



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 05:20 pm BST

PDB ID : 7OUI / pdb\_00007oui  
EMDB ID : EMD-13078  
Title : Structure of C2S2M2-type Photosystem supercomplex from *Arabidopsis thaliana* (digitonin-extracted)  
Authors : Graca, A.T.; Hall, M.; Persson, K.; Schroder, W.P.  
Deposited on : 2021-06-11  
Resolution : 2.79 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.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

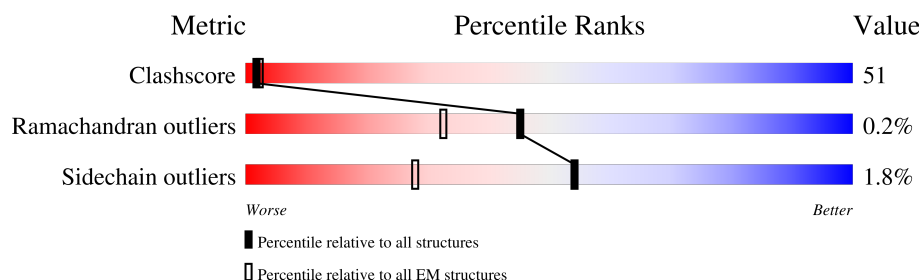
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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.






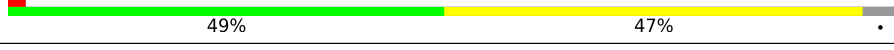




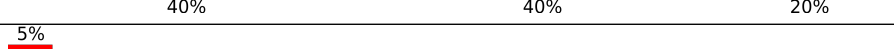
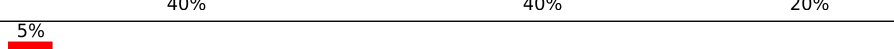
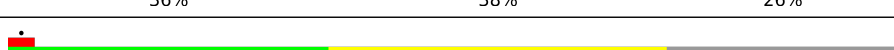
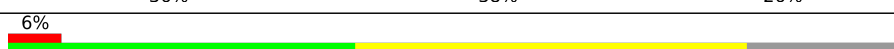
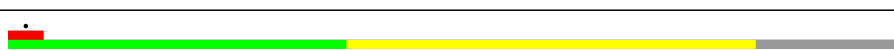
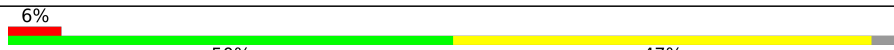
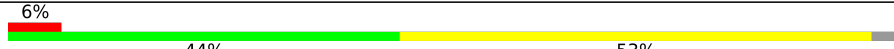
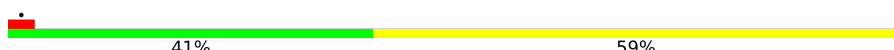
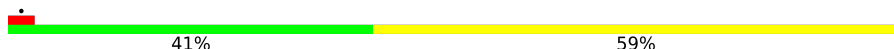



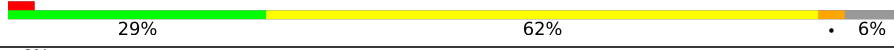

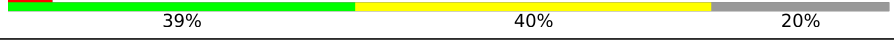


| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | 1     | 266    | <div> <div>76%</div> <div> <div>30%</div> <div>43%</div> <div>24%</div> </div> </div> |
| 1   | 3     | 266    | <div> <div>76%</div> <div> <div>30%</div> <div>43%</div> <div>24%</div> </div> </div> |
| 1   | 5     | 266    | <div> <div>76%</div> <div> <div>30%</div> <div>43%</div> <div>24%</div> </div> </div> |
| 1   | 7     | 266    | <div> <div>76%</div> <div> <div>30%</div> <div>43%</div> <div>24%</div> </div> </div> |
| 2   | 2     | 243    | <div> <div>84%</div> <div> <div>28%</div> <div>56%</div> <div>16%</div> </div> </div> |
| 2   | 6     | 243    | <div> <div>84%</div> <div> <div>28%</div> <div>56%</div> <div>16%</div> </div> </div> |
| 3   | 4     | 212    | <div> <div>92%</div> <div> <div>40%</div> <div>56%</div> <div>.</div> </div> </div>   |
| 3   | 8     | 212    | <div> <div>92%</div> <div> <div>40%</div> <div>56%</div> <div>.</div> </div> </div>   |





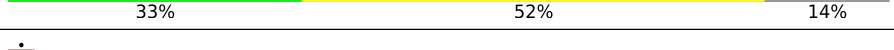
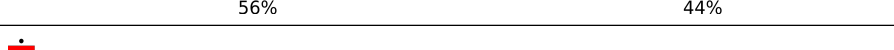
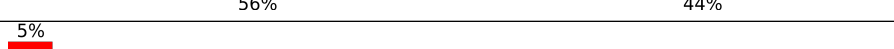
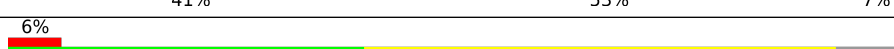
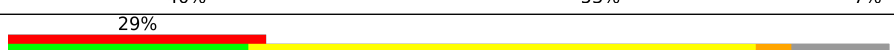
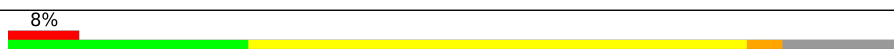
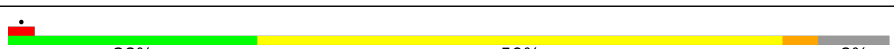
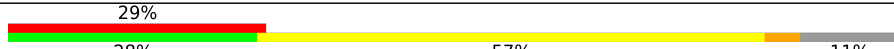
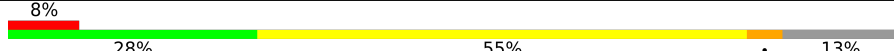
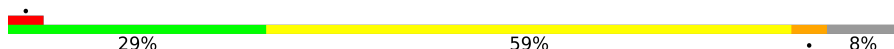




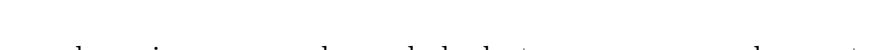
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | A     | 352    |    |
| 4   | a     | 352    |    |
| 5   | B     | 508    |    |
| 5   | b     | 508    |    |
| 6   | C     | 459    |    |
| 6   | c     | 459    |    |
| 7   | D     | 352    |    |
| 7   | d     | 352    |    |
| 8   | E     | 83     |    |
| 8   | e     | 83     |    |
| 9   | F     | 39     |    |
| 9   | f     | 39     |  |
| 10  | H     | 72     |  |
| 10  | h     | 72     |  |
| 11  | I     | 36     |  |
| 11  | i     | 36     |  |
| 12  | K     | 37     |  |
| 12  | k     | 37     |  |
| 13  | L     | 38     |  |
| 13  | l     | 38     |  |
| 14  | M     | 34     |  |
| 14  | m     | 34     |  |
| 15  | O     | 247    |  |
| 15  | o     | 247    |  |
| 16  | T     | 33     |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 16  | t     | 33     |    |
| 17  | W     | 54     |    |
| 17  | w     | 54     |    |
| 18  | X     | 42     |    |
| 18  | x     | 42     |    |
| 19  | Z     | 62     |    |
| 19  | z     | 62     |    |
| 20  | S     | 232    |    |
| 20  | s     | 232    |    |
| 21  | G     | 232    |    |
| 21  | N     | 232    |    |
| 21  | Y     | 232    |  |
| 21  | g     | 232    |  |
| 21  | n     | 232    |  |
| 21  | y     | 232    |  |
| 22  | R     | 250    |  |
| 22  | r     | 250    |  |
| 23  | U     | 28     |  |
| 23  | u     | 28     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CHL  | 1     | 301 | X         | -        | -       | -                |
| 24  | CHL  | 1     | 302 | X         | -        | -       | -                |
| 24  | CHL  | 2     | 601 | X         | -        | -       | -                |
| 24  | CHL  | 2     | 603 | X         | -        | X       | -                |
| 24  | CHL  | 5     | 301 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CHL  | 5     | 302 | X         | -        | -       | -                |
| 24  | CHL  | 6     | 601 | X         | -        | -       | -                |
| 24  | CHL  | 6     | 603 | X         | -        | -       | -                |
| 24  | CHL  | G     | 601 | X         | -        | -       | -                |
| 24  | CHL  | G     | 605 | X         | -        | -       | -                |
| 24  | CHL  | G     | 606 | X         | -        | -       | -                |
| 24  | CHL  | G     | 607 | X         | -        | -       | -                |
| 24  | CHL  | G     | 608 | X         | -        | -       | -                |
| 24  | CHL  | G     | 609 | X         | -        | -       | -                |
| 24  | CHL  | N     | 601 | X         | -        | -       | -                |
| 24  | CHL  | N     | 605 | X         | -        | -       | -                |
| 24  | CHL  | N     | 606 | X         | -        | -       | -                |
| 24  | CHL  | N     | 607 | X         | -        | X       | -                |
| 24  | CHL  | N     | 608 | X         | -        | -       | -                |
| 24  | CHL  | N     | 609 | X         | -        | X       | -                |
| 24  | CHL  | R     | 605 | X         | -        | -       | -                |
| 24  | CHL  | R     | 606 | X         | -        | -       | -                |
| 24  | CHL  | R     | 607 | X         | -        | -       | -                |
| 24  | CHL  | R     | 613 | X         | -        | -       | -                |
| 24  | CHL  | S     | 302 | X         | -        | -       | -                |
| 24  | CHL  | S     | 306 | X         | -        | -       | -                |
| 24  | CHL  | S     | 307 | X         | -        | -       | -                |
| 24  | CHL  | S     | 308 | X         | -        | -       | -                |
| 24  | CHL  | Y     | 302 | X         | -        | X       | -                |
| 24  | CHL  | Y     | 306 | X         | -        | -       | -                |
| 24  | CHL  | Y     | 307 | X         | -        | -       | -                |
| 24  | CHL  | Y     | 308 | X         | -        | -       | -                |
| 24  | CHL  | Y     | 309 | X         | -        | -       | -                |
| 24  | CHL  | Y     | 310 | X         | -        | -       | -                |
| 24  | CHL  | g     | 601 | X         | -        | -       | -                |
| 24  | CHL  | g     | 605 | X         | -        | -       | -                |
| 24  | CHL  | g     | 606 | X         | -        | -       | -                |
| 24  | CHL  | g     | 607 | X         | -        | -       | -                |
| 24  | CHL  | g     | 608 | X         | -        | -       | -                |
| 24  | CHL  | g     | 609 | X         | -        | -       | -                |
| 24  | CHL  | n     | 601 | X         | -        | -       | -                |
| 24  | CHL  | n     | 605 | X         | -        | -       | -                |
| 24  | CHL  | n     | 606 | X         | -        | -       | -                |
| 24  | CHL  | n     | 607 | X         | -        | X       | -                |
| 24  | CHL  | n     | 608 | X         | -        | -       | -                |
| 24  | CHL  | n     | 609 | X         | -        | X       | -                |
| 24  | CHL  | r     | 605 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CHL  | r     | 606 | X         | -        | -       | -                |
| 24  | CHL  | r     | 607 | X         | -        | -       | -                |
| 24  | CHL  | r     | 613 | X         | -        | -       | -                |
| 24  | CHL  | s     | 302 | X         | -        | -       | -                |
| 24  | CHL  | s     | 306 | X         | -        | -       | -                |
| 24  | CHL  | s     | 307 | X         | -        | -       | -                |
| 24  | CHL  | s     | 308 | X         | -        | -       | -                |
| 24  | CHL  | y     | 302 | X         | -        | X       | -                |
| 24  | CHL  | y     | 306 | X         | -        | -       | -                |
| 24  | CHL  | y     | 307 | X         | -        | -       | -                |
| 24  | CHL  | y     | 308 | X         | -        | -       | -                |
| 24  | CHL  | y     | 309 | X         | -        | -       | -                |
| 24  | CHL  | y     | 310 | X         | -        | -       | -                |
| 25  | CLA  | 2     | 602 | X         | -        | -       | -                |
| 25  | CLA  | 2     | 604 | X         | -        | -       | -                |
| 25  | CLA  | 2     | 605 | X         | -        | -       | -                |
| 25  | CLA  | 6     | 602 | X         | -        | -       | -                |
| 25  | CLA  | 6     | 604 | X         | -        | -       | -                |
| 25  | CLA  | 6     | 605 | X         | -        | -       | -                |
| 25  | CLA  | A     | 401 | X         | -        | -       | -                |
| 25  | CLA  | A     | 402 | X         | -        | -       | -                |
| 25  | CLA  | A     | 405 | X         | -        | -       | -                |
| 25  | CLA  | B     | 601 | X         | -        | -       | -                |
| 25  | CLA  | B     | 602 | X         | -        | -       | -                |
| 25  | CLA  | B     | 603 | X         | -        | -       | -                |
| 25  | CLA  | B     | 604 | X         | -        | -       | -                |
| 25  | CLA  | B     | 605 | X         | -        | -       | -                |
| 25  | CLA  | B     | 606 | X         | -        | -       | -                |
| 25  | CLA  | B     | 607 | X         | -        | -       | -                |
| 25  | CLA  | B     | 608 | X         | -        | -       | -                |
| 25  | CLA  | B     | 609 | X         | -        | -       | -                |
| 25  | CLA  | B     | 610 | X         | -        | -       | -                |
| 25  | CLA  | B     | 611 | X         | -        | -       | -                |
| 25  | CLA  | B     | 612 | X         | -        | -       | -                |
| 25  | CLA  | B     | 613 | X         | -        | -       | -                |
| 25  | CLA  | B     | 614 | X         | -        | -       | -                |
| 25  | CLA  | B     | 615 | X         | -        | -       | -                |
| 25  | CLA  | B     | 616 | X         | -        | -       | -                |
| 25  | CLA  | C     | 501 | X         | -        | -       | -                |
| 25  | CLA  | C     | 502 | X         | -        | -       | -                |
| 25  | CLA  | C     | 503 | X         | -        | -       | -                |
| 25  | CLA  | C     | 504 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | C     | 505 | X         | -        | -       | -                |
| 25  | CLA  | C     | 506 | X         | -        | -       | -                |
| 25  | CLA  | C     | 507 | X         | -        | -       | -                |
| 25  | CLA  | C     | 508 | X         | -        | -       | -                |
| 25  | CLA  | C     | 509 | X         | -        | -       | -                |
| 25  | CLA  | C     | 510 | X         | -        | X       | -                |
| 25  | CLA  | C     | 511 | X         | -        | -       | -                |
| 25  | CLA  | C     | 512 | X         | -        | -       | -                |
| 25  | CLA  | C     | 513 | X         | -        | -       | -                |
| 25  | CLA  | D     | 401 | X         | -        | -       | -                |
| 25  | CLA  | D     | 402 | X         | -        | -       | -                |
| 25  | CLA  | D     | 403 | X         | -        | -       | -                |
| 25  | CLA  | G     | 602 | X         | -        | -       | -                |
| 25  | CLA  | G     | 603 | X         | -        | -       | -                |
| 25  | CLA  | G     | 604 | X         | -        | -       | -                |
| 25  | CLA  | G     | 610 | X         | -        | X       | -                |
| 25  | CLA  | G     | 611 | X         | -        | -       | -                |
| 25  | CLA  | G     | 612 | X         | -        | -       | -                |
| 25  | CLA  | G     | 613 | X         | -        | -       | -                |
| 25  | CLA  | G     | 614 | X         | -        | -       | -                |
| 25  | CLA  | N     | 602 | X         | -        | X       | -                |
| 25  | CLA  | N     | 603 | X         | -        | X       | -                |
| 25  | CLA  | N     | 604 | X         | -        | -       | -                |
| 25  | CLA  | N     | 610 | X         | -        | X       | -                |
| 25  | CLA  | N     | 611 | X         | -        | -       | -                |
| 25  | CLA  | N     | 612 | X         | -        | -       | -                |
| 25  | CLA  | N     | 613 | X         | -        | X       | -                |
| 25  | CLA  | N     | 614 | X         | -        | -       | -                |
| 25  | CLA  | R     | 601 | X         | -        | -       | -                |
| 25  | CLA  | R     | 602 | X         | -        | -       | -                |
| 25  | CLA  | R     | 603 | X         | -        | -       | -                |
| 25  | CLA  | R     | 604 | X         | -        | -       | -                |
| 25  | CLA  | R     | 608 | X         | -        | -       | -                |
| 25  | CLA  | R     | 609 | X         | -        | -       | -                |
| 25  | CLA  | R     | 610 | X         | -        | -       | -                |
| 25  | CLA  | R     | 611 | X         | -        | -       | -                |
| 25  | CLA  | R     | 612 | X         | -        | -       | -                |
| 25  | CLA  | R     | 614 | X         | -        | -       | -                |
| 25  | CLA  | S     | 303 | X         | -        | -       | -                |
| 25  | CLA  | S     | 304 | X         | -        | -       | -                |
| 25  | CLA  | S     | 305 | X         | -        | -       | -                |
| 25  | CLA  | S     | 309 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | S     | 310 | X         | -        | -       | -                |
| 25  | CLA  | S     | 311 | X         | -        | -       | -                |
| 25  | CLA  | S     | 312 | X         | -        | -       | -                |
| 25  | CLA  | S     | 313 | X         | -        | -       | -                |
| 25  | CLA  | S     | 314 | X         | -        | -       | -                |
| 25  | CLA  | Y     | 303 | X         | -        | X       | -                |
| 25  | CLA  | Y     | 304 | X         | -        | X       | -                |
| 25  | CLA  | Y     | 305 | X         | -        | -       | -                |
| 25  | CLA  | Y     | 311 | X         | -        | X       | -                |
| 25  | CLA  | Y     | 312 | X         | -        | -       | -                |
| 25  | CLA  | Y     | 313 | X         | -        | -       | -                |
| 25  | CLA  | Y     | 314 | X         | -        | -       | -                |
| 25  | CLA  | Y     | 315 | X         | -        | -       | -                |
| 25  | CLA  | a     | 402 | X         | -        | -       | -                |
| 25  | CLA  | a     | 403 | X         | -        | -       | -                |
| 25  | CLA  | a     | 406 | X         | -        | -       | -                |
| 25  | CLA  | b     | 601 | X         | -        | -       | -                |
| 25  | CLA  | b     | 602 | X         | -        | -       | -                |
| 25  | CLA  | b     | 603 | X         | -        | -       | -                |
| 25  | CLA  | b     | 604 | X         | -        | -       | -                |
| 25  | CLA  | b     | 605 | X         | -        | -       | -                |
| 25  | CLA  | b     | 606 | X         | -        | -       | -                |
| 25  | CLA  | b     | 607 | X         | -        | -       | -                |
| 25  | CLA  | b     | 608 | X         | -        | -       | -                |
| 25  | CLA  | b     | 609 | X         | -        | -       | -                |
| 25  | CLA  | b     | 610 | X         | -        | -       | -                |
| 25  | CLA  | b     | 611 | X         | -        | -       | -                |
| 25  | CLA  | b     | 612 | X         | -        | -       | -                |
| 25  | CLA  | b     | 613 | X         | -        | -       | -                |
| 25  | CLA  | b     | 614 | X         | -        | -       | -                |
| 25  | CLA  | b     | 615 | X         | -        | -       | -                |
| 25  | CLA  | b     | 616 | X         | -        | -       | -                |
| 25  | CLA  | c     | 501 | X         | -        | -       | -                |
| 25  | CLA  | c     | 502 | X         | -        | -       | -                |
| 25  | CLA  | c     | 503 | X         | -        | -       | -                |
| 25  | CLA  | c     | 504 | X         | -        | -       | -                |
| 25  | CLA  | c     | 505 | X         | -        | -       | -                |
| 25  | CLA  | c     | 506 | X         | -        | -       | -                |
| 25  | CLA  | c     | 507 | X         | -        | -       | -                |
| 25  | CLA  | c     | 508 | X         | -        | -       | -                |
| 25  | CLA  | c     | 509 | X         | -        | -       | -                |
| 25  | CLA  | c     | 510 | X         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | c     | 511 | X         | -        | X       | -                |
| 25  | CLA  | c     | 512 | X         | -        | -       | -                |
| 25  | CLA  | c     | 513 | X         | -        | -       | -                |
| 25  | CLA  | d     | 401 | X         | -        | -       | -                |
| 25  | CLA  | d     | 402 | X         | -        | -       | -                |
| 25  | CLA  | d     | 403 | X         | -        | -       | -                |
| 25  | CLA  | g     | 602 | X         | -        | -       | -                |
| 25  | CLA  | g     | 603 | X         | -        | -       | -                |
| 25  | CLA  | g     | 604 | X         | -        | -       | -                |
| 25  | CLA  | g     | 610 | X         | -        | X       | -                |
| 25  | CLA  | g     | 611 | X         | -        | -       | -                |
| 25  | CLA  | g     | 612 | X         | -        | -       | -                |
| 25  | CLA  | g     | 613 | X         | -        | -       | -                |
| 25  | CLA  | g     | 614 | X         | -        | -       | -                |
| 25  | CLA  | n     | 602 | X         | -        | X       | -                |
| 25  | CLA  | n     | 603 | X         | -        | X       | -                |
| 25  | CLA  | n     | 604 | X         | -        | -       | -                |
| 25  | CLA  | n     | 610 | X         | -        | X       | -                |
| 25  | CLA  | n     | 611 | X         | -        | -       | -                |
| 25  | CLA  | n     | 612 | X         | -        | -       | -                |
| 25  | CLA  | n     | 613 | X         | -        | X       | -                |
| 25  | CLA  | n     | 614 | X         | -        | -       | -                |
| 25  | CLA  | r     | 601 | X         | -        | -       | -                |
| 25  | CLA  | r     | 602 | X         | -        | -       | -                |
| 25  | CLA  | r     | 603 | X         | -        | -       | -                |
| 25  | CLA  | r     | 604 | X         | -        | -       | -                |
| 25  | CLA  | r     | 608 | X         | -        | -       | -                |
| 25  | CLA  | r     | 609 | X         | -        | -       | -                |
| 25  | CLA  | r     | 610 | X         | -        | -       | -                |
| 25  | CLA  | r     | 611 | X         | -        | -       | -                |
| 25  | CLA  | r     | 612 | X         | -        | -       | -                |
| 25  | CLA  | r     | 614 | X         | -        | -       | -                |
| 25  | CLA  | s     | 303 | X         | -        | -       | -                |
| 25  | CLA  | s     | 304 | X         | -        | -       | -                |
| 25  | CLA  | s     | 305 | X         | -        | -       | -                |
| 25  | CLA  | s     | 309 | X         | -        | -       | -                |
| 25  | CLA  | s     | 310 | X         | -        | -       | -                |
| 25  | CLA  | s     | 311 | X         | -        | -       | -                |
| 25  | CLA  | s     | 312 | X         | -        | -       | -                |
| 25  | CLA  | s     | 313 | X         | -        | -       | -                |
| 25  | CLA  | s     | 314 | X         | -        | -       | -                |
| 25  | CLA  | y     | 303 | X         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | y     | 304 | X         | -        | -       | -                |
| 25  | CLA  | y     | 305 | X         | -        | -       | -                |
| 25  | CLA  | y     | 311 | X         | -        | X       | -                |
| 25  | CLA  | y     | 312 | X         | -        | -       | -                |
| 25  | CLA  | y     | 313 | X         | -        | -       | -                |
| 25  | CLA  | y     | 314 | X         | -        | -       | -                |
| 25  | CLA  | y     | 315 | X         | -        | -       | -                |
| 28  | BCR  | t     | 101 | -         | -        | X       | -                |
| 32  | AJP  | A     | 412 | X         | -        | -       | -                |
| 32  | AJP  | B     | 624 | X         | -        | -       | -                |
| 32  | AJP  | G     | 618 | X         | -        | -       | -                |
| 32  | AJP  | N     | 619 | X         | -        | -       | -                |
| 32  | AJP  | N     | 620 | X         | -        | -       | -                |
| 32  | AJP  | S     | 319 | X         | -        | -       | -                |
| 32  | AJP  | Y     | 320 | X         | -        | -       | -                |
| 32  | AJP  | Y     | 321 | X         | -        | -       | -                |
| 32  | AJP  | Y     | 322 | X         | -        | -       | -                |
| 32  | AJP  | Y     | 323 | X         | -        | -       | -                |
| 32  | AJP  | Y     | 324 | X         | -        | -       | -                |
| 32  | AJP  | a     | 413 | X         | -        | -       | -                |
| 32  | AJP  | b     | 624 | X         | -        | -       | -                |
| 32  | AJP  | g     | 618 | X         | -        | -       | -                |
| 32  | AJP  | n     | 619 | X         | -        | -       | -                |
| 32  | AJP  | n     | 620 | X         | -        | -       | -                |
| 32  | AJP  | s     | 319 | X         | -        | -       | -                |
| 32  | AJP  | y     | 320 | X         | -        | -       | -                |
| 32  | AJP  | y     | 321 | X         | -        | -       | -                |
| 32  | AJP  | y     | 322 | X         | -        | -       | -                |
| 32  | AJP  | y     | 323 | X         | -        | -       | -                |
| 32  | AJP  | y     | 324 | X         | -        | -       | -                |
| 33  | BCT  | A     | 413 | -         | -        | X       | -                |
| 39  | LUT  | s     | 316 | -         | -        | X       | -                |
| 41  | XAT  | r     | 616 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 85897 atoms, of which 1470 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, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 996 | 250 | 286 | 5 |         |       |
| 1   | 3     | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 996 | 250 | 286 | 5 |         |       |
| 1   | 5     | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 996 | 250 | 286 | 5 |         |       |
| 1   | 7     | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 996 | 250 | 286 | 5 |         |       |

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1593  | 1040 | 258 | 290 | 5 |         |       |
| 2   | 6     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1593  | 1040 | 258 | 290 | 5 |         |       |

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 4     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1597  | 1048 | 262 | 283 | 4 |         |       |
| 3   | 8     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1597  | 1048 | 262 | 283 | 4 |         |       |

- Molecule 4 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | A     | 326      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2548  | 1664 | 419 | 452 | 13 |         |       |
| 4   | a     | 326      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2548  | 1664 | 419 | 452 | 13 |         |       |

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | B     | 487      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3810  | 2495 | 644 | 659 | 12 |         |       |
| 5   | b     | 487      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3810  | 2495 | 644 | 659 | 12 |         |       |

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | C     | 433      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3373  | 2221 | 563 | 578 | 11 |         |       |
| 6   | c     | 433      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3373  | 2221 | 563 | 578 | 11 |         |       |

- Molecule 7 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | D     | 342      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2722  | 1800 | 445 | 465 | 12 |         |       |
| 7   | d     | 342      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2722  | 1800 | 445 | 465 | 12 |         |       |

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 8   | E     | 66       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 543   | 357 | 88 | 98 |         |       |
| 8   | e     | 66       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 543   | 357 | 88 | 98 |         |       |

- Molecule 9 is a protein called Cytochrome b559 subunit beta (PsbF).

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | F     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 224   | 147 | 40 | 36 | 1 |         |       |
| 9   | f     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 224   | 147 | 40 | 36 | 1 |         |       |

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



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | H     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 293 | 70 | 81 | 2 |         |       |
| 10  | h     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 293 | 70 | 81 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | I     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 286   | 195 | 44 | 46 | 1 |         |       |
| 11  | i     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 286   | 195 | 44 | 46 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | K     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 211 | 44 | 45 | 1 |         |       |
| 12  | k     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 211 | 44 | 45 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | L     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 200 | 47 | 55 |   |         |       |
| 13  | l     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 200 | 47 | 55 |   |         |       |

- Molecule 14 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | M     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 250   | 173 | 35 | 41 | 1 |         |       |
| 14  | m     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 250   | 173 | 35 | 41 | 1 |         |       |

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 969 | 241 | 302 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | o     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 969 | 241 | 302 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | T     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 168 | 33 | 37 | 1 |         |       |
| 16  | t     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 168 | 33 | 37 | 1 |         |       |

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | W     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 282 | 61 | 83 | 1 |         |       |
| 17  | w     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 282 | 61 | 83 | 1 |         |       |

- Molecule 18 is a protein called (thale cress) hypothetical protein.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 18  | X     | 36       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 248   | 162 | 39 | 47 |  |         |       |
| 18  | x     | 36       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 248   | 162 | 39 | 47 |  |         |       |

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 313 | 69 | 81 | 1 |         |       |
| 19  | z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 313 | 69 | 81 | 1 |         |       |

- Molecule 20 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | S     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1670  | 1091 | 272 | 303 | 4 |         |       |
| 20  | s     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1670  | 1091 | 272 | 303 | 4 |         |       |

- Molecule 21 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | G     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1562  | 1010 | 255 | 292 | 5 |         |       |
| 21  | N     | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1536  | 994  | 251 | 286 | 5 |         |       |
| 21  | Y     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1621  | 1048 | 266 | 302 | 5 |         |       |
| 21  | g     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1562  | 1010 | 255 | 292 | 5 |         |       |
| 21  | n     | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1536  | 994  | 251 | 286 | 5 |         |       |
| 21  | y     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1621  | 1048 | 266 | 302 | 5 |         |       |

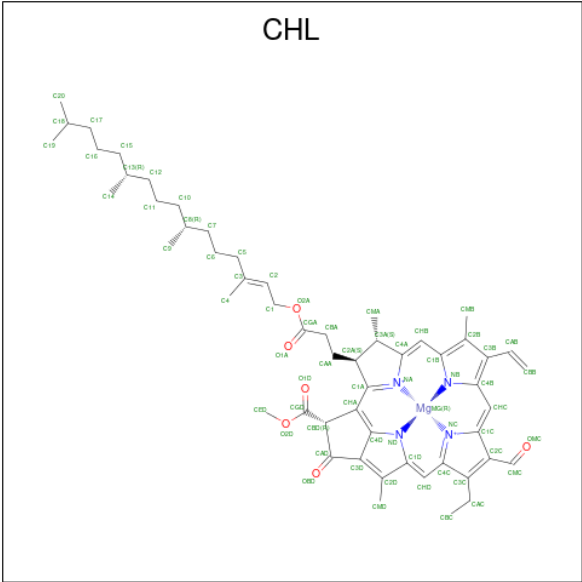
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | R     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1183 | 298 | 343 | 3 |         |       |
| 22  | r     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1183 | 298 | 343 | 3 |         |       |

- Molecule 23 is a protein called Photosystem II 5 kDa protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | U     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 194   | 122 | 36 | 33 | 3 |         |       |
| 23  | u     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 194   | 122 | 36 | 33 | 3 |         |       |

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24  | 1     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | 1     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | 2     | 1        | Total<br>64 | C<br>53 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | 2     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 24  | G     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 39 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 24  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 24  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 24  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 53 | 1  | 4 | 6 |         |
| 24  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |

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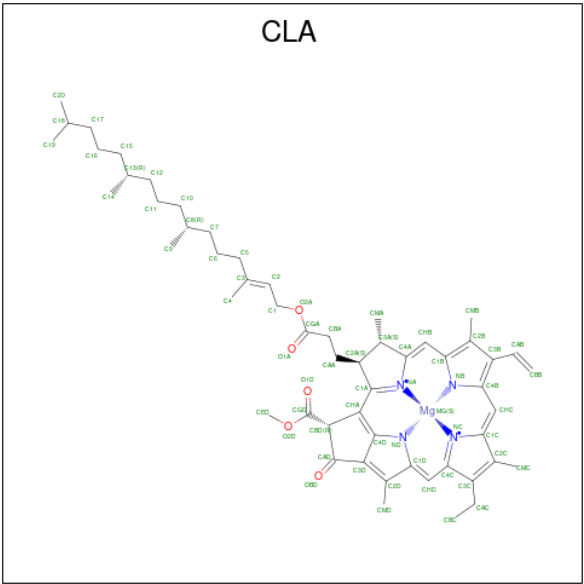
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 24  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 39 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 39 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 24  | y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 24  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 24  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 24  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |

- Molecule 25 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 25  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | D     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | S     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | G     | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | Y     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | R     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 6     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | s     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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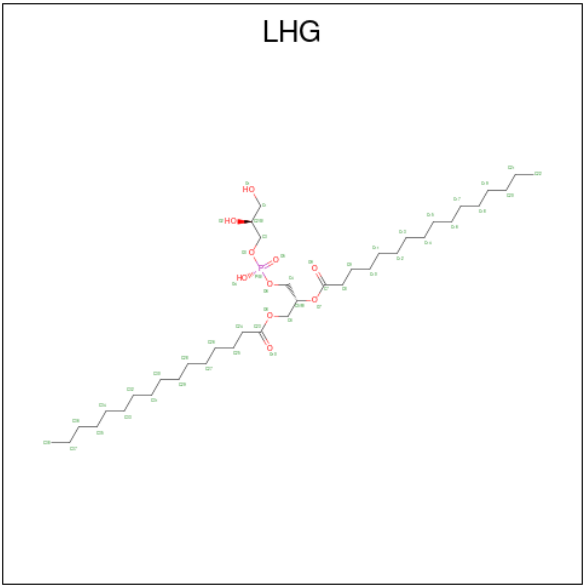
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 25  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | g     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | n     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | y     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | r     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 25  | r     | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 25  | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- 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  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms        |         |         |                   |   | AltConf |
|-----|-------|----------|--------------|---------|---------|-------------------|---|---------|
| 26  | B     | 1        | Total<br>46  | C<br>35 | O<br>10 | P<br>1            | 0 |         |
| 26  | C     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | C     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | C     | 1        | Total<br>123 | C<br>38 | H<br>74 | O<br>10<br>P<br>1 | 0 |         |
| 26  | D     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | L     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | S     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | S     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | N     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | Y     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | Y     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | R     | 1        | Total<br>42  | C<br>31 | O<br>10 | P<br>1            | 0 |         |
| 26  | 6     | 1        | Total<br>47  | C<br>36 | O<br>10 | P<br>1            | 0 |         |
| 26  | b     | 1        | Total<br>47  | C<br>36 | O<br>10 | P<br>1            | 0 |         |
| 26  | b     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | b     | 1        | Total<br>46  | C<br>35 | O<br>10 | P<br>1            | 0 |         |
| 26  | c     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | c     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | c     | 1        | Total<br>123 | C<br>38 | H<br>74 | O<br>10<br>P<br>1 | 0 |         |
| 26  | d     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |
| 26  | l     | 1        | Total<br>49  | C<br>38 | O<br>10 | P<br>1            | 0 |         |

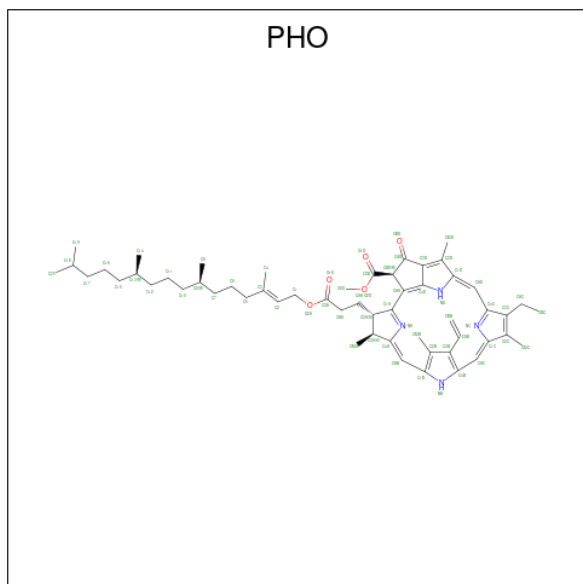
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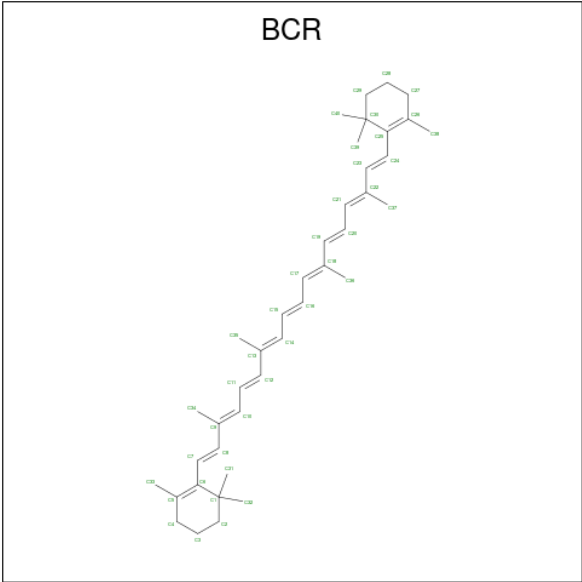
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | s     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | s     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 27  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 27  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



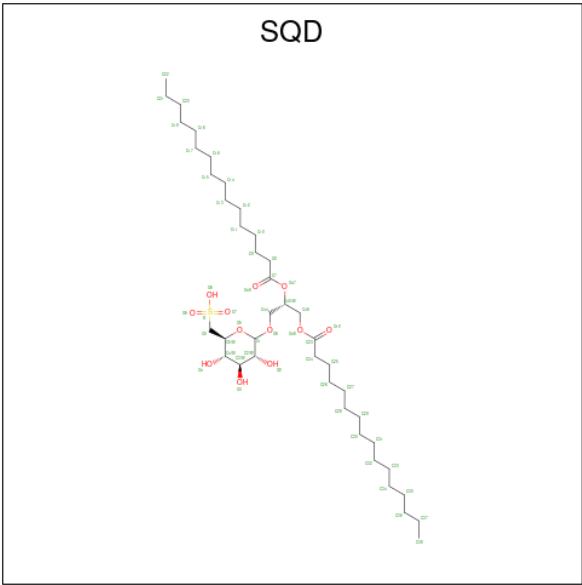
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | D     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | H     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | I     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | K     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | T     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | Z     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | a     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 28  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 28  | b     | 1        | Total C<br>40 40 | 0       |
| 28  | c     | 1        | Total C<br>40 40 | 0       |
| 28  | d     | 1        | Total C<br>40 40 | 0       |
| 28  | h     | 1        | Total C<br>40 40 | 0       |
| 28  | i     | 1        | Total C<br>40 40 | 0       |
| 28  | k     | 1        | Total C<br>40 40 | 0       |
| 28  | t     | 1        | Total C<br>40 40 | 0       |
| 28  | z     | 1        | Total C<br>40 40 | 0       |

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



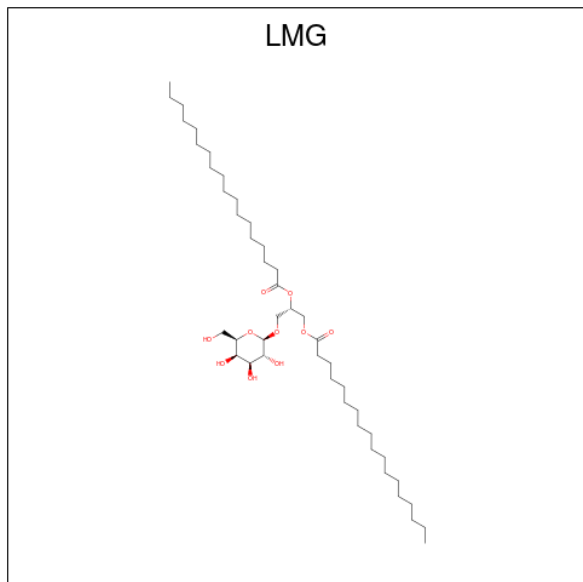
| Mol | Chain | Residues | Atoms                     | AltConf |
|-----|-------|----------|---------------------------|---------|
| 29  | A     | 1        | Total C O S<br>50 37 12 1 | 0       |
| 29  | A     | 1        | Total C O S<br>54 41 12 1 | 0       |
| 29  | L     | 1        | Total C O S<br>42 29 12 1 | 0       |

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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



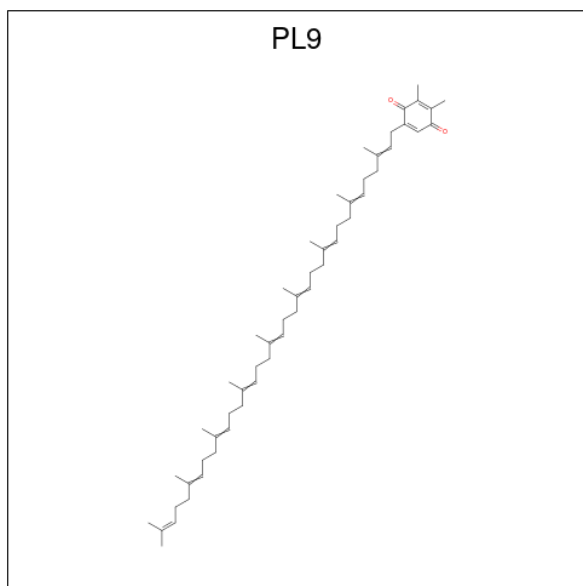
| Mol | Chain | Residues | Atoms |    |    |  | AltConf |
|-----|-------|----------|-------|----|----|--|---------|
| 30  | A     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 48    | 38 | 10 |  |         |
| 30  | A     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 40    | 30 | 10 |  |         |
| 30  | B     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 51    | 41 | 10 |  |         |
| 30  | B     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 55    | 45 | 10 |  |         |
| 30  | C     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 51    | 41 | 10 |  |         |
| 30  | D     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 46    | 36 | 10 |  |         |

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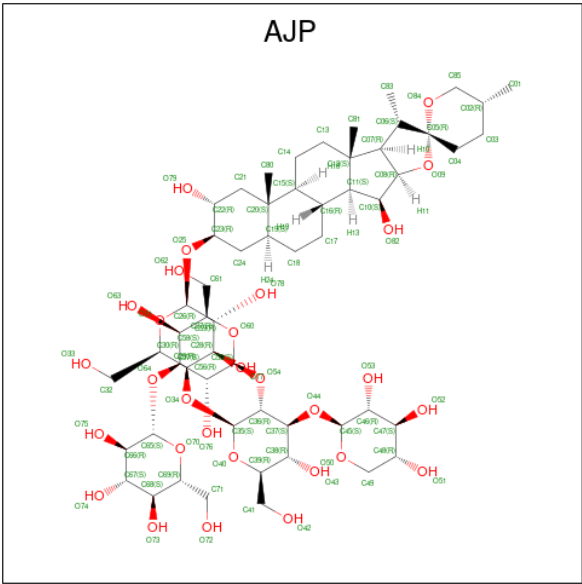
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 30  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 30  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 30  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 30  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 30  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 30  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |

- Molecule 31 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 31  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 31  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 31  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |

- Molecule 32 is Digitonin (CCD ID: AJP) (formula: C<sub>56</sub>H<sub>92</sub>O<sub>29</sub>) (labeled as "Ligand of Interest" by depositor).



