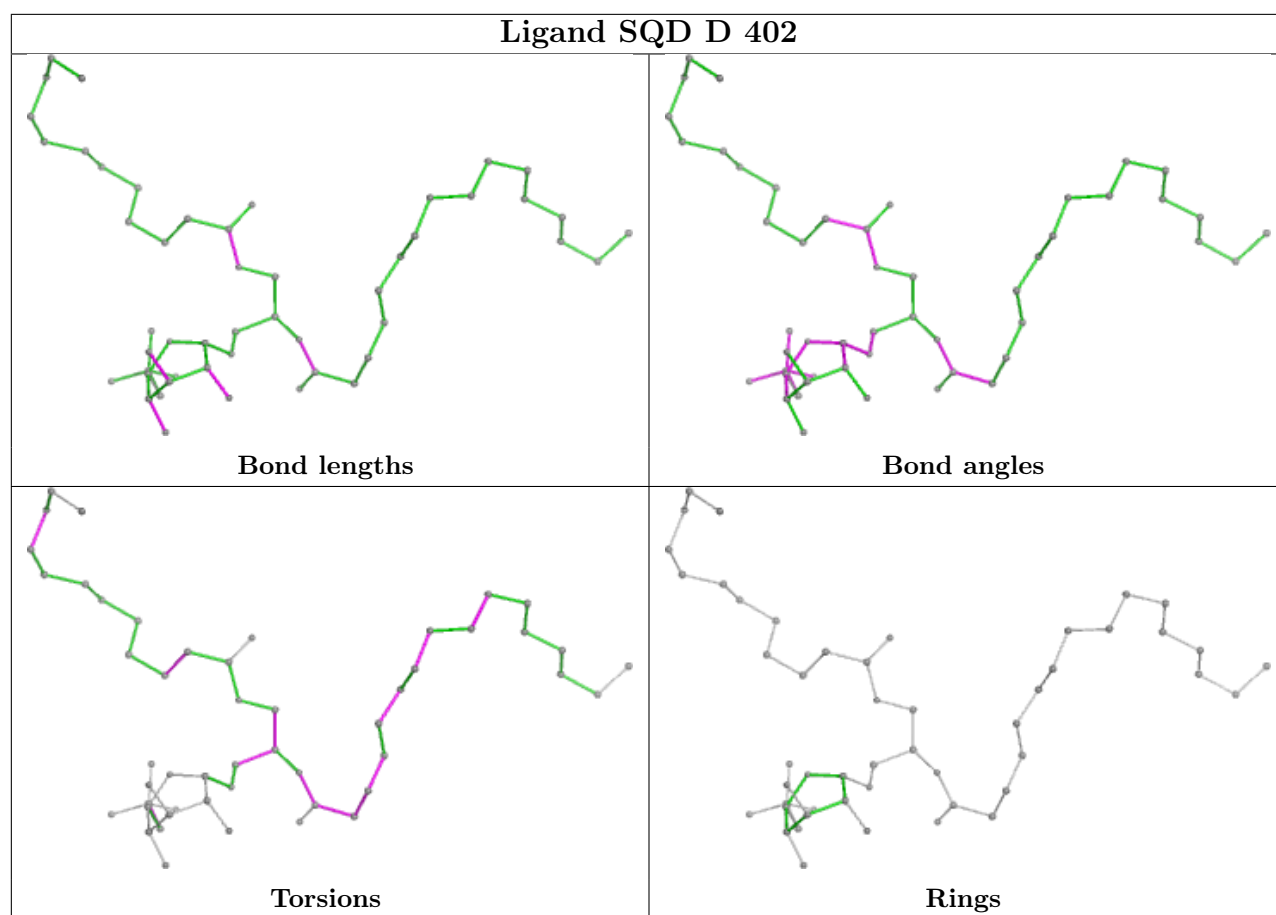


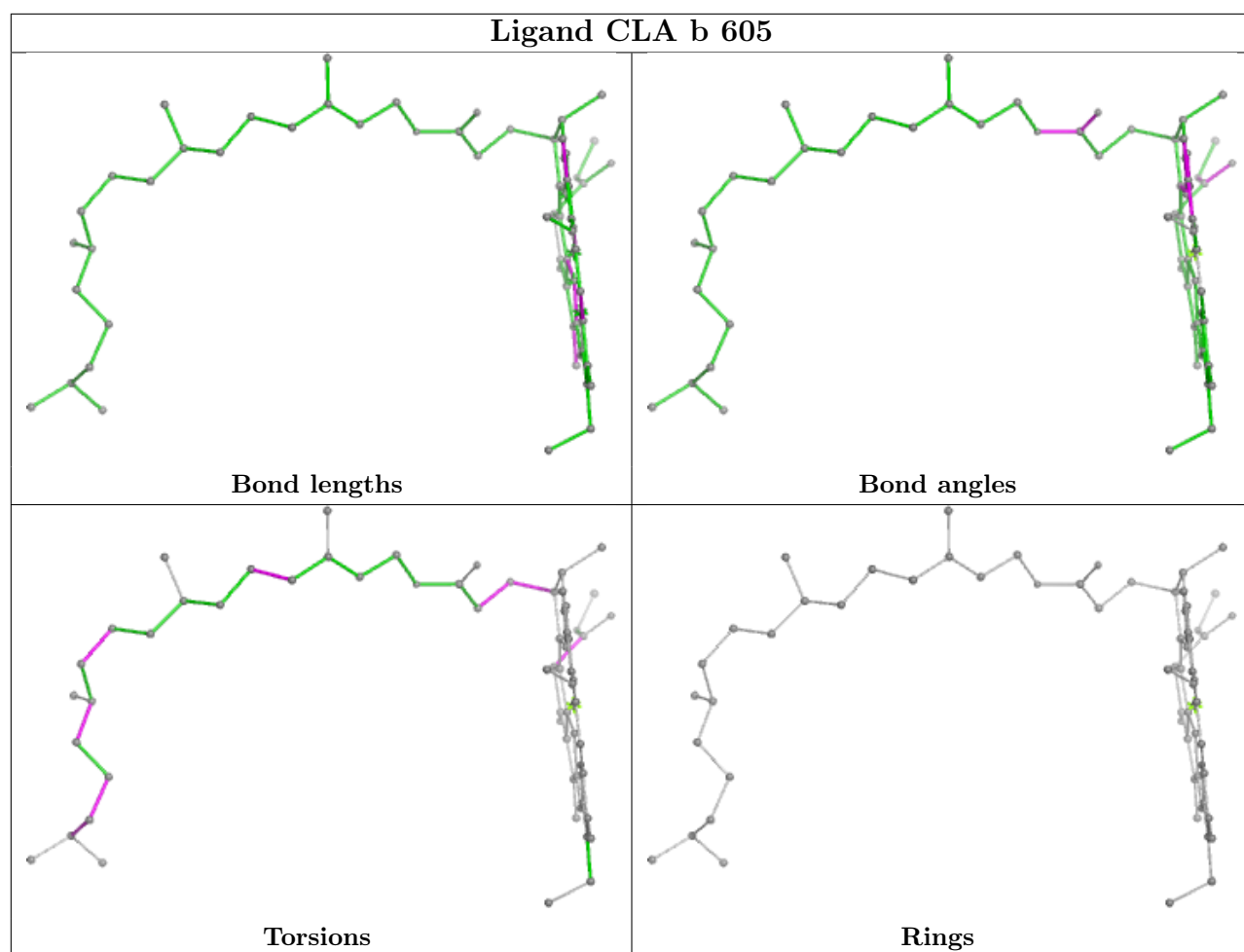
Rings

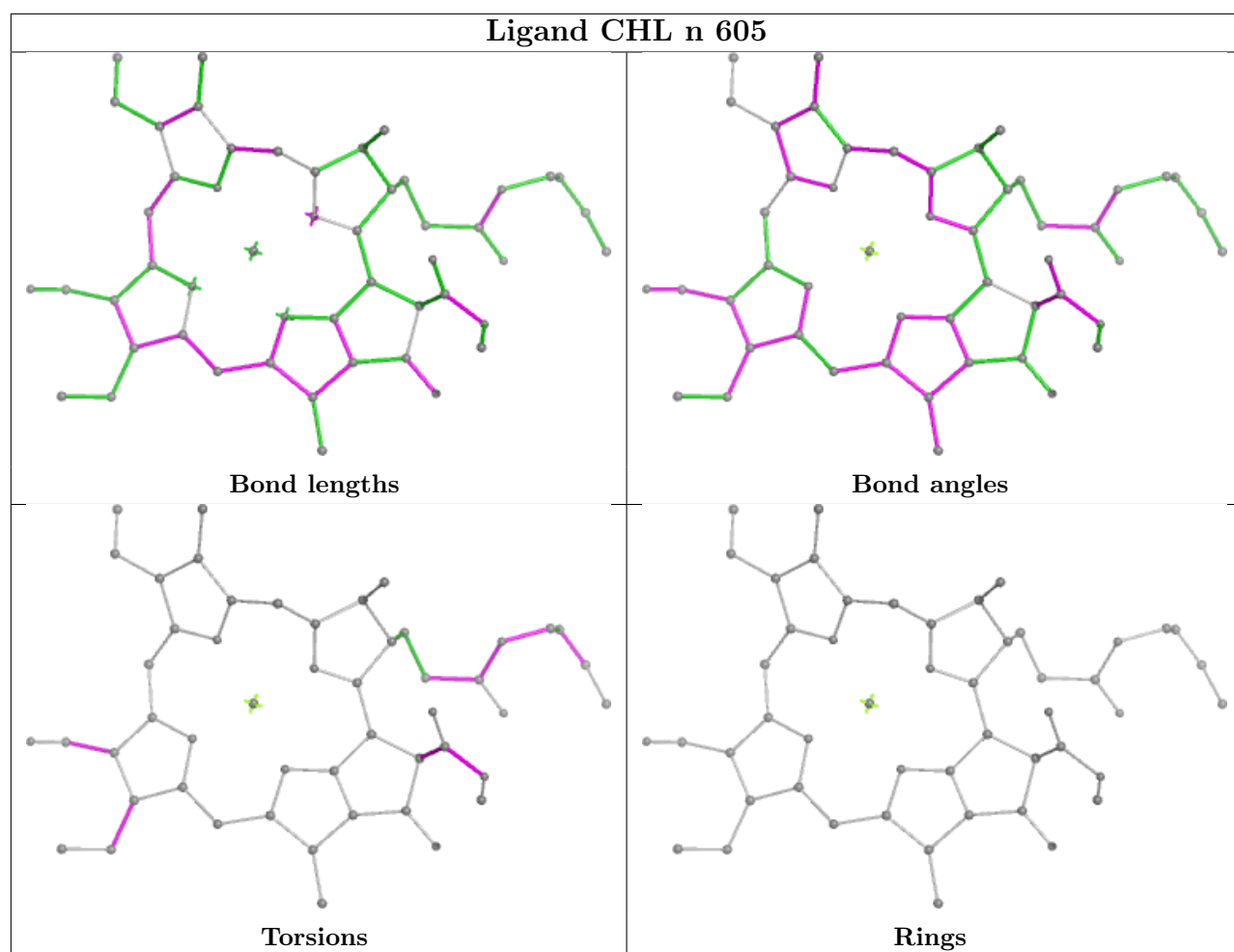


## Ligand CLA r 309

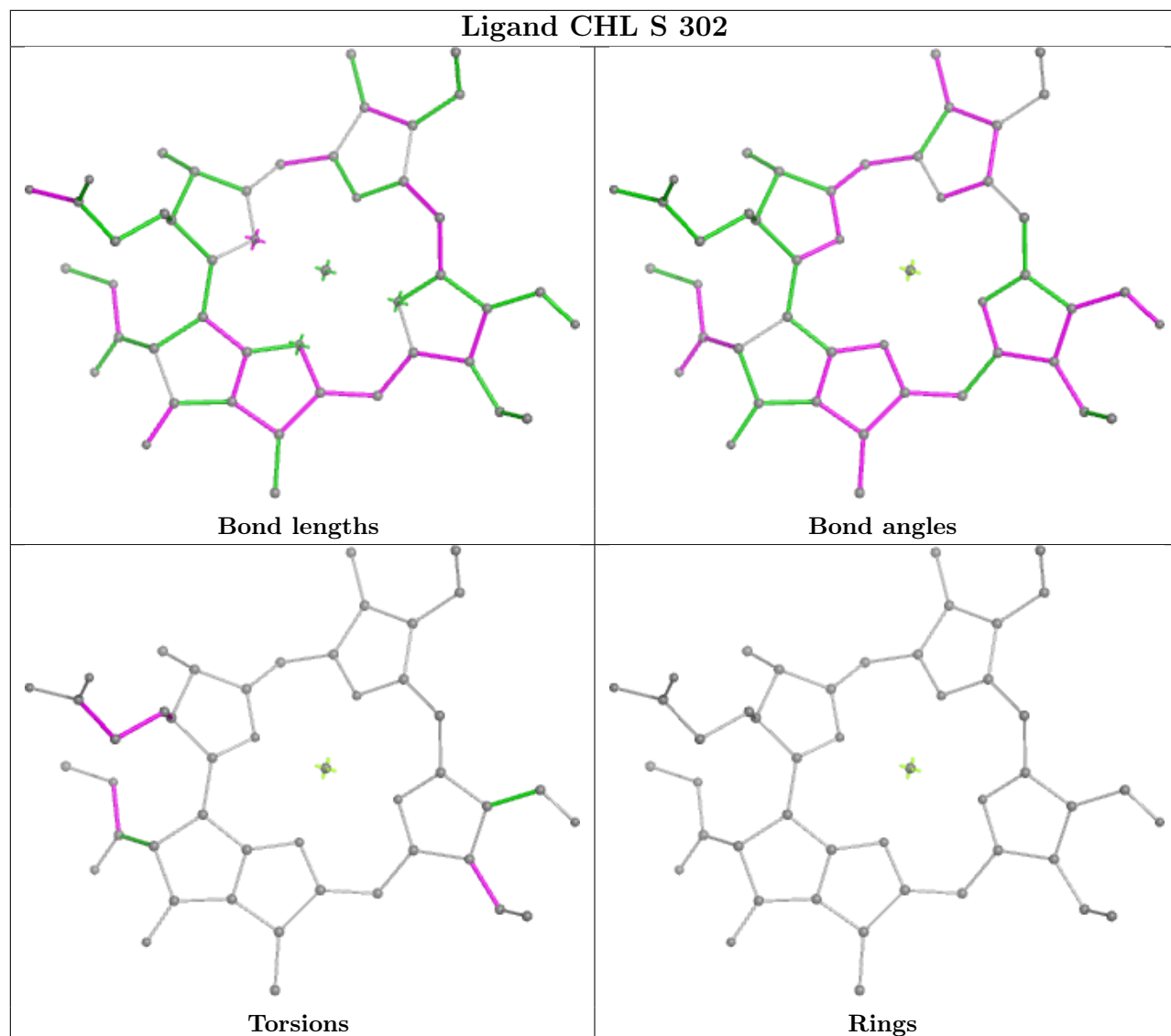


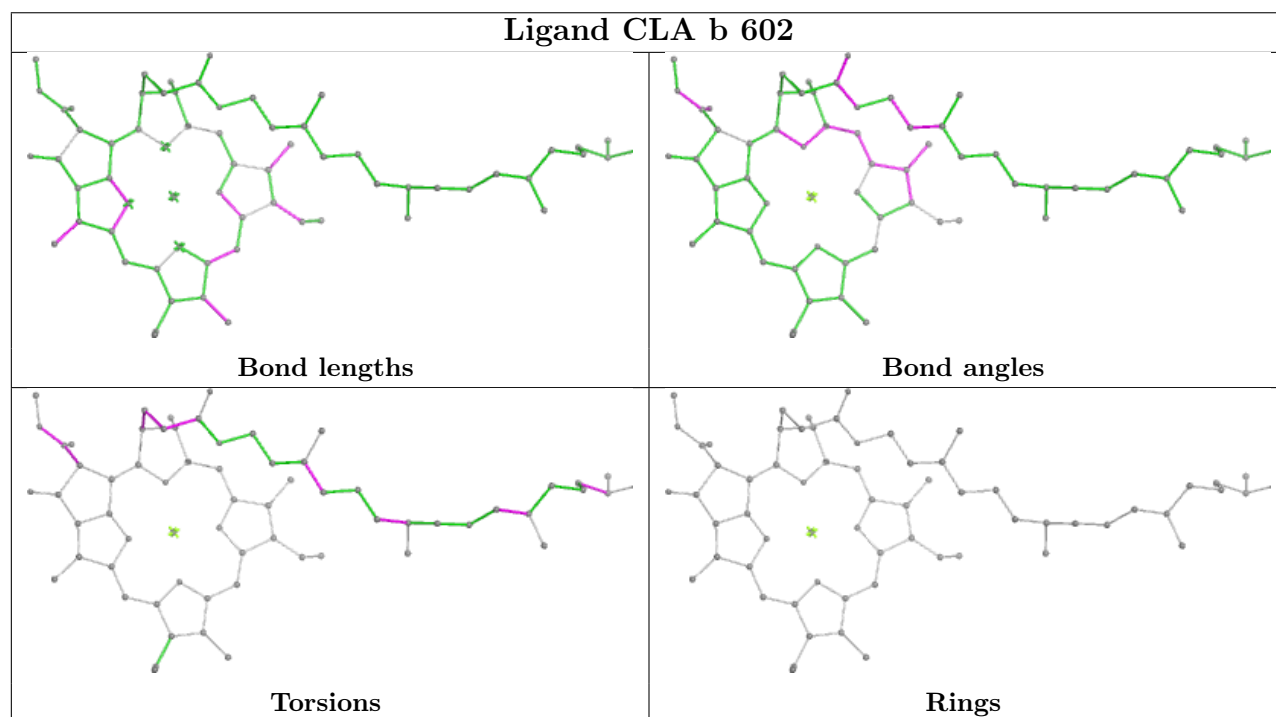
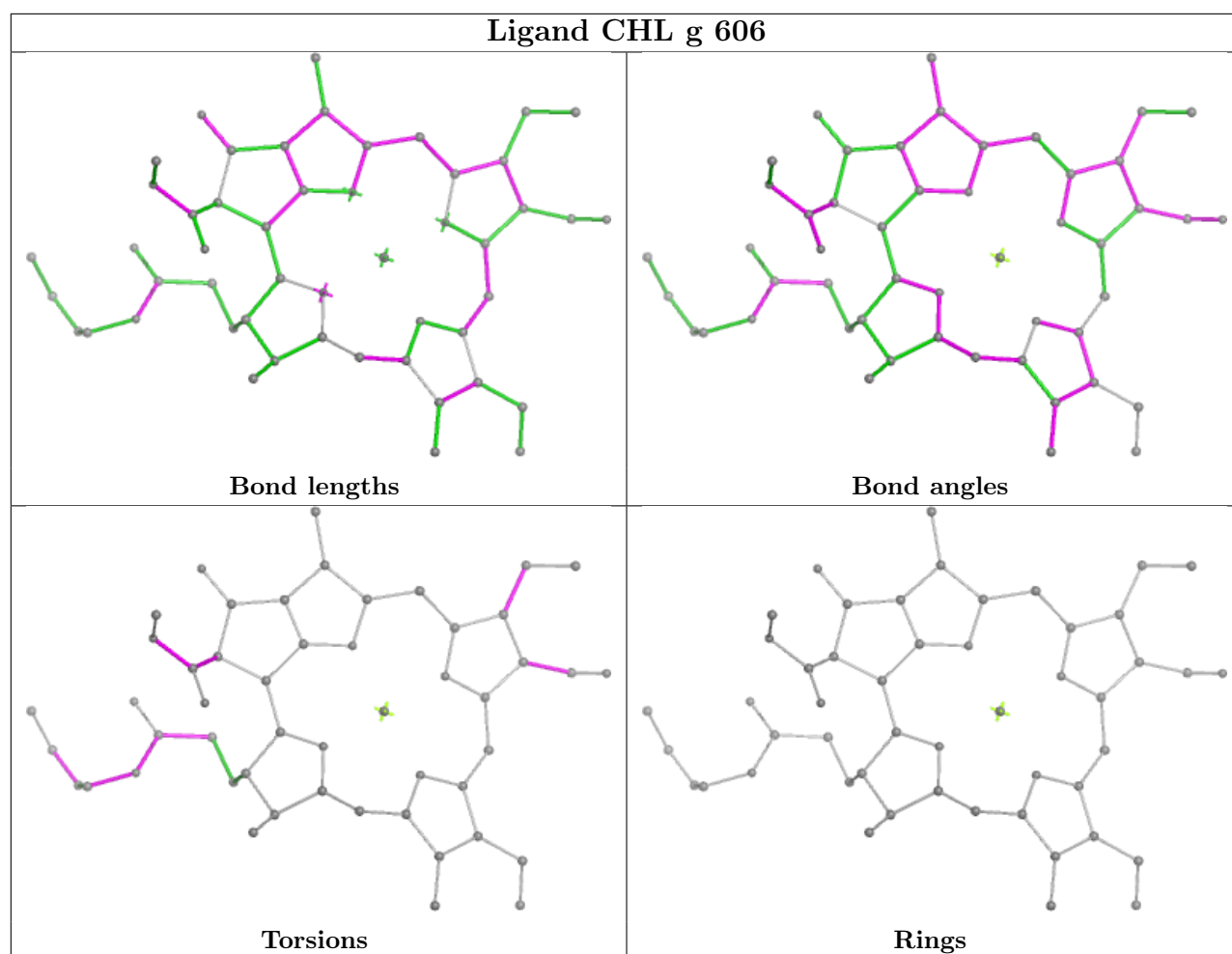




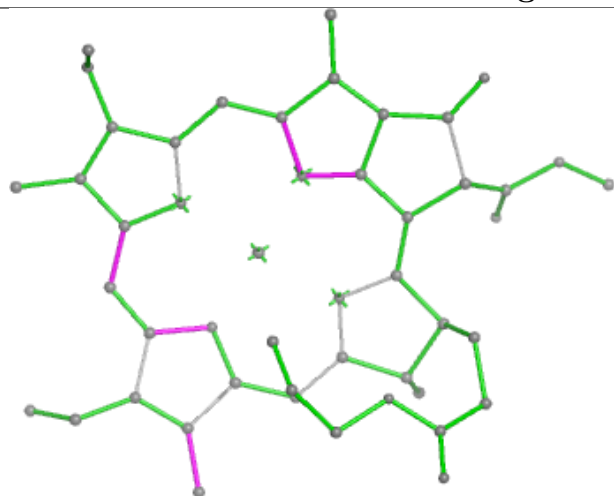


## Ligand CHL S 302

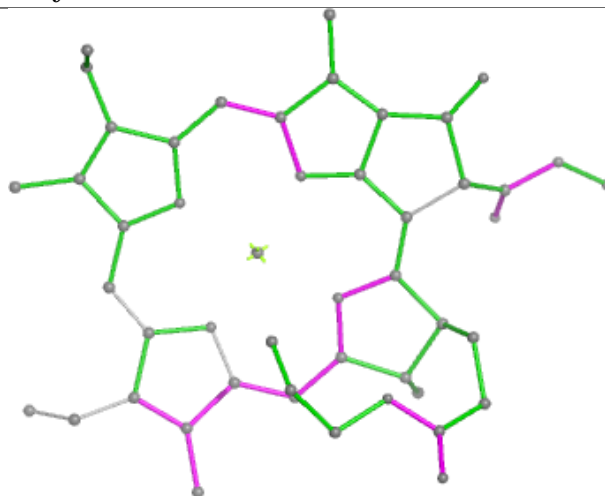




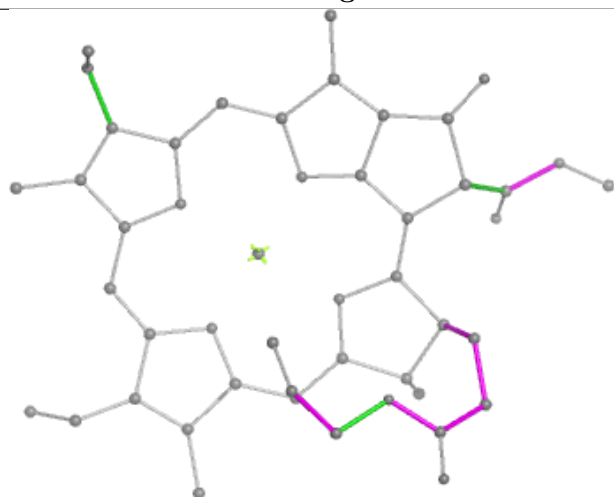
## Ligand CLA y 613



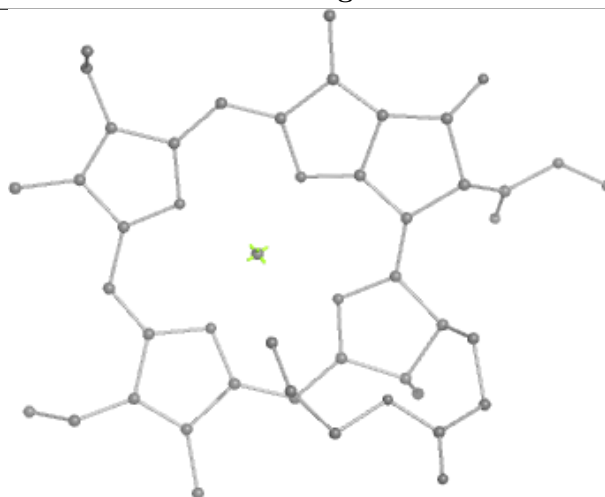
Bond lengths



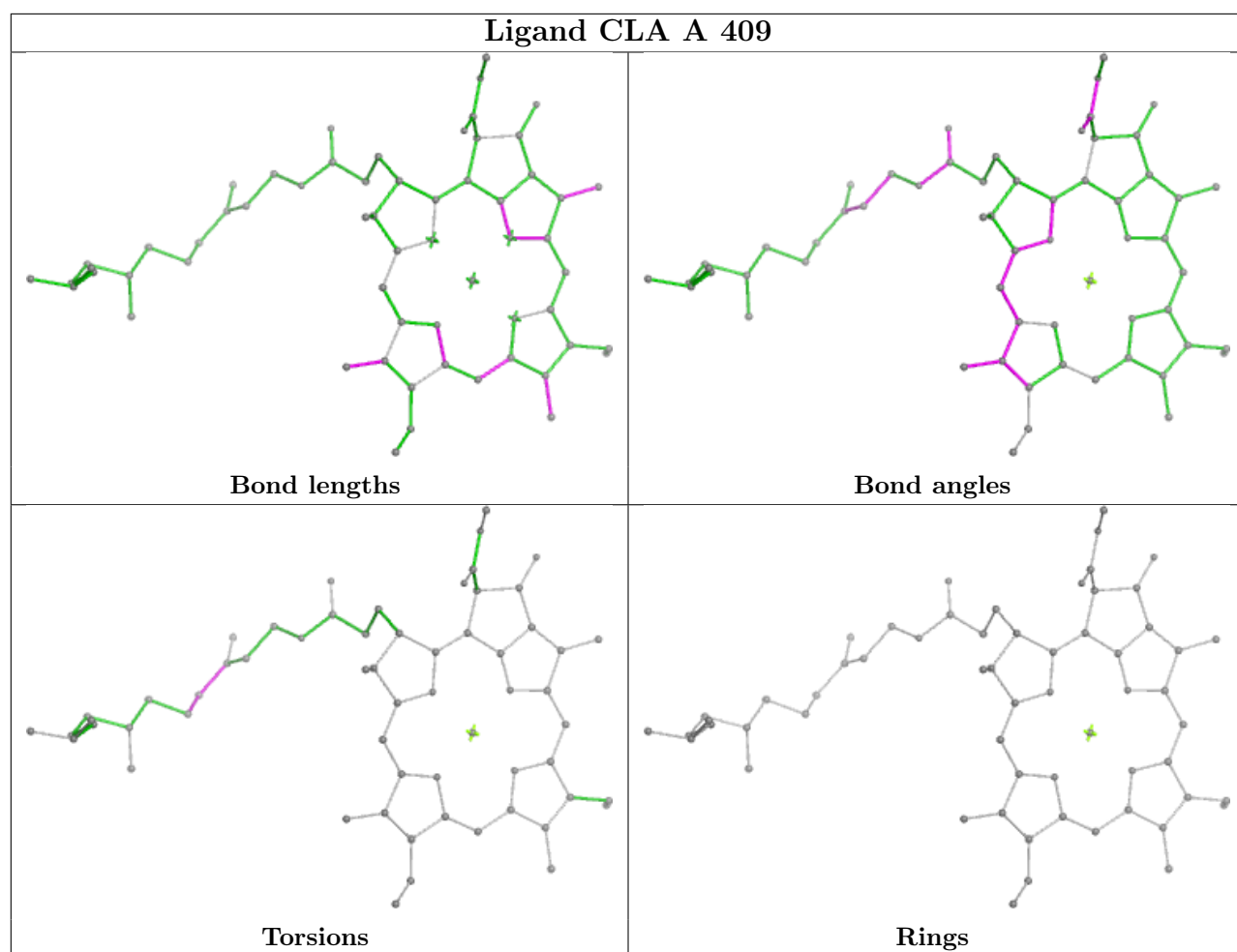
Bond angles



Torsions

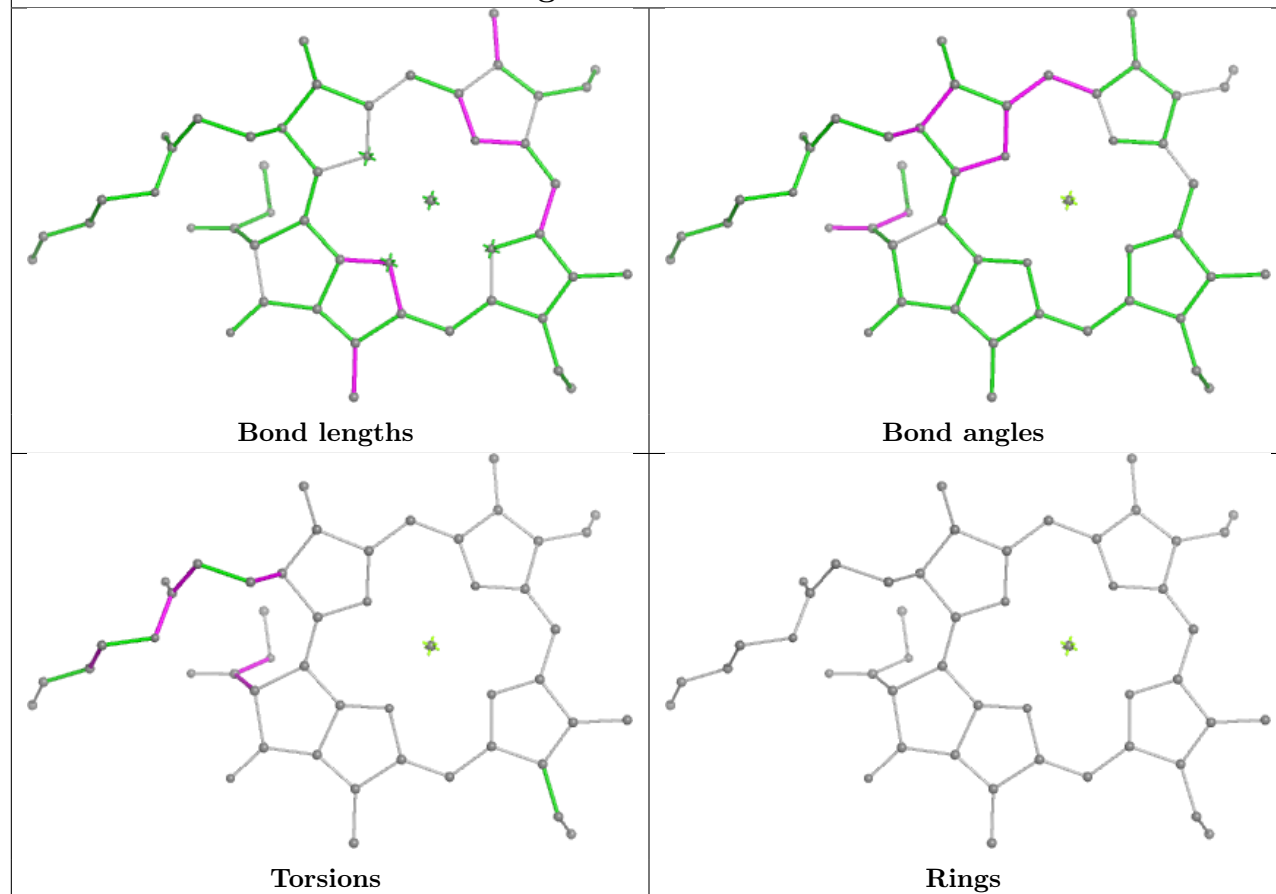


Rings

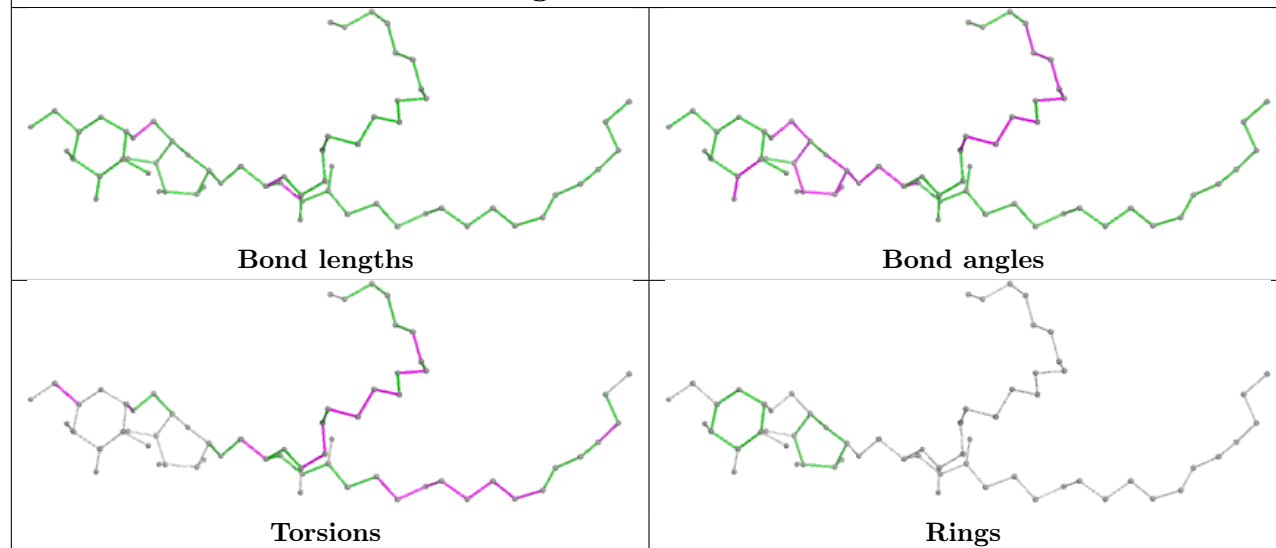


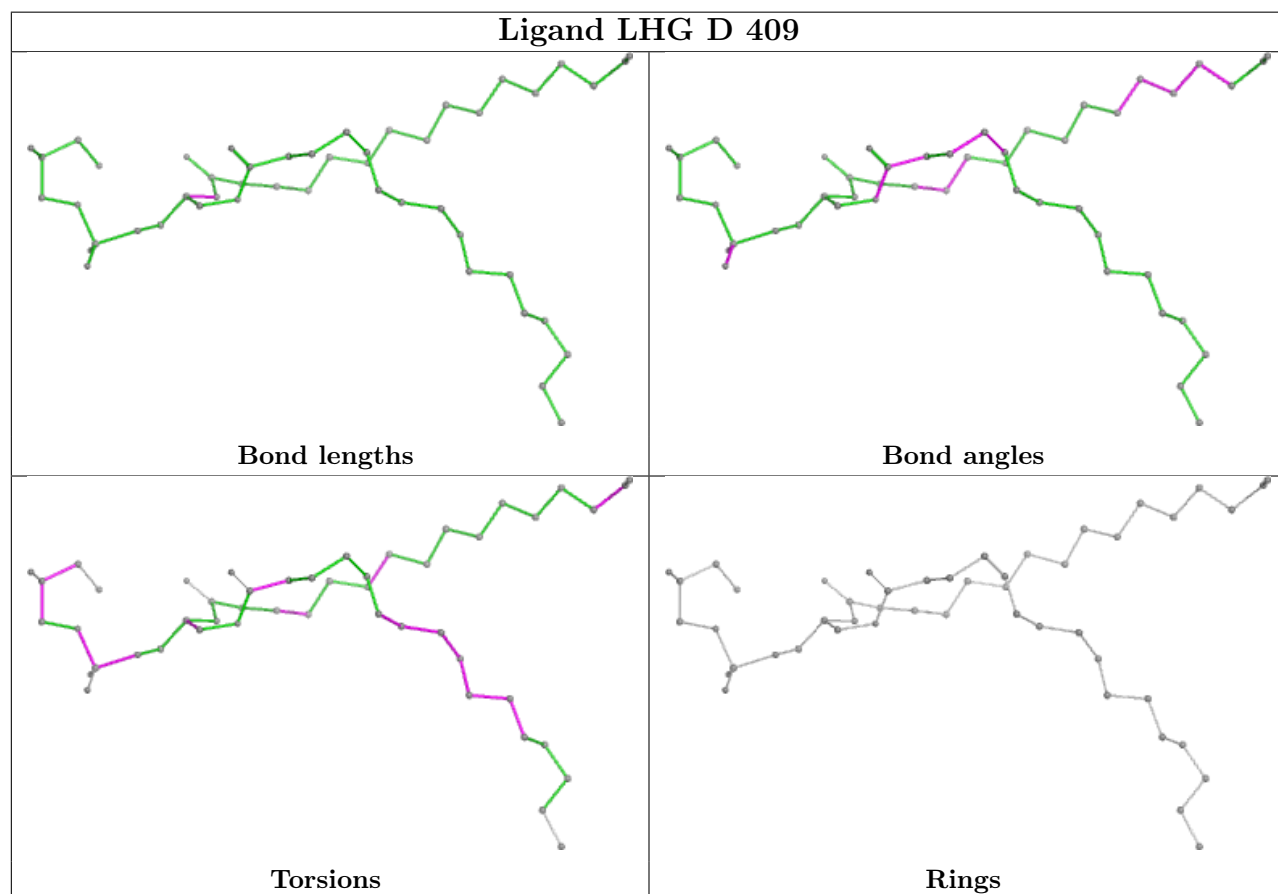
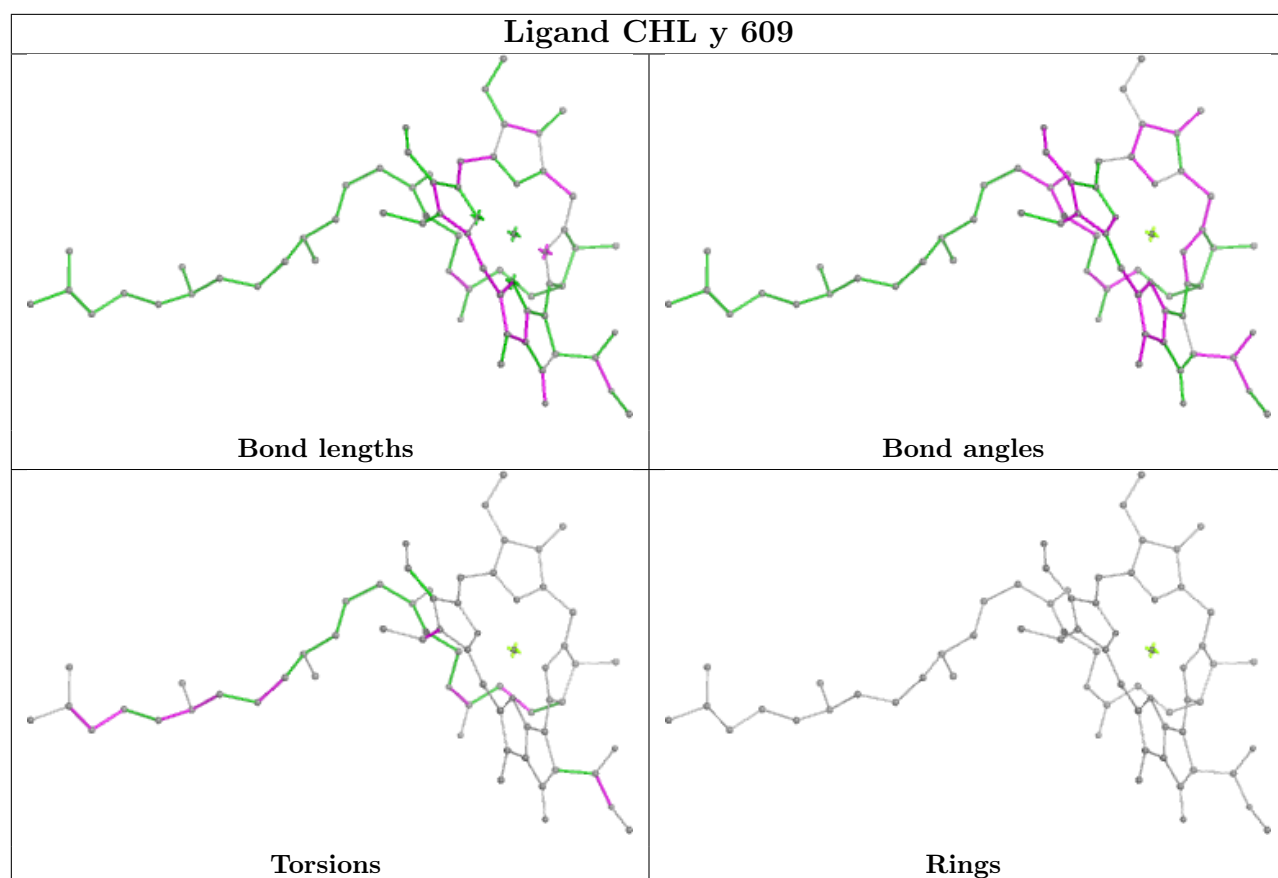