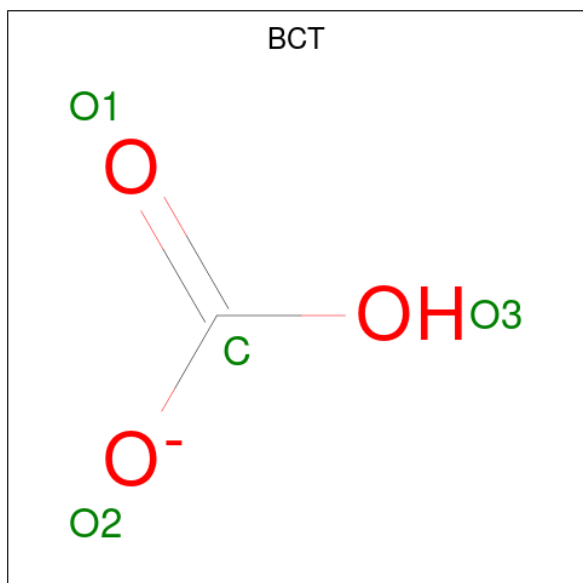
| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 32  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 177   | 56 | 92 | 29 |         |
| 32  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 177   | 56 | 92 | 29 |         |
| 32  | S     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | G     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | N     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | N     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | Y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | Y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | Y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | Y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | Y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | a     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 177   | 56 | 92 | 29 |         |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 32  | b     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 177   | 56 | 92 | 29 |         |
| 32  | s     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | g     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | n     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | n     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |
| 32  | y     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 95    | 33 | 53 | 9  |         |

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 33  | A     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

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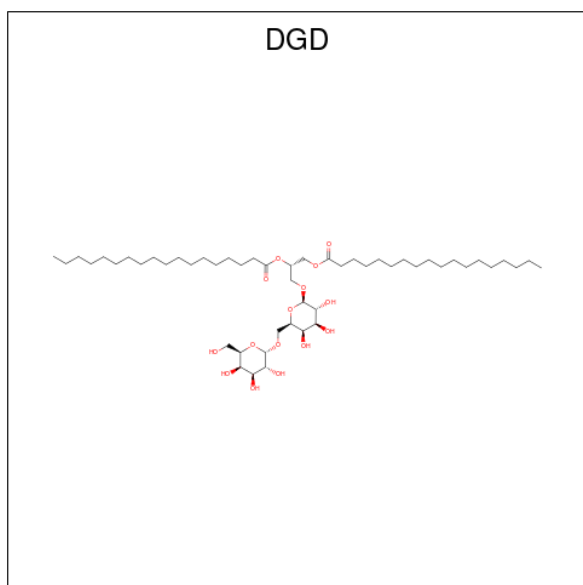
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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 33  | a     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    |  | AltConf |
|-----|-------|----------|-------|----|--|---------|
| 34  | A     | 1        | Total | Fe |  | 0       |
|     |       |          | 1     | 1  |  |         |
| 34  | a     | 1        | Total | Fe |  | 0       |
|     |       |          | 1     | 1  |  |         |

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |
| 35  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |
| 35  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 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 |         |

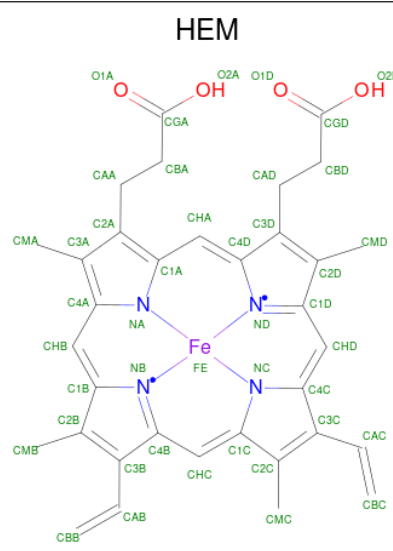
- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 36  | A     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 36  | B     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 36  | a     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 36  | b     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

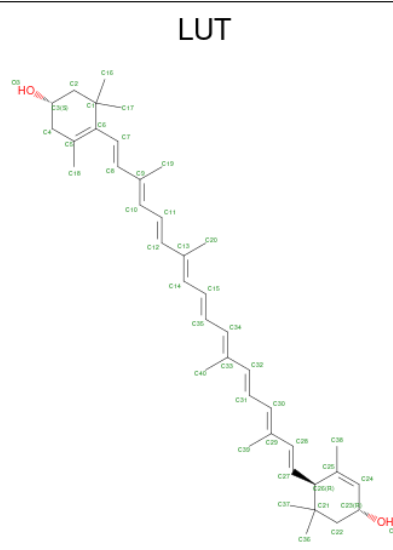
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 37  | D     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 37  | d     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 38  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 38  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



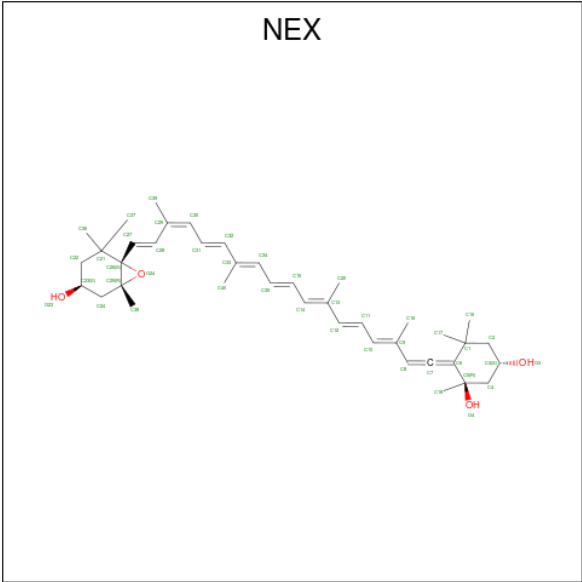
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 39  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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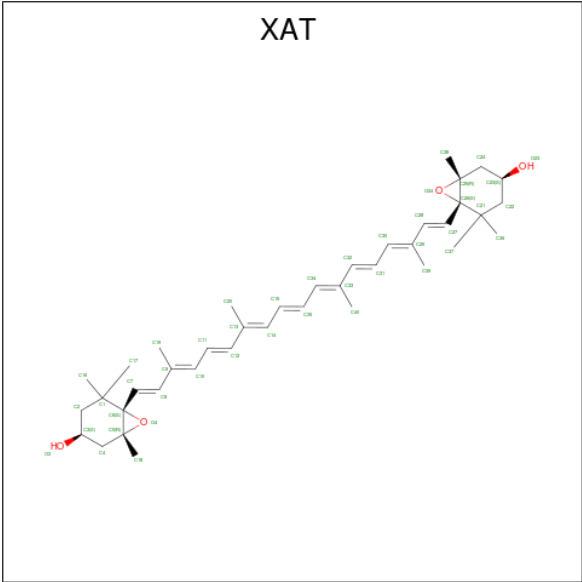
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 39  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | s     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | s     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-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 |
|-----|-------|----------|-------|----|---|---------|
| 40  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | s     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 40  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 41 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 |
|-----|-------|----------|-------|----|---|---------|
| 41  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 41  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 42 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 42  | A     | 23       | Total | O  | 0       |
|     |       |          | 23    | 23 |         |
| 42  | B     | 10       | Total | O  | 0       |
|     |       |          | 10    | 10 |         |
| 42  | C     | 14       | Total | O  | 0       |
|     |       |          | 14    | 14 |         |
| 42  | D     | 14       | Total | O  | 0       |
|     |       |          | 14    | 14 |         |
| 42  | H     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 42  | I     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 42  | L     | 3        | Total | O  | 0       |
|     |       |          | 3     | 3  |         |
| 42  | M     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 42  | T     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 42  | W     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |

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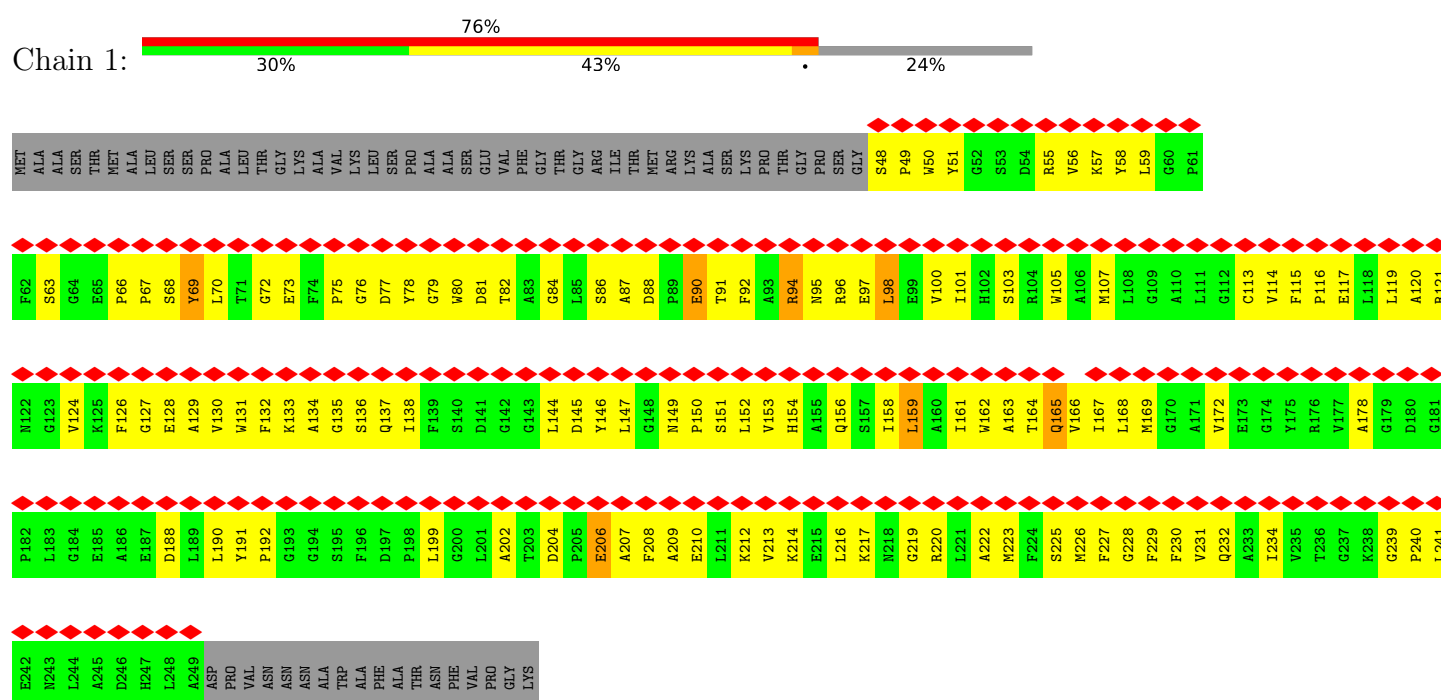
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 42  | a     | 23       | Total<br>23 | O<br>23 | 0       |
| 42  | b     | 10       | Total<br>10 | O<br>10 | 0       |
| 42  | c     | 14       | Total<br>14 | O<br>14 | 0       |
| 42  | d     | 14       | Total<br>14 | O<br>14 | 0       |
| 42  | h     | 1        | Total<br>1  | O<br>1  | 0       |
| 42  | i     | 1        | Total<br>1  | O<br>1  | 0       |
| 42  | l     | 3        | Total<br>3  | O<br>3  | 0       |
| 42  | m     | 2        | Total<br>2  | O<br>2  | 0       |
| 42  | t     | 1        | Total<br>1  | O<br>1  | 0       |
| 42  | w     | 1        | Total<br>1  | O<br>1  | 0       |

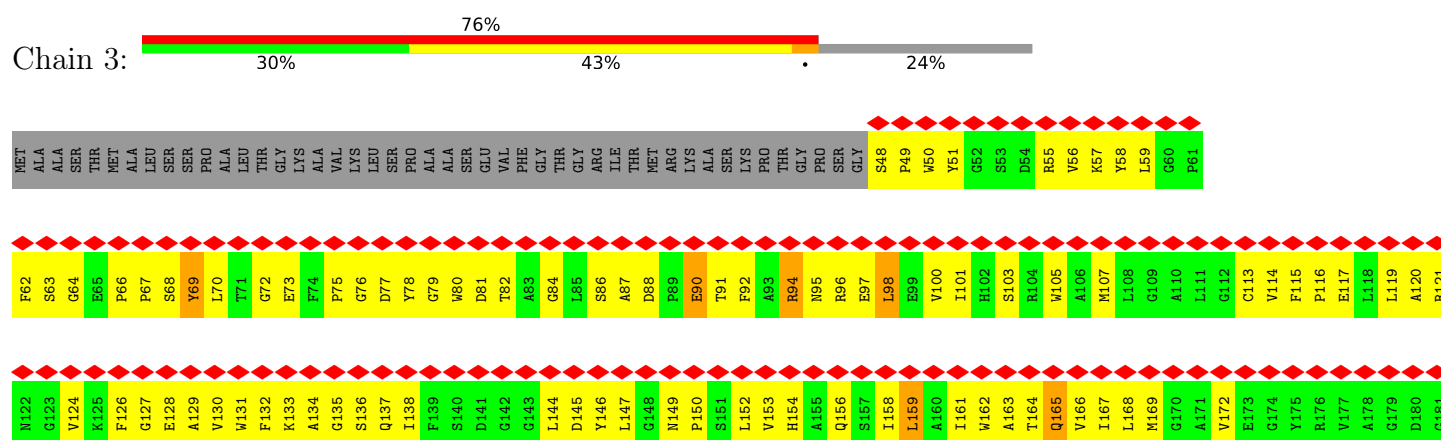
### 3 Residue-property plots [i](#)

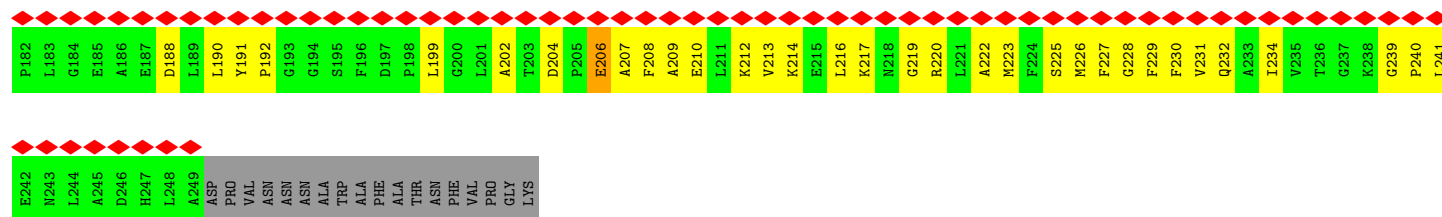
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

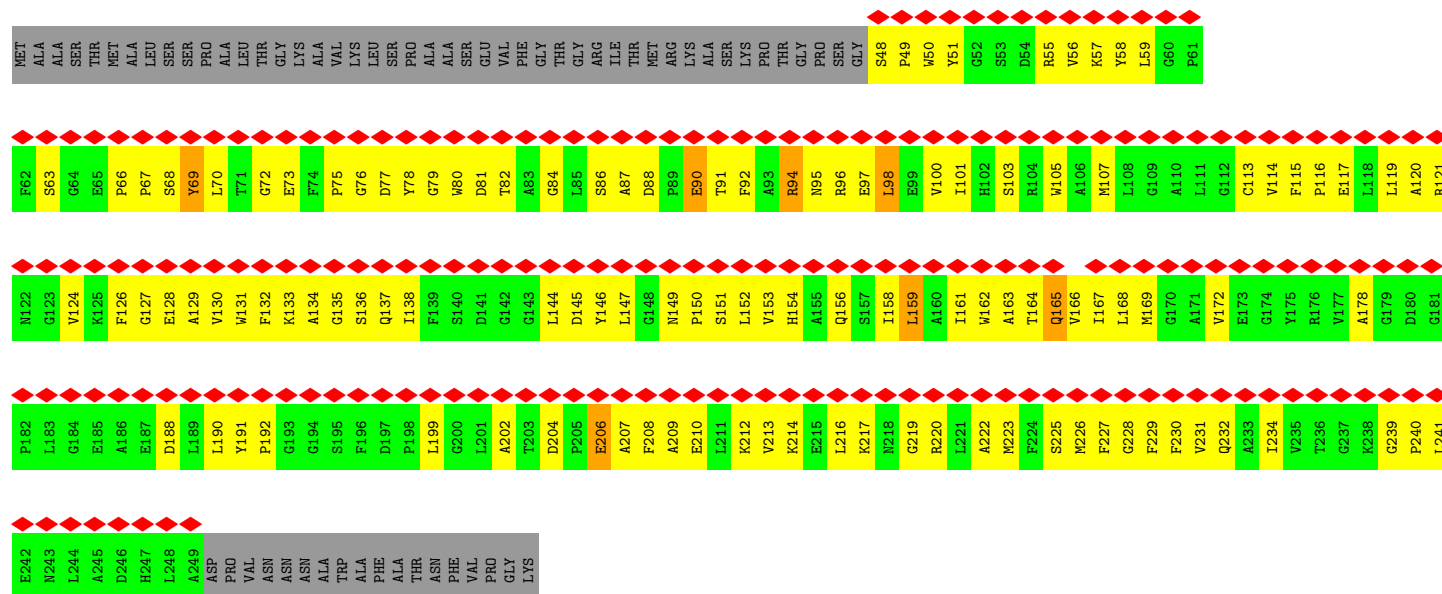
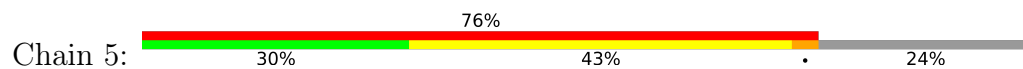


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

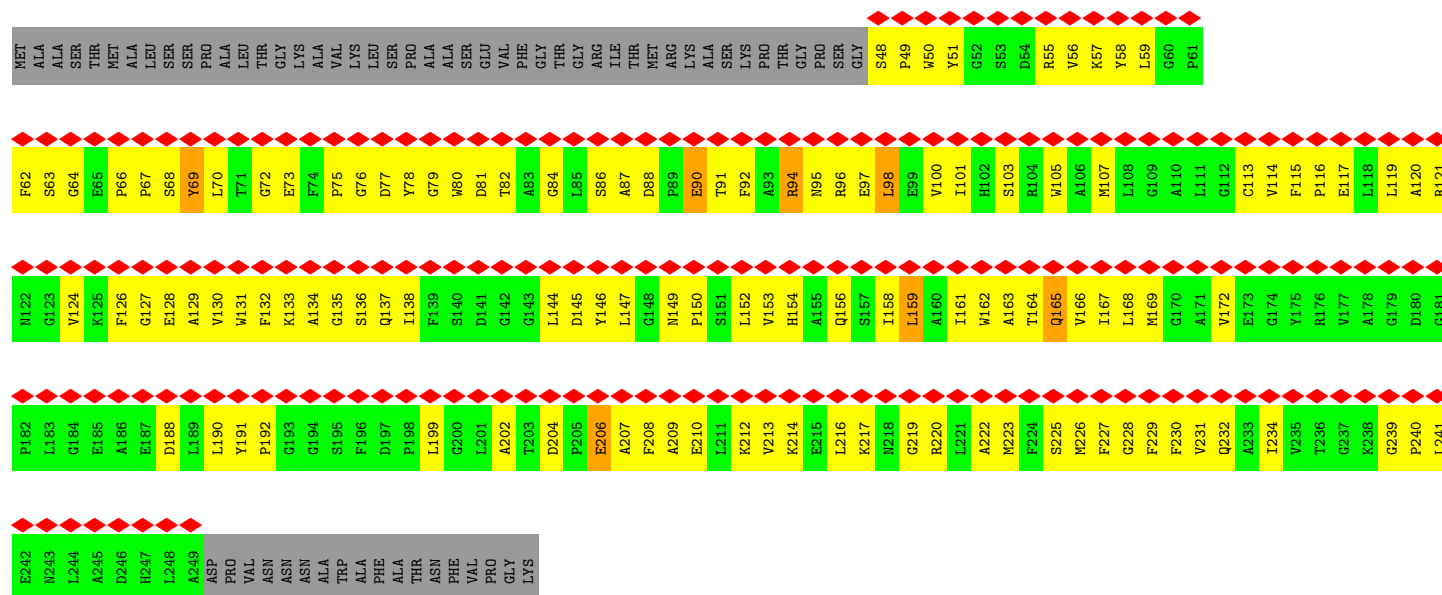
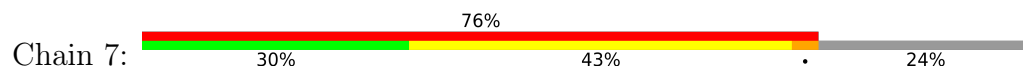




- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

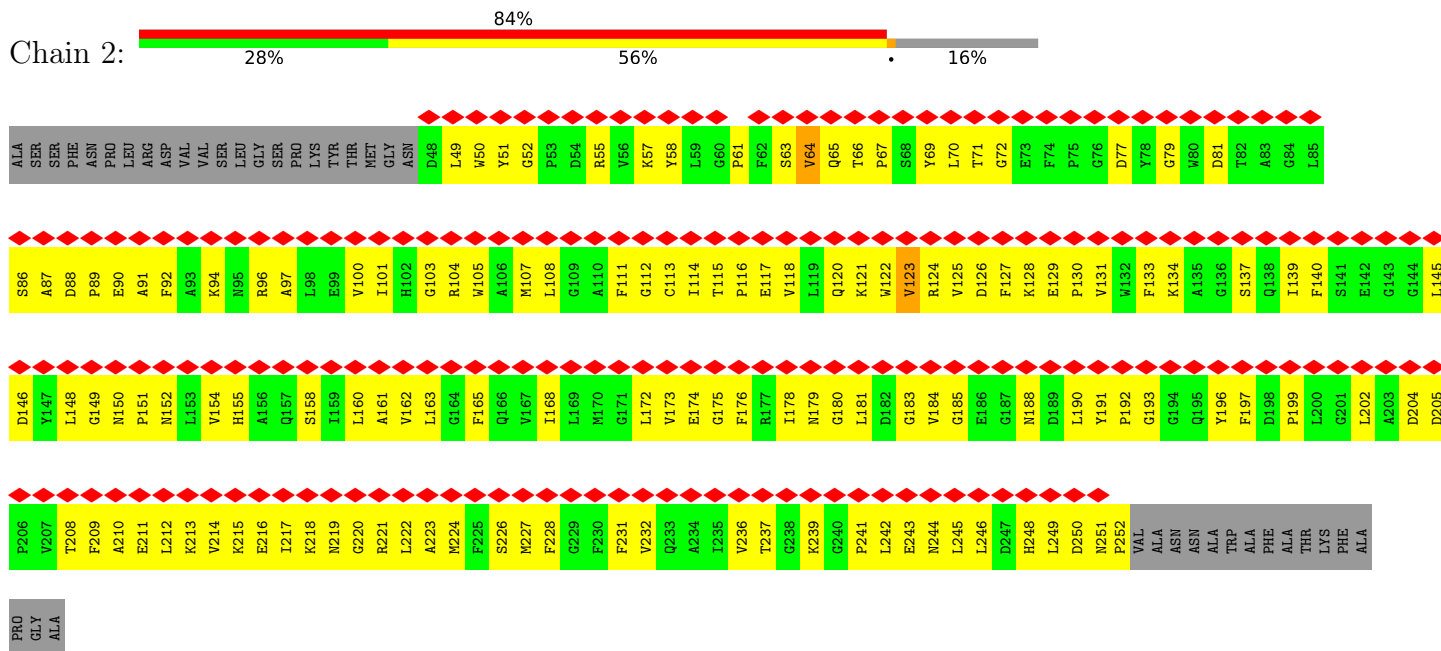


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

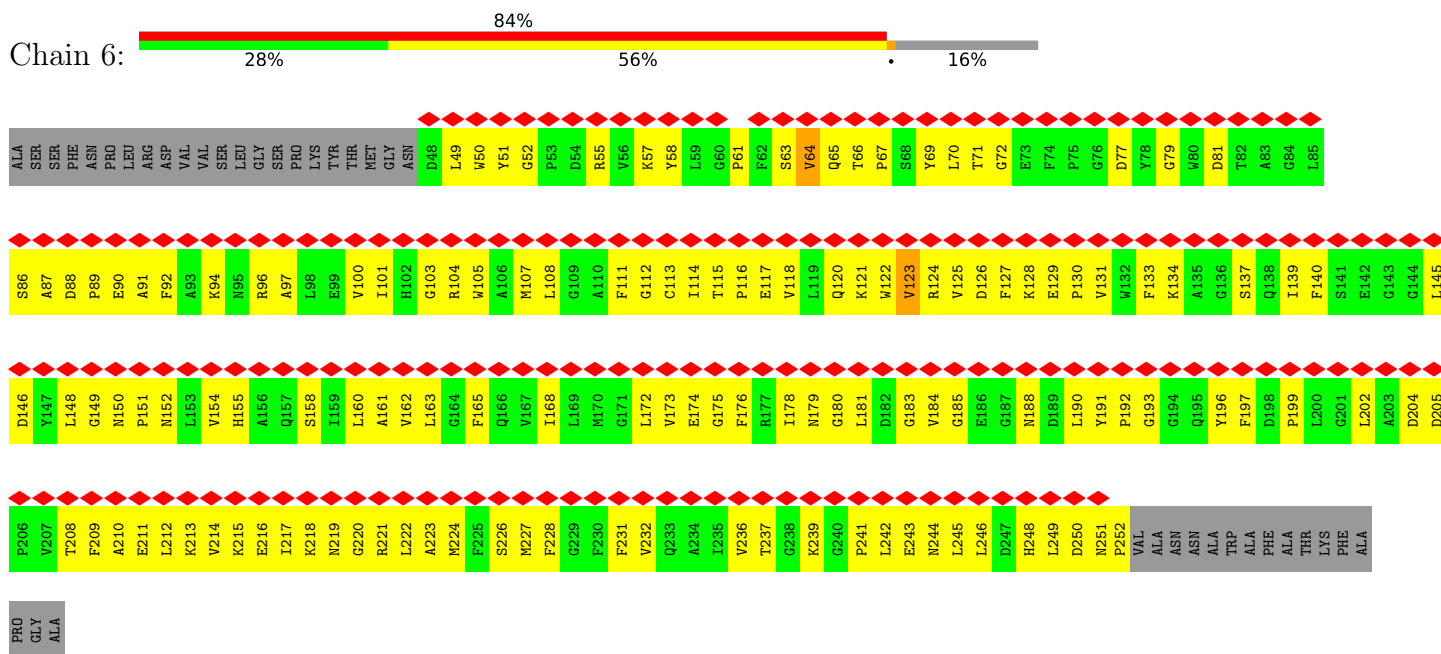




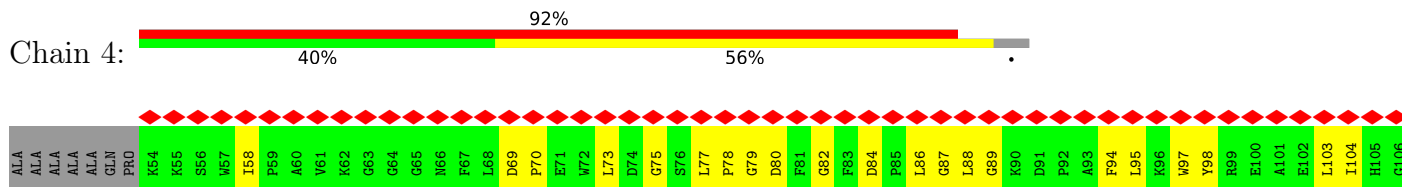
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

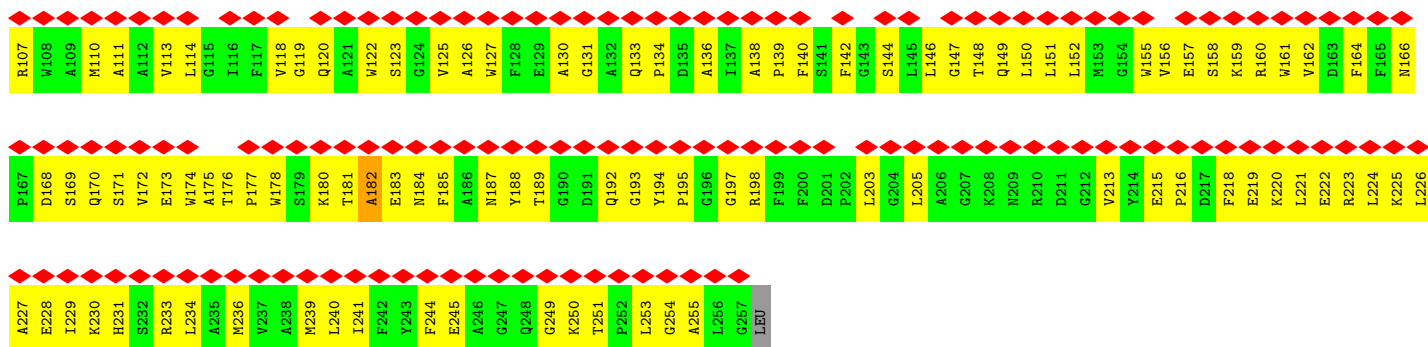


- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

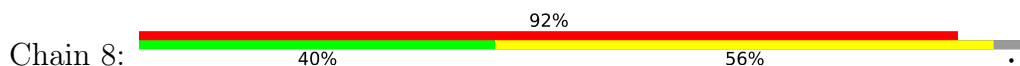


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

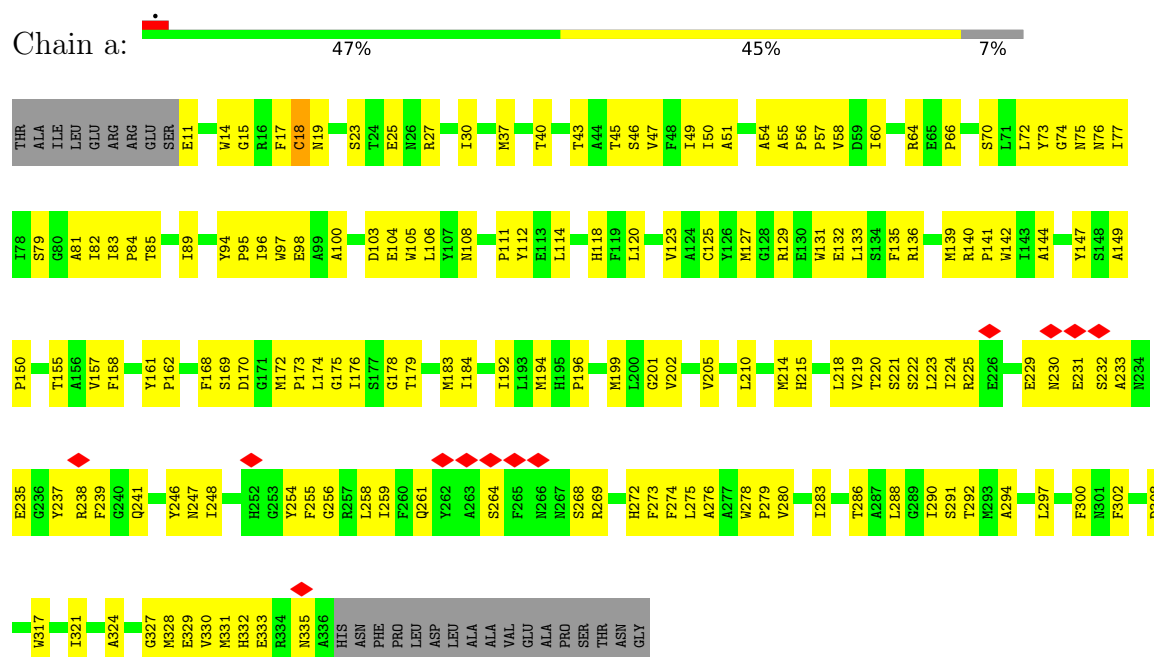




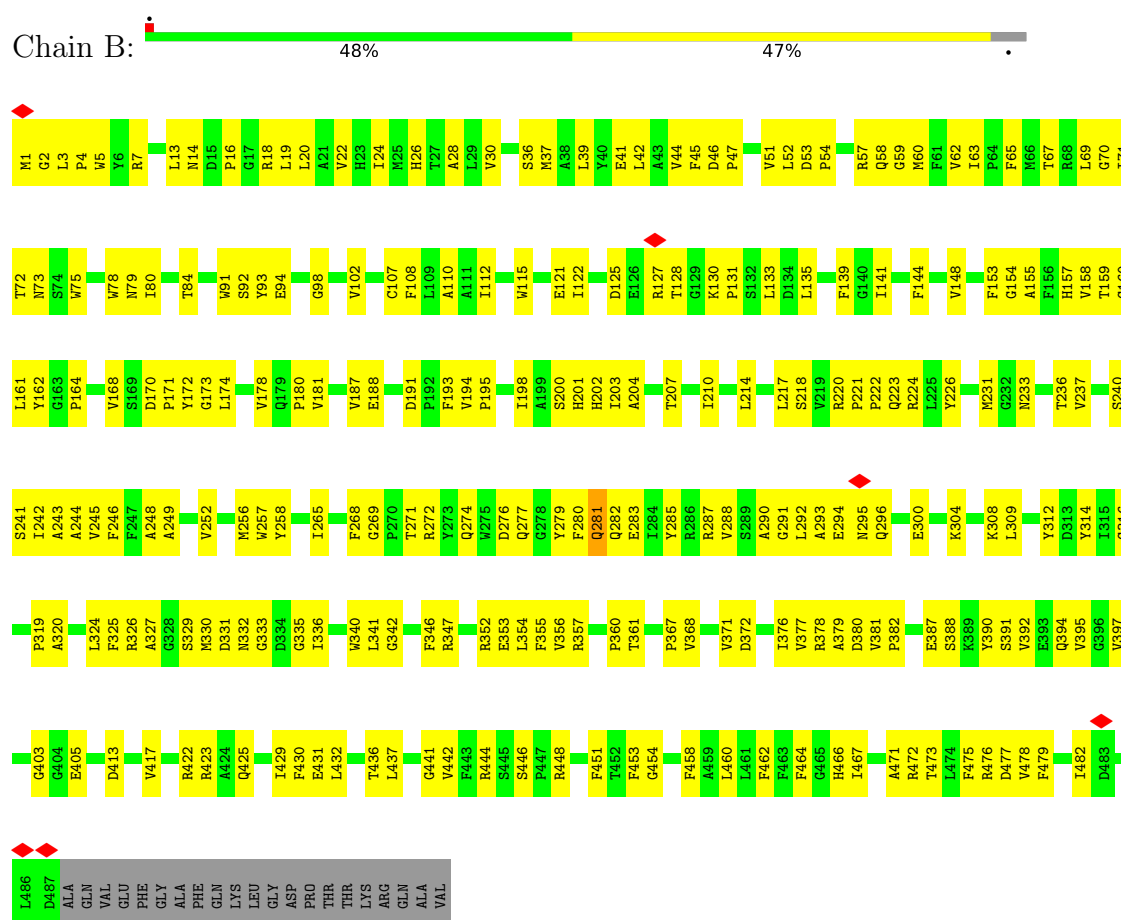
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic



- Molecule 4: Photosystem II protein D1

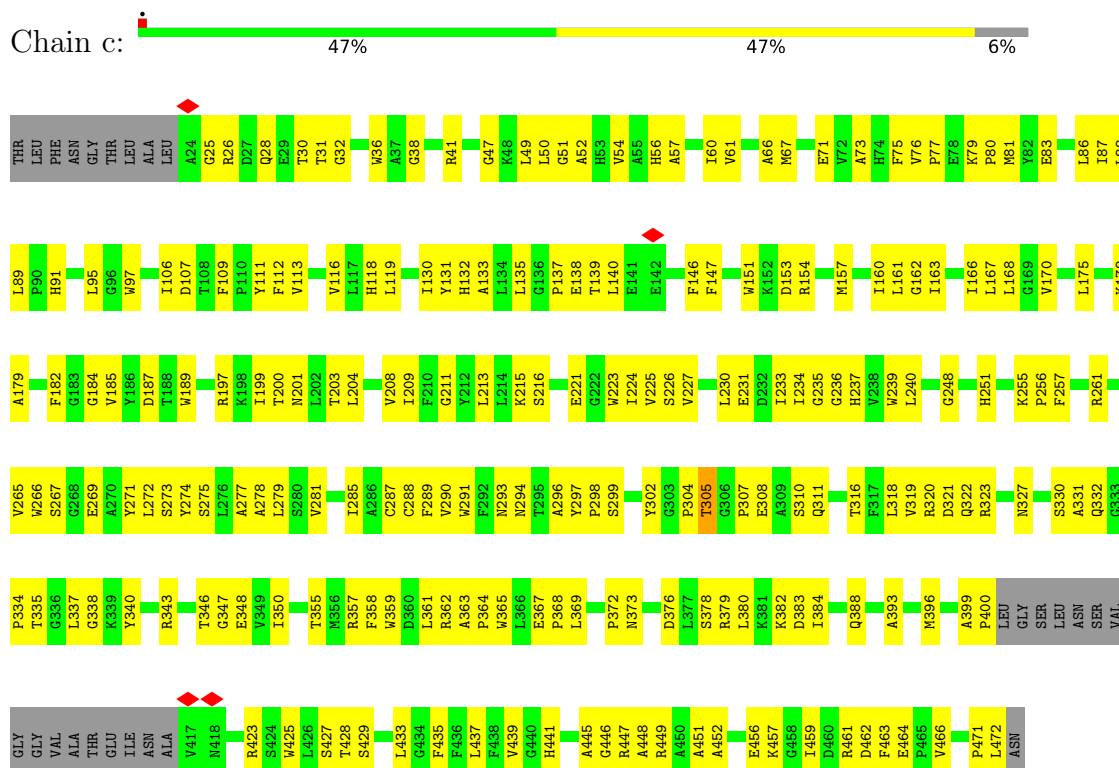


- Molecule 5: Photosystem II CP47 reaction center protein

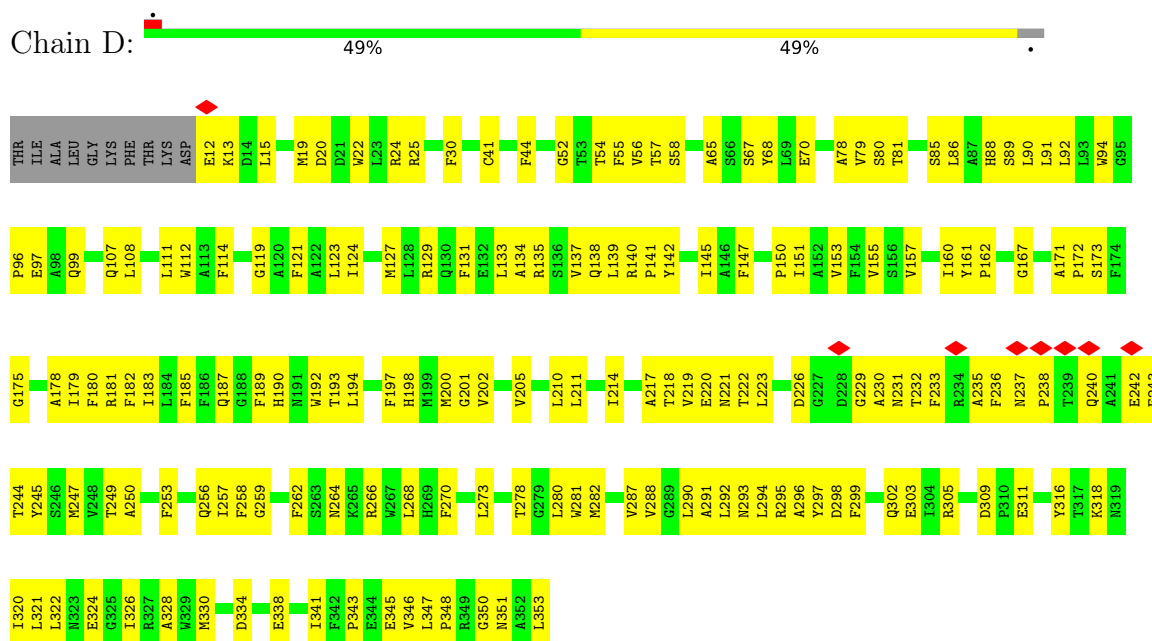


- Molecule 5: Photosystem II CP47 reaction center protein

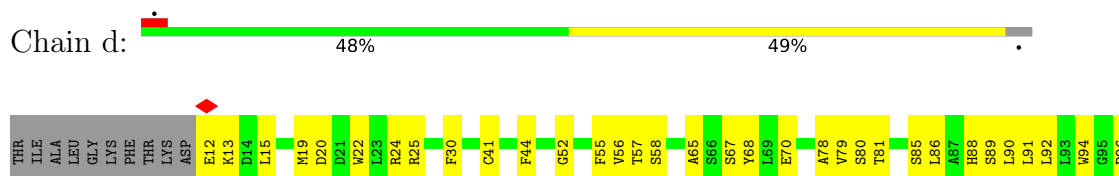


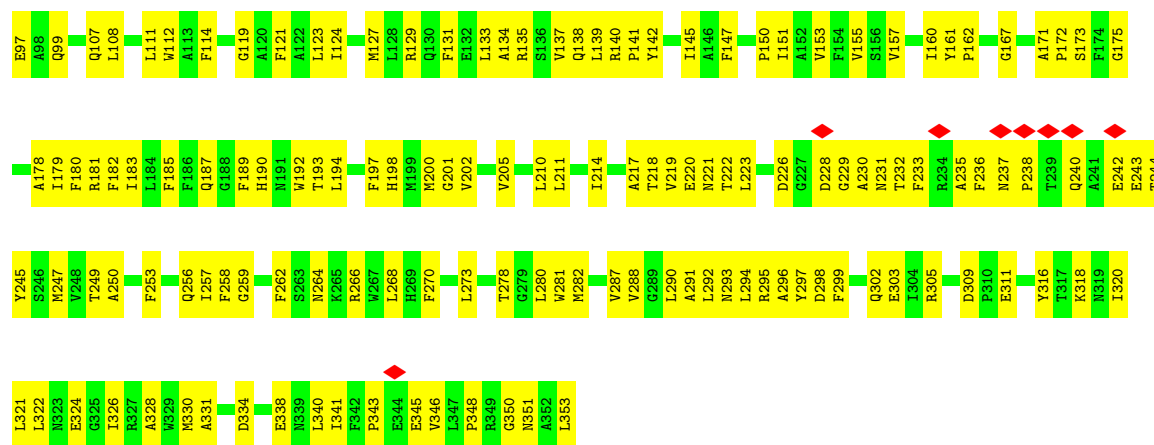


• Molecule 7: Photosystem II D2 protein

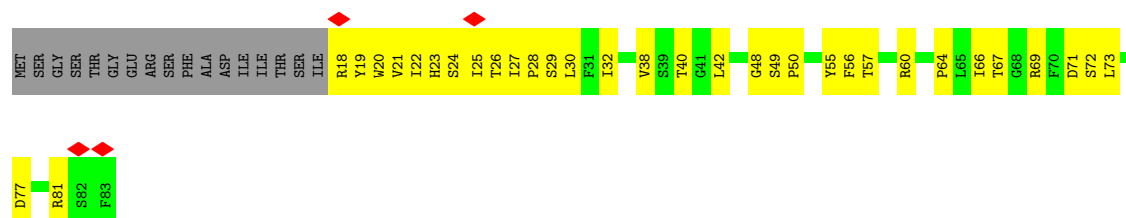
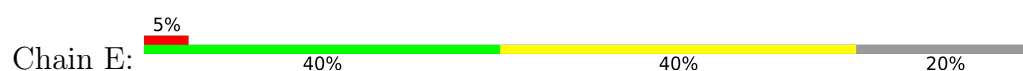


• Molecule 7: Photosystem II D2 protein

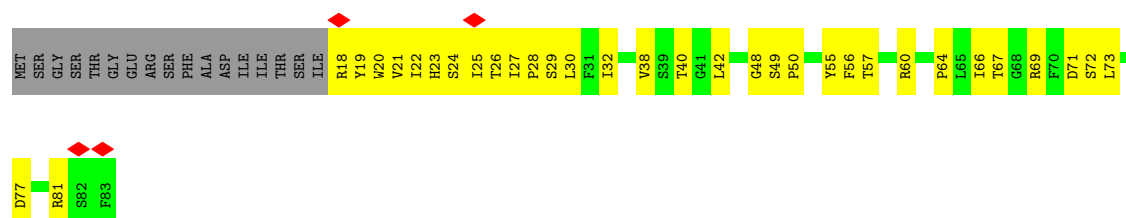




• Molecule 8: Cytochrome b559 subunit alpha



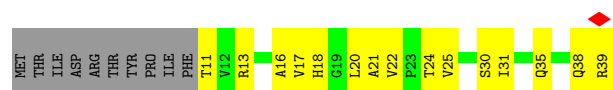
• Molecule 8: Cytochrome b559 subunit alpha



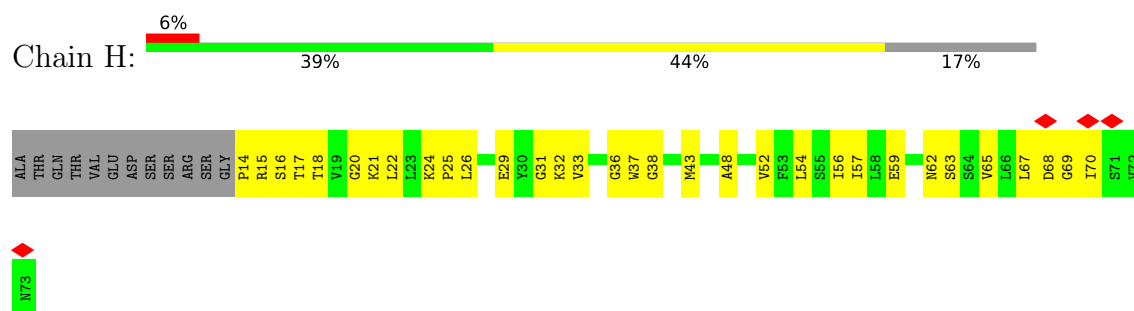
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



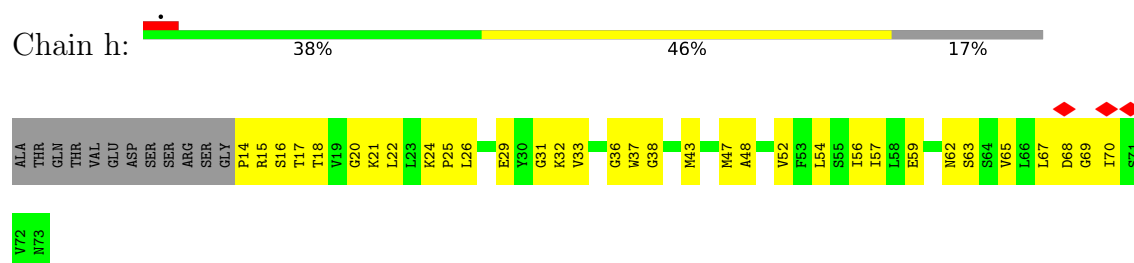
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



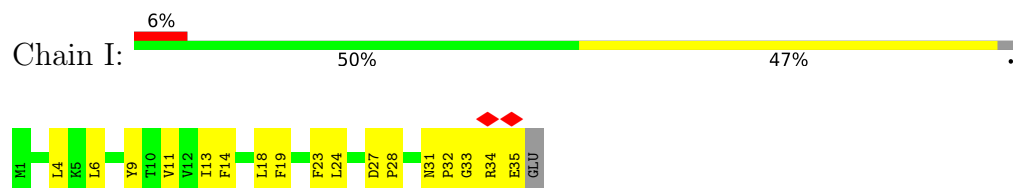
- Molecule 10: Photosystem II reaction center protein H



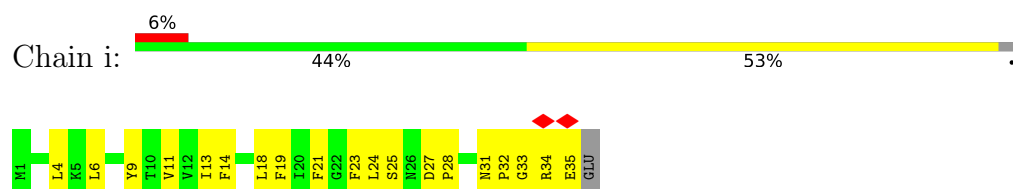
- Molecule 10: Photosystem II reaction center protein H



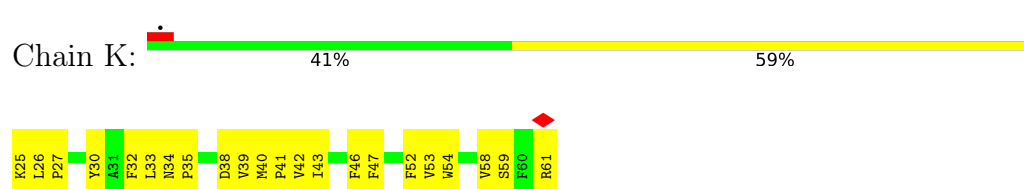
- Molecule 11: Photosystem II reaction center protein I



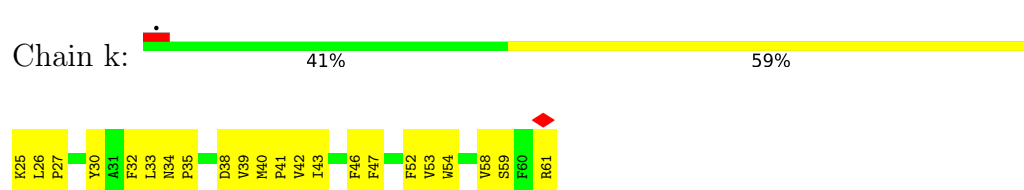
- Molecule 11: Photosystem II reaction center protein I



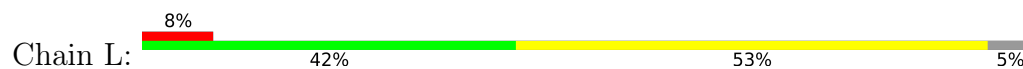
- Molecule 12: Photosystem II reaction center protein K



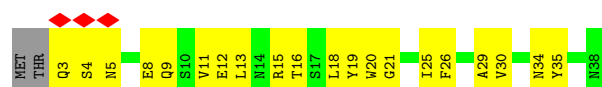
- Molecule 12: Photosystem II reaction center protein K



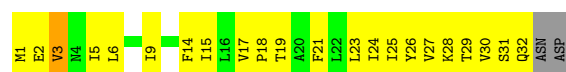
- Molecule 13: Photosystem II reaction center protein L



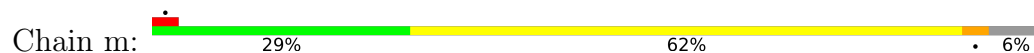
- Molecule 13: Photosystem II reaction center protein L



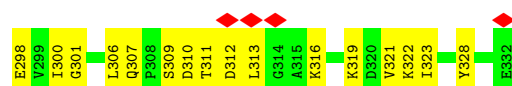
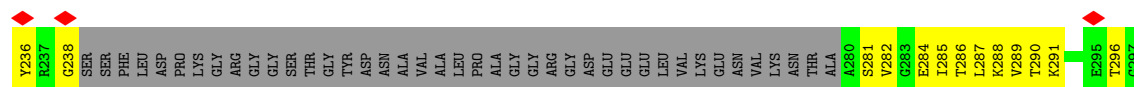
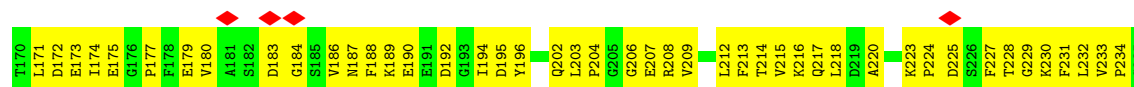
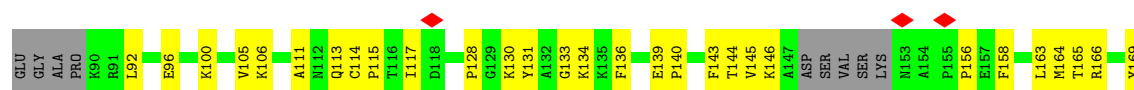
- Molecule 14: Photosystem II reaction center protein M



- Molecule 14: Photosystem II reaction center protein M

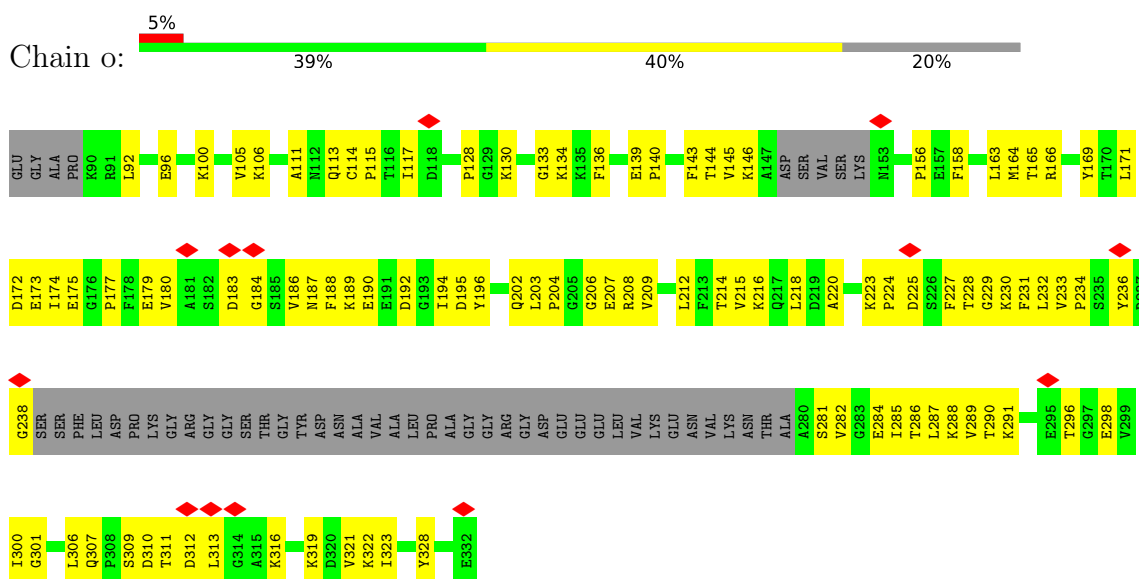


- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic

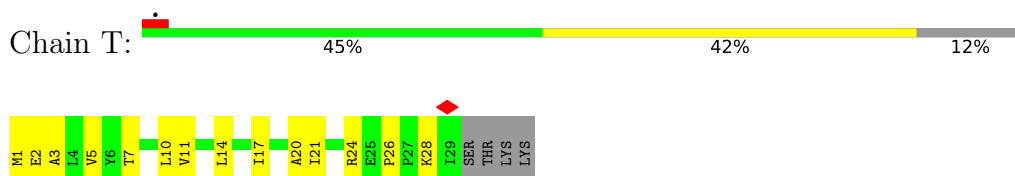


- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic

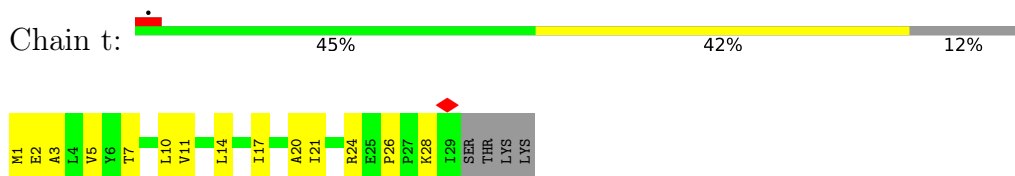




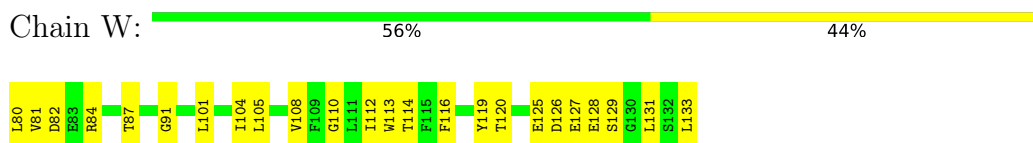
- Molecule 16: Photosystem II reaction center protein T



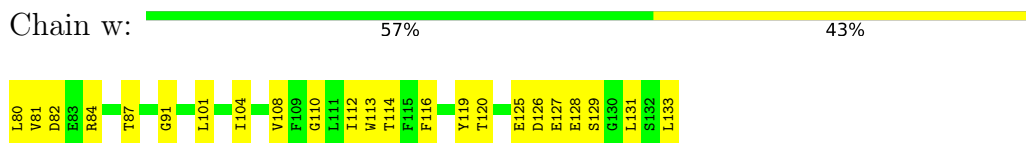
- Molecule 16: Photosystem II reaction center protein T