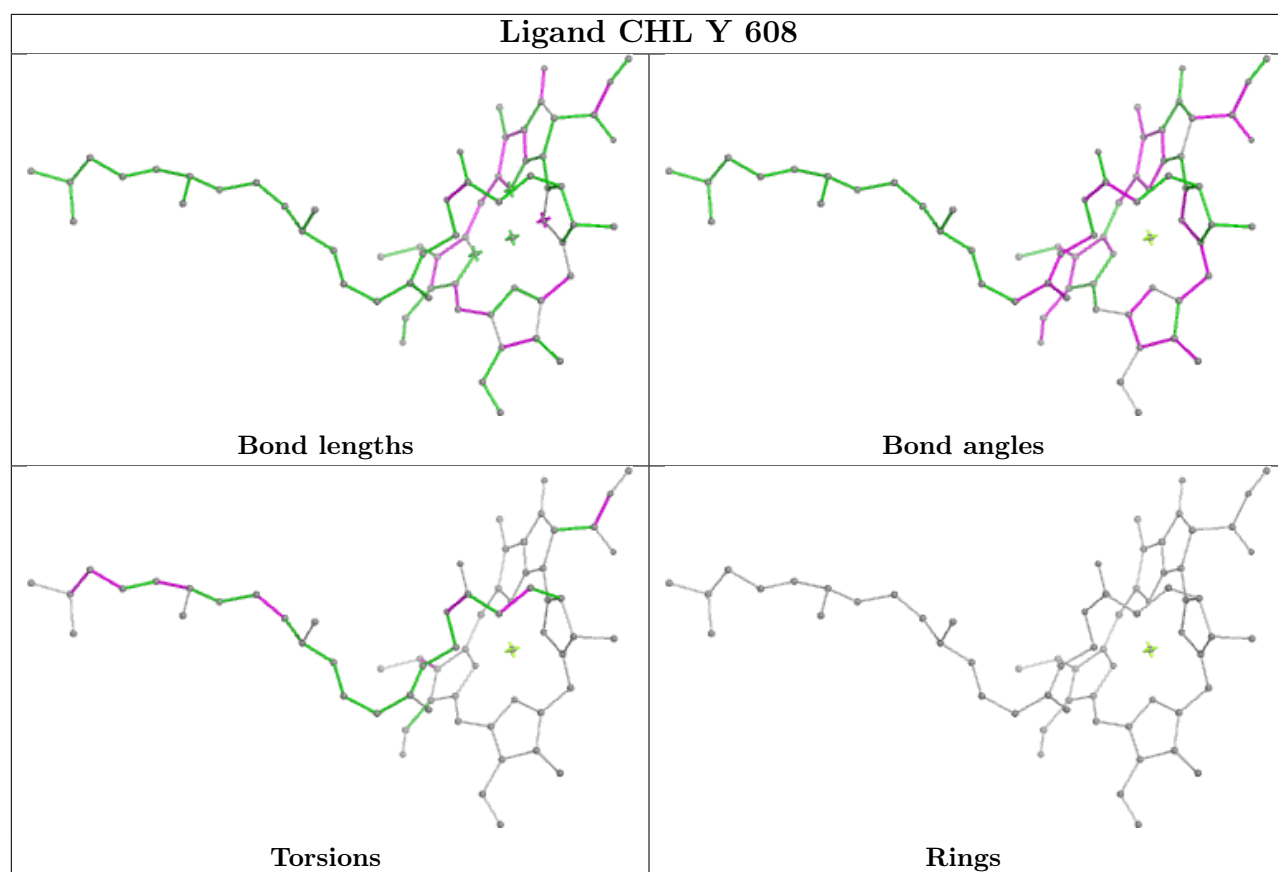
## Ligand CLA r 311



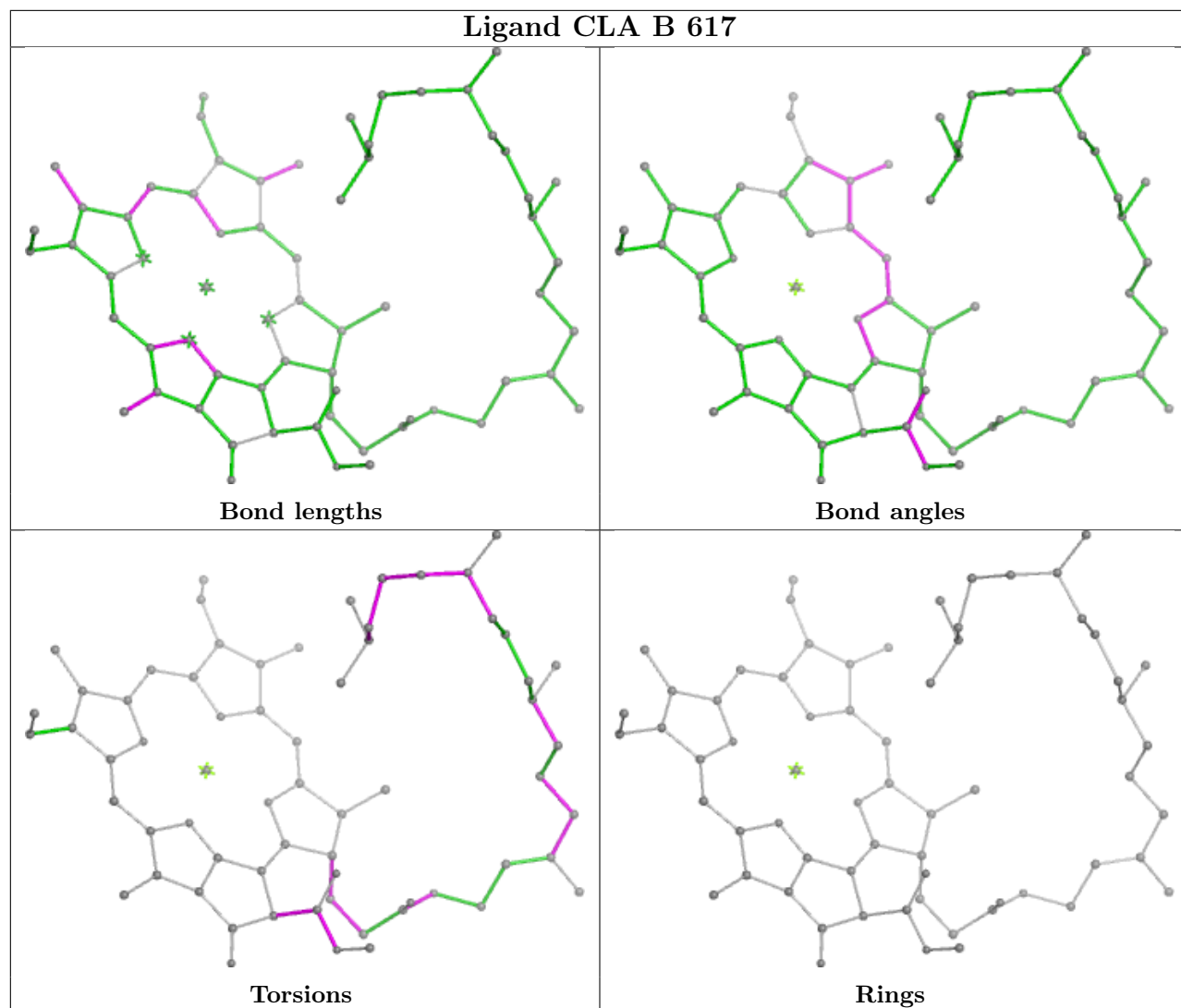
## Ligand DGD h 102

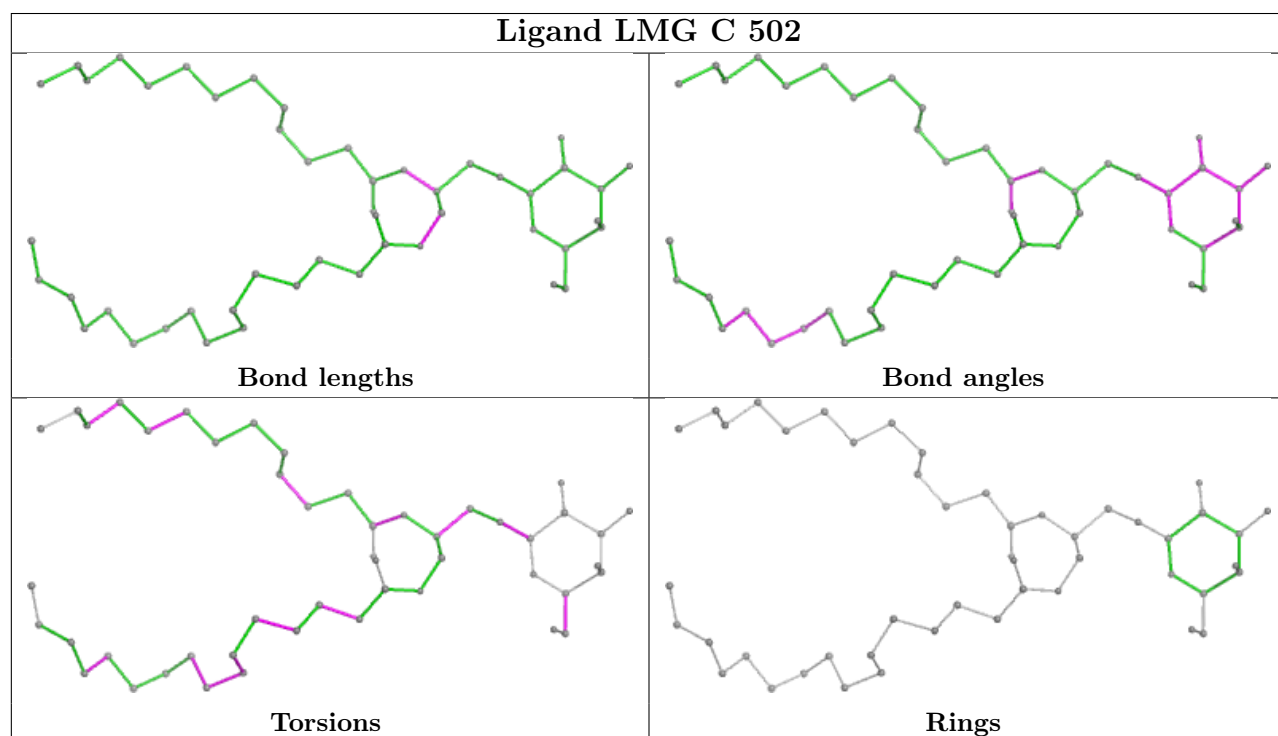
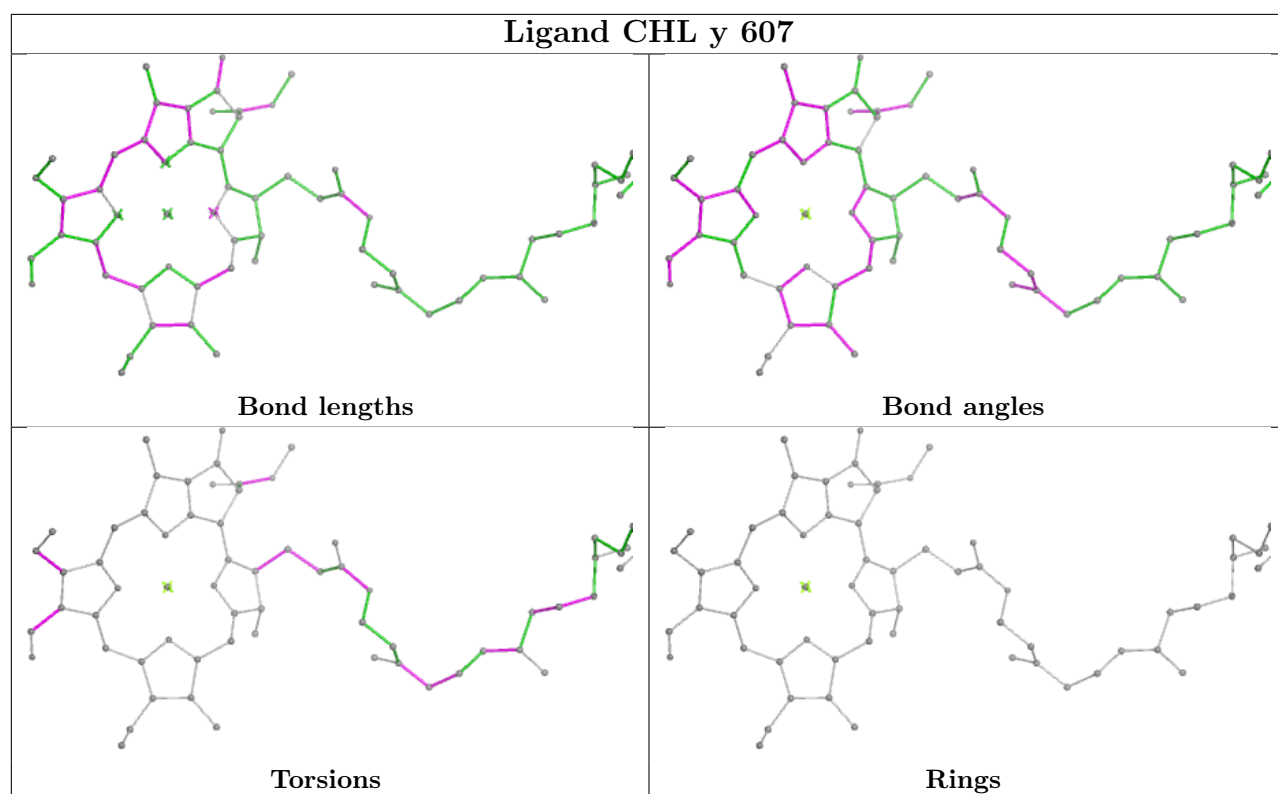


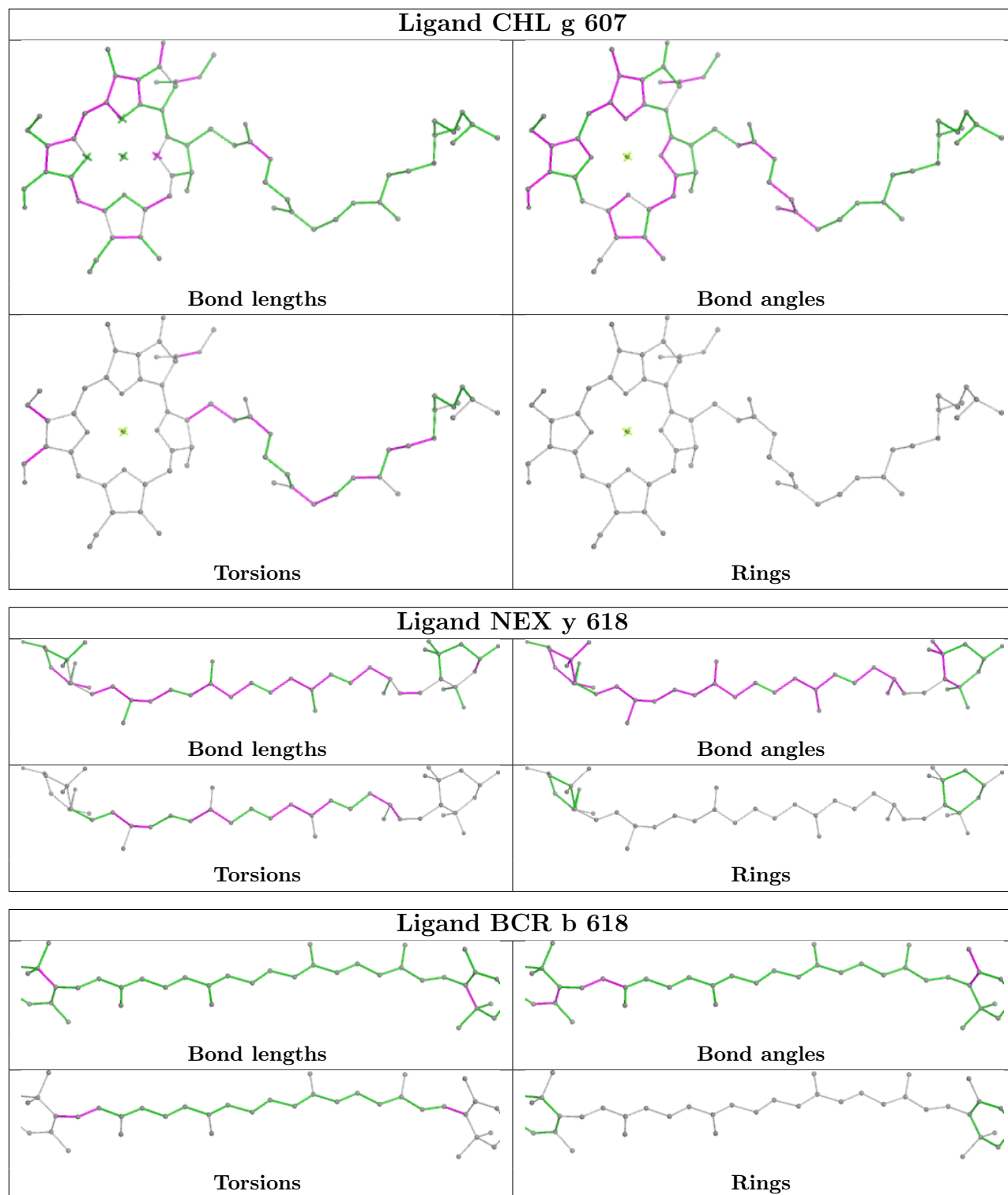


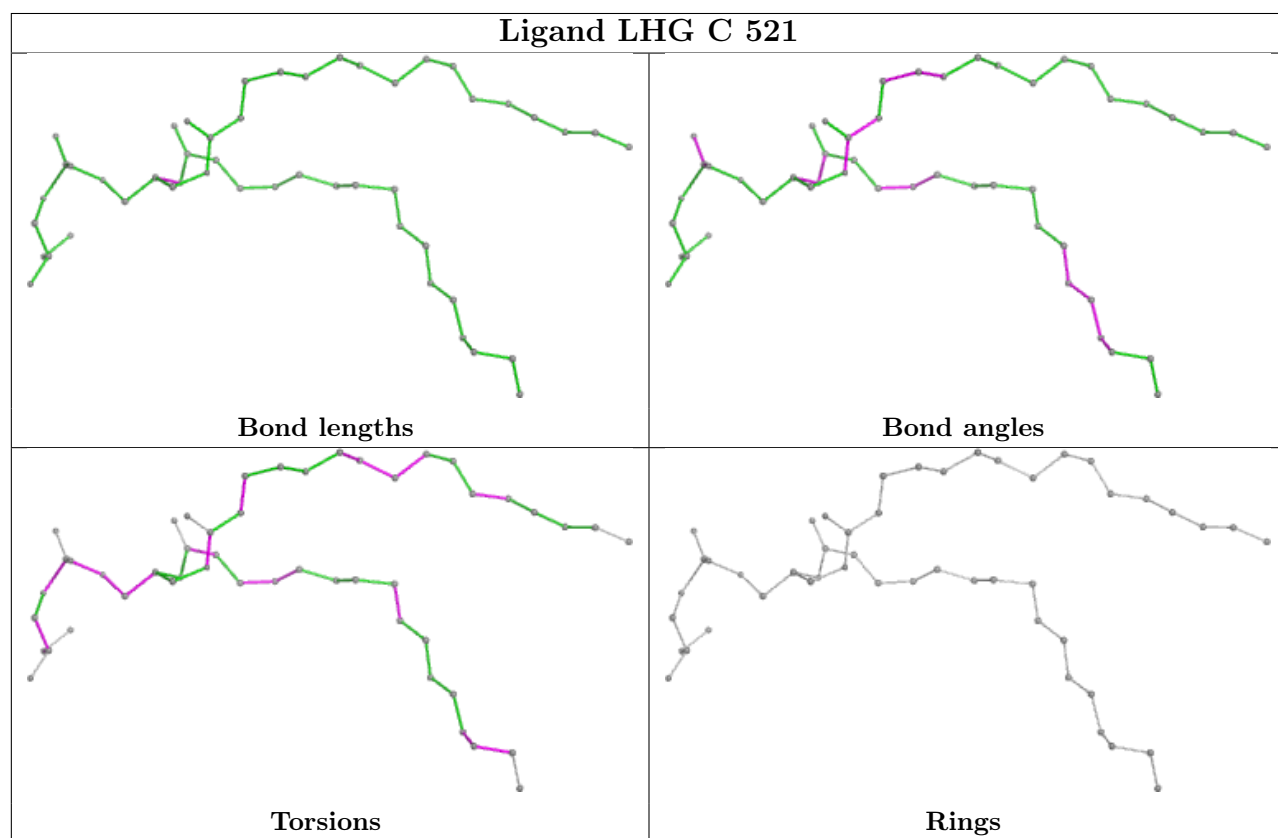
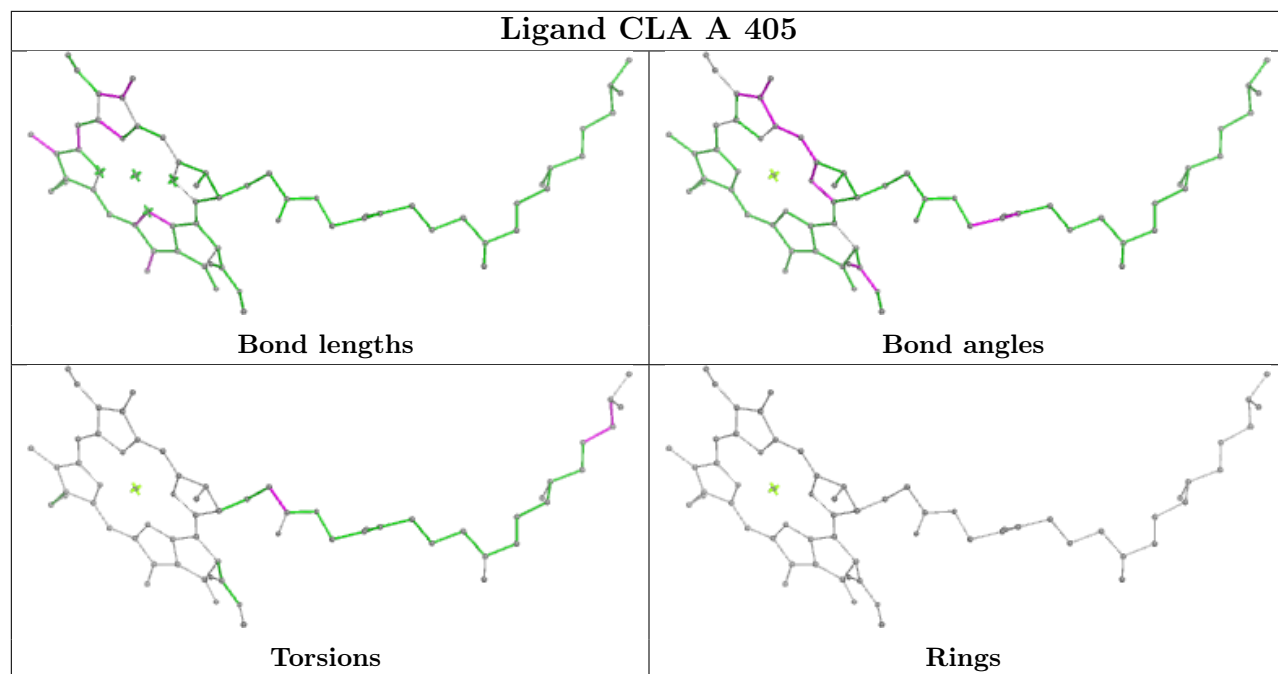


## Ligand CLA B 617

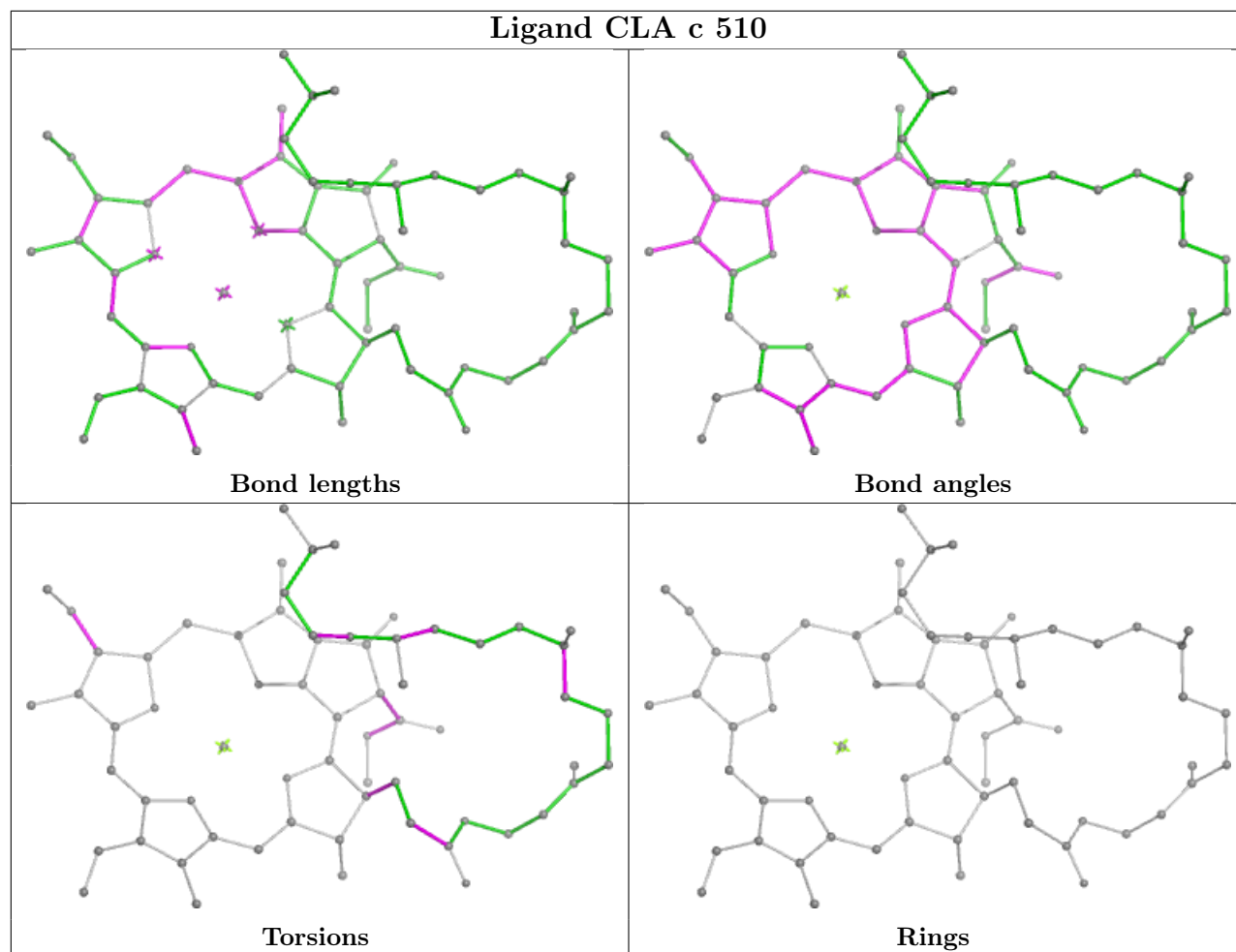




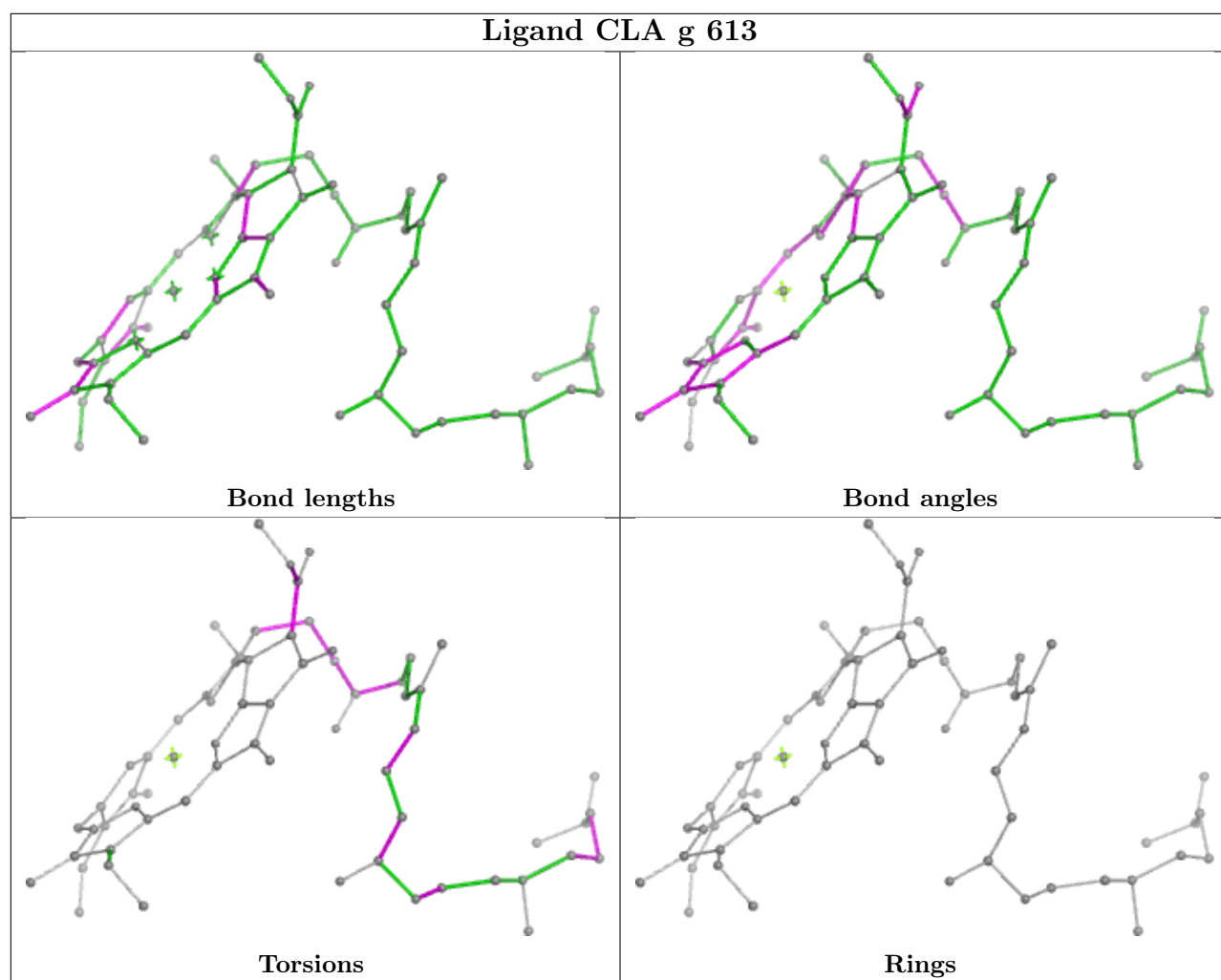




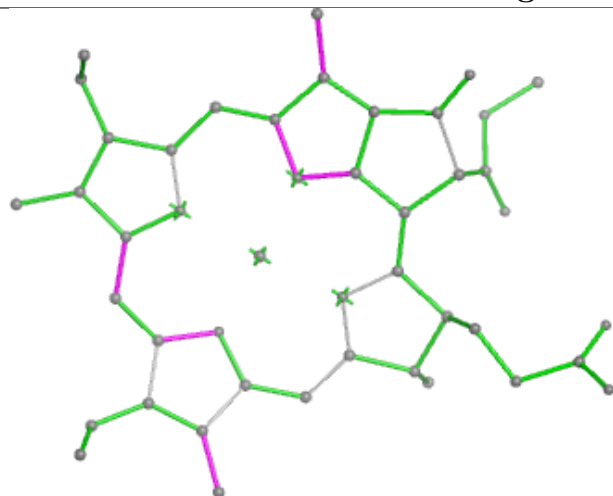
## Ligand CLA c 510



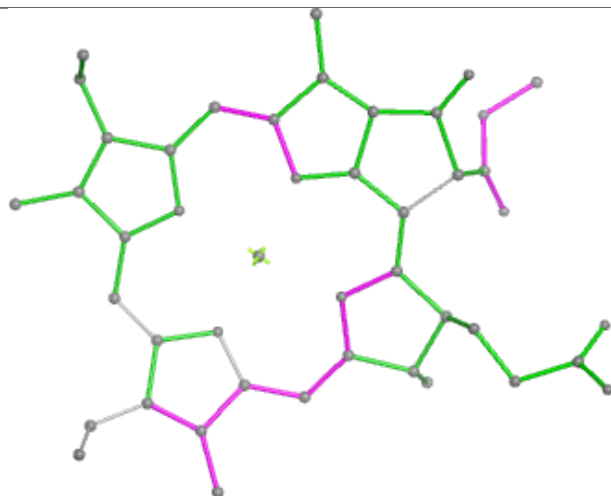




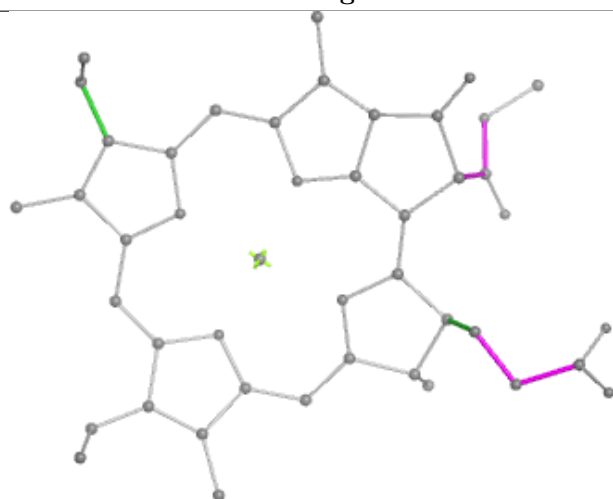
## Ligand CLA S 308



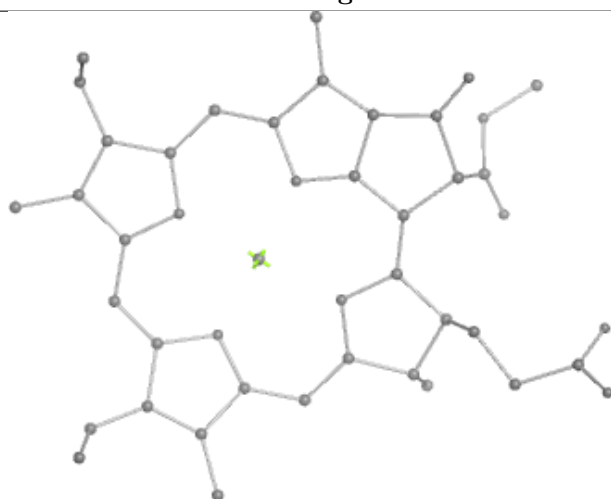
Bond lengths



Bond angles

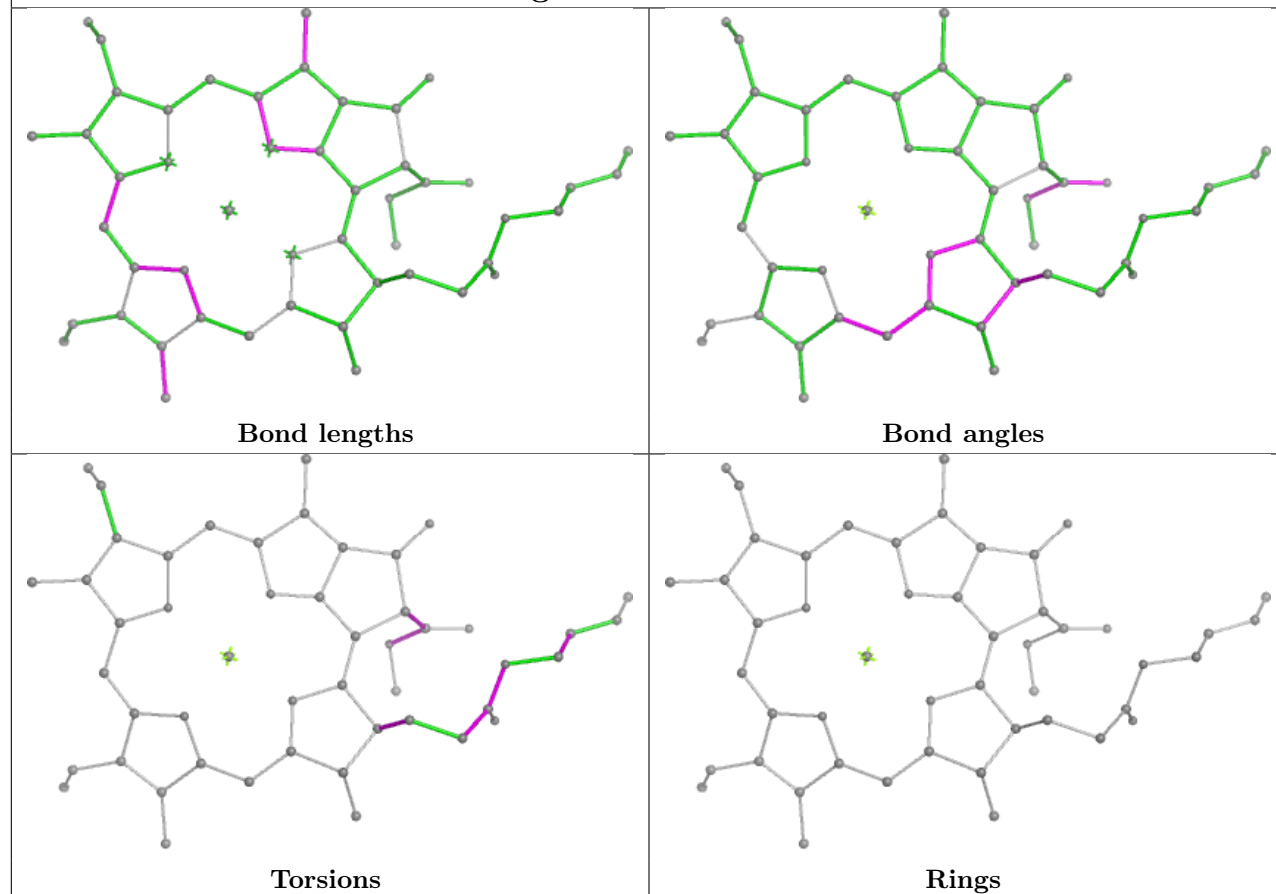


Torsions

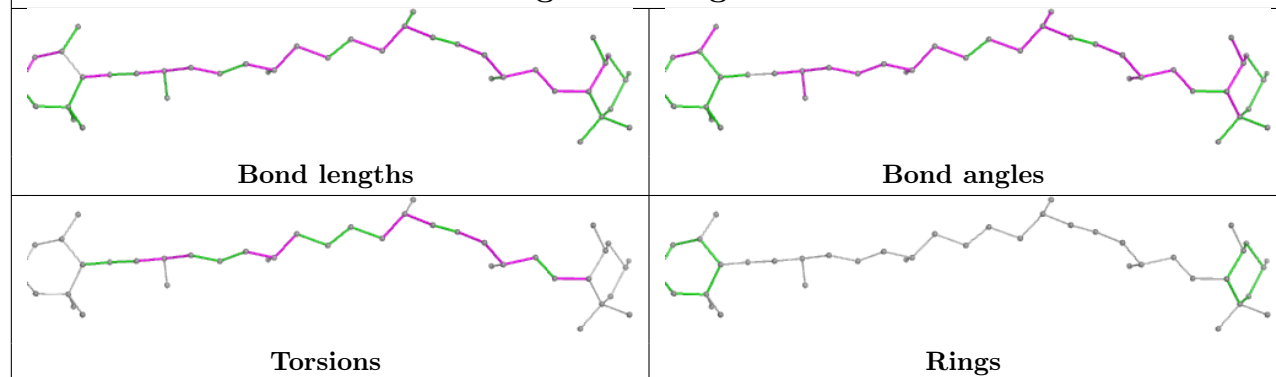


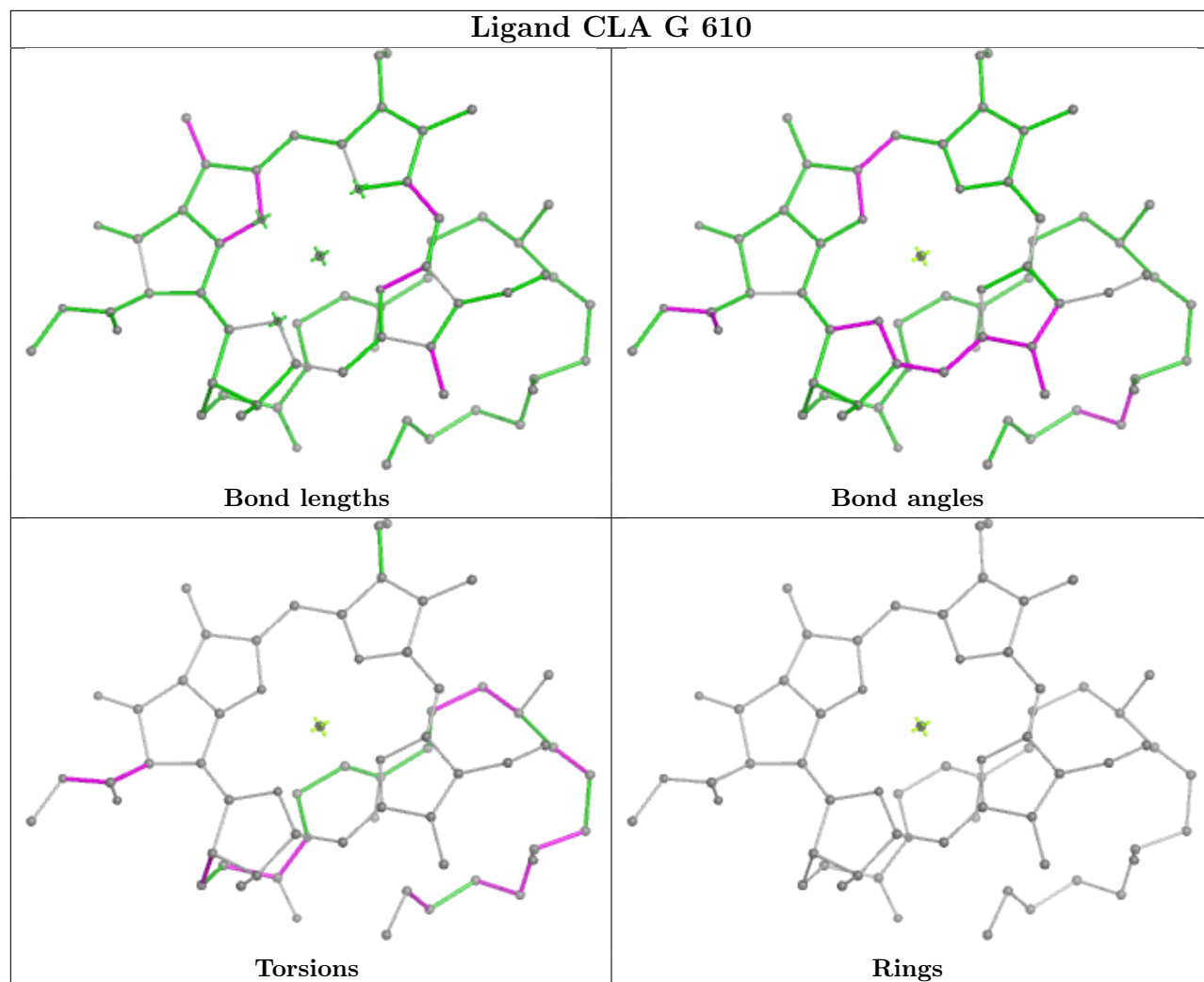
Rings

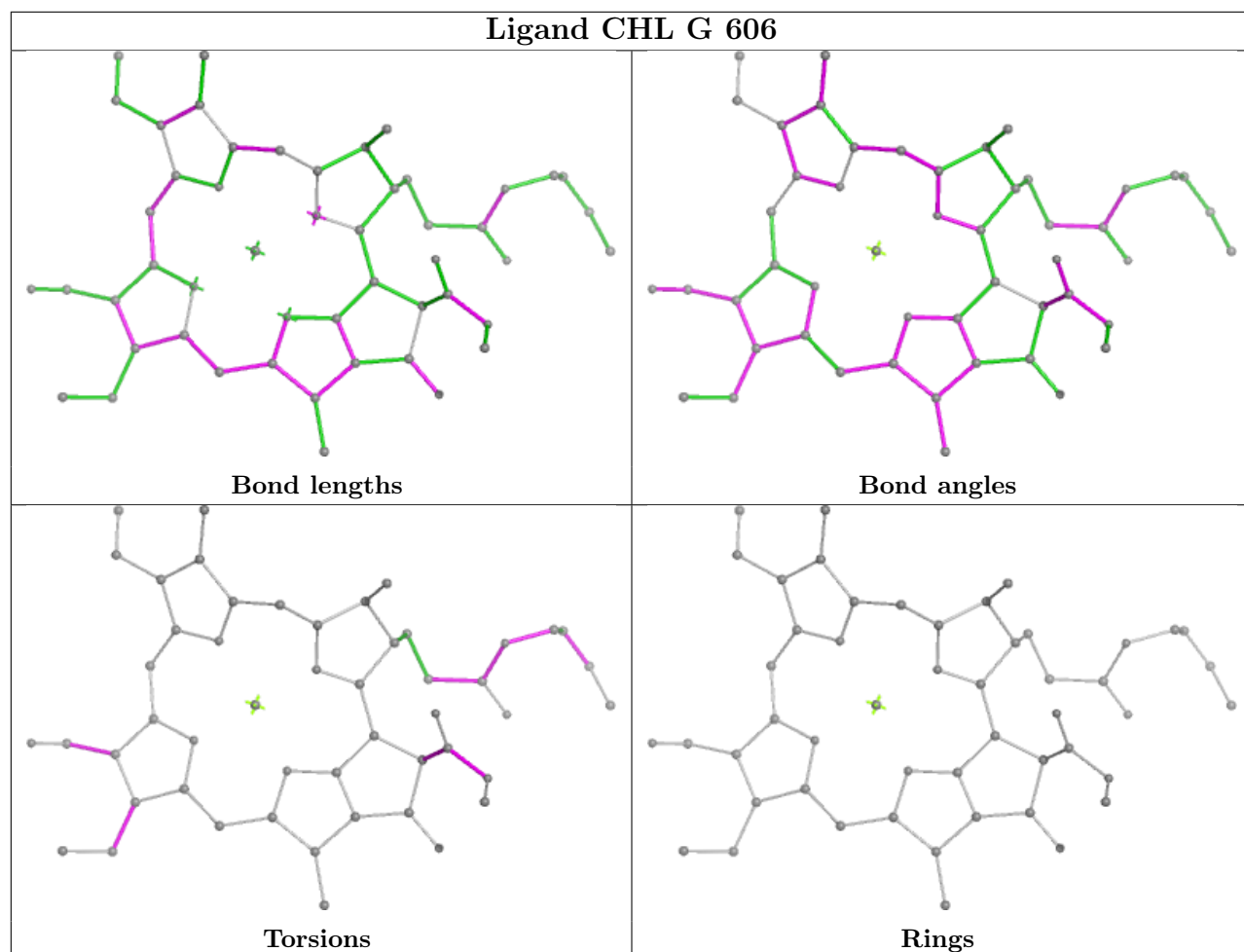
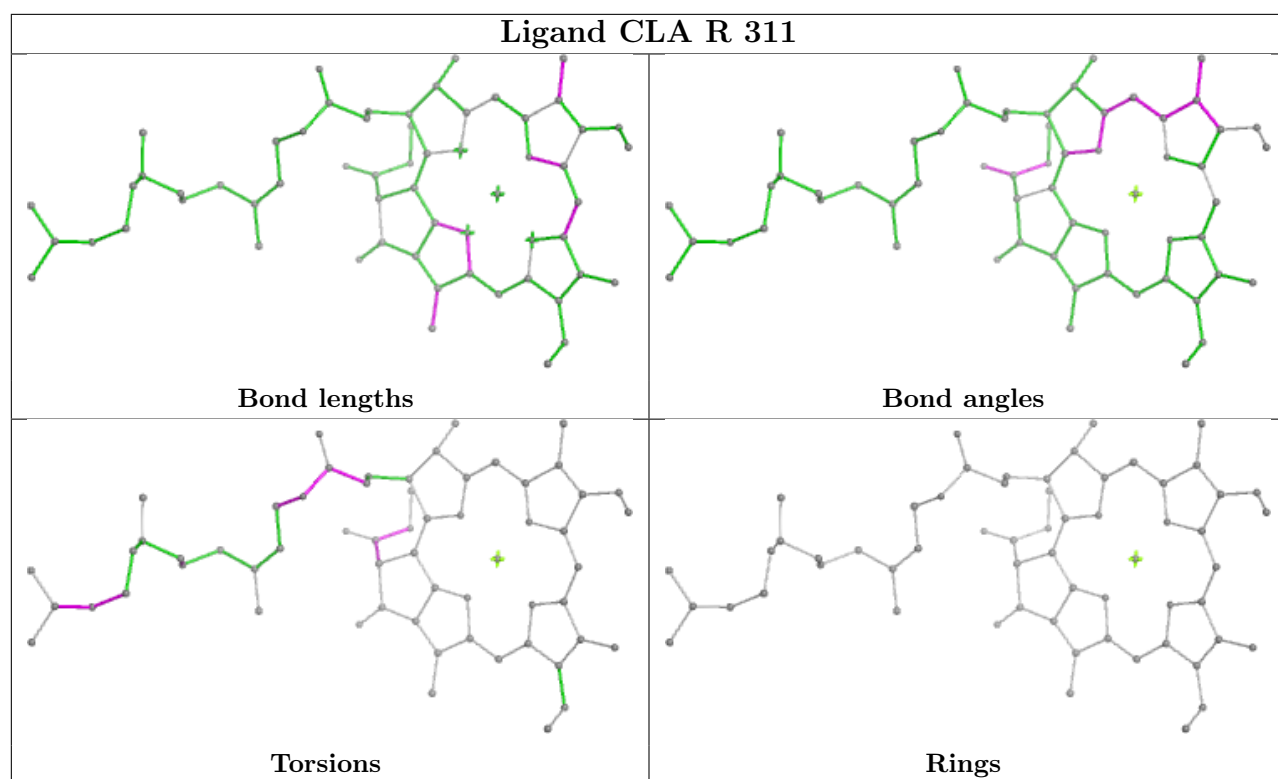
## Ligand CLA R 310

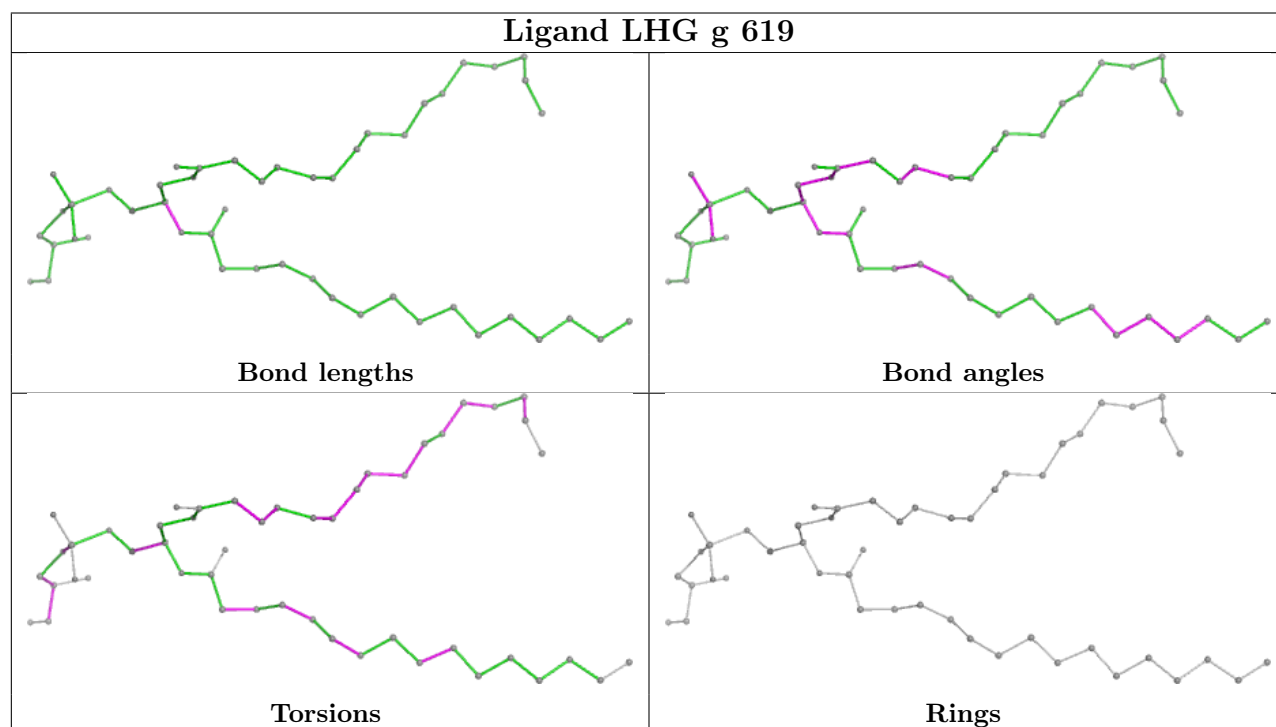
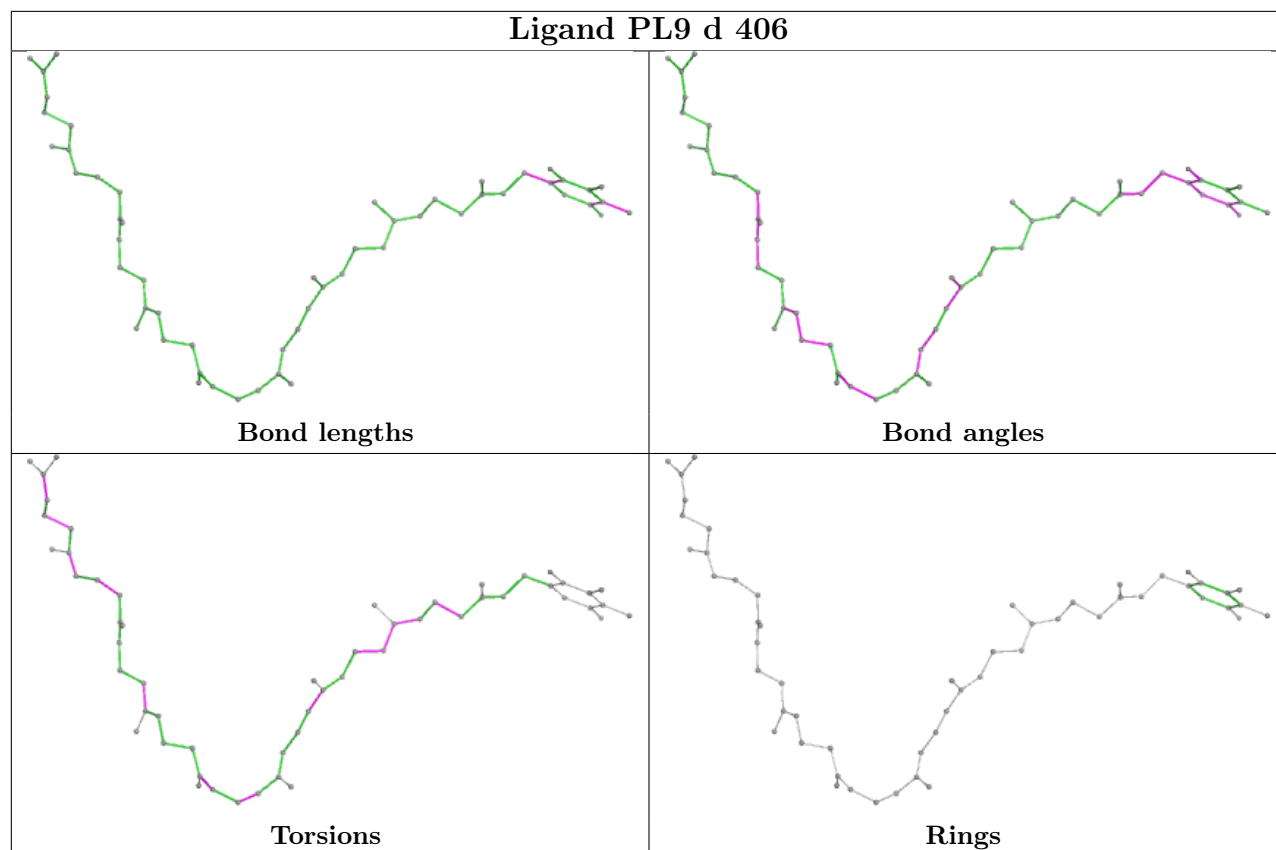


## Ligand LUT g 616

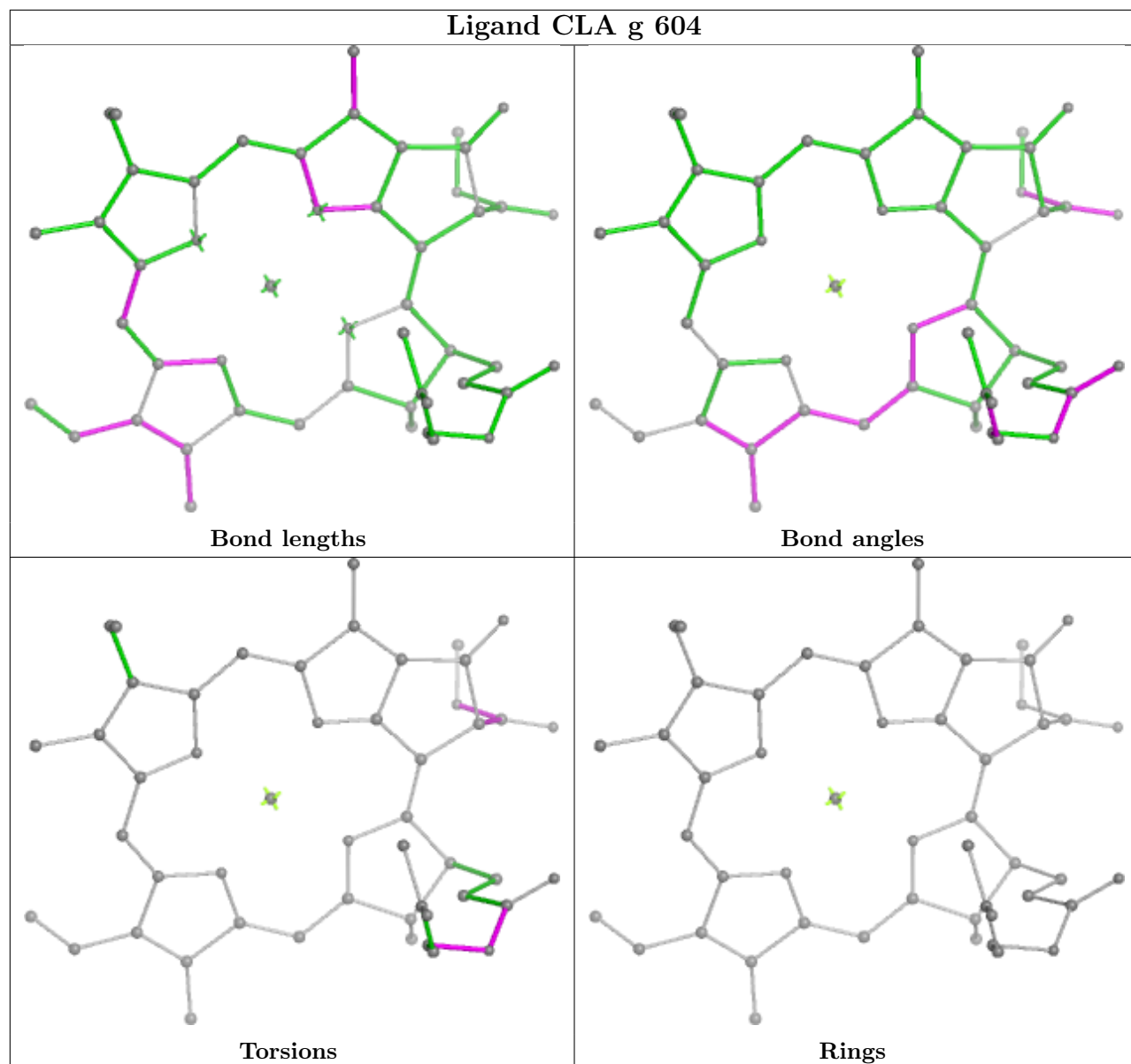


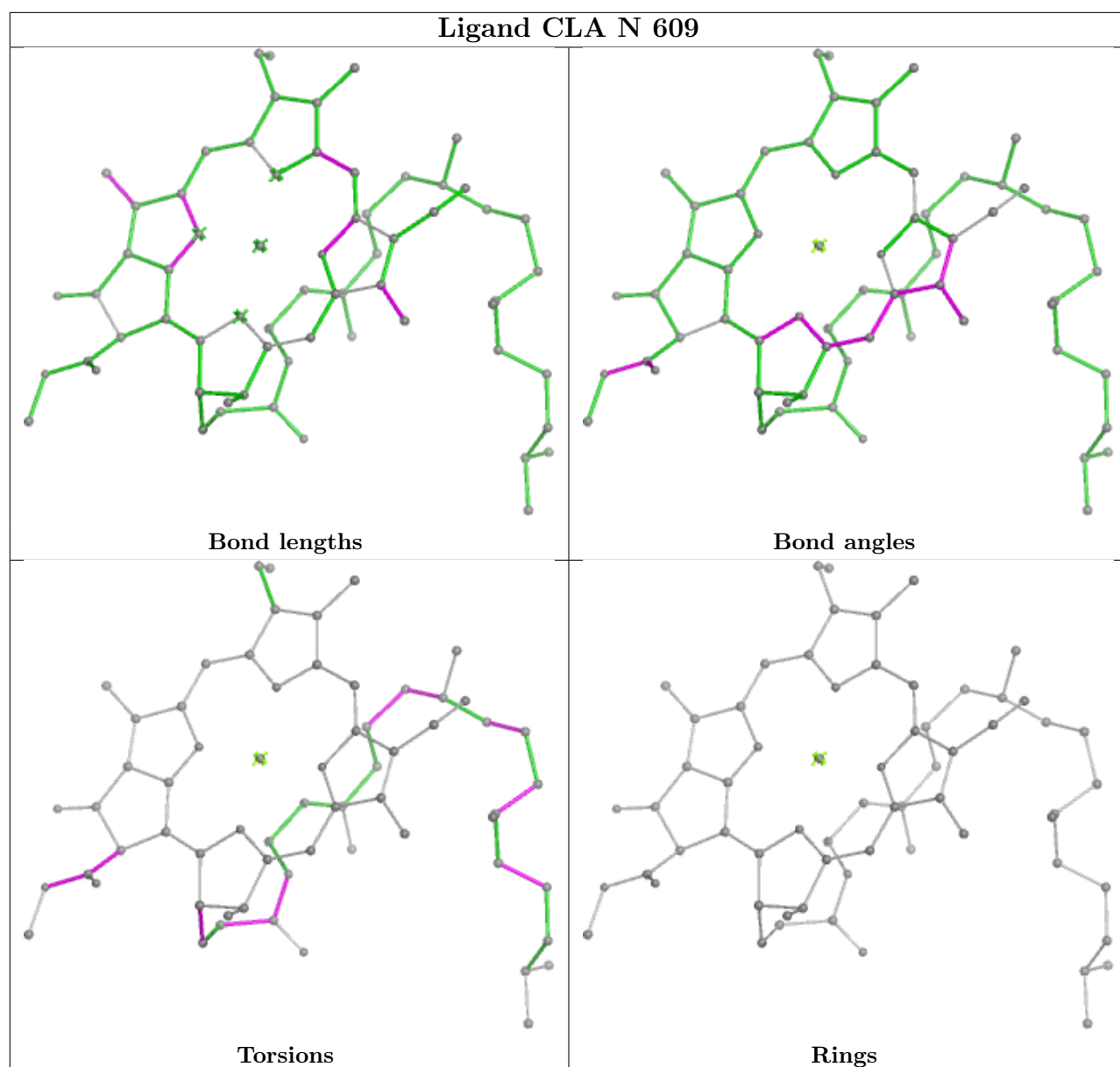






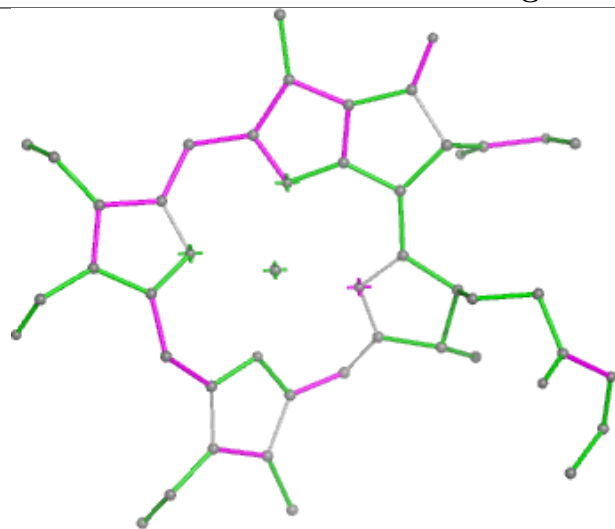
## Ligand CLA g 604



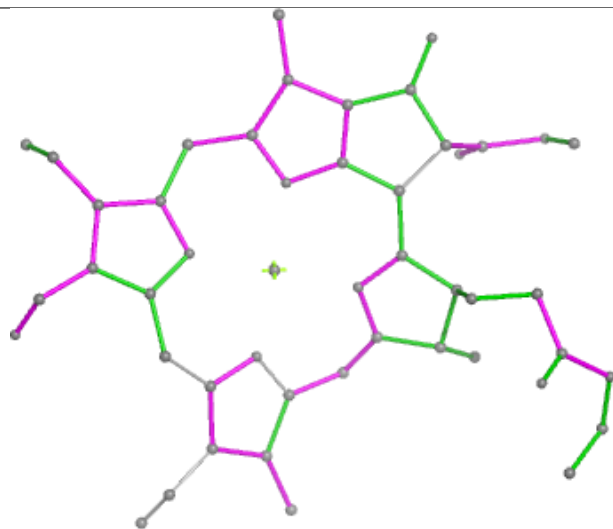




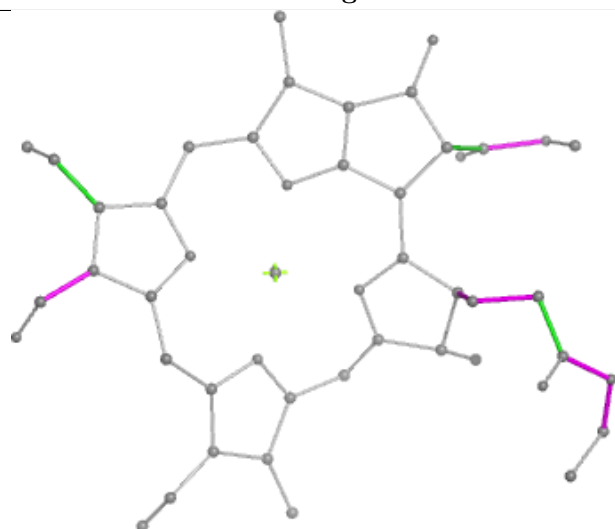
## Ligand CHL s 301



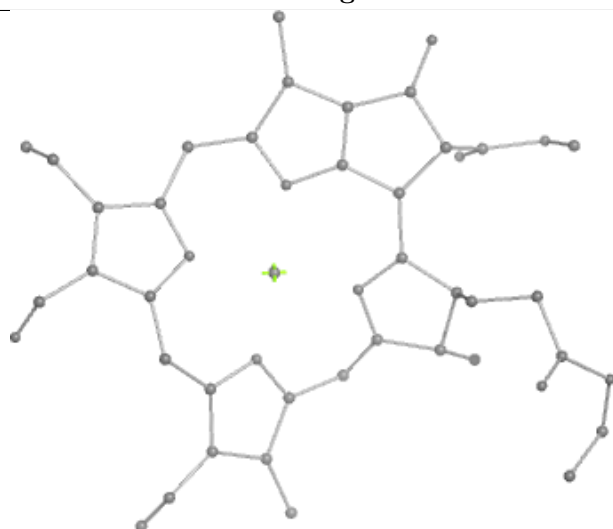
Bond lengths



Bond angles

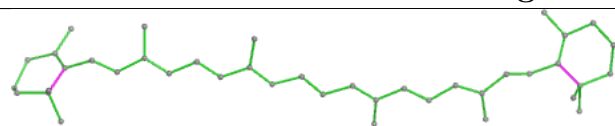


Torsions

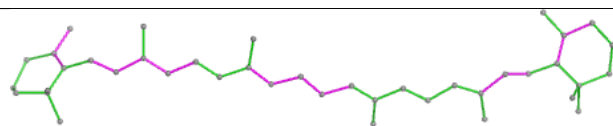


Rings

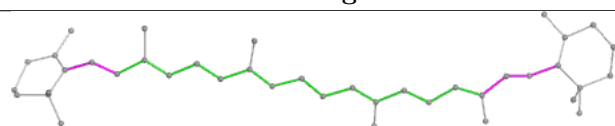
## Ligand BCR b 616



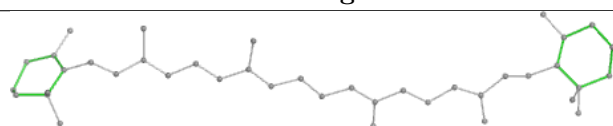
Bond lengths



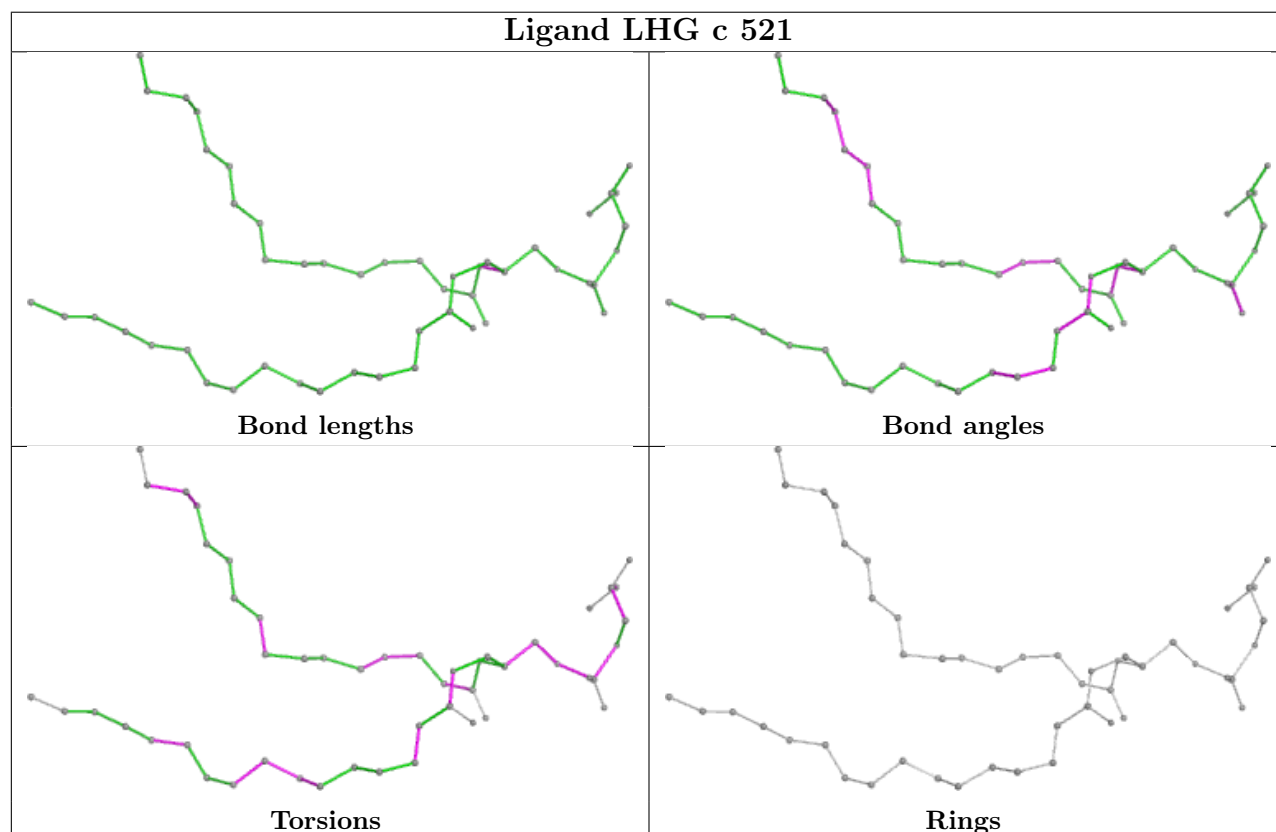
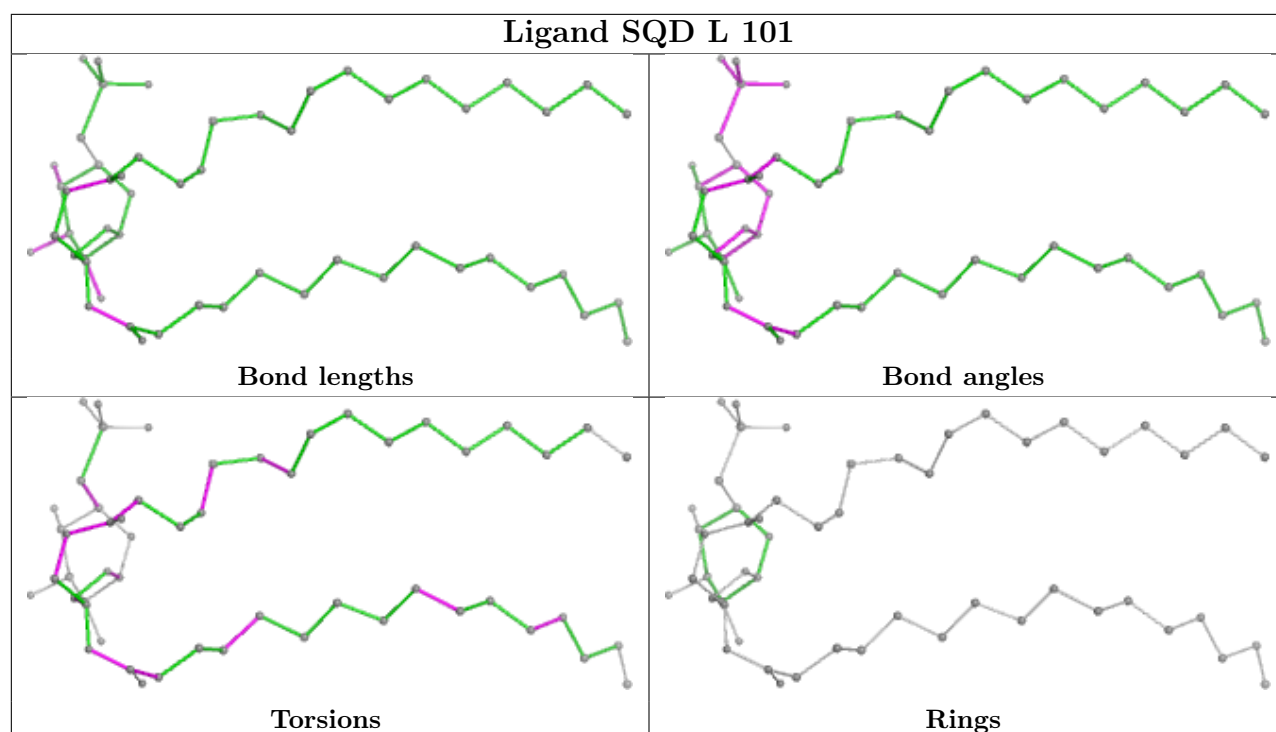
Bond angles

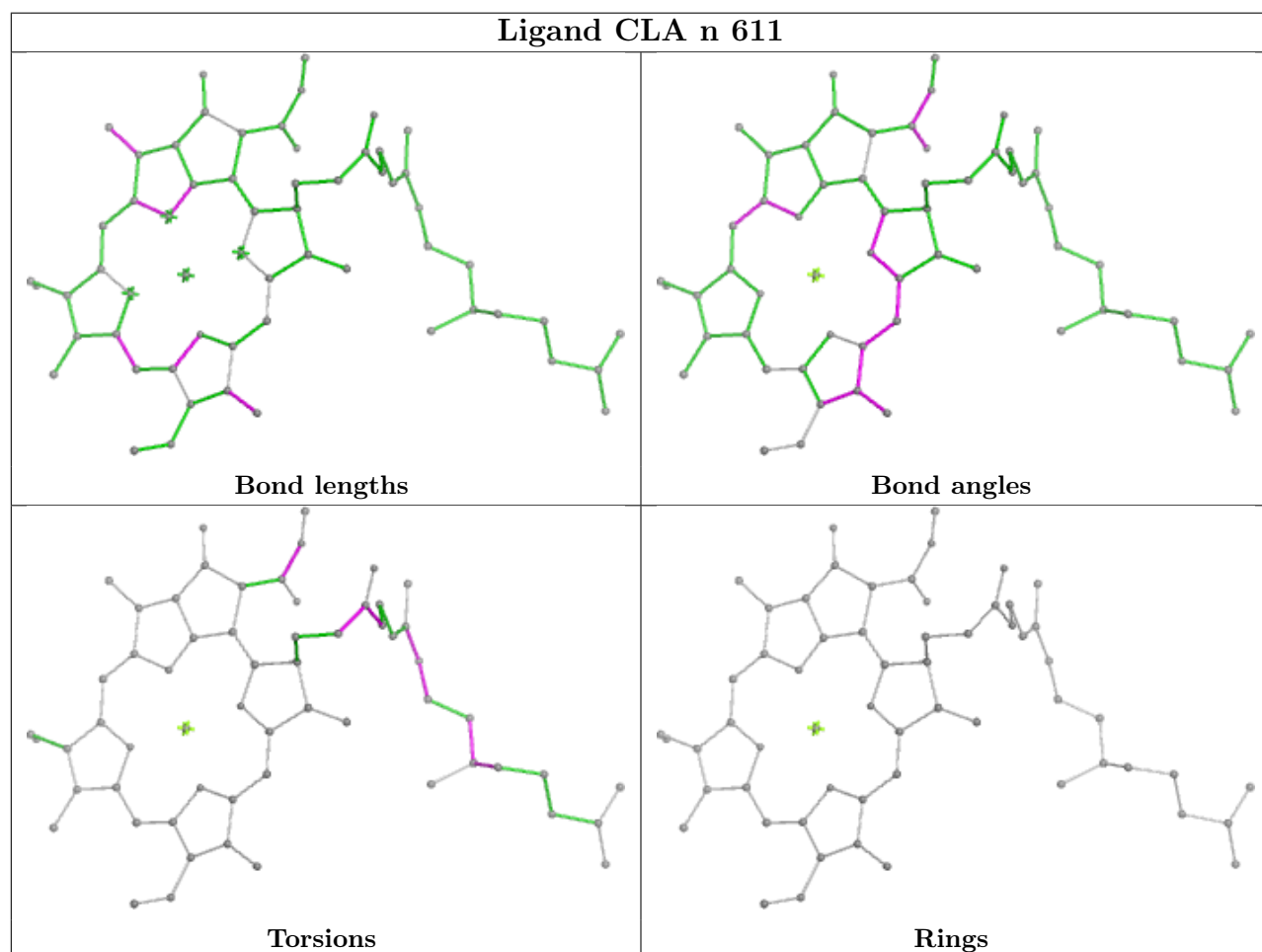
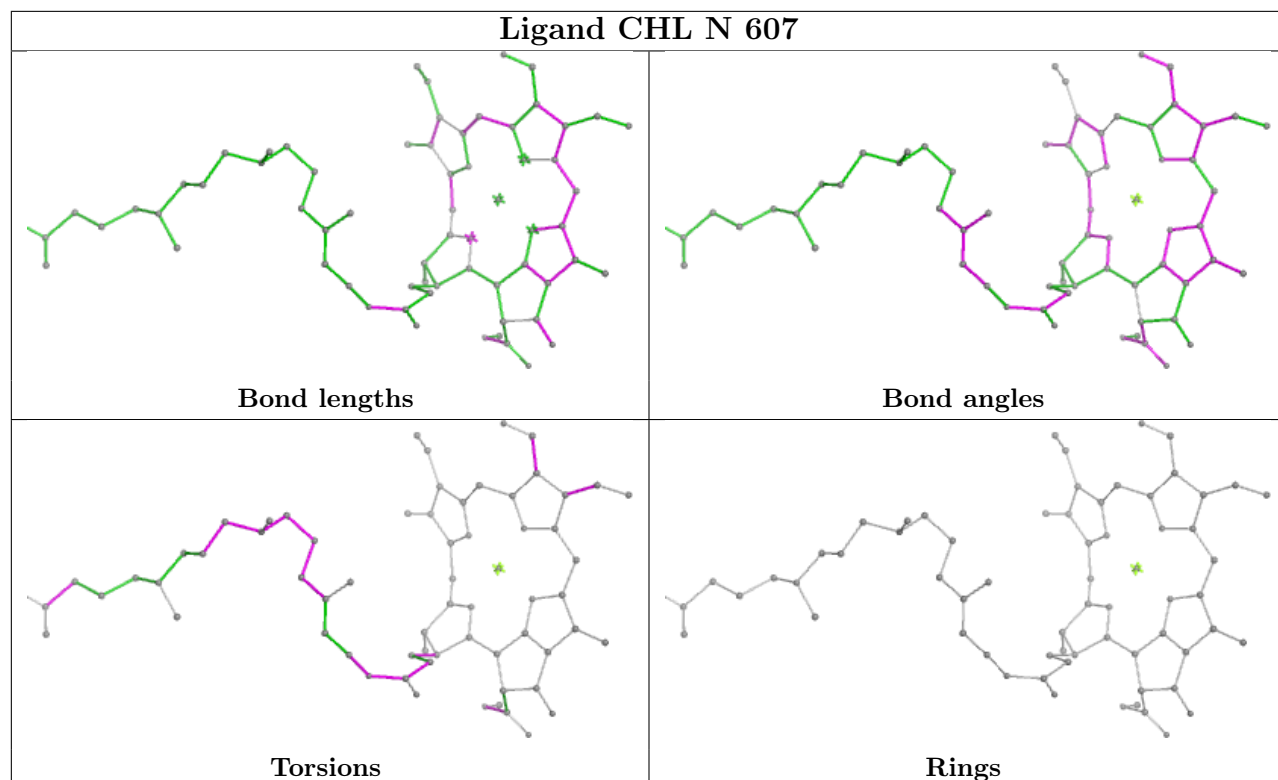