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



- Molecule 17: Photosystem II reaction center W protein, chloroplastic

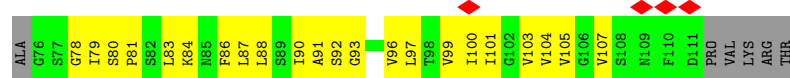


- Molecule 18: (thale cress) hypothetical protein

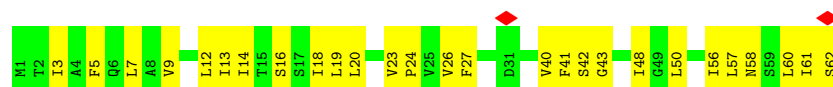




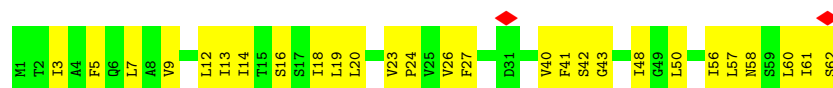
- Molecule 18: (thale cress) hypothetical protein



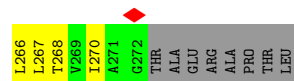
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

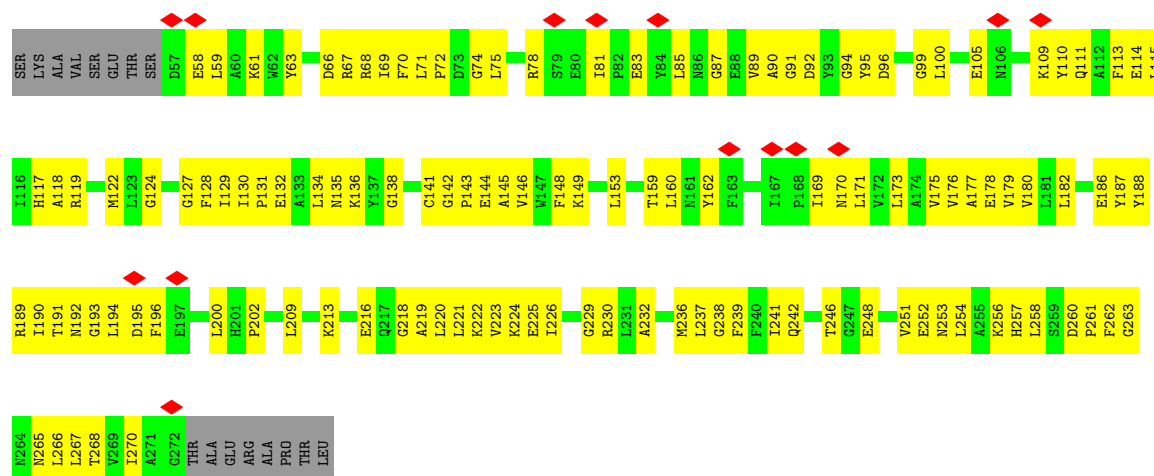


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

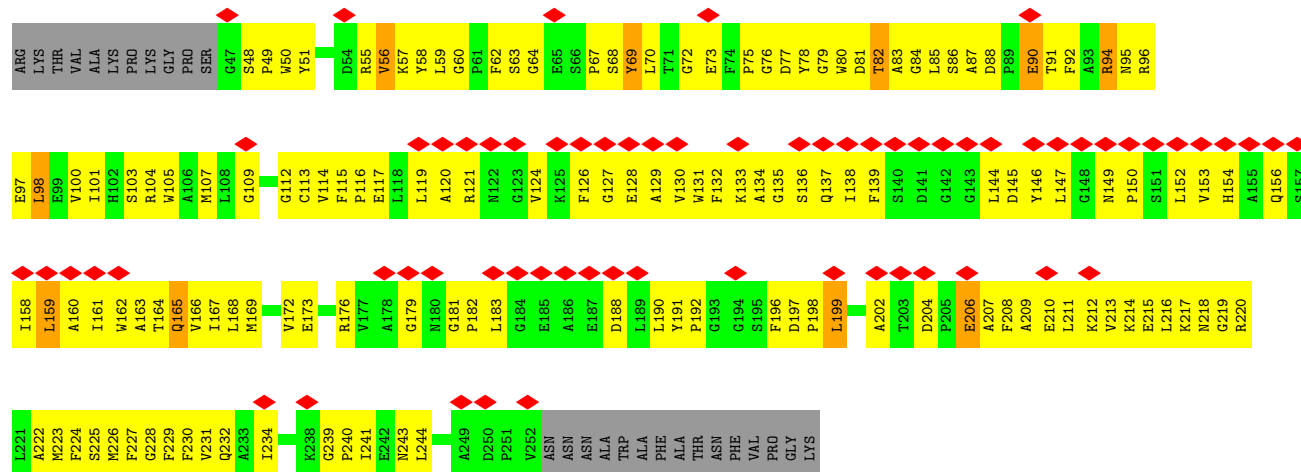


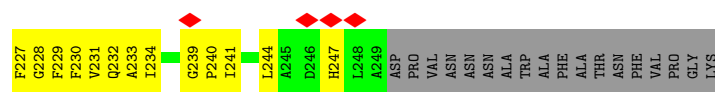
- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic



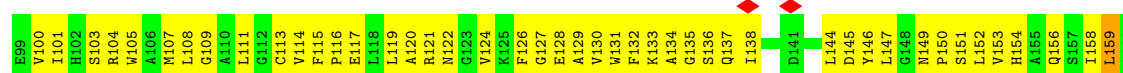
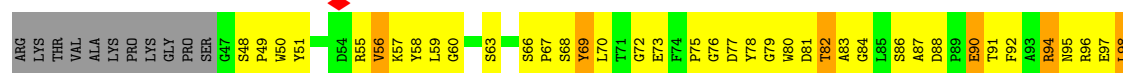
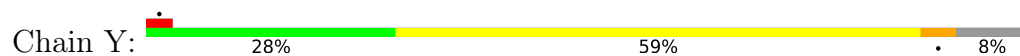


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

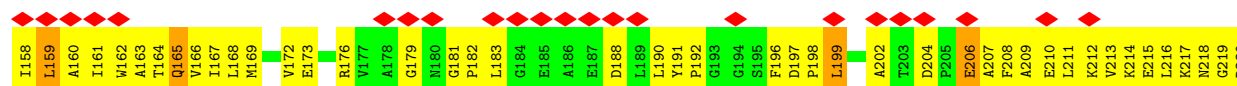
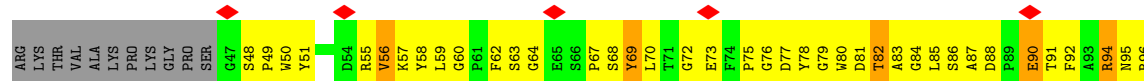




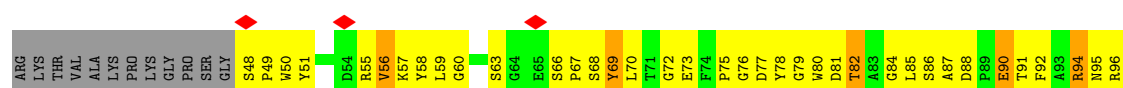
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

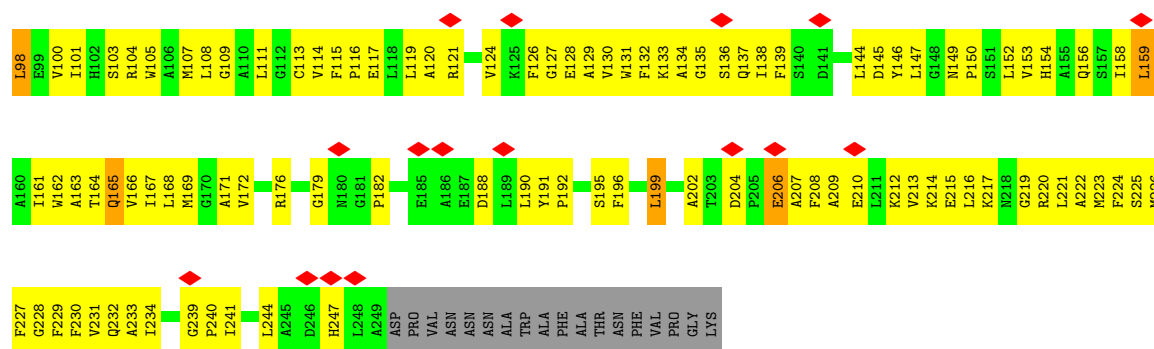


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



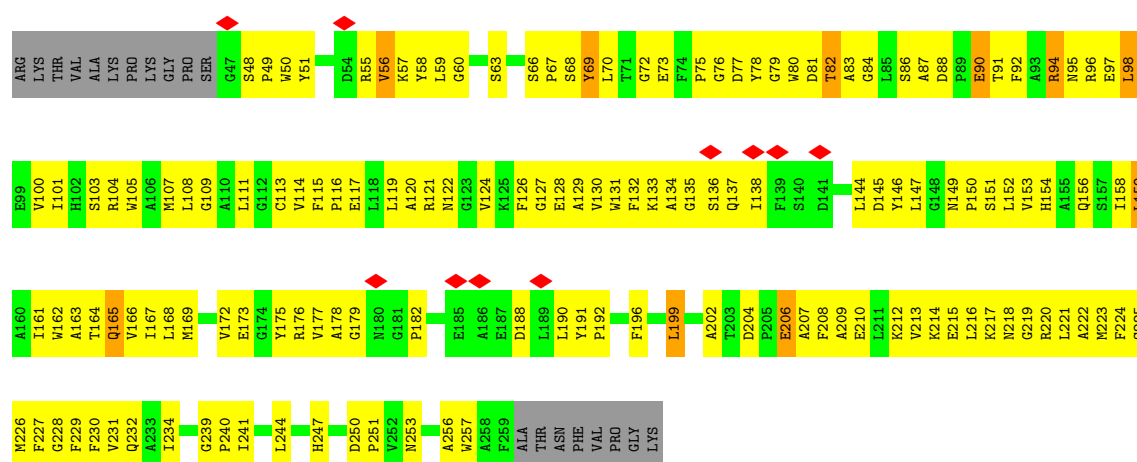
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic





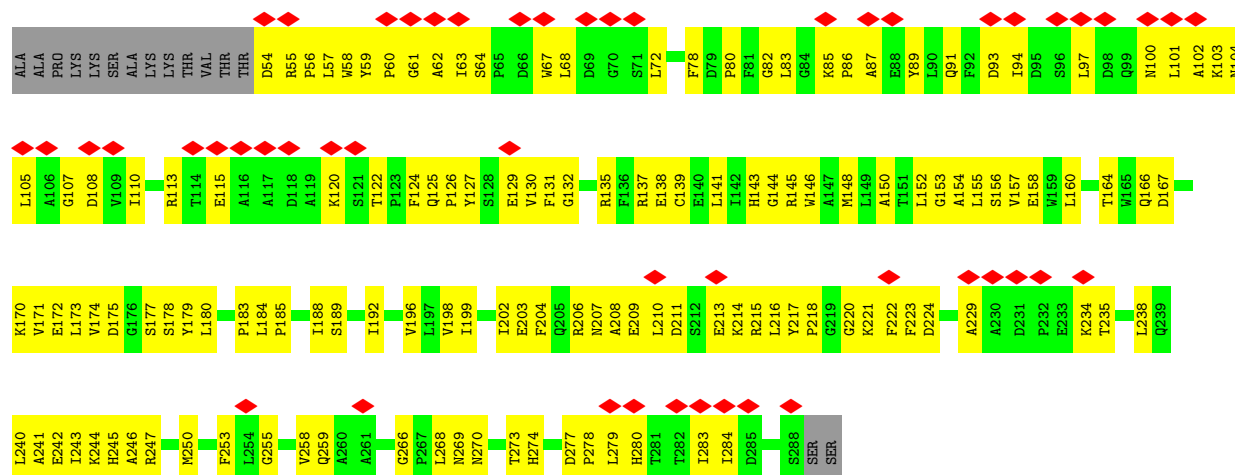
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 29% 59% 8%

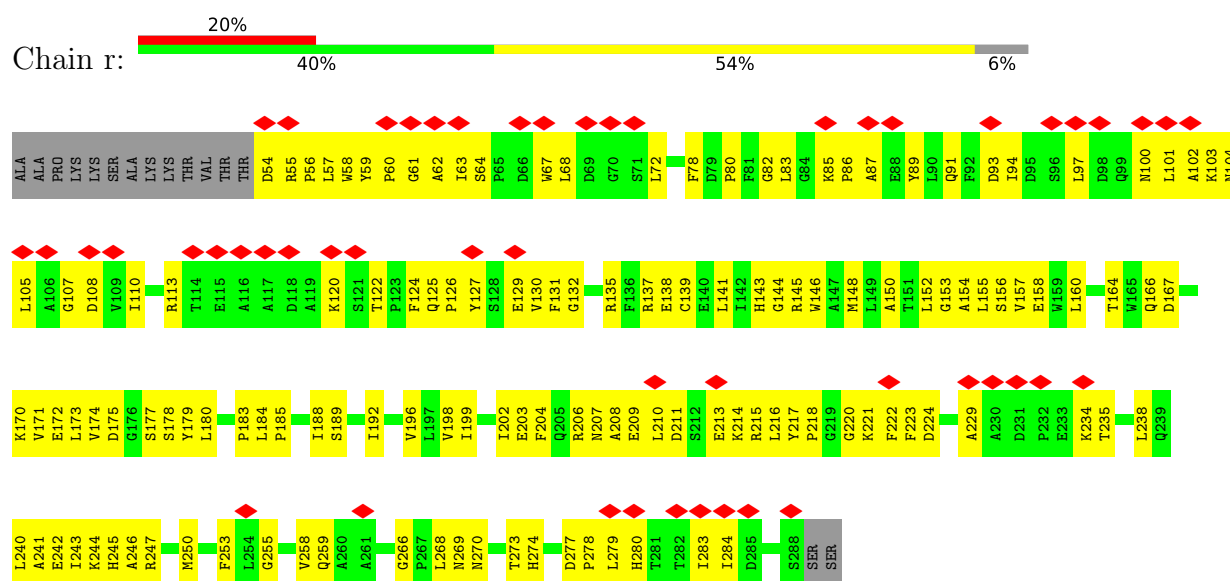


- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

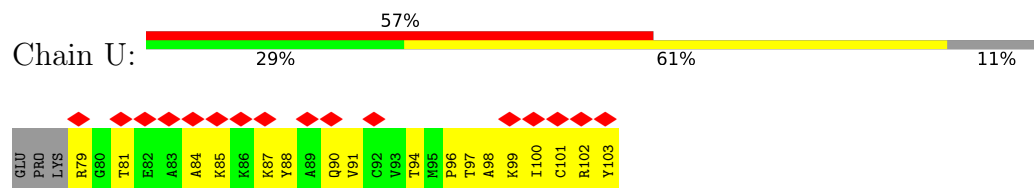
Chain R: 20% 39% 55% 6%



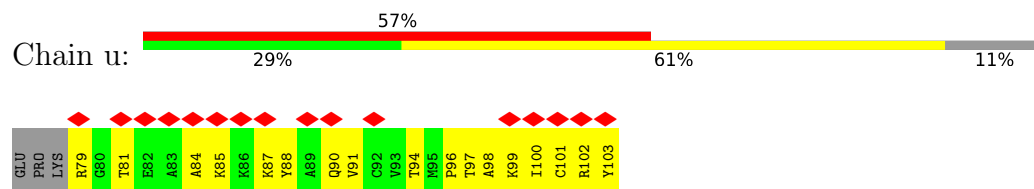
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 100712                    | 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 ( $e^-/\text{\AA}^2$ ) | 1.49                      | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 33.682                    | Depositor |
| Minimum map value                    | -19.496                   | Depositor |
| Average map value                    | -0.004                    | Depositor |
| Map value standard deviation         | 0.976                     | Depositor |
| Recommended contour level            | 4                         | Depositor |
| Map size ( $\text{\AA}$ )            | 410.0, 410.0, 410.0       | wwPDB     |
| Map dimensions                       | 500, 500, 500             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.82, 0.82, 0.82          | Depositor |

## 5 Model quality [i](#)

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

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

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   | 1     | 0.19         | 0/1582      | 0.45        | 0/2150      |
| 1   | 3     | 0.19         | 0/1582      | 0.45        | 0/2150      |
| 1   | 5     | 0.19         | 0/1582      | 0.45        | 0/2150      |
| 1   | 7     | 0.19         | 0/1582      | 0.45        | 0/2150      |
| 2   | 2     | 0.17         | 0/1640      | 0.42        | 0/2229      |
| 2   | 6     | 0.17         | 0/1640      | 0.42        | 0/2229      |
| 3   | 4     | 0.17         | 0/1652      | 0.43        | 0/2242      |
| 3   | 8     | 0.17         | 0/1652      | 0.43        | 0/2242      |
| 4   | A     | 0.12         | 0/2626      | 0.34        | 0/3580      |
| 4   | a     | 0.12         | 0/2626      | 0.34        | 0/3580      |
| 5   | B     | 0.12         | 0/3940      | 0.29        | 0/5368      |
| 5   | b     | 0.12         | 0/3940      | 0.29        | 0/5368      |
| 6   | C     | 0.11         | 0/3487      | 0.26        | 0/4750      |
| 6   | c     | 0.11         | 0/3487      | 0.26        | 0/4750      |
| 7   | D     | 0.12         | 0/2815      | 0.28        | 0/3837      |
| 7   | d     | 0.12         | 0/2815      | 0.28        | 0/3837      |
| 8   | E     | 0.10         | 0/561       | 0.29        | 0/763       |
| 8   | e     | 0.10         | 0/561       | 0.29        | 0/763       |
| 9   | F     | 0.09         | 0/229       | 0.24        | 0/311       |
| 9   | f     | 0.09         | 0/229       | 0.24        | 0/311       |
| 10  | H     | 0.10         | 0/455       | 0.36        | 0/619       |
| 10  | h     | 0.10         | 0/455       | 0.35        | 0/619       |
| 11  | I     | 0.13         | 0/294       | 0.38        | 0/397       |
| 11  | i     | 0.12         | 0/294       | 0.38        | 0/397       |
| 12  | K     | 0.10         | 0/312       | 0.27        | 0/428       |
| 12  | k     | 0.10         | 0/312       | 0.27        | 0/428       |
| 13  | L     | 0.09         | 0/310       | 0.20        | 0/421       |
| 13  | l     | 0.09         | 0/310       | 0.20        | 0/421       |
| 14  | M     | 0.11         | 0/254       | 0.28        | 0/347       |
| 14  | m     | 0.11         | 0/254       | 0.28        | 0/347       |
| 15  | O     | 0.10         | 0/1548      | 0.31        | 0/2091      |



| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 15  | o     | 0.10         | 0/1548  | 0.31        | 0/2091  |
| 16  | T     | 0.09         | 0/246   | 0.22        | 0/333   |
| 16  | t     | 0.09         | 0/246   | 0.22        | 0/333   |
| 17  | W     | 0.10         | 0/438   | 0.26        | 0/594   |
| 17  | w     | 0.10         | 0/438   | 0.26        | 0/594   |
| 18  | X     | 0.09         | 0/250   | 0.23        | 0/339   |
| 18  | x     | 0.10         | 0/250   | 0.23        | 0/339   |
| 19  | Z     | 0.15         | 0/474   | 0.30        | 0/649   |
| 19  | z     | 0.15         | 0/474   | 0.30        | 0/649   |
| 20  | S     | 0.12         | 0/1715  | 0.29        | 0/2328  |
| 20  | s     | 0.12         | 0/1715  | 0.30        | 0/2328  |
| 21  | G     | 0.19         | 0/1607  | 0.44        | 0/2184  |
| 21  | N     | 0.19         | 0/1580  | 0.44        | 0/2146  |
| 21  | Y     | 0.19         | 0/1669  | 0.44        | 0/2270  |
| 21  | g     | 0.19         | 0/1607  | 0.44        | 0/2184  |
| 21  | n     | 0.19         | 0/1580  | 0.44        | 0/2146  |
| 21  | y     | 0.19         | 0/1669  | 0.44        | 0/2270  |
| 22  | R     | 0.15         | 0/1878  | 0.34        | 0/2561  |
| 22  | r     | 0.15         | 0/1878  | 0.34        | 0/2561  |
| 23  | U     | 0.08         | 0/196   | 0.27        | 0/261   |
| 23  | u     | 0.09         | 0/196   | 0.27        | 0/261   |
| All | All   | 0.14         | 0/66680 | 0.35        | 0/90696 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1537  | 0        | 1480     | 181     | 0            |
| 1   | 3     | 1537  | 0        | 1480     | 182     | 0            |
| 1   | 5     | 1537  | 0        | 1480     | 179     | 0            |
| 1   | 7     | 1537  | 0        | 1480     | 183     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 2     | 1593  | 0        | 1543     | 287     | 0            |
| 2   | 6     | 1593  | 0        | 1543     | 292     | 0            |
| 3   | 4     | 1597  | 0        | 1534     | 197     | 0            |
| 3   | 8     | 1597  | 0        | 1534     | 200     | 0            |
| 4   | A     | 2548  | 0        | 2460     | 229     | 0            |
| 4   | a     | 2548  | 0        | 2460     | 233     | 0            |
| 5   | B     | 3810  | 0        | 3688     | 326     | 0            |
| 5   | b     | 3810  | 0        | 3688     | 327     | 0            |
| 6   | C     | 3373  | 0        | 3302     | 277     | 0            |
| 6   | c     | 3373  | 0        | 3302     | 284     | 0            |
| 7   | D     | 2722  | 0        | 2615     | 251     | 0            |
| 7   | d     | 2722  | 0        | 2615     | 255     | 0            |
| 8   | E     | 543   | 0        | 519      | 38      | 0            |
| 8   | e     | 543   | 0        | 519      | 37      | 0            |
| 9   | F     | 224   | 0        | 233      | 14      | 0            |
| 9   | f     | 224   | 0        | 233      | 14      | 0            |
| 10  | H     | 446   | 0        | 471      | 58      | 0            |
| 10  | h     | 446   | 0        | 471      | 60      | 0            |
| 11  | I     | 286   | 0        | 295      | 32      | 0            |
| 11  | i     | 286   | 0        | 295      | 32      | 0            |
| 12  | K     | 301   | 0        | 313      | 28      | 0            |
| 12  | k     | 301   | 0        | 313      | 28      | 0            |
| 13  | L     | 302   | 0        | 291      | 29      | 0            |
| 13  | l     | 302   | 0        | 291      | 30      | 0            |
| 14  | M     | 250   | 0        | 279      | 41      | 0            |
| 14  | m     | 250   | 0        | 279      | 41      | 0            |
| 15  | O     | 1516  | 0        | 1494     | 133     | 0            |
| 15  | o     | 1516  | 0        | 1494     | 131     | 0            |
| 16  | T     | 239   | 0        | 255      | 19      | 0            |
| 16  | t     | 239   | 0        | 255      | 20      | 0            |
| 17  | W     | 427   | 0        | 405      | 33      | 0            |
| 17  | w     | 427   | 0        | 405      | 34      | 0            |
| 18  | X     | 248   | 0        | 266      | 43      | 0            |
| 18  | x     | 248   | 0        | 266      | 43      | 0            |
| 19  | Z     | 464   | 0        | 495      | 38      | 0            |
| 19  | z     | 464   | 0        | 495      | 40      | 0            |
| 20  | S     | 1670  | 0        | 1647     | 186     | 0            |
| 20  | s     | 1670  | 0        | 1647     | 188     | 0            |
| 21  | G     | 1562  | 0        | 1501     | 302     | 0            |
| 21  | N     | 1536  | 0        | 1478     | 293     | 0            |
| 21  | Y     | 1621  | 0        | 1546     | 306     | 0            |
| 21  | g     | 1562  | 0        | 1501     | 300     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | n     | 1536  | 0        | 1478     | 295     | 0            |
| 21  | y     | 1621  | 0        | 1546     | 307     | 0            |
| 22  | R     | 1827  | 0        | 1777     | 212     | 0            |
| 22  | r     | 1827  | 0        | 1777     | 211     | 0            |
| 23  | U     | 194   | 0        | 206      | 36      | 0            |
| 23  | u     | 194   | 0        | 206      | 35      | 0            |
| 24  | 1     | 92    | 0        | 62       | 18      | 0            |
| 24  | 2     | 110   | 0        | 91       | 29      | 0            |
| 24  | 5     | 92    | 0        | 62       | 17      | 0            |
| 24  | 6     | 110   | 0        | 91       | 30      | 0            |
| 24  | G     | 335   | 0        | 296      | 78      | 0            |
| 24  | N     | 348   | 0        | 321      | 117     | 0            |
| 24  | R     | 195   | 0        | 146      | 23      | 0            |
| 24  | S     | 184   | 0        | 124      | 28      | 0            |
| 24  | Y     | 344   | 0        | 308      | 94      | 0            |
| 24  | g     | 335   | 0        | 296      | 77      | 0            |
| 24  | n     | 348   | 0        | 321      | 116     | 0            |
| 24  | r     | 195   | 0        | 146      | 24      | 0            |
| 24  | s     | 184   | 0        | 124      | 33      | 0            |
| 24  | y     | 344   | 0        | 308      | 93      | 0            |
| 25  | 2     | 163   | 0        | 142      | 33      | 0            |
| 25  | 6     | 163   | 0        | 142      | 37      | 0            |
| 25  | A     | 190   | 0        | 203      | 39      | 0            |
| 25  | B     | 1040  | 0        | 1150     | 147     | 0            |
| 25  | C     | 840   | 0        | 923      | 145     | 0            |
| 25  | D     | 180   | 0        | 183      | 41      | 0            |
| 25  | G     | 472   | 0        | 464      | 110     | 0            |
| 25  | N     | 473   | 0        | 468      | 139     | 0            |
| 25  | R     | 543   | 0        | 490      | 113     | 0            |
| 25  | S     | 465   | 0        | 393      | 90      | 0            |
| 25  | Y     | 470   | 0        | 465      | 123     | 0            |
| 25  | a     | 190   | 0        | 203      | 39      | 0            |
| 25  | b     | 1040  | 0        | 1150     | 149     | 0            |
| 25  | c     | 840   | 0        | 923      | 157     | 0            |
| 25  | d     | 180   | 0        | 183      | 42      | 0            |
| 25  | g     | 472   | 0        | 464      | 115     | 0            |
| 25  | n     | 473   | 0        | 468      | 136     | 0            |
| 25  | r     | 543   | 0        | 490      | 121     | 0            |
| 25  | s     | 465   | 0        | 393      | 92      | 0            |
| 25  | y     | 470   | 0        | 465      | 120     | 0            |
| 26  | 2     | 47    | 0        | 67       | 14      | 0            |
| 26  | 6     | 47    | 0        | 67       | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | B     | 142   | 0        | 206      | 18      | 0            |
| 26  | C     | 147   | 74       | 222      | 10      | 0            |
| 26  | D     | 49    | 0        | 74       | 10      | 0            |
| 26  | L     | 49    | 0        | 74       | 5       | 0            |
| 26  | N     | 49    | 0        | 74       | 11      | 0            |
| 26  | R     | 42    | 0        | 56       | 14      | 0            |
| 26  | S     | 98    | 0        | 148      | 13      | 0            |
| 26  | Y     | 98    | 0        | 146      | 20      | 0            |
| 26  | b     | 142   | 0        | 206      | 18      | 0            |
| 26  | c     | 147   | 74       | 222      | 10      | 0            |
| 26  | d     | 49    | 0        | 74       | 10      | 0            |
| 26  | l     | 49    | 0        | 74       | 5       | 0            |
| 26  | n     | 49    | 0        | 74       | 10      | 0            |
| 26  | r     | 42    | 0        | 56       | 16      | 0            |
| 26  | s     | 98    | 0        | 148      | 15      | 0            |
| 26  | y     | 98    | 0        | 146      | 20      | 0            |
| 27  | A     | 128   | 0        | 148      | 27      | 0            |
| 27  | a     | 128   | 0        | 148      | 28      | 0            |
| 28  | A     | 40    | 0        | 56       | 4       | 0            |
| 28  | B     | 120   | 0        | 168      | 18      | 0            |
| 28  | C     | 40    | 0        | 56       | 7       | 0            |
| 28  | D     | 40    | 0        | 56       | 3       | 0            |
| 28  | H     | 40    | 0        | 56       | 6       | 0            |
| 28  | I     | 40    | 0        | 56       | 20      | 0            |
| 28  | K     | 40    | 0        | 56       | 7       | 0            |
| 28  | T     | 40    | 0        | 54       | 20      | 0            |
| 28  | Z     | 40    | 0        | 56       | 5       | 0            |
| 28  | a     | 40    | 0        | 56       | 5       | 0            |
| 28  | b     | 120   | 0        | 168      | 19      | 0            |
| 28  | c     | 40    | 0        | 56       | 7       | 0            |
| 28  | d     | 40    | 0        | 56       | 3       | 0            |
| 28  | h     | 40    | 0        | 56       | 8       | 0            |
| 28  | i     | 40    | 0        | 56       | 20      | 0            |
| 28  | k     | 40    | 0        | 56       | 9       | 0            |
| 28  | t     | 40    | 0        | 54       | 21      | 0            |
| 28  | z     | 40    | 0        | 56       | 5       | 0            |
| 29  | A     | 104   | 0        | 145      | 13      | 0            |
| 29  | L     | 96    | 0        | 126      | 25      | 0            |
| 29  | a     | 104   | 0        | 145      | 12      | 0            |
| 29  | l     | 96    | 0        | 126      | 25      | 0            |
| 30  | A     | 88    | 0        | 116      | 6       | 0            |
| 30  | B     | 106   | 0        | 158      | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | C     | 51    | 0        | 72       | 4       | 0            |
| 30  | D     | 46    | 0        | 62       | 3       | 0            |
| 30  | a     | 88    | 0        | 116      | 6       | 0            |
| 30  | b     | 106   | 0        | 158      | 10      | 0            |
| 30  | c     | 51    | 0        | 72       | 4       | 0            |
| 30  | d     | 46    | 0        | 62       | 3       | 0            |
| 31  | A     | 13    | 0        | 7        | 2       | 0            |
| 31  | D     | 55    | 0        | 80       | 6       | 0            |
| 31  | a     | 13    | 0        | 7        | 2       | 0            |
| 31  | d     | 55    | 0        | 80       | 6       | 0            |
| 32  | A     | 85    | 92       | 0        | 0       | 0            |
| 32  | B     | 85    | 92       | 0        | 0       | 0            |
| 32  | G     | 42    | 53       | 0        | 0       | 0            |
| 32  | N     | 84    | 106      | 0        | 3       | 0            |
| 32  | S     | 42    | 53       | 0        | 2       | 0            |
| 32  | Y     | 210   | 265      | 0        | 7       | 0            |
| 32  | a     | 85    | 92       | 0        | 0       | 0            |
| 32  | b     | 85    | 92       | 0        | 0       | 0            |
| 32  | g     | 42    | 53       | 0        | 0       | 0            |
| 32  | n     | 84    | 106      | 0        | 3       | 0            |
| 32  | s     | 42    | 53       | 0        | 2       | 0            |
| 32  | y     | 210   | 265      | 0        | 7       | 0            |
| 33  | A     | 4     | 0        | 1        | 2       | 0            |
| 33  | a     | 4     | 0        | 1        | 1       | 0            |
| 34  | A     | 1     | 0        | 0        | 0       | 0            |
| 34  | a     | 1     | 0        | 0        | 0       | 0            |
| 35  | A     | 59    | 0        | 76       | 3       | 0            |
| 35  | B     | 62    | 0        | 82       | 5       | 0            |
| 35  | C     | 117   | 0        | 150      | 18      | 0            |
| 35  | a     | 59    | 0        | 76       | 3       | 0            |
| 35  | b     | 62    | 0        | 82       | 6       | 0            |
| 35  | c     | 117   | 0        | 150      | 17      | 0            |
| 36  | A     | 1     | 0        | 0        | 0       | 0            |
| 36  | B     | 1     | 0        | 0        | 0       | 0            |
| 36  | a     | 1     | 0        | 0        | 0       | 0            |
| 36  | b     | 1     | 0        | 0        | 0       | 0            |
| 37  | D     | 1     | 0        | 0        | 1       | 0            |
| 37  | d     | 1     | 0        | 0        | 1       | 0            |
| 38  | F     | 43    | 0        | 30       | 7       | 0            |
| 38  | f     | 43    | 0        | 30       | 8       | 0            |
| 39  | G     | 84    | 0        | 112      | 30      | 0            |
| 39  | N     | 84    | 0        | 112      | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | R     | 42    | 0        | 56       | 6       | 0            |
| 39  | S     | 84    | 0        | 112      | 27      | 0            |
| 39  | Y     | 84    | 0        | 112      | 25      | 0            |
| 39  | g     | 84    | 0        | 112      | 30      | 0            |
| 39  | n     | 84    | 0        | 112      | 27      | 0            |
| 39  | r     | 42    | 0        | 56       | 8       | 0            |
| 39  | s     | 84    | 0        | 112      | 29      | 0            |
| 39  | y     | 84    | 0        | 112      | 25      | 0            |
| 40  | G     | 44    | 0        | 56       | 15      | 0            |
| 40  | N     | 44    | 0        | 56       | 15      | 0            |
| 40  | R     | 44    | 0        | 56       | 8       | 0            |
| 40  | S     | 44    | 0        | 56       | 6       | 0            |
| 40  | Y     | 44    | 0        | 56       | 7       | 0            |
| 40  | g     | 44    | 0        | 56       | 15      | 0            |
| 40  | n     | 44    | 0        | 56       | 13      | 0            |
| 40  | r     | 44    | 0        | 56       | 10      | 0            |
| 40  | s     | 44    | 0        | 56       | 5       | 0            |
| 40  | y     | 44    | 0        | 56       | 10      | 0            |
| 41  | R     | 44    | 0        | 56       | 20      | 0            |
| 41  | r     | 44    | 0        | 56       | 22      | 0            |
| 42  | A     | 23    | 0        | 0        | 0       | 0            |
| 42  | B     | 10    | 0        | 0        | 3       | 0            |
| 42  | C     | 14    | 0        | 0        | 1       | 0            |
| 42  | D     | 14    | 0        | 0        | 0       | 0            |
| 42  | H     | 1     | 0        | 0        | 0       | 0            |
| 42  | I     | 1     | 0        | 0        | 0       | 0            |
| 42  | L     | 3     | 0        | 0        | 2       | 0            |
| 42  | M     | 1     | 0        | 0        | 0       | 0            |
| 42  | T     | 1     | 0        | 0        | 0       | 0            |
| 42  | W     | 1     | 0        | 0        | 0       | 0            |
| 42  | a     | 23    | 0        | 0        | 1       | 0            |
| 42  | b     | 10    | 0        | 0        | 3       | 0            |
| 42  | c     | 14    | 0        | 0        | 1       | 0            |
| 42  | d     | 14    | 0        | 0        | 0       | 0            |
| 42  | h     | 1     | 0        | 0        | 0       | 0            |
| 42  | i     | 1     | 0        | 0        | 0       | 0            |
| 42  | l     | 3     | 0        | 0        | 2       | 0            |
| 42  | m     | 2     | 0        | 0        | 0       | 0            |
| 42  | t     | 1     | 0        | 0        | 0       | 0            |
| 42  | w     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 84427 | 1470     | 83152    | 8481    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 51.