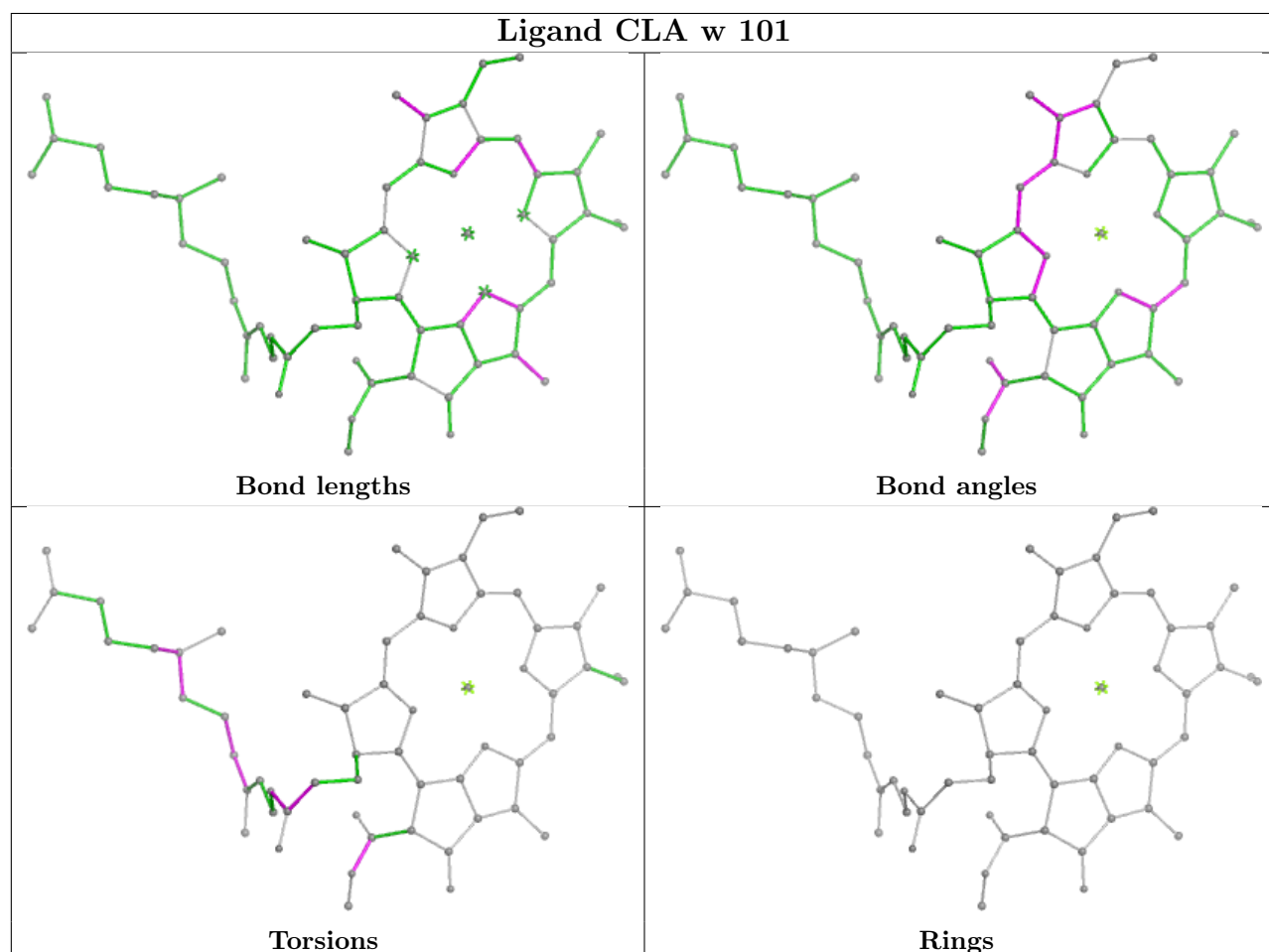
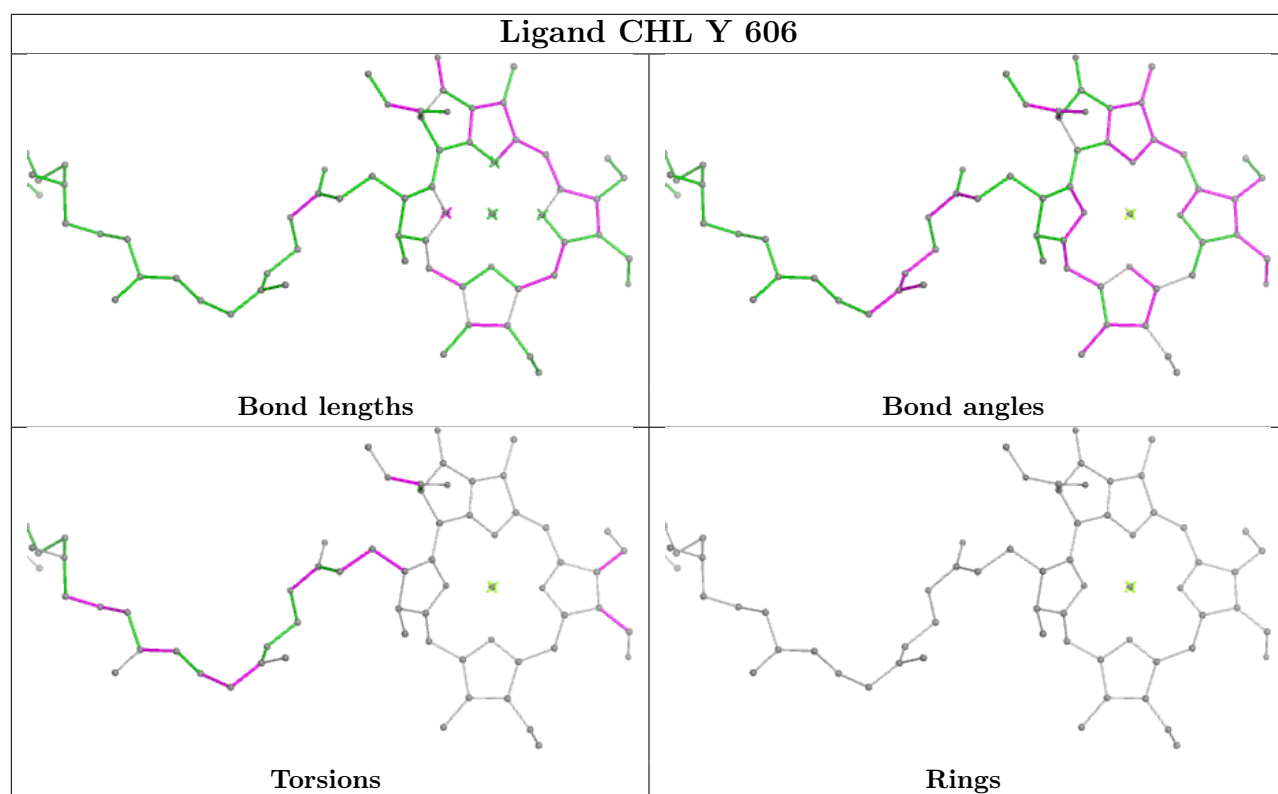
Torsions

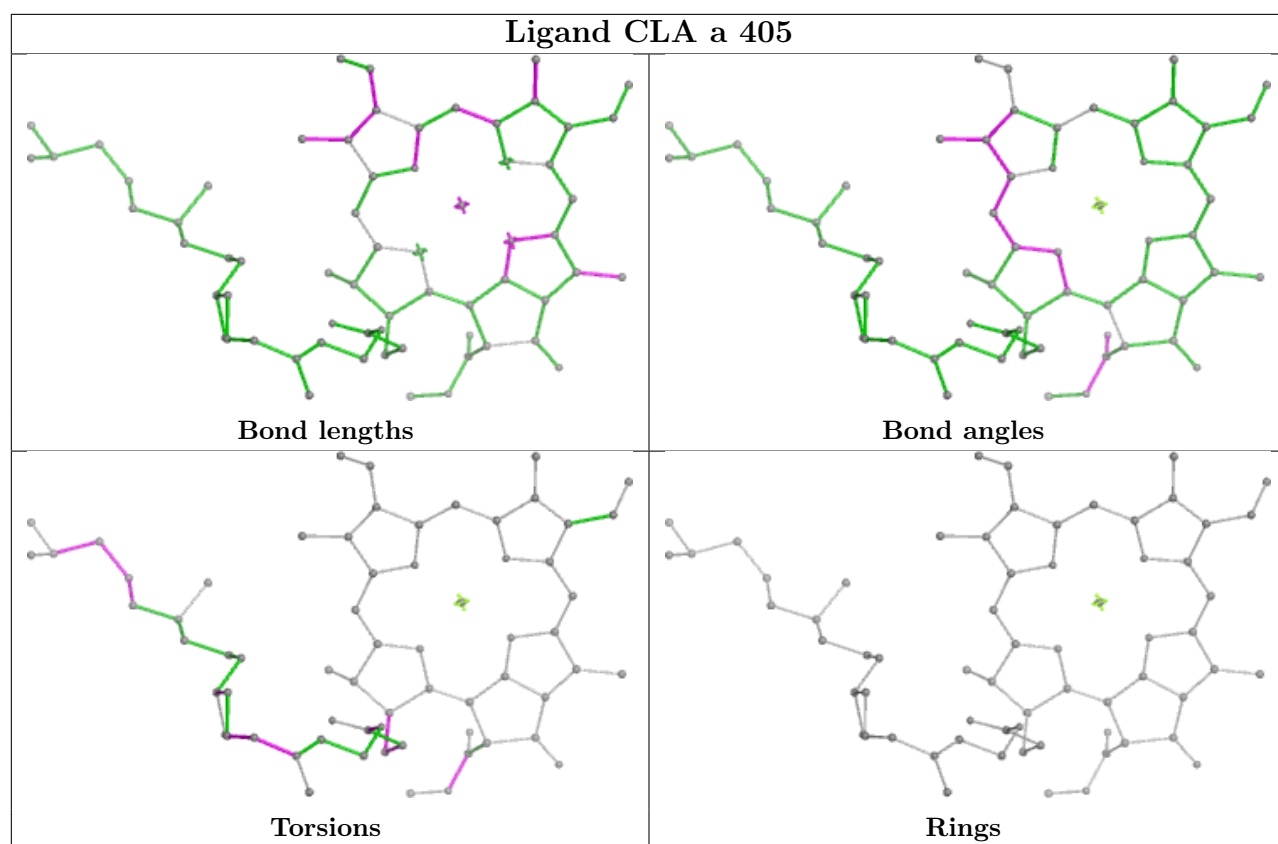


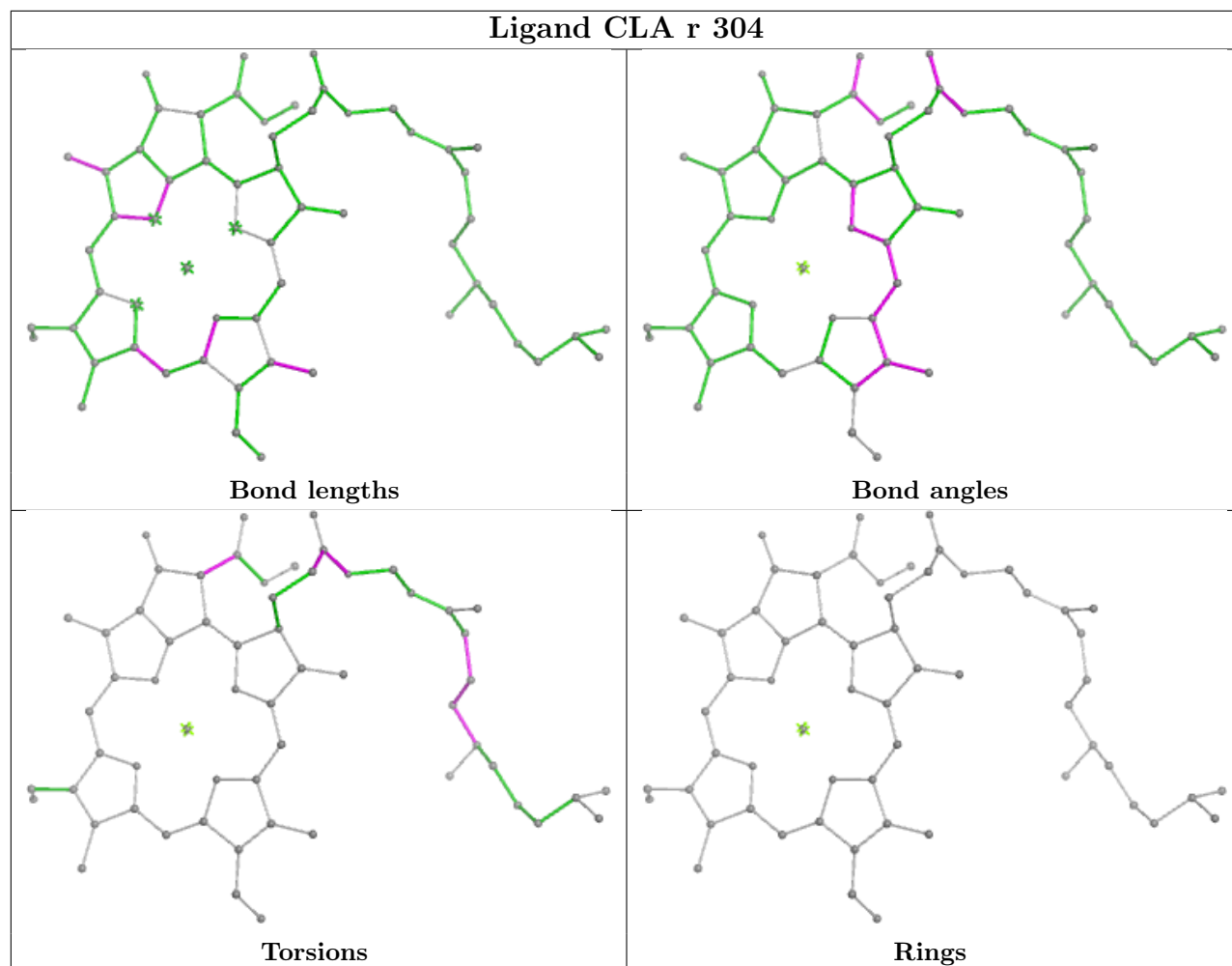
Rings

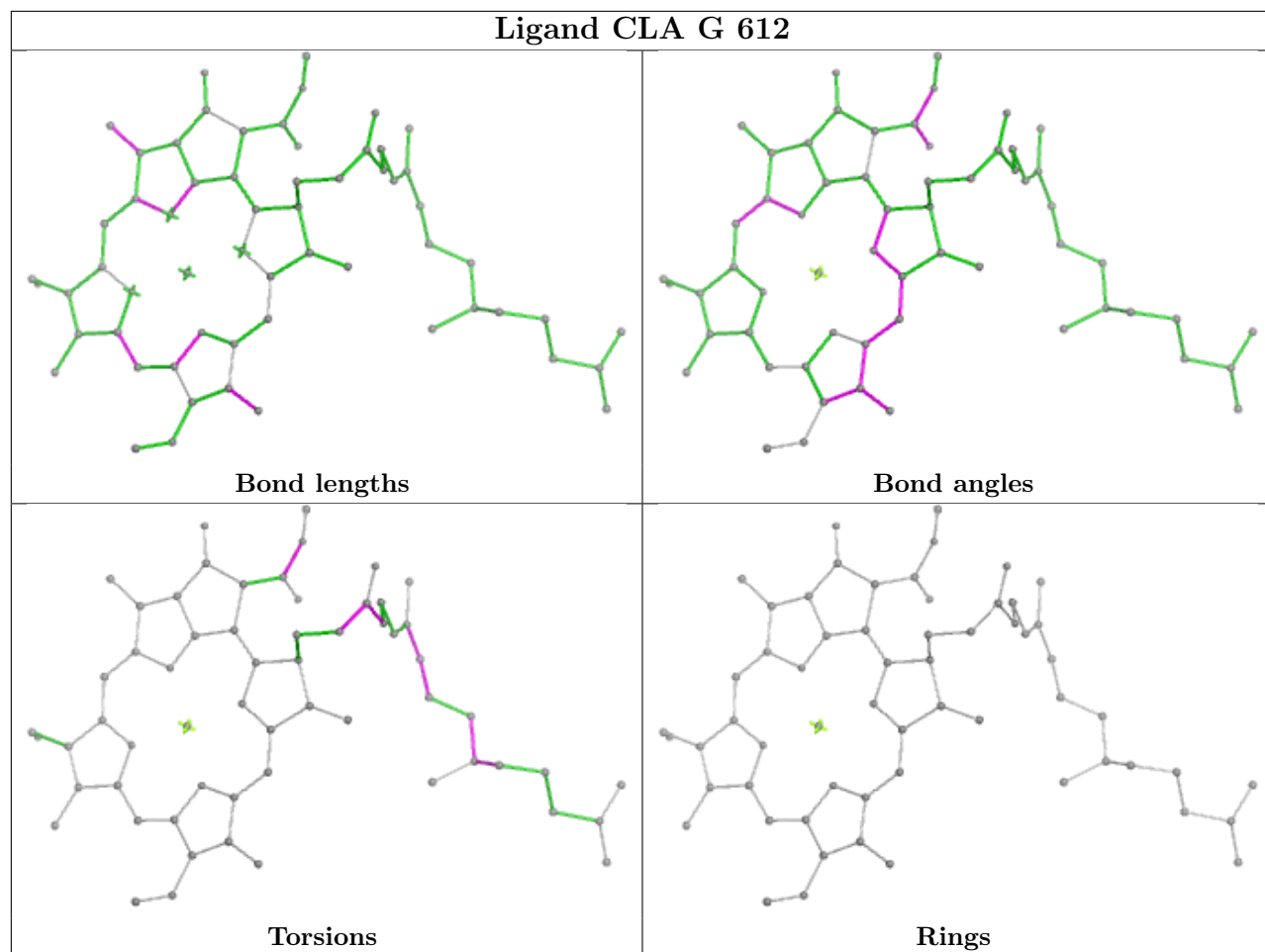


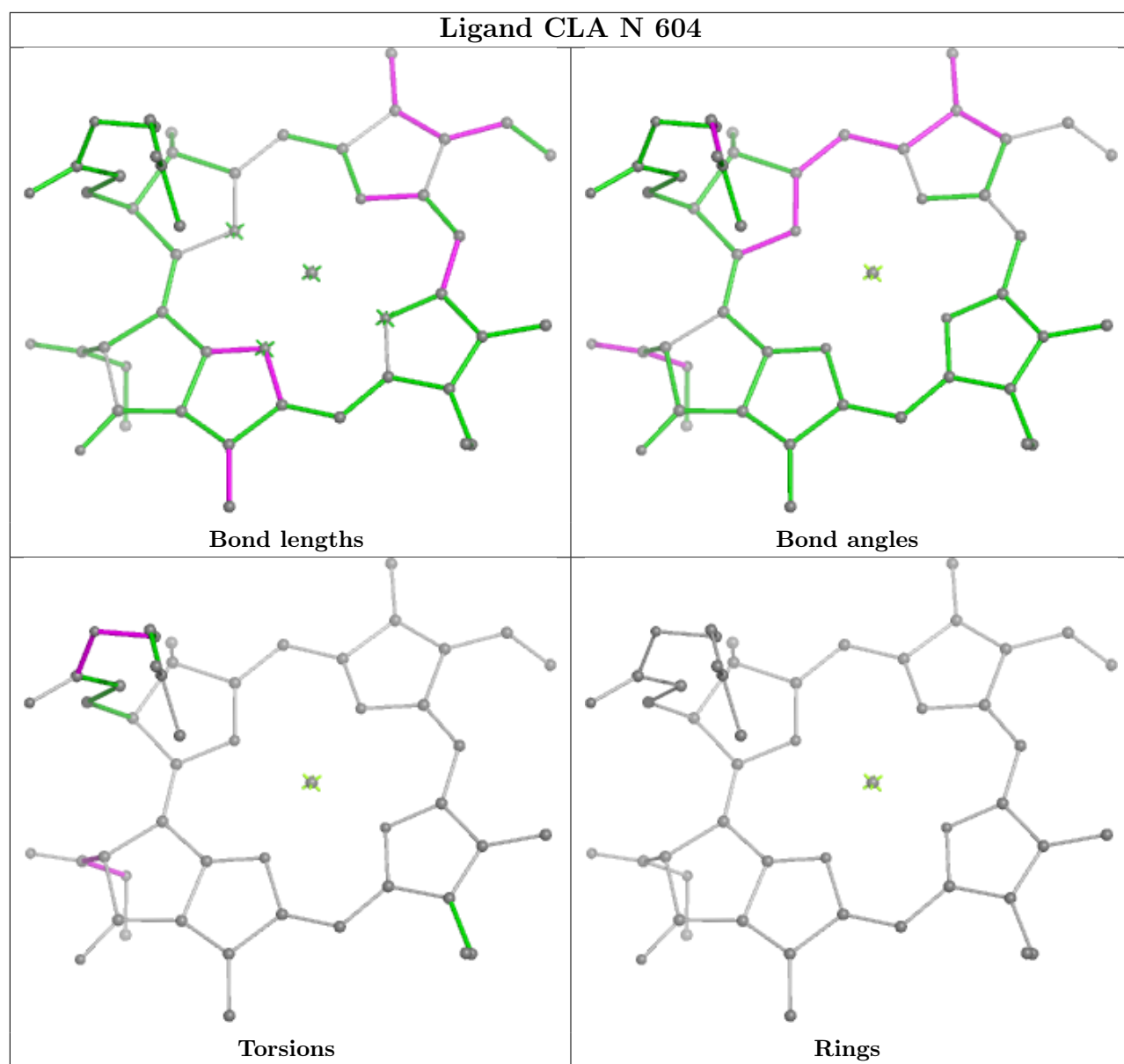






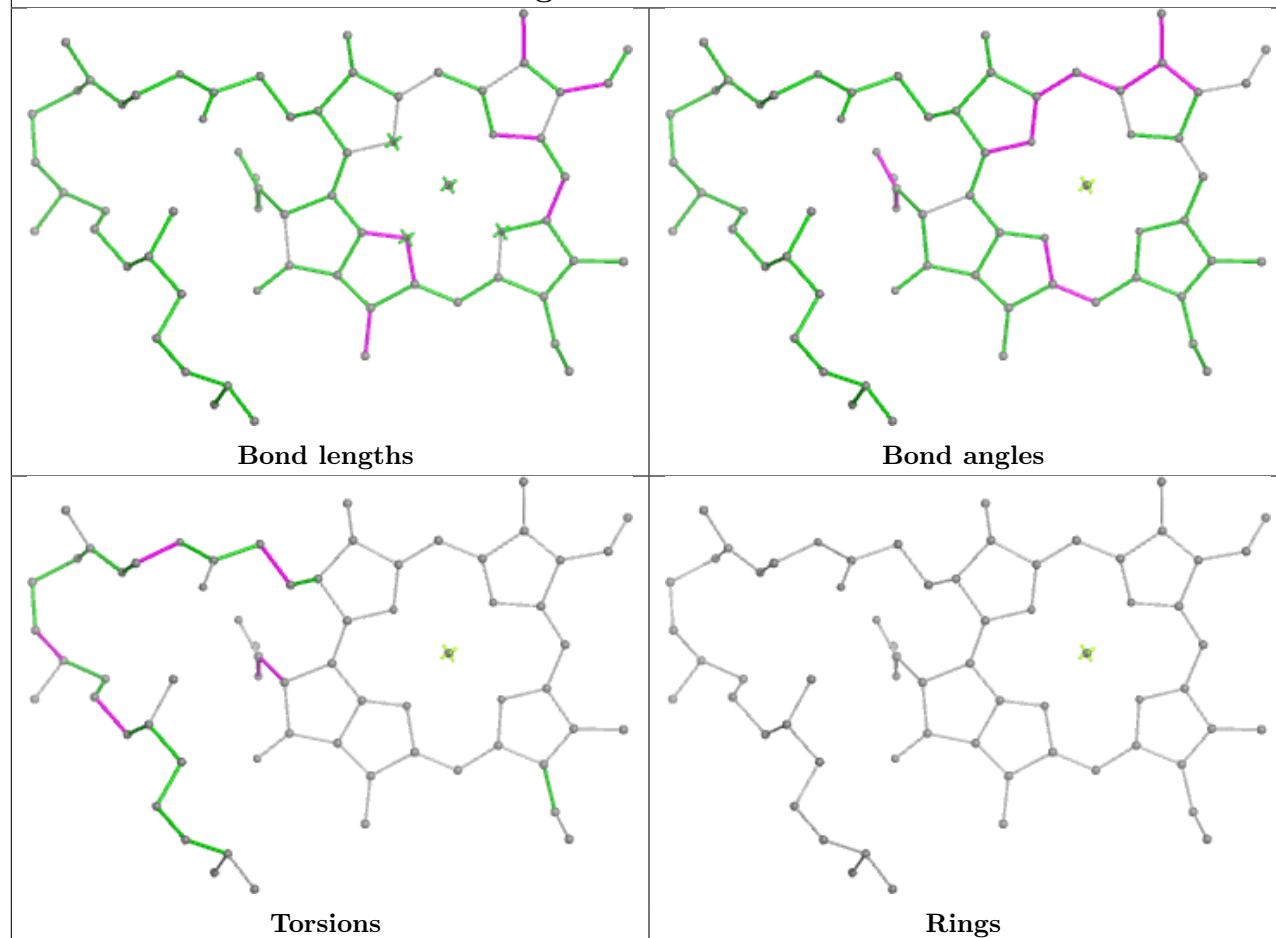




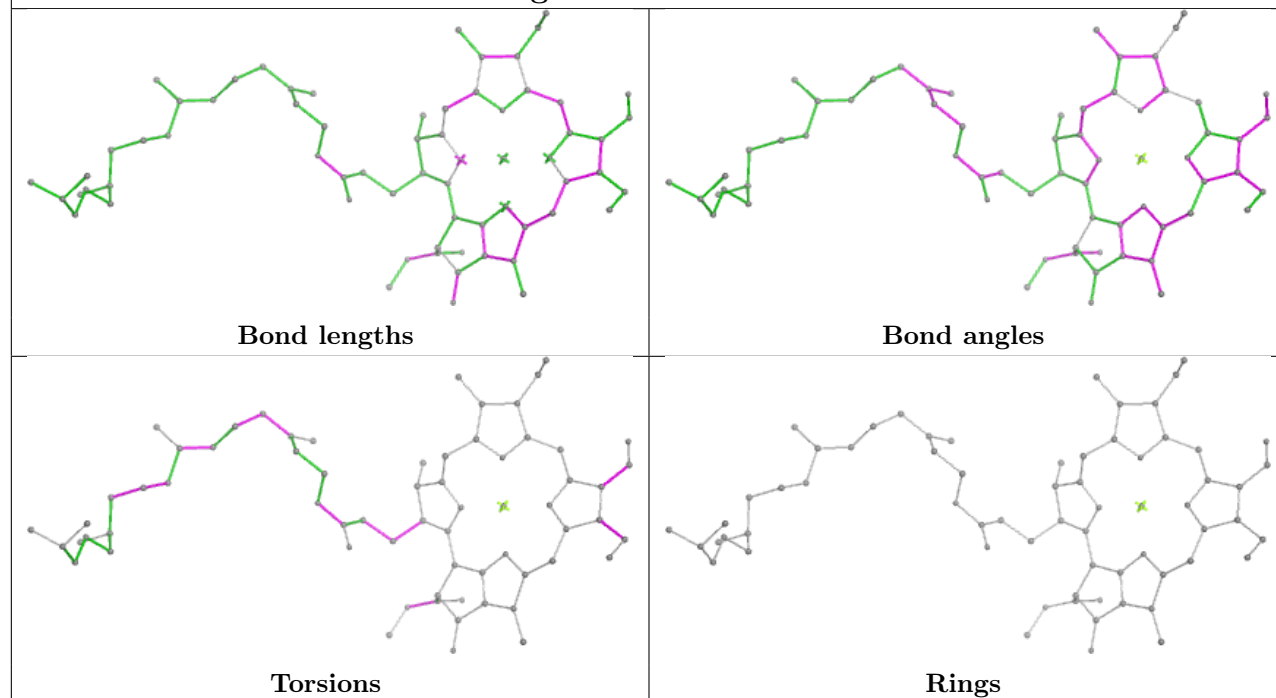


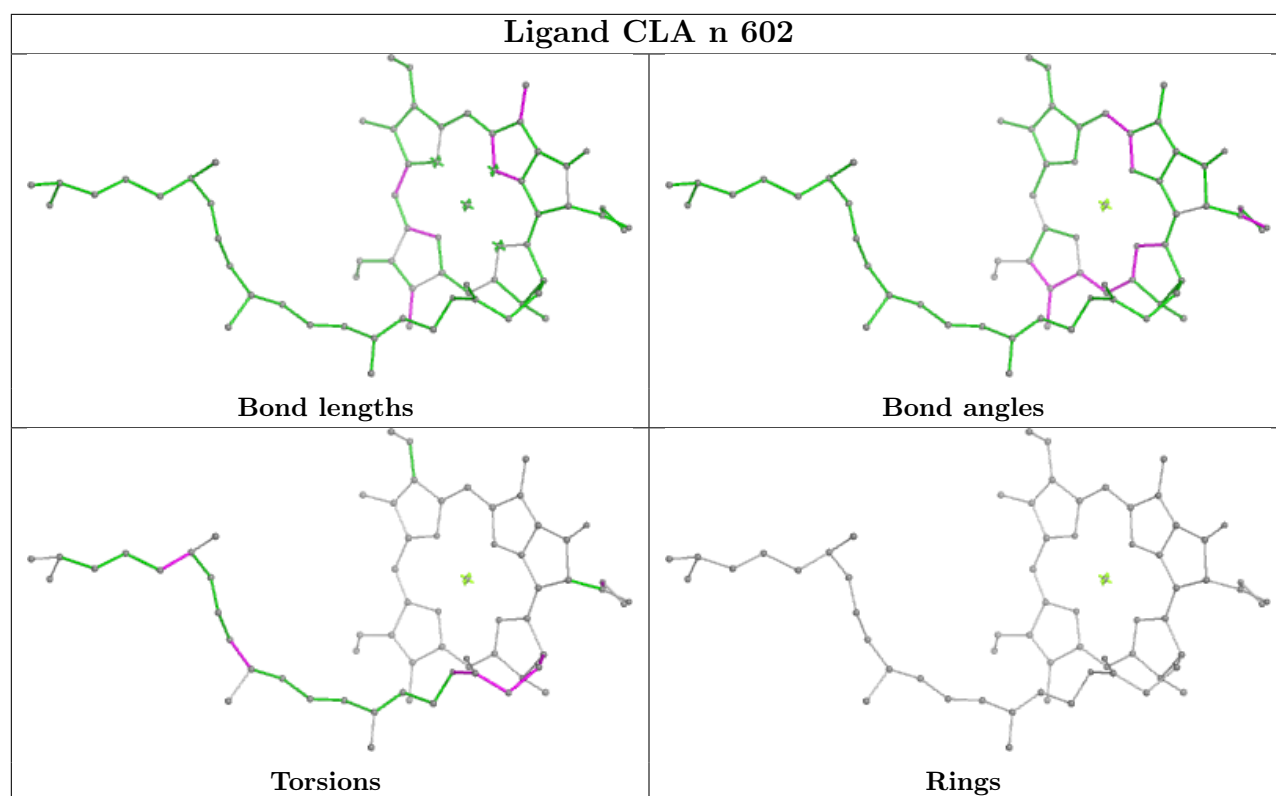


## Ligand CLA b 609

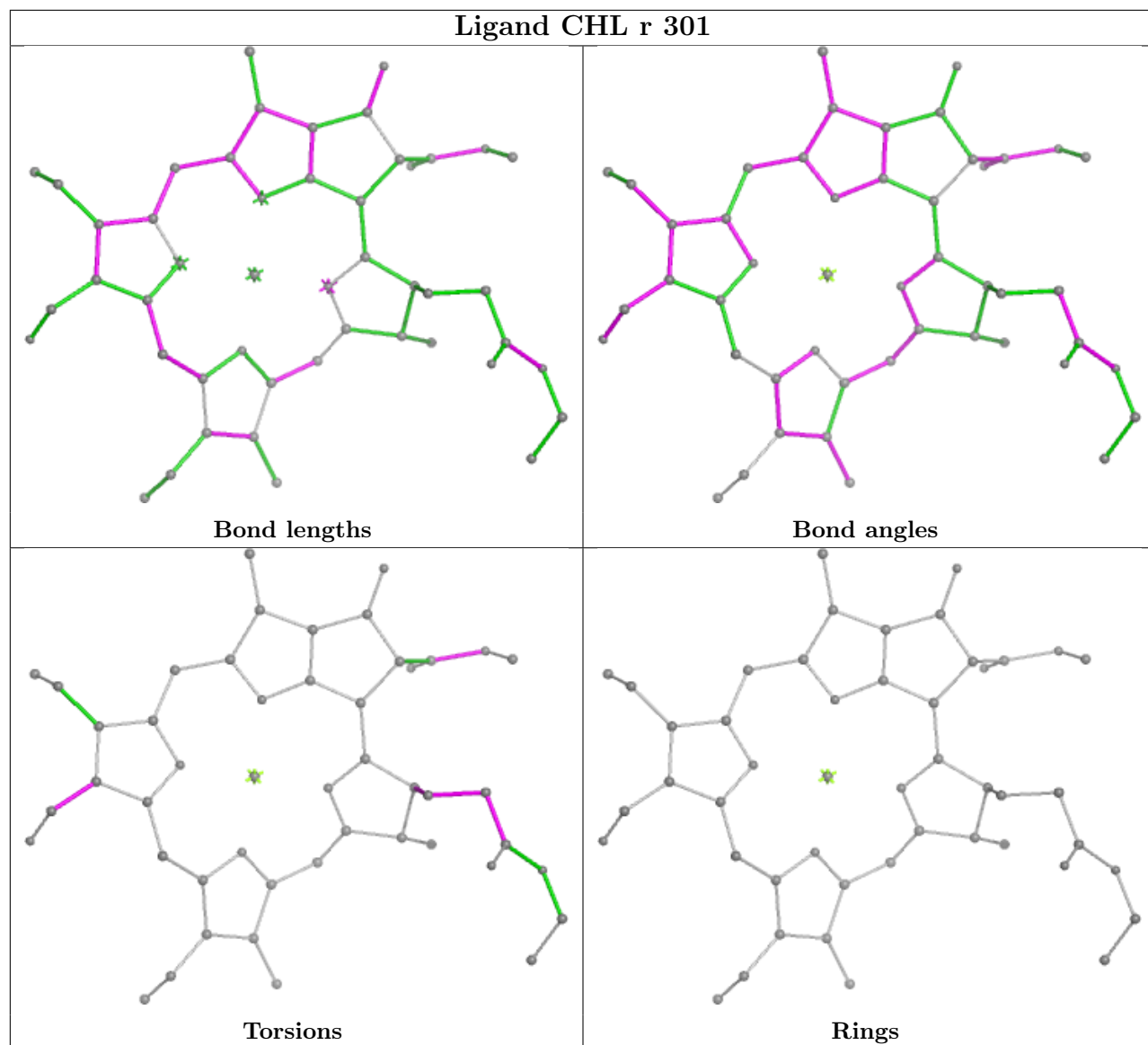


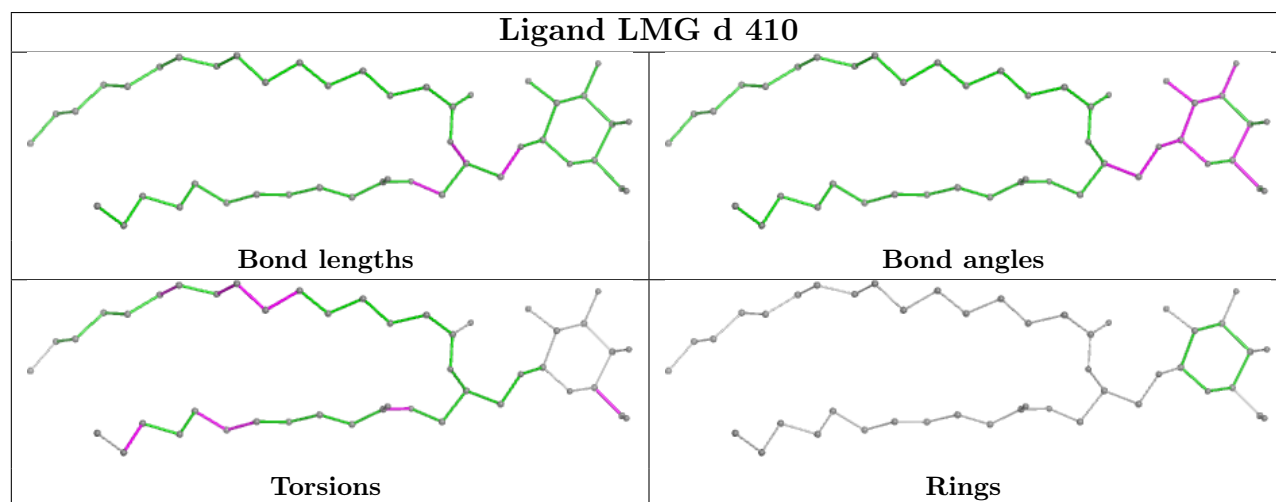
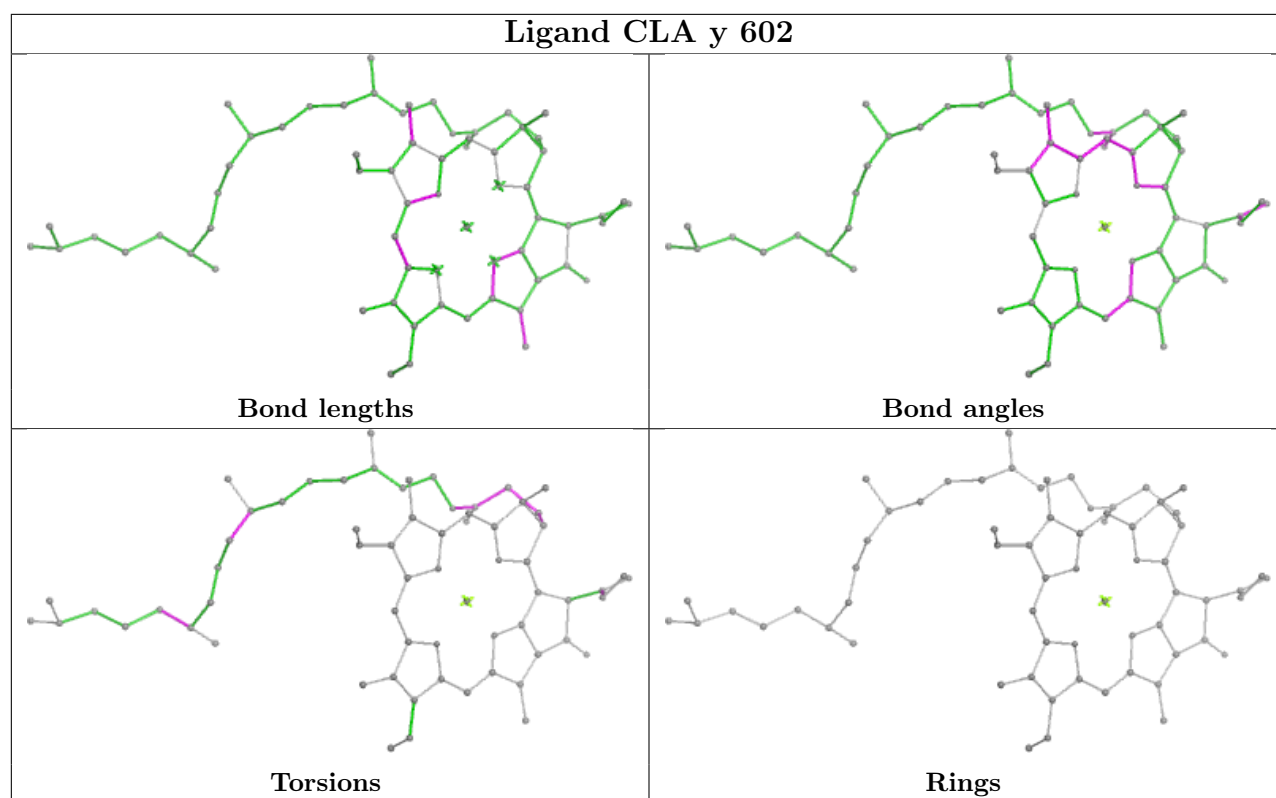
## Ligand CHL G 607



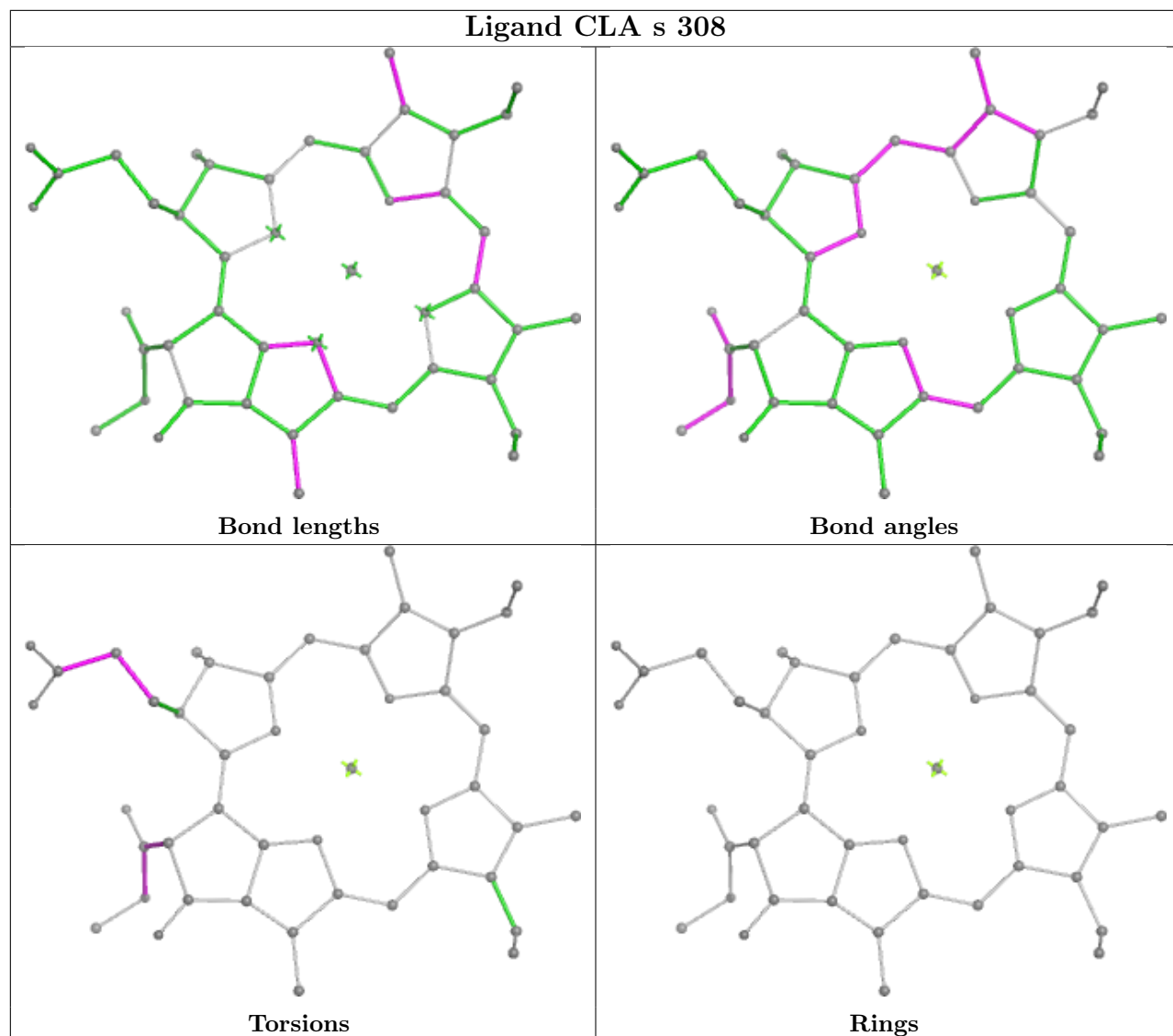


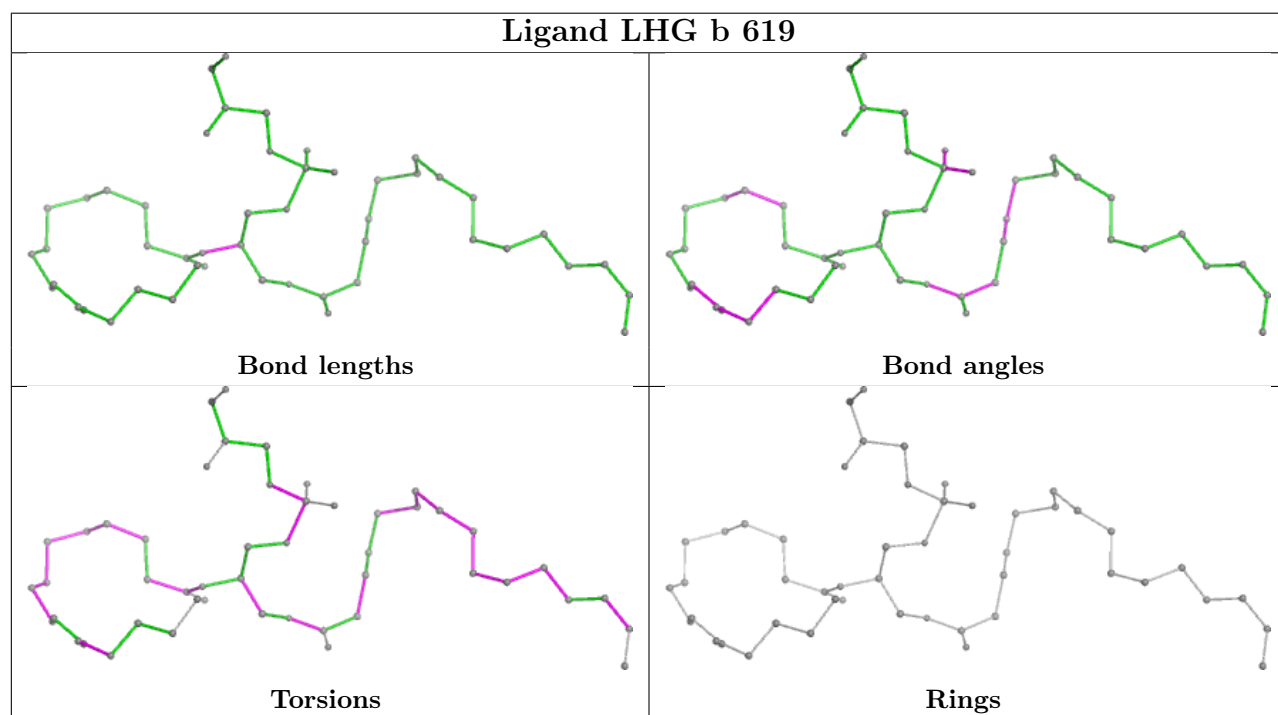
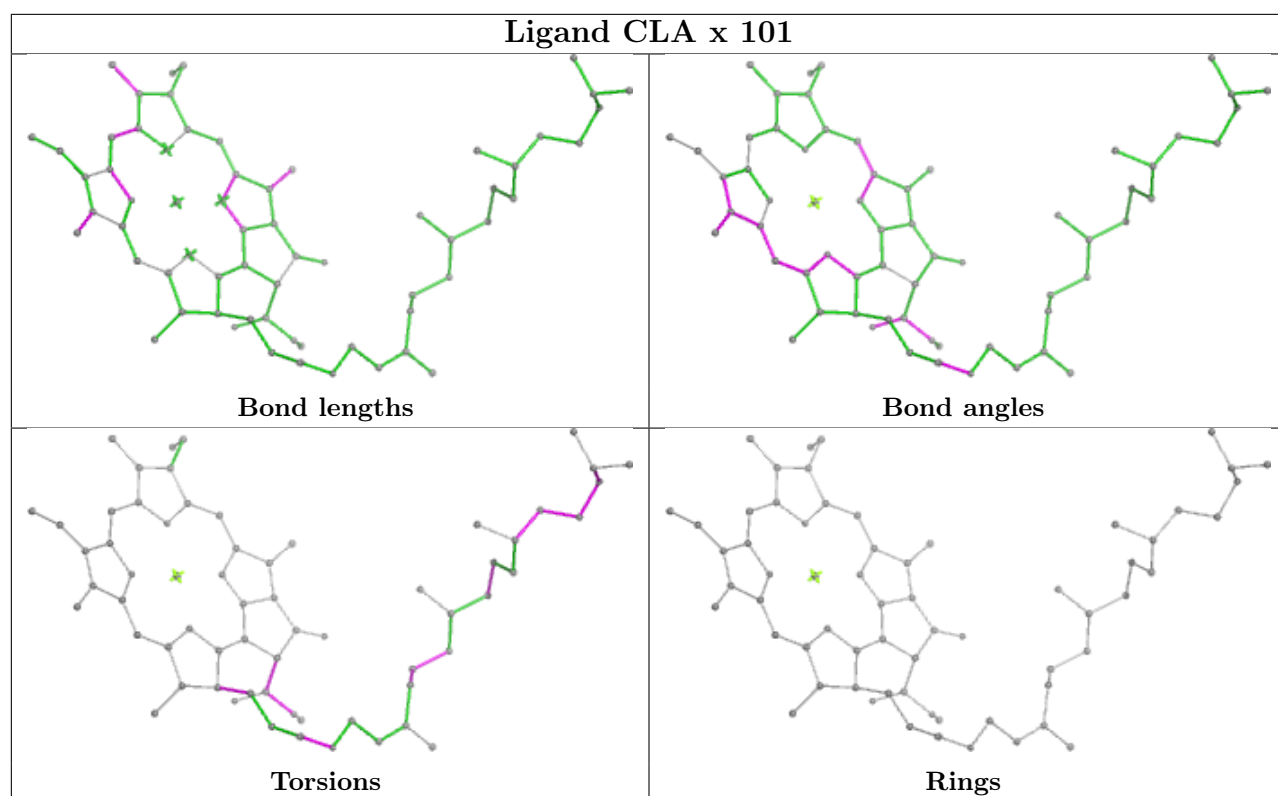
## Ligand CHL r 301

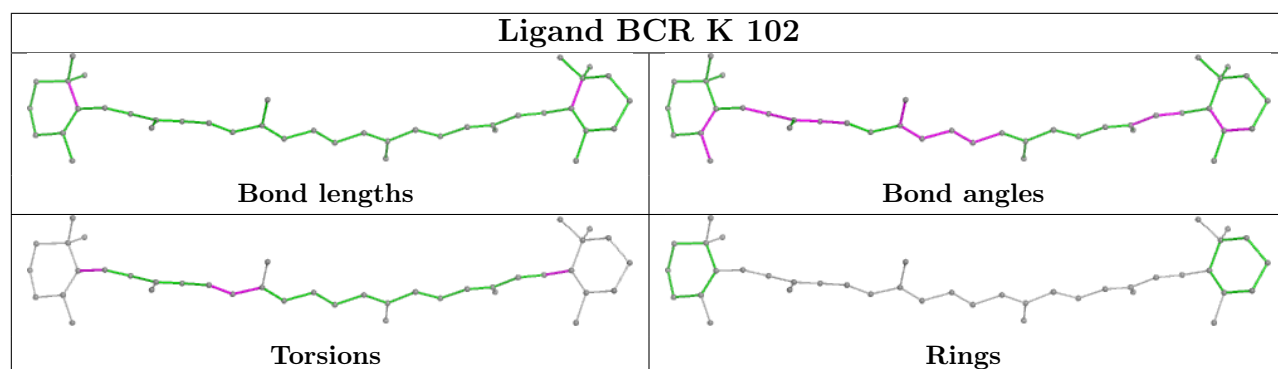
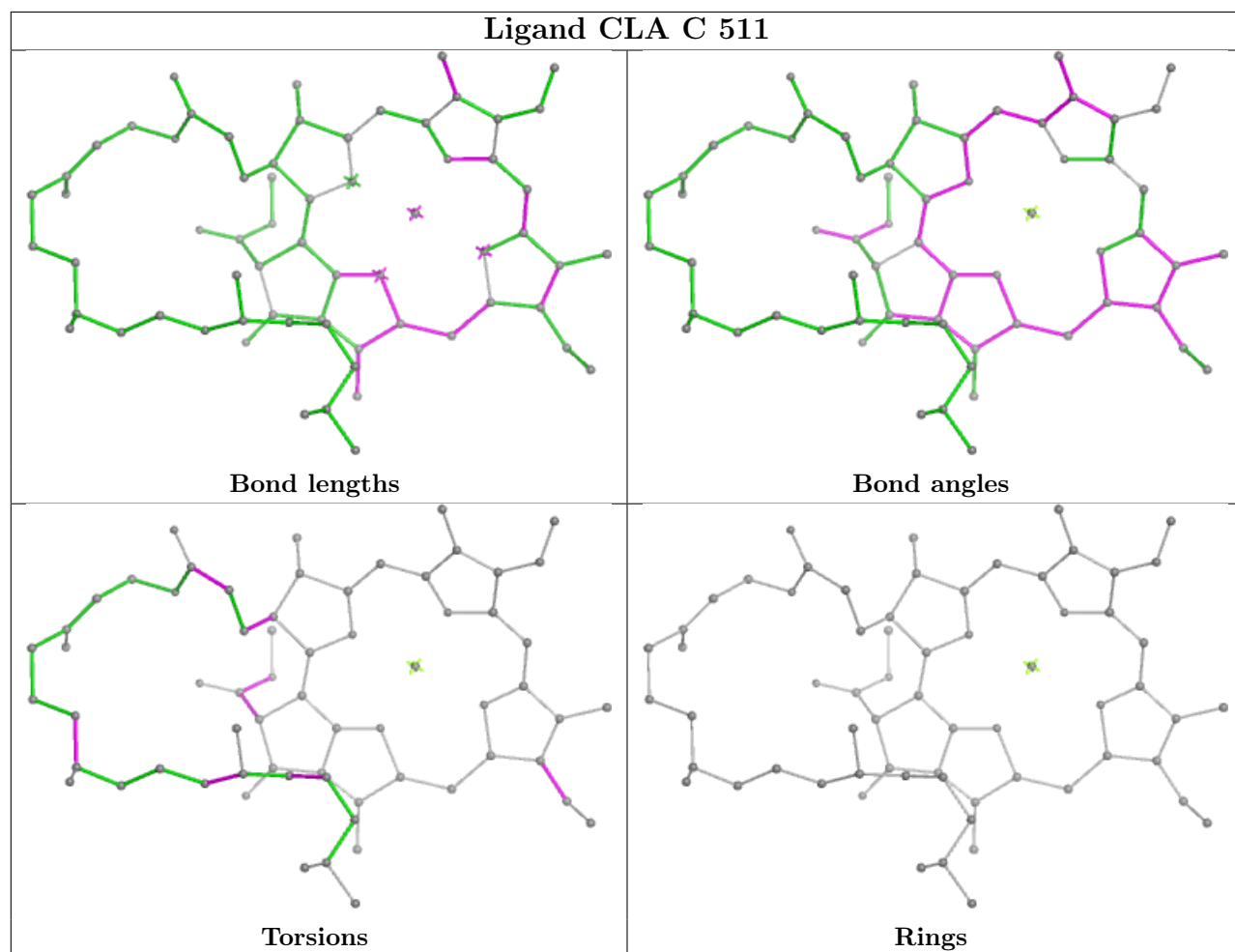
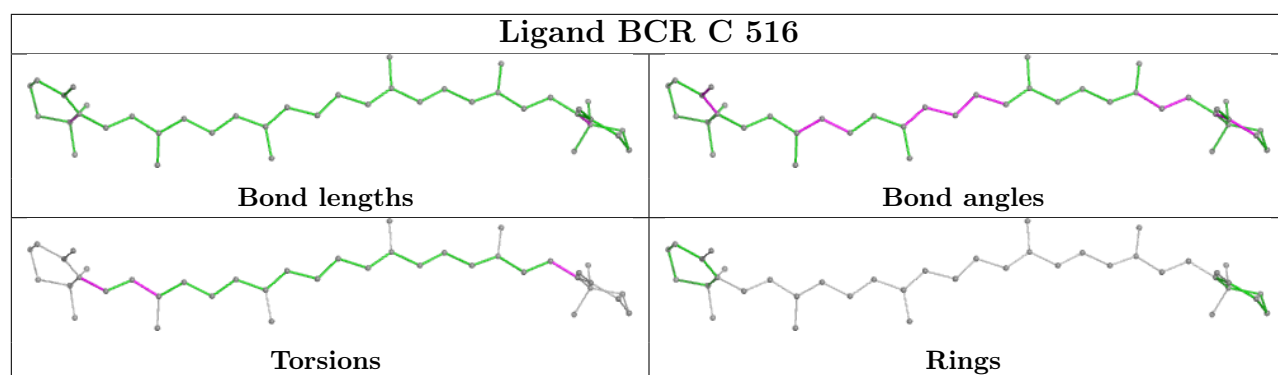


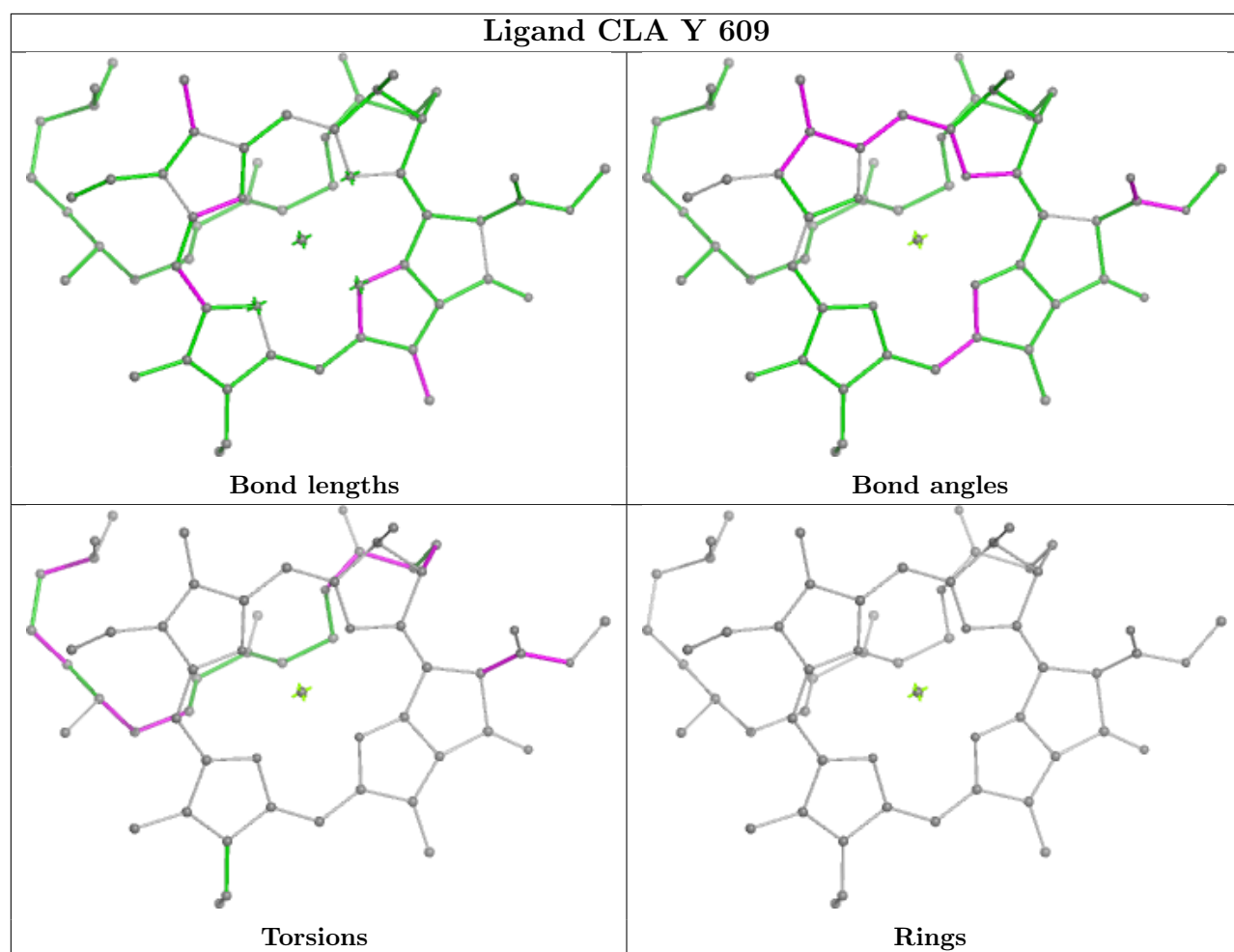


## Ligand CLA s 308



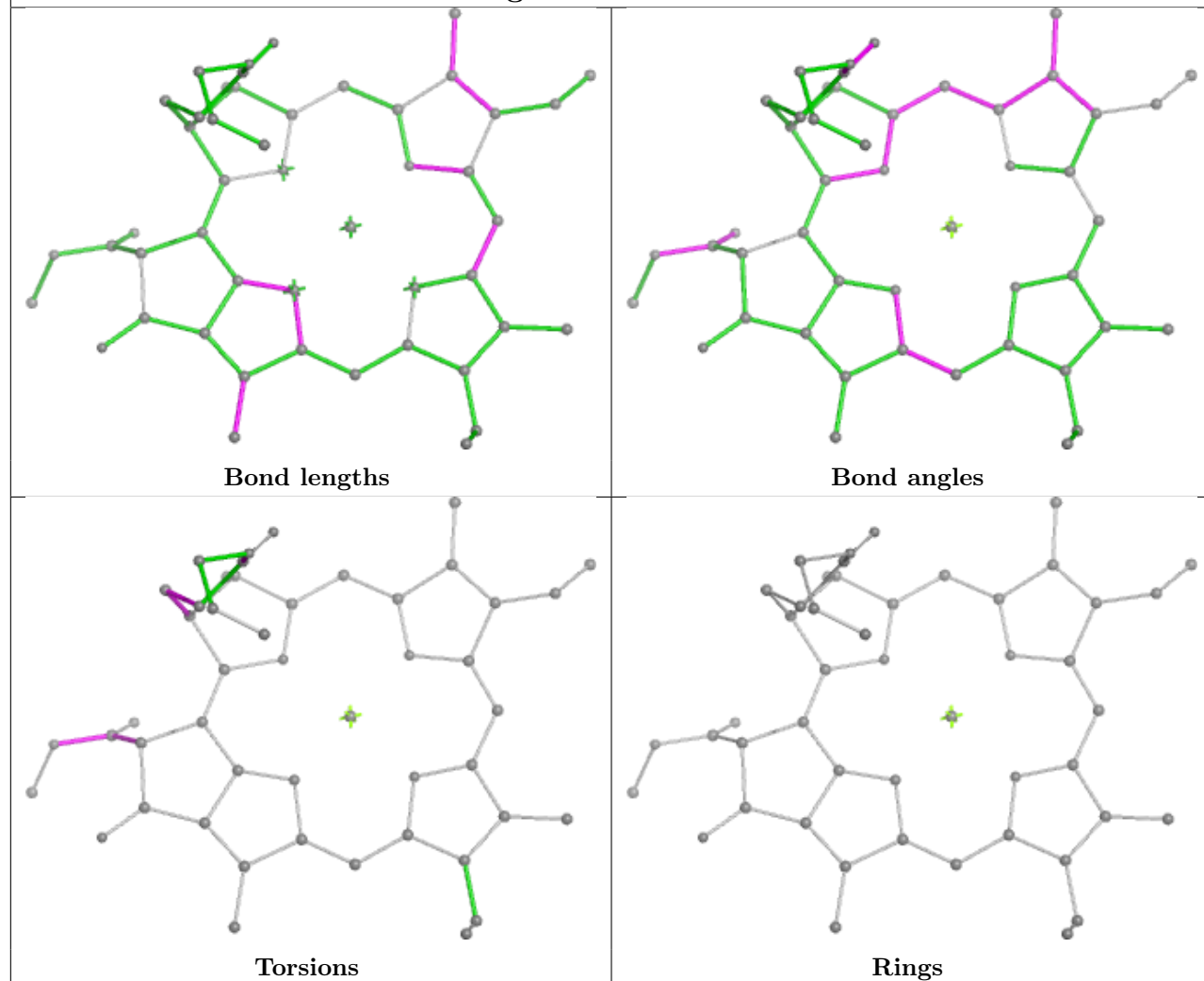




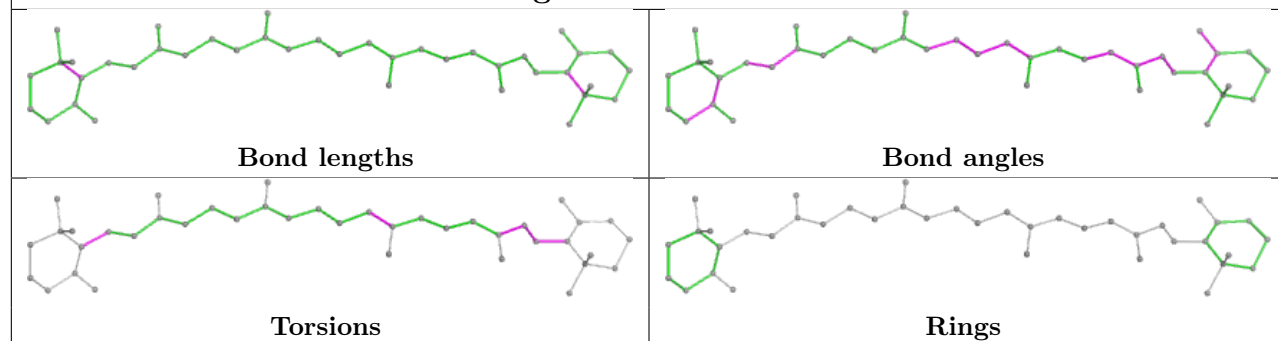


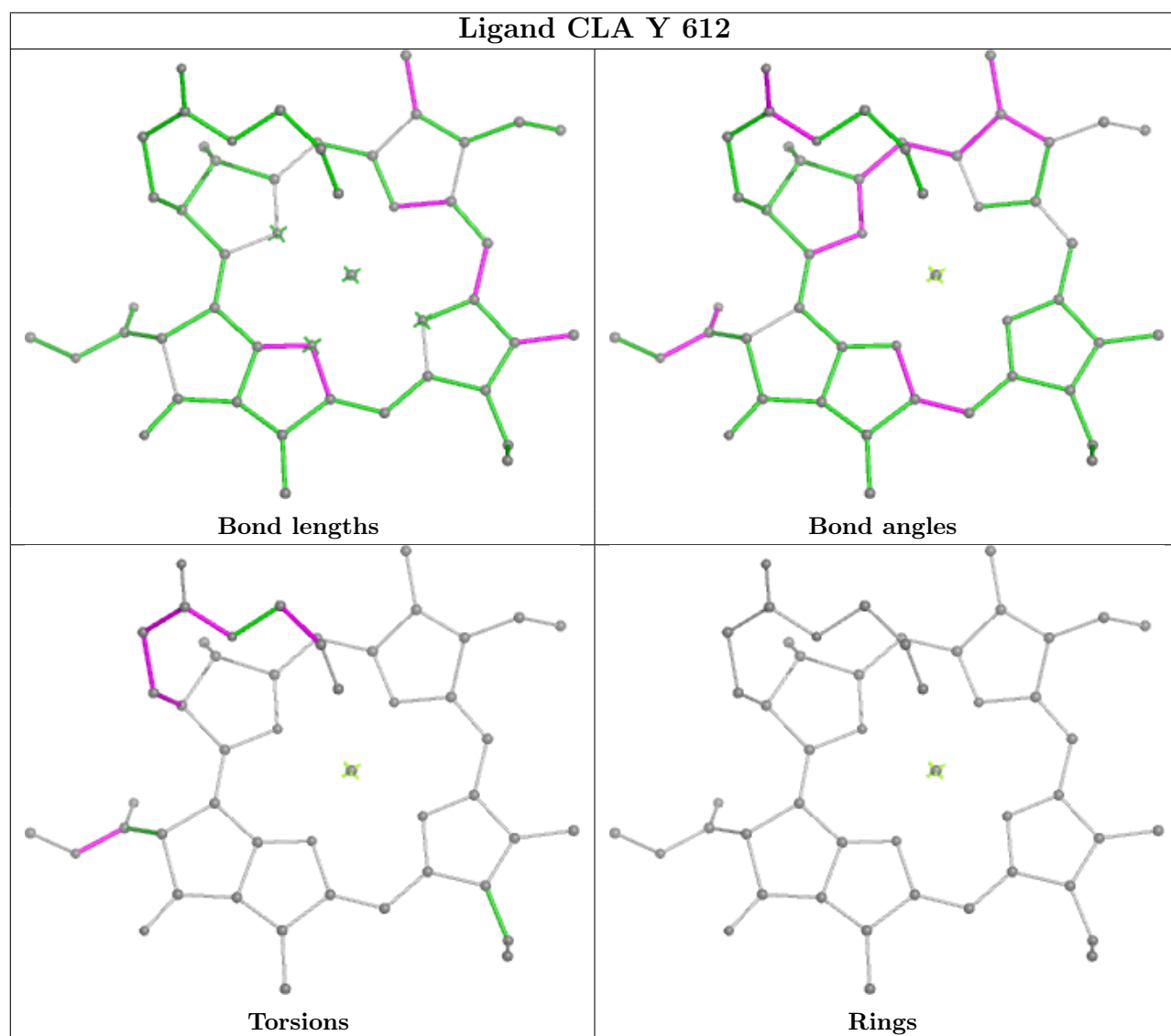
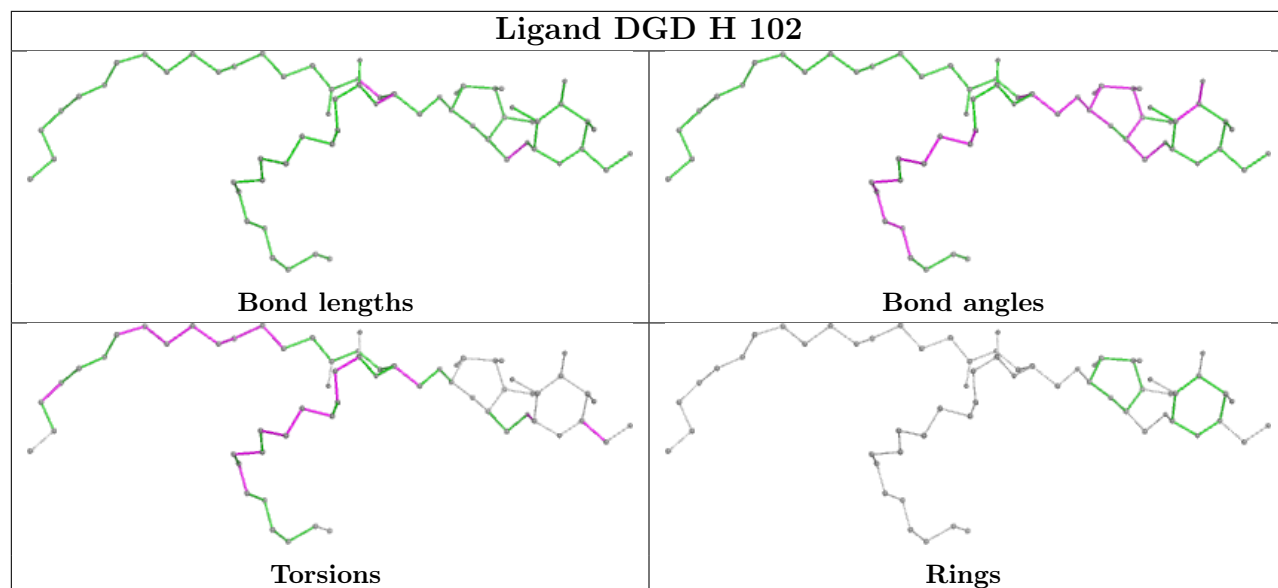


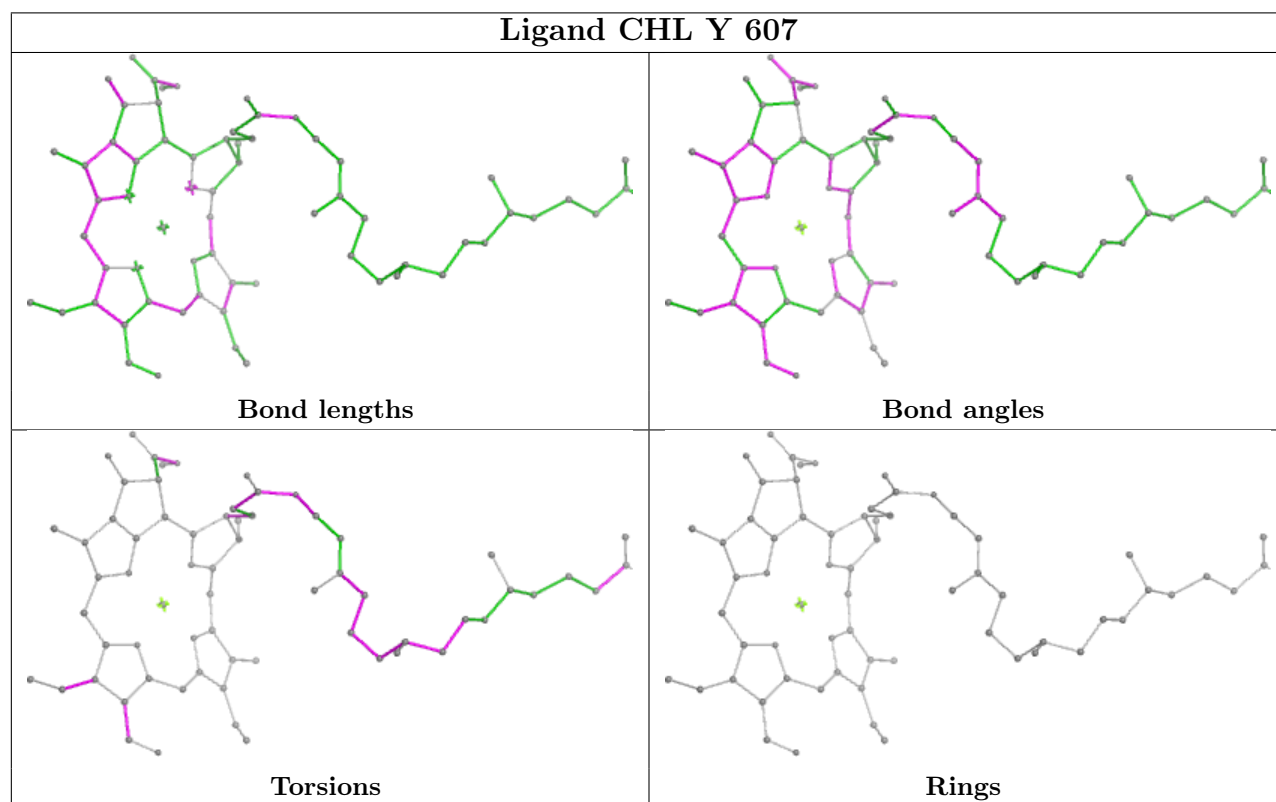
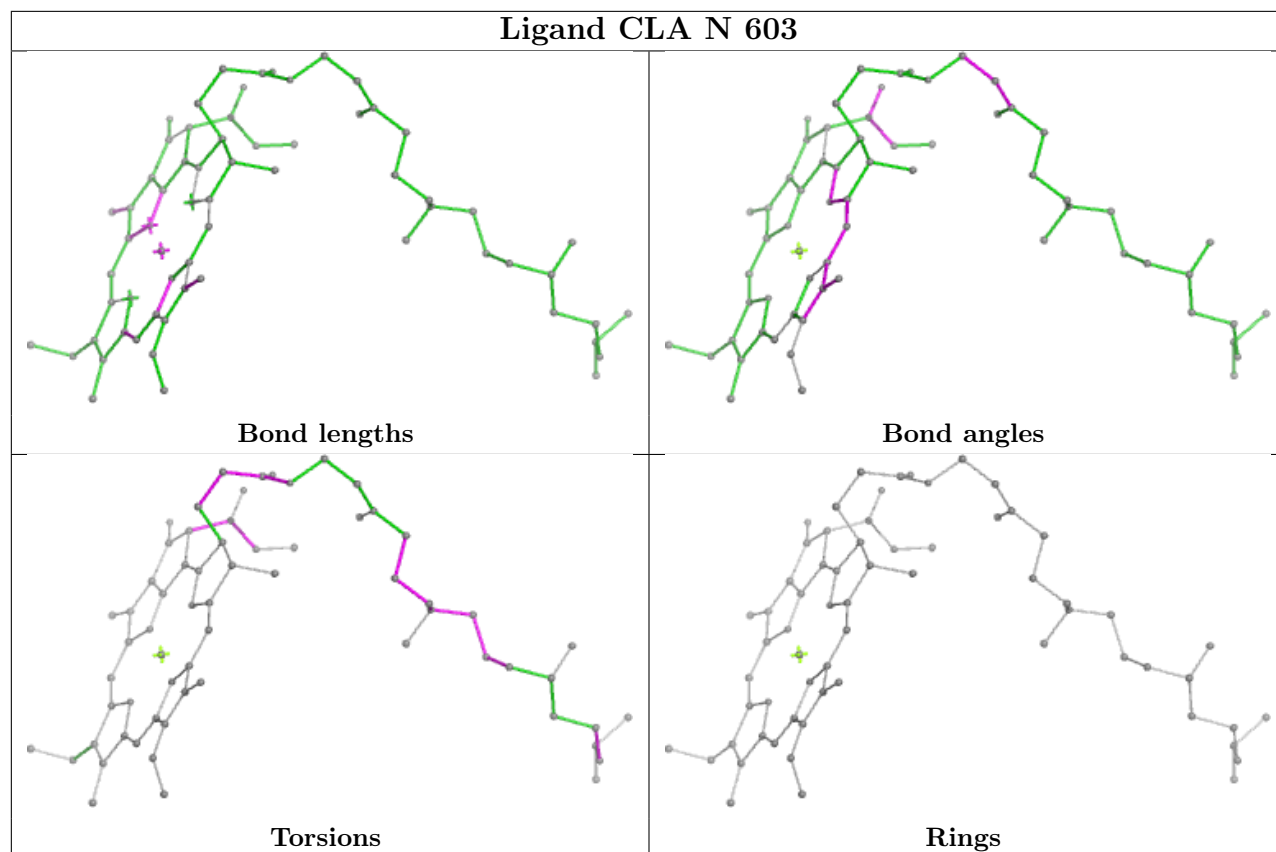
## Ligand CLA r 305

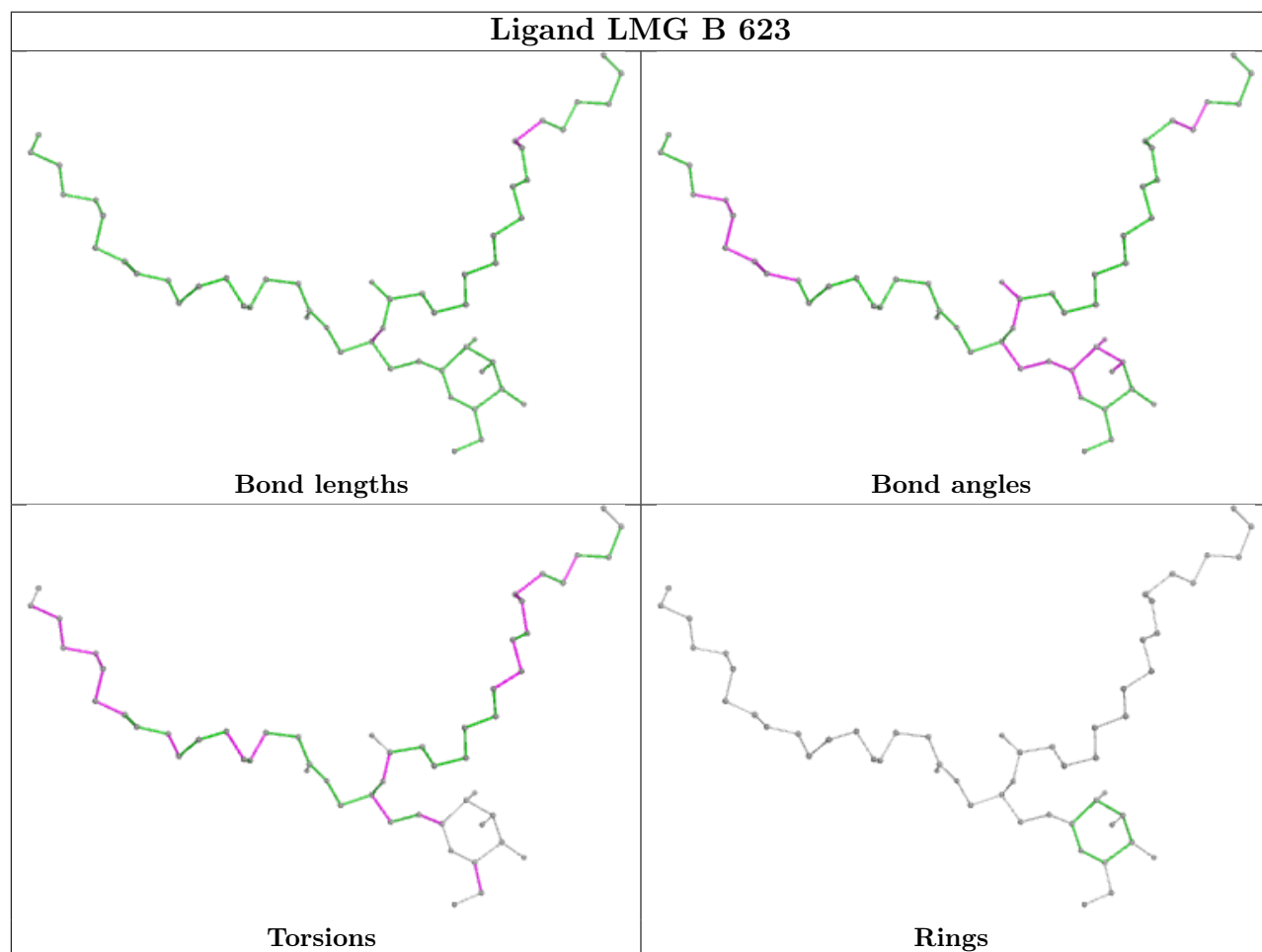
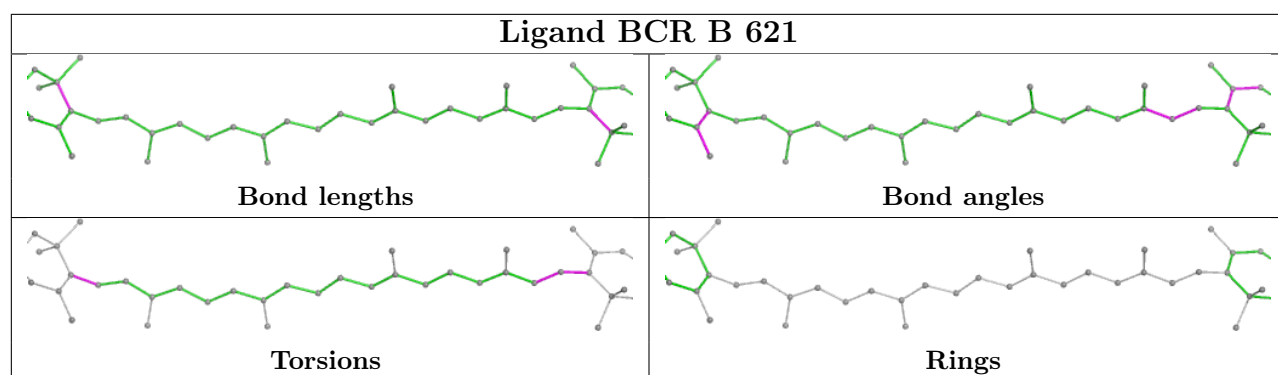