All (8481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:196:TYR:HB2  | 15:O:212:LEU:HD21 | 1.21                     | 1.19              |
| 10:h:56:ILE:HD13  | 18:x:84:LYS:HE3   | 1.25                     | 1.17              |
| 21:n:138:ILE:HG21 | 24:n:606:CHL:HBC1 | 1.23                     | 1.17              |
| 22:r:144:GLY:HA3  | 22:r:246:ALA:HB1  | 1.28                     | 1.16              |
| 22:R:144:GLY:HA3  | 22:R:246:ALA:HB1  | 1.28                     | 1.14              |
| 21:g:97:GLU:HG3   | 21:g:190:LEU:HD21 | 1.31                     | 1.13              |
| 21:n:97:GLU:HG3   | 21:n:190:LEU:HD21 | 1.31                     | 1.13              |
| 21:y:138:ILE:HG21 | 24:y:307:CHL:HBC1 | 1.26                     | 1.12              |
| 21:G:97:GLU:HG3   | 21:G:190:LEU:HD21 | 1.31                     | 1.12              |
| 2:2:175:GLY:HA3   | 2:2:181:LEU:HD11  | 1.32                     | 1.12              |
| 1:5:178:ALA:HA    | 2:6:64:VAL:HG21   | 1.12                     | 1.12              |
| 24:n:609:CHL:HAA2 | 21:y:82:THR:HG21  | 1.28                     | 1.12              |
| 21:Y:97:GLU:HG3   | 21:Y:190:LEU:HD21 | 1.31                     | 1.11              |
| 21:G:138:ILE:HG21 | 24:G:606:CHL:HBC1 | 1.17                     | 1.11              |
| 1:1:97:GLU:HG3    | 1:1:190:LEU:HD21  | 1.31                     | 1.11              |
| 1:5:97:GLU:HG3    | 1:5:190:LEU:HD21  | 1.31                     | 1.11              |
| 1:7:97:GLU:HG3    | 1:7:190:LEU:HD21  | 1.31                     | 1.11              |
| 21:n:97:GLU:HA    | 21:n:190:LEU:HD11 | 1.33                     | 1.11              |
| 21:Y:138:ILE:HG21 | 24:Y:307:CHL:HBC1 | 1.26                     | 1.11              |
| 2:6:97:ALA:HA     | 2:6:190:LEU:HD21  | 1.32                     | 1.11              |
| 21:G:97:GLU:HA    | 21:G:190:LEU:HD11 | 1.33                     | 1.10              |
| 24:N:609:CHL:HAA2 | 21:Y:82:THR:HG21  | 1.28                     | 1.10              |
| 21:N:138:ILE:HG21 | 24:N:606:CHL:HBC1 | 1.23                     | 1.09              |
| 21:Y:97:GLU:HA    | 21:Y:190:LEU:HD11 | 1.33                     | 1.09              |
| 21:N:97:GLU:HG3   | 21:N:190:LEU:HD21 | 1.31                     | 1.09              |
| 10:H:56:ILE:HD13  | 18:X:84:LYS:HE3   | 1.25                     | 1.09              |
| 21:N:97:GLU:HA    | 21:N:190:LEU:HD11 | 1.33                     | 1.09              |
| 15:o:196:TYR:HB2  | 15:o:212:LEU:HD21 | 1.21                     | 1.09              |
| 21:G:76:GLY:HA3   | 21:G:216:LEU:HD23 | 1.35                     | 1.08              |
| 21:N:76:GLY:HA3   | 21:N:216:LEU:HD23 | 1.35                     | 1.08              |
| 21:y:76:GLY:HA3   | 21:y:216:LEU:HD23 | 1.35                     | 1.08              |
| 1:1:178:ALA:HA    | 2:2:64:VAL:HG21   | 1.12                     | 1.08              |
| 1:5:97:GLU:HA     | 1:5:190:LEU:HD11  | 1.33                     | 1.08              |
| 1:1:76:GLY:HA3    | 1:1:216:LEU:HD23  | 1.35                     | 1.08              |
| 1:3:97:GLU:HG3    | 1:3:190:LEU:HD21  | 1.31                     | 1.08              |
| 21:y:98:LEU:HD22  | 25:y:304:CLA:HAA2 | 1.35                     | 1.08              |
| 24:y:308:CHL:H8   | 24:y:308:CHL:H41  | 1.33                     | 1.07              |
| 2:6:175:GLY:HA3   | 2:6:181:LEU:HD11  | 1.32                     | 1.07              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Y:308:CHL:H8   | 24:Y:308:CHL:H41  | 1.33                     | 1.07              |
| 1:7:76:GLY:HA3    | 1:7:216:LEU:HD23  | 1.35                     | 1.07              |
| 21:g:138:ILE:HG21 | 24:g:606:CHL:HBC1 | 1.17                     | 1.07              |
| 21:Y:76:GLY:HA3   | 21:Y:216:LEU:HD23 | 1.35                     | 1.07              |
| 5:B:72:THR:HG23   | 5:B:80:ILE:HG22   | 1.36                     | 1.06              |
| 1:7:97:GLU:HA     | 1:7:190:LEU:HD11  | 1.33                     | 1.06              |
| 21:g:97:GLU:HA    | 21:g:190:LEU:HD11 | 1.33                     | 1.06              |
| 21:y:97:GLU:HA    | 21:y:190:LEU:HD11 | 1.33                     | 1.06              |
| 21:y:97:GLU:HG3   | 21:y:190:LEU:HD21 | 1.31                     | 1.06              |
| 21:n:76:GLY:HA3   | 21:n:216:LEU:HD23 | 1.35                     | 1.06              |
| 1:3:97:GLU:HA     | 1:3:190:LEU:HD11  | 1.33                     | 1.06              |
| 24:n:607:CHL:H11  | 24:y:302:CHL:H191 | 1.37                     | 1.06              |
| 2:2:97:ALA:HA     | 2:2:190:LEU:HD21  | 1.32                     | 1.05              |
| 1:1:97:GLU:HA     | 1:1:190:LEU:HD11  | 1.33                     | 1.05              |
| 1:3:76:GLY:HA3    | 1:3:216:LEU:HD23  | 1.35                     | 1.05              |
| 23:u:85:LYS:HG2   | 23:u:101:CYS:HB3  | 1.36                     | 1.05              |
| 5:b:72:THR:HG23   | 5:b:80:ILE:HG22   | 1.36                     | 1.05              |
| 21:Y:98:LEU:HD22  | 25:Y:304:CLA:HAA2 | 1.35                     | 1.04              |
| 21:Y:60:GLY:HA3   | 24:Y:302:CHL:HMC  | 1.39                     | 1.04              |
| 21:g:76:GLY:HA3   | 21:g:216:LEU:HD23 | 1.35                     | 1.03              |
| 1:3:55:ARG:HH12   | 1:3:72:GLY:HA3    | 1.23                     | 1.03              |
| 1:5:76:GLY:HA3    | 1:5:216:LEU:HD23  | 1.35                     | 1.03              |
| 1:7:55:ARG:HH12   | 1:7:72:GLY:HA3    | 1.23                     | 1.03              |
| 2:6:178:ILE:HD11  | 1:7:62:PHE:HA     | 1.41                     | 1.03              |
| 3:8:73:LEU:HG     | 3:8:82:GLY:HA2    | 1.41                     | 1.02              |
| 3:8:133:GLN:HG2   | 3:8:134:PRO:HD3   | 1.41                     | 1.02              |
| 21:g:55:ARG:HH12  | 21:g:72:GLY:HA3   | 1.23                     | 1.02              |
| 21:y:60:GLY:HA3   | 24:y:302:CHL:HMC  | 1.39                     | 1.02              |
| 25:y:311:CLA:H51  | 25:y:313:CLA:HMA1 | 1.37                     | 1.02              |
| 23:U:85:LYS:HG2   | 23:U:101:CYS:HB3  | 1.36                     | 1.02              |
| 25:B:607:CLA:H171 | 25:B:613:CLA:H161 | 1.38                     | 1.02              |
| 3:4:133:GLN:HG2   | 3:4:134:PRO:HD3   | 1.42                     | 1.02              |
| 21:Y:55:ARG:HH12  | 21:Y:72:GLY:HA3   | 1.23                     | 1.02              |
| 1:1:55:ARG:HH12   | 1:1:72:GLY:HA3    | 1.23                     | 1.01              |
| 25:Y:311:CLA:H51  | 25:Y:313:CLA:HMA1 | 1.37                     | 1.01              |
| 3:8:78:PRO:HG3    | 3:8:225:LYS:HB3   | 1.38                     | 1.01              |
| 24:N:607:CHL:H11  | 24:Y:302:CHL:H191 | 1.38                     | 1.01              |
| 21:n:55:ARG:HH12  | 21:n:72:GLY:HA3   | 1.23                     | 1.01              |
| 15:o:130:LYS:HE2  | 15:o:177:PRO:HB2  | 1.43                     | 1.01              |
| 2:2:89:PRO:HA     | 2:2:92:PHE:HD2    | 1.22                     | 1.01              |
| 1:5:55:ARG:HH12   | 1:5:72:GLY:HA3    | 1.23                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:55:ARG:HH12  | 21:G:72:GLY:HA3   | 1.23                     | 1.00              |
| 2:2:179:ASN:HA    | 24:2:603:CHL:HMC  | 1.43                     | 1.00              |
| 2:6:89:PRO:HA     | 2:6:92:PHE:HD2    | 1.22                     | 1.00              |
| 25:b:607:CLA:H171 | 25:b:613:CLA:H161 | 1.38                     | 1.00              |
| 21:N:55:ARG:HH12  | 21:N:72:GLY:HA3   | 1.23                     | 1.00              |
| 3:4:78:PRO:HG3    | 3:4:225:LYS:HB3   | 1.38                     | 1.00              |
| 2:6:120:GLN:HG3   | 2:6:125:VAL:HA    | 1.44                     | 1.00              |
| 23:U:97:THR:HA    | 23:U:102:ARG:HH21 | 1.26                     | 0.99              |
| 3:4:103:LEU:HD11  | 3:4:194:TYR:HD1   | 1.28                     | 0.99              |
| 2:2:120:GLN:HG3   | 2:2:125:VAL:HA    | 1.44                     | 0.99              |
| 22:R:58:TRP:HE1   | 25:R:601:CLA:HAA1 | 1.26                     | 0.99              |
| 7:d:15:LEU:HD11   | 18:x:103:VAL:HG13 | 1.42                     | 0.99              |
| 5:b:272:ARG:HH12  | 5:b:361:THR:HG21  | 1.26                     | 0.99              |
| 7:d:173:SER:HB2   | 7:d:178:ALA:HB1   | 1.45                     | 0.99              |
| 23:u:97:THR:HA    | 23:u:102:ARG:HH21 | 1.26                     | 0.99              |
| 2:2:178:ILE:HD11  | 1:3:62:PHE:HA     | 1.41                     | 0.99              |
| 7:D:15:LEU:HD11   | 18:X:103:VAL:HG13 | 1.42                     | 0.99              |
| 15:O:130:LYS:HE2  | 15:O:177:PRO:HB2  | 1.43                     | 0.99              |
| 3:8:222:GLU:HG2   | 3:8:225:LYS:HD3   | 1.45                     | 0.99              |
| 7:D:173:SER:HB2   | 7:D:178:ALA:HB1   | 1.45                     | 0.98              |
| 22:r:58:TRP:HE1   | 25:r:601:CLA:HAA1 | 1.26                     | 0.98              |
| 3:4:73:LEU:HG     | 3:4:82:GLY:HA2    | 1.41                     | 0.98              |
| 10:h:18:THR:HA    | 10:h:21:LYS:HD3   | 1.46                     | 0.98              |
| 3:4:222:GLU:HG2   | 3:4:225:LYS:HD3   | 1.45                     | 0.98              |
| 20:S:72:PRO:HG2   | 20:S:75:LEU:HD13  | 1.43                     | 0.98              |
| 5:B:272:ARG:HH12  | 5:B:361:THR:HG21  | 1.26                     | 0.98              |
| 11:i:33:GLY:O     | 11:i:34:ARG:HG3   | 1.64                     | 0.98              |
| 5:B:243:ALA:HA    | 5:B:246:PHE:CE1   | 2.00                     | 0.97              |
| 5:b:53:ASP:OD2    | 5:b:58:GLN:NE2    | 1.97                     | 0.97              |
| 21:y:55:ARG:HH12  | 21:y:72:GLY:HA3   | 1.23                     | 0.97              |
| 21:Y:251:PRO:HB2  | 25:Y:315:CLA:HMA1 | 1.46                     | 0.97              |
| 40:Y:318:NEX:H28  | 40:Y:318:NEX:H361 | 1.45                     | 0.97              |
| 2:6:179:ASN:HA    | 24:6:603:CHL:HMC  | 1.43                     | 0.97              |
| 1:3:67:PRO:HG2    | 1:3:70:LEU:HD12   | 1.47                     | 0.97              |
| 2:6:145:LEU:HD22  | 2:6:154:VAL:HG22  | 1.47                     | 0.97              |
| 3:8:103:LEU:HD11  | 3:8:194:TYR:HD1   | 1.28                     | 0.97              |
| 20:s:59:LEU:HD11  | 20:s:216:GLU:HG3  | 1.47                     | 0.97              |
| 25:B:604:CLA:H142 | 25:B:615:CLA:HMA1 | 1.46                     | 0.97              |
| 21:N:67:PRO:HG2   | 21:N:70:LEU:HD12  | 1.47                     | 0.97              |
| 29:L:101:SQD:H132 | 29:L:101:SQD:H271 | 1.47                     | 0.96              |
| 6:c:151:TRP:HB2   | 17:w:133:LEU:HD21 | 1.48                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:67:PRO:HG2   | 21:n:70:LEU:HD12  | 1.47                     | 0.96              |
| 10:H:18:THR:HA    | 10:H:21:LYS:HD3   | 1.46                     | 0.96              |
| 21:y:67:PRO:HG2   | 21:y:70:LEU:HD12  | 1.47                     | 0.96              |
| 1:5:209:ALA:HA    | 1:5:212:LYS:HG3   | 1.48                     | 0.96              |
| 20:S:236:MET:HE2  | 39:S:316:LUT:H12  | 1.48                     | 0.96              |
| 21:G:67:PRO:HG2   | 21:G:70:LEU:HD12  | 1.47                     | 0.96              |
| 21:Y:67:PRO:HG2   | 21:Y:70:LEU:HD12  | 1.47                     | 0.96              |
| 5:b:243:ALA:HA    | 5:b:246:PHE:CE1   | 1.99                     | 0.96              |
| 21:N:138:ILE:HG13 | 21:N:144:LEU:HB2  | 1.48                     | 0.96              |
| 1:5:138:ILE:HG13  | 1:5:144:LEU:HB2   | 1.48                     | 0.96              |
| 2:2:145:LEU:HD22  | 2:2:154:VAL:HG22  | 1.46                     | 0.96              |
| 25:b:604:CLA:H142 | 25:b:615:CLA:HMA1 | 1.46                     | 0.96              |
| 1:3:209:ALA:HA    | 1:3:212:LYS:HG3   | 1.48                     | 0.95              |
| 5:B:53:ASP:OD2    | 5:B:58:GLN:NE2    | 1.97                     | 0.95              |
| 21:g:209:ALA:HA   | 21:g:212:LYS:HG3  | 1.48                     | 0.95              |
| 24:n:607:CHL:H203 | 25:y:303:CLA:H161 | 1.47                     | 0.95              |
| 11:I:33:GLY:O     | 11:I:34:ARG:HG3   | 1.64                     | 0.95              |
| 20:s:236:MET:HE2  | 39:s:316:LUT:H12  | 1.47                     | 0.95              |
| 21:y:209:ALA:HA   | 21:y:212:LYS:HG3  | 1.48                     | 0.95              |
| 7:D:183:ILE:HG23  | 25:D:402:CLA:HAC1 | 1.48                     | 0.95              |
| 20:s:72:PRO:HG2   | 20:s:75:LEU:HD13  | 1.43                     | 0.95              |
| 20:S:59:LEU:HD11  | 20:S:216:GLU:HG3  | 1.47                     | 0.95              |
| 1:7:209:ALA:HA    | 1:7:212:LYS:HG3   | 1.48                     | 0.95              |
| 21:g:98:LEU:HD22  | 25:g:603:CLA:HAA1 | 1.47                     | 0.95              |
| 21:y:138:ILE:HG13 | 21:y:144:LEU:HB2  | 1.48                     | 0.95              |
| 21:N:209:ALA:HA   | 21:N:212:LYS:HG3  | 1.48                     | 0.95              |
| 21:Y:138:ILE:HG13 | 21:Y:144:LEU:HB2  | 1.48                     | 0.95              |
| 21:Y:209:ALA:HA   | 21:Y:212:LYS:HG3  | 1.48                     | 0.95              |
| 1:1:209:ALA:HA    | 1:1:212:LYS:HG3   | 1.48                     | 0.94              |
| 21:g:138:ILE:HG13 | 21:g:144:LEU:HB2  | 1.48                     | 0.94              |
| 24:r:607:CHL:HAB  | 24:r:607:CHL:H112 | 1.49                     | 0.94              |
| 24:N:607:CHL:H203 | 25:Y:303:CLA:H161 | 1.47                     | 0.94              |
| 21:Y:122:ASN:HB3  | 32:Y:320:AJP:C80  | 1.97                     | 0.94              |
| 40:y:318:NEX:H28  | 40:y:318:NEX:H361 | 1.45                     | 0.94              |
| 7:d:183:ILE:HG23  | 25:d:402:CLA:HAC1 | 1.48                     | 0.94              |
| 1:7:67:PRO:HG2    | 1:7:70:LEU:HD12   | 1.47                     | 0.94              |
| 21:y:251:PRO:HB2  | 25:y:315:CLA:HMA1 | 1.46                     | 0.94              |
| 5:B:460:LEU:HD11  | 7:D:288:VAL:HG21  | 1.48                     | 0.94              |
| 21:G:209:ALA:HA   | 21:G:212:LYS:HG3  | 1.48                     | 0.94              |
| 4:a:235:GLU:HB3   | 7:d:264:ASN:HD21  | 1.32                     | 0.94              |
| 21:G:91:THR:OG1   | 21:N:84:GLY:O     | 1.85                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:122:ASN:HB3  | 32:y:320:AJP:C80  | 1.97                     | 0.94              |
| 21:G:98:LEU:HD22  | 25:G:603:CLA:HAA1 | 1.47                     | 0.94              |
| 21:G:138:ILE:HG13 | 21:G:144:LEU:HB2  | 1.48                     | 0.94              |
| 25:G:611:CLA:HHC  | 25:G:611:CLA:HBB1 | 1.49                     | 0.94              |
| 21:n:138:ILE:HG13 | 21:n:144:LEU:HB2  | 1.48                     | 0.94              |
| 21:g:91:THR:OG1   | 21:n:84:GLY:O     | 1.85                     | 0.93              |
| 20:S:225:GLU:HB2  | 25:S:310:CLA:C1B  | 1.97                     | 0.93              |
| 4:a:225:ARG:HD3   | 22:r:102:ALA:HB1  | 1.50                     | 0.93              |
| 1:1:67:PRO:HG2    | 1:1:70:LEU:HD12   | 1.47                     | 0.93              |
| 6:C:151:TRP:HB2   | 17:W:133:LEU:HD21 | 1.48                     | 0.93              |
| 21:g:67:PRO:HG2   | 21:g:70:LEU:HD12  | 1.47                     | 0.93              |
| 5:b:460:LEU:HD11  | 7:d:288:VAL:HG21  | 1.48                     | 0.93              |
| 29:l:102:SQD:H132 | 29:l:102:SQD:H271 | 1.47                     | 0.93              |
| 1:1:138:ILE:HG13  | 1:1:144:LEU:HB2   | 1.48                     | 0.93              |
| 1:1:168:LEU:O     | 1:1:172:VAL:HG23  | 1.68                     | 0.93              |
| 1:3:168:LEU:O     | 1:3:172:VAL:HG23  | 1.68                     | 0.93              |
| 1:7:138:ILE:HG13  | 1:7:144:LEU:HB2   | 1.48                     | 0.93              |
| 24:R:607:CHL:HAB  | 24:R:607:CHL:H112 | 1.49                     | 0.93              |
| 20:s:225:GLU:HB2  | 25:s:310:CLA:C1B  | 1.97                     | 0.93              |
| 21:g:168:LEU:O    | 21:g:172:VAL:HG23 | 1.68                     | 0.93              |
| 21:n:168:LEU:O    | 21:n:172:VAL:HG23 | 1.69                     | 0.93              |
| 21:n:209:ALA:HA   | 21:n:212:LYS:HG3  | 1.48                     | 0.93              |
| 1:3:138:ILE:HG13  | 1:3:144:LEU:HB2   | 1.48                     | 0.92              |
| 1:5:168:LEU:O     | 1:5:172:VAL:HG23  | 1.69                     | 0.92              |
| 25:g:611:CLA:HHC  | 25:g:611:CLA:HBB1 | 1.49                     | 0.92              |
| 21:y:168:LEU:O    | 21:y:172:VAL:HG23 | 1.69                     | 0.92              |
| 1:5:67:PRO:HG2    | 1:5:70:LEU:HD12   | 1.47                     | 0.92              |
| 1:7:168:LEU:O     | 1:7:172:VAL:HG23  | 1.69                     | 0.92              |
| 3:4:103:LEU:HD13  | 3:4:193:GLY:HA3   | 1.52                     | 0.92              |
| 2:2:174:GLU:CG    | 1:3:59:LEU:HD22   | 1.99                     | 0.92              |
| 1:5:178:ALA:CA    | 2:6:64:VAL:HG21   | 1.99                     | 0.92              |
| 21:N:168:LEU:O    | 21:N:172:VAL:HG23 | 1.68                     | 0.92              |
| 3:8:103:LEU:HD13  | 3:8:193:GLY:HA3   | 1.52                     | 0.92              |
| 15:o:298:GLU:OE1  | 15:o:328:TYR:OH   | 1.86                     | 0.92              |
| 28:T:101:BCR:H362 | 28:T:101:BCR:H292 | 1.52                     | 0.92              |
| 21:Y:168:LEU:O    | 21:Y:172:VAL:HG23 | 1.68                     | 0.92              |
| 4:A:235:GLU:HB3   | 7:D:264:ASN:HD21  | 1.32                     | 0.92              |
| 2:6:174:GLU:CG    | 1:7:59:LEU:HD22   | 1.99                     | 0.92              |
| 2:6:178:ILE:CD1   | 1:7:62:PHE:HA     | 2.00                     | 0.92              |
| 3:8:77:LEU:HG     | 3:8:78:PRO:HD2    | 1.51                     | 0.92              |
| 15:o:113:GLN:HE21 | 17:w:80:LEU:HD11  | 1.35                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:70:GLY:HA2    | 5:B:178:VAL:HG11  | 1.50                     | 0.92              |
| 21:y:104:ARG:HB3  | 25:y:311:CLA:HBC3 | 1.52                     | 0.92              |
| 5:b:70:GLY:HA2    | 5:b:178:VAL:HG11  | 1.50                     | 0.91              |
| 1:1:178:ALA:CA    | 2:2:64:VAL:HG21   | 1.99                     | 0.91              |
| 2:2:178:ILE:CD1   | 1:3:62:PHE:HA     | 2.00                     | 0.91              |
| 3:4:77:LEU:HG     | 3:4:78:PRO:HD2    | 1.51                     | 0.91              |
| 4:A:225:ARG:HD3   | 22:R:102:ALA:HB1  | 1.50                     | 0.91              |
| 21:G:168:LEU:O    | 21:G:172:VAL:HG23 | 1.68                     | 0.91              |
| 15:O:298:GLU:OE1  | 15:O:328:TYR:OH   | 1.86                     | 0.91              |
| 10:h:17:THR:HG23  | 10:h:20:GLY:H     | 1.34                     | 0.91              |
| 25:6:605:CLA:HAA1 | 25:6:605:CLA:HBD  | 1.51                     | 0.91              |
| 21:Y:104:ARG:HB3  | 25:Y:311:CLA:HBC3 | 1.52                     | 0.91              |
| 3:4:194:TYR:HE2   | 3:4:221:LEU:HB2   | 1.35                     | 0.91              |
| 1:1:55:ARG:NH1    | 1:1:72:GLY:HA3    | 1.86                     | 0.91              |
| 20:s:115:LEU:HD12 | 20:s:200:LEU:HD13 | 1.53                     | 0.91              |
| 10:H:17:THR:HG23  | 10:H:20:GLY:H     | 1.34                     | 0.90              |
| 25:N:613:CLA:H143 | 25:N:613:CLA:H8   | 1.54                     | 0.90              |
| 25:c:511:CLA:H162 | 19:z:20:LEU:HD12  | 1.53                     | 0.90              |
| 21:G:55:ARG:NH1   | 21:G:72:GLY:HA3   | 1.86                     | 0.90              |
| 1:7:55:ARG:NH1    | 1:7:72:GLY:HA3    | 1.86                     | 0.90              |
| 4:a:192:ILE:HG21  | 25:a:402:CLA:HHD  | 1.53                     | 0.90              |
| 5:b:141:ILE:HG21  | 25:b:615:CLA:HBB1 | 1.53                     | 0.90              |
| 6:c:163:ILE:HG21  | 25:c:512:CLA:HAB  | 1.53                     | 0.90              |
| 2:6:55:ARG:NH1    | 2:6:77:ASP:O      | 2.05                     | 0.90              |
| 1:3:55:ARG:NH1    | 1:3:72:GLY:HA3    | 1.86                     | 0.90              |
| 15:O:196:TYR:HB2  | 15:O:212:LEU:CD2  | 2.02                     | 0.90              |
| 25:2:605:CLA:HBD  | 25:2:605:CLA:HAA1 | 1.51                     | 0.90              |
| 7:d:187:GLN:HB2   | 25:d:402:CLA:HBC1 | 1.53                     | 0.90              |
| 15:o:145:VAL:HG11 | 15:o:203:LEU:HD11 | 1.54                     | 0.90              |
| 2:2:55:ARG:NH1    | 2:2:77:ASP:O      | 2.05                     | 0.90              |
| 25:C:511:CLA:H162 | 19:Z:20:LEU:HD12  | 1.54                     | 0.90              |
| 4:A:220:THR:O     | 7:D:140:ARG:NH2   | 2.04                     | 0.89              |
| 6:C:163:ILE:HG21  | 25:C:512:CLA:HAB  | 1.53                     | 0.89              |
| 21:N:55:ARG:NH1   | 21:N:72:GLY:HA3   | 1.86                     | 0.89              |
| 7:D:187:GLN:HB2   | 25:D:402:CLA:HBC1 | 1.53                     | 0.89              |
| 25:c:501:CLA:HHB  | 28:i:101:BCR:H271 | 1.54                     | 0.89              |
| 25:n:613:CLA:H143 | 25:n:613:CLA:H8   | 1.53                     | 0.89              |
| 2:2:145:LEU:HD23  | 2:2:154:VAL:HA    | 1.55                     | 0.89              |
| 2:2:174:GLU:HB3   | 1:3:62:PHE:CB     | 2.03                     | 0.89              |
| 1:5:55:ARG:NH1    | 1:5:72:GLY:HA3    | 1.86                     | 0.89              |
| 3:8:194:TYR:HE2   | 3:8:221:LEU:HB2   | 1.35                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:t:101:BCR:H362 | 28:t:101:BCR:H292 | 1.52                     | 0.89              |
| 2:6:179:ASN:HA    | 24:6:603:CHL:CMC  | 2.03                     | 0.89              |
| 4:a:220:THR:O     | 7:d:140:ARG:NH2   | 2.04                     | 0.89              |
| 11:I:34:ARG:HH11  | 11:I:35:GLU:HG2   | 1.38                     | 0.89              |
| 1:7:114:VAL:HG13  | 1:7:241:LEU:HD11  | 1.55                     | 0.89              |
| 25:C:501:CLA:HBB  | 28:I:101:BCR:H271 | 1.54                     | 0.89              |
| 2:6:145:LEU:HD23  | 2:6:154:VAL:HA    | 1.55                     | 0.89              |
| 2:6:174:GLU:HB3   | 1:7:62:PHE:CB     | 2.03                     | 0.89              |
| 21:y:55:ARG:NH1   | 21:y:72:GLY:HA3   | 1.86                     | 0.89              |
| 20:S:115:LEU:HD12 | 20:S:200:LEU:HD13 | 1.53                     | 0.89              |
| 21:Y:55:ARG:NH1   | 21:Y:72:GLY:HA3   | 1.86                     | 0.89              |
| 4:A:192:ILE:HG21  | 25:A:401:CLA:HHD  | 1.53                     | 0.89              |
| 1:5:114:VAL:HG13  | 1:5:241:LEU:HD11  | 1.55                     | 0.89              |
| 3:8:103:LEU:HD11  | 3:8:194:TYR:CD1   | 2.08                     | 0.89              |
| 5:B:141:ILE:HG21  | 25:B:615:CLA:HBB1 | 1.53                     | 0.89              |
| 15:o:196:TYR:HB2  | 15:o:212:LEU:CD2  | 2.02                     | 0.89              |
| 21:n:55:ARG:NH1   | 21:n:72:GLY:HA3   | 1.86                     | 0.89              |
| 25:G:611:CLA:HBC1 | 26:Y:301:LHG:H292 | 1.56                     | 0.88              |
| 11:i:34:ARG:HH11  | 11:i:35:GLU:HG2   | 1.38                     | 0.88              |
| 21:g:55:ARG:NH1   | 21:g:72:GLY:HA3   | 1.86                     | 0.88              |
| 1:3:114:VAL:HG13  | 1:3:241:LEU:HD11  | 1.55                     | 0.88              |
| 15:O:145:VAL:HG11 | 15:O:203:LEU:HD11 | 1.54                     | 0.88              |
| 2:6:188:ASN:O     | 24:6:603:CHL:HBC1 | 1.73                     | 0.88              |
| 25:y:304:CLA:HMC3 | 25:y:304:CLA:HBC3 | 1.55                     | 0.88              |
| 6:c:221:GLU:O     | 6:c:226:SER:OG    | 1.91                     | 0.88              |
| 2:2:179:ASN:HA    | 24:2:603:CHL:CMC  | 2.03                     | 0.88              |
| 25:a:406:CLA:HMC1 | 11:i:11:VAL:HG11  | 1.56                     | 0.88              |
| 25:r:610:CLA:HBC3 | 26:r:618:LHG:HC5  | 1.55                     | 0.88              |
| 2:2:188:ASN:O     | 24:2:603:CHL:HBC1 | 1.73                     | 0.88              |
| 15:O:113:GLN:HE21 | 17:W:80:LEU:HD11  | 1.35                     | 0.88              |
| 25:g:611:CLA:HBC1 | 26:y:301:LHG:H292 | 1.56                     | 0.88              |
| 25:R:614:CLA:HBC3 | 25:R:614:CLA:HHD  | 1.56                     | 0.88              |
| 3:4:103:LEU:HD11  | 3:4:194:TYR:CD1   | 2.08                     | 0.87              |
| 25:S:310:CLA:H51  | 25:S:312:CLA:HMA1 | 1.56                     | 0.87              |
| 4:a:76:ASN:HB2    | 13:l:34:ASN:HD22  | 1.40                     | 0.87              |
| 21:g:98:LEU:HD22  | 25:g:603:CLA:CAA  | 2.04                     | 0.87              |
| 3:4:177:PRO:HG3   | 25:R:610:CLA:HBB2 | 1.57                     | 0.87              |
| 21:G:94:ARG:HG3   | 21:N:82:THR:O     | 1.74                     | 0.87              |
| 25:s:310:CLA:H51  | 25:s:312:CLA:HMA1 | 1.56                     | 0.87              |
| 3:8:177:PRO:HG3   | 25:r:610:CLA:HBB2 | 1.57                     | 0.87              |
| 4:a:74:GLY:HA3    | 7:d:305:ARG:NH1   | 1.90                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:n:610:CLA:H52  | 39:n:615:LUT:H28  | 1.57                     | 0.87              |
| 5:B:472:ARG:HA    | 5:B:479:PHE:CE2   | 2.10                     | 0.87              |
| 25:A:405:CLA:HMC1 | 11:I:11:VAL:HG11  | 1.56                     | 0.87              |
| 21:G:231:VAL:HG11 | 25:G:613:CLA:HAC2 | 1.56                     | 0.87              |
| 6:c:457:LYS:HE2   | 7:d:230:ALA:HB2   | 1.57                     | 0.87              |
| 6:C:221:GLU:O     | 6:C:226:SER:OG    | 1.91                     | 0.86              |
| 6:C:457:LYS:HE2   | 7:D:230:ALA:HB2   | 1.57                     | 0.86              |
| 22:R:58:TRP:NE1   | 25:R:601:CLA:HAA1 | 1.90                     | 0.86              |
| 1:1:114:VAL:HG13  | 1:1:241:LEU:HD11  | 1.55                     | 0.86              |
| 8:E:27:ILE:HG23   | 8:E:28:PRO:HD3    | 1.57                     | 0.86              |
| 21:n:231:VAL:HG21 | 25:n:613:CLA:HAC1 | 1.57                     | 0.86              |
| 21:y:250:ASP:OD2  | 21:y:253:ASN:N    | 2.09                     | 0.86              |
| 25:S:313:CLA:HBB  | 39:S:315:LUT:H3   | 1.56                     | 0.86              |
| 8:e:27:ILE:HG23   | 8:e:28:PRO:HD3    | 1.58                     | 0.86              |
| 24:G:601:CHL:H122 | 24:Y:308:CHL:HAB  | 1.58                     | 0.86              |
| 24:Y:308:CHL:HHD  | 24:Y:308:CHL:HBC2 | 1.56                     | 0.86              |
| 3:8:174:TRP:CE3   | 3:8:180:LYS:HD2   | 2.11                     | 0.86              |
| 21:G:98:LEU:HD22  | 25:G:603:CLA:CAA  | 2.04                     | 0.86              |
| 5:b:472:ARG:HA    | 5:b:479:PHE:CE2   | 2.10                     | 0.86              |
| 4:A:76:ASN:HB2    | 13:L:34:ASN:HD22  | 1.40                     | 0.86              |
| 21:G:243:ASN:ND2  | 25:G:613:CLA:O1D  | 2.09                     | 0.86              |
| 21:G:232:GLN:HE21 | 25:G:613:CLA:C4D  | 1.85                     | 0.86              |
| 12:k:40:MET:HA    | 12:k:43:ILE:HD12  | 1.57                     | 0.86              |
| 25:s:313:CLA:HBB  | 39:s:315:LUT:H3   | 1.56                     | 0.86              |
| 21:Y:109:GLY:HA2  | 39:Y:317:LUT:H181 | 1.58                     | 0.86              |
| 7:d:183:ILE:CG2   | 25:d:402:CLA:HAC1 | 2.06                     | 0.86              |
| 22:r:58:TRP:NE1   | 25:r:601:CLA:HAA1 | 1.90                     | 0.86              |
| 25:R:610:CLA:HBC3 | 26:R:618:LHG:HC5  | 1.55                     | 0.86              |
| 3:8:221:LEU:O     | 3:8:225:LYS:HG3   | 1.76                     | 0.86              |
| 21:y:109:GLY:HA2  | 39:y:317:LUT:H181 | 1.58                     | 0.86              |
| 7:D:55:PHE:O      | 8:E:49:SER:OG     | 1.94                     | 0.86              |
| 20:S:246:THR:HG22 | 20:S:248:GLU:HG2  | 1.57                     | 0.86              |
| 24:y:308:CHL:HHD  | 24:y:308:CHL:HBC2 | 1.56                     | 0.86              |
| 3:4:221:LEU:O     | 3:4:225:LYS:HG3   | 1.76                     | 0.85              |
| 24:N:607:CHL:H18  | 24:N:609:CHL:H71  | 1.57                     | 0.85              |
| 25:Y:304:CLA:HMC3 | 25:Y:304:CLA:HBC3 | 1.55                     | 0.85              |
| 21:g:94:ARG:HG3   | 21:n:82:THR:O     | 1.74                     | 0.85              |
| 21:g:243:ASN:ND2  | 25:g:613:CLA:O1D  | 2.09                     | 0.85              |
| 24:g:601:CHL:H122 | 24:y:308:CHL:HAB  | 1.58                     | 0.85              |
| 25:n:602:CLA:H52  | 25:n:602:CLA:HMB3 | 1.58                     | 0.85              |
| 21:n:104:ARG:HB3  | 25:n:610:CLA:HBC3 | 1.58                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:614:CLA:HBC3 | 25:r:614:CLA:HHD  | 1.56                     | 0.85              |
| 4:A:74:GLY:HA3    | 7:D:305:ARG:NH1   | 1.90                     | 0.85              |
| 21:N:104:ARG:HB3  | 25:N:610:CLA:HBC3 | 1.59                     | 0.85              |
| 1:1:220:ARG:HA    | 1:1:223:MET:HE3   | 1.59                     | 0.85              |
| 20:s:89:VAL:HG11  | 20:s:111:GLN:NE2  | 1.91                     | 0.85              |
| 25:N:602:CLA:HMB3 | 25:N:602:CLA:H52  | 1.58                     | 0.85              |
| 21:Y:98:LEU:CD2   | 25:Y:304:CLA:HAA2 | 2.07                     | 0.85              |
| 2:6:120:GLN:OE1   | 2:6:129:GLU:HG3   | 1.76                     | 0.85              |
| 21:n:220:ARG:HA   | 21:n:223:MET:HE3  | 1.59                     | 0.85              |
| 5:B:277:GLN:NE2   | 35:B:626:DGD:O5E  | 2.10                     | 0.85              |
| 7:D:183:ILE:CG2   | 25:D:402:CLA:HAC1 | 2.06                     | 0.85              |
| 21:N:159:LEU:HD11 | 21:Y:257:TRP:CG   | 2.11                     | 0.85              |
| 12:K:40:MET:HA    | 12:K:43:ILE:HD12  | 1.57                     | 0.85              |
| 20:s:246:THR:HG22 | 20:s:248:GLU:HG2  | 1.57                     | 0.85              |
| 5:B:51:VAL:HG13   | 5:B:308:LYS:HG3   | 1.58                     | 0.85              |
| 26:D:406:LHG:H321 | 16:T:21:ILE:HD11  | 1.58                     | 0.85              |
| 18:X:84:LYS:O     | 18:X:87:LEU:HG    | 1.76                     | 0.85              |
| 25:N:610:CLA:H52  | 39:N:615:LUT:H28  | 1.57                     | 0.85              |
| 21:Y:250:ASP:OD2  | 21:Y:253:ASN:N    | 2.09                     | 0.85              |
| 2:2:120:GLN:OE1   | 2:2:129:GLU:HG3   | 1.76                     | 0.84              |
| 15:O:290:THR:HG22 | 15:O:291:LYS:H    | 1.41                     | 0.84              |
| 21:G:220:ARG:HA   | 21:G:223:MET:HE3  | 1.59                     | 0.84              |
| 2:6:117:GLU:HB2   | 2:6:241:PRO:HG2   | 1.58                     | 0.84              |
| 24:n:607:CHL:H18  | 24:n:609:CHL:H71  | 1.57                     | 0.84              |
| 2:2:146:ASP:O     | 2:2:152:ASN:ND2   | 2.11                     | 0.84              |
| 21:N:231:VAL:HG21 | 25:N:613:CLA:HAC1 | 1.57                     | 0.84              |
| 2:6:174:GLU:HG2   | 1:7:59:LEU:HD22   | 1.59                     | 0.84              |
| 26:d:406:LHG:H321 | 16:t:21:ILE:HD11  | 1.58                     | 0.84              |
| 18:x:84:LYS:O     | 18:x:87:LEU:HG    | 1.76                     | 0.84              |
| 21:y:98:LEU:CD2   | 25:y:304:CLA:HAA2 | 2.07                     | 0.84              |
| 1:3:220:ARG:HA    | 1:3:223:MET:HE3   | 1.59                     | 0.84              |
| 21:Y:98:LEU:HD22  | 25:Y:304:CLA:CAA  | 2.07                     | 0.84              |
| 5:b:460:LEU:CD1   | 7:d:288:VAL:HG21  | 2.07                     | 0.84              |
| 7:d:56:VAL:HG21   | 7:d:111:LEU:CD1   | 2.08                     | 0.84              |
| 3:4:175:ALA:HB2   | 22:R:59:TYR:HE2   | 1.41                     | 0.84              |
| 5:b:51:VAL:HG13   | 5:b:308:LYS:HG3   | 1.58                     | 0.84              |
| 15:o:202:GLN:HE21 | 15:o:206:GLY:HA2  | 1.43                     | 0.84              |
| 5:B:460:LEU:CD1   | 7:D:288:VAL:HG21  | 2.07                     | 0.84              |
| 13:L:5:ASN:ND2    | 13:L:8:GLU:OE1    | 2.10                     | 0.84              |
| 21:Y:220:ARG:HA   | 21:Y:223:MET:HE3  | 1.59                     | 0.84              |
| 7:d:55:PHE:O      | 8:e:49:SER:OG     | 1.93                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:220:ARG:HA   | 21:N:223:MET:HE3  | 1.59                     | 0.84              |
| 3:4:174:TRP:CE3   | 3:4:180:LYS:HD2   | 2.11                     | 0.84              |
| 1:5:220:ARG:HA    | 1:5:223:MET:HE3   | 1.59                     | 0.84              |
| 25:c:502:CLA:HAA1 | 25:c:502:CLA:HBD  | 1.60                     | 0.84              |
| 15:o:309:SER:N    | 15:o:319:LYS:O    | 2.10                     | 0.84              |
| 21:g:220:ARG:HA   | 21:g:223:MET:HE3  | 1.59                     | 0.84              |
| 23:u:84:ALA:HB1   | 23:u:100:ILE:HG23 | 1.57                     | 0.84              |
| 25:B:615:CLA:H193 | 25:B:616:CLA:HBC3 | 1.59                     | 0.84              |
| 7:D:56:VAL:HG21   | 7:D:111:LEU:CD1   | 2.08                     | 0.84              |
| 20:S:89:VAL:HG11  | 20:S:111:GLN:NE2  | 1.91                     | 0.84              |
| 25:B:604:CLA:H41  | 25:B:604:CLA:H92  | 1.59                     | 0.84              |
| 26:C:518:LHG:H161 | 25:Y:312:CLA:HAB  | 1.58                     | 0.84              |
| 15:O:228:THR:HG22 | 15:O:284:GLU:OE2  | 1.77                     | 0.84              |
| 23:U:84:ALA:HB1   | 23:U:100:ILE:HG23 | 1.57                     | 0.84              |
| 1:5:165:GLN:NE2   | 24:5:302:CHL:NB   | 2.26                     | 0.84              |
| 2:6:89:PRO:HA     | 2:6:92:PHE:CD2    | 2.10                     | 0.84              |
| 5:b:277:GLN:NE2   | 35:b:626:DGD:O5E  | 2.10                     | 0.84              |
| 21:g:231:VAL:HG11 | 25:g:613:CLA:HAC2 | 1.56                     | 0.84              |
| 21:n:232:GLN:HE21 | 25:n:613:CLA:C4D  | 1.82                     | 0.84              |
| 15:O:309:SER:N    | 15:O:319:LYS:O    | 2.10                     | 0.83              |
| 2:6:146:ASP:O     | 2:6:152:ASN:ND2   | 2.11                     | 0.83              |
| 21:n:158:ILE:HD11 | 21:y:257:TRP:HE3  | 1.43                     | 0.83              |
| 21:y:98:LEU:HD22  | 25:y:304:CLA:CAA  | 2.07                     | 0.83              |
| 25:r:604:CLA:CHC  | 40:r:617:NEX:H222 | 2.08                     | 0.83              |
| 2:2:117:GLU:HB2   | 2:2:241:PRO:HG2   | 1.58                     | 0.83              |
| 25:R:604:CLA:CHC  | 40:R:617:NEX:H222 | 2.08                     | 0.83              |
| 1:7:220:ARG:HA    | 1:7:223:MET:HE3   | 1.59                     | 0.83              |
| 3:8:175:ALA:HB2   | 22:r:59:TYR:HE2   | 1.41                     | 0.83              |
| 5:b:174:LEU:HD21  | 5:b:309:LEU:HD13  | 1.60                     | 0.83              |
| 5:b:326:ARG:NH2   | 7:d:298:ASP:OD1   | 2.11                     | 0.83              |
| 25:b:615:CLA:H193 | 25:b:616:CLA:HBC3 | 1.59                     | 0.83              |
| 2:2:174:GLU:HG2   | 1:3:59:LEU:HD22   | 1.59                     | 0.83              |
| 2:2:220:GLY:CA    | 25:2:602:CLA:HAC1 | 2.08                     | 0.83              |
| 1:3:130:VAL:O     | 1:3:134:ALA:N     | 2.12                     | 0.83              |
| 25:C:502:CLA:HAA1 | 25:C:502:CLA:HBD  | 1.60                     | 0.83              |
| 26:c:518:LHG:H161 | 25:y:312:CLA:HAB  | 1.58                     | 0.83              |
| 21:n:159:LEU:HD11 | 21:y:257:TRP:CG   | 2.11                     | 0.83              |
| 21:y:165:GLN:OE1  | 21:y:165:GLN:HA   | 1.79                     | 0.83              |
| 21:N:109:GLY:HA2  | 39:N:616:LUT:H181 | 1.60                     | 0.83              |
| 6:c:310:SER:HB3   | 6:c:355:THR:HG22  | 1.60                     | 0.83              |
| 1:1:165:GLN:OE1   | 1:1:165:GLN:HA    | 1.79                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:612:CLA:HHB  | 39:R:615:LUT:H42  | 1.61                     | 0.83              |
| 25:b:604:CLA:H41  | 25:b:604:CLA:H92  | 1.59                     | 0.83              |
| 13:l:5:ASN:ND2    | 13:l:8:GLU:OE1    | 2.10                     | 0.83              |
| 25:S:312:CLA:HBA1 | 25:S:312:CLA:HMA2 | 1.61                     | 0.83              |
| 7:d:226:ASP:HB2   | 7:d:235:ALA:HB1   | 1.58                     | 0.83              |
| 22:r:120:LYS:N    | 22:r:126:PRO:O    | 2.11                     | 0.83              |
| 5:B:326:ARG:NH2   | 7:D:298:ASP:OD1   | 2.11                     | 0.83              |
| 6:C:331:ALA:O     | 15:O:196:TYR:OH   | 1.97                     | 0.83              |
| 15:O:202:GLN:HE21 | 15:O:206:GLY:HA2  | 1.43                     | 0.83              |
| 1:5:130:VAL:O     | 1:5:134:ALA:N     | 2.12                     | 0.83              |
| 21:n:130:VAL:O    | 21:n:134:ALA:N    | 2.12                     | 0.83              |
| 2:2:89:PRO:HA     | 2:2:92:PHE:CD2    | 2.10                     | 0.83              |
| 22:R:120:LYS:N    | 22:R:126:PRO:O    | 2.11                     | 0.83              |
| 5:B:233:ASN:O     | 5:B:236:THR:HG22  | 1.79                     | 0.83              |
| 5:b:233:ASN:O     | 5:b:236:THR:HG22  | 1.79                     | 0.83              |
| 1:1:213:VAL:O     | 1:1:217:LYS:HG3   | 1.79                     | 0.83              |
| 1:3:213:VAL:O     | 1:3:217:LYS:HG3   | 1.79                     | 0.83              |
| 7:D:226:ASP:HB2   | 7:D:235:ALA:HB1   | 1.58                     | 0.83              |
| 15:o:290:THR:HG22 | 15:o:291:LYS:H    | 1.41                     | 0.83              |
| 21:y:130:VAL:O    | 21:y:134:ALA:N    | 2.12                     | 0.83              |
| 21:Y:213:VAL:O    | 21:Y:217:LYS:HG3  | 1.79                     | 0.82              |
| 22:R:158:GLU:HB3  | 22:R:268:LEU:HD12 | 1.60                     | 0.82              |
| 14:M:31:SER:HG    | 14:m:31:SER:HG    | 0.97                     | 0.82              |
| 19:Z:19:LEU:HD21  | 19:Z:43:GLY:HA3   | 1.61                     | 0.82              |
| 27:a:405:PHO:HBC3 | 7:d:280:LEU:HD12  | 1.61                     | 0.82              |
| 21:g:165:GLN:OE1  | 21:g:165:GLN:HA   | 1.79                     | 0.82              |
| 21:y:220:ARG:HA   | 21:y:223:MET:HE3  | 1.59                     | 0.82              |
| 25:r:612:CLA:HHB  | 39:r:615:LUT:H42  | 1.61                     | 0.82              |
| 5:B:159:THR:OG1   | 5:B:161:LEU:HD23  | 1.79                     | 0.82              |
| 21:Y:130:VAL:O    | 21:Y:134:ALA:N    | 2.12                     | 0.82              |
| 1:5:213:VAL:O     | 1:5:217:LYS:HG3   | 1.79                     | 0.82              |
| 2:6:173:VAL:O     | 2:6:176:PHE:HB2   | 1.80                     | 0.82              |
| 20:s:118:ALA:HB1  | 20:s:229:GLY:HA3  | 1.61                     | 0.82              |
| 27:A:404:PHO:HBC3 | 7:D:280:LEU:HD12  | 1.61                     | 0.82              |
| 21:N:158:ILE:HD11 | 21:Y:257:TRP:HE3  | 1.43                     | 0.82              |
| 21:G:146:TYR:CE2  | 25:G:604:CLA:H2   | 2.15                     | 0.82              |
| 21:G:213:VAL:O    | 21:G:217:LYS:HG3  | 1.79                     | 0.82              |
| 21:N:130:VAL:O    | 21:N:134:ALA:N    | 2.12                     | 0.82              |
| 22:R:137:ARG:HH21 | 25:R:602:CLA:HED3 | 1.44                     | 0.82              |
| 15:o:228:THR:HG22 | 15:o:284:GLU:OE2  | 1.77                     | 0.82              |
| 21:g:130:VAL:O    | 21:g:134:ALA:N    | 2.12                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3:97:GLU:HG3    | 1:3:190:LEU:CD2   | 2.10                     | 0.82              |
| 5:B:174:LEU:HD21  | 5:B:309:LEU:HD13  | 1.60                     | 0.82              |
| 2:6:220:GLY:CA    | 25:6:602:CLA:HAC1 | 2.08                     | 0.82              |
| 1:1:165:GLN:NE2   | 24:1:302:CHL:NB   | 2.26                     | 0.82              |
| 5:B:157:HIS:CD2   | 5:B:164:PRO:HD2   | 2.15                     | 0.82              |
| 21:N:213:VAL:O    | 21:N:217:LYS:HG3  | 1.79                     | 0.82              |
| 21:Y:165:GLN:OE1  | 21:Y:165:GLN:HA   | 1.79                     | 0.82              |
| 5:b:157:HIS:CD2   | 5:b:164:PRO:HD2   | 2.15                     | 0.82              |
| 5:b:159:THR:OG1   | 5:b:161:LEU:HD23  | 1.79                     | 0.82              |
| 8:e:27:ILE:CG2    | 8:e:28:PRO:HD3    | 2.09                     | 0.82              |
| 22:r:158:GLU:HB3  | 22:r:268:LEU:HD12 | 1.60                     | 0.82              |
| 1:1:130:VAL:O     | 1:1:134:ALA:N     | 2.12                     | 0.82              |
| 25:N:603:CLA:H191 | 24:N:607:CHL:H111 | 1.61                     | 0.82              |
| 22:R:269:ASN:O    | 22:R:273:THR:HG23 | 1.80                     | 0.82              |
| 1:7:97:GLU:HG3    | 1:7:190:LEU:CD2   | 2.10                     | 0.82              |
| 1:7:130:VAL:O     | 1:7:134:ALA:N     | 2.12                     | 0.82              |
| 4:a:278:TRP:HB3   | 4:a:279:PRO:HD3   | 1.62                     | 0.82              |
| 21:n:109:GLY:HA2  | 39:n:616:LUT:H181 | 1.60                     | 0.82              |
| 21:n:165:GLN:OE1  | 21:n:165:GLN:HA   | 1.79                     | 0.82              |
| 21:y:97:GLU:HG3   | 21:y:190:LEU:CD2  | 2.10                     | 0.82              |
| 21:y:104:ARG:HB3  | 25:y:311:CLA:CBC  | 2.10                     | 0.82              |
| 5:B:482:ILE:HG21  | 7:D:139:LEU:HD23  | 1.61                     | 0.82              |
| 20:S:68:ARG:HH22  | 26:S:301:LHG:HC12 | 1.45                     | 0.82              |
| 25:S:303:CLA:H71  | 25:S:304:CLA:HMA1 | 1.62                     | 0.82              |
| 40:N:617:NEX:H12  | 40:N:617:NEX:H191 | 1.59                     | 0.82              |
| 22:R:58:TRP:CE3   | 22:R:60:PRO:HG3   | 2.15                     | 0.82              |
| 21:g:82:THR:HG22  | 24:y:310:CHL:HED3 | 1.61                     | 0.82              |
| 21:n:213:VAL:O    | 21:n:217:LYS:HG3  | 1.79                     | 0.82              |
| 40:n:617:NEX:H12  | 40:n:617:NEX:H191 | 1.60                     | 0.82              |
| 21:y:213:VAL:O    | 21:y:217:LYS:HG3  | 1.79                     | 0.82              |
| 22:r:58:TRP:CE3   | 22:r:60:PRO:HG3   | 2.15                     | 0.82              |
| 1:1:97:GLU:HG3    | 1:1:190:LEU:CD2   | 2.09                     | 0.82              |
| 21:G:130:VAL:O    | 21:G:134:ALA:N    | 2.12                     | 0.82              |
| 21:N:165:GLN:OE1  | 21:N:165:GLN:HA   | 1.79                     | 0.82              |
| 23:U:96:PRO:O     | 23:U:97:THR:OG1   | 1.97                     | 0.82              |
| 25:s:312:CLA:HMA2 | 25:s:312:CLA:HBA1 | 1.61                     | 0.82              |
| 8:E:27:ILE:CG2    | 8:E:28:PRO:HD3    | 2.09                     | 0.81              |
| 21:Y:138:ILE:HG21 | 24:Y:307:CHL:CBC  | 2.10                     | 0.81              |
| 2:2:175:GLY:HA3   | 2:2:181:LEU:CD1   | 2.10                     | 0.81              |
| 4:A:278:TRP:HB3   | 4:A:279:PRO:HD3   | 1.62                     | 0.81              |
| 1:7:213:VAL:O     | 1:7:217:LYS:HG3   | 1.79                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:z:19:LEU:HD21  | 19:z:43:GLY:HA3   | 1.61                     | 0.81              |
| 21:g:146:TYR:CE2  | 25:g:604:CLA:H2   | 2.15                     | 0.81              |
| 25:r:610:CLA:CMB  | 26:r:618:LHG:HC2  | 2.10                     | 0.81              |
| 23:u:96:PRO:O     | 23:u:97:THR:OG1   | 1.97                     | 0.81              |
| 2:2:204:ASP:O     | 2:2:208:THR:HG23  | 1.80                     | 0.81              |
| 20:S:119:ARG:HD3  | 25:S:310:CLA:CHD  | 2.11                     | 0.81              |
| 5:b:388:SER:HA    | 7:d:345:GLU:OE1   | 1.81                     | 0.81              |
| 6:c:331:ALA:O     | 15:o:196:TYR:OH   | 1.97                     | 0.81              |
| 21:g:213:VAL:O    | 21:g:217:LYS:HG3  | 1.79                     | 0.81              |
| 20:S:118:ALA:HB1  | 20:S:229:GLY:HA3  | 1.61                     | 0.81              |
| 21:G:107:MET:HG2  | 21:G:222:ALA:CB   | 2.11                     | 0.81              |
| 25:R:610:CLA:CMB  | 26:R:618:LHG:HC2  | 2.10                     | 0.81              |
| 2:6:184:VAL:HB    | 2:6:196:TYR:HE2   | 1.45                     | 0.81              |
| 21:y:161:ILE:O    | 21:y:165:GLN:HB2  | 1.81                     | 0.81              |
| 4:A:57:PRO:HD3    | 4:A:73:TYR:CE2    | 2.16                     | 0.81              |
| 5:B:296:GLN:HE22  | 5:B:304:LYS:HD2   | 1.45                     | 0.81              |
| 15:O:232:LEU:HD23 | 15:O:282:VAL:HG12 | 1.63                     | 0.81              |
| 1:5:161:ILE:O     | 1:5:165:GLN:HB2   | 1.81                     | 0.81              |
| 21:g:97:GLU:HG3   | 21:g:190:LEU:CD2  | 2.10                     | 0.81              |
| 21:y:138:ILE:HG21 | 24:y:307:CHL:CBC  | 2.10                     | 0.81              |
| 1:3:107:MET:HG2   | 1:3:222:ALA:CB    | 2.11                     | 0.81              |
| 21:N:107:MET:HG2  | 21:N:222:ALA:CB   | 2.11                     | 0.81              |
| 21:Y:104:ARG:HB3  | 25:Y:311:CLA:CBC  | 2.10                     | 0.81              |
| 1:5:153:VAL:HG13  | 24:5:301:CHL:C1D  | 2.10                     | 0.81              |
| 2:6:130:PRO:O     | 2:6:134:LYS:N     | 2.14                     | 0.81              |
| 2:6:204:ASP:O     | 2:6:208:THR:HG23  | 1.80                     | 0.81              |
| 1:1:161:ILE:O     | 1:1:165:GLN:HB2   | 1.81                     | 0.81              |
| 21:G:165:GLN:OE1  | 21:G:165:GLN:HA   | 1.79                     | 0.81              |
| 6:c:178:LYS:NZ    | 6:c:184:GLY:O     | 2.14                     | 0.81              |
| 5:B:388:SER:HA    | 7:D:345:GLU:OE1   | 1.81                     | 0.81              |
| 20:S:175:VAL:O    | 20:S:179:VAL:HG23 | 1.80                     | 0.81              |
| 1:5:165:GLN:OE1   | 1:5:165:GLN:HA    | 1.79                     | 0.81              |
| 1:7:165:GLN:HA    | 1:7:165:GLN:OE1   | 1.79                     | 0.81              |
| 25:s:305:CLA:CHC  | 40:s:317:NEX:H222 | 2.11                     | 0.81              |
| 22:r:269:ASN:O    | 22:r:273:THR:HG23 | 1.80                     | 0.81              |
| 2:2:49:LEU:O      | 2:2:55:ARG:HA     | 1.80                     | 0.81              |
| 2:2:184:VAL:HB    | 2:2:196:TYR:HE2   | 1.45                     | 0.81              |
| 1:3:161:ILE:O     | 1:3:165:GLN:HB2   | 1.81                     | 0.81              |
| 19:Z:26:VAL:HG21  | 19:Z:40:VAL:CG2   | 2.11                     | 0.81              |
| 20:s:119:ARG:HD3  | 25:s:310:CLA:CHD  | 2.11                     | 0.81              |
| 21:n:104:ARG:HB3  | 25:n:610:CLA:CBC  | 2.11                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:y:315:CLA:HBC1 | 39:y:316:LUT:H162 | 1.63                     | 0.81              |
| 1:1:153:VAL:HG13  | 24:1:301:CHL:C1D  | 2.10                     | 0.80              |
| 1:3:165:GLN:OE1   | 1:3:165:GLN:HA    | 1.79                     | 0.80              |
| 6:C:310:SER:HB3   | 6:C:355:THR:HG22  | 1.60                     | 0.80              |
| 21:N:104:ARG:HB3  | 25:N:610:CLA:CBC  | 2.11                     | 0.80              |
| 21:Y:107:MET:HG2  | 21:Y:222:ALA:CB   | 2.11                     | 0.80              |
| 2:6:49:LEU:O      | 2:6:55:ARG:HA     | 1.80                     | 0.80              |
| 1:7:107:MET:HG2   | 1:7:222:ALA:CB    | 2.11                     | 0.80              |
| 1:7:161:ILE:O     | 1:7:165:GLN:HB2   | 1.81                     | 0.80              |
| 21:g:107:MET:HG2  | 21:g:222:ALA:CB   | 2.11                     | 0.80              |
| 21:n:161:ILE:O    | 21:n:165:GLN:HB2  | 1.81                     | 0.80              |
| 21:y:138:ILE:CG2  | 24:y:307:CHL:HBC1 | 2.11                     | 0.80              |
| 22:r:72:LEU:HB3   | 22:r:137:ARG:HH12 | 1.46                     | 0.80              |
| 3:4:229:ILE:HG13  | 3:4:230:LYS:H     | 1.45                     | 0.80              |
| 6:C:265:VAL:HG22  | 17:W:131:LEU:HD12 | 1.63                     | 0.80              |
| 21:Y:138:ILE:CG2  | 24:Y:307:CHL:HBC1 | 2.11                     | 0.80              |
| 1:5:97:GLU:HG3    | 1:5:190:LEU:CD2   | 2.10                     | 0.80              |
| 25:n:603:CLA:H191 | 24:n:607:CHL:H111 | 1.61                     | 0.80              |
| 2:2:130:PRO:O     | 2:2:134:LYS:N     | 2.14                     | 0.80              |
| 6:C:178:LYS:NZ    | 6:C:184:GLY:O     | 2.14                     | 0.80              |
| 21:G:55:ARG:HH12  | 21:G:72:GLY:CA    | 1.95                     | 0.80              |
| 21:n:107:MET:HG2  | 21:n:222:ALA:CB   | 2.11                     | 0.80              |
| 21:Y:55:ARG:HH12  | 21:Y:72:GLY:CA    | 1.95                     | 0.80              |
| 21:Y:161:ILE:O    | 21:Y:165:GLN:HB2  | 1.81                     | 0.80              |
| 4:a:57:PRO:HD3    | 4:a:73:TYR:CE2    | 2.16                     | 0.80              |
| 4:a:223:LEU:HB2   | 7:d:140:ARG:HH21  | 1.46                     | 0.80              |
| 5:b:296:GLN:HE22  | 5:b:304:LYS:HD2   | 1.46                     | 0.80              |
| 13:l:8:GLU:HB3    | 29:l:102:SQD:H62  | 1.63                     | 0.80              |
| 1:1:107:MET:HG2   | 1:1:222:ALA:CB    | 2.11                     | 0.80              |
| 2:2:173:VAL:O     | 2:2:176:PHE:HB2   | 1.80                     | 0.80              |
| 21:G:82:THR:HG22  | 24:Y:310:CHL:HED3 | 1.61                     | 0.80              |
| 21:N:161:ILE:O    | 21:N:165:GLN:HB2  | 1.81                     | 0.80              |
| 1:3:135:GLY:O     | 1:3:138:ILE:HG22  | 1.82                     | 0.80              |
| 21:G:161:ILE:O    | 21:G:165:GLN:HB2  | 1.81                     | 0.80              |
| 21:N:231:VAL:HG11 | 25:N:613:CLA:HHD  | 1.63                     | 0.80              |
| 21:n:55:ARG:HH12  | 21:n:72:GLY:CA    | 1.95                     | 0.80              |
| 25:y:312:CLA:H122 | 25:y:313:CLA:H141 | 1.64                     | 0.80              |
| 25:G:610:CLA:H52  | 39:G:615:LUT:H30  | 1.63                     | 0.80              |
| 1:5:55:ARG:HH12   | 1:5:72:GLY:CA     | 1.95                     | 0.80              |
| 1:5:107:MET:HG2   | 1:5:222:ALA:CB    | 2.11                     | 0.80              |
| 5:b:482:ILE:HG21  | 7:d:139:LEU:HD23  | 1.61                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:s:132:GLU:HA   | 20:s:145:ALA:HB1  | 1.63                     | 0.80              |
| 20:s:175:VAL:O    | 20:s:179:VAL:HG23 | 1.80                     | 0.80              |
| 25:s:303:CLA:H71  | 25:s:304:CLA:HMA1 | 1.62                     | 0.80              |
| 4:A:223:LEU:HB2   | 7:D:140:ARG:HH21  | 1.46                     | 0.80              |
| 25:B:605:CLA:HMA1 | 25:B:606:CLA:H3A  | 1.64                     | 0.80              |
| 21:Y:97:GLU:HG3   | 21:Y:190:LEU:CD2  | 2.10                     | 0.80              |
| 1:5:135:GLY:O     | 1:5:138:ILE:HG22  | 1.82                     | 0.80              |
| 19:z:26:VAL:HG21  | 19:z:40:VAL:CG2   | 2.11                     | 0.80              |
| 21:n:97:GLU:HG3   | 21:n:190:LEU:CD2  | 2.09                     | 0.80              |
| 21:n:231:VAL:HG11 | 25:n:613:CLA:HHD  | 1.63                     | 0.80              |
| 22:r:137:ARG:HH21 | 25:r:602:CLA:HED3 | 1.44                     | 0.80              |
| 21:G:97:GLU:HG3   | 21:G:190:LEU:CD2  | 2.10                     | 0.80              |
| 21:N:135:GLY:O    | 21:N:138:ILE:HG22 | 1.82                     | 0.80              |
| 25:d:403:CLA:H112 | 10:h:48:ALA:HB1   | 1.63                     | 0.80              |
| 20:s:68:ARG:HH22  | 26:s:301:LHG:HC12 | 1.45                     | 0.80              |
| 21:y:199:LEU:HG   | 39:y:316:LUT:H221 | 1.64                     | 0.80              |
| 25:G:602:CLA:H121 | 25:G:602:CLA:H93  | 1.64                     | 0.80              |
| 21:N:55:ARG:HH12  | 21:N:72:GLY:CA    | 1.95                     | 0.80              |
| 21:Y:135:GLY:O    | 21:Y:138:ILE:HG22 | 1.82                     | 0.80              |
| 5:b:467:ILE:HD12  | 7:d:127:MET:HE2   | 1.64                     | 0.80              |
| 17:W:125:GLU:O    | 17:W:129:SER:OG   | 1.98                     | 0.79              |
| 21:Y:226:MET:HG2  | 39:Y:317:LUT:H12  | 1.62                     | 0.79              |
| 17:w:125:GLU:O    | 17:w:129:SER:OG   | 1.98                     | 0.79              |
| 21:g:161:ILE:O    | 21:g:165:GLN:HB2  | 1.81                     | 0.79              |
| 21:n:135:GLY:O    | 21:n:138:ILE:HG22 | 1.82                     | 0.79              |
| 21:n:182:PRO:HB3  | 40:n:617:NEX:H171 | 1.63                     | 0.79              |
| 21:y:55:ARG:HH12  | 21:y:72:GLY:CA    | 1.95                     | 0.79              |
| 1:1:55:ARG:HH12   | 1:1:72:GLY:CA     | 1.95                     | 0.79              |
| 1:1:135:GLY:O     | 1:1:138:ILE:HG22  | 1.82                     | 0.79              |
| 21:G:135:GLY:O    | 21:G:138:ILE:HG22 | 1.82                     | 0.79              |
| 3:8:229:ILE:HG13  | 3:8:230:LYS:H     | 1.45                     | 0.79              |
| 21:y:135:GLY:O    | 21:y:138:ILE:HG22 | 1.82                     | 0.79              |
| 25:S:305:CLA:CHC  | 40:S:317:NEX:H222 | 2.11                     | 0.79              |
| 5:b:173:GLY:HA3   | 5:b:265:ILE:HD11  | 1.64                     | 0.79              |
| 21:y:107:MET:HG2  | 21:y:222:ALA:CB   | 2.11                     | 0.79              |
| 25:D:403:CLA:H112 | 10:H:48:ALA:HB1   | 1.63                     | 0.79              |
| 20:S:132:GLU:HA   | 20:S:145:ALA:HB1  | 1.63                     | 0.79              |
| 2:6:175:GLY:HA3   | 2:6:181:LEU:CD1   | 2.10                     | 0.79              |
| 15:o:232:LEU:HD23 | 15:o:282:VAL:HG12 | 1.63                     | 0.79              |
| 22:r:85:LYS:HG2   | 22:r:86:PRO:HD2   | 1.65                     | 0.79              |
| 1:3:55:ARG:HH12   | 1:3:72:GLY:CA     | 1.95                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Y:315:CLA:HBC1 | 39:Y:316:LUT:H162 | 1.62                     | 0.79              |
| 22:R:85:LYS:HG2   | 22:R:86:PRO:HD2   | 1.65                     | 0.79              |
| 2:6:193:GLY:HA2   | 2:6:197:PHE:HD2   | 1.48                     | 0.79              |
| 5:b:277:GLN:HB2   | 23:u:99:LYS:HG2   | 1.65                     | 0.79              |
| 21:g:135:GLY:O    | 21:g:138:ILE:HG22 | 1.82                     | 0.79              |
| 21:g:165:GLN:HE22 | 24:g:606:CHL:C1B  | 1.96                     | 0.79              |
| 4:A:139:MET:HE3   | 7:D:222:THR:CG2   | 2.13                     | 0.79              |
| 7:D:108:LEU:HD23  | 8:E:66:ILE:HD13   | 1.64                     | 0.79              |
| 21:N:182:PRO:HB3  | 40:N:617:NEX:H171 | 1.63                     | 0.79              |
| 21:G:165:GLN:HE22 | 24:G:606:CHL:C1B  | 1.96                     | 0.79              |
| 1:5:153:VAL:HA    | 24:5:301:CHL:C4D  | 2.13                     | 0.79              |
| 21:N:97:GLU:HG3   | 21:N:190:LEU:CD2  | 2.10                     | 0.79              |
| 21:N:164:THR:HG21 | 24:N:606:CHL:HED3 | 1.64                     | 0.79              |
| 1:5:138:ILE:HD12  | 1:5:144:LEU:HD13  | 1.65                     | 0.79              |
| 5:b:73:ASN:ND2    | 5:b:79:ASN:OD1    | 2.16                     | 0.79              |
| 7:D:20:ASP:OD2    | 7:D:24:ARG:NH1    | 2.15                     | 0.79              |
| 21:N:138:ILE:HD12 | 21:N:144:LEU:HD13 | 1.65                     | 0.79              |
| 1:7:55:ARG:HH12   | 1:7:72:GLY:CA     | 1.95                     | 0.79              |
| 1:7:135:GLY:O     | 1:7:138:ILE:HG22  | 1.82                     | 0.79              |
| 28:h:101:BCR:H403 | 28:h:101:BCR:H23C | 1.65                     | 0.79              |
| 15:o:207:GLU:OE1  | 15:o:209:VAL:HG23 | 1.83                     | 0.79              |
| 25:g:610:CLA:H52  | 39:g:615:LUT:H30  | 1.63                     | 0.79              |
| 21:y:226:MET:HG2  | 39:y:317:LUT:H12  | 1.62                     | 0.79              |
| 22:r:214:LYS:NZ   | 22:r:218:PRO:O    | 2.13                     | 0.79              |
| 2:2:205:ASP:O     | 2:2:208:THR:OG1   | 2.01                     | 0.79              |
| 4:a:139:MET:HE3   | 7:d:222:THR:CG2   | 2.13                     | 0.79              |
| 6:c:265:VAL:HG22  | 17:w:131:LEU:HD12 | 1.63                     | 0.79              |
| 1:1:153:VAL:HA    | 24:1:301:CHL:C4D  | 2.13                     | 0.78              |
| 8:E:77:ASP:O      | 8:E:81:ARG:HG3    | 1.83                     | 0.78              |
| 21:Y:138:ILE:HD12 | 21:Y:144:LEU:HD13 | 1.65                     | 0.78              |
| 21:Y:199:LEU:HG   | 39:Y:316:LUT:H221 | 1.64                     | 0.78              |
| 4:a:288:LEU:O     | 4:a:292:THR:HG23  | 1.84                     | 0.78              |
| 8:e:77:ASP:O      | 8:e:81:ARG:HG3    | 1.83                     | 0.78              |
| 21:g:55:ARG:HH12  | 21:g:72:GLY:CA    | 1.95                     | 0.78              |
| 5:B:73:ASN:ND2    | 5:B:79:ASN:OD1    | 2.16                     | 0.78              |
| 5:B:277:GLN:HB2   | 23:U:99:LYS:HG2   | 1.65                     | 0.78              |
| 13:L:8:GLU:HB3    | 29:L:101:SQD:H62  | 1.63                     | 0.78              |
| 3:8:122:TRP:HA    | 3:8:127:TRP:HD1   | 1.48                     | 0.78              |
| 3:8:175:ALA:HB2   | 22:r:59:TYR:CE2   | 2.19                     | 0.78              |
| 25:b:605:CLA:HMA1 | 25:b:606:CLA:H3A  | 1.64                     | 0.78              |
| 7:d:20:ASP:OD2    | 7:d:24:ARG:NH1    | 2.15                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:122:TRP:HA    | 3:4:127:TRP:HD1   | 1.48                     | 0.78              |
| 15:O:207:GLU:OE1  | 15:O:209:VAL:HG23 | 1.83                     | 0.78              |
| 4:a:60:ILE:HD12   | 4:a:84:PRO:HD2    | 1.64                     | 0.78              |
| 21:g:138:ILE:HD12 | 21:g:144:LEU:HD13 | 1.65                     | 0.78              |
| 21:g:215:GLU:HG3  | 25:g:610:CLA:NB   | 1.99                     | 0.78              |
| 5:B:173:GLY:HA3   | 5:B:265:ILE:HD11  | 1.64                     | 0.78              |
| 11:I:34:ARG:HD2   | 11:I:35:GLU:HG3   | 1.63                     | 0.78              |
| 25:Y:312:CLA:H122 | 25:Y:313:CLA:H141 | 1.64                     | 0.78              |
| 2:6:205:ASP:O     | 2:6:208:THR:OG1   | 2.01                     | 0.78              |
| 2:2:70:LEU:HD13   | 2:2:79:GLY:HA2    | 1.65                     | 0.78              |
| 25:2:602:CLA:HBD  | 25:2:602:CLA:HAA1 | 1.65                     | 0.78              |
| 5:B:42:LEU:HD13   | 5:B:94:GLU:HG3    | 1.66                     | 0.78              |
| 21:G:138:ILE:HD12 | 21:G:144:LEU:HD13 | 1.65                     | 0.78              |
| 25:N:610:CLA:H51  | 25:N:612:CLA:HMA1 | 1.66                     | 0.78              |
| 22:R:72:LEU:HB3   | 22:R:137:ARG:HH12 | 1.46                     | 0.78              |
| 5:b:360:PRO:O     | 5:b:361:THR:HG22  | 1.84                     | 0.78              |
| 10:h:56:ILE:HD13  | 18:x:84:LYS:CE    | 2.12                     | 0.78              |
| 11:i:34:ARG:HD2   | 11:i:35:GLU:HG3   | 1.63                     | 0.78              |
| 4:A:89:ILE:HD11   | 4:A:108:ASN:HB3   | 1.66                     | 0.78              |
| 5:B:360:PRO:O     | 5:B:361:THR:HG22  | 1.84                     | 0.78              |
| 24:N:609:CHL:CAA  | 21:Y:82:THR:HG21  | 2.13                     | 0.78              |
| 21:y:138:ILE:HD12 | 21:y:144:LEU:HD13 | 1.65                     | 0.78              |
| 3:4:170:GLN:HB2   | 3:4:183:GLU:HG2   | 1.63                     | 0.78              |
| 28:H:101:BCR:H403 | 28:H:101:BCR:H23C | 1.65                     | 0.78              |
| 2:6:70:LEU:HD13   | 2:6:79:GLY:HA2    | 1.65                     | 0.78              |
| 21:n:138:ILE:HD12 | 21:n:144:LEU:HD13 | 1.65                     | 0.78              |
| 2:2:193:GLY:HA2   | 2:2:197:PHE:HD2   | 1.48                     | 0.78              |
| 5:B:272:ARG:NH1   | 5:B:276:ASP:OD2   | 2.17                     | 0.78              |
| 6:C:449:ARG:HH12  | 11:I:28:PRO:HG3   | 1.48                     | 0.78              |
| 21:G:97:GLU:CA    | 21:G:190:LEU:HD11 | 2.14                     | 0.78              |
| 1:7:57:LYS:HZ1    | 1:7:66:PRO:HG3    | 1.48                     | 0.78              |
| 3:8:138:ALA:HB3   | 3:8:140:PHE:CE2   | 2.19                     | 0.78              |
| 3:8:170:GLN:HB2   | 3:8:183:GLU:HG2   | 1.63                     | 0.78              |
| 6:c:97:TRP:CH2    | 30:c:520:LMG:H172 | 2.19                     | 0.78              |
| 20:s:132:GLU:HG2  | 20:s:251:VAL:HB   | 1.66                     | 0.78              |
| 20:S:132:GLU:HG2  | 20:S:251:VAL:HB   | 1.66                     | 0.78              |
| 22:R:214:LYS:NZ   | 22:R:218:PRO:O    | 2.13                     | 0.78              |
| 2:6:152:ASN:O     | 2:6:154:VAL:HG23  | 1.84                     | 0.78              |
| 5:b:478:VAL:O     | 7:d:140:ARG:HD3   | 1.84                     | 0.78              |
| 6:c:449:ARG:HH12  | 11:i:28:PRO:HG3   | 1.48                     | 0.78              |
| 7:d:108:LEU:HD23  | 8:e:66:ILE:HD13   | 1.64                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:467:ILE:HD12  | 7:D:127:MET:HE2   | 1.64                     | 0.77              |
| 6:C:322:GLN:HE22  | 6:C:384:ILE:HD12  | 1.49                     | 0.77              |
| 7:D:292:LEU:HB2   | 7:D:294:LEU:HD13  | 1.66                     | 0.77              |
| 5:b:51:VAL:HG13   | 5:b:308:LYS:CG    | 2.14                     | 0.77              |
| 21:g:84:GLY:O     | 21:y:91:THR:OG1   | 2.02                     | 0.77              |
| 21:g:97:GLU:CA    | 21:g:190:LEU:HD11 | 2.14                     | 0.77              |
| 25:n:610:CLA:H51  | 25:n:612:CLA:HMA1 | 1.66                     | 0.77              |
| 19:Z:26:VAL:HG21  | 19:Z:40:VAL:HG21  | 1.66                     | 0.77              |
| 21:N:206:GLU:OE1  | 21:N:206:GLU:N    | 2.18                     | 0.77              |
| 1:7:206:GLU:N     | 1:7:206:GLU:OE1   | 2.18                     | 0.77              |
| 25:g:602:CLA:H121 | 25:g:602:CLA:H93  | 1.64                     | 0.77              |
| 25:n:612:CLA:HHC  | 25:n:612:CLA:HBB1 | 1.65                     | 0.77              |
| 1:1:138:ILE:HD12  | 1:1:144:LEU:HD13  | 1.65                     | 0.77              |
| 2:2:239:LYS:HD2   | 2:2:242:LEU:CD1   | 2.14                     | 0.77              |
| 4:A:60:ILE:HD12   | 4:A:84:PRO:HD2    | 1.64                     | 0.77              |
| 5:B:280:PHE:CD2   | 5:B:312:TYR:HB3   | 2.19                     | 0.77              |
| 6:C:97:TRP:CH2    | 30:C:520:LMG:H172 | 2.19                     | 0.77              |
| 14:M:31:SER:O     | 14:M:32:GLN:HG2   | 1.85                     | 0.77              |
| 2:6:239:LYS:HD2   | 2:6:242:LEU:CD1   | 2.14                     | 0.77              |
| 5:b:42:LEU:HD13   | 5:b:94:GLU:HG3    | 1.66                     | 0.77              |
| 1:1:206:GLU:OE1   | 1:1:206:GLU:N     | 2.18                     | 0.77              |
| 5:B:51:VAL:HG13   | 5:B:308:LYS:CG    | 2.14                     | 0.77              |
| 21:N:232:GLN:HE21 | 25:N:613:CLA:C4D  | 1.82                     | 0.77              |
| 3:8:155:TRP:CD1   | 3:8:159:LYS:HZ1   | 2.03                     | 0.77              |
| 21:y:206:GLU:OE1  | 21:y:206:GLU:N    | 2.18                     | 0.77              |
| 1:3:206:GLU:OE1   | 1:3:206:GLU:N     | 2.18                     | 0.77              |
| 4:A:292:THR:HG22  | 6:C:428:THR:HG23  | 1.66                     | 0.77              |
| 24:N:607:CHL:H203 | 25:Y:303:CLA:C16  | 2.14                     | 0.77              |
| 25:s:303:CLA:HAB  | 39:s:316:LUT:H30  | 1.66                     | 0.77              |
| 1:1:97:GLU:CA     | 1:1:190:LEU:HD11  | 2.14                     | 0.77              |
| 4:A:335:ASN:HA    | 7:D:351:ASN:HD22  | 1.50                     | 0.77              |
| 25:B:603:CLA:H2   | 25:B:605:CLA:H91  | 1.65                     | 0.77              |
| 4:a:335:ASN:HA    | 7:d:351:ASN:HD22  | 1.50                     | 0.77              |
| 25:b:603:CLA:H2   | 25:b:605:CLA:H91  | 1.65                     | 0.77              |
| 6:c:369:LEU:HD21  | 6:c:384:ILE:HG12  | 1.66                     | 0.77              |
| 25:g:614:CLA:HBD  | 25:g:614:CLA:HAA1 | 1.67                     | 0.77              |
| 3:4:175:ALA:HB2   | 22:R:59:TYR:CE2   | 2.19                     | 0.77              |
| 15:O:169:TYR:OH   | 17:W:80:LEU:HA    | 1.84                     | 0.77              |
| 25:N:612:CLA:HHC  | 25:N:612:CLA:HBB1 | 1.64                     | 0.77              |
| 22:R:238:LEU:HB3  | 25:R:609:CLA:H3A  | 1.66                     | 0.77              |
| 1:7:97:GLU:CA     | 1:7:190:LEU:HD11  | 2.14                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:c:322:GLN:HE22  | 6:c:384:ILE:HD12  | 1.49                     | 0.77              |
| 21:g:232:GLN:HE21 | 25:g:613:CLA:C4D  | 1.85                     | 0.77              |
| 3:4:138:ALA:HB3   | 3:4:140:PHE:CE2   | 2.19                     | 0.77              |
| 4:A:288:LEU:O     | 4:A:292:THR:HG23  | 1.84                     | 0.77              |
| 21:G:215:GLU:HG3  | 25:G:610:CLA:NB   | 1.99                     | 0.77              |
| 40:G:617:NEX:H28  | 40:G:617:NEX:H361 | 1.67                     | 0.77              |
| 21:Y:206:GLU:OE1  | 21:Y:206:GLU:N    | 2.18                     | 0.77              |
| 21:g:64:GLY:HA3   | 21:y:178:ALA:HA   | 1.66                     | 0.77              |
| 21:g:206:GLU:N    | 21:g:206:GLU:OE1  | 2.18                     | 0.77              |
| 21:n:179:GLY:HA2  | 24:n:608:CHL:HAC1 | 1.67                     | 0.77              |
| 25:r:603:CLA:C14  | 25:r:603:CLA:HMB2 | 2.14                     | 0.77              |
| 5:B:451:PHE:HE2   | 25:B:604:CLA:HMA3 | 1.50                     | 0.77              |
| 5:B:478:VAL:O     | 7:D:140:ARG:HD3   | 1.84                     | 0.77              |
| 25:R:603:CLA:C14  | 25:R:603:CLA:HMB2 | 2.14                     | 0.77              |
| 1:5:206:GLU:OE1   | 1:5:206:GLU:N     | 2.18                     | 0.77              |
| 4:a:292:THR:HG22  | 6:c:428:THR:HG23  | 1.66                     | 0.77              |
| 2:2:122:TRP:O     | 2:2:123:VAL:HG23  | 1.85                     | 0.77              |
| 21:G:64:GLY:HA3   | 21:Y:178:ALA:HA   | 1.66                     | 0.77              |
| 21:Y:231:VAL:HG21 | 25:Y:314:CLA:HAC2 | 1.66                     | 0.77              |
| 2:6:122:TRP:O     | 2:6:123:VAL:HG23  | 1.85                     | 0.77              |
| 2:6:127:PHE:HE2   | 2:6:145:LEU:HB2   | 1.50                     | 0.77              |
| 1:7:138:ILE:HD12  | 1:7:144:LEU:HD13  | 1.65                     | 0.77              |
| 1:1:57:LYS:HZ1    | 1:1:66:PRO:HG3    | 1.50                     | 0.76              |
| 1:3:138:ILE:HD12  | 1:3:144:LEU:HD13  | 1.65                     | 0.76              |
| 6:C:369:LEU:HD21  | 6:C:384:ILE:HG12  | 1.66                     | 0.76              |
| 18:X:84:LYS:HA    | 18:X:87:LEU:CD2   | 2.15                     | 0.76              |
| 21:G:196:PHE:HE2  | 24:G:608:CHL:HBC2 | 1.50                     | 0.76              |
| 21:N:97:GLU:CA    | 21:N:190:LEU:HD11 | 2.14                     | 0.76              |
| 7:d:292:LEU:HB2   | 7:d:294:LEU:HD13  | 1.66                     | 0.76              |
| 18:x:84:LYS:HA    | 18:x:87:LEU:CD2   | 2.14                     | 0.76              |
| 22:r:238:LEU:HB3  | 25:r:609:CLA:H3A  | 1.67                     | 0.76              |
| 25:S:303:CLA:HAB  | 39:S:316:LUT:H30  | 1.66                     | 0.76              |
| 26:d:406:LHG:H182 | 16:t:17:ILE:HD11  | 1.66                     | 0.76              |
| 21:G:84:GLY:O     | 21:Y:91:THR:OG1   | 2.02                     | 0.76              |
| 5:b:272:ARG:NH1   | 5:b:276:ASP:OD2   | 2.17                     | 0.76              |
| 21:n:164:THR:HG21 | 24:n:606:CHL:HED3 | 1.65                     | 0.76              |
| 6:C:86:LEU:HD13   | 6:C:89:LEU:HD12   | 1.68                     | 0.76              |
| 19:Z:48:ILE:HG12  | 26:S:318:LHG:H222 | 1.67                     | 0.76              |
| 22:R:68:LEU:HD11  | 25:R:602:CLA:CGD  | 2.16                     | 0.76              |
| 4:a:89:ILE:HD11   | 4:a:108:ASN:HB3   | 1.66                     | 0.76              |
| 5:b:280:PHE:CD2   | 5:b:312:TYR:HB3   | 2.19                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:m:31:SER:O     | 14:m:32:GLN:HG2   | 1.85                     | 0.76              |
| 21:g:196:PHE:HE2  | 24:g:608:CHL:HBC2 | 1.50                     | 0.76              |
| 21:n:97:GLU:CA    | 21:n:190:LEU:HD11 | 2.14                     | 0.76              |
| 21:n:206:GLU:OE1  | 21:n:206:GLU:N    | 2.18                     | 0.76              |
| 1:3:220:ARG:HA    | 1:3:223:MET:CE    | 2.15                     | 0.76              |
| 25:g:610:CLA:H41  | 25:g:612:CLA:HMA2 | 1.68                     | 0.76              |
| 21:n:220:ARG:HA   | 21:n:223:MET:CE   | 2.15                     | 0.76              |
| 2:2:152:ASN:O     | 2:2:154:VAL:HG23  | 1.84                     | 0.76              |
| 2:2:211:GLU:HA    | 2:2:214:VAL:HG12  | 1.68                     | 0.76              |
| 3:4:219:GLU:CG    | 3:4:222:GLU:HB2   | 2.15                     | 0.76              |
| 21:G:206:GLU:N    | 21:G:206:GLU:OE1  | 2.18                     | 0.76              |
| 25:G:614:CLA:HBD  | 25:G:614:CLA:HAA1 | 1.67                     | 0.76              |
| 21:N:220:ARG:HA   | 21:N:223:MET:CE   | 2.15                     | 0.76              |
| 21:Y:220:ARG:HA   | 21:Y:223:MET:CE   | 2.15                     | 0.76              |
| 2:6:211:GLU:HA    | 2:6:214:VAL:HG12  | 1.68                     | 0.76              |
| 5:b:162:TYR:HA    | 26:b:621:LHG:HC2  | 1.68                     | 0.76              |
| 25:c:502:CLA:HMC2 | 25:c:510:CLA:HBB1 | 1.67                     | 0.76              |
| 19:z:48:ILE:HG12  | 26:s:318:LHG:H222 | 1.67                     | 0.76              |
| 20:s:141:CYS:HB3  | 25:s:305:CLA:OBD  | 1.85                     | 0.76              |
| 25:n:603:CLA:HMC3 | 25:n:603:CLA:HBC3 | 1.68                     | 0.76              |
| 1:1:220:ARG:HA    | 1:1:223:MET:CE    | 2.15                     | 0.76              |
| 4:A:328:MET:HG2   | 7:D:326:ILE:HG12  | 1.68                     | 0.76              |
| 5:b:392:VAL:HG13  | 5:b:397:VAL:HG22  | 1.68                     | 0.76              |
| 19:z:26:VAL:HG21  | 19:z:40:VAL:HG21  | 1.66                     | 0.76              |
| 5:B:223:GLN:HA    | 10:H:33:VAL:HG11  | 1.67                     | 0.76              |
| 26:D:406:LHG:H182 | 16:T:17:ILE:HD11  | 1.66                     | 0.76              |
| 8:E:60:ARG:CZ     | 8:E:64:PRO:HG3    | 2.16                     | 0.76              |
| 24:N:607:CHL:H192 | 25:Y:303:CLA:H151 | 1.68                     | 0.76              |
| 2:6:69:TYR:CE1    | 2:6:70:LEU:HG     | 2.20                     | 0.76              |
| 2:6:160:LEU:HD23  | 2:6:163:LEU:HD12  | 1.68                     | 0.76              |
| 3:8:219:GLU:CG    | 3:8:222:GLU:HB2   | 2.15                     | 0.76              |
| 5:B:162:TYR:HA    | 26:B:621:LHG:HC2  | 1.68                     | 0.76              |
| 15:O:236:TYR:HB2  | 15:O:310:ASP:OD2  | 1.86                     | 0.76              |
| 25:N:603:CLA:HMC3 | 25:N:603:CLA:HBC3 | 1.68                     | 0.76              |
| 25:N:603:CLA:H101 | 24:N:609:CHL:H141 | 1.68                     | 0.76              |
| 21:y:227:PHE:HD2  | 25:y:303:CLA:H202 | 1.51                     | 0.76              |
| 1:3:97:GLU:CA     | 1:3:190:LEU:HD11  | 2.14                     | 0.76              |
| 5:B:341:LEU:HD12  | 5:B:429:ILE:HG22  | 1.68                     | 0.76              |
| 25:a:402:CLA:HMC3 | 25:a:402:CLA:HBC3 | 1.68                     | 0.76              |
| 24:n:607:CHL:H203 | 25:y:303:CLA:C16  | 2.14                     | 0.76              |
| 21:y:146:TYR:HB3  | 21:y:152:LEU:HD13 | 1.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:69:TYR:CE1    | 2:2:70:LEU:HG     | 2.20                     | 0.75              |
| 5:B:392:VAL:HG13  | 5:B:397:VAL:HG22  | 1.68                     | 0.75              |
| 2:6:175:GLY:CA    | 2:6:181:LEU:HD11  | 2.15                     | 0.75              |
| 5:b:272:ARG:NH1   | 5:b:361:THR:HG21  | 2.01                     | 0.75              |
| 21:y:97:GLU:CA    | 21:y:190:LEU:HD11 | 2.14                     | 0.75              |
| 23:u:88:TYR:HB2   | 23:u:100:ILE:HG21 | 1.68                     | 0.75              |
| 3:8:225:LYS:HA    | 3:8:228:GLU:OE1   | 1.86                     | 0.75              |
| 1:1:146:TYR:HB3   | 1:1:152:LEU:HD13  | 1.68                     | 0.75              |
| 1:3:146:TYR:HB3   | 1:3:152:LEU:HD13  | 1.68                     | 0.75              |
| 5:B:121:GLU:O     | 10:H:24:LYS:HE2   | 1.86                     | 0.75              |
| 5:B:377:VAL:HG11  | 7:D:343:PRO:HG3   | 1.69                     | 0.75              |
| 6:C:215:LYS:HG2   | 6:C:221:GLU:HB3   | 1.69                     | 0.75              |
| 15:O:180:VAL:HA   | 15:O:186:VAL:HG12 | 1.68                     | 0.75              |
| 21:G:220:ARG:HA   | 21:G:223:MET:CE   | 2.15                     | 0.75              |
| 25:R:604:CLA:CHB  | 41:R:616:XAT:H42  | 2.17                     | 0.75              |
| 1:5:57:LYS:HZ1    | 1:5:66:PRO:HG3    | 1.51                     | 0.75              |
| 15:o:236:TYR:HB2  | 15:o:310:ASP:OD2  | 1.85                     | 0.75              |
| 40:g:617:NEX:H28  | 40:g:617:NEX:H361 | 1.67                     | 0.75              |
| 21:y:231:VAL:HG21 | 25:y:314:CLA:HAC2 | 1.66                     | 0.75              |
| 25:r:610:CLA:HMB3 | 26:r:618:LHG:HC2  | 1.68                     | 0.75              |
| 15:O:92:LEU:HB3   | 15:O:96:GLU:HG3   | 1.68                     | 0.75              |
| 2:6:88:ASP:HB3    | 2:6:91:ALA:CB     | 2.17                     | 0.75              |
| 2:6:239:LYS:HD2   | 2:6:242:LEU:HD12  | 1.68                     | 0.75              |
| 15:o:169:TYR:OH   | 17:w:80:LEU:HA    | 1.84                     | 0.75              |
| 21:g:220:ARG:HA   | 21:g:223:MET:CE   | 2.15                     | 0.75              |
| 25:A:401:CLA:HMC3 | 25:A:401:CLA:HBC3 | 1.68                     | 0.75              |
| 5:B:127:ARG:HG3   | 5:B:128:THR:HG23  | 1.69                     | 0.75              |
| 20:S:141:CYS:HB3  | 25:S:305:CLA:OBD  | 1.85                     | 0.75              |
| 25:6:602:CLA:HBD  | 25:6:602:CLA:HAA1 | 1.65                     | 0.75              |
| 10:h:56:ILE:HA    | 18:x:84:LYS:HE2   | 1.69                     | 0.75              |
| 21:n:132:PHE:HB2  | 24:n:607:CHL:H2A  | 1.68                     | 0.75              |
| 22:r:68:LEU:HD11  | 25:r:602:CLA:CGD  | 2.16                     | 0.75              |
| 2:2:175:GLY:CA    | 2:2:181:LEU:HD11  | 2.15                     | 0.75              |
| 3:4:225:LYS:HA    | 3:4:228:GLU:OE1   | 1.86                     | 0.75              |
| 3:4:226:LEU:HD12  | 3:4:229:ILE:HD11  | 1.67                     | 0.75              |
| 3:8:226:LEU:HD12  | 3:8:229:ILE:HD11  | 1.67                     | 0.75              |
| 5:b:377:VAL:HG11  | 7:d:343:PRO:HG3   | 1.69                     | 0.75              |
| 6:c:215:LYS:HG2   | 6:c:221:GLU:HB3   | 1.68                     | 0.75              |
| 8:e:60:ARG:CZ     | 8:e:64:PRO:HG3    | 2.16                     | 0.75              |
| 21:N:132:PHE:HB2  | 24:N:607:CHL:H2A  | 1.68                     | 0.75              |
| 21:N:146:TYR:HB3  | 21:N:152:LEU:HD13 | 1.68                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:220:ARG:HA    | 1:5:223:MET:CE    | 2.15                     | 0.75              |
| 25:n:603:CLA:H101 | 24:n:609:CHL:H141 | 1.68                     | 0.75              |
| 21:y:220:ARG:HA   | 21:y:223:MET:CE   | 2.15                     | 0.75              |
| 2:2:127:PHE:HE2   | 2:2:145:LEU:HB2   | 1.50                     | 0.75              |
| 27:A:403:PHO:HMB1 | 27:A:403:PHO:HBB1 | 1.68                     | 0.75              |
| 26:B:625:LHG:O4   | 7:D:142:TYR:OH    | 2.04                     | 0.75              |
| 22:R:72:LEU:HB3   | 22:R:137:ARG:NH1  | 2.01                     | 0.75              |
| 6:c:86:LEU:HD13   | 6:c:89:LEU:HD12   | 1.68                     | 0.75              |
| 21:g:146:TYR:HB3  | 21:g:152:LEU:HD13 | 1.68                     | 0.75              |
| 21:y:105:TRP:HE1  | 24:y:309:CHL:HED2 | 1.52                     | 0.75              |
| 2:2:127:PHE:HB3   | 2:2:140:PHE:CE2   | 2.22                     | 0.75              |
| 3:4:133:GLN:HG2   | 3:4:134:PRO:CD    | 2.17                     | 0.75              |
| 3:4:221:LEU:HD12  | 3:4:222:GLU:N     | 2.02                     | 0.75              |
| 8:E:23:HIS:O      | 8:E:27:ILE:HG22   | 1.87                     | 0.75              |
| 21:G:84:GLY:CA    | 21:Y:94:ARG:HG2   | 2.17                     | 0.75              |
| 21:N:179:GLY:HA2  | 24:N:608:CHL:HAC1 | 1.67                     | 0.75              |
| 21:Y:227:PHE:HD2  | 25:Y:303:CLA:H202 | 1.51                     | 0.75              |
| 1:7:146:TYR:HB3   | 1:7:152:LEU:HD13  | 1.68                     | 0.75              |
| 8:e:23:HIS:O      | 8:e:27:ILE:HG22   | 1.87                     | 0.75              |
| 15:o:92:LEU:HB3   | 15:o:96:GLU:HG3   | 1.68                     | 0.75              |
| 3:4:107:ARG:O     | 3:4:110:MET:HG3   | 1.87                     | 0.74              |
| 25:C:502:CLA:HMC2 | 25:C:510:CLA:HBB1 | 1.67                     | 0.74              |
| 21:G:169:MET:HG3  | 24:G:609:CHL:HMC  | 1.69                     | 0.74              |
| 24:G:608:CHL:H12  | 24:G:608:CHL:H151 | 1.69                     | 0.74              |
| 24:Y:308:CHL:HBC3 | 32:Y:322:AJP:O82  | 1.86                     | 0.74              |
| 1:5:146:TYR:HB3   | 1:5:152:LEU:HD13  | 1.68                     | 0.74              |
| 24:s:307:CHL:HBC2 | 32:s:319:AJP:O82  | 1.87                     | 0.74              |
| 24:n:607:CHL:H192 | 25:y:303:CLA:H151 | 1.68                     | 0.74              |
| 2:2:88:ASP:HB3    | 2:2:91:ALA:CB     | 2.17                     | 0.74              |
| 2:2:130:PRO:HG2   | 2:2:133:PHE:HB2   | 1.70                     | 0.74              |
| 2:2:130:PRO:HD3   | 2:2:239:LYS:HE2   | 1.69                     | 0.74              |
| 21:Y:105:TRP:HE1  | 24:Y:309:CHL:HED2 | 1.52                     | 0.74              |
| 2:6:130:PRO:HG2   | 2:6:133:PHE:HB2   | 1.70                     | 0.74              |
| 1:7:220:ARG:HA    | 1:7:223:MET:CE    | 2.15                     | 0.74              |
| 3:8:221:LEU:HD12  | 3:8:222:GLU:N     | 2.02                     | 0.74              |
| 5:b:360:PRO:O     | 42:b:701:HOH:O    | 2.05                     | 0.74              |
| 15:o:180:VAL:HA   | 15:o:186:VAL:HG12 | 1.68                     | 0.74              |
| 21:y:117:GLU:OE2  | 21:y:239:GLY:HA3  | 1.88                     | 0.74              |
| 2:2:239:LYS:HD2   | 2:2:242:LEU:HD12  | 1.68                     | 0.74              |
| 4:A:230:ASN:OD1   | 22:R:100:ASN:HA   | 1.87                     | 0.74              |
| 22:R:214:LYS:HG3  | 22:R:218:PRO:O    | 1.86                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:6:126:ASP:HA    | 2:6:148:LEU:HG    | 1.70                     | 0.74              |
| 5:b:223:GLN:HA    | 10:h:33:VAL:HG11  | 1.67                     | 0.74              |
| 25:b:604:CLA:HBD  | 25:b:604:CLA:HBA1 | 1.70                     | 0.74              |
| 25:n:613:CLA:H141 | 25:n:614:CLA:HMD1 | 1.68                     | 0.74              |
| 22:r:214:LYS:HG3  | 22:r:218:PRO:O    | 1.86                     | 0.74              |
| 2:2:126:ASP:HA    | 2:2:148:LEU:HG    | 1.70                     | 0.74              |
| 1:3:57:LYS:HZ1    | 1:3:66:PRO:HG3    | 1.51                     | 0.74              |
| 25:A:405:CLA:CMC  | 11:I:11:VAL:HG11  | 2.17                     | 0.74              |
| 21:N:117:GLU:OE2  | 21:N:239:GLY:HA3  | 1.87                     | 0.74              |
| 21:N:227:PHE:HD2  | 25:N:602:CLA:H202 | 1.52                     | 0.74              |
| 2:6:127:PHE:HB3   | 2:6:140:PHE:CE2   | 2.22                     | 0.74              |
| 2:6:130:PRO:HD3   | 2:6:239:LYS:HE2   | 1.69                     | 0.74              |
| 3:8:107:ARG:O     | 3:8:110:MET:HG3   | 1.87                     | 0.74              |
| 5:b:214:LEU:HD11  | 25:r:608:CLA:H51  | 1.69                     | 0.74              |
| 18:x:87:LEU:CD1   | 18:x:88:LEU:HD22  | 2.18                     | 0.74              |
| 25:r:604:CLA:CHB  | 41:r:616:XAT:H42  | 2.17                     | 0.74              |
| 1:1:57:LYS:NZ     | 1:1:66:PRO:HG3    | 2.02                     | 0.74              |
| 18:X:87:LEU:CD1   | 18:X:88:LEU:HD22  | 2.18                     | 0.74              |
| 25:G:610:CLA:H41  | 25:G:612:CLA:HMA2 | 1.68                     | 0.74              |
| 25:R:610:CLA:HMB3 | 26:R:618:LHG:HC2  | 1.68                     | 0.74              |
| 5:b:451:PHE:HE2   | 25:b:604:CLA:HMA3 | 1.50                     | 0.74              |
| 24:n:609:CHL:H72  | 24:y:302:CHL:H111 | 1.69                     | 0.74              |
| 24:y:308:CHL:HBC3 | 32:y:322:AJP:O82  | 1.86                     | 0.74              |
| 22:r:72:LEU:HB3   | 22:r:137:ARG:NH1  | 2.01                     | 0.74              |
| 1:3:117:GLU:OE2   | 1:3:239:GLY:HA3   | 1.88                     | 0.74              |
| 5:B:282:GLN:CD    | 23:U:100:ILE:HD11 | 2.13                     | 0.74              |
| 38:F:101:HEM:HBB2 | 38:F:101:HEM:HHC  | 1.70                     | 0.74              |
| 25:N:613:CLA:H141 | 25:N:614:CLA:HMD1 | 1.68                     | 0.74              |
| 4:a:328:MET:HG2   | 7:d:326:ILE:HG12  | 1.68                     | 0.74              |
| 6:c:30:THR:HG23   | 6:c:31:THR:HG23   | 1.68                     | 0.74              |
| 21:g:132:PHE:HB2  | 24:g:607:CHL:HMA3 | 1.68                     | 0.74              |
| 21:n:227:PHE:HD2  | 25:n:602:CLA:H202 | 1.52                     | 0.74              |
| 5:B:360:PRO:O     | 42:B:701:HOH:O    | 2.05                     | 0.74              |
| 10:H:56:ILE:HA    | 18:X:84:LYS:HE2   | 1.68                     | 0.74              |
| 24:N:609:CHL:H72  | 24:Y:302:CHL:H111 | 1.69                     | 0.74              |
| 25:a:406:CLA:CMC  | 11:i:11:VAL:HG11  | 2.17                     | 0.74              |
| 5:b:121:GLU:O     | 10:h:24:LYS:HE2   | 1.86                     | 0.74              |
| 5:b:127:ARG:HG3   | 5:b:128:THR:HG23  | 1.69                     | 0.74              |
| 1:1:117:GLU:OE2   | 1:1:239:GLY:HA3   | 1.88                     | 0.74              |
| 2:2:246:LEU:O     | 2:2:249:LEU:HG    | 1.88                     | 0.74              |
| 1:3:146:TYR:O     | 1:3:152:LEU:HD12  | 1.88                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:272:ARG:NH1   | 5:B:361:THR:HG21  | 2.01                     | 0.74              |
| 10:H:56:ILE:HD13  | 18:X:84:LYS:CE    | 2.12                     | 0.74              |
| 21:G:146:TYR:HB3  | 21:G:152:LEU:HD13 | 1.68                     | 0.74              |
| 21:Y:146:TYR:O    | 21:Y:152:LEU:HD12 | 1.88                     | 0.74              |
| 2:6:88:ASP:HB3    | 2:6:91:ALA:HB3    | 1.70                     | 0.74              |
| 26:b:625:LHG:O4   | 7:d:142:TYR:OH    | 2.04                     | 0.74              |
| 24:n:609:CHL:CAA  | 21:y:82:THR:HG21  | 2.13                     | 0.74              |
| 5:B:214:LEU:HD11  | 25:R:608:CLA:H51  | 1.69                     | 0.74              |
| 21:N:104:ARG:NH1  | 24:N:608:CHL:OBD  | 2.20                     | 0.74              |
| 4:a:230:ASN:OD1   | 22:r:100:ASN:HA   | 1.87                     | 0.74              |
| 24:S:307:CHL:HBC2 | 32:S:319:AJP:O82  | 1.87                     | 0.74              |
| 2:6:246:LEU:O     | 2:6:249:LEU:HG    | 1.88                     | 0.74              |