## Ligand BCR d 405

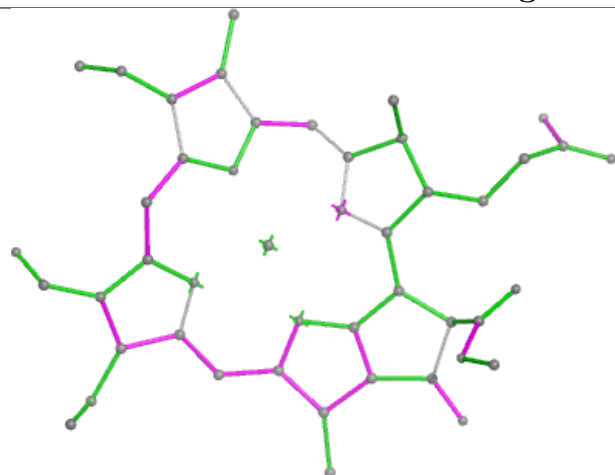




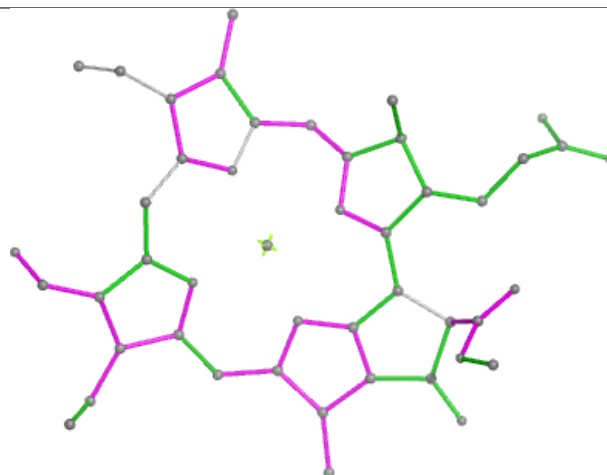




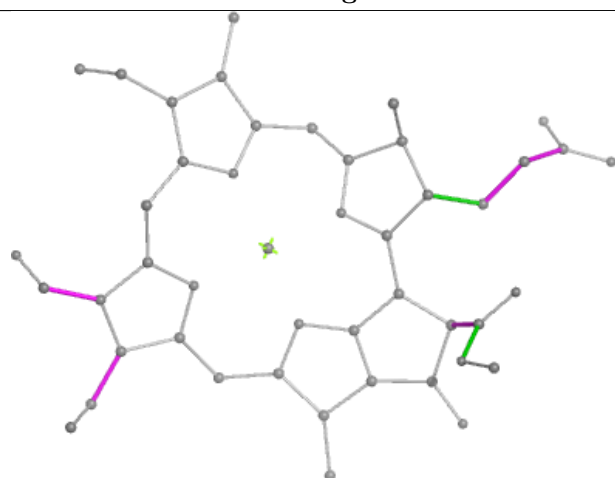
## Ligand CHL S 306



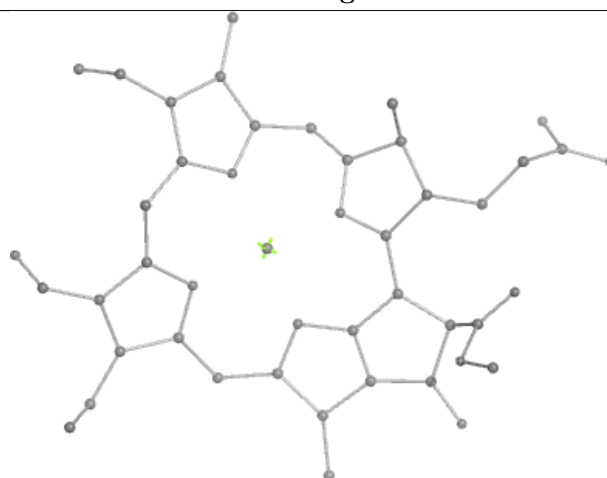
Bond lengths



Bond angles

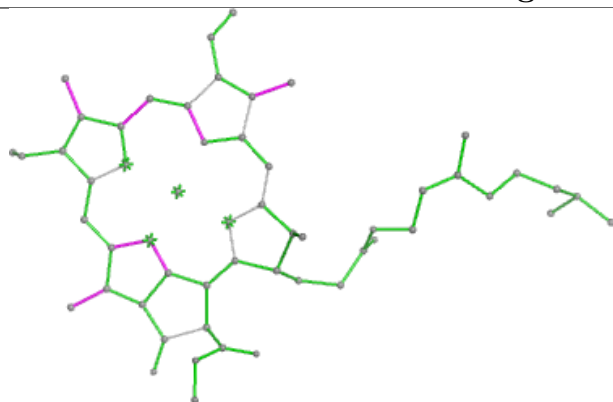


Torsions

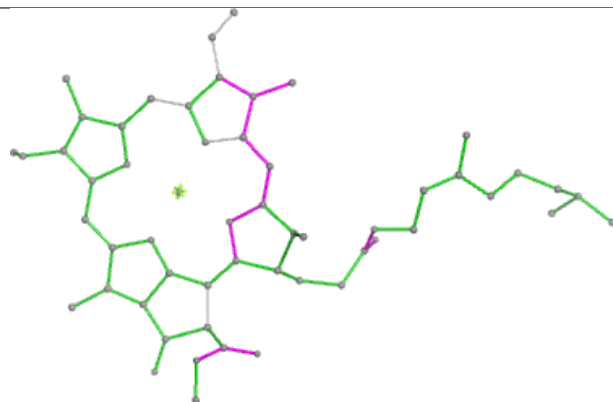


Rings

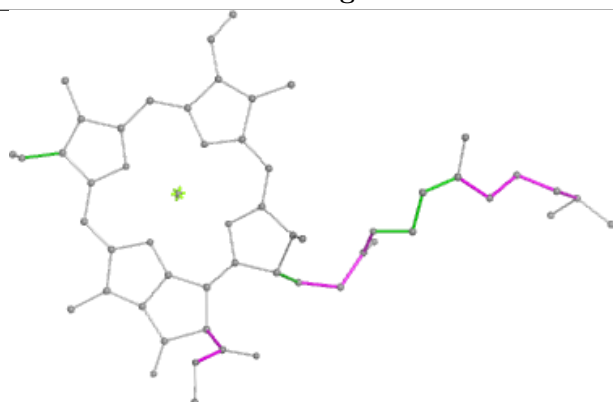
## Ligand CLA S 310



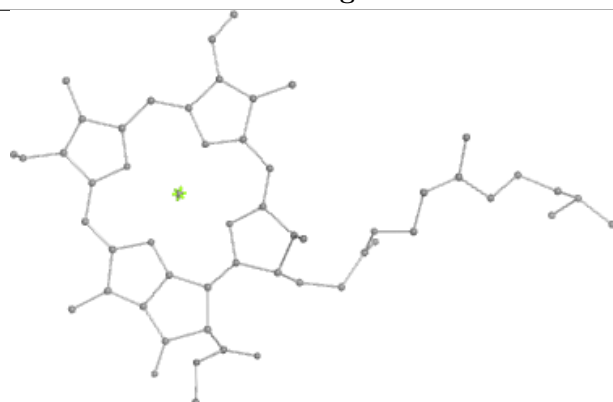
Bond lengths



Bond angles

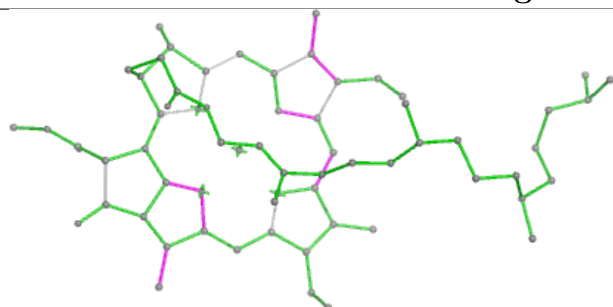


Torsions

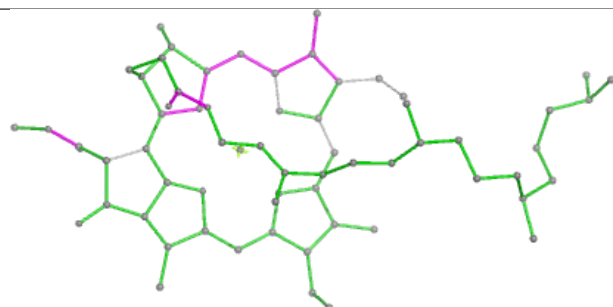


Rings

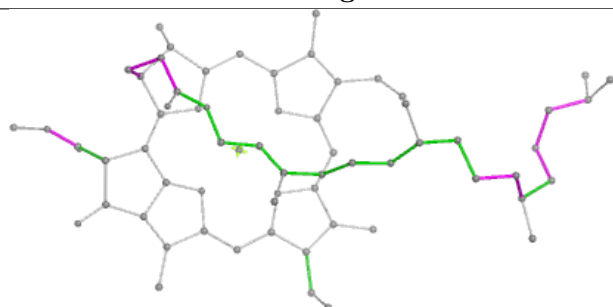
## Ligand CLA C 507



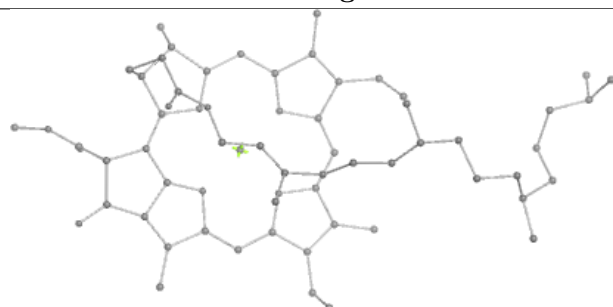
Bond lengths



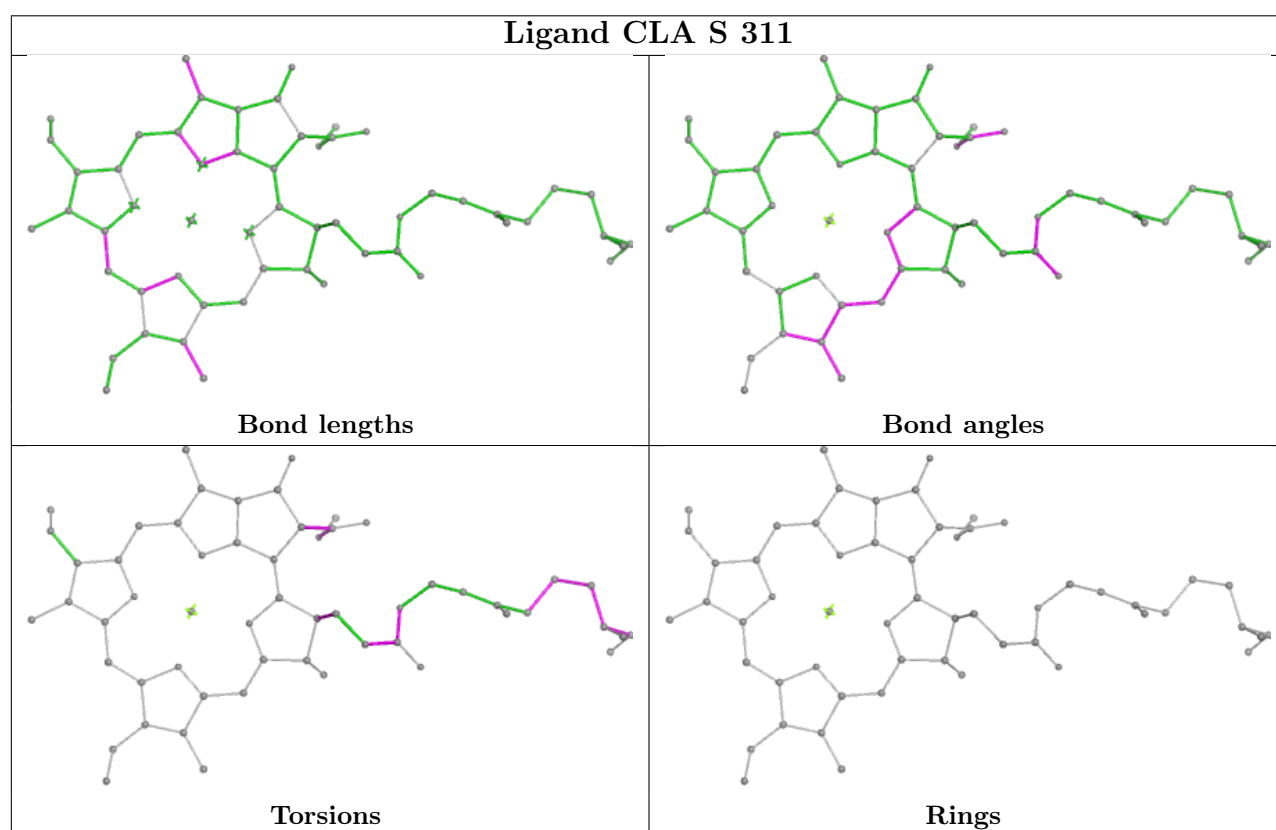
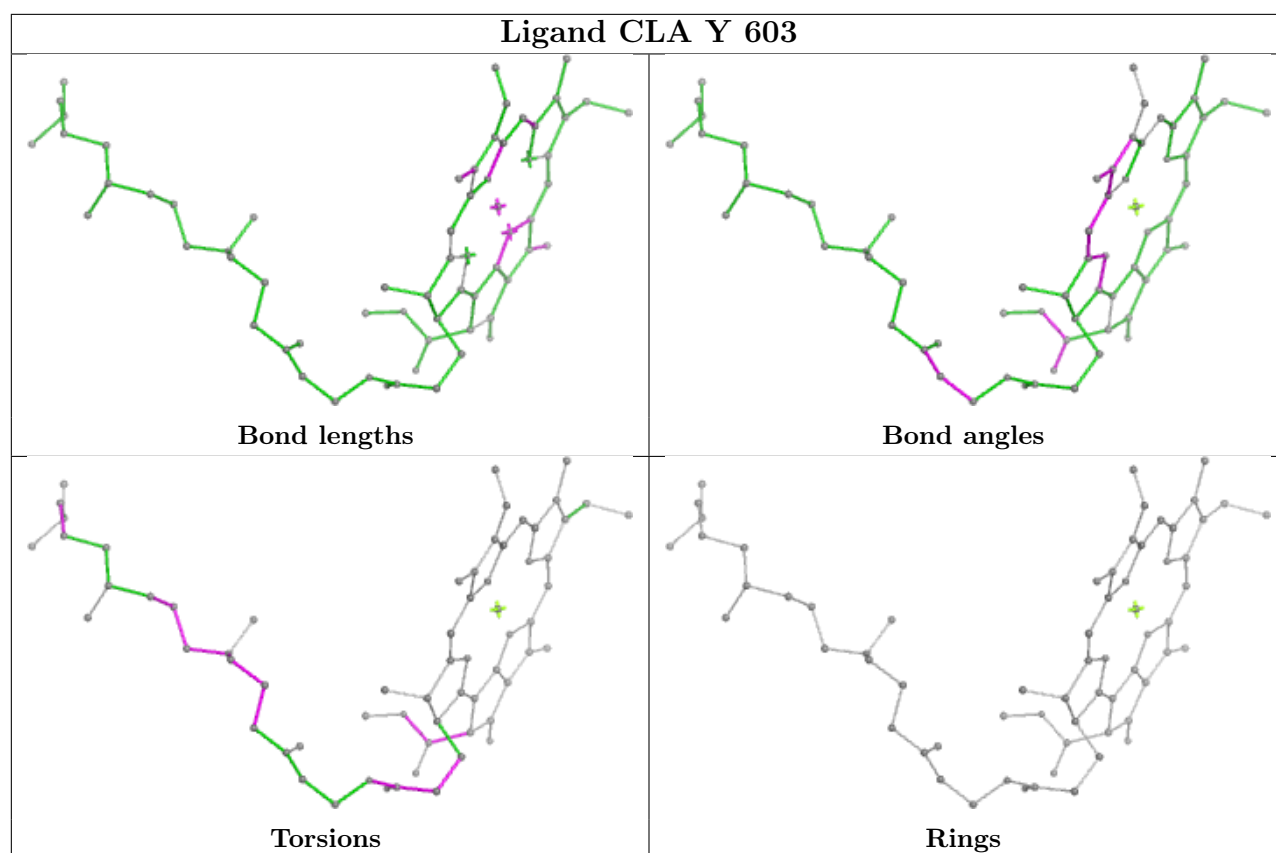
Bond angles

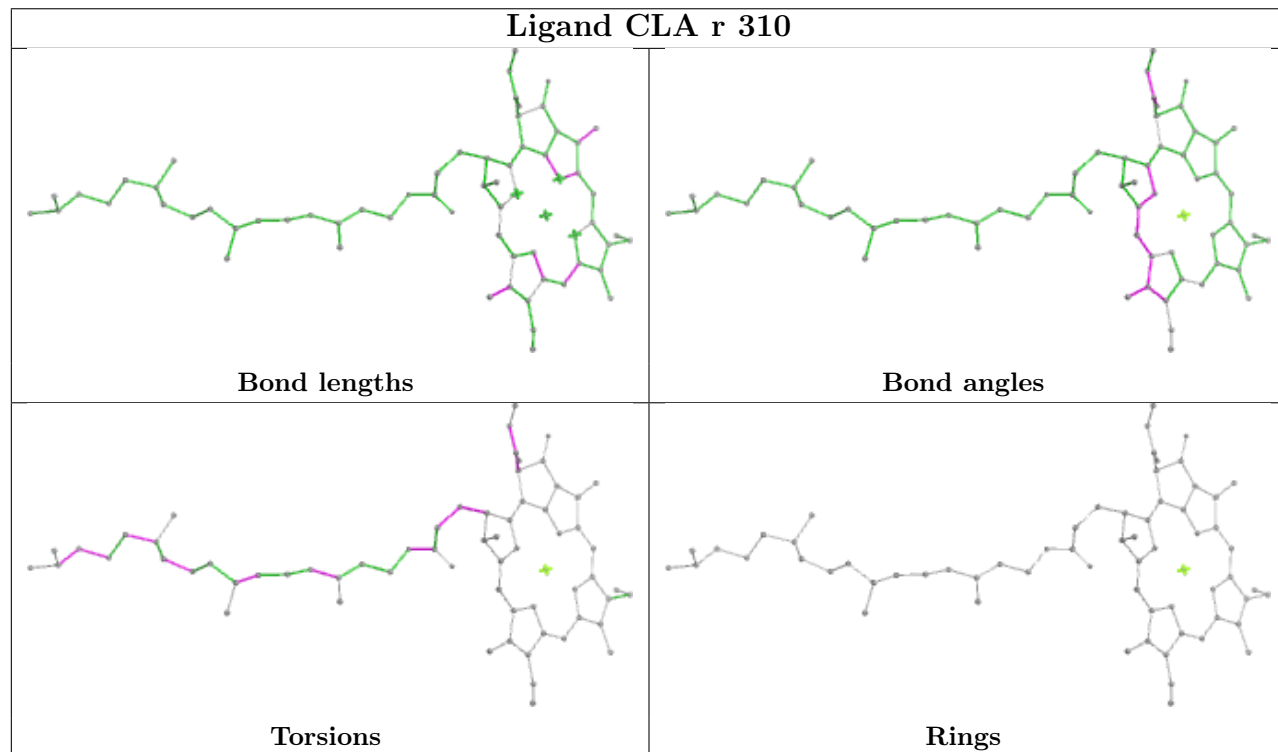
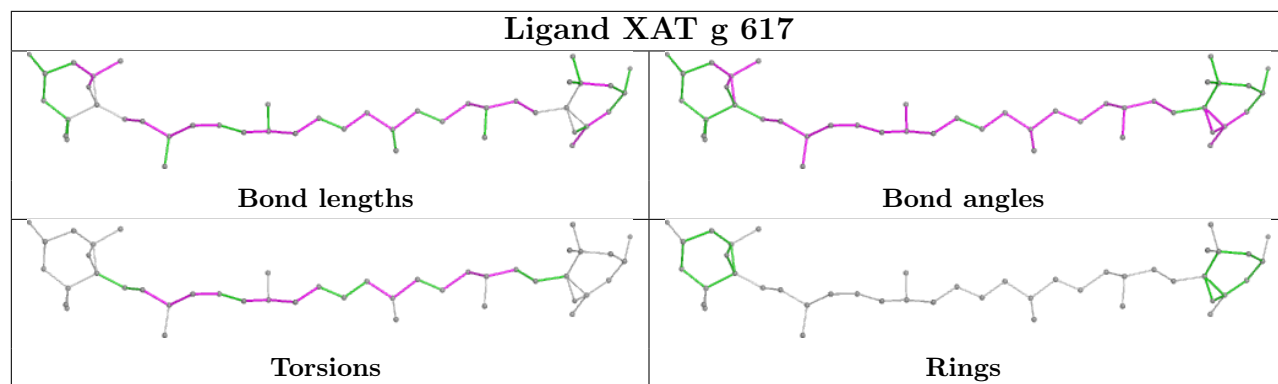


Torsions

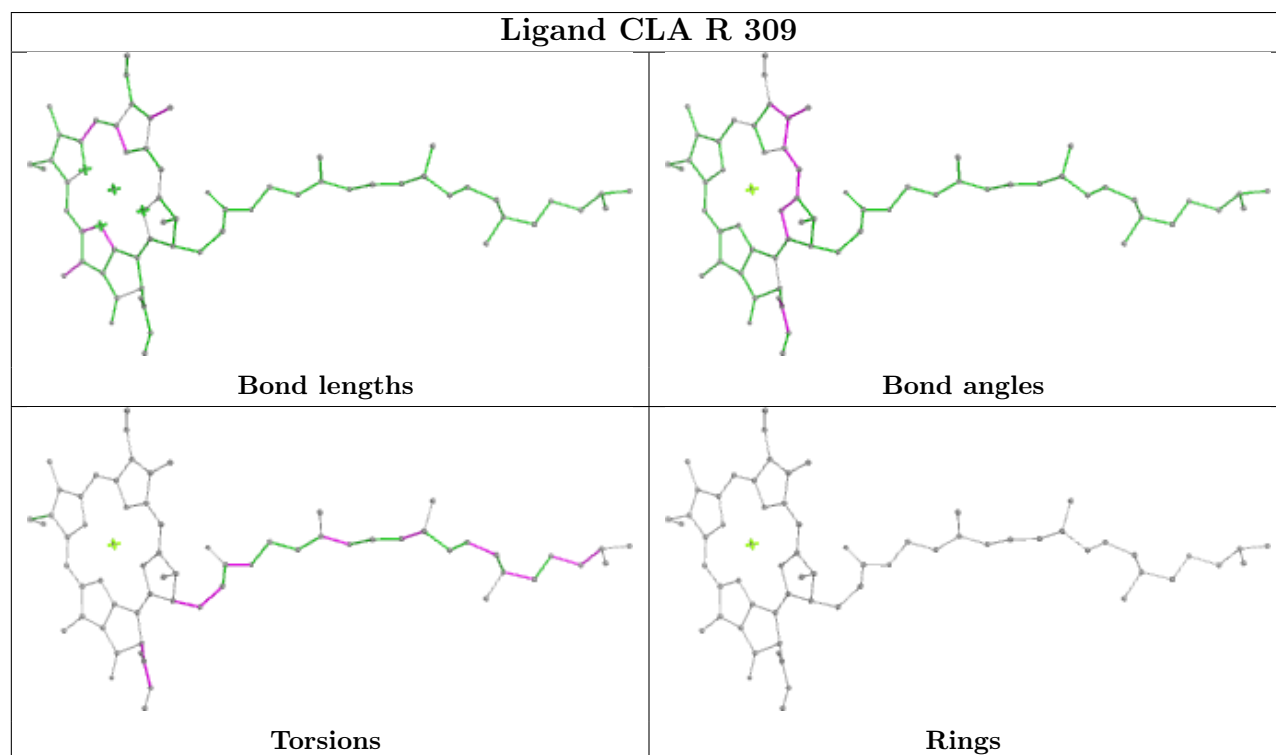
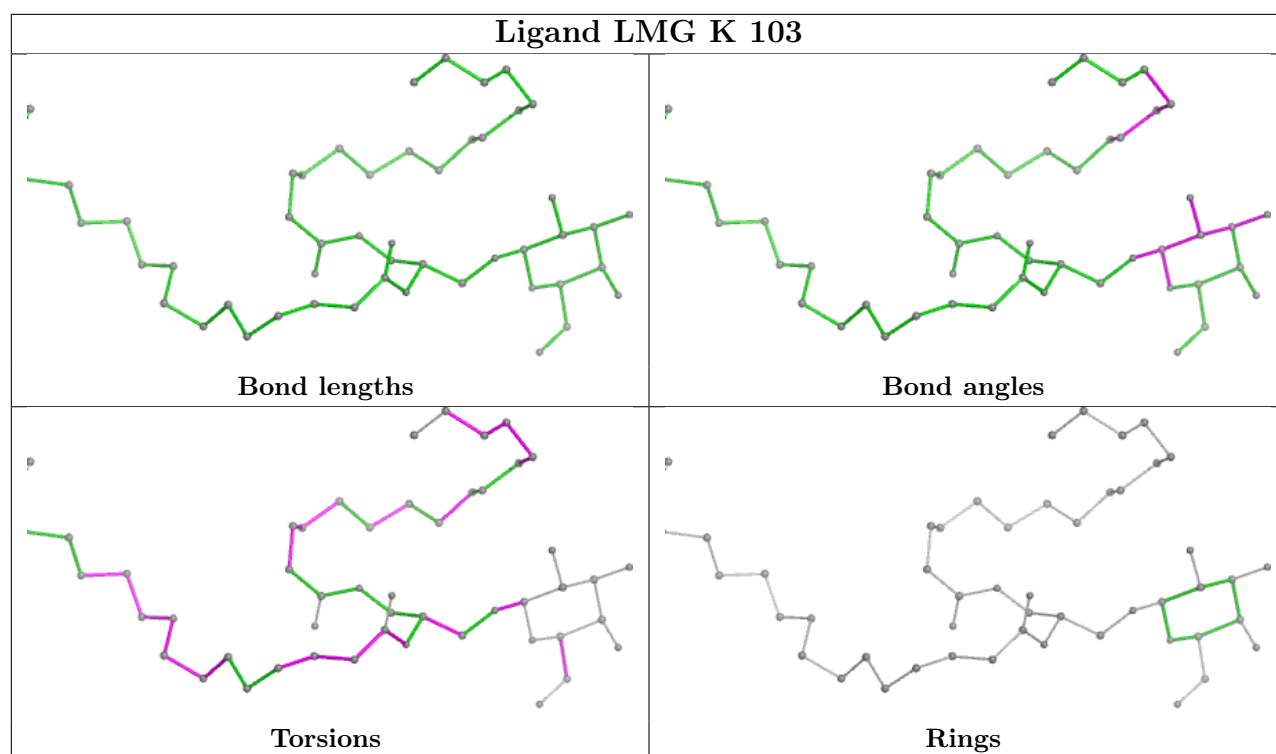