| 25:a:402:CLA:H52  | 25:a:403:CLA:HAB  | 1.70                     | 0.74              |
| 21:n:159:LEU:HD11 | 21:y:257:TRP:CB   | 2.18                     | 0.74              |
| 6:C:30:THR:HG23   | 6:C:31:THR:HG23   | 1.69                     | 0.73              |
| 21:N:146:TYR:O    | 21:N:152:LEU:HD12 | 1.88                     | 0.73              |
| 21:Y:59:LEU:HD23  | 24:Y:302:CHL:C2B  | 2.18                     | 0.73              |
| 21:Y:97:GLU:CA    | 21:Y:190:LEU:HD11 | 2.14                     | 0.73              |
| 25:c:504:CLA:C1C  | 35:c:516:DGD:HB51 | 2.18                     | 0.73              |
| 21:y:59:LEU:HD23  | 24:y:302:CHL:C2B  | 2.18                     | 0.73              |
| 21:Y:107:MET:HG2  | 21:Y:222:ALA:HB2  | 1.70                     | 0.73              |
| 24:R:607:CHL:HBB2 | 40:R:617:NEX:H12  | 1.71                     | 0.73              |
| 1:5:97:GLU:CA     | 1:5:190:LEU:HD11  | 2.14                     | 0.73              |
| 2:6:155:HIS:NE2   | 2:6:161:ALA:HB2   | 2.03                     | 0.73              |
| 5:b:341:LEU:HD12  | 5:b:429:ILE:HG22  | 1.68                     | 0.73              |
| 25:N:603:CLA:HAB  | 39:N:616:LUT:C35  | 2.19                     | 0.73              |
| 21:Y:146:TYR:HB3  | 21:Y:152:LEU:HD13 | 1.68                     | 0.73              |
| 5:b:282:GLN:CD    | 23:u:100:ILE:HD11 | 2.13                     | 0.73              |
| 1:1:107:MET:HG2   | 1:1:222:ALA:HB2   | 1.70                     | 0.73              |
| 17:W:110:GLY:O    | 17:W:114:THR:HG23 | 1.89                     | 0.73              |
| 21:G:103:SER:HB2  | 21:G:219:GLY:HA3  | 1.71                     | 0.73              |
| 21:G:132:PHE:HB2  | 24:G:607:CHL:HMA3 | 1.68                     | 0.73              |
| 21:N:159:LEU:HD11 | 21:Y:257:TRP:CB   | 2.18                     | 0.73              |
| 23:U:88:TYR:HB2   | 23:U:100:ILE:HG21 | 1.68                     | 0.73              |
| 1:5:70:LEU:HD13   | 1:5:79:GLY:HA2    | 1.71                     | 0.73              |
| 7:d:56:VAL:HG21   | 7:d:111:LEU:HD12  | 1.69                     | 0.73              |
| 20:s:192:ASN:OD1  | 20:s:195:ASP:HA   | 1.87                     | 0.73              |
| 21:g:169:MET:HG3  | 24:g:609:CHL:HMC  | 1.69                     | 0.73              |
| 1:3:57:LYS:NZ     | 1:3:66:PRO:HG3    | 2.02                     | 0.73              |
| 5:B:14:ASN:ND2    | 22:R:97:LEU:O     | 2.18                     | 0.73              |
| 25:B:604:CLA:HBD  | 25:B:604:CLA:HBA1 | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:D:56:VAL:HG21   | 7:D:111:LEU:HD12  | 1.69                     | 0.73              |
| 21:G:107:MET:HG2  | 21:G:222:ALA:HB2  | 1.70                     | 0.73              |
| 21:G:146:TYR:O    | 21:G:152:LEU:HD12 | 1.88                     | 0.73              |
| 22:R:93:ASP:HB2   | 22:R:108:ASP:H    | 1.53                     | 0.73              |
| 1:5:57:LYS:NZ     | 1:5:66:PRO:HG3    | 2.02                     | 0.73              |
| 3:8:133:GLN:HG2   | 3:8:134:PRO:CD    | 2.16                     | 0.73              |
| 25:d:401:CLA:HAB  | 25:d:402:CLA:H72  | 1.69                     | 0.73              |
| 21:n:103:SER:HB2  | 21:n:219:GLY:HA3  | 1.71                     | 0.73              |
| 21:y:107:MET:HG2  | 21:y:222:ALA:HB2  | 1.70                     | 0.73              |
| 1:1:103:SER:HB2   | 1:1:219:GLY:HA3   | 1.71                     | 0.73              |
| 3:4:219:GLU:HG3   | 3:4:222:GLU:HB2   | 1.69                     | 0.73              |
| 10:H:62:ASN:OD1   | 10:H:63:SER:N     | 2.22                     | 0.73              |
| 15:O:183:ASP:OD2  | 15:O:223:LYS:NZ   | 2.21                     | 0.73              |
| 1:5:146:TYR:O     | 1:5:152:LEU:HD12  | 1.88                     | 0.73              |
| 38:f:101:HEM:HBB2 | 38:f:101:HEM:HHC  | 1.70                     | 0.73              |
| 21:g:70:LEU:HD13  | 21:g:79:GLY:HA2   | 1.71                     | 0.73              |
| 21:g:117:GLU:OE2  | 21:g:239:GLY:HA3  | 1.88                     | 0.73              |
| 21:n:146:TYR:HB3  | 21:n:152:LEU:HD13 | 1.69                     | 0.73              |
| 21:n:146:TYR:O    | 21:n:152:LEU:HD12 | 1.88                     | 0.73              |
| 21:y:146:TYR:O    | 21:y:152:LEU:HD12 | 1.88                     | 0.73              |
| 2:2:160:LEU:HD23  | 2:2:163:LEU:HD12  | 1.68                     | 0.73              |
| 25:R:612:CLA:H101 | 25:R:612:CLA:HAB  | 1.71                     | 0.73              |
| 1:7:57:LYS:NZ     | 1:7:66:PRO:HG3    | 2.02                     | 0.73              |
| 1:7:117:GLU:OE2   | 1:7:239:GLY:HA3   | 1.88                     | 0.73              |
| 21:G:117:GLU:OE2  | 21:G:239:GLY:HA3  | 1.88                     | 0.73              |
| 21:N:107:MET:HG2  | 21:N:222:ALA:HB2  | 1.70                     | 0.73              |
| 21:Y:103:SER:HB2  | 21:Y:219:GLY:HA3  | 1.71                     | 0.73              |
| 27:a:404:PHO:HBB1 | 27:a:404:PHO:HMB1 | 1.68                     | 0.73              |
| 5:b:397:VAL:HG23  | 5:b:417:VAL:HG11  | 1.71                     | 0.73              |
| 6:c:225:VAL:HG22  | 6:c:289:PHE:CE1   | 2.24                     | 0.73              |
| 21:n:117:GLU:OE2  | 21:n:239:GLY:HA3  | 1.87                     | 0.73              |
| 21:y:70:LEU:HD13  | 21:y:79:GLY:HA2   | 1.71                     | 0.73              |
| 2:2:50:TRP:CD1    | 2:2:213:LYS:HD3   | 2.24                     | 0.73              |
| 1:3:70:LEU:HD13   | 1:3:79:GLY:HA2    | 1.71                     | 0.73              |
| 1:3:103:SER:HB2   | 1:3:219:GLY:HA3   | 1.71                     | 0.73              |
| 4:A:95:PRO:HG2    | 4:A:98:GLU:HG2    | 1.71                     | 0.73              |
| 25:C:504:CLA:C1C  | 35:C:516:DGD:HB51 | 2.18                     | 0.73              |
| 1:5:103:SER:HB2   | 1:5:219:GLY:HA3   | 1.71                     | 0.73              |
| 2:6:214:VAL:HA    | 2:6:217:ILE:HD11  | 1.69                     | 0.73              |
| 3:8:142:PHE:CE1   | 3:8:146:LEU:HD11  | 2.24                     | 0.73              |
| 3:8:221:LEU:HA    | 3:8:224:LEU:CD2   | 2.19                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:c:513:CLA:HBA1 | 25:c:513:CLA:HBD  | 1.71                     | 0.73              |
| 17:w:110:GLY:O    | 17:w:114:THR:HG23 | 1.89                     | 0.73              |
| 21:g:103:SER:HB2  | 21:g:219:GLY:HA3  | 1.71                     | 0.73              |
| 24:g:606:CHL:HBA1 | 40:g:617:NEX:H403 | 1.71                     | 0.73              |
| 24:r:607:CHL:HBB2 | 40:r:617:NEX:H12  | 1.71                     | 0.73              |
| 2:2:220:GLY:HA3   | 25:2:602:CLA:HAC1 | 1.71                     | 0.73              |
| 25:B:614:CLA:H8   | 28:B:617:BCR:H362 | 1.70                     | 0.73              |
| 20:S:192:ASN:OD1  | 20:S:195:ASP:HA   | 1.87                     | 0.73              |
| 21:G:215:GLU:HG3  | 25:G:610:CLA:C4B  | 2.19                     | 0.73              |
| 21:N:103:SER:HB2  | 21:N:219:GLY:HA3  | 1.71                     | 0.73              |
| 1:7:70:LEU:HD13   | 1:7:79:GLY:HA2    | 1.71                     | 0.73              |
| 4:a:95:PRO:HG2    | 4:a:98:GLU:HG2    | 1.71                     | 0.73              |
| 4:a:317:TRP:CZ3   | 7:d:181:ARG:HD3   | 2.24                     | 0.73              |
| 5:b:172:TYR:CE2   | 5:b:283:GLU:HB2   | 2.24                     | 0.73              |
| 15:o:310:ASP:OD1  | 15:o:311:THR:N    | 2.22                     | 0.73              |
| 18:x:84:LYS:HA    | 18:x:87:LEU:HD23  | 1.71                     | 0.73              |
| 21:g:84:GLY:CA    | 21:y:94:ARG:HG2   | 2.17                     | 0.73              |
| 24:g:608:CHL:H12  | 24:g:608:CHL:H151 | 1.69                     | 0.73              |
| 22:r:127:TYR:CD2  | 22:r:135:ARG:HD2  | 2.24                     | 0.73              |
| 5:b:285:TYR:CE1   | 23:u:90:GLN:HG3   | 2.23                     | 0.72              |
| 22:r:54:ASP:OD2   | 22:r:56:PRO:HD2   | 1.88                     | 0.72              |
| 2:2:214:VAL:HA    | 2:2:217:ILE:HD11  | 1.69                     | 0.72              |
| 5:B:285:TYR:CE1   | 23:U:90:GLN:HG3   | 2.23                     | 0.72              |
| 21:G:197:ASP:OD1  | 25:G:610:CLA:HAA1 | 1.89                     | 0.72              |
| 21:Y:70:LEU:HD13  | 21:Y:79:GLY:HA2   | 1.71                     | 0.72              |
| 22:R:54:ASP:OD2   | 22:R:56:PRO:HD2   | 1.88                     | 0.72              |
| 2:6:50:TRP:CD1    | 2:6:213:LYS:HD3   | 2.24                     | 0.72              |
| 15:o:183:ASP:OD2  | 15:o:223:LYS:NZ   | 2.21                     | 0.72              |
| 21:n:107:MET:HG2  | 21:n:222:ALA:HB2  | 1.70                     | 0.72              |
| 22:r:93:ASP:HB2   | 22:r:108:ASP:H    | 1.53                     | 0.72              |
| 1:1:146:TYR:O     | 1:1:152:LEU:HD12  | 1.88                     | 0.72              |
| 5:B:172:TYR:CE2   | 5:B:283:GLU:HB2   | 2.24                     | 0.72              |
| 5:B:382:PRO:HB3   | 7:D:345:GLU:OE2   | 1.90                     | 0.72              |
| 18:X:84:LYS:HA    | 18:X:87:LEU:HD23  | 1.71                     | 0.72              |
| 20:S:63:TYR:CE2   | 20:S:219:ALA:HB1  | 2.25                     | 0.72              |
| 20:S:72:PRO:CG    | 20:S:75:LEU:HD13  | 2.19                     | 0.72              |
| 2:6:213:LYS:O     | 2:6:217:ILE:HG12  | 1.89                     | 0.72              |
| 1:7:103:SER:HB2   | 1:7:219:GLY:HA3   | 1.71                     | 0.72              |
| 1:7:107:MET:HG2   | 1:7:222:ALA:HB2   | 1.70                     | 0.72              |
| 21:g:107:MET:HG2  | 21:g:222:ALA:HB2  | 1.70                     | 0.72              |
| 21:n:70:LEU:HD13  | 21:n:79:GLY:HA2   | 1.71                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:104:ARG:NH1  | 24:n:608:CHL:OBD  | 2.20                     | 0.72              |
| 6:C:57:ALA:O      | 6:C:61:VAL:HG23   | 1.89                     | 0.72              |
| 21:N:70:LEU:HD13  | 21:N:79:GLY:HA2   | 1.71                     | 0.72              |
| 2:6:130:PRO:HG2   | 2:6:133:PHE:CD2   | 2.25                     | 0.72              |
| 25:b:614:CLA:H8   | 28:b:617:BCR:H362 | 1.70                     | 0.72              |
| 21:g:146:TYR:O    | 21:g:152:LEU:HD12 | 1.88                     | 0.72              |
| 3:4:221:LEU:HA    | 3:4:224:LEU:CD2   | 2.19                     | 0.72              |
| 4:A:331:MET:CE    | 7:D:321:LEU:HB3   | 2.20                     | 0.72              |
| 25:A:401:CLA:H52  | 25:A:402:CLA:HAB  | 1.70                     | 0.72              |
| 5:B:128:THR:HG21  | 22:R:94:ILE:HD13  | 1.72                     | 0.72              |
| 21:G:215:GLU:HG3  | 25:G:610:CLA:C1B  | 2.19                     | 0.72              |
| 21:Y:117:GLU:OE2  | 21:Y:239:GLY:HA3  | 1.88                     | 0.72              |
| 21:Y:169:MET:HG3  | 24:Y:310:CHL:CMC  | 2.19                     | 0.72              |
| 1:5:107:MET:HG2   | 1:5:222:ALA:HB2   | 1.70                     | 0.72              |
| 2:6:174:GLU:HB3   | 1:7:62:PHE:HB3    | 1.70                     | 0.72              |
| 6:c:216:SER:OG    | 6:c:221:GLU:OE1   | 2.06                     | 0.72              |
| 5:B:70:GLY:HA2    | 5:B:178:VAL:CG1   | 2.20                     | 0.72              |
| 14:M:17:VAL:HB    | 14:M:18:PRO:HD3   | 1.72                     | 0.72              |
| 21:N:127:GLY:O    | 21:N:128:GLU:HG2  | 1.90                     | 0.72              |
| 1:5:117:GLU:OE2   | 1:5:239:GLY:HA3   | 1.88                     | 0.72              |
| 25:c:508:CLA:H141 | 25:c:510:CLA:H18  | 1.72                     | 0.72              |
| 4:A:283:ILE:HG13  | 27:A:403:PHO:HBC3 | 1.72                     | 0.72              |
| 3:8:73:LEU:HG     | 3:8:82:GLY:CA     | 2.20                     | 0.72              |
| 23:u:85:LYS:HG2   | 23:u:101:CYS:CB   | 2.19                     | 0.72              |
| 2:2:88:ASP:HB3    | 2:2:91:ALA:HB3    | 1.70                     | 0.72              |
| 4:A:317:TRP:CZ3   | 7:D:181:ARG:HD3   | 2.24                     | 0.72              |
| 5:B:397:VAL:HG23  | 5:B:417:VAL:HG11  | 1.71                     | 0.72              |
| 1:7:127:GLY:O     | 1:7:128:GLU:HG2   | 1.90                     | 0.72              |
| 5:b:14:ASN:ND2    | 22:r:97:LEU:O     | 2.18                     | 0.72              |
| 10:h:62:ASN:OD1   | 10:h:63:SER:N     | 2.22                     | 0.72              |
| 21:g:215:GLU:HG3  | 25:g:610:CLA:C1B  | 2.19                     | 0.72              |
| 2:2:174:GLU:HB3   | 1:3:62:PHE:HB3    | 1.70                     | 0.72              |
| 1:3:107:MET:HG2   | 1:3:222:ALA:HB2   | 1.70                     | 0.72              |
| 25:C:504:CLA:H42  | 35:C:516:DGD:HB32 | 1.72                     | 0.72              |
| 24:G:606:CHL:HBA1 | 40:G:617:NEX:H403 | 1.71                     | 0.72              |
| 21:Y:215:GLU:HG3  | 25:Y:311:CLA:NB   | 2.04                     | 0.72              |
| 21:g:82:THR:CG2   | 24:y:310:CHL:HED3 | 2.20                     | 0.72              |
| 21:y:169:MET:HG3  | 24:y:310:CHL:CMC  | 2.19                     | 0.72              |
| 25:D:401:CLA:HAB  | 25:D:402:CLA:H72  | 1.69                     | 0.72              |
| 4:a:283:ILE:HG13  | 27:a:404:PHO:HBC3 | 1.72                     | 0.72              |
| 15:o:306:LEU:HD21 | 15:o:322:LYS:HE2  | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:103:SER:HB2  | 21:y:219:GLY:HA3  | 1.71                     | 0.72              |
| 21:y:127:GLY:O    | 21:y:128:GLU:HG2  | 1.90                     | 0.72              |
| 2:2:130:PRO:HG2   | 2:2:133:PHE:CD2   | 2.25                     | 0.71              |
| 5:B:141:ILE:CG2   | 25:B:615:CLA:HBB1 | 2.19                     | 0.71              |
| 6:C:293:ASN:OD1   | 35:C:515:DGD:HE61 | 1.90                     | 0.71              |
| 11:I:23:PHE:HB3   | 28:I:101:BCR:HC32 | 1.72                     | 0.71              |
| 20:S:63:TYR:OH    | 20:S:90:ALA:HB2   | 1.90                     | 0.71              |
| 4:a:329:GLU:HA    | 4:a:332:HIS:NE2   | 2.05                     | 0.71              |
| 6:c:130:ILE:HG22  | 19:z:27:PHE:HD2   | 1.55                     | 0.71              |
| 25:C:513:CLA:HBA1 | 25:C:513:CLA:HBD  | 1.71                     | 0.71              |
| 21:G:231:VAL:HG11 | 25:G:613:CLA:HHD  | 1.73                     | 0.71              |
| 4:a:308:ASP:OD1   | 8:e:55:TYR:HB2    | 1.90                     | 0.71              |
| 4:A:329:GLU:HA    | 4:A:332:HIS:NE2   | 2.05                     | 0.71              |
| 6:C:225:VAL:HG22  | 6:C:289:PHE:CE1   | 2.24                     | 0.71              |
| 15:O:310:ASP:OD1  | 15:O:311:THR:N    | 2.22                     | 0.71              |
| 2:6:104:ARG:NE    | 24:6:603:CHL:HBD  | 2.05                     | 0.71              |
| 2:6:218:LYS:O     | 2:6:221:ARG:HG2   | 1.91                     | 0.71              |
| 2:6:220:GLY:HA3   | 25:6:602:CLA:HAC1 | 1.71                     | 0.71              |
| 1:7:146:TYR:O     | 1:7:152:LEU:HD12  | 1.88                     | 0.71              |
| 20:s:63:TYR:OH    | 20:s:90:ALA:HB2   | 1.90                     | 0.71              |
| 2:2:218:LYS:O     | 2:2:221:ARG:HG2   | 1.91                     | 0.71              |
| 21:G:70:LEU:HD13  | 21:G:79:GLY:HA2   | 1.71                     | 0.71              |
| 14:m:17:VAL:HB    | 14:m:18:PRO:HD3   | 1.72                     | 0.71              |
| 21:y:215:GLU:HG3  | 25:y:311:CLA:NB   | 2.04                     | 0.71              |
| 1:1:70:LEU:HD13   | 1:1:79:GLY:HA2    | 1.71                     | 0.71              |
| 2:2:120:GLN:HA    | 2:2:124:ARG:O     | 1.90                     | 0.71              |
| 2:2:155:HIS:NE2   | 2:2:161:ALA:HB2   | 2.03                     | 0.71              |
| 3:4:142:PHE:CE1   | 3:4:146:LEU:HD11  | 2.24                     | 0.71              |
| 4:A:229:GLU:O     | 4:A:232:SER:HB2   | 1.90                     | 0.71              |
| 2:6:113:CYS:SG    | 2:6:131:VAL:HG21  | 2.30                     | 0.71              |
| 25:c:504:CLA:H42  | 35:c:516:DGD:HB32 | 1.72                     | 0.71              |
| 20:s:246:THR:CG2  | 20:s:248:GLU:HG2  | 2.21                     | 0.71              |
| 25:n:613:CLA:H8   | 25:n:613:CLA:C14  | 2.21                     | 0.71              |
| 15:O:306:LEU:HD21 | 15:O:322:LYS:HE2  | 1.70                     | 0.71              |
| 22:R:127:TYR:CD2  | 22:R:135:ARG:HD2  | 2.24                     | 0.71              |
| 3:8:219:GLU:HG3   | 3:8:222:GLU:HB2   | 1.69                     | 0.71              |
| 5:b:460:LEU:HD11  | 7:d:288:VAL:CG2   | 2.21                     | 0.71              |
| 6:c:131:TYR:OH    | 20:s:74:GLY:HA3   | 1.90                     | 0.71              |
| 6:c:293:ASN:OD1   | 35:c:515:DGD:HE61 | 1.90                     | 0.71              |
| 20:s:63:TYR:CE2   | 20:s:219:ALA:HB1  | 2.25                     | 0.71              |
| 22:r:246:ALA:O    | 22:r:250:MET:HG3  | 1.91                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:127:GLY:O     | 1:1:128:GLU:HG2   | 1.90                     | 0.71              |
| 20:S:141:CYS:SG   | 20:S:162:TYR:HA   | 2.31                     | 0.71              |
| 25:N:610:CLA:HMC1 | 39:N:615:LUT:C31  | 2.21                     | 0.71              |
| 1:5:128:GLU:HB2   | 1:5:137:GLN:HB2   | 1.73                     | 0.71              |
| 11:i:23:PHE:HB3   | 28:i:101:BCR:HC32 | 1.72                     | 0.71              |
| 25:n:603:CLA:HAB  | 39:n:616:LUT:C35  | 2.19                     | 0.71              |
| 22:r:124:PHE:HD1  | 25:r:614:CLA:CHC  | 2.03                     | 0.71              |
| 2:2:104:ARG:NE    | 24:2:603:CHL:HBD  | 2.04                     | 0.71              |
| 1:3:127:GLY:O     | 1:3:128:GLU:HG2   | 1.90                     | 0.71              |
| 3:4:94:PHE:HB3    | 3:4:98:TYR:HE2    | 1.56                     | 0.71              |
| 25:A:405:CLA:HHD  | 28:A:406:BCR:H362 | 1.72                     | 0.71              |
| 6:C:131:TYR:OH    | 20:S:74:GLY:HA3   | 1.90                     | 0.71              |
| 1:7:138:ILE:HB    | 1:7:144:LEU:HD12  | 1.73                     | 0.71              |
| 4:a:331:MET:CE    | 7:d:321:LEU:HB3   | 2.20                     | 0.71              |
| 5:b:382:PRO:HB3   | 7:d:345:GLU:OE2   | 1.90                     | 0.71              |
| 6:c:57:ALA:O      | 6:c:61:VAL:HG23   | 1.89                     | 0.71              |
| 21:g:215:GLU:HG3  | 25:g:610:CLA:C4B  | 2.19                     | 0.71              |
| 21:n:128:GLU:HB2  | 21:n:137:GLN:HB2  | 1.73                     | 0.71              |
| 2:2:213:LYS:O     | 2:2:217:ILE:HG12  | 1.89                     | 0.71              |
| 21:N:107:MET:HE1  | 25:N:610:CLA:HHC  | 1.73                     | 0.71              |
| 25:N:613:CLA:H8   | 25:N:613:CLA:C14  | 2.21                     | 0.71              |
| 5:b:70:GLY:HA2    | 5:b:178:VAL:CG1   | 2.20                     | 0.71              |
| 7:d:57:THR:HG21   | 8:e:50:PRO:HD3    | 1.73                     | 0.71              |
| 20:s:141:CYS:SG   | 20:s:162:TYR:HA   | 2.31                     | 0.71              |
| 21:g:127:GLY:O    | 21:g:128:GLU:HG2  | 1.90                     | 0.71              |
| 21:g:128:GLU:HB2  | 21:g:137:GLN:HB2  | 1.73                     | 0.71              |
| 21:g:197:ASP:OD1  | 25:g:610:CLA:HAA1 | 1.89                     | 0.71              |
| 25:r:612:CLA:H101 | 25:r:612:CLA:HAB  | 1.71                     | 0.71              |
| 1:3:138:ILE:HB    | 1:3:144:LEU:HD12  | 1.73                     | 0.71              |
| 3:4:168:ASP:HA    | 3:4:185:PHE:CZ    | 2.26                     | 0.71              |
| 4:A:335:ASN:HA    | 7:D:351:ASN:ND2   | 2.05                     | 0.71              |
| 2:6:97:ALA:CB     | 2:6:190:LEU:HD11  | 2.21                     | 0.71              |
| 4:a:229:GLU:O     | 4:a:232:SER:HB2   | 1.90                     | 0.71              |
| 25:a:406:CLA:HHD  | 28:a:407:BCR:H362 | 1.73                     | 0.71              |
| 21:g:231:VAL:HG11 | 25:g:613:CLA:HHD  | 1.72                     | 0.71              |
| 21:y:138:ILE:HB   | 21:y:144:LEU:HD12 | 1.73                     | 0.71              |
| 21:N:231:VAL:HG11 | 25:N:613:CLA:HAC1 | 1.73                     | 0.70              |
| 40:Y:318:NEX:H28  | 40:Y:318:NEX:C36  | 2.21                     | 0.70              |
| 5:b:128:THR:HG21  | 22:r:94:ILE:HD13  | 1.72                     | 0.70              |
| 5:b:272:ARG:HB2   | 5:b:319:PRO:HG2   | 1.73                     | 0.70              |
| 19:z:14:ILE:O     | 19:z:18:ILE:HD12  | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:73:GLU:HG2   | 21:g:73:GLU:O     | 1.91                     | 0.70              |
| 21:n:107:MET:HE1  | 25:n:610:CLA:HHC  | 1.73                     | 0.70              |
| 21:n:127:GLY:O    | 21:n:128:GLU:HG2  | 1.90                     | 0.70              |
| 1:3:128:GLU:HB2   | 1:3:137:GLN:HB2   | 1.73                     | 0.70              |
| 21:N:165:GLN:HE22 | 24:N:606:CHL:C1B  | 2.04                     | 0.70              |
| 1:5:73:GLU:O      | 1:5:73:GLU:HG2    | 1.91                     | 0.70              |
| 4:a:333:GLU:O     | 7:d:350:GLY:HA3   | 1.91                     | 0.70              |
| 5:b:141:ILE:CG2   | 25:b:615:CLA:HBB1 | 2.20                     | 0.70              |
| 25:g:610:CLA:HBB1 | 39:g:615:LUT:H32  | 1.73                     | 0.70              |
| 40:y:318:NEX:H28  | 40:y:318:NEX:C36  | 2.21                     | 0.70              |
| 2:2:217:ILE:HD12  | 25:2:604:CLA:CAD  | 2.21                     | 0.70              |
| 5:B:460:LEU:HD11  | 7:D:288:VAL:CG2   | 2.21                     | 0.70              |
| 15:O:163:LEU:O    | 15:O:164:MET:HE2  | 1.91                     | 0.70              |
| 20:S:246:THR:CG2  | 20:S:248:GLU:HG2  | 2.21                     | 0.70              |
| 21:N:138:ILE:HB   | 21:N:144:LEU:HD12 | 1.73                     | 0.70              |
| 2:6:120:GLN:HA    | 2:6:124:ARG:O     | 1.90                     | 0.70              |
| 3:8:113:VAL:HG13  | 3:8:114:LEU:HD12  | 1.72                     | 0.70              |
| 4:a:74:GLY:HA3    | 7:d:305:ARG:HH12  | 1.54                     | 0.70              |
| 4:a:183:MET:HB3   | 25:a:402:CLA:HBC2 | 1.73                     | 0.70              |
| 3:4:219:GLU:OE1   | 3:4:219:GLU:N     | 2.25                     | 0.70              |
| 4:A:183:MET:HB3   | 25:A:401:CLA:HBC2 | 1.73                     | 0.70              |
| 21:G:82:THR:CG2   | 24:Y:310:CHL:HED3 | 2.20                     | 0.70              |
| 21:N:128:GLU:HB2  | 21:N:137:GLN:HB2  | 1.73                     | 0.70              |
| 3:8:219:GLU:OE1   | 3:8:219:GLU:N     | 2.24                     | 0.70              |
| 6:c:163:ILE:HG21  | 25:c:512:CLA:CAB  | 2.21                     | 0.70              |
| 26:d:406:LHG:HC62 | 13:l:16:THR:HG23  | 1.73                     | 0.70              |
| 20:s:202:PRO:HG3  | 24:s:308:CHL:HBC2 | 1.74                     | 0.70              |
| 25:n:610:CLA:HMC1 | 39:n:615:LUT:C31  | 2.21                     | 0.70              |
| 2:2:97:ALA:CB     | 2:2:190:LEU:HD11  | 2.21                     | 0.70              |
| 4:A:333:GLU:O     | 7:D:350:GLY:HA3   | 1.91                     | 0.70              |
| 25:C:508:CLA:H141 | 25:C:510:CLA:H18  | 1.72                     | 0.70              |
| 25:C:510:CLA:ND   | 25:C:510:CLA:H172 | 2.07                     | 0.70              |
| 21:G:138:ILE:HB   | 21:G:144:LEU:HD12 | 1.73                     | 0.70              |
| 21:N:215:GLU:HG3  | 25:N:610:CLA:C4B  | 2.22                     | 0.70              |
| 22:R:246:ALA:O    | 22:R:250:MET:HG3  | 1.91                     | 0.70              |
| 1:5:127:GLY:O     | 1:5:128:GLU:HG2   | 1.90                     | 0.70              |
| 3:8:168:ASP:HA    | 3:8:185:PHE:CZ    | 2.26                     | 0.70              |
| 6:c:151:TRP:CB    | 17:w:133:LEU:HD21 | 2.21                     | 0.70              |
| 28:k:101:BCR:C33  | 19:z:12:LEU:HD23  | 2.22                     | 0.70              |
| 16:t:14:LEU:HD12  | 28:t:101:BCR:H343 | 1.73                     | 0.70              |
| 2:2:113:CYS:SG    | 2:2:131:VAL:HG21  | 2.30                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:241:SER:OG    | 25:B:612:CLA:OBD  | 2.06                     | 0.70              |
| 6:C:369:LEU:HD22  | 6:C:380:LEU:HD23  | 1.74                     | 0.70              |
| 16:T:1:MET:HG2    | 16:T:3:ALA:H      | 1.57                     | 0.70              |
| 16:T:14:LEU:HD12  | 28:T:101:BCR:H343 | 1.73                     | 0.70              |
| 22:R:184:LEU:HD23 | 24:y:306:CHL:HAA2 | 1.74                     | 0.70              |
| 25:6:604:CLA:HAA1 | 25:6:604:CLA:HBD  | 1.74                     | 0.70              |
| 3:8:94:PHE:HB3    | 3:8:98:TYR:HE2    | 1.56                     | 0.70              |
| 4:a:335:ASN:HA    | 7:d:351:ASN:ND2   | 2.05                     | 0.70              |
| 7:d:194:LEU:HD23  | 7:d:296:ALA:O     | 1.92                     | 0.70              |
| 25:g:610:CLA:H2   | 39:g:615:LUT:H28  | 1.73                     | 0.70              |
| 21:n:165:GLN:HE22 | 24:n:606:CHL:C1B  | 2.04                     | 0.70              |
| 21:n:215:GLU:HG3  | 25:n:610:CLA:C4B  | 2.22                     | 0.70              |
| 3:4:113:VAL:HG13  | 3:4:114:LEU:HD12  | 1.72                     | 0.70              |
| 3:4:122:TRP:O     | 3:4:126:ALA:N     | 2.25                     | 0.70              |
| 6:C:130:ILE:HG22  | 19:Z:27:PHE:HD2   | 1.55                     | 0.70              |
| 7:D:15:LEU:HD11   | 18:X:103:VAL:CG1  | 2.21                     | 0.70              |
| 22:R:124:PHE:HD1  | 25:R:614:CLA:CHC  | 2.03                     | 0.70              |
| 3:8:225:LYS:HA    | 3:8:228:GLU:CD    | 2.17                     | 0.70              |
| 15:o:163:LEU:O    | 15:o:164:MET:HE2  | 1.91                     | 0.70              |
| 25:2:604:CLA:HBD  | 25:2:604:CLA:HAA1 | 1.74                     | 0.70              |
| 3:4:225:LYS:HA    | 3:4:228:GLU:CD    | 2.17                     | 0.70              |
| 25:B:615:CLA:H91  | 25:B:615:CLA:H172 | 1.73                     | 0.70              |
| 21:G:127:GLY:O    | 21:G:128:GLU:HG2  | 1.90                     | 0.70              |
| 21:N:73:GLU:O     | 21:N:73:GLU:HG2   | 1.91                     | 0.70              |
| 21:Y:127:GLY:O    | 21:Y:128:GLU:HG2  | 1.90                     | 0.70              |
| 22:R:93:ASP:HB2   | 22:R:108:ASP:N    | 2.06                     | 0.70              |
| 4:a:235:GLU:OE1   | 7:d:266:ARG:HB2   | 1.92                     | 0.70              |
| 5:b:332:ASN:ND2   | 30:b:620:LMG:O4   | 2.25                     | 0.70              |
| 2:2:104:ARG:CZ    | 24:2:603:CHL:HBD  | 2.22                     | 0.70              |
| 4:A:308:ASP:OD1   | 8:E:55:TYR:HB2    | 1.90                     | 0.70              |
| 7:D:57:THR:HG21   | 8:E:50:PRO:HD3    | 1.73                     | 0.70              |
| 21:G:98:LEU:CD2   | 25:G:603:CLA:HAA1 | 2.21                     | 0.70              |
| 25:G:610:CLA:HBB1 | 39:G:615:LUT:H32  | 1.73                     | 0.70              |
| 25:b:604:CLA:H142 | 25:b:615:CLA:CMA  | 2.21                     | 0.70              |
| 21:y:202:ALA:HB1  | 21:y:208:PHE:HD1  | 1.57                     | 0.70              |
| 4:A:232:SER:HB3   | 5:B:4:PRO:HD3     | 1.74                     | 0.70              |
| 5:B:442:VAL:HG23  | 5:B:444:ARG:HH12  | 1.57                     | 0.70              |
| 6:C:163:ILE:HG21  | 25:C:512:CLA:CAB  | 2.21                     | 0.70              |
| 6:C:327:ASN:HD21  | 15:O:192:ASP:HB2  | 1.57                     | 0.70              |
| 19:Z:14:ILE:O     | 19:Z:18:ILE:HD12  | 1.91                     | 0.70              |
| 21:N:202:ALA:HB1  | 21:N:208:PHE:HD1  | 1.57                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:R:129:GLU:OE1  | 22:R:132:GLY:N    | 2.25                     | 0.70              |
| 4:a:75:ASN:HB2    | 4:a:79:SER:OG     | 1.92                     | 0.70              |
| 20:s:119:ARG:HD3  | 25:s:310:CLA:HHD  | 1.74                     | 0.70              |
| 21:g:98:LEU:CD2   | 25:g:603:CLA:HAA1 | 2.21                     | 0.70              |
| 21:y:73:GLU:O     | 21:y:73:GLU:HG2   | 1.91                     | 0.70              |
| 4:A:74:GLY:HA3    | 7:D:305:ARG:HH12  | 1.54                     | 0.69              |
| 5:B:272:ARG:HB2   | 5:B:319:PRO:HG2   | 1.73                     | 0.69              |
| 6:C:255:LYS:NZ    | 17:W:127:GLU:OE2  | 2.22                     | 0.69              |
| 7:D:78:ALA:HB2    | 7:D:175:GLY:HA3   | 1.74                     | 0.69              |
| 29:L:101:SQD:H251 | 29:L:101:SQD:H111 | 1.74                     | 0.69              |
| 14:M:28:LYS:HB2   | 14:m:27:VAL:CG1   | 2.22                     | 0.69              |
| 2:6:104:ARG:CZ    | 24:6:603:CHL:HBD  | 2.22                     | 0.69              |
| 1:7:128:GLU:HB2   | 1:7:137:GLN:HB2   | 1.73                     | 0.69              |
| 4:a:232:SER:HB3   | 5:b:4:PRO:HD3     | 1.74                     | 0.69              |
| 5:b:121:GLU:OE2   | 10:h:16:SER:OG    | 2.08                     | 0.69              |
| 29:l:102:SQD:H251 | 29:l:102:SQD:H111 | 1.74                     | 0.69              |
| 5:B:332:ASN:ND2   | 30:B:620:LMG:O4   | 2.25                     | 0.69              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:C1B  | 2.22                     | 0.69              |
| 21:N:215:GLU:HG3  | 25:N:610:CLA:NB   | 2.06                     | 0.69              |
| 25:c:510:CLA:ND   | 25:c:510:CLA:H172 | 2.07                     | 0.69              |
| 20:s:72:PRO:CG    | 20:s:75:LEU:HD13  | 2.19                     | 0.69              |
| 20:s:109:LYS:O    | 20:s:113:PHE:HD2  | 1.75                     | 0.69              |
| 21:g:138:ILE:HB   | 21:g:144:LEU:HD12 | 1.73                     | 0.69              |
| 21:n:215:GLU:HG3  | 25:n:610:CLA:NB   | 2.06                     | 0.69              |
| 1:3:138:ILE:CG1   | 1:3:144:LEU:HB2   | 2.23                     | 0.69              |
| 7:D:298:ASP:HA    | 7:D:316:TYR:OH    | 1.92                     | 0.69              |
| 28:K:101:BCR:C33  | 19:Z:12:LEU:HD23  | 2.22                     | 0.69              |
| 25:G:610:CLA:H2   | 39:G:615:LUT:H28  | 1.73                     | 0.69              |
| 21:Y:73:GLU:O     | 21:Y:73:GLU:HG2   | 1.91                     | 0.69              |
| 7:d:78:ALA:HB2    | 7:d:175:GLY:HA3   | 1.74                     | 0.69              |
| 21:y:128:GLU:HB2  | 21:y:137:GLN:HB2  | 1.73                     | 0.69              |
| 21:y:131:TRP:HB2  | 39:y:317:LUT:H21  | 1.75                     | 0.69              |
| 22:r:93:ASP:HB2   | 22:r:108:ASP:N    | 2.06                     | 0.69              |
| 25:B:603:CLA:HAB  | 25:B:605:CLA:H152 | 1.74                     | 0.69              |
| 20:S:109:LYS:O    | 20:S:113:PHE:HD2  | 1.75                     | 0.69              |
| 2:6:178:ILE:HD12  | 1:7:62:PHE:HD1    | 1.58                     | 0.69              |
| 4:a:133:LEU:HD23  | 7:d:257:ILE:HG12  | 1.74                     | 0.69              |
| 7:d:298:ASP:HA    | 7:d:316:TYR:OH    | 1.92                     | 0.69              |
| 15:o:230:LYS:HD3  | 15:o:284:GLU:OE1  | 1.93                     | 0.69              |
| 21:n:202:ALA:HB1  | 21:n:208:PHE:HD1  | 1.57                     | 0.69              |
| 1:1:138:ILE:HB    | 1:1:144:LEU:HD12  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:235:GLU:OE1   | 7:D:266:ARG:HB2   | 1.92                     | 0.69              |
| 21:G:82:THR:HG21  | 24:Y:310:CHL:HAA1 | 1.74                     | 0.69              |
| 24:Y:306:CHL:HAA2 | 22:r:184:LEU:HD23 | 1.74                     | 0.69              |
| 25:b:613:CLA:HED2 | 25:b:613:CLA:H2   | 1.74                     | 0.69              |
| 21:g:82:THR:HG21  | 24:y:310:CHL:HAA1 | 1.74                     | 0.69              |
| 26:D:406:LHG:HC62 | 13:L:16:THR:HG23  | 1.73                     | 0.69              |
| 21:N:138:ILE:CG1  | 21:N:144:LEU:HB2  | 2.22                     | 0.69              |
| 21:Y:131:TRP:HB2  | 39:Y:317:LUT:H21  | 1.74                     | 0.69              |
| 21:Y:138:ILE:HB   | 21:Y:144:LEU:HD12 | 1.73                     | 0.69              |
| 1:5:202:ALA:HB1   | 1:5:208:PHE:HD1   | 1.57                     | 0.69              |
| 2:6:210:ALA:HA    | 2:6:213:LYS:NZ    | 2.07                     | 0.69              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:C1B  | 2.22                     | 0.69              |
| 21:n:231:VAL:HG11 | 25:n:613:CLA:HAC1 | 1.73                     | 0.69              |
| 1:1:128:GLU:HB2   | 1:1:137:GLN:HB2   | 1.73                     | 0.69              |
| 2:2:104:ARG:NE    | 24:2:603:CHL:CBD  | 2.55                     | 0.69              |
| 6:C:154:ARG:HG2   | 6:C:266:TRP:CE3   | 2.28                     | 0.69              |
| 7:D:194:LEU:HD23  | 7:D:296:ALA:O     | 1.92                     | 0.69              |
| 20:s:144:GLU:HB3  | 20:s:153:LEU:HD21 | 1.73                     | 0.69              |
| 2:2:178:ILE:HD12  | 1:3:62:PHE:HD1    | 1.57                     | 0.69              |
| 2:2:210:ALA:HA    | 2:2:213:LYS:NZ    | 2.07                     | 0.69              |
| 3:4:155:TRP:CD1   | 3:4:159:LYS:HZ1   | 2.10                     | 0.69              |
| 3:4:219:GLU:O     | 3:4:219:GLU:HG2   | 1.93                     | 0.69              |
| 4:A:46:SER:O      | 4:A:50:ILE:HG12   | 1.93                     | 0.69              |
| 26:L:102:LHG:H102 | 26:L:102:LHG:HC61 | 1.74                     | 0.69              |
| 14:M:27:VAL:CG1   | 14:m:28:LYS:HB2   | 2.22                     | 0.69              |
| 15:O:309:SER:OG   | 15:O:319:LYS:N    | 2.20                     | 0.69              |
| 25:N:603:CLA:H191 | 24:N:607:CHL:C11  | 2.22                     | 0.69              |
| 21:Y:128:GLU:HB2  | 21:Y:137:GLN:HB2  | 1.73                     | 0.69              |
| 22:R:156:SER:HB3  | 25:R:604:CLA:HHD  | 1.75                     | 0.69              |
| 1:5:138:ILE:HB    | 1:5:144:LEU:HD12  | 1.73                     | 0.69              |
| 1:7:138:ILE:CG1   | 1:7:144:LEU:HB2   | 2.23                     | 0.69              |
| 1:7:202:ALA:HB1   | 1:7:208:PHE:HD1   | 1.57                     | 0.69              |
| 25:a:403:CLA:HBB  | 27:a:404:PHO:H203 | 1.74                     | 0.69              |
| 25:b:606:CLA:CHC  | 26:b:622:LHG:H272 | 2.23                     | 0.69              |
| 6:c:154:ARG:HG2   | 6:c:266:TRP:CE3   | 2.28                     | 0.69              |
| 7:d:56:VAL:HG21   | 7:d:111:LEU:HD11  | 1.75                     | 0.69              |
| 16:t:1:MET:HG2    | 16:t:3:ALA:H      | 1.57                     | 0.69              |
| 17:w:116:PHE:O    | 17:w:120:THR:HG23 | 1.93                     | 0.69              |
| 21:n:138:ILE:CG1  | 21:n:144:LEU:HB2  | 2.22                     | 0.69              |
| 25:n:602:CLA:HMC3 | 25:n:602:CLA:HBC2 | 1.75                     | 0.69              |
| 25:n:603:CLA:H191 | 24:n:607:CHL:C11  | 2.22                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:156:SER:HB3  | 25:r:604:CLA:HHD  | 1.75                     | 0.69              |
| 2:2:150:ASN:O     | 2:2:154:VAL:HG21  | 1.92                     | 0.69              |
| 3:4:157:GLU:O     | 3:4:161:TRP:HD1   | 1.76                     | 0.69              |
| 3:4:176:THR:OG1   | 3:4:180:LYS:HA    | 1.93                     | 0.69              |
| 3:4:219:GLU:HB2   | 3:4:222:GLU:HB2   | 1.75                     | 0.69              |
| 7:D:162:PRO:HB3   | 7:D:171:ALA:HB2   | 1.75                     | 0.69              |
| 21:Y:104:ARG:NH1  | 24:Y:309:CHL:OBD  | 2.20                     | 0.69              |
| 6:c:369:LEU:HD22  | 6:c:380:LEU:HD23  | 1.74                     | 0.69              |
| 21:g:202:ALA:HB1  | 21:g:208:PHE:HD1  | 1.57                     | 0.69              |
| 4:A:75:ASN:HB2    | 4:A:79:SER:OG     | 1.92                     | 0.69              |
| 17:W:116:PHE:O    | 17:W:120:THR:HG23 | 1.93                     | 0.69              |
| 1:5:178:ALA:HA    | 2:6:64:VAL:CG2    | 2.07                     | 0.69              |
| 2:6:150:ASN:O     | 2:6:154:VAL:HG21  | 1.93                     | 0.69              |
| 3:8:176:THR:OG1   | 3:8:180:LYS:HA    | 1.93                     | 0.69              |
| 3:8:224:LEU:O     | 3:8:228:GLU:OE1   | 2.10                     | 0.69              |
| 21:g:87:ALA:HB1   | 21:y:90:GLU:CB    | 2.23                     | 0.69              |
| 21:g:211:LEU:HB3  | 25:g:610:CLA:HMA1 | 1.74                     | 0.69              |
| 21:n:138:ILE:CG2  | 24:n:606:CHL:HBC1 | 2.14                     | 0.69              |
| 1:1:73:GLU:HG2    | 1:1:73:GLU:O      | 1.91                     | 0.68              |
| 1:3:202:ALA:HB1   | 1:3:208:PHE:HD1   | 1.57                     | 0.68              |
| 4:A:133:LEU:HD23  | 7:D:257:ILE:HG12  | 1.74                     | 0.68              |
| 6:C:281:VAL:O     | 6:C:285:ILE:HG13  | 1.94                     | 0.68              |
| 20:S:202:PRO:HG3  | 24:S:308:CHL:HBC2 | 1.74                     | 0.68              |
| 21:G:128:GLU:HB2  | 21:G:137:GLN:HB2  | 1.73                     | 0.68              |
| 22:R:202:ILE:HD12 | 24:R:607:CHL:HMA3 | 1.75                     | 0.68              |
| 2:6:217:ILE:HD12  | 25:6:604:CLA:CAD  | 2.21                     | 0.68              |
| 12:k:32:PHE:HZ    | 19:z:9:VAL:HG11   | 1.58                     | 0.68              |
| 3:4:224:LEU:O     | 3:4:228:GLU:OE1   | 2.10                     | 0.68              |
| 4:A:176:ILE:HD13  | 25:A:402:CLA:HED3 | 1.75                     | 0.68              |
| 25:B:606:CLA:CHC  | 26:B:622:LHG:H272 | 2.23                     | 0.68              |
| 25:B:613:CLA:HED2 | 25:B:613:CLA:H2   | 1.74                     | 0.68              |
| 21:G:87:ALA:HB1   | 21:Y:90:GLU:CB    | 2.23                     | 0.68              |
| 21:Y:244:LEU:HD22 | 39:Y:316:LUT:H163 | 1.75                     | 0.68              |
| 2:6:174:GLU:OE1   | 1:7:62:PHE:HD2    | 1.76                     | 0.68              |
| 3:8:219:GLU:HB2   | 3:8:222:GLU:HB2   | 1.75                     | 0.68              |
| 6:c:26:ARG:NH2    | 6:c:41:ARG:O      | 2.26                     | 0.68              |
| 6:c:281:VAL:O     | 6:c:285:ILE:HG13  | 1.94                     | 0.68              |
| 6:C:26:ARG:NH2    | 6:C:41:ARG:O      | 2.26                     | 0.68              |
| 20:S:236:MET:HE2  | 39:S:316:LUT:C12  | 2.23                     | 0.68              |
| 21:G:138:ILE:CG1  | 21:G:144:LEU:HB2  | 2.23                     | 0.68              |
| 21:G:211:LEU:HB3  | 25:G:610:CLA:HMA1 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:N:609:CHL:HAA2 | 21:Y:82:THR:CG2   | 2.17                     | 0.68              |
| 21:Y:256:ALA:HB2  | 25:Y:314:CLA:CAD  | 2.23                     | 0.68              |
| 23:U:85:LYS:HG2   | 23:U:101:CYS:CB   | 2.19                     | 0.68              |
| 3:8:122:TRP:O     | 3:8:126:ALA:N     | 2.25                     | 0.68              |
| 20:s:225:GLU:HB2  | 25:s:310:CLA:CHB  | 2.22                     | 0.68              |
| 21:n:73:GLU:O     | 21:n:73:GLU:HG2   | 1.91                     | 0.68              |
| 22:r:198:VAL:O    | 22:r:202:ILE:HG23 | 1.94                     | 0.68              |
| 2:2:131:VAL:O     | 2:2:134:LYS:HB2   | 1.94                     | 0.68              |
| 2:2:251:ASN:HB3   | 25:2:605:CLA:HBB  | 1.75                     | 0.68              |
| 21:G:73:GLU:HG2   | 21:G:73:GLU:O     | 1.91                     | 0.68              |
| 21:N:234:ILE:HG21 | 32:N:620:AJP:C81  | 2.23                     | 0.68              |
| 3:8:183:GLU:HB3   | 3:8:185:PHE:CD1   | 2.28                     | 0.68              |
| 7:d:162:PRO:HB3   | 7:d:171:ALA:HB2   | 1.75                     | 0.68              |
| 21:Y:56:VAL:HB    | 24:Y:302:CHL:HBC1 | 1.76                     | 0.68              |
| 3:8:157:GLU:O     | 3:8:161:TRP:HD1   | 1.76                     | 0.68              |
| 5:b:162:TYR:O     | 25:b:606:CLA:HHD  | 1.93                     | 0.68              |
| 6:c:346:THR:OG1   | 6:c:348:GLU:OE1   | 2.09                     | 0.68              |
| 25:c:504:CLA:CHC  | 35:c:516:DGD:HB51 | 2.24                     | 0.68              |
| 26:l:103:LHG:H102 | 26:l:103:LHG:HC61 | 1.74                     | 0.68              |
| 21:g:59:LEU:HD23  | 24:g:601:CHL:C2B  | 2.24                     | 0.68              |
| 21:y:104:ARG:NH1  | 24:y:309:CHL:OBD  | 2.20                     | 0.68              |
| 21:y:127:GLY:HA3  | 21:y:137:GLN:HG3  | 1.76                     | 0.68              |
| 3:4:73:LEU:HG     | 3:4:82:GLY:CA     | 2.20                     | 0.68              |
| 3:4:183:GLU:HB3   | 3:4:185:PHE:CD1   | 2.28                     | 0.68              |
| 29:L:101:SQD:H122 | 14:m:23:LEU:HD13  | 1.74                     | 0.68              |
| 20:S:59:LEU:CD1   | 20:S:216:GLU:HG3  | 2.24                     | 0.68              |
| 20:S:262:PHE:HE2  | 25:S:314:CLA:H3A  | 1.59                     | 0.68              |
| 21:Y:231:VAL:HG11 | 25:Y:314:CLA:HAC2 | 1.73                     | 0.68              |
| 2:6:251:ASN:HB3   | 25:6:605:CLA:HBB  | 1.75                     | 0.68              |
| 1:7:73:GLU:HG2    | 1:7:73:GLU:O      | 1.91                     | 0.68              |
| 4:a:176:ILE:HD13  | 25:a:403:CLA:HED3 | 1.75                     | 0.68              |
| 5:b:442:VAL:HG23  | 5:b:444:ARG:HH12  | 1.57                     | 0.68              |
| 20:s:113:PHE:O    | 20:s:117:HIS:ND1  | 2.26                     | 0.68              |
| 21:y:138:ILE:CG1  | 21:y:144:LEU:HB2  | 2.23                     | 0.68              |
| 1:1:138:ILE:CG1   | 1:1:144:LEU:HB2   | 2.23                     | 0.68              |
| 1:1:202:ALA:HB1   | 1:1:208:PHE:HD1   | 1.57                     | 0.68              |
| 21:G:60:GLY:HA3   | 24:G:601:CHL:CMC  | 2.23                     | 0.68              |
| 25:N:602:CLA:HMC3 | 25:N:602:CLA:HBC2 | 1.75                     | 0.68              |
| 22:R:153:GLY:HA2  | 25:R:604:CLA:C4C  | 2.24                     | 0.68              |
| 25:R:603:CLA:C1D  | 25:R:608:CLA:H92  | 1.95                     | 0.68              |
| 24:6:601:CHL:H12  | 26:6:606:LHG:H181 | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:a:46:SER:O      | 4:a:50:ILE:HG12   | 1.93                     | 0.68              |
| 25:b:615:CLA:H91  | 25:b:615:CLA:H172 | 1.73                     | 0.68              |
| 26:s:301:LHG:H272 | 25:s:311:CLA:HBB2 | 1.76                     | 0.68              |
| 21:n:138:ILE:HB   | 21:n:144:LEU:HD12 | 1.73                     | 0.68              |
| 21:y:231:VAL:HG11 | 25:y:314:CLA:HAC2 | 1.73                     | 0.68              |
| 25:r:601:CLA:C4C  | 26:r:618:LHG:HC92 | 2.24                     | 0.68              |
| 1:3:127:GLY:HA3   | 1:3:137:GLN:HG3   | 1.76                     | 0.68              |
| 5:B:162:TYR:O     | 25:B:606:CLA:HHD  | 1.93                     | 0.68              |
| 25:B:615:CLA:H51  | 25:B:616:CLA:H203 | 1.75                     | 0.68              |
| 21:G:231:VAL:HG21 | 25:G:613:CLA:CAC  | 2.24                     | 0.68              |
| 21:N:127:GLY:HA3  | 21:N:137:GLN:HG3  | 1.76                     | 0.68              |
| 21:Y:151:SER:HB2  | 22:r:185:PRO:HD3  | 1.76                     | 0.68              |
| 22:R:198:VAL:O    | 22:R:202:ILE:HG23 | 1.94                     | 0.68              |
| 5:b:91:TRP:HE1    | 26:b:622:LHG:HC61 | 1.58                     | 0.68              |
| 21:y:56:VAL:HB    | 24:y:302:CHL:HBC1 | 1.76                     | 0.68              |
| 21:y:59:LEU:HD23  | 24:y:302:CHL:C1B  | 2.24                     | 0.68              |
| 21:y:256:ALA:HB2  | 25:y:314:CLA:CAD  | 2.24                     | 0.68              |
| 2:2:174:GLU:OE1   | 1:3:62:PHE:HD2    | 1.76                     | 0.68              |
| 21:G:59:LEU:HD23  | 24:G:601:CHL:C2B  | 2.24                     | 0.68              |
| 5:b:462:PHE:CZ    | 25:b:613:CLA:HMB3 | 2.29                     | 0.68              |
| 25:b:603:CLA:HAB  | 25:b:605:CLA:H152 | 1.74                     | 0.68              |
| 25:y:313:CLA:HBB1 | 39:y:316:LUT:C14  | 2.24                     | 0.68              |
| 22:r:224:ASP:OD1  | 39:r:615:LUT:O23  | 2.12                     | 0.68              |
| 1:3:73:GLU:O      | 1:3:73:GLU:HG2    | 1.91                     | 0.68              |
| 15:O:230:LYS:HD3  | 15:O:284:GLU:OE1  | 1.93                     | 0.68              |
| 20:S:144:GLU:HB3  | 20:S:153:LEU:HD21 | 1.73                     | 0.68              |
| 20:S:225:GLU:HB2  | 25:S:310:CLA:CHB  | 2.22                     | 0.68              |
| 26:S:301:LHG:H272 | 25:S:311:CLA:HBB2 | 1.76                     | 0.68              |
| 2:6:128:LYS:HD3   | 2:6:133:PHE:HB3   | 1.76                     | 0.68              |
| 2:6:131:VAL:O     | 2:6:134:LYS:HB2   | 1.94                     | 0.68              |
| 2:6:168:ILE:O     | 2:6:172:LEU:HG    | 1.94                     | 0.68              |
| 21:g:60:GLY:HA3   | 24:g:601:CHL:CMC  | 2.24                     | 0.68              |
| 21:n:234:ILE:HG21 | 32:n:620:AJP:C81  | 2.23                     | 0.68              |
| 21:y:176:ARG:NH2  | 24:y:310:CHL:O1D  | 2.27                     | 0.68              |
| 2:2:168:ILE:O     | 2:2:172:LEU:HG    | 1.94                     | 0.67              |
| 1:3:115:PHE:CZ    | 1:3:119:LEU:HD21  | 2.29                     | 0.67              |
| 6:C:216:SER:OG    | 6:C:221:GLU:OE1   | 2.06                     | 0.67              |
| 25:C:504:CLA:CHC  | 35:C:516:DGD:HB51 | 2.24                     | 0.67              |
| 21:G:85:LEU:HD13  | 25:G:602:CLA:H42  | 1.75                     | 0.67              |
| 21:G:202:ALA:HB1  | 21:G:208:PHE:HD1  | 1.57                     | 0.67              |
| 21:Y:202:ALA:HB1  | 21:Y:208:PHE:HD1  | 1.57                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Y:309:CHL:H11  | 39:Y:316:LUT:H383 | 1.75                     | 0.67              |
| 25:Y:313:CLA:HBB1 | 39:Y:316:LUT:C14  | 2.24                     | 0.67              |
| 22:R:173:LEU:HD13 | 22:R:188:ILE:HG13 | 1.76                     | 0.67              |
| 1:7:115:PHE:CZ    | 1:7:119:LEU:HD21  | 2.29                     | 0.67              |
| 3:8:229:ILE:O     | 3:8:233:ARG:HD3   | 1.94                     | 0.67              |
| 7:d:15:LEU:HD11   | 18:x:103:VAL:CG1  | 2.21                     | 0.67              |
| 3:4:229:ILE:O     | 3:4:233:ARG:HD3   | 1.94                     | 0.67              |
| 6:C:224:ILE:O     | 6:C:227:VAL:HG23  | 1.95                     | 0.67              |
| 25:C:513:CLA:HMD1 | 20:S:75:LEU:HD11  | 1.77                     | 0.67              |
| 14:M:23:LEU:HD13  | 29:l:102:SQD:H122 | 1.74                     | 0.67              |
| 6:c:327:ASN:HD21  | 15:o:192:ASP:HB2  | 1.57                     | 0.67              |
| 21:g:85:LEU:HD13  | 25:g:602:CLA:H42  | 1.75                     | 0.67              |
| 22:r:202:ILE:HD12 | 24:r:607:CHL:HMA3 | 1.75                     | 0.67              |
| 22:r:211:ASP:OD1  | 22:r:213:GLU:HG2  | 1.94                     | 0.67              |
| 6:C:373:ASN:OD1   | 15:O:111:ALA:HA   | 1.95                     | 0.67              |
| 20:S:119:ARG:HD3  | 25:S:310:CLA:HHD  | 1.74                     | 0.67              |
| 21:N:138:ILE:CG2  | 24:N:606:CHL:HBC1 | 2.14                     | 0.67              |
| 2:6:70:LEU:CD1    | 2:6:79:GLY:HA2    | 2.23                     | 0.67              |
| 3:8:73:LEU:CG     | 3:8:82:GLY:HA2    | 2.22                     | 0.67              |
| 6:c:224:ILE:O     | 6:c:227:VAL:HG23  | 1.95                     | 0.67              |
| 6:c:255:LYS:NZ    | 17:w:127:GLU:OE2  | 2.22                     | 0.67              |
| 6:c:335:THR:HG23  | 6:c:337:LEU:H     | 1.58                     | 0.67              |
| 7:d:94:TRP:HE1    | 18:x:87:LEU:HD22  | 1.59                     | 0.67              |
| 21:y:115:PHE:CZ   | 21:y:119:LEU:HD21 | 2.29                     | 0.67              |
| 2:2:70:LEU:CD1    | 2:2:79:GLY:HA2    | 2.23                     | 0.67              |
| 3:4:177:PRO:HG3   | 25:R:610:CLA:CBB  | 2.25                     | 0.67              |
| 5:B:159:THR:HA    | 5:B:181:VAL:O     | 1.94                     | 0.67              |
| 21:G:138:ILE:HG21 | 24:G:606:CHL:CBC  | 2.10                     | 0.67              |
| 21:N:115:PHE:CZ   | 21:N:119:LEU:HD21 | 2.30                     | 0.67              |
| 25:R:601:CLA:C4C  | 26:R:618:LHG:HC92 | 2.24                     | 0.67              |
| 1:5:138:ILE:CG1   | 1:5:144:LEU:HB2   | 2.22                     | 0.67              |
| 4:a:196:PRO:HG3   | 4:a:300:PHE:CE2   | 2.29                     | 0.67              |
| 20:s:236:MET:HE2  | 39:s:316:LUT:C12  | 2.23                     | 0.67              |
| 21:n:115:PHE:CZ   | 21:n:119:LEU:HD21 | 2.30                     | 0.67              |
| 4:A:246:TYR:CE2   | 4:A:248:ILE:HG12  | 2.29                     | 0.67              |
| 5:B:91:TRP:HE1    | 26:B:622:LHG:HC61 | 1.58                     | 0.67              |
| 6:C:457:LYS:HE2   | 7:D:230:ALA:CB    | 2.24                     | 0.67              |
| 25:C:501:CLA:CHC  | 25:C:503:CLA:H71  | 2.24                     | 0.67              |
| 7:D:94:TRP:HE1    | 18:X:87:LEU:HD22  | 1.59                     | 0.67              |
| 21:N:131:TRP:HB3  | 39:N:616:LUT:H41  | 1.76                     | 0.67              |
| 21:Y:127:GLY:HA3  | 21:Y:137:GLN:HG3  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:115:PHE:CZ    | 1:5:119:LEU:HD21  | 2.30                     | 0.67              |
| 13:l:13:LEU:HB2   | 14:m:25:ILE:HG22  | 1.77                     | 0.67              |
| 15:o:309:SER:OG   | 15:o:319:LYS:N    | 2.20                     | 0.67              |
| 24:y:309:CHL:H11  | 39:y:316:LUT:H383 | 1.75                     | 0.67              |
| 22:r:153:GLY:HA2  | 25:r:604:CLA:C4C  | 2.24                     | 0.67              |
| 23:u:97:THR:HA    | 23:u:102:ARG:NH2  | 2.06                     | 0.67              |
| 25:C:505:CLA:HAA1 | 25:C:505:CLA:HBD  | 1.76                     | 0.67              |
| 7:D:56:VAL:HG21   | 7:D:111:LEU:HD11  | 1.75                     | 0.67              |
| 10:H:25:PRO:HG3   | 22:R:122:THR:HB   | 1.77                     | 0.67              |
| 12:K:32:PHE:HZ    | 19:Z:9:VAL:HG11   | 1.58                     | 0.67              |
| 21:N:153:VAL:HG13 | 24:N:605:CHL:CHD  | 2.25                     | 0.67              |
| 21:Y:59:LEU:HD23  | 24:Y:302:CHL:C1B  | 2.24                     | 0.67              |
| 21:Y:138:ILE:CG1  | 21:Y:144:LEU:HB2  | 2.23                     | 0.67              |
| 3:8:219:GLU:HG2   | 3:8:219:GLU:O     | 1.93                     | 0.67              |
| 3:8:226:LEU:HD12  | 3:8:229:ILE:CD1   | 2.24                     | 0.67              |
| 6:c:373:ASN:OD1   | 15:o:111:ALA:HA   | 1.95                     | 0.67              |
| 21:g:138:ILE:CG1  | 21:g:144:LEU:HB2  | 2.22                     | 0.67              |
| 21:y:56:VAL:HB    | 24:y:302:CHL:CBC  | 2.25                     | 0.67              |
| 5:B:462:PHE:CZ    | 25:B:613:CLA:HMB3 | 2.29                     | 0.67              |
| 6:C:335:THR:HG23  | 6:C:337:LEU:H     | 1.58                     | 0.67              |
| 24:S:302:CHL:HHC  | 24:S:302:CHL:HBB1 | 1.77                     | 0.67              |
| 21:Y:176:ARG:NH2  | 24:Y:310:CHL:O1D  | 2.27                     | 0.67              |
| 1:7:127:GLY:HA3   | 1:7:137:GLN:HG3   | 1.76                     | 0.67              |
| 4:a:246:TYR:CE2   | 4:a:248:ILE:HG12  | 2.29                     | 0.67              |
| 5:b:201:HIS:HE1   | 25:b:602:CLA:ND   | 1.93                     | 0.67              |
| 21:n:75:PRO:HG3   | 21:n:212:LYS:HD3  | 1.77                     | 0.67              |
| 25:n:613:CLA:H141 | 25:n:614:CLA:CMD  | 2.25                     | 0.67              |
| 25:r:602:CLA:HMC1 | 41:r:616:XAT:C31  | 2.25                     | 0.67              |
| 1:1:127:GLY:HA3   | 1:1:137:GLN:HG3   | 1.76                     | 0.67              |
| 3:4:226:LEU:HD12  | 3:4:229:ILE:CD1   | 2.24                     | 0.67              |
| 4:A:255:PHE:CE2   | 4:A:264:SER:HB3   | 2.30                     | 0.67              |
| 20:S:146:VAL:HG11 | 20:S:149:LYS:HZ3  | 1.60                     | 0.67              |
| 25:b:615:CLA:H51  | 25:b:616:CLA:H203 | 1.75                     | 0.67              |
| 6:c:472:LEU:HD11  | 16:t:26:PRO:HB3   | 1.77                     | 0.67              |
| 25:c:501:CLA:CHC  | 25:c:503:CLA:H71  | 2.24                     | 0.67              |
| 22:r:170:LYS:O    | 22:r:174:VAL:HG22 | 1.95                     | 0.67              |
| 25:r:604:CLA:HBB  | 41:r:616:XAT:H42  | 1.77                     | 0.67              |
| 3:4:175:ALA:O     | 3:4:177:PRO:HD3   | 1.95                     | 0.67              |
| 5:B:352:ARG:CZ    | 5:B:372:ASP:HB2   | 2.25                     | 0.67              |
| 6:C:151:TRP:CB    | 17:W:133:LEU:HD21 | 2.21                     | 0.67              |
| 21:N:107:MET:CE   | 25:N:610:CLA:HHC  | 2.25                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:R:170:LYS:O    | 22:R:174:VAL:HG22 | 1.95                     | 0.67              |
| 22:R:185:PRO:HD3  | 21:y:151:SER:HB2  | 1.76                     | 0.67              |
| 22:R:220:GLY:CA   | 22:R:224:ASP:HB3  | 2.25                     | 0.67              |
| 25:6:604:CLA:C1C  | 26:6:606:LHG:HC5  | 2.25                     | 0.67              |
| 3:8:175:ALA:O     | 3:8:177:PRO:HD3   | 1.95                     | 0.67              |
| 4:a:255:PHE:CE2   | 4:a:264:SER:HB3   | 2.30                     | 0.67              |
| 5:b:423:ARG:NH2   | 5:b:430:PHE:O     | 2.28                     | 0.67              |
| 21:g:127:GLY:HA3  | 21:g:137:GLN:HG3  | 1.76                     | 0.67              |
| 21:n:107:MET:CE   | 25:n:610:CLA:HHC  | 2.25                     | 0.67              |
| 2:2:120:GLN:NE2   | 2:2:125:VAL:HG23  | 2.09                     | 0.67              |
| 2:2:129:GLU:HB2   | 2:2:239:LYS:CE    | 2.24                     | 0.67              |
| 25:B:604:CLA:H142 | 25:B:615:CLA:CMA  | 2.21                     | 0.67              |
| 6:C:472:LEU:HD11  | 16:T:26:PRO:HB3   | 1.77                     | 0.67              |
| 24:S:308:CHL:HHC  | 24:S:308:CHL:HBB1 | 1.77                     | 0.67              |
| 2:6:117:GLU:HG2   | 2:6:239:LYS:HB3   | 1.76                     | 0.67              |
| 2:6:129:GLU:HB2   | 2:6:239:LYS:CE    | 2.24                     | 0.67              |
| 5:b:159:THR:HA    | 5:b:181:VAL:O     | 1.94                     | 0.67              |
| 25:b:615:CLA:CMB  | 25:b:615:CLA:H201 | 2.25                     | 0.67              |
| 21:g:100:VAL:CB   | 21:g:190:LEU:HD13 | 2.25                     | 0.67              |
| 21:g:115:PHE:CZ   | 21:g:119:LEU:HD21 | 2.30                     | 0.67              |
| 25:n:603:CLA:H171 | 24:n:607:CHL:H193 | 1.77                     | 0.67              |
| 2:2:128:LYS:HD3   | 2:2:133:PHE:HB3   | 1.75                     | 0.66              |
| 24:2:601:CHL:H12  | 26:2:606:LHG:H181 | 1.75                     | 0.66              |
| 4:A:196:PRO:HG3   | 4:A:300:PHE:CE2   | 2.29                     | 0.66              |
| 25:A:402:CLA:HHB  | 27:A:403:PHO:H203 | 1.74                     | 0.66              |
| 21:G:75:PRO:HG3   | 21:G:212:LYS:HD3  | 1.77                     | 0.66              |
| 21:Y:107:MET:HE1  | 25:Y:311:CLA:HHC  | 1.77                     | 0.66              |
| 25:R:604:CLA:HHB  | 41:R:616:XAT:H42  | 1.77                     | 0.66              |
| 1:5:100:VAL:CB    | 1:5:190:LEU:HD13  | 2.25                     | 0.66              |
| 2:6:120:GLN:NE2   | 2:6:125:VAL:HG23  | 2.09                     | 0.66              |
| 25:6:605:CLA:CBC  | 26:6:606:LHG:H362 | 2.25                     | 0.66              |
| 4:a:225:ARG:HD3   | 22:r:102:ALA:CB   | 2.24                     | 0.66              |
| 20:s:59:LEU:CD1   | 20:s:216:GLU:HG3  | 2.24                     | 0.66              |
| 25:s:304:CLA:HMC2 | 39:s:316:LUT:C13  | 2.26                     | 0.66              |
| 21:n:127:GLY:HA3  | 21:n:137:GLN:HG3  | 1.76                     | 0.66              |
| 24:n:609:CHL:HAA2 | 21:y:82:THR:CG2   | 2.17                     | 0.66              |
| 24:y:307:CHL:HHC  | 24:y:308:CHL:C2C  | 2.25                     | 0.66              |
| 22:r:220:GLY:CA   | 22:r:224:ASP:HB3  | 2.25                     | 0.66              |
| 1:1:115:PHE:CZ    | 1:1:119:LEU:HD21  | 2.29                     | 0.66              |
| 2:2:128:LYS:HE3   | 2:2:140:PHE:CZ    | 2.31                     | 0.66              |
| 4:A:231:GLU:HG2   | 5:B:1:MET:HA      | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:615:CLA:HMB1 | 25:B:615:CLA:H201 | 1.76                     | 0.66              |
| 20:S:128:PHE:CE2  | 20:S:236:MET:HE1  | 2.31                     | 0.66              |
| 25:G:603:CLA:HAB  | 39:G:616:LUT:C35  | 2.25                     | 0.66              |
| 21:Y:75:PRO:HG3   | 21:Y:212:LYS:HD3  | 1.77                     | 0.66              |
| 24:Y:307:CHL:HHC  | 24:Y:308:CHL:C2C  | 2.25                     | 0.66              |
| 2:6:128:LYS:HE3   | 2:6:140:PHE:CZ    | 2.31                     | 0.66              |
| 4:a:237:TYR:HB3   | 7:d:264:ASN:OD1   | 1.96                     | 0.66              |
| 25:c:511:CLA:H3A  | 28:k:101:BCR:H271 | 1.78                     | 0.66              |
| 15:o:139:GLU:OE1  | 17:w:80:LEU:N     | 2.28                     | 0.66              |
| 21:n:100:VAL:CB   | 21:n:190:LEU:HD13 | 2.26                     | 0.66              |
| 21:n:131:TRP:HB3  | 39:n:616:LUT:H41  | 1.77                     | 0.66              |
| 25:n:613:CLA:H142 | 25:n:613:CLA:H2   | 1.76                     | 0.66              |
| 25:2:604:CLA:C1C  | 26:2:606:LHG:HC5  | 2.25                     | 0.66              |
| 1:3:75:PRO:HG3    | 1:3:212:LYS:HD3   | 1.77                     | 0.66              |
| 25:C:501:CLA:HMB1 | 28:I:101:BCR:H23C | 1.77                     | 0.66              |
| 25:G:604:CLA:HBB1 | 39:G:616:LUT:H181 | 1.78                     | 0.66              |
| 15:o:133:GLY:O    | 15:o:134:LYS:HE2  | 1.96                     | 0.66              |
| 22:r:173:LEU:HD13 | 22:r:188:ILE:HG13 | 1.76                     | 0.66              |
| 3:4:245:GLU:HB2   | 3:4:250:LYS:HB3   | 1.77                     | 0.66              |
| 26:B:625:LHG:O9   | 26:L:102:LHG:HC81 | 1.96                     | 0.66              |
| 15:O:146:LYS:HB2  | 15:O:158:PHE:CD1  | 2.31                     | 0.66              |
| 21:N:75:PRO:HG3   | 21:N:212:LYS:HD3  | 1.77                     | 0.66              |
| 21:Y:115:PHE:CZ   | 21:Y:119:LEU:HD21 | 2.30                     | 0.66              |
| 15:o:140:PRO:HD2  | 15:o:169:TYR:CD2  | 2.30                     | 0.66              |
| 20:s:246:THR:HG21 | 20:s:253:ASN:OD1  | 1.95                     | 0.66              |
| 1:1:165:GLN:HE22  | 24:1:302:CHL:C1B  | 2.08                     | 0.66              |
| 2:2:117:GLU:HG2   | 2:2:239:LYS:HB3   | 1.76                     | 0.66              |
| 25:C:511:CLA:H3A  | 28:K:101:BCR:H271 | 1.78                     | 0.66              |
| 20:S:113:PHE:CE1  | 25:S:304:CLA:HBD  | 2.31                     | 0.66              |
| 25:S:304:CLA:HMC2 | 39:S:316:LUT:C13  | 2.26                     | 0.66              |
| 21:G:127:GLY:HA3  | 21:G:137:GLN:HG3  | 1.76                     | 0.66              |
| 24:G:606:CHL:HBC2 | 24:G:607:CHL:CHD  | 2.25                     | 0.66              |
| 25:N:603:CLA:C17  | 24:N:607:CHL:H193 | 2.25                     | 0.66              |
| 21:Y:107:MET:CE   | 25:Y:311:CLA:HHC  | 2.26                     | 0.66              |
| 22:R:103:LYS:HE3  | 22:R:105:LEU:HD11 | 1.78                     | 0.66              |
| 22:R:211:ASP:OD1  | 22:R:213:GLU:HG2  | 1.94                     | 0.66              |
| 3:8:245:GLU:HB2   | 3:8:250:LYS:HB3   | 1.77                     | 0.66              |
| 4:a:292:THR:CG2   | 6:c:428:THR:HG23  | 2.25                     | 0.66              |
| 25:b:615:CLA:H201 | 25:b:615:CLA:HMB1 | 1.76                     | 0.66              |
| 21:n:153:VAL:HG13 | 24:n:605:CHL:CHD  | 2.25                     | 0.66              |
| 25:n:603:CLA:C17  | 24:n:607:CHL:H193 | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:75:PRO:HG3   | 21:y:212:LYS:HD3  | 1.77                     | 0.66              |
| 1:3:100:VAL:CB    | 1:3:190:LEU:HD13  | 2.25                     | 0.66              |
| 5:B:44:VAL:HG23   | 5:B:60:MET:HE1    | 1.77                     | 0.66              |
| 21:G:115:PHE:CZ   | 21:G:119:LEU:HD21 | 2.30                     | 0.66              |
| 21:Y:231:VAL:HG11 | 25:Y:314:CLA:HHD  | 1.78                     | 0.66              |
| 5:b:352:ARG:CZ    | 5:b:372:ASP:HB2   | 2.25                     | 0.66              |
| 25:c:501:CLA:HMB1 | 28:i:101:BCR:H23C | 1.77                     | 0.66              |
| 20:s:128:PHE:CE2  | 20:s:236:MET:HE1  | 2.31                     | 0.66              |
| 24:s:308:CHL:HHC  | 24:s:308:CHL:HBB1 | 1.77                     | 0.66              |
| 21:y:244:LEU:HD22 | 39:y:316:LUT:H163 | 1.75                     | 0.66              |
| 25:2:605:CLA:CBC  | 26:2:606:LHG:H362 | 2.25                     | 0.66              |
| 3:4:73:LEU:CG     | 3:4:82:GLY:HA2    | 2.22                     | 0.66              |
| 4:A:235:GLU:HB3   | 7:D:264:ASN:ND2   | 2.08                     | 0.66              |
| 4:A:292:THR:CG2   | 6:C:428:THR:HG23  | 2.25                     | 0.66              |
| 29:L:101:SQD:H92  | 29:L:101:SQD:C23  | 2.26                     | 0.66              |
| 15:O:169:TYR:OH   | 17:W:80:LEU:HD23  | 1.95                     | 0.66              |
| 20:S:246:THR:HG21 | 20:S:253:ASN:OD1  | 1.95                     | 0.66              |
| 25:N:613:CLA:H142 | 25:N:613:CLA:H2   | 1.76                     | 0.66              |
| 24:5:302:CHL:HHC  | 24:5:302:CHL:HBB1 | 1.78                     | 0.66              |
| 5:b:44:VAL:HG23   | 5:b:60:MET:HE1    | 1.77                     | 0.66              |
| 20:s:262:PHE:HE2  | 25:s:314:CLA:H3A  | 1.59                     | 0.66              |
| 24:g:606:CHL:HBC2 | 24:g:607:CHL:CHD  | 2.25                     | 0.66              |
| 2:2:116:PRO:HG3   | 2:2:134:LYS:HE3   | 1.76                     | 0.66              |
| 5:B:45:PHE:CE2    | 5:B:47:PRO:HB3    | 2.31                     | 0.66              |
| 5:B:121:GLU:OE2   | 10:H:16:SER:OG    | 2.08                     | 0.66              |
| 5:B:475:PHE:HB2   | 5:B:479:PHE:CE2   | 2.31                     | 0.66              |
| 25:B:615:CLA:H201 | 25:B:615:CLA:CMB  | 2.25                     | 0.66              |
| 7:D:175:GLY:O     | 7:D:179:ILE:HG12  | 1.96                     | 0.66              |
| 13:L:13:LEU:HB2   | 14:M:25:ILE:HG22  | 1.77                     | 0.66              |
| 25:G:610:CLA:C4   | 25:G:612:CLA:HMA2 | 2.26                     | 0.66              |
| 22:R:130:VAL:HG23 | 22:R:131:PHE:HD1  | 1.61                     | 0.66              |
| 24:R:613:CHL:HHC  | 24:R:613:CHL:HBB1 | 1.78                     | 0.66              |
| 3:8:194:TYR:CE2   | 3:8:221:LEU:HB2   | 2.24                     | 0.66              |
| 15:o:146:LYS:HB2  | 15:o:158:PHE:CD1  | 2.31                     | 0.66              |
| 21:g:231:VAL:HG21 | 25:g:613:CLA:CAC  | 2.24                     | 0.66              |
| 2:2:130:PRO:CD    | 2:2:239:LYS:HE2   | 2.25                     | 0.66              |
| 3:4:194:TYR:CE2   | 3:4:221:LEU:HB2   | 2.24                     | 0.66              |
| 4:A:225:ARG:HD3   | 22:R:102:ALA:CB   | 2.24                     | 0.66              |
| 5:B:478:VAL:HG13  | 7:D:140:ARG:HG2   | 1.78                     | 0.66              |
| 1:5:127:GLY:HA3   | 1:5:137:GLN:HG3   | 1.76                     | 0.66              |
| 20:s:113:PHE:CE1  | 25:s:304:CLA:HBD  | 2.31                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:107:MET:CE   | 25:y:311:CLA:HHC  | 2.26                     | 0.66              |
| 4:A:139:MET:HE3   | 7:D:222:THR:HG22  | 1.78                     | 0.66              |
| 15:O:133:GLY:O    | 15:O:134:LYS:HE2  | 1.96                     | 0.66              |
| 15:O:139:GLU:OE1  | 17:W:80:LEU:N     | 2.28                     | 0.66              |
| 20:S:113:PHE:O    | 20:S:117:HIS:ND1  | 2.26                     | 0.66              |
| 25:R:604:CLA:HHB  | 41:R:616:XAT:H22  | 1.78                     | 0.66              |
| 4:a:224:ILE:HD13  | 5:b:482:ILE:HG13  | 1.78                     | 0.66              |
| 4:a:231:GLU:HG2   | 5:b:1:MET:HA      | 1.77                     | 0.66              |
| 21:y:100:VAL:CB   | 21:y:190:LEU:HD13 | 2.26                     | 0.66              |
| 1:1:100:VAL:CB    | 1:1:190:LEU:HD13  | 2.25                     | 0.65              |
| 5:B:423:ARG:NH2   | 5:B:430:PHE:O     | 2.28                     | 0.65              |
| 25:N:613:CLA:H141 | 25:N:614:CLA:CMD  | 2.25                     | 0.65              |
| 21:Y:56:VAL:HB    | 24:Y:302:CHL:CBC  | 2.25                     | 0.65              |
| 25:R:602:CLA:HMC1 | 41:R:616:XAT:C31  | 2.25                     | 0.65              |
| 5:b:161:LEU:HD21  | 30:b:623:LMG:O3   | 1.96                     | 0.65              |
| 6:c:162:GLY:HA2   | 6:c:248:GLY:HA2   | 1.79                     | 0.65              |
| 25:c:512:CLA:C1B  | 28:c:514:BCR:H401 | 2.27                     | 0.65              |
| 10:h:52:VAL:O     | 10:h:56:ILE:HG12  | 1.97                     | 0.65              |
| 2:2:117:GLU:CB    | 2:2:241:PRO:HG2   | 2.26                     | 0.65              |
| 5:B:128:THR:HG21  | 22:R:94:ILE:CD1   | 2.26                     | 0.65              |
| 14:M:1:MET:HB2    | 14:M:3:VAL:HG13   | 1.78                     | 0.65              |
| 20:S:135:ASN:ND2  | 20:S:141:CYS:H    | 1.95                     | 0.65              |
| 21:G:104:ARG:NH1  | 24:G:608:CHL:OBD  | 2.28                     | 0.65              |
| 21:N:100:VAL:CB   | 21:N:190:LEU:HD13 | 2.26                     | 0.65              |
| 25:N:603:CLA:H101 | 24:N:609:CHL:C14  | 2.26                     | 0.65              |
| 21:Y:100:VAL:CB   | 21:Y:190:LEU:HD13 | 2.26                     | 0.65              |
| 2:6:117:GLU:CB    | 2:6:241:PRO:HG2   | 2.26                     | 0.65              |
| 3:8:86:LEU:HB3    | 3:8:88:LEU:HD13   | 1.77                     | 0.65              |
| 3:8:177:PRO:HG3   | 25:r:610:CLA:CBB  | 2.25                     | 0.65              |
| 5:b:45:PHE:CE2    | 5:b:47:PRO:HB3    | 2.31                     | 0.65              |
| 6:c:457:LYS:HE2   | 7:d:230:ALA:CB    | 2.24                     | 0.65              |
| 25:g:603:CLA:HAB  | 39:g:616:LUT:C35  | 2.25                     | 0.65              |
| 22:r:214:LYS:HA   | 22:r:217:TYR:O    | 1.97                     | 0.65              |
| 25:r:604:CLA:HHB  | 41:r:616:XAT:H22  | 1.78                     | 0.65              |
| 4:A:173:PRO:HB2   | 4:A:178:GLY:HA3   | 1.79                     | 0.65              |
| 2:6:116:PRO:HG3   | 2:6:134:LYS:HE3   | 1.76                     | 0.65              |
| 5:b:388:SER:HB2   | 5:b:391:SER:HB2   | 1.77                     | 0.65              |
| 6:c:60:ILE:HA     | 25:c:510:CLA:HMC3 | 1.79                     | 0.65              |
| 6:c:278:ALA:CB    | 25:c:507:CLA:HMA1 | 2.27                     | 0.65              |
| 10:h:25:PRO:HG3   | 22:r:122:THR:HB   | 1.77                     | 0.65              |
| 29:l:102:SQD:H251 | 29:l:102:SQD:C10  | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:o:169:TYR:OH   | 17:w:80:LEU:HD23  | 1.95                     | 0.65              |
| 21:n:209:ALA:O    | 21:n:212:LYS:HB2  | 1.96                     | 0.65              |
| 25:y:304:CLA:H122 | 25:y:304:CLA:H203 | 1.78                     | 0.65              |
| 24:1:302:CHL:HHC  | 24:1:302:CHL:HBB1 | 1.78                     | 0.65              |
| 2:2:137:SER:HA    | 2:2:140:PHE:CD2   | 2.32                     | 0.65              |
| 2:2:223:ALA:HB3   | 25:2:602:CLA:HMC2 | 1.78                     | 0.65              |
| 1:3:209:ALA:O     | 1:3:212:LYS:HB2   | 1.96                     | 0.65              |
| 3:4:86:LEU:HB3    | 3:4:88:LEU:HD13   | 1.77                     | 0.65              |
| 3:4:136:ALA:HB1   | 3:4:140:PHE:HZ    | 1.61                     | 0.65              |
| 21:G:224:PHE:CD2  | 26:Y:301:LHG:H281 | 2.31                     | 0.65              |
| 22:R:138:GLU:HB2  | 22:R:216:LEU:HD11 | 1.79                     | 0.65              |
| 2:6:125:VAL:HG13  | 2:6:148:LEU:CD1   | 2.26                     | 0.65              |
| 6:c:305:THR:HG22  | 6:c:307:PRO:HD2   | 1.79                     | 0.65              |
| 25:c:505:CLA:HBD  | 25:c:505:CLA:HAA1 | 1.77                     | 0.65              |
| 7:d:194:LEU:HD22  | 7:d:316:TYR:HE1   | 1.61                     | 0.65              |
| 15:o:117:ILE:CG2  | 15:o:298:GLU:HB3  | 2.27                     | 0.65              |
| 21:n:227:PHE:O    | 21:n:231:VAL:HG23 | 1.97                     | 0.65              |
| 21:y:209:ALA:O    | 21:y:212:LYS:HB2  | 1.96                     | 0.65              |
| 22:r:130:VAL:HG23 | 22:r:131:PHE:HD1  | 1.61                     | 0.65              |
| 10:H:52:VAL:HG22  | 18:X:88:LEU:HD12  | 1.78                     | 0.65              |
| 15:O:140:PRO:HD2  | 15:O:169:TYR:CD2  | 2.30                     | 0.65              |
| 21:G:227:PHE:O    | 21:G:231:VAL:HG23 | 1.97                     | 0.65              |
| 21:N:209:ALA:O    | 21:N:212:LYS:HB2  | 1.97                     | 0.65              |
| 1:5:75:PRO:HG3    | 1:5:212:LYS:HD3   | 1.77                     | 0.65              |
| 1:5:227:PHE:O     | 1:5:231:VAL:HG23  | 1.97                     | 0.65              |
| 25:a:406:CLA:HHD  | 28:a:407:BCR:C36  | 2.27                     | 0.65              |
| 25:b:608:CLA:H152 | 25:b:609:CLA:H203 | 1.78                     | 0.65              |
| 6:c:133:ALA:HB1   | 25:c:511:CLA:HMA2 | 1.78                     | 0.65              |
| 25:d:403:CLA:H52  | 18:x:91:ALA:CB    | 2.27                     | 0.65              |
| 25:r:612:CLA:CHB  | 39:r:615:LUT:H42  | 2.25                     | 0.65              |
| 1:3:227:PHE:O     | 1:3:231:VAL:HG23  | 1.97                     | 0.65              |
| 5:B:161:LEU:HD21  | 30:B:623:LMG:O3   | 1.96                     | 0.65              |
| 25:B:608:CLA:H152 | 25:B:609:CLA:H203 | 1.78                     | 0.65              |
| 6:C:162:GLY:HA2   | 6:C:248:GLY:HA2   | 1.78                     | 0.65              |
| 29:L:101:SQD:H251 | 29:L:101:SQD:C11  | 2.27                     | 0.65              |
| 1:7:100:VAL:CB    | 1:7:190:LEU:HD13  | 2.25                     | 0.65              |
| 6:c:362:ARG:HG3   | 6:c:367:GLU:CD    | 2.22                     | 0.65              |
| 25:c:511:CLA:H143 | 19:z:20:LEU:HD11  | 1.79                     | 0.65              |
| 20:s:128:PHE:HE2  | 20:s:236:MET:HE1  | 1.62                     | 0.65              |
| 21:g:138:ILE:HG21 | 24:g:606:CHL:CBC  | 2.10                     | 0.65              |
| 21:g:227:PHE:O    | 21:g:231:VAL:HG23 | 1.97                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:n:603:CLA:H101 | 24:n:609:CHL:C14  | 2.26                     | 0.65              |
| 2:2:125:VAL:HG13  | 2:2:148:LEU:CD1   | 2.26                     | 0.65              |
| 6:C:87:ILE:HD13   | 25:C:504:CLA:CMB  | 2.27                     | 0.65              |
| 6:C:346:THR:OG1   | 6:C:348:GLU:OE1   | 2.09                     | 0.65              |
| 20:S:128:PHE:HE2  | 20:S:236:MET:HE1  | 1.61                     | 0.65              |
| 25:R:612:CLA:CHB  | 39:R:615:LUT:H42  | 2.25                     | 0.65              |
| 3:8:78:PRO:CG     | 3:8:225:LYS:HE2   | 2.27                     | 0.65              |
| 26:b:625:LHG:O9   | 26:l:103:LHG:HC81 | 1.96                     | 0.65              |
| 6:c:87:ILE:HD13   | 25:c:504:CLA:CMB  | 2.27                     | 0.65              |
| 25:g:604:CLA:HBB1 | 39:g:616:LUT:H181 | 1.78                     | 0.65              |
| 24:g:606:CHL:HBB1 | 24:g:606:CHL:HHC  | 1.78                     | 0.65              |
| 24:r:613:CHL:HHC  | 24:r:613:CHL:HBB1 | 1.78                     | 0.65              |
| 1:1:75:PRO:HG3    | 1:1:212:LYS:HD3   | 1.77                     | 0.65              |
| 5:B:274:GLN:HG2   | 5:B:279:TYR:CD2   | 2.32                     | 0.65              |
| 5:B:277:GLN:HA    | 23:U:98:ALA:HA    | 1.79                     | 0.65              |
| 6:C:305:THR:HG22  | 6:C:307:PRO:HD2   | 1.79                     | 0.65              |
| 6:C:362:ARG:HG3   | 6:C:367:GLU:CD    | 2.22                     | 0.65              |
| 7:D:194:LEU:HD22  | 7:D:316:TYR:HE1   | 1.61                     | 0.65              |
| 29:L:101:SQD:H251 | 29:L:101:SQD:C10  | 2.26                     | 0.65              |
| 21:G:231:VAL:HG21 | 25:G:613:CLA:HAC2 | 1.79                     | 0.65              |
| 21:N:227:PHE:O    | 21:N:231:VAL:HG23 | 1.97                     | 0.65              |
| 1:5:153:VAL:HG13  | 24:5:301:CHL:CHD  | 2.27                     | 0.65              |
| 2:6:130:PRO:CD    | 2:6:239:LYS:HE2   | 2.25                     | 0.65              |
| 2:6:145:LEU:CD2   | 2:6:154:VAL:HA    | 2.27                     | 0.65              |
| 24:n:606:CHL:HBC2 | 24:n:607:CHL:CHD  | 2.27                     | 0.65              |
| 21:y:94:ARG:NE    | 21:y:94:ARG:HA    | 2.12                     | 0.65              |
| 5:B:98:GLY:O      | 5:B:102:VAL:HG23  | 1.97                     | 0.65              |
| 6:C:378:SER:O     | 6:C:382:LYS:HG2   | 1.97                     | 0.65              |
| 8:E:73:LEU:HD23   | 8:E:77:ASP:OD2    | 1.97                     | 0.65              |
| 10:H:52:VAL:O     | 10:H:56:ILE:HG12  | 1.97                     | 0.65              |
| 25:N:603:CLA:H171 | 24:N:607:CHL:H193 | 1.77                     | 0.65              |
| 25:Y:304:CLA:H122 | 25:Y:304:CLA:H203 | 1.78                     | 0.65              |
| 22:R:214:LYS:HA   | 22:R:217:TYR:O    | 1.97                     | 0.65              |
| 24:s:302:CHL:HHC  | 24:s:302:CHL:HBB1 | 1.77                     | 0.65              |
| 21:g:209:ALA:O    | 21:g:212:LYS:HB2  | 1.97                     | 0.65              |
| 24:y:302:CHL:HMB3 | 26:y:319:LHG:H161 | 1.79                     | 0.65              |
| 22:r:139:CYS:O    | 22:r:143:HIS:ND1  | 2.29                     | 0.65              |
| 3:4:77:LEU:CG     | 3:4:78:PRO:HD2    | 2.26                     | 0.65              |
| 25:A:405:CLA:HHD  | 28:A:406:BCR:C36  | 2.27                     | 0.65              |
| 5:B:201:HIS:HE1   | 25:B:602:CLA:ND   | 1.93                     | 0.65              |
| 18:X:87:LEU:HD11  | 18:X:88:LEU:HD22  | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:100:VAL:CB   | 21:G:190:LEU:HD13 | 2.25                     | 0.65              |
| 24:N:606:CHL:HBC2 | 24:N:607:CHL:CHD  | 2.27                     | 0.65              |
| 22:R:224:ASP:OD1  | 39:R:615:LUT:O23  | 2.12                     | 0.65              |
| 1:5:165:GLN:HE22  | 24:5:302:CHL:C1B  | 2.08                     | 0.65              |
| 2:6:137:SER:HA    | 2:6:140:PHE:CD2   | 2.32                     | 0.65              |
| 1:7:75:PRO:HG3    | 1:7:212:LYS:HD3   | 1.77                     | 0.65              |
| 1:7:94:ARG:NE     | 1:7:94:ARG:HA     | 2.12                     | 0.65              |
| 3:8:175:ALA:HB1   | 25:r:601:CLA:HHC  | 1.78                     | 0.65              |
| 5:b:98:GLY:O      | 5:b:102:VAL:HG23  | 1.97                     | 0.65              |
| 25:b:606:CLA:HMC1 | 26:b:622:LHG:H292 | 1.80                     | 0.65              |
| 8:e:73:LEU:HD23   | 8:e:77:ASP:OD2    | 1.97                     | 0.65              |
| 20:s:135:ASN:ND2  | 20:s:141:CYS:H    | 1.94                     | 0.65              |
| 21:g:75:PRO:HG3   | 21:g:212:LYS:HD3  | 1.77                     | 0.65              |
| 21:y:107:MET:HE1  | 25:y:311:CLA:HHC  | 1.78                     | 0.65              |
| 21:y:227:PHE:O    | 21:y:231:VAL:HG23 | 1.97                     | 0.65              |
| 21:y:231:VAL:HG11 | 25:y:314:CLA:HHD  | 1.78                     | 0.65              |
| 1:1:227:PHE:O     | 1:1:231:VAL:HG23  | 1.97                     | 0.64              |
| 3:4:78:PRO:CD     | 3:4:225:LYS:HE2   | 2.27                     | 0.64              |
| 4:A:237:TYR:HB3   | 7:D:264:ASN:OD1   | 1.96                     | 0.64              |
| 5:B:72:THR:HG23   | 5:B:80:ILE:CG2    | 2.22                     | 0.64              |
| 5:B:336:ILE:HD12  | 5:B:436:THR:HG21  | 1.77                     | 0.64              |
| 6:C:133:ALA:HB1   | 25:C:511:CLA:HMA2 | 1.78                     | 0.64              |
| 6:C:272:LEU:HD21  | 25:C:508:CLA:CHB  | 2.27                     | 0.64              |
| 25:C:512:CLA:C1B  | 28:C:514:BCR:H401 | 2.27                     | 0.64              |
| 21:G:62:PHE:C     | 21:Y:178:ALA:HB2  | 2.22                     | 0.64              |
| 24:N:607:CHL:H142 | 24:N:607:CHL:H93  | 1.79                     | 0.64              |
| 22:R:209:GLU:CD   | 22:R:214:LYS:HD2  | 2.22                     | 0.64              |
| 5:b:475:PHE:HB2   | 5:b:479:PHE:CE2   | 2.31                     | 0.64              |
| 29:l:102:SQD:H92  | 29:l:102:SQD:C23  | 2.26                     | 0.64              |
| 21:g:104:ARG:NH1  | 24:g:608:CHL:OBD  | 2.28                     | 0.64              |
| 22:r:103:LYS:HE3  | 22:r:105:LEU:HD11 | 1.78                     | 0.64              |
| 15:O:117:ILE:CG2  | 15:O:298:GLU:HB3  | 2.27                     | 0.64              |
| 21:N:94:ARG:NE    | 21:N:94:ARG:HA    | 2.12                     | 0.64              |
| 21:Y:94:ARG:NE    | 21:Y:94:ARG:HA    | 2.12                     | 0.64              |
| 21:Y:209:ALA:O    | 21:Y:212:LYS:HB2  | 1.96                     | 0.64              |
| 21:Y:215:GLU:HG3  | 25:Y:311:CLA:C4B  | 2.27                     | 0.64              |
| 21:Y:227:PHE:O    | 21:Y:231:VAL:HG23 | 1.97                     | 0.64              |
| 1:7:227:PHE:O     | 1:7:231:VAL:HG23  | 1.97                     | 0.64              |
| 4:a:173:PRO:HB2   | 4:a:178:GLY:HA3   | 1.79                     | 0.64              |
| 7:d:175:GLY:O     | 7:d:179:ILE:HG12  | 1.96                     | 0.64              |
| 14:m:1:MET:HB2    | 14:m:3:VAL:HG13   | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:164:THR:HG21 | 24:g:606:CHL:O1D  | 1.97                     | 0.64              |
| 25:n:603:CLA:H192 | 24:n:607:CHL:H172 | 1.79                     | 0.64              |
| 22:r:208:ALA:O    | 22:r:210:LEU:HD12 | 1.97                     | 0.64              |
| 1:1:94:ARG:NE     | 1:1:94:ARG:HA     | 2.12                     | 0.64              |
| 1:1:153:VAL:HG13  | 24:1:301:CHL:CHD  | 2.27                     | 0.64              |
| 3:4:78:PRO:CG     | 3:4:225:LYS:HE2   | 2.27                     | 0.64              |
| 5:B:388:SER:HB2   | 5:B:391:SER:HB2   | 1.78                     | 0.64              |
| 6:C:278:ALA:CB    | 25:C:507:CLA:HMA1 | 2.27                     | 0.64              |
| 7:D:189:PHE:O     | 7:D:295:ARG:NH1   | 2.31                     | 0.64              |
| 28:K:101:BCR:H332 | 19:Z:12:LEU:HD23  | 1.79                     | 0.64              |
| 28:T:101:BCR:H271 | 5:b:39:LEU:CD1    | 2.28                     | 0.64              |
| 21:G:94:ARG:NE    | 21:G:94:ARG:HA    | 2.12                     | 0.64              |
| 24:N:607:CHL:C1   | 24:Y:302:CHL:H191 | 2.23                     | 0.64              |
| 24:Y:310:CHL:HHC  | 24:Y:310:CHL:HBB1 | 1.79                     | 0.64              |
| 1:5:162:TRP:O     | 1:5:166:VAL:HG23  | 1.98                     | 0.64              |
| 1:5:209:ALA:O     | 1:5:212:LYS:HB2   | 1.96                     | 0.64              |
| 2:6:223:ALA:HB3   | 25:6:602:CLA:HMC2 | 1.79                     | 0.64              |
| 1:7:209:ALA:O     | 1:7:212:LYS:HB2   | 1.96                     | 0.64              |
| 5:b:128:THR:HG21  | 22:r:94:ILE:CD1   | 2.26                     | 0.64              |
| 21:g:224:PHE:CD2  | 26:y:301:LHG:H281 | 2.31                     | 0.64              |
| 24:g:601:CHL:HHB  | 24:y:310:CHL:HMB3 | 1.79                     | 0.64              |
| 21:n:231:VAL:CG1  | 25:n:613:CLA:HHD  | 2.26                     | 0.64              |
| 24:n:607:CHL:H93  | 24:n:607:CHL:H142 | 1.79                     | 0.64              |
| 20:S:135:ASN:OD1  | 20:S:145:ALA:HB2  | 1.97                     | 0.64              |
| 21:N:132:PHE:CE1  | 21:N:133:LYS:HG3  | 2.33                     | 0.64              |
| 22:R:103:LYS:HE3  | 22:R:105:LEU:HD21 | 1.79                     | 0.64              |
| 24:5:301:CHL:HHC  | 24:5:301:CHL:HBB1 | 1.80                     | 0.64              |
| 5:b:335:GLY:HA3   | 5:b:432:LEU:HB3   | 1.80                     | 0.64              |
| 6:c:272:LEU:HD21  | 25:c:508:CLA:CHB  | 2.27                     | 0.64              |
| 6:c:428:THR:HG22  | 35:c:516:DGD:HBW1 | 1.78                     | 0.64              |
| 15:o:158:PHE:CE2  | 15:o:322:LYS:HE3  | 2.33                     | 0.64              |
| 20:s:135:ASN:OD1  | 20:s:145:ALA:HB2  | 1.97                     | 0.64              |
| 22:r:68:LEU:HD11  | 25:r:602:CLA:O2D  | 1.97                     | 0.64              |
| 22:r:209:GLU:CD   | 22:r:214:LYS:HD2  | 2.23                     | 0.64              |
| 4:A:135:PHE:CE1   | 6:C:449:ARG:HG2   | 2.33                     | 0.64              |
| 25:B:607:CLA:H171 | 25:B:613:CLA:C16  | 2.23                     | 0.64              |
| 6:C:52:ALA:HB1    | 25:C:509:CLA:HBB1 | 1.80                     | 0.64              |
| 21:N:158:ILE:CD1  | 21:Y:257:TRP:HE3  | 2.11                     | 0.64              |
| 21:Y:57:LYS:HB2   | 21:Y:63:SER:OG    | 1.98                     | 0.64              |
| 21:Y:179:GLY:HA2  | 24:Y:309:CHL:HAC1 | 1.79                     | 0.64              |
| 3:8:136:ALA:HB1   | 3:8:140:PHE:HZ    | 1.61                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:336:ILE:HD12  | 5:b:436:THR:HG21  | 1.77                     | 0.64              |
| 18:x:87:LEU:HD11  | 18:x:88:LEU:HD22  | 1.79                     | 0.64              |
| 25:r:601:CLA:C4D  | 26:r:618:LHG:H102 | 2.03                     | 0.64              |
| 1:1:51:TYR:CE2    | 1:1:209:ALA:HB1   | 2.33                     | 0.64              |
| 2:2:145:LEU:CD2   | 2:2:154:VAL:HA    | 2.27                     | 0.64              |
| 7:D:52:GLY:HA3    | 7:D:79:VAL:HG22   | 1.79                     | 0.64              |
| 24:G:606:CHL:HBB1 | 24:G:606:CHL:HHC  | 1.78                     | 0.64              |
| 25:G:610:CLA:HMC1 | 39:G:615:LUT:C31  | 2.27                     | 0.64              |
| 3:8:77:LEU:CG     | 3:8:78:PRO:HD2    | 2.26                     | 0.64              |
| 3:8:224:LEU:O     | 3:8:227:ALA:HB3   | 1.98                     | 0.64              |
| 5:b:241:SER:OG    | 25:b:612:CLA:OBD  | 2.06                     | 0.64              |
| 5:b:274:GLN:HG2   | 5:b:279:TYR:CD2   | 2.32                     | 0.64              |
| 5:b:291:GLY:HA2   | 5:b:294:GLU:OE2   | 1.98                     | 0.64              |
| 15:o:130:LYS:HD2  | 15:o:179:GLU:HB2  | 1.80                     | 0.64              |
| 24:n:607:CHL:C1   | 24:y:302:CHL:H191 | 2.23                     | 0.64              |
| 21:y:215:GLU:HG3  | 25:y:311:CLA:C4B  | 2.27                     | 0.64              |
| 1:3:132:PHE:CE1   | 1:3:133:LYS:HG3   | 2.33                     | 0.64              |
| 24:G:601:CHL:HHB  | 24:Y:310:CHL:HMB3 | 1.79                     | 0.64              |
| 22:R:122:THR:OG1  | 22:R:125:GLN:O    | 2.16                     | 0.64              |
| 22:R:220:GLY:HA2  | 22:R:224:ASP:N    | 2.13                     | 0.64              |
| 1:5:94:ARG:HA     | 1:5:94:ARG:NE     | 2.12                     | 0.64              |
| 5:b:478:VAL:HG13  | 7:d:140:ARG:HG2   | 1.78                     | 0.64              |
| 25:g:610:CLA:C4   | 25:g:612:CLA:HMA2 | 2.26                     | 0.64              |
| 25:g:610:CLA:HMC1 | 39:g:615:LUT:C31  | 2.27                     | 0.64              |