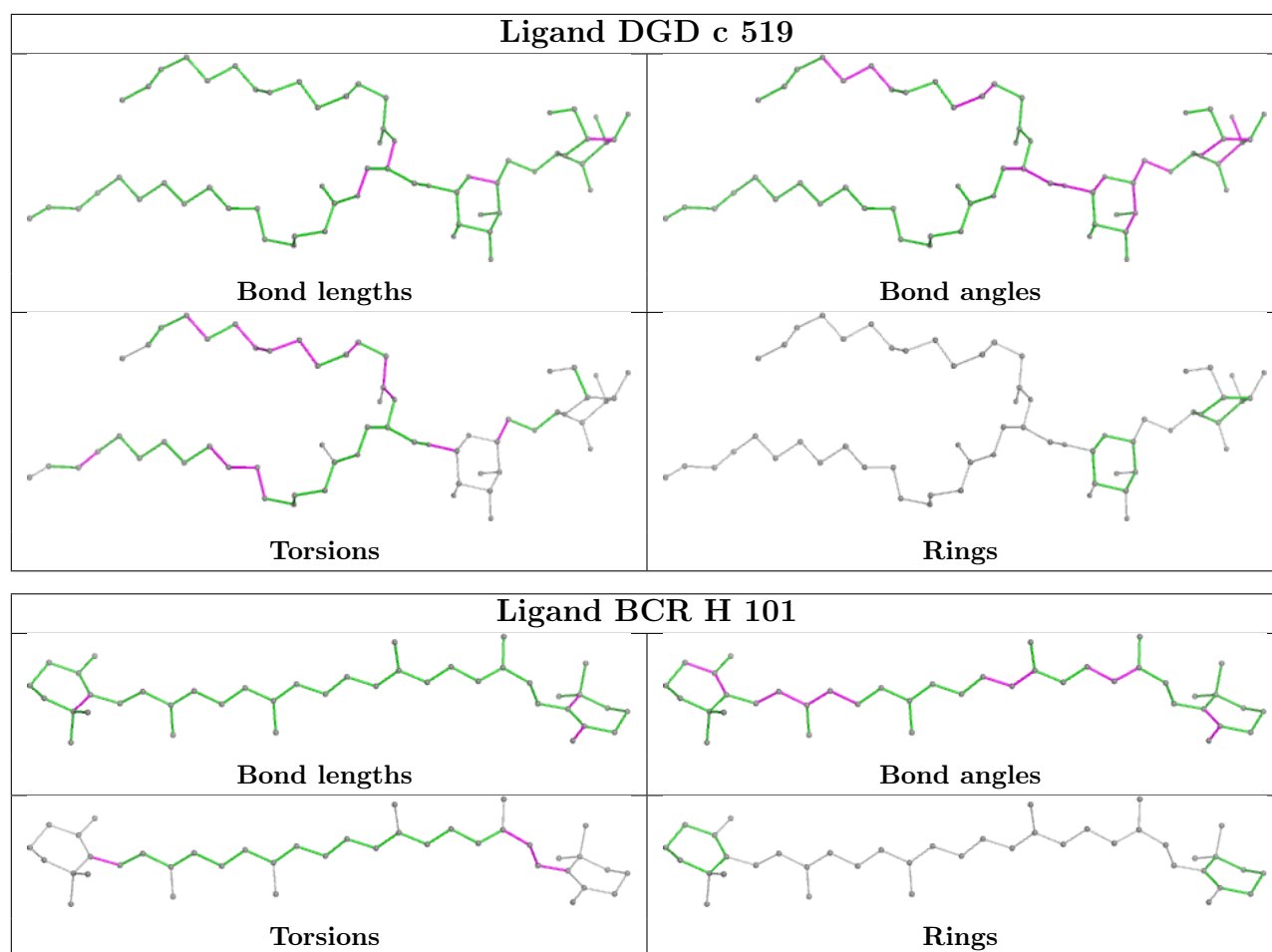
Rings

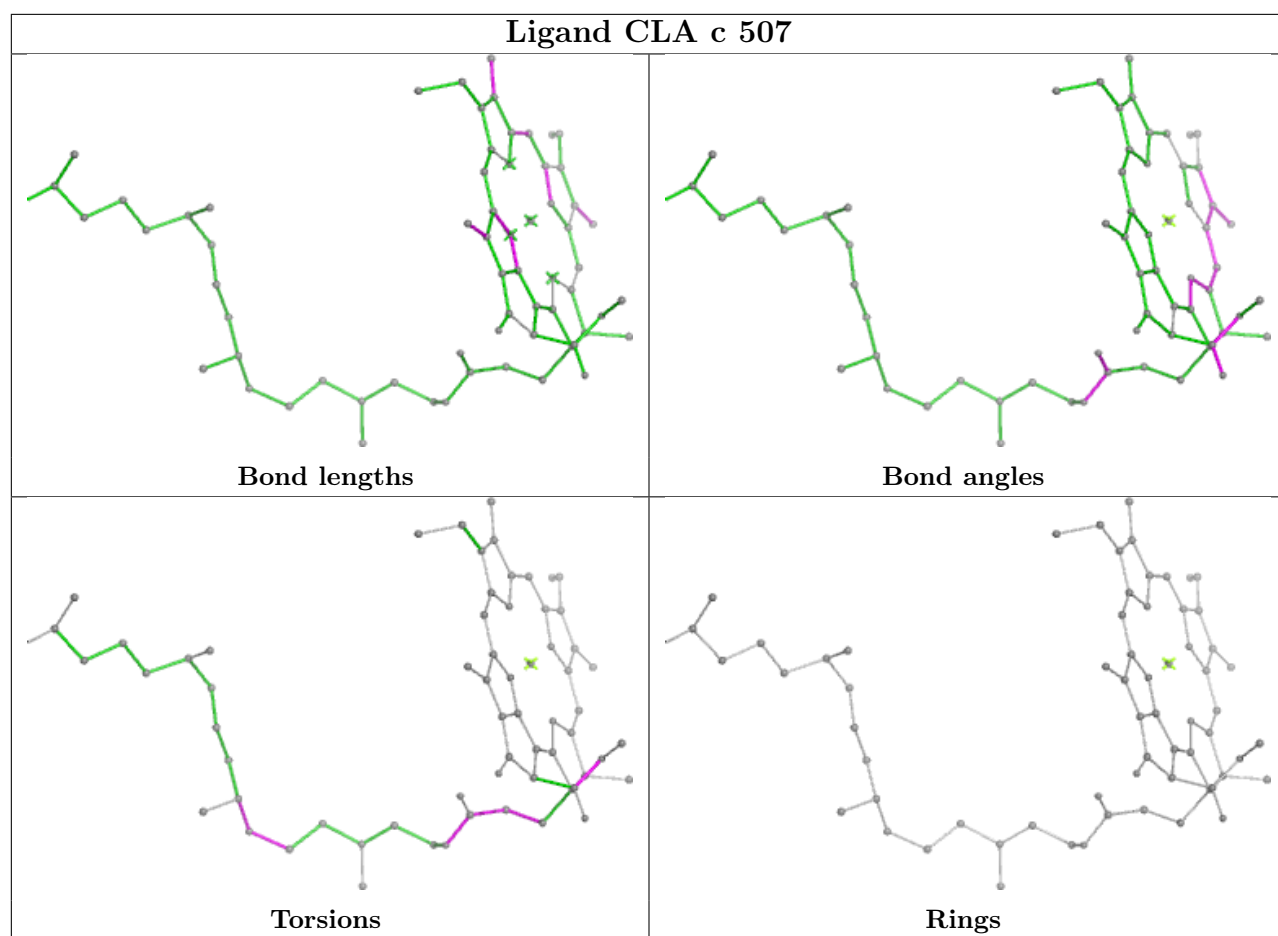




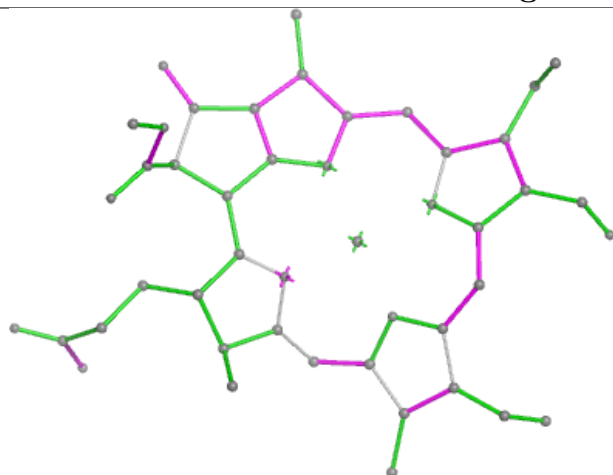




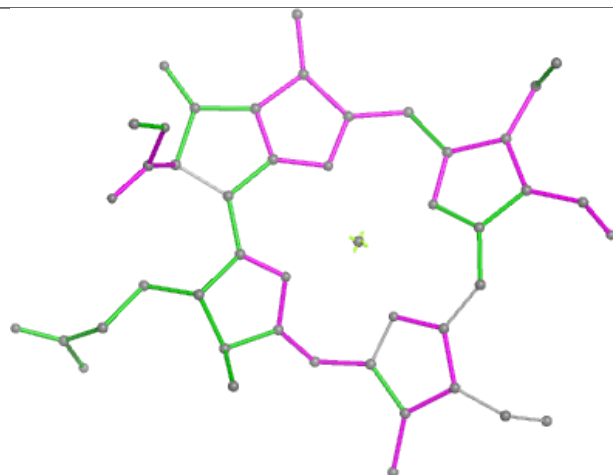




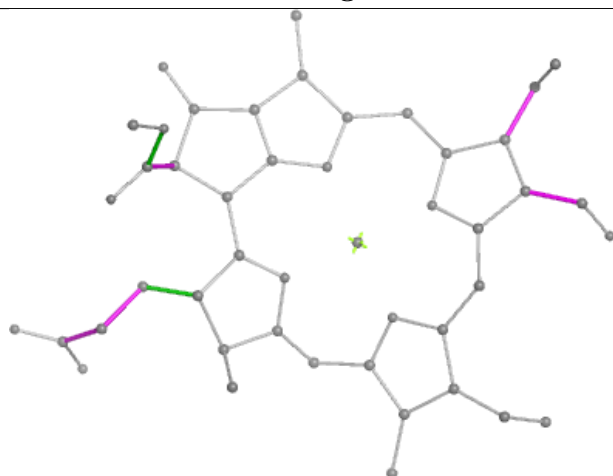
## Ligand CHL s 306



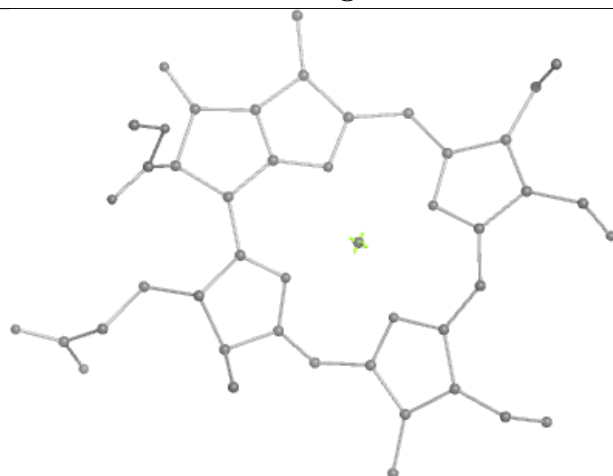
Bond lengths



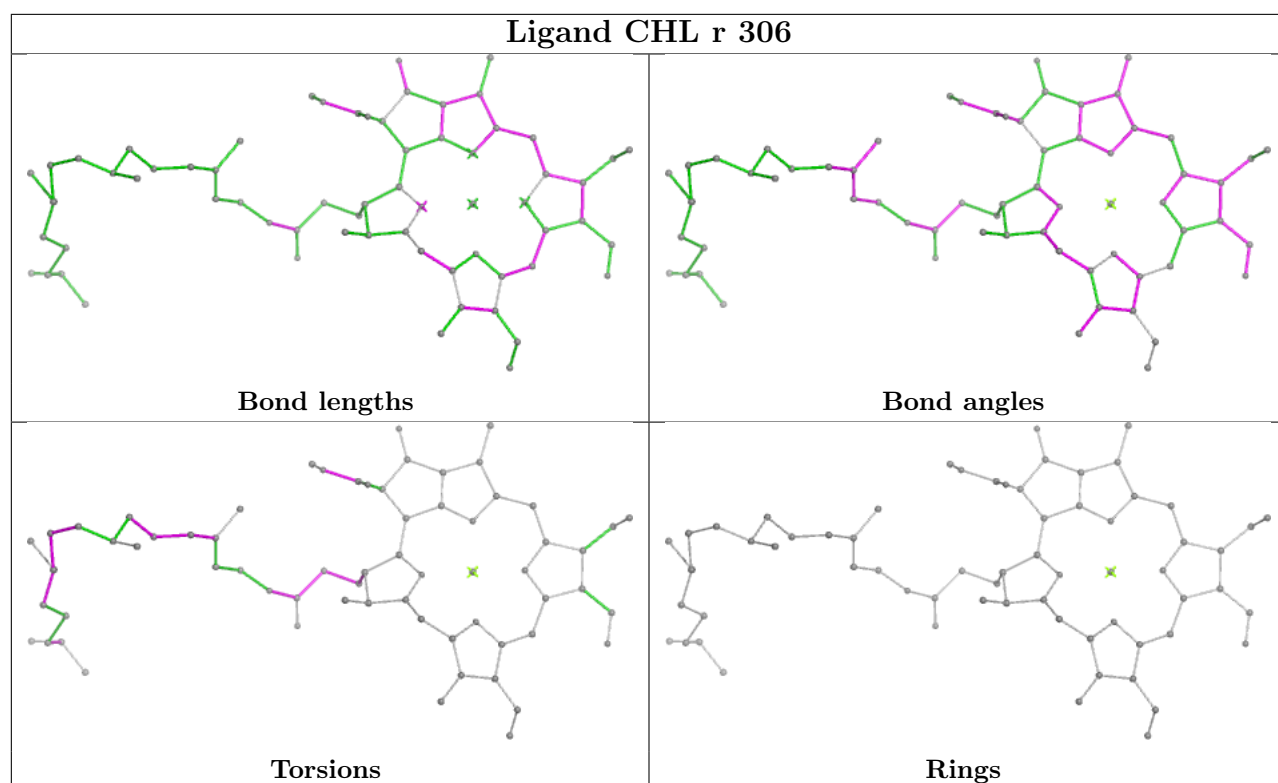
Bond angles

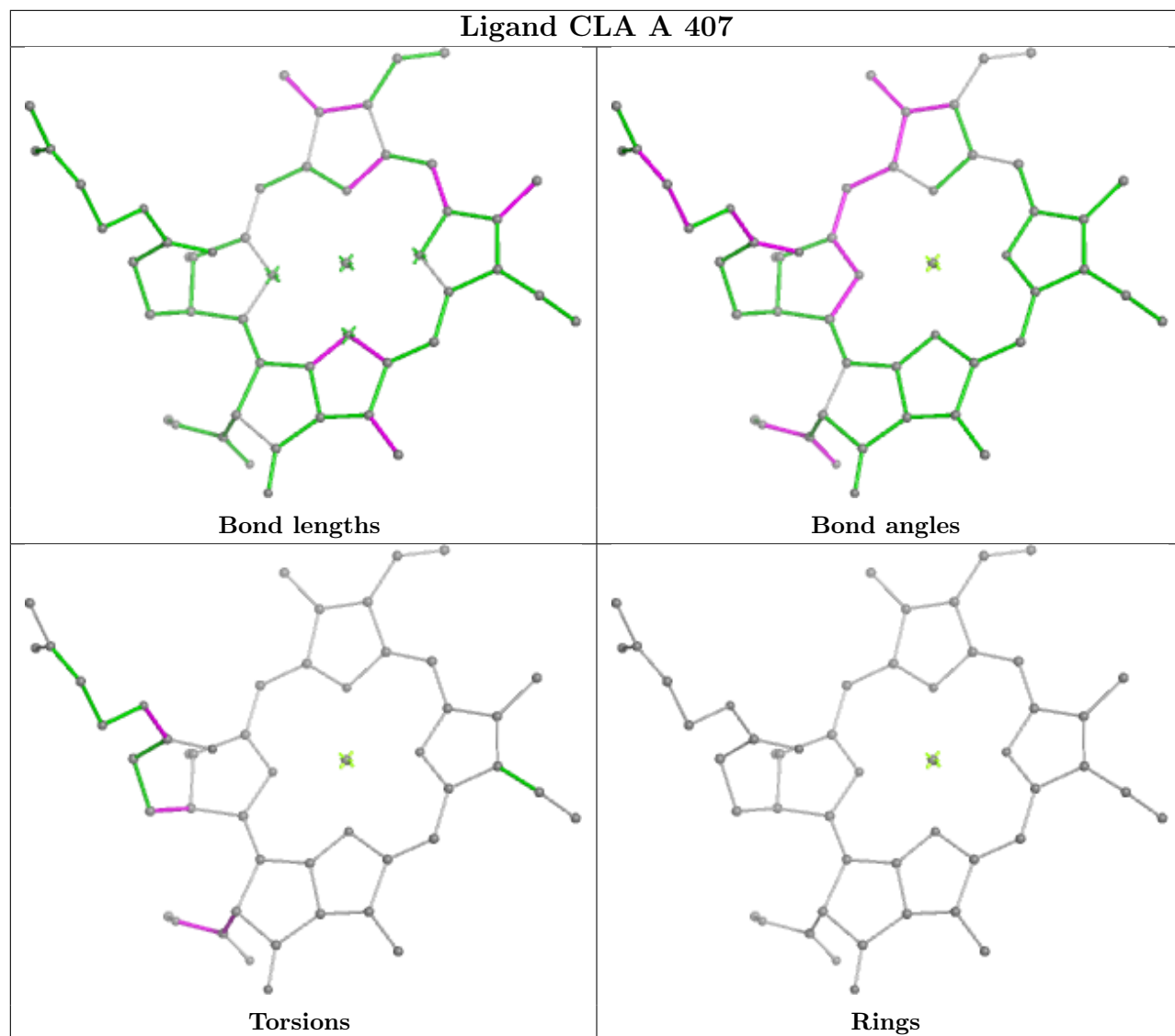


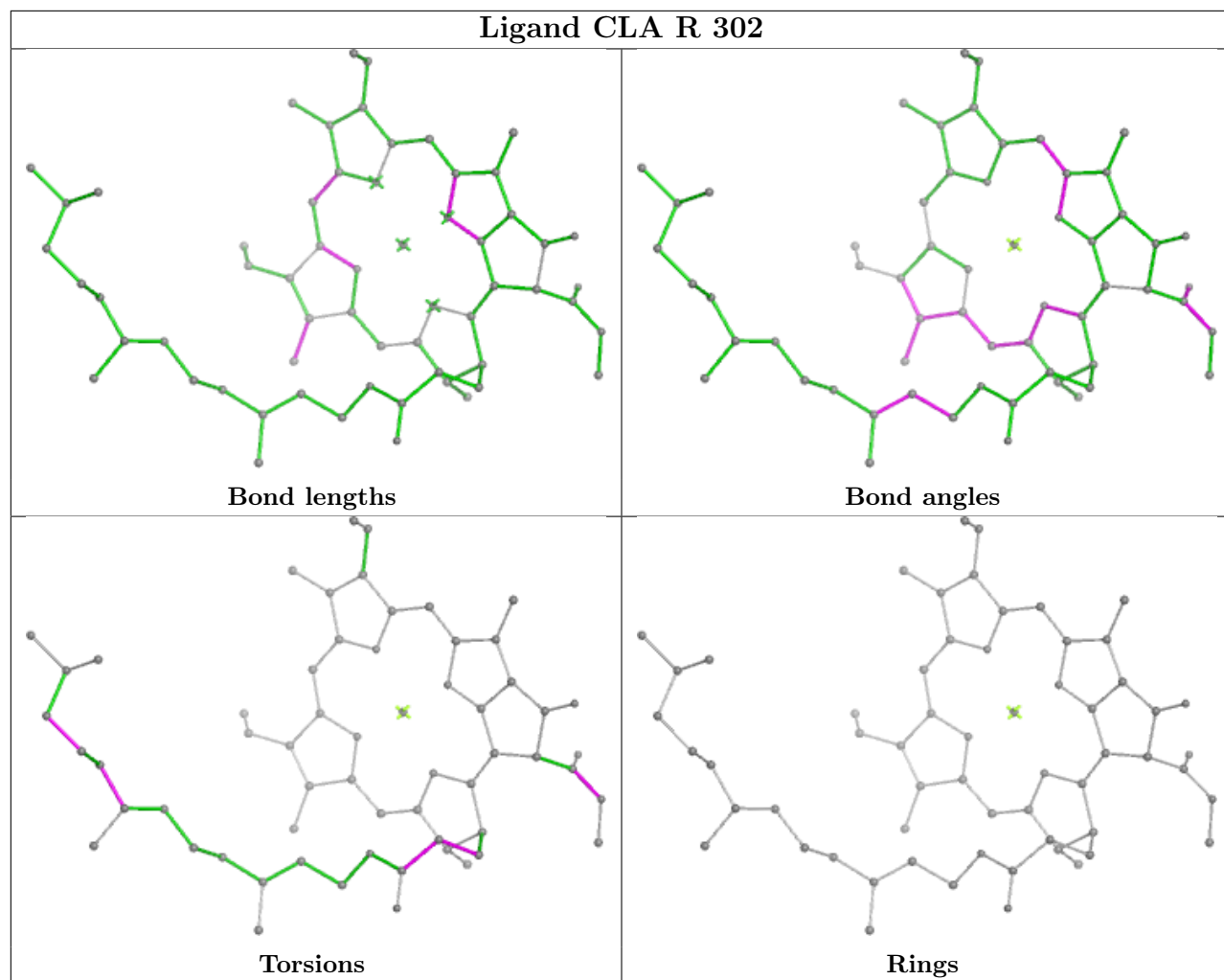
Torsions

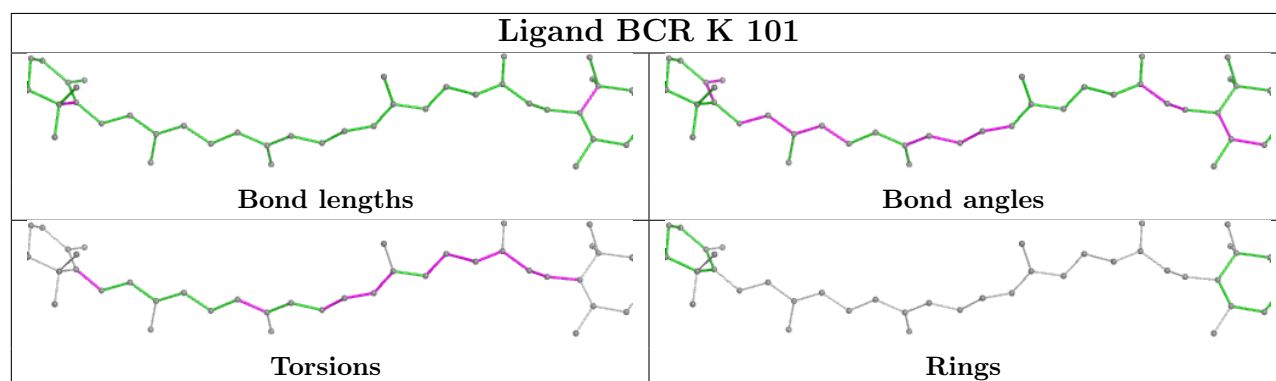
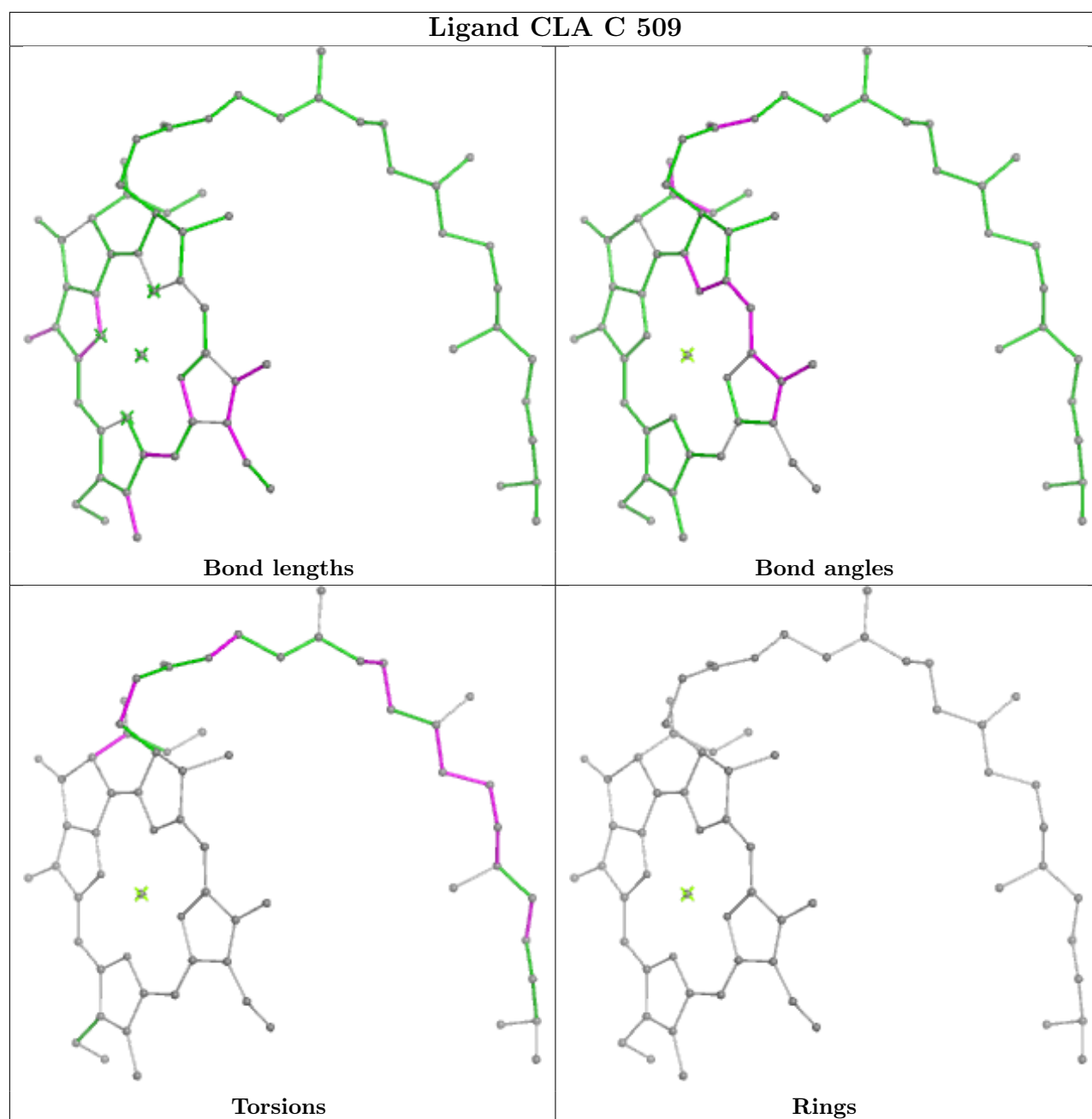


Rings



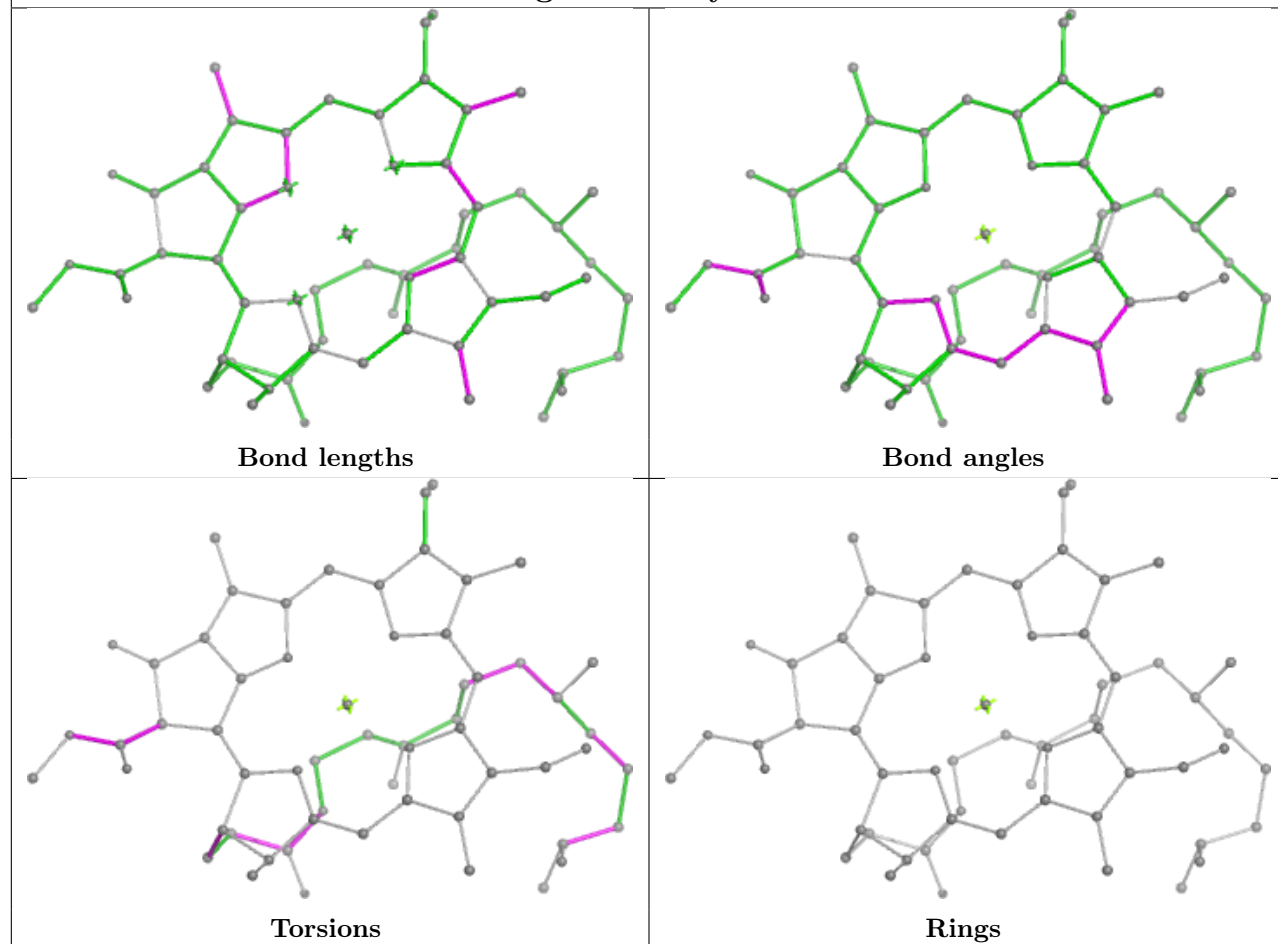




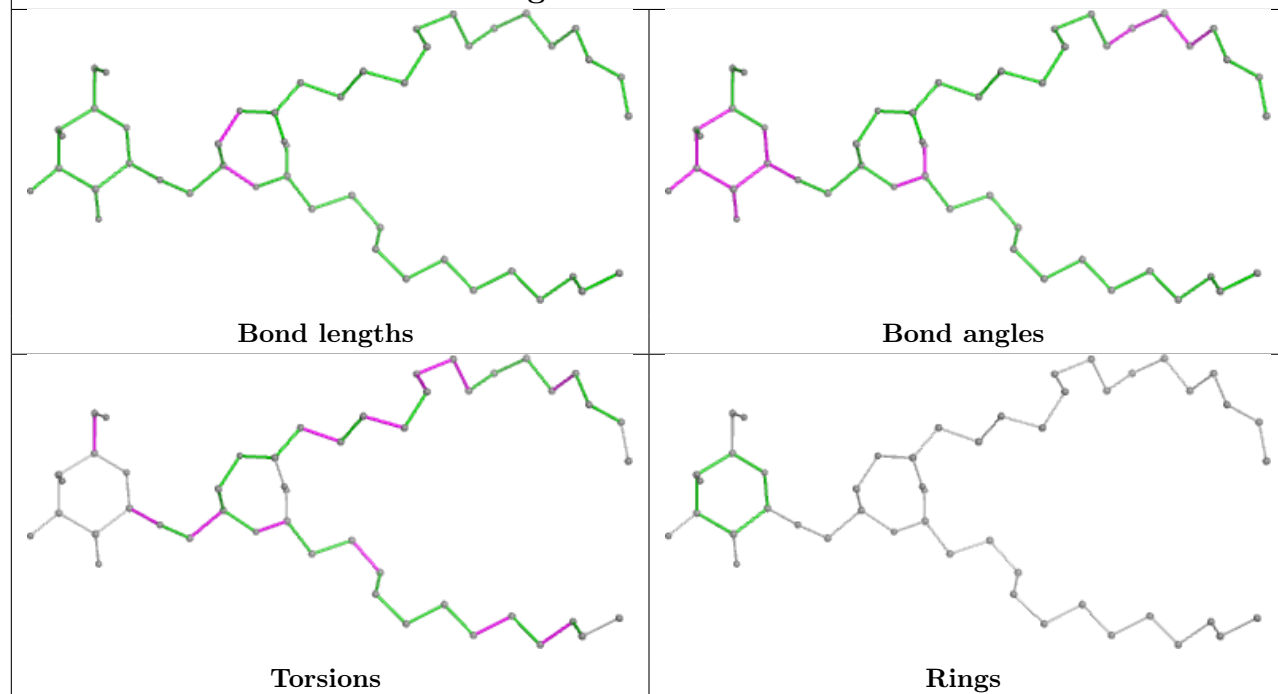




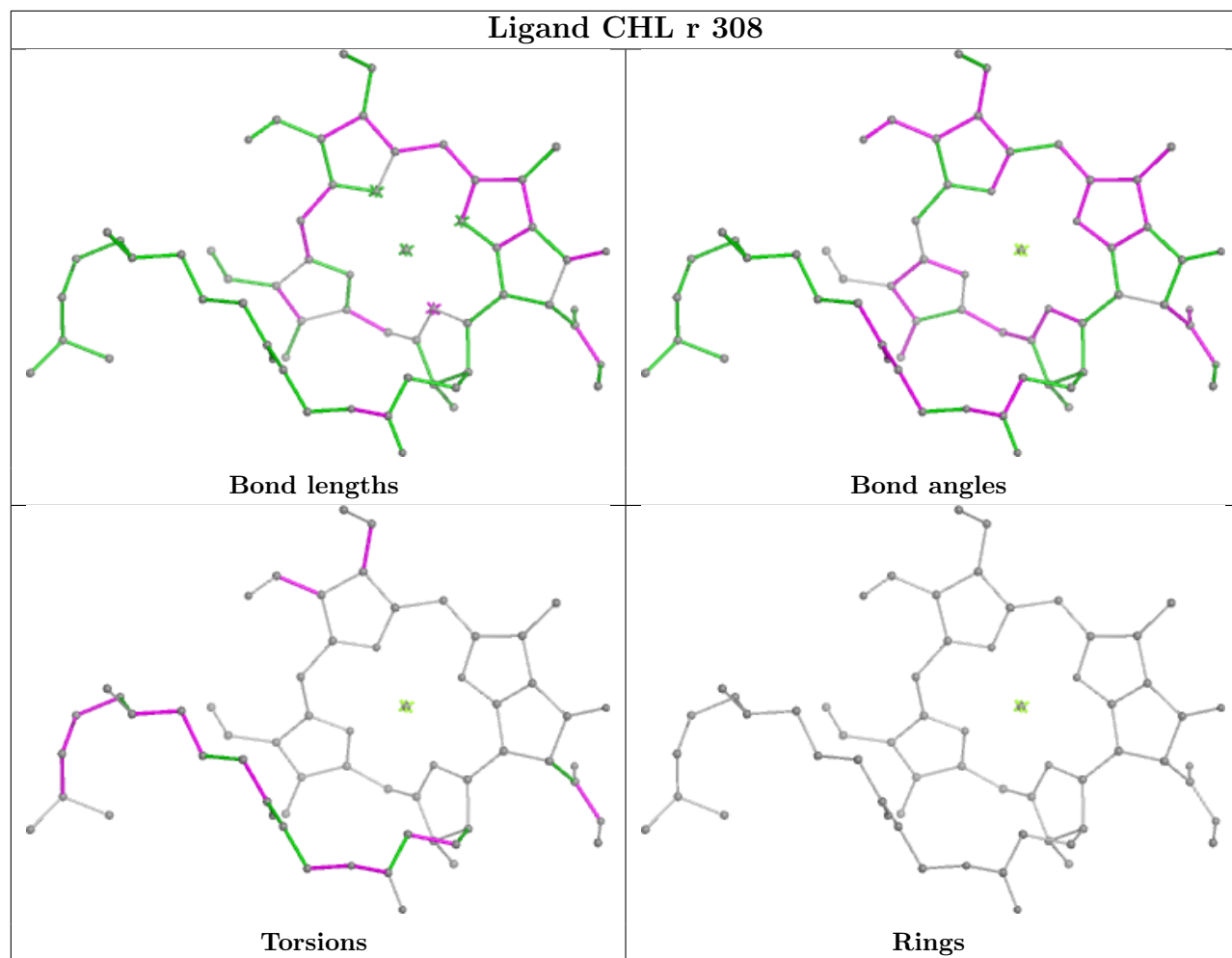
## Ligand CLA y 610



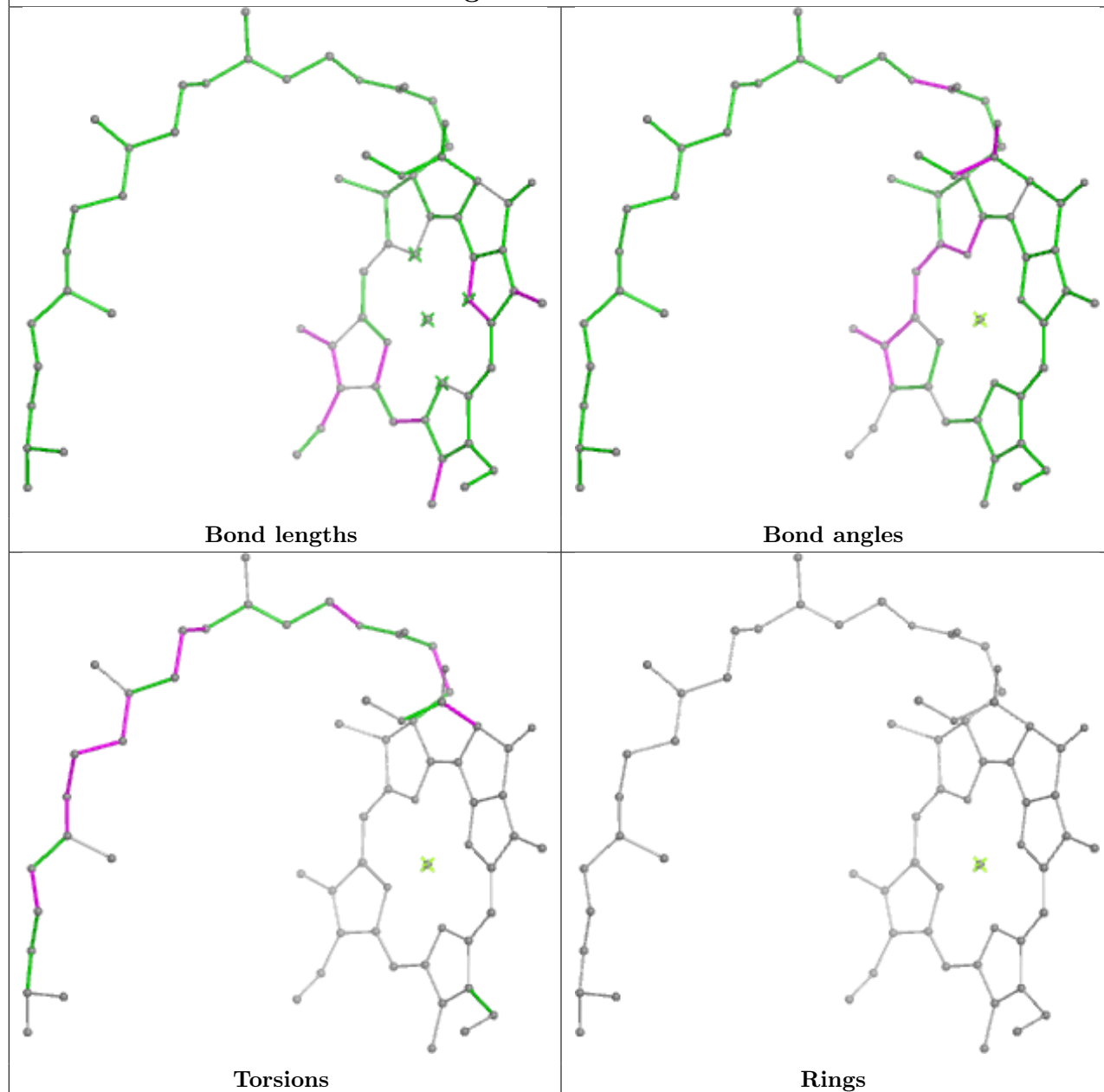
## Ligand LMG w 102

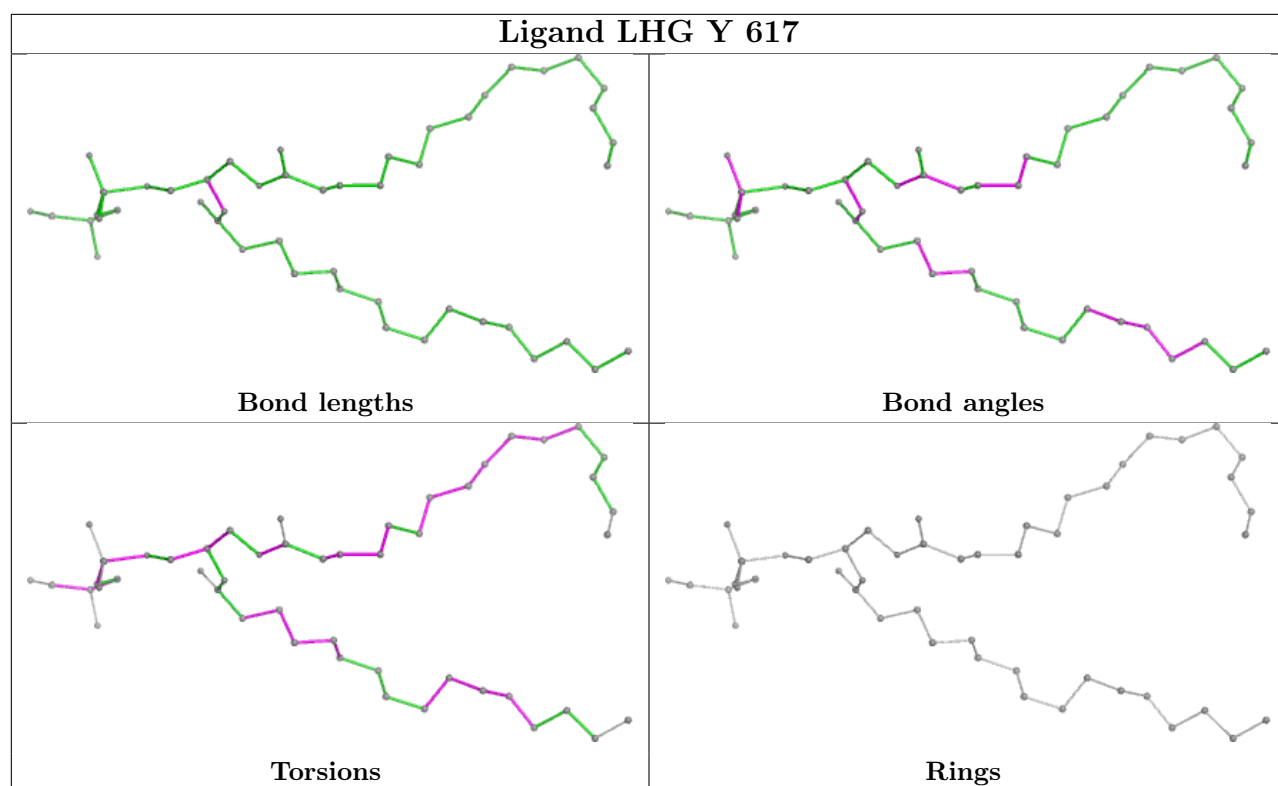


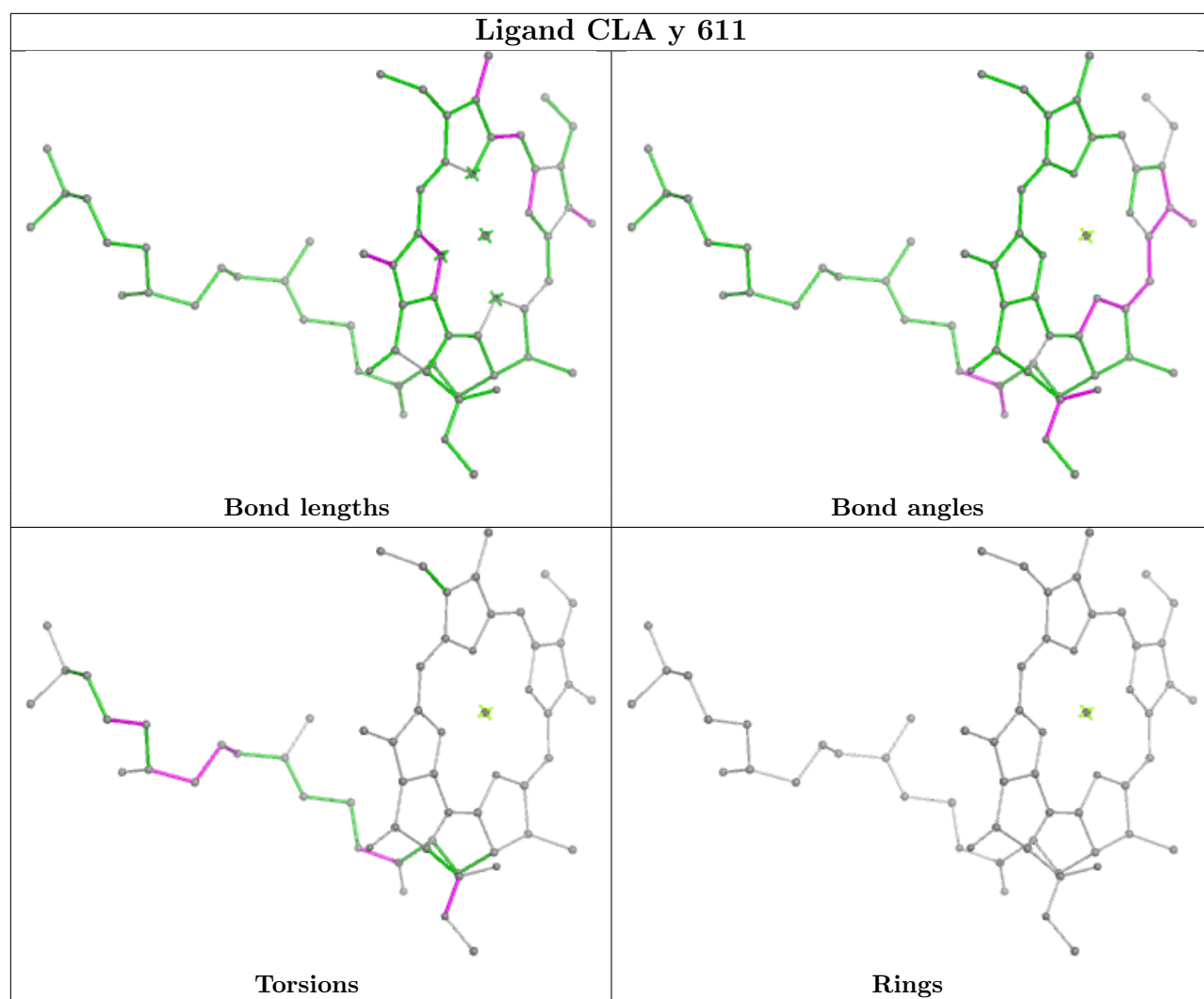
## Ligand CHL r 308

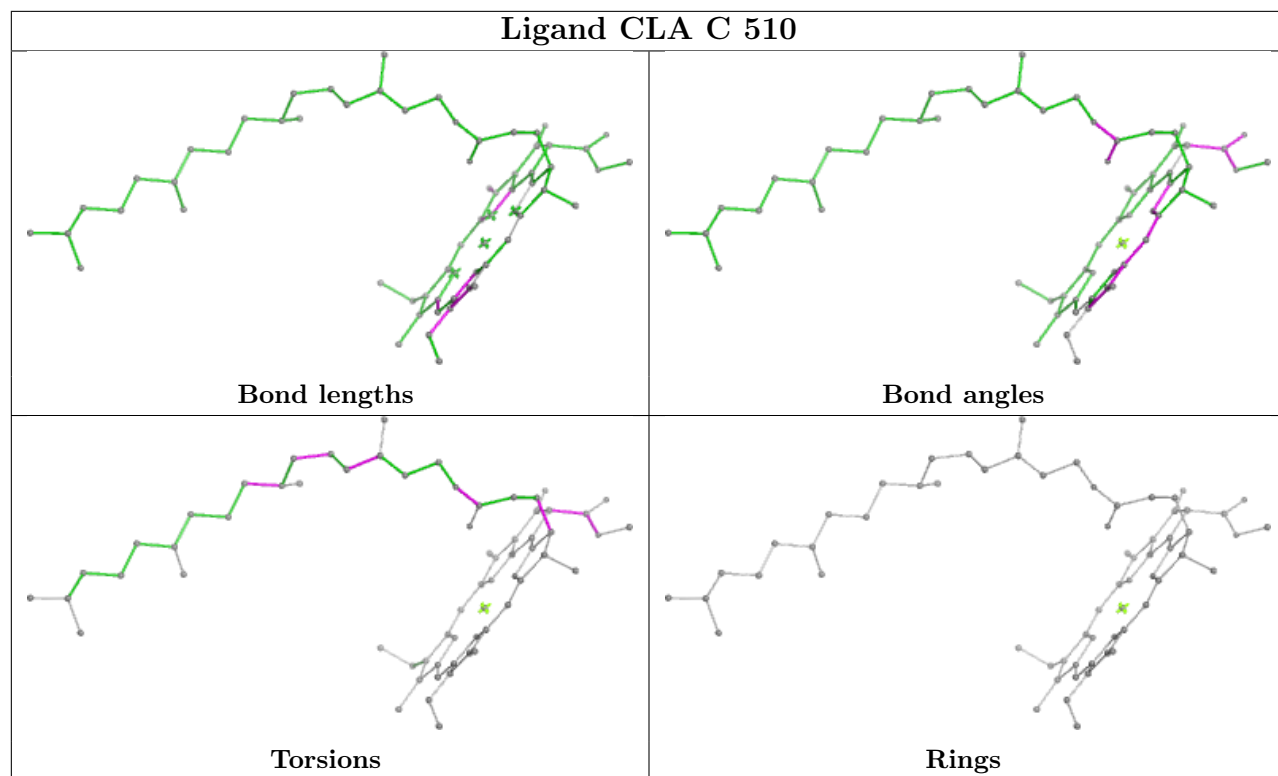


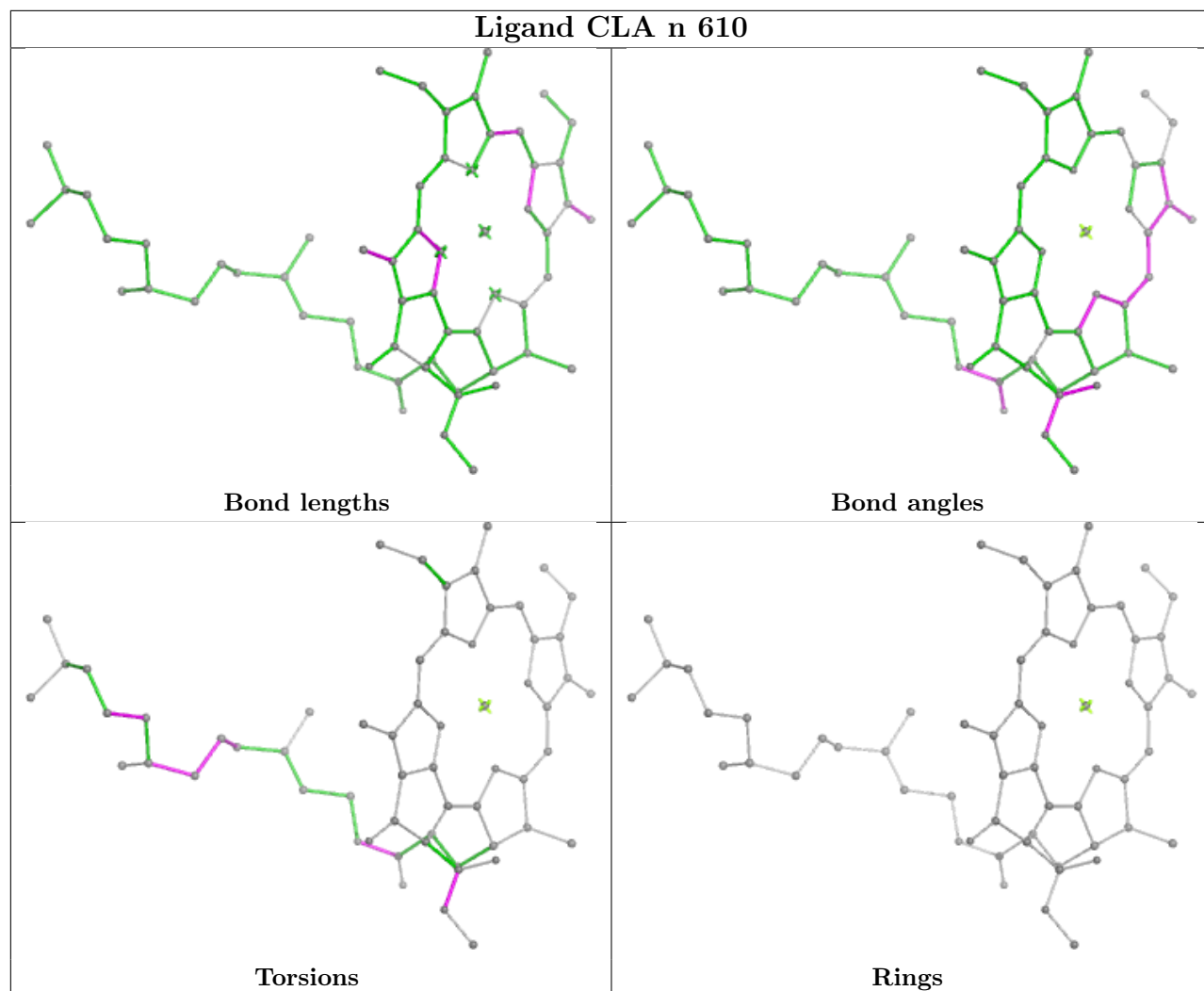
## Ligand CLA c 508

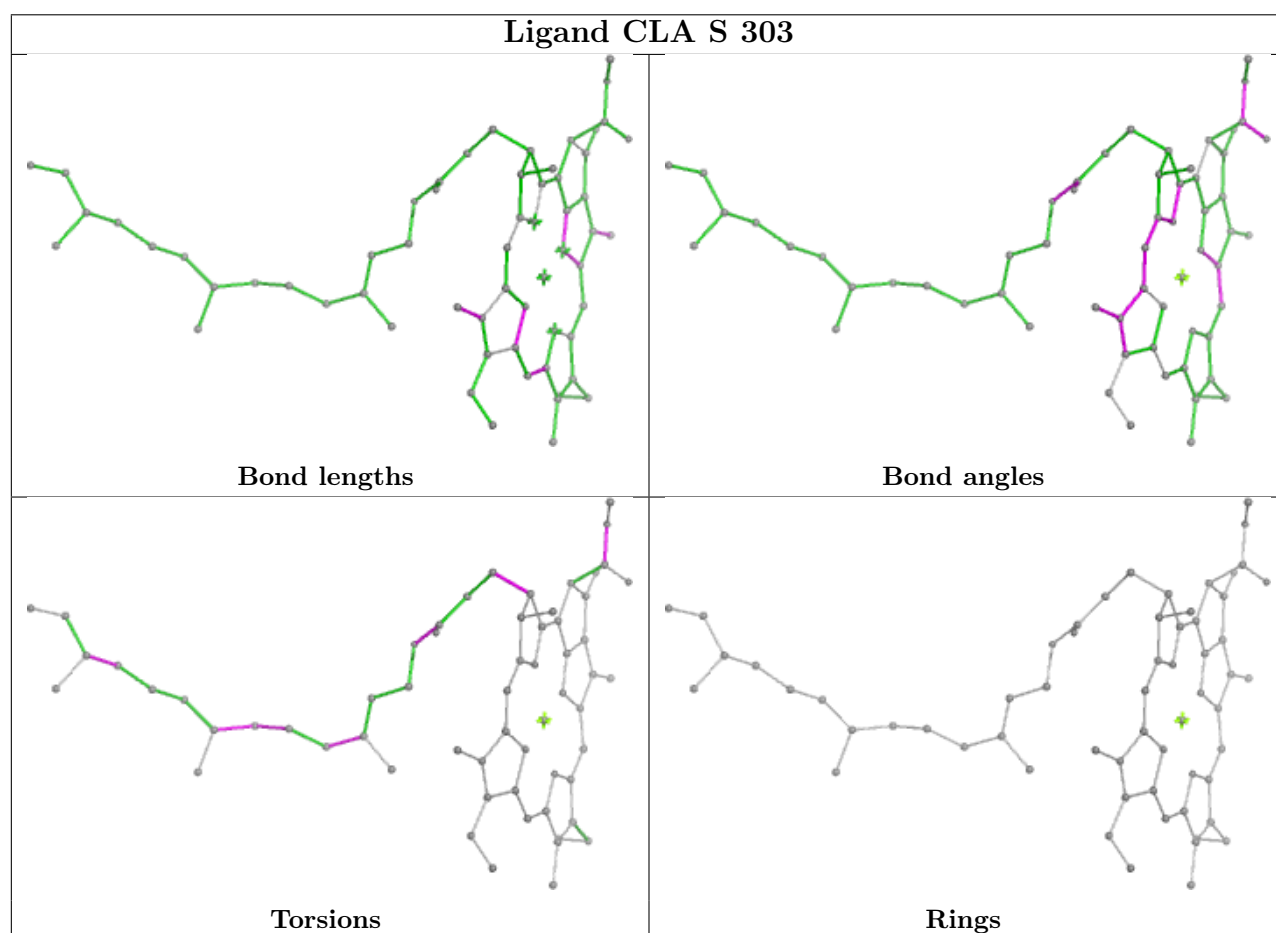
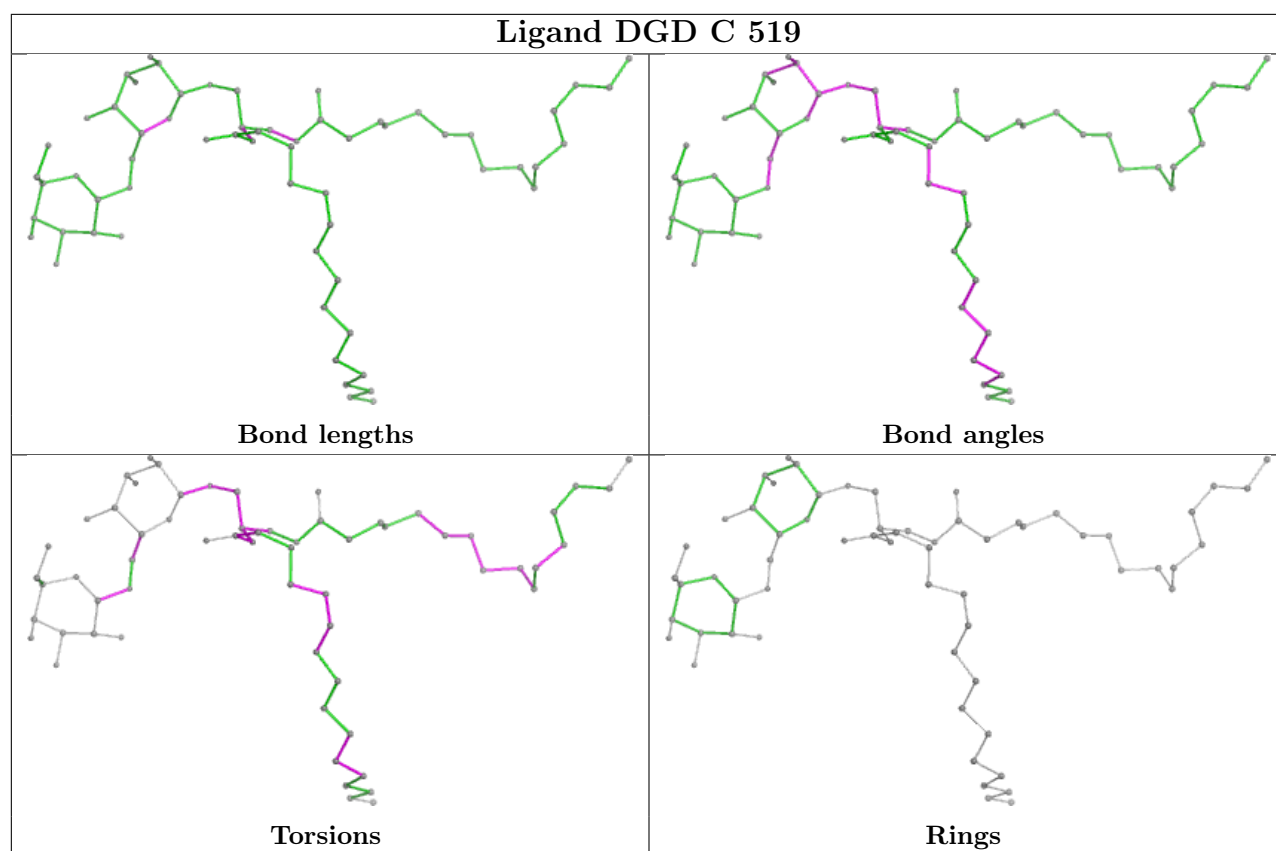