| 21:n:57:LYS:HB2   | 21:n:63:SER:OG    | 1.98                     | 0.64              |
| 21:y:86:SER:OG    | 25:y:303:CLA:O1A  | 2.16                     | 0.64              |
| 1:1:209:ALA:O     | 1:1:212:LYS:HB2   | 1.96                     | 0.64              |
| 1:3:202:ALA:HB1   | 1:3:208:PHE:CD1   | 2.33                     | 0.64              |
| 3:4:175:ALA:HB1   | 25:R:601:CLA:HHC  | 1.78                     | 0.64              |
| 4:A:224:ILE:HD13  | 5:B:482:ILE:HG13  | 1.78                     | 0.64              |
| 5:B:335:GLY:HA3   | 5:B:432:LEU:HB3   | 1.80                     | 0.64              |
| 25:B:606:CLA:HMC1 | 26:B:622:LHG:H292 | 1.80                     | 0.64              |
| 6:C:138:GLU:HG3   | 6:C:139:THR:HG23  | 1.80                     | 0.64              |
| 6:C:255:LYS:HG3   | 6:C:256:PRO:HD2   | 1.80                     | 0.64              |
| 7:D:185:PHE:HA    | 7:D:330:MET:HE1   | 1.80                     | 0.64              |
| 21:G:51:TYR:CE2   | 21:G:209:ALA:HB1  | 2.33                     | 0.64              |
| 21:N:57:LYS:HB2   | 21:N:63:SER:OG    | 1.98                     | 0.64              |
| 25:Y:314:CLA:HAA1 | 25:Y:314:CLA:HBD  | 1.79                     | 0.64              |
| 22:R:208:ALA:O    | 22:R:210:LEU:HD12 | 1.97                     | 0.64              |
| 2:6:220:GLY:HA2   | 25:6:602:CLA:HAC1 | 1.80                     | 0.64              |
| 5:b:277:GLN:HA    | 23:u:98:ALA:HA    | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:c:513:CLA:OBD  | 20:s:72:PRO:HB2   | 1.97                     | 0.64              |
| 7:d:185:PHE:HA    | 7:d:330:MET:HE1   | 1.80                     | 0.64              |
| 29:l:102:SQD:H251 | 29:l:102:SQD:C11  | 2.27                     | 0.64              |
| 21:g:62:PHE:C     | 21:y:178:ALA:HB2  | 2.22                     | 0.64              |
| 21:n:202:ALA:HB1  | 21:n:208:PHE:CD1  | 2.33                     | 0.64              |
| 22:r:138:GLU:HB2  | 22:r:216:LEU:HD11 | 1.79                     | 0.64              |
| 22:r:220:GLY:HA2  | 22:r:224:ASP:N    | 2.13                     | 0.64              |
| 1:3:57:LYS:HB2    | 1:3:63:SER:OG     | 1.98                     | 0.64              |
| 4:A:332:HIS:HB3   | 7:D:322:LEU:HD21  | 1.80                     | 0.64              |
| 5:B:39:LEU:CD1    | 28:t:101:BCR:H271 | 2.28                     | 0.64              |
| 6:C:60:ILE:HA     | 25:C:510:CLA:HMC3 | 1.79                     | 0.64              |
| 25:D:403:CLA:H52  | 18:X:91:ALA:CB    | 2.27                     | 0.64              |
| 21:G:209:ALA:O    | 21:G:212:LYS:HB2  | 1.97                     | 0.64              |
| 21:N:162:TRP:O    | 21:N:166:VAL:HG23 | 1.98                     | 0.64              |
| 3:8:229:ILE:HG13  | 3:8:230:LYS:N     | 2.13                     | 0.64              |
| 6:c:138:GLU:HG3   | 6:c:139:THR:HG23  | 1.80                     | 0.64              |
| 6:c:199:ILE:O     | 6:c:200:THR:HG22  | 1.98                     | 0.64              |
| 25:c:510:CLA:HMA2 | 25:c:510:CLA:H2   | 1.80                     | 0.64              |
| 10:h:52:VAL:HG22  | 18:x:88:LEU:HD12  | 1.78                     | 0.64              |
| 11:i:34:ARG:NH1   | 11:i:35:GLU:HG2   | 2.11                     | 0.64              |
| 20:s:128:PHE:HE1  | 39:s:316:LUT:H173 | 1.63                     | 0.64              |
| 25:s:304:CLA:HMA2 | 25:s:304:CLA:HBA1 | 1.80                     | 0.64              |
| 21:n:132:PHE:CE1  | 21:n:133:LYS:HG3  | 2.33                     | 0.64              |
| 21:n:224:PHE:CD1  | 25:n:602:CLA:H201 | 2.33                     | 0.64              |
| 21:y:162:TRP:O    | 21:y:166:VAL:HG23 | 1.98                     | 0.64              |
| 21:y:179:GLY:HA2  | 24:y:309:CHL:HAC1 | 1.79                     | 0.64              |
| 1:1:132:PHE:CE1   | 1:1:133:LYS:HG3   | 2.33                     | 0.64              |
| 5:B:291:GLY:HA2   | 5:B:294:GLU:OE2   | 1.98                     | 0.64              |
| 25:C:513:CLA:OBD  | 20:S:72:PRO:HB2   | 1.97                     | 0.64              |
| 25:S:313:CLA:HAA1 | 25:S:313:CLA:HBD  | 1.80                     | 0.64              |
| 21:N:80:TRP:CE3   | 39:N:616:LUT:H383 | 2.33                     | 0.64              |
| 4:a:139:MET:HE3   | 7:d:222:THR:HG22  | 1.78                     | 0.64              |
| 6:c:185:VAL:HG23  | 6:c:230:LEU:HD13  | 1.80                     | 0.64              |
| 6:c:348:GLU:OE2   | 15:o:106:LYS:HA   | 1.98                     | 0.64              |
| 7:d:211:LEU:HA    | 7:d:214:ILE:HG22  | 1.80                     | 0.64              |
| 13:l:11:VAL:HG11  | 14:m:25:ILE:HD12  | 1.80                     | 0.64              |
| 21:g:51:TYR:CE2   | 21:g:209:ALA:HB1  | 2.33                     | 0.64              |
| 21:g:231:VAL:HG21 | 25:g:613:CLA:HAC2 | 1.79                     | 0.64              |
| 22:r:103:LYS:HE3  | 22:r:105:LEU:HD21 | 1.79                     | 0.64              |
| 2:2:120:GLN:CG    | 2:2:125:VAL:HA    | 2.26                     | 0.63              |
| 11:I:34:ARG:NH1   | 11:I:35:GLU:HG2   | 2.11                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:K:32:PHE:CZ    | 19:Z:9:VAL:HG11   | 2.33                     | 0.63              |
| 21:G:57:LYS:HB2   | 21:G:63:SER:OG    | 1.98                     | 0.63              |
| 21:G:213:VAL:HG12 | 25:G:611:CLA:HED1 | 1.80                     | 0.63              |
| 21:N:231:VAL:CG1  | 25:N:613:CLA:HHD  | 2.26                     | 0.63              |
| 25:N:603:CLA:H192 | 24:N:607:CHL:H172 | 1.79                     | 0.63              |
| 1:7:51:TYR:CE2    | 1:7:209:ALA:HB1   | 2.33                     | 0.63              |
| 3:8:78:PRO:CD     | 3:8:225:LYS:HE2   | 2.27                     | 0.63              |
| 6:c:73:ALA:HB2    | 12:k:26:LEU:HG    | 1.80                     | 0.63              |
| 7:d:189:PHE:O     | 7:d:295:ARG:NH1   | 2.31                     | 0.63              |
| 12:k:32:PHE:CZ    | 19:z:9:VAL:HG11   | 2.33                     | 0.63              |
| 21:g:172:VAL:HG21 | 40:g:617:NEX:H34  | 1.80                     | 0.63              |
| 24:n:607:CHL:H142 | 24:n:607:CHL:C9   | 2.28                     | 0.63              |
| 6:C:308:GLU:HA    | 6:C:361:LEU:HD22  | 1.80                     | 0.63              |
| 25:C:511:CLA:H143 | 19:Z:20:LEU:HD11  | 1.79                     | 0.63              |
| 25:C:512:CLA:HBC3 | 25:C:512:CLA:HHD  | 1.80                     | 0.63              |
| 15:O:130:LYS:HD2  | 15:O:179:GLU:HB2  | 1.80                     | 0.63              |
| 16:T:2:GLU:O      | 16:T:5:VAL:HG22   | 1.98                     | 0.63              |
| 21:G:132:PHE:CE1  | 21:G:133:LYS:HG3  | 2.33                     | 0.63              |
| 21:G:164:THR:HG21 | 24:G:606:CHL:O1D  | 1.97                     | 0.63              |
| 21:N:202:ALA:HB1  | 21:N:208:PHE:CD1  | 2.33                     | 0.63              |
| 21:Y:164:THR:HG21 | 24:Y:307:CHL:O1D  | 1.98                     | 0.63              |
| 1:5:132:PHE:CE1   | 1:5:133:LYS:HG3   | 2.33                     | 0.63              |
| 2:6:51:TYR:HA     | 2:6:55:ARG:HD3    | 1.80                     | 0.63              |
| 4:a:172:MET:HE1   | 25:a:403:CLA:HBC2 | 1.79                     | 0.63              |
| 5:b:472:ARG:HA    | 5:b:479:PHE:CZ    | 2.33                     | 0.63              |
| 7:d:13:LYS:HA     | 7:d:13:LYS:HE2    | 1.80                     | 0.63              |
| 16:t:2:GLU:O      | 16:t:5:VAL:HG22   | 1.98                     | 0.63              |
| 21:g:138:ILE:HD13 | 24:g:606:CHL:CBC  | 2.28                     | 0.63              |
| 1:1:162:TRP:O     | 1:1:166:VAL:HG23  | 1.98                     | 0.63              |
| 6:C:428:THR:HG22  | 35:C:516:DGD:HBW1 | 1.78                     | 0.63              |
| 25:C:510:CLA:HMA2 | 25:C:510:CLA:H2   | 1.80                     | 0.63              |
| 21:G:138:ILE:HD13 | 24:G:606:CHL:CBC  | 2.28                     | 0.63              |
| 21:G:162:TRP:O    | 21:G:166:VAL:HG23 | 1.98                     | 0.63              |
| 21:Y:202:ALA:HB1  | 21:Y:208:PHE:CD1  | 2.33                     | 0.63              |
| 3:8:174:TRP:HE3   | 3:8:180:LYS:HD2   | 1.63                     | 0.63              |
| 4:a:290:ILE:HG13  | 25:a:402:CLA:HED3 | 1.80                     | 0.63              |
| 7:d:52:GLY:HA3    | 7:d:79:VAL:HG22   | 1.79                     | 0.63              |
| 21:g:97:GLU:CG    | 21:g:190:LEU:HD21 | 2.20                     | 0.63              |
| 25:g:603:CLA:HAB  | 39:g:616:LUT:C34  | 2.28                     | 0.63              |
| 21:y:51:TYR:CE2   | 21:y:209:ALA:HB1  | 2.33                     | 0.63              |
| 1:1:49:PRO:O      | 1:1:55:ARG:HG2    | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:C:112:PHE:O     | 6:C:116:VAL:HG23  | 1.98                     | 0.63              |
| 6:C:185:VAL:HG23  | 6:C:230:LEU:HD13  | 1.81                     | 0.63              |
| 6:C:304:PRO:O     | 6:C:305:THR:HB    | 1.99                     | 0.63              |
| 11:I:23:PHE:HB3   | 28:I:101:BCR:C3   | 2.29                     | 0.63              |
| 20:S:128:PHE:HE1  | 39:S:316:LUT:H173 | 1.63                     | 0.63              |
| 25:G:603:CLA:HAB  | 39:G:616:LUT:C34  | 2.29                     | 0.63              |
| 25:N:603:CLA:H203 | 24:N:607:CHL:C19  | 2.29                     | 0.63              |
| 23:U:97:THR:HA    | 23:U:102:ARG:NH2  | 2.06                     | 0.63              |
| 1:7:132:PHE:CE1   | 1:7:133:LYS:HG3   | 2.33                     | 0.63              |
| 3:8:78:PRO:HG3    | 3:8:225:LYS:HE2   | 1.79                     | 0.63              |
| 6:c:308:GLU:HA    | 6:c:361:LEU:HD22  | 1.80                     | 0.63              |
| 6:c:378:SER:O     | 6:c:382:LYS:HG2   | 1.98                     | 0.63              |
| 21:g:213:VAL:HG12 | 25:g:611:CLA:HED1 | 1.81                     | 0.63              |
| 21:g:218:ASN:OD1  | 25:g:611:CLA:HMD2 | 1.98                     | 0.63              |
| 21:n:162:TRP:O    | 21:n:166:VAL:HG23 | 1.98                     | 0.63              |
| 22:r:129:GLU:OE1  | 22:r:132:GLY:N    | 2.25                     | 0.63              |
| 2:2:220:GLY:HA2   | 25:2:602:CLA:HAC1 | 1.80                     | 0.63              |
| 1:3:94:ARG:NE     | 1:3:94:ARG:HA     | 2.12                     | 0.63              |
| 4:A:172:MET:HE1   | 25:A:402:CLA:HBC2 | 1.79                     | 0.63              |
| 25:B:601:CLA:HBB2 | 28:H:101:BCR:H351 | 1.81                     | 0.63              |
| 6:C:38:GLY:HA3    | 25:C:511:CLA:HMD2 | 1.80                     | 0.63              |
| 15:O:190:GLU:OE2  | 15:O:216:LYS:HA   | 1.99                     | 0.63              |
| 25:S:304:CLA:HMA2 | 25:S:304:CLA:HBA1 | 1.80                     | 0.63              |
| 24:G:605:CHL:HHC  | 24:G:605:CHL:HBB1 | 1.81                     | 0.63              |
| 3:8:155:TRP:CE2   | 25:r:601:CLA:HMB1 | 2.34                     | 0.63              |
| 4:a:132:GLU:O     | 4:a:136:ARG:HG2   | 1.99                     | 0.63              |
| 15:o:158:PHE:CD2  | 15:o:322:LYS:HE3  | 2.33                     | 0.63              |
| 21:y:57:LYS:HB2   | 21:y:63:SER:OG    | 1.98                     | 0.63              |
| 24:y:310:CHL:HBB1 | 24:y:310:CHL:HHC  | 1.79                     | 0.63              |
| 1:3:97:GLU:CG     | 1:3:190:LEU:HD21  | 2.20                     | 0.63              |
| 4:A:147:TYR:O     | 4:A:150:PRO:HD2   | 1.98                     | 0.63              |
| 6:C:199:ILE:O     | 6:C:200:THR:HG22  | 1.98                     | 0.63              |
| 6:C:348:GLU:OE2   | 15:O:106:LYS:HA   | 1.98                     | 0.63              |
| 21:N:51:TYR:CE2   | 21:N:209:ALA:HB1  | 2.33                     | 0.63              |
| 21:Y:51:TYR:CE2   | 21:Y:209:ALA:HB1  | 2.33                     | 0.63              |
| 24:Y:302:CHL:HMB3 | 26:Y:319:LHG:H161 | 1.79                     | 0.63              |
| 1:5:57:LYS:HB2    | 1:5:63:SER:OG     | 1.98                     | 0.63              |
| 1:7:114:VAL:CG1   | 1:7:241:LEU:HD11  | 2.27                     | 0.63              |
| 3:8:159:LYS:HZ2   | 25:r:601:CLA:HMB2 | 1.62                     | 0.63              |
| 4:a:135:PHE:CE1   | 6:c:449:ARG:HG2   | 2.33                     | 0.63              |
| 5:b:60:MET:SD     | 5:b:63:ILE:HD12   | 2.39                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:122:ILE:CG2   | 10:h:20:GLY:HA2   | 2.29                     | 0.63              |
| 21:g:162:TRP:O    | 21:g:166:VAL:HG23 | 1.98                     | 0.63              |
| 22:r:67:TRP:HZ3   | 22:r:82:GLY:HA2   | 1.63                     | 0.63              |
| 5:B:141:ILE:HG21  | 25:B:615:CLA:HHC  | 1.81                     | 0.63              |
| 13:L:11:VAL:HG11  | 14:M:25:ILE:HD12  | 1.80                     | 0.63              |
| 15:O:158:PHE:CD2  | 15:O:322:LYS:HE3  | 2.33                     | 0.63              |
| 21:G:196:PHE:CE2  | 24:G:608:CHL:HBC2 | 2.33                     | 0.63              |
| 21:G:202:ALA:HB1  | 21:G:208:PHE:CD1  | 2.33                     | 0.63              |
| 21:N:49:PRO:O     | 21:N:55:ARG:HG2   | 1.99                     | 0.63              |
| 2:6:120:GLN:CG    | 2:6:125:VAL:HA    | 2.26                     | 0.63              |
| 6:c:112:PHE:O     | 6:c:116:VAL:HG23  | 1.98                     | 0.63              |
| 26:c:518:LHG:O4   | 25:y:312:CLA:H3A  | 1.99                     | 0.63              |
| 7:d:322:LEU:O     | 7:d:326:ILE:HG13  | 1.99                     | 0.63              |
| 21:n:94:ARG:NE    | 21:n:94:ARG:HA    | 2.12                     | 0.63              |
| 22:r:122:THR:OG1  | 22:r:125:GLN:O    | 2.16                     | 0.63              |
| 2:2:51:TYR:HA     | 2:2:55:ARG:HD3    | 1.80                     | 0.63              |
| 2:2:117:GLU:HB3   | 2:2:121:LYS:NZ    | 2.13                     | 0.63              |
| 1:3:49:PRO:O      | 1:3:55:ARG:HG2    | 1.99                     | 0.63              |
| 1:3:162:TRP:O     | 1:3:166:VAL:HG23  | 1.98                     | 0.63              |
| 3:4:155:TRP:CE2   | 25:R:601:CLA:HMB1 | 2.34                     | 0.63              |
| 3:4:229:ILE:HG13  | 3:4:230:LYS:N     | 2.13                     | 0.63              |
| 6:C:73:ALA:HB2    | 12:K:26:LEU:HG    | 1.80                     | 0.63              |
| 6:C:168:LEU:HD13  | 25:C:507:CLA:H43  | 1.81                     | 0.63              |
| 21:G:94:ARG:HG2   | 21:N:84:GLY:N     | 2.14                     | 0.63              |
| 21:G:204:ASP:HB3  | 21:G:207:ALA:HB3  | 1.81                     | 0.63              |
| 40:G:617:NEX:H361 | 40:G:617:NEX:C28  | 2.29                     | 0.63              |
| 21:N:224:PHE:CD1  | 25:N:602:CLA:H201 | 2.33                     | 0.63              |
| 21:Y:132:PHE:CE1  | 21:Y:133:LYS:HG3  | 2.33                     | 0.63              |
| 25:Y:304:CLA:O2A  | 25:Y:304:CLA:H2A  | 1.99                     | 0.63              |
| 22:R:68:LEU:HD11  | 25:R:602:CLA:O2D  | 1.98                     | 0.63              |
| 1:7:49:PRO:O      | 1:7:55:ARG:HG2    | 1.99                     | 0.63              |
| 4:a:147:TYR:O     | 4:a:150:PRO:HD2   | 1.98                     | 0.63              |
| 14:m:26:TYR:CZ    | 14:m:30:VAL:HG11  | 2.34                     | 0.63              |
| 21:g:57:LYS:HB2   | 21:g:63:SER:OG    | 1.98                     | 0.63              |
| 25:g:614:CLA:HMC1 | 25:g:614:CLA:HBC3 | 1.80                     | 0.63              |
| 21:y:132:PHE:CE1  | 21:y:133:LYS:HG3  | 2.33                     | 0.63              |
| 21:y:202:ALA:HB1  | 21:y:208:PHE:CD1  | 2.33                     | 0.63              |
| 3:4:224:LEU:O     | 3:4:227:ALA:HB3   | 1.98                     | 0.63              |
| 5:B:122:ILE:CG2   | 10:H:20:GLY:HA2   | 2.29                     | 0.63              |
| 5:B:122:ILE:HG21  | 10:H:20:GLY:HA2   | 1.81                     | 0.63              |
| 21:Y:162:TRP:O    | 21:Y:166:VAL:HG23 | 1.98                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:51:TYR:CE2    | 1:5:209:ALA:HB1   | 2.33                     | 0.63              |
| 1:7:162:TRP:O     | 1:7:166:VAL:HG23  | 1.98                     | 0.63              |
| 5:b:141:ILE:HG21  | 25:b:615:CLA:HHC  | 1.81                     | 0.63              |
| 28:k:101:BCR:H332 | 19:z:12:LEU:HD23  | 1.78                     | 0.63              |
| 20:s:144:GLU:CB   | 20:s:153:LEU:HD21 | 2.29                     | 0.63              |
| 21:g:94:ARG:NE    | 21:g:94:ARG:HA    | 2.12                     | 0.63              |
| 21:g:202:ALA:HB1  | 21:g:208:PHE:CD1  | 2.33                     | 0.63              |
| 25:y:314:CLA:HAA1 | 25:y:314:CLA:HBD  | 1.79                     | 0.63              |
| 1:3:51:TYR:CE2    | 1:3:209:ALA:HB1   | 2.33                     | 0.62              |
| 3:4:78:PRO:HG3    | 3:4:225:LYS:HE2   | 1.79                     | 0.62              |
| 6:C:289:PHE:CE2   | 25:C:501:CLA:H12  | 2.34                     | 0.62              |
| 6:C:369:LEU:HD11  | 6:C:388:GLN:OE1   | 1.99                     | 0.62              |
| 7:D:295:ARG:HG3   | 7:D:297:TYR:HB2   | 1.81                     | 0.62              |
| 21:G:84:GLY:N     | 21:Y:94:ARG:HG2   | 2.14                     | 0.62              |
| 21:Y:204:ASP:HB3  | 21:Y:207:ALA:HB3  | 1.81                     | 0.62              |
| 24:Y:302:CHL:H8   | 24:Y:302:CHL:H143 | 1.81                     | 0.62              |
| 2:6:117:GLU:HB3   | 2:6:121:LYS:NZ    | 2.13                     | 0.62              |
| 5:b:157:HIS:HE1   | 25:b:606:CLA:C4A  | 2.09                     | 0.62              |
| 25:b:605:CLA:HMB2 | 25:b:606:CLA:O2A  | 1.99                     | 0.62              |
| 15:o:130:LYS:CE   | 15:o:177:PRO:HB2  | 2.25                     | 0.62              |
| 20:s:232:ALA:O    | 20:s:236:MET:HG2  | 1.99                     | 0.62              |
| 21:g:196:PHE:CE2  | 24:g:608:CHL:HBC2 | 2.33                     | 0.62              |
| 25:n:603:CLA:H203 | 24:n:607:CHL:C19  | 2.29                     | 0.62              |
| 21:y:164:THR:HG21 | 24:y:307:CHL:O1D  | 1.98                     | 0.62              |
| 1:1:202:ALA:HB1   | 1:1:208:PHE:CD1   | 2.33                     | 0.62              |
| 2:2:130:PRO:CG    | 2:2:133:PHE:HB2   | 2.29                     | 0.62              |
| 5:B:472:ARG:HA    | 5:B:479:PHE:CZ    | 2.33                     | 0.62              |
| 8:E:67:THR:O      | 23:U:102:ARG:HD3  | 1.99                     | 0.62              |
| 21:G:218:ASN:OD1  | 25:G:611:CLA:HMD2 | 1.98                     | 0.62              |
| 21:Y:49:PRO:O     | 21:Y:55:ARG:HG2   | 1.99                     | 0.62              |
| 21:Y:231:VAL:HG21 | 25:Y:314:CLA:CAC  | 2.30                     | 0.62              |
| 22:R:67:TRP:HZ3   | 22:R:82:GLY:HA2   | 1.63                     | 0.62              |
| 2:6:69:TYR:CD1    | 2:6:70:LEU:HG     | 2.35                     | 0.62              |
| 25:b:601:CLA:HBB2 | 28:h:101:BCR:H351 | 1.81                     | 0.62              |
| 6:c:267:SER:HA    | 17:w:133:LEU:HD23 | 1.81                     | 0.62              |
| 14:m:1:MET:CB     | 14:m:3:VAL:HG13   | 2.28                     | 0.62              |
| 21:g:132:PHE:CE1  | 21:g:133:LYS:HG3  | 2.33                     | 0.62              |
| 1:1:57:LYS:HB2    | 1:1:63:SER:OG     | 1.98                     | 0.62              |
| 24:1:301:CHL:HHC  | 24:1:301:CHL:HBB1 | 1.80                     | 0.62              |
| 1:3:114:VAL:CG1   | 1:3:241:LEU:HD11  | 2.27                     | 0.62              |
| 4:A:132:GLU:O     | 4:A:136:ARG:HG2   | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:94:ARG:NH2   | 21:G:97:GLU:OE1   | 2.33                     | 0.62              |
| 21:G:172:VAL:HG21 | 40:G:617:NEX:H34  | 1.80                     | 0.62              |
| 21:N:164:THR:CG2  | 24:N:606:CHL:HED3 | 2.28                     | 0.62              |
| 24:N:607:CHL:H12  | 32:Y:321:AJP:C21  | 2.29                     | 0.62              |
| 40:N:617:NEX:H191 | 40:N:617:NEX:C12  | 2.30                     | 0.62              |
| 1:5:49:PRO:O      | 1:5:55:ARG:HG2    | 1.99                     | 0.62              |
| 1:7:94:ARG:NH2    | 1:7:97:GLU:OE1    | 2.33                     | 0.62              |
| 4:a:232:SER:OG    | 5:b:7:ARG:HD2     | 2.00                     | 0.62              |
| 6:c:38:GLY:HA3    | 25:c:511:CLA:HMD2 | 1.80                     | 0.62              |
| 24:g:605:CHL:HBB1 | 24:g:605:CHL:HHC  | 1.81                     | 0.62              |
| 21:n:80:TRP:CE3   | 39:n:616:LUT:H383 | 2.33                     | 0.62              |
| 21:n:204:ASP:HB3  | 21:n:207:ALA:HB3  | 1.81                     | 0.62              |
| 1:3:204:ASP:HB3   | 1:3:207:ALA:HB3   | 1.81                     | 0.62              |
| 5:B:39:LEU:HB3    | 28:t:101:BCR:C38  | 2.28                     | 0.62              |
| 5:B:157:HIS:HE1   | 25:B:606:CLA:C4A  | 2.09                     | 0.62              |
| 25:C:511:CLA:HBD  | 25:C:511:CLA:HAA1 | 1.81                     | 0.62              |
| 14:M:1:MET:CB     | 14:M:3:VAL:HG13   | 2.28                     | 0.62              |
| 28:T:101:BCR:C38  | 5:b:39:LEU:HB3    | 2.28                     | 0.62              |
| 20:S:232:ALA:O    | 20:S:236:MET:HG2  | 1.99                     | 0.62              |
| 21:G:49:PRO:O     | 21:G:55:ARG:HG2   | 1.99                     | 0.62              |
| 24:N:607:CHL:H142 | 24:N:607:CHL:C9   | 2.28                     | 0.62              |
| 1:5:94:ARG:NH2    | 1:5:97:GLU:OE1    | 2.33                     | 0.62              |
| 1:7:202:ALA:HB1   | 1:7:208:PHE:CD1   | 2.33                     | 0.62              |
| 6:c:255:LYS:HG3   | 6:c:256:PRO:HD2   | 1.80                     | 0.62              |
| 6:c:304:PRO:O     | 6:c:305:THR:HB    | 1.99                     | 0.62              |
| 25:s:313:CLA:HAA1 | 25:s:313:CLA:HBD  | 1.80                     | 0.62              |
| 21:g:94:ARG:NH2   | 21:g:97:GLU:OE1   | 2.33                     | 0.62              |
| 21:g:94:ARG:HG2   | 21:n:84:GLY:N     | 2.14                     | 0.62              |
| 21:g:131:TRP:HB3  | 39:g:616:LUT:H41  | 1.82                     | 0.62              |
| 24:n:607:CHL:H12  | 32:y:321:AJP:C21  | 2.29                     | 0.62              |
| 25:y:303:CLA:HAB  | 39:y:317:LUT:H32  | 1.81                     | 0.62              |
| 6:C:279:LEU:HD12  | 25:C:509:CLA:HED3 | 1.81                     | 0.62              |
| 7:D:13:LYS:HA     | 7:D:13:LYS:HE2    | 1.80                     | 0.62              |
| 7:D:211:LEU:HA    | 7:D:214:ILE:HG22  | 1.80                     | 0.62              |
| 18:X:84:LYS:O     | 18:X:88:LEU:HD23  | 1.99                     | 0.62              |
| 1:5:114:VAL:CG1   | 1:5:241:LEU:HD11  | 2.28                     | 0.62              |
| 1:5:202:ALA:HB1   | 1:5:208:PHE:CD1   | 2.33                     | 0.62              |
| 2:6:232:VAL:HG13  | 2:6:243:GLU:OE1   | 2.00                     | 0.62              |
| 6:c:52:ALA:HB1    | 25:c:509:CLA:HBB1 | 1.80                     | 0.62              |
| 21:n:51:TYR:CE2   | 21:n:209:ALA:HB1  | 2.33                     | 0.62              |
| 21:n:94:ARG:NH2   | 21:n:97:GLU:OE1   | 2.33                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:164:THR:CG2  | 24:n:606:CHL:HED3 | 2.29                     | 0.62              |
| 21:n:232:GLN:NE2  | 25:n:613:CLA:C4D  | 2.40                     | 0.62              |
| 5:B:60:MET:SD     | 5:B:63:ILE:HD12   | 2.39                     | 0.62              |
| 25:B:605:CLA:HMB2 | 25:B:606:CLA:O2A  | 1.99                     | 0.62              |
| 26:C:518:LHG:O4   | 25:Y:312:CLA:H3A  | 1.99                     | 0.62              |
| 7:D:86:LEU:HD13   | 7:D:91:LEU:HD21   | 1.80                     | 0.62              |
| 15:O:158:PHE:CE2  | 15:O:322:LYS:HE3  | 2.33                     | 0.62              |
| 25:G:614:CLA:HMC1 | 25:G:614:CLA:HBC3 | 1.80                     | 0.62              |
| 21:N:204:ASP:HB3  | 21:N:207:ALA:HB3  | 1.81                     | 0.62              |
| 21:Y:86:SER:OG    | 25:Y:303:CLA:O1A  | 2.16                     | 0.62              |
| 21:Y:94:ARG:NH2   | 21:Y:97:GLU:OE1   | 2.33                     | 0.62              |
| 1:5:86:SER:HB3    | 1:5:92:PHE:HD1    | 1.65                     | 0.62              |
| 4:a:332:HIS:HB3   | 7:d:322:LEU:HD21  | 1.80                     | 0.62              |
| 6:c:168:LEU:HD13  | 25:c:507:CLA:H43  | 1.81                     | 0.62              |
| 11:i:23:PHE:HB3   | 28:i:101:BCR:C3   | 2.29                     | 0.62              |
| 21:g:49:PRO:O     | 21:g:55:ARG:HG2   | 1.99                     | 0.62              |
| 21:g:131:TRP:HB2  | 39:g:616:LUT:H21  | 1.82                     | 0.62              |
| 21:n:90:GLU:OE1   | 21:n:90:GLU:HA    | 2.00                     | 0.62              |
| 21:y:49:PRO:O     | 21:y:55:ARG:HG2   | 1.99                     | 0.62              |
| 4:A:131:TRP:CH2   | 25:C:505:CLA:HAA2 | 2.35                     | 0.62              |
| 6:C:267:SER:HA    | 17:W:133:LEU:HD23 | 1.81                     | 0.62              |
| 6:C:350:ILE:HG21  | 6:C:359:TRP:HB2   | 1.82                     | 0.62              |
| 21:G:90:GLU:OE1   | 21:G:90:GLU:HA    | 2.00                     | 0.62              |
| 22:R:173:LEU:CD1  | 22:R:188:ILE:HG13 | 2.30                     | 0.62              |
| 1:7:57:LYS:HB2    | 1:7:63:SER:OG     | 1.98                     | 0.62              |
| 3:8:219:GLU:CB    | 3:8:222:GLU:HB2   | 2.30                     | 0.62              |
| 6:c:289:PHE:CE2   | 25:c:501:CLA:H12  | 2.34                     | 0.62              |
| 6:c:369:LEU:HD11  | 6:c:388:GLN:OE1   | 1.99                     | 0.62              |
| 25:c:512:CLA:HBC3 | 25:c:512:CLA:HHD  | 1.80                     | 0.62              |
| 18:x:84:LYS:O     | 18:x:88:LEU:HD23  | 1.99                     | 0.62              |
| 25:r:601:CLA:HHB  | 26:r:618:LHG:H132 | 1.81                     | 0.62              |
| 1:1:86:SER:HB3    | 1:1:92:PHE:HD1    | 1.65                     | 0.62              |
| 2:2:120:GLN:HB3   | 2:2:129:GLU:OE2   | 2.00                     | 0.62              |
| 1:3:94:ARG:NH2    | 1:3:97:GLU:OE1    | 2.33                     | 0.62              |
| 4:A:232:SER:OG    | 5:B:7:ARG:HD2     | 2.00                     | 0.62              |
| 12:K:53:VAL:CG2   | 28:Z:101:BCR:H21C | 2.30                     | 0.62              |
| 14:M:26:TYR:CZ    | 14:M:30:VAL:HG11  | 2.34                     | 0.62              |
| 3:8:139:PRO:HB2   | 22:r:280:HIS:NE2  | 2.15                     | 0.62              |
| 4:a:131:TRP:CH2   | 25:c:505:CLA:HAA2 | 2.35                     | 0.62              |
| 21:n:86:SER:HB3   | 21:n:92:PHE:HD1   | 1.65                     | 0.62              |
| 22:r:173:LEU:CD1  | 22:r:188:ILE:HG13 | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:204:ASP:HB3   | 1:1:207:ALA:HB3   | 1.81                     | 0.62              |
| 2:2:69:TYR:CD1    | 2:2:70:LEU:HG     | 2.35                     | 0.62              |
| 3:4:222:GLU:HA    | 3:4:225:LYS:CG    | 2.30                     | 0.62              |
| 25:C:501:CLA:H171 | 25:C:507:CLA:H122 | 1.82                     | 0.62              |
| 12:K:58:VAL:O     | 12:K:58:VAL:HG12  | 1.99                     | 0.62              |
| 21:G:86:SER:HB3   | 21:G:92:PHE:HD1   | 1.65                     | 0.62              |
| 2:6:130:PRO:CG    | 2:6:133:PHE:HB2   | 2.29                     | 0.62              |
| 5:b:157:HIS:NE2   | 5:b:164:PRO:HD2   | 2.15                     | 0.62              |
| 25:c:511:CLA:HAA1 | 25:c:511:CLA:HBD  | 1.81                     | 0.62              |
| 8:e:67:THR:O      | 23:u:102:ARG:HD3  | 1.99                     | 0.62              |
| 20:s:132:GLU:CG   | 20:s:251:VAL:HB   | 2.30                     | 0.62              |
| 21:n:49:PRO:O     | 21:n:55:ARG:HG2   | 1.99                     | 0.62              |
| 24:n:606:CHL:HBC2 | 24:n:607:CHL:HHD  | 1.82                     | 0.62              |
| 21:y:231:VAL:HG21 | 25:y:314:CLA:CAC  | 2.29                     | 0.62              |
| 24:y:302:CHL:H143 | 24:y:302:CHL:H8   | 1.81                     | 0.62              |
| 5:B:141:ILE:HG13  | 5:B:217:LEU:HD21  | 1.82                     | 0.62              |
| 6:C:163:ILE:O     | 6:C:167:LEU:HD23  | 2.00                     | 0.62              |
| 6:C:288:CYS:SG    | 35:C:515:DGD:HB32 | 2.40                     | 0.62              |
| 10:H:56:ILE:CD1   | 18:X:84:LYS:HE3   | 2.16                     | 0.62              |
| 20:S:144:GLU:CB   | 20:S:153:LEU:HD21 | 2.29                     | 0.62              |
| 20:S:218:GLY:O    | 20:S:222:LYS:HG3  | 2.00                     | 0.62              |
| 21:Y:86:SER:HB3   | 21:Y:92:PHE:HD1   | 1.65                     | 0.62              |
| 21:Y:90:GLU:OE1   | 21:Y:90:GLU:HA    | 2.00                     | 0.62              |
| 21:Y:215:GLU:HG3  | 25:Y:311:CLA:C1B  | 2.30                     | 0.62              |
| 2:6:100:VAL:HG22  | 2:6:216:GLU:OE2   | 2.00                     | 0.62              |
| 3:8:205:LEU:HB3   | 3:8:220:LYS:NZ    | 2.15                     | 0.62              |
| 4:a:81:ALA:HB2    | 4:a:175:GLY:HA3   | 1.82                     | 0.62              |
| 25:b:609:CLA:HAA1 | 10:h:43:MET:SD    | 2.40                     | 0.62              |
| 25:c:507:CLA:H142 | 28:i:101:BCR:H362 | 1.81                     | 0.62              |
| 7:d:305:ARG:HD3   | 14:m:1:MET:HE1    | 1.82                     | 0.62              |
| 15:o:285:ILE:HG12 | 15:o:287:LEU:HD11 | 1.82                     | 0.62              |
| 40:g:617:NEX:H361 | 40:g:617:NEX:C28  | 2.29                     | 0.62              |
| 22:r:283:ILE:HG13 | 25:r:612:CLA:HMD3 | 1.81                     | 0.62              |
| 1:1:94:ARG:NH2    | 1:1:97:GLU:OE1    | 2.33                     | 0.61              |
| 1:1:138:ILE:CD1   | 24:1:302:CHL:HMD3 | 2.30                     | 0.61              |
| 2:2:117:GLU:HG3   | 2:2:239:LYS:HD3   | 1.82                     | 0.61              |
| 2:2:232:VAL:HG13  | 2:2:243:GLU:OE1   | 2.00                     | 0.61              |
| 3:4:139:PRO:HB2   | 22:R:280:HIS:NE2  | 2.15                     | 0.61              |
| 6:C:199:ILE:HG23  | 6:C:231:GLU:HG3   | 1.82                     | 0.61              |
| 7:D:305:ARG:HH11  | 14:M:1:MET:HE2    | 1.65                     | 0.61              |
| 11:I:6:LEU:HD23   | 17:W:101:LEU:HD23 | 1.80                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:90:GLU:OE1   | 21:N:90:GLU:HA    | 2.00                     | 0.61              |
| 22:R:172:GLU:OE1  | 22:R:177:SER:HA   | 2.00                     | 0.61              |
| 22:R:283:ILE:HG13 | 25:R:612:CLA:HMD3 | 1.81                     | 0.61              |
| 25:R:601:CLA:HHB  | 26:R:618:LHG:H132 | 1.81                     | 0.61              |
| 1:5:138:ILE:CD1   | 24:5:302:CHL:HMD3 | 2.30                     | 0.61              |
| 6:c:199:ILE:HG23  | 6:c:231:GLU:HG3   | 1.82                     | 0.61              |
| 6:c:251:HIS:CE1   | 25:c:506:CLA:HMA3 | 2.35                     | 0.61              |
| 6:c:288:CYS:SG    | 35:c:515:DGD:HB32 | 2.40                     | 0.61              |
| 25:c:501:CLA:H171 | 25:c:507:CLA:H122 | 1.82                     | 0.61              |
| 7:d:295:ARG:HG3   | 7:d:297:TYR:HB2   | 1.81                     | 0.61              |
| 12:k:53:VAL:CG2   | 28:z:101:BCR:H21C | 2.30                     | 0.61              |
| 28:t:101:BCR:H292 | 28:t:101:BCR:C36  | 2.29                     | 0.61              |
| 24:n:607:CHL:H202 | 24:n:609:CHL:C4   | 2.30                     | 0.61              |
| 21:y:94:ARG:NH2   | 21:y:97:GLU:OE1   | 2.33                     | 0.61              |
| 22:r:172:GLU:OE1  | 22:r:177:SER:HA   | 2.00                     | 0.61              |
| 3:4:205:LEU:HB3   | 3:4:220:LYS:NZ    | 2.15                     | 0.61              |
| 3:4:222:GLU:HG2   | 3:4:225:LYS:CD    | 2.27                     | 0.61              |
| 14:M:15:ILE:O     | 14:M:19:THR:OG1   | 2.18                     | 0.61              |
| 21:N:94:ARG:NH2   | 21:N:97:GLU:OE1   | 2.33                     | 0.61              |
| 27:a:404:PHO:HBB1 | 27:a:404:PHO:CMB  | 2.30                     | 0.61              |
| 11:i:6:LEU:HD23   | 17:w:101:LEU:HD23 | 1.80                     | 0.61              |
| 21:y:204:ASP:HB3  | 21:y:207:ALA:HB3  | 1.81                     | 0.61              |
| 1:1:90:GLU:OE1    | 1:1:90:GLU:HA     | 2.00                     | 0.61              |
| 2:2:96:ARG:O      | 2:2:100:VAL:HG23  | 2.00                     | 0.61              |
| 24:2:601:CHL:CGD  | 26:2:606:LHG:H142 | 2.30                     | 0.61              |
| 5:B:153:PHE:O     | 5:B:158:VAL:HG23  | 2.00                     | 0.61              |
| 7:D:133:LEU:O     | 7:D:137:VAL:HG22  | 2.01                     | 0.61              |
| 21:G:215:GLU:CG   | 25:G:610:CLA:C1B  | 2.78                     | 0.61              |
| 25:R:601:CLA:C4D  | 26:R:618:LHG:H102 | 2.03                     | 0.61              |
| 2:6:181:LEU:HD13  | 24:6:603:CHL:CAB  | 2.30                     | 0.61              |
| 24:6:601:CHL:CGD  | 26:6:606:LHG:H142 | 2.30                     | 0.61              |
| 21:g:84:GLY:N     | 21:y:94:ARG:HG2   | 2.14                     | 0.61              |
| 21:g:215:GLU:CG   | 25:g:610:CLA:C1B  | 2.78                     | 0.61              |
| 25:n:613:CLA:HMC3 | 25:n:613:CLA:HBC2 | 1.81                     | 0.61              |
| 21:y:224:PHE:HE2  | 25:y:314:CLA:HAB  | 1.65                     | 0.61              |
| 2:2:100:VAL:HG22  | 2:2:216:GLU:OE2   | 2.00                     | 0.61              |
| 3:4:219:GLU:CB    | 3:4:222:GLU:HB2   | 2.30                     | 0.61              |
| 4:A:290:ILE:HG13  | 25:A:401:CLA:HED3 | 1.80                     | 0.61              |
| 5:B:75:TRP:CD1    | 5:B:92:SER:HG     | 2.19                     | 0.61              |
| 7:D:322:LEU:O     | 7:D:326:ILE:HG13  | 1.99                     | 0.61              |
| 20:S:196:PHE:HD2  | 24:S:308:CHL:HBC3 | 1.66                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:208:PHE:CE2  | 21:G:212:LYS:HE3  | 2.36                     | 0.61              |
| 21:Y:231:VAL:CG1  | 25:Y:314:CLA:HHD  | 2.31                     | 0.61              |
| 22:R:139:CYS:O    | 22:R:143:HIS:ND1  | 2.29                     | 0.61              |
| 2:6:117:GLU:HG3   | 2:6:239:LYS:HD3   | 1.82                     | 0.61              |
| 6:c:279:LEU:HD12  | 25:c:509:CLA:HED3 | 1.81                     | 0.61              |
| 15:o:190:GLU:OE2  | 15:o:216:LYS:HA   | 1.99                     | 0.61              |
| 1:1:208:PHE:CE2   | 1:1:212:LYS:HE3   | 2.36                     | 0.61              |
| 1:3:78:TYR:OH     | 1:3:217:LYS:NZ    | 2.20                     | 0.61              |
| 6:C:237:HIS:HE1   | 25:C:501:CLA:ND   | 1.98                     | 0.61              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:C2B  | 2.30                     | 0.61              |
| 24:Y:307:CHL:HMB2 | 24:Y:310:CHL:OMC  | 2.01                     | 0.61              |
| 22:R:178:SER:OG   | 22:R:183:PRO:HA   | 2.00                     | 0.61              |
| 22:R:274:HIS:O    | 22:R:278:PRO:HA   | 2.01                     | 0.61              |
| 2:6:221:ARG:NH1   | 2:6:222:LEU:HD21  | 2.16                     | 0.61              |
| 3:8:222:GLU:HA    | 3:8:225:LYS:CG    | 2.30                     | 0.61              |
| 5:b:122:ILE:HG21  | 10:h:20:GLY:HA2   | 1.81                     | 0.61              |
| 6:c:153:ASP:O     | 6:c:157:MET:HG2   | 2.00                     | 0.61              |
| 6:c:350:ILE:HG21  | 6:c:359:TRP:HB2   | 1.82                     | 0.61              |
| 10:h:18:THR:O     | 10:h:21:LYS:HB2   | 2.00                     | 0.61              |
| 20:s:196:PHE:CD2  | 24:s:308:CHL:HBC3 | 2.36                     | 0.61              |
| 21:y:215:GLU:HG3  | 25:y:311:CLA:C1B  | 2.30                     | 0.61              |
| 3:4:142:PHE:CZ    | 3:4:146:LEU:HD11  | 2.36                     | 0.61              |
| 5:B:282:GLN:NE2   | 23:U:100:ILE:HD11 | 2.15                     | 0.61              |
| 15:O:227:PHE:CE2  | 15:O:287:LEU:HD13 | 2.36                     | 0.61              |
| 20:S:182:LEU:HD23 | 24:S:306:CHL:HMA1 | 1.82                     | 0.61              |
| 20:S:196:PHE:CD2  | 24:S:308:CHL:HBC3 | 2.36                     | 0.61              |
| 20:S:267:LEU:HD13 | 25:S:314:CLA:HED1 | 1.81                     | 0.61              |
| 21:G:199:LEU:HG   | 39:G:615:LUT:H221 | 1.83                     | 0.61              |
| 24:G:601:CHL:HMD3 | 26:Y:301:LHG:HC61 | 1.83                     | 0.61              |
| 25:Y:303:CLA:HBA1 | 39:Y:317:LUT:H382 | 1.83                     | 0.61              |
| 1:5:97:GLU:CG     | 1:5:190:LEU:HD21  | 2.20                     | 0.61              |
| 1:5:208:PHE:CE2   | 1:5:212:LYS:HE3   | 2.36                     | 0.61              |
| 2:6:104:ARG:NE    | 24:6:603:CHL:CBD  | 2.55                     | 0.61              |
| 1:7:191:TYR:CE2   | 1:7:212:LYS:HE2   | 2.36                     | 0.61              |
| 4:a:235:GLU:HB3   | 7:d:264:ASN:ND2   | 2.08                     | 0.61              |
| 6:c:227:VAL:HG21  | 28:i:101:BCR:H292 | 1.82                     | 0.61              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:C2B  | 2.30                     | 0.61              |
| 21:y:191:TYR:CE2  | 21:y:212:LYS:HE2  | 2.36                     | 0.61              |
| 1:3:86:SER:HB3    | 1:3:92:PHE:HD1    | 1.65                     | 0.61              |
| 5:B:161:LEU:HD21  | 30:B:623:LMG:C2   | 2.31                     | 0.61              |
| 5:B:272:ARG:NH2   | 42:B:702:HOH:O    | 2.11                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:K:101:BCR:H343 | 19:Z:13:ILE:HD13  | 1.81                     | 0.61              |
| 21:N:191:TYR:CE2  | 21:N:212:LYS:HE2  | 2.36                     | 0.61              |
| 21:N:208:PHE:CE2  | 21:N:212:LYS:HE3  | 2.36                     | 0.61              |
| 2:6:208:THR:O     | 2:6:212:LEU:HG    | 2.01                     | 0.61              |
| 1:7:90:GLU:OE1    | 1:7:90:GLU:HA     | 2.00                     | 0.61              |
| 5:b:141:ILE:HG13  | 5:b:217:LEU:HD21  | 1.82                     | 0.61              |
| 7:d:86:LEU:HD13   | 7:d:91:LEU:HD21   | 1.80                     | 0.61              |
| 21:g:204:ASP:HB3  | 21:g:207:ALA:HB3  | 1.81                     | 0.61              |
| 21:g:208:PHE:CE2  | 21:g:212:LYS:HE3  | 2.36                     | 0.61              |
| 24:g:601:CHL:HMD3 | 26:y:301:LHG:HC61 | 1.83                     | 0.61              |
| 25:B:609:CLA:HAA1 | 10:H:43:MET:SD    | 2.40                     | 0.61              |
| 26:C:518:LHG:H352 | 25:Y:315:CLA:HBB1 | 1.82                     | 0.61              |
| 10:H:18:THR:O     | 10:H:21:LYS:HB2   | 2.00                     | 0.61              |
| 20:S:113:PHE:HE1  | 25:S:304:CLA:HBD  | 1.66                     | 0.61              |
| 21:G:131:TRP:HB2  | 39:G:616:LUT:H21  | 1.82                     | 0.61              |
| 2:6:224:MET:HG2   | 25:6:602:CLA:HMC3 | 1.83                     | 0.61              |
| 1:7:204:ASP:HB3   | 1:7:207:ALA:HB3   | 1.81                     | 0.61              |
| 3:8:221:LEU:HA    | 3:8:224:LEU:HD21  | 1.82                     | 0.61              |
| 4:a:172:MET:CE    | 25:a:403:CLA:HBC2 | 2.30                     | 0.61              |
| 26:c:518:LHG:H352 | 25:y:315:CLA:HBB1 | 1.82                     | 0.61              |
| 28:k:101:BCR:H343 | 19:z:13:ILE:HD13  | 1.81                     | 0.61              |
| 15:o:143:PHE:CD2  | 17:w:81:VAL:HG11  | 2.36                     | 0.61              |
| 20:s:196:PHE:HD2  | 24:s:308:CHL:HBC3 | 1.65                     | 0.61              |
| 21:g:191:TYR:CE2  | 21:g:212:LYS:HE2  | 2.36                     | 0.61              |
| 25:n:603:CLA:H203 | 24:n:607:CHL:H172 | 1.82                     | 0.61              |
| 22:r:103:LYS:HG2  | 22:r:105:LEU:HD11 | 1.83                     | 0.61              |
| 2:2:221:ARG:NH1   | 2:2:222:LEU:HD21  | 2.16                     | 0.61              |
| 3:4:157:GLU:HG3   | 3:4:161:TRP:HE1   | 1.66                     | 0.61              |
| 4:A:219:VAL:HG13  | 4:A:246:TYR:CD1   | 2.36                     | 0.61              |
| 27:A:403:PHO:HBB1 | 27:A:403:PHO:CMB  | 2.30                     | 0.61              |
| 25:A:405:CLA:HMC1 | 11:I:11:VAL:CG1   | 2.30                     | 0.61              |
| 5:B:157:HIS:NE2   | 5:B:164:PRO:HD2   | 2.15                     | 0.61              |
| 5:B:157:HIS:HB2   | 25:B:606:CLA:C4C  | 2.31                     | 0.61              |
| 5:B:346:PHE:O     | 5:B:354:LEU:N     | 2.32                     | 0.61              |
| 6:C:153:ASP:O     | 6:C:157:MET:HG2   | 2.00                     | 0.61              |
| 7:D:30:PHE:O      | 7:D:129:ARG:NH1   | 2.33                     | 0.61              |
| 7:D:127:MET:SD    | 7:D:151:ILE:HD12  | 2.41                     | 0.61              |
| 11:I:24:LEU:HD13  | 28:I:101:BCR:HC41 | 1.83                     | 0.61              |
| 15:O:285:ILE:HG12 | 15:O:287:LEU:HD11 | 1.82                     | 0.61              |
| 20:S:132:GLU:CG   | 20:S:251:VAL:HB   | 2.30                     | 0.61              |
| 21:G:131:TRP:HB3  | 39:G:616:LUT:H41  | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:86:SER:HB3   | 21:N:92:PHE:HD1   | 1.65                     | 0.61              |
| 21:N:199:LEU:HG   | 39:N:615:LUT:H221 | 1.83                     | 0.61              |
| 24:N:607:CHL:H202 | 24:N:609:CHL:C4   | 2.30                     | 0.61              |
| 25:Y:303:CLA:HAB  | 39:Y:317:LUT:H32  | 1.81                     | 0.61              |
| 22:R:103:LYS:HG2  | 22:R:105:LEU:HD11 | 1.83                     | 0.61              |
| 1:5:90:GLU:HA     | 1:5:90:GLU:OE1    | 2.00                     | 0.61              |
| 1:5:138:ILE:HD11  | 24:5:302:CHL:HMD3 | 1.83                     | 0.61              |
| 2:6:96:ARG:O      | 2:6:100:VAL:HG23  | 2.00                     | 0.61              |
| 2:6:120:GLN:HB3   | 2:6:129:GLU:OE