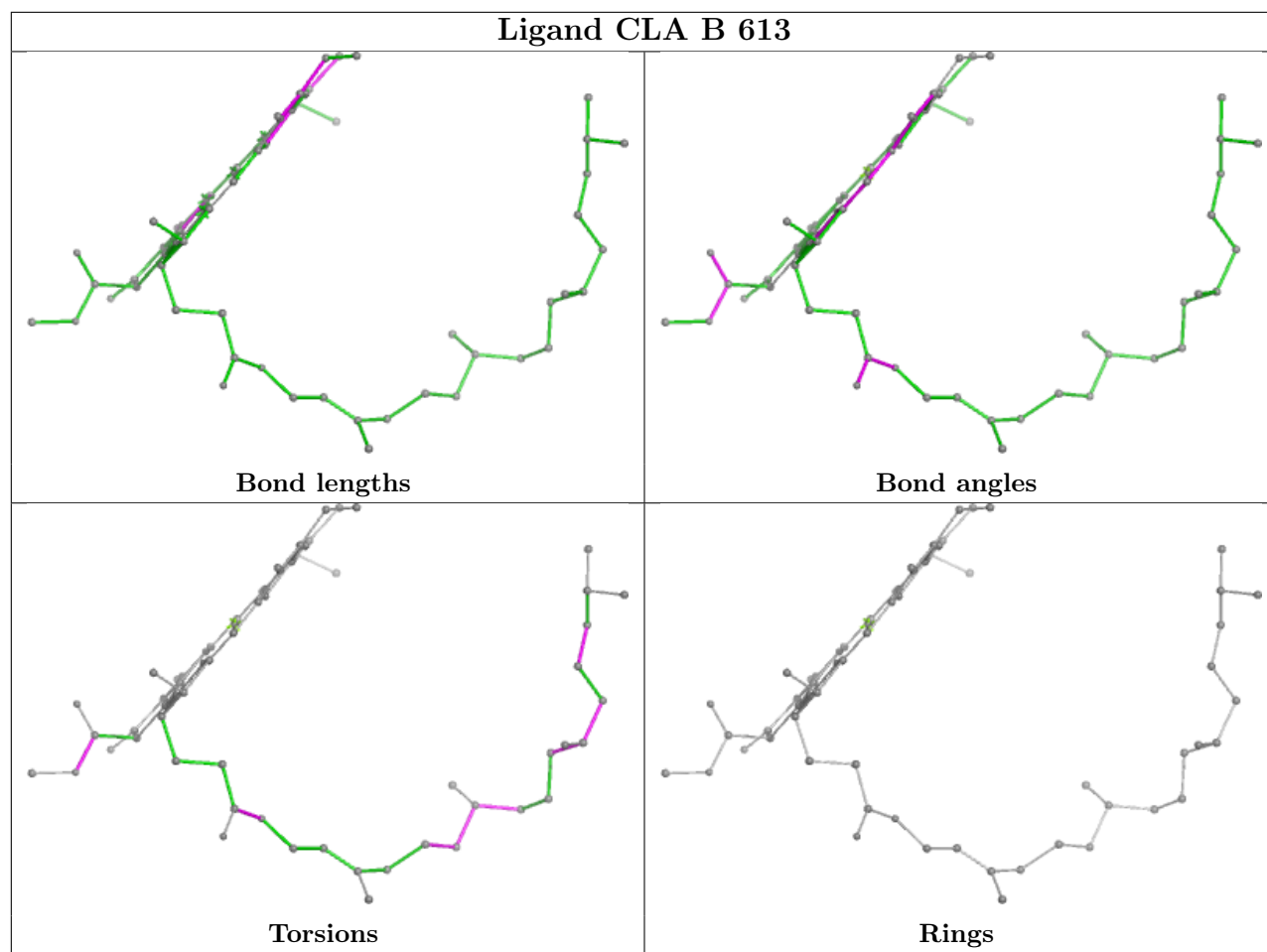
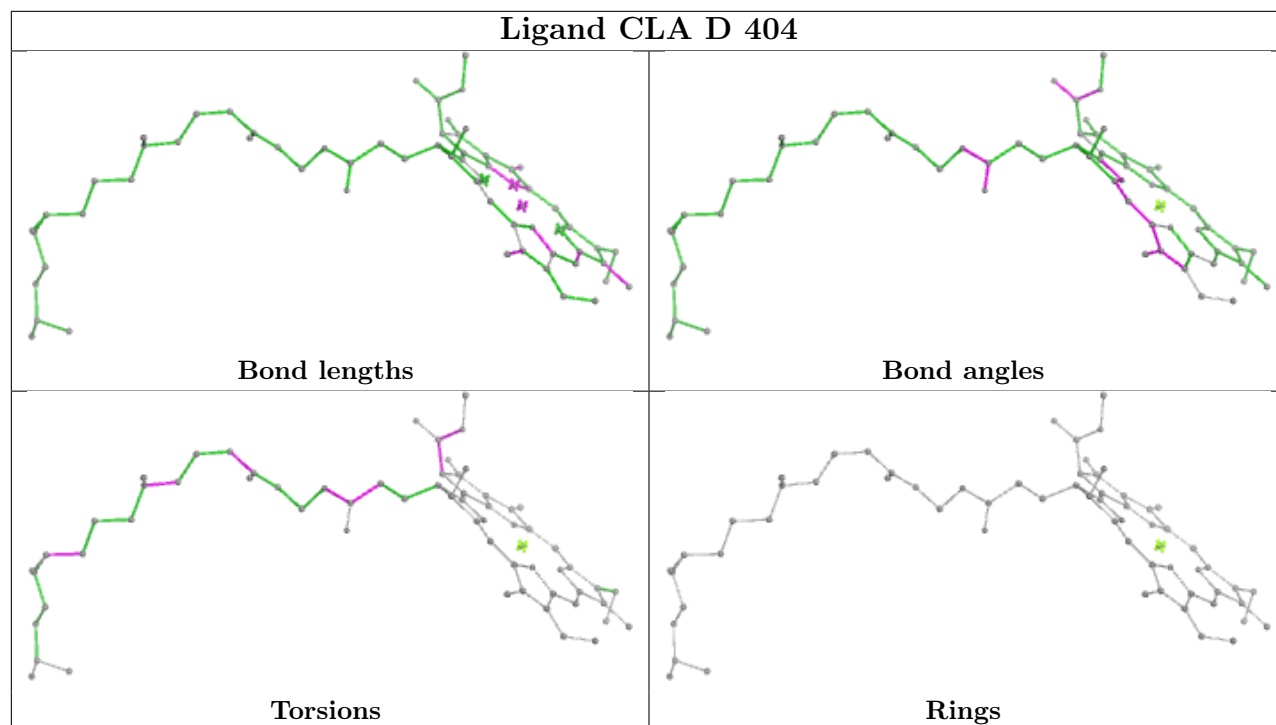


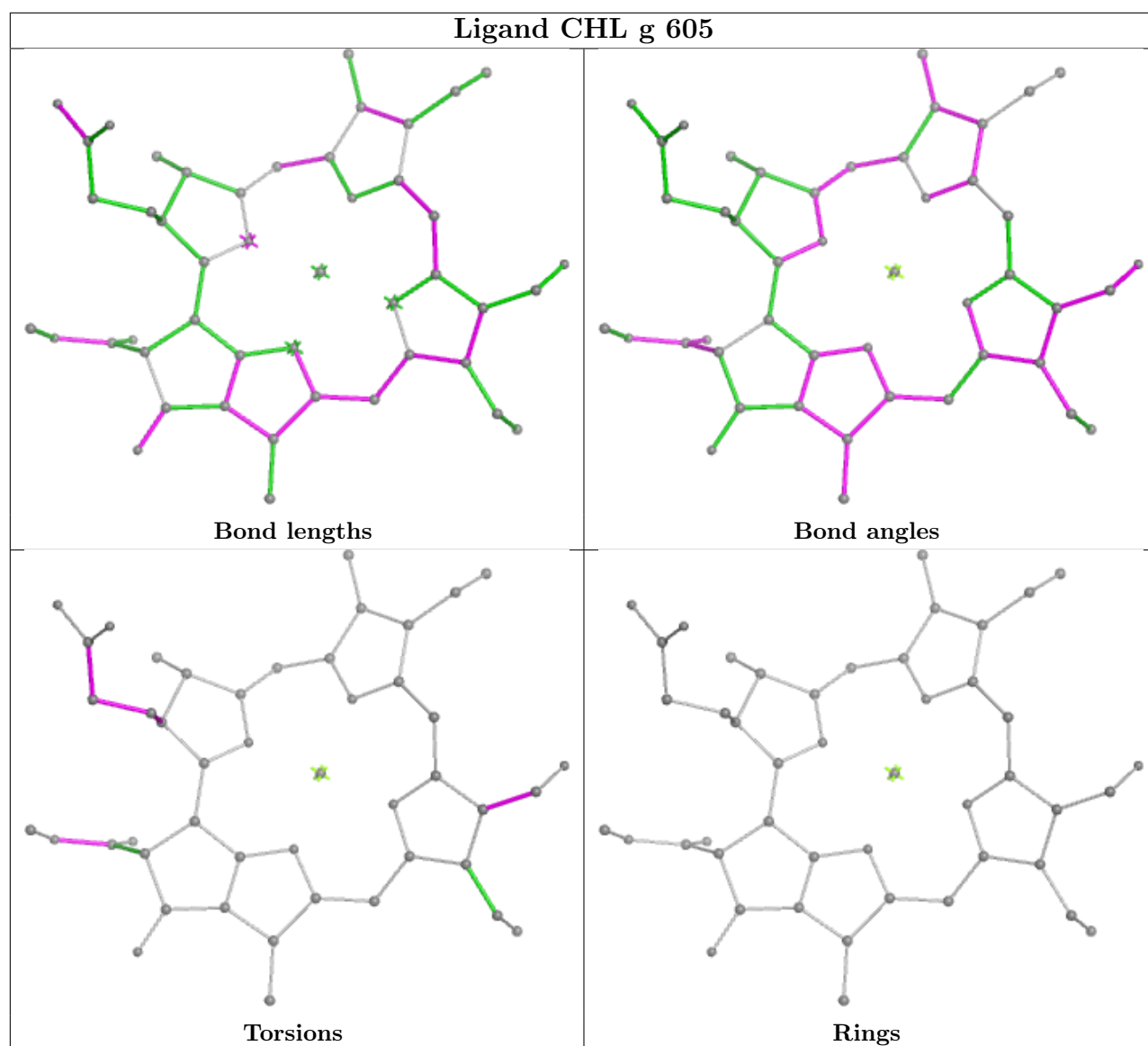












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

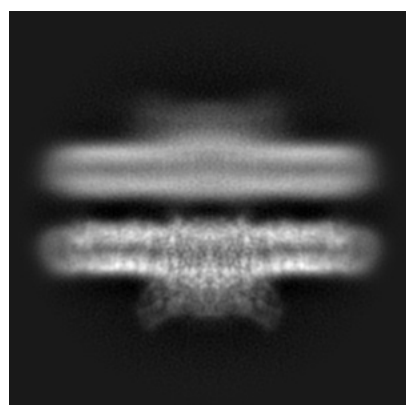
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10865. These allow visual inspection of the internal detail of the map and identification of artifacts.

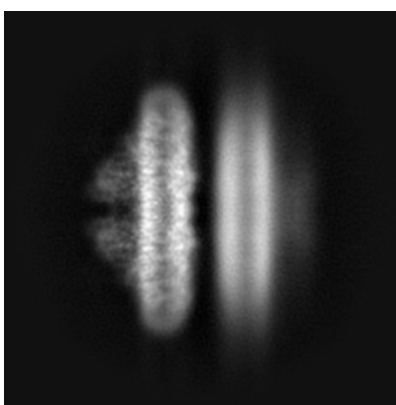
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

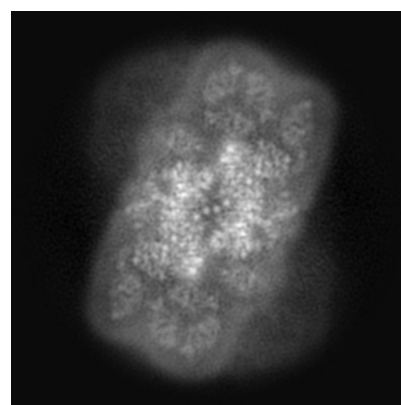
#### 6.1.1 Primary map



X



Y

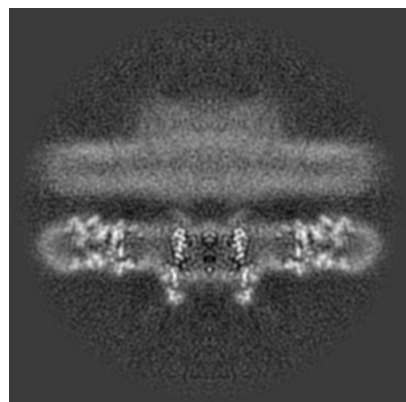


Z

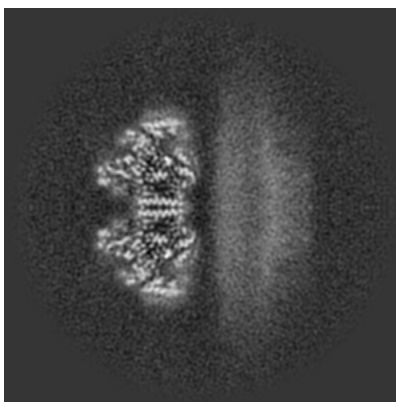
The images above show the map projected in three orthogonal directions.

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

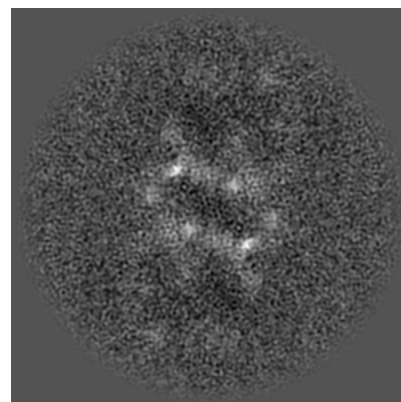
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

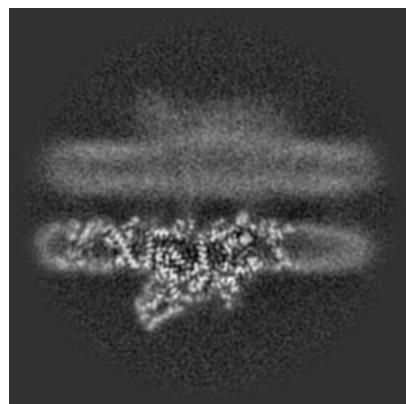


Z Index: 170

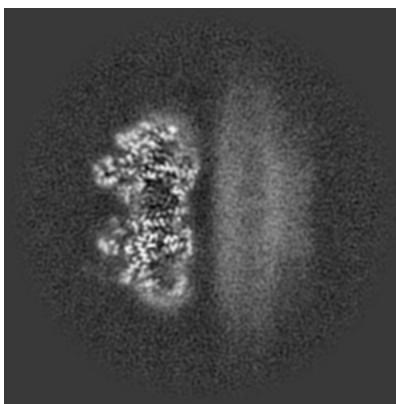
The images above show central slices of the map in three orthogonal directions.

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

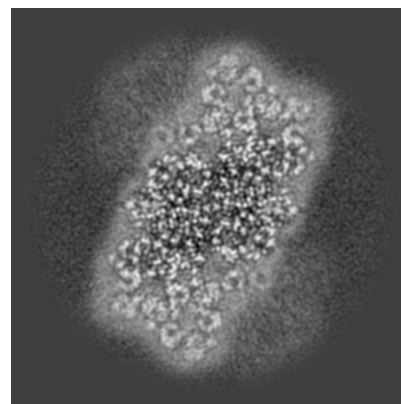
### 6.3.1 Primary map



X Index: 156



Y Index: 166

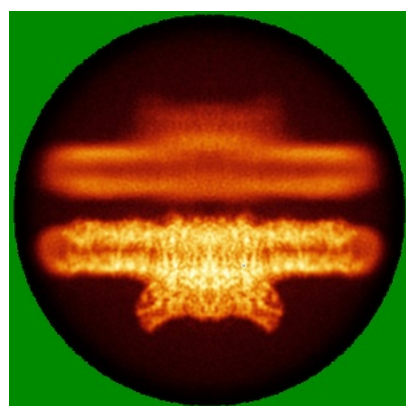


Z Index: 121

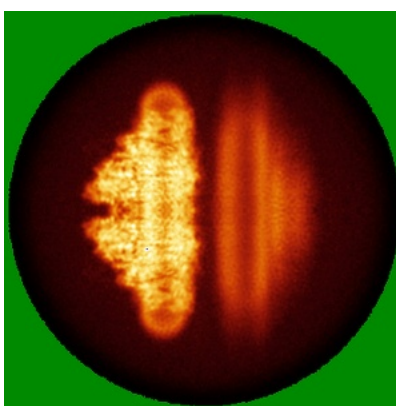
The images above show the largest variance slices of the map in three orthogonal directions.

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

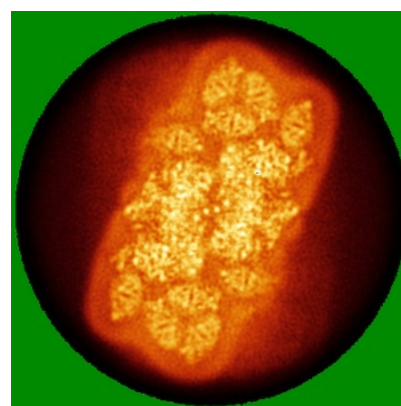
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

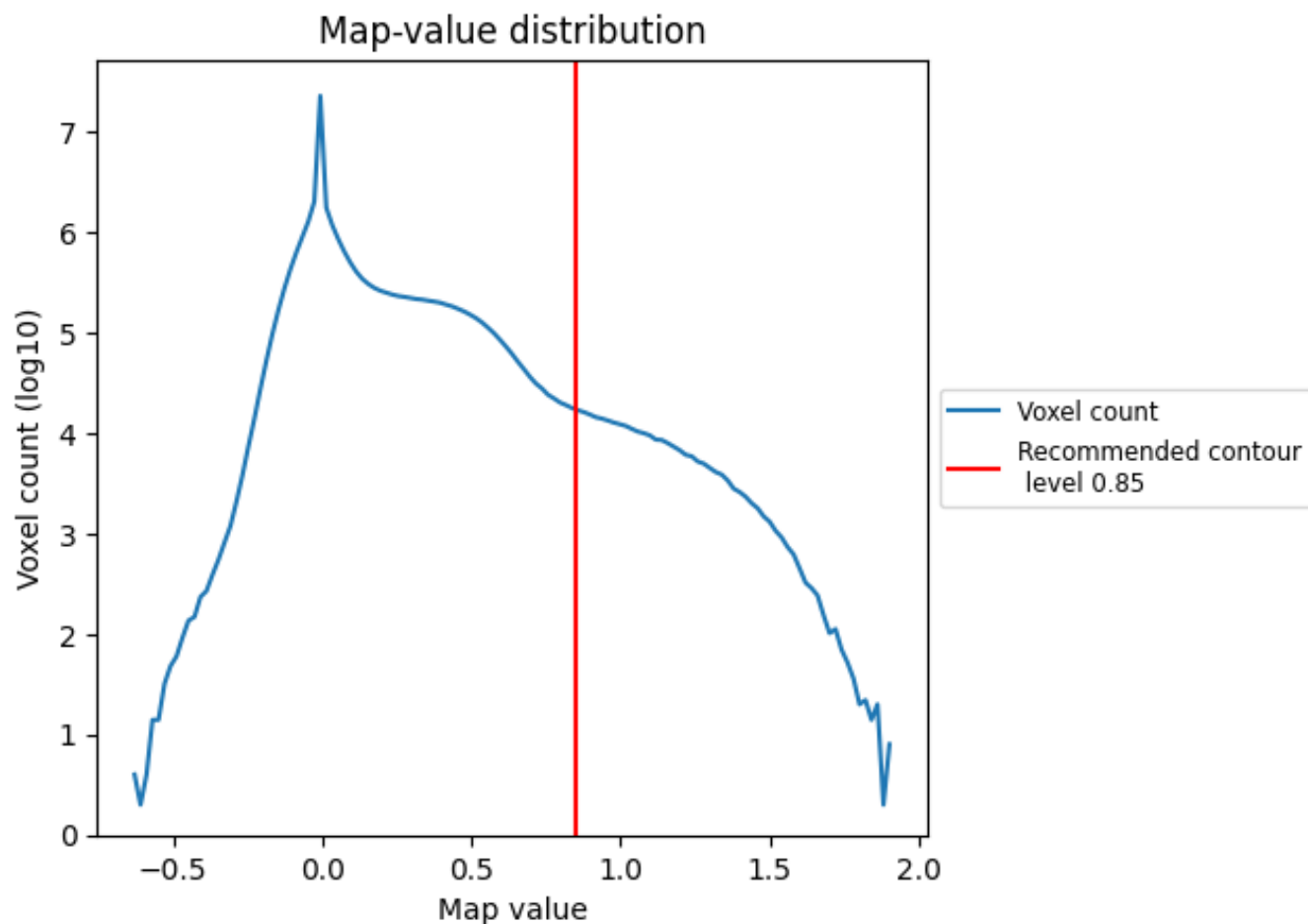
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

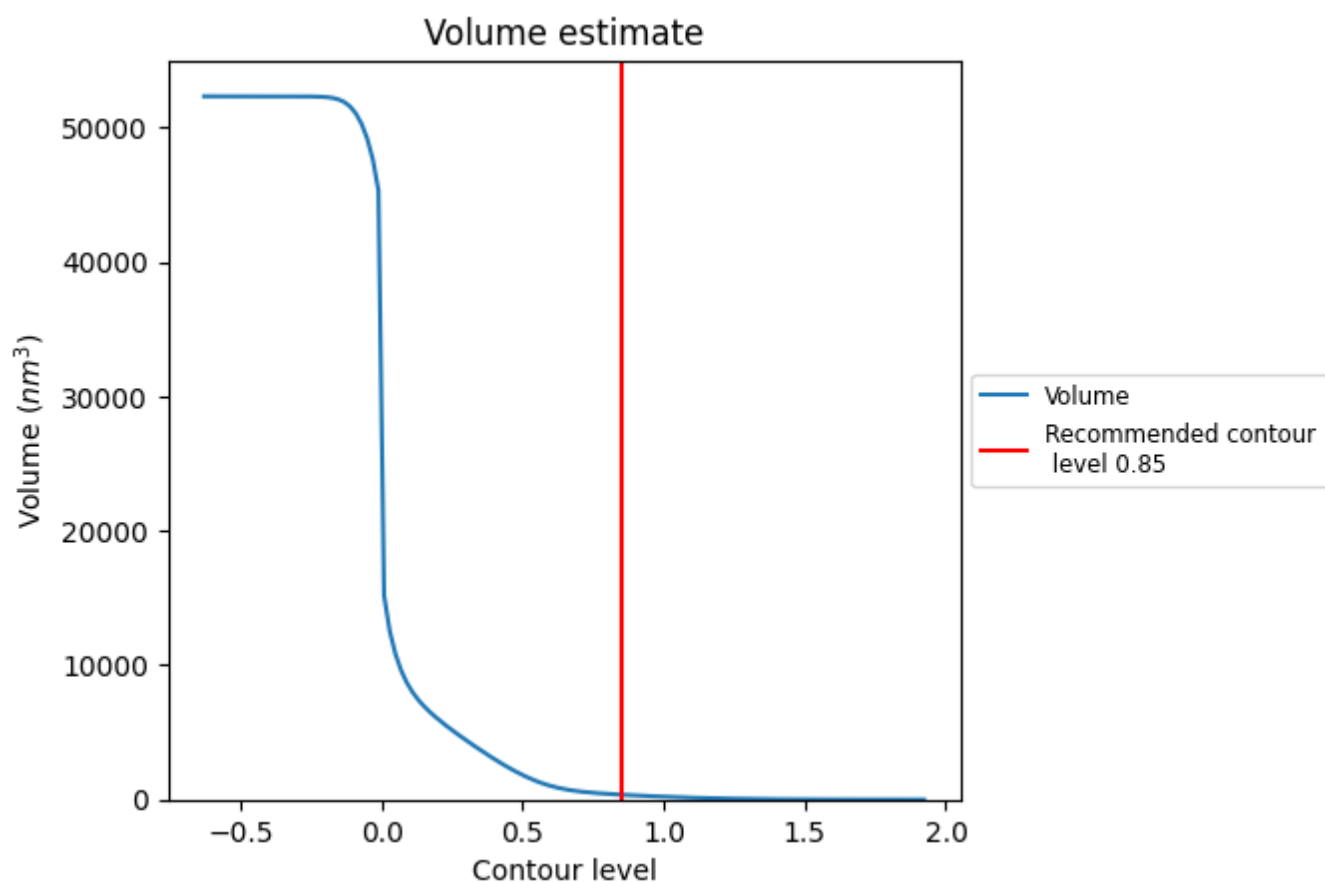
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

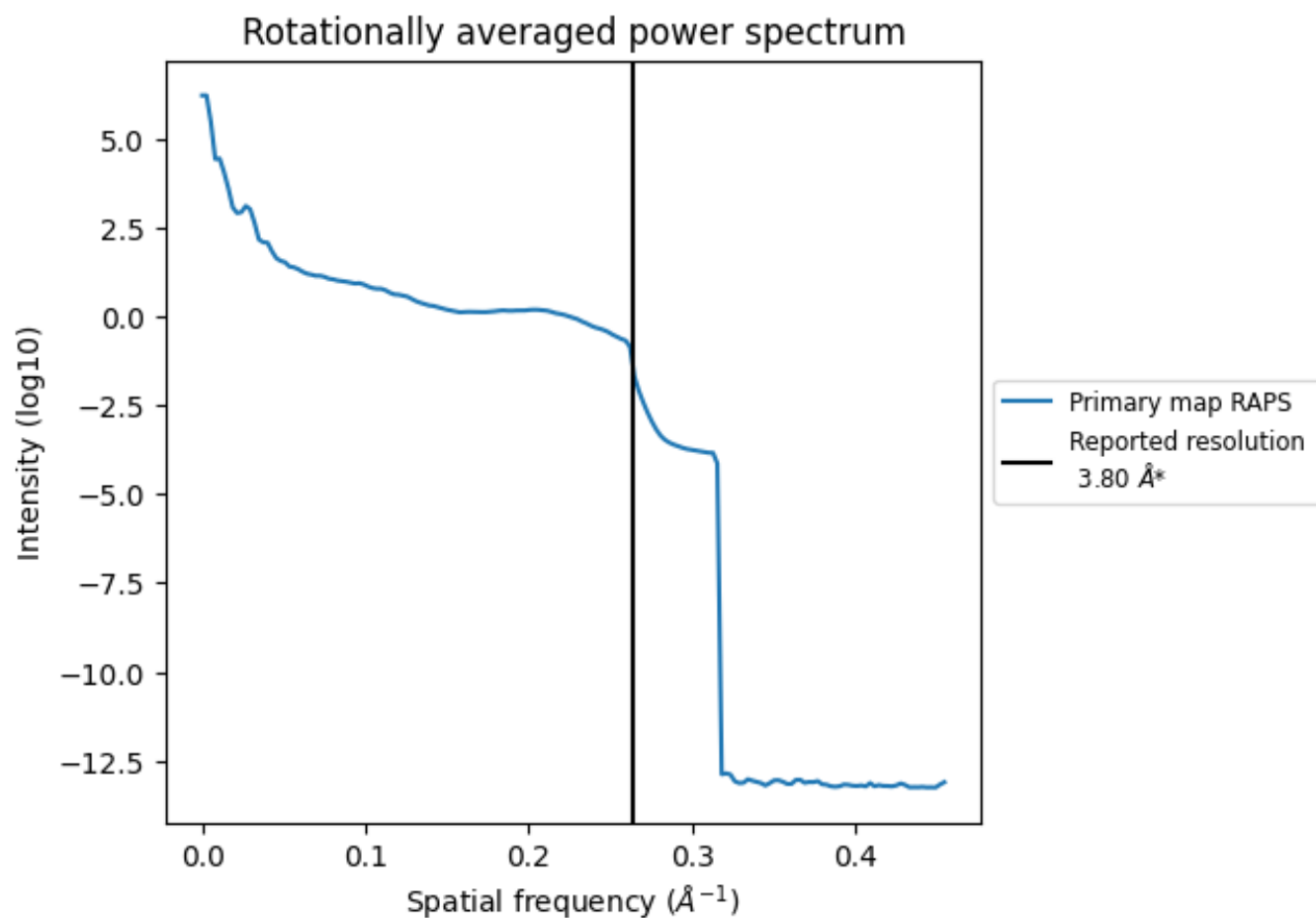
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm<sup>3</sup>; this corresponds to an approximate mass of 325 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>



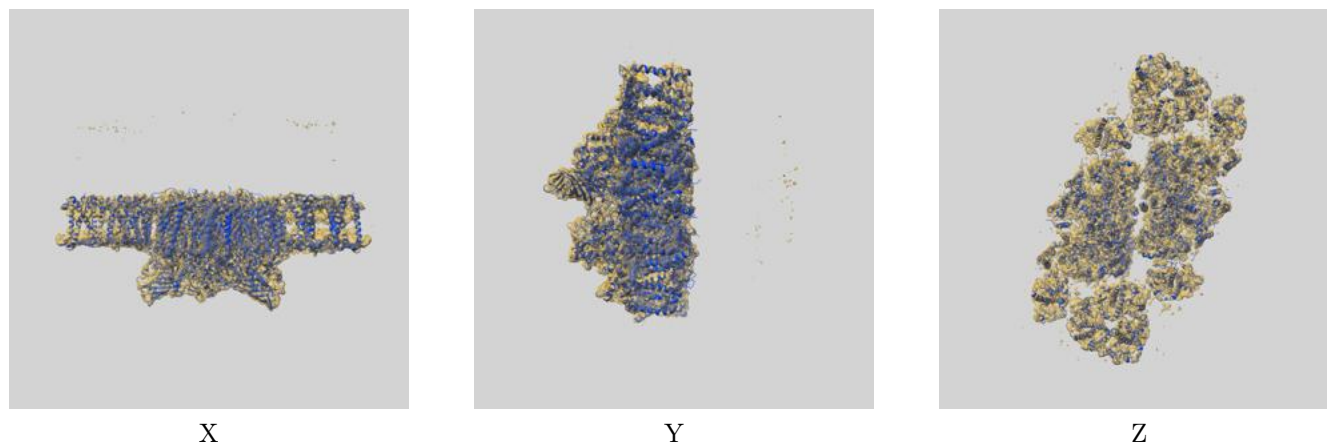
## 8 Fourier-Shell correlation

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

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

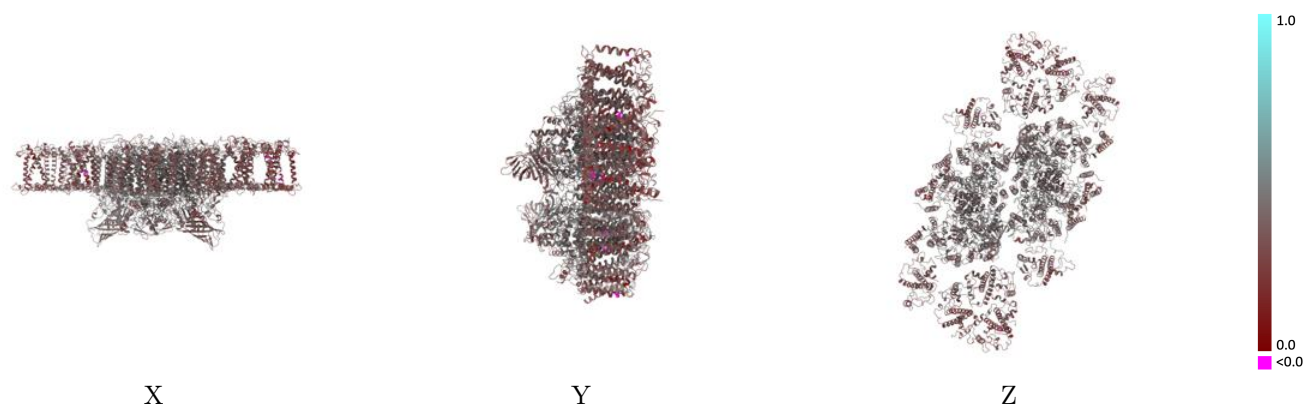
This section contains information regarding the fit between EMDB map EMD-10865 and PDB model 6YP7. Per-residue inclusion information can be found in section [3](#) on page [38](#).

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



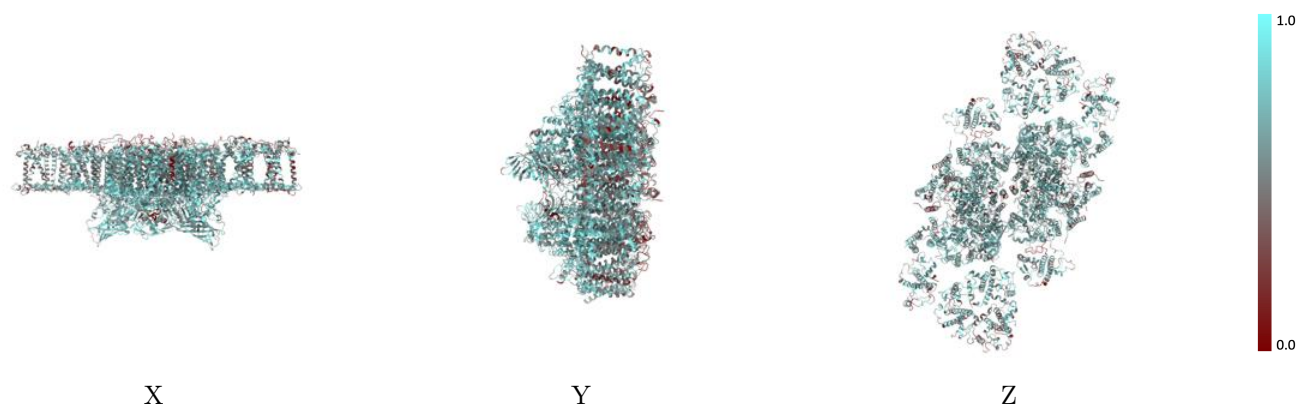
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



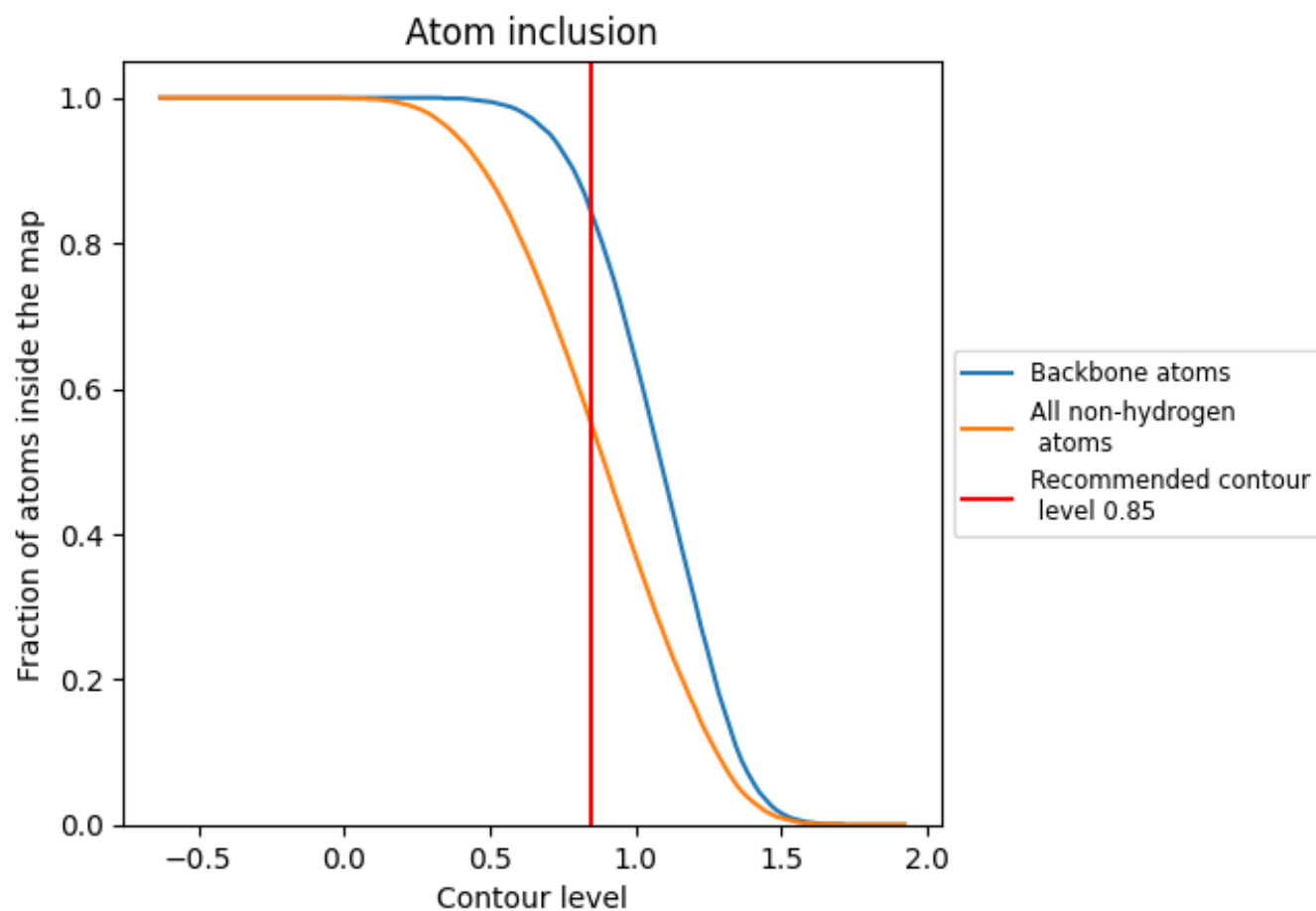
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 55% 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 (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.5490   |  0.3820   |
| A     |  0.6070   |  0.4440   |
| B     |  0.6110   |  0.4330   |
| C     |  0.6010   |  0.4200   |
| D     |  0.5870   |  0.4380   |
| E     |  0.6390   |  0.3060   |
| F     |  0.5960   |  0.3180   |
| G     |  0.4520   |  0.2780   |
| H     |  0.5190   |  0.3920   |
| I     |  0.5270   |  0.4460   |
| J     |  0.2670   |  0.3740   |
| K     |  0.4340   |  0.4020   |
| L     |  0.4010   |  0.4420   |
| M     |  0.3530   |  0.3940   |
| N     |  0.4790  |  0.2880  |
| O     |  0.5690 |  0.4020 |
| R     |  0.4710 |  0.3470 |
| S     |  0.5430 |  0.3340 |
| T     |  0.3670 |  0.4390 |
| W     |  0.4440 |  0.3460 |
| X     |  0.5220 |  0.3380 |
| Y     |  0.5450 |  0.3440 |
| Z     |  0.5280 |  0.3270 |
| a     |  0.6190 |  0.4440 |
| b     |  0.6220 |  0.4350 |
| c     |  0.6050 |  0.4220 |
| d     |  0.5890 |  0.4410 |
| e     |  0.6740 |  0.3500 |
| f     |  0.5960 |  0.3260 |
| g     |  0.4420 |  0.2710 |
| h     |  0.5360 |  0.4140 |
| i     |  0.6040 |  0.4440 |
| j     |  0.2790 |  0.3520 |
| k     |  0.4300 |  0.4000 |
| l     |  0.3950 |  0.4490 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| m     |  0.4160 |  0.3850 |
| n     |  0.4890 |  0.2920 |
| o     |  0.5420 |  0.3560 |
| r     |  0.4680 |  0.3520 |
| s     |  0.5430 |  0.3330 |
| t     |  0.4960 |  0.4360 |
| w     |  0.4700 |  0.4050 |
| x     |  0.5250 |  0.3640 |
| y     |  0.5440 |  0.3470 |
| z     |  0.5410 |  0.3310 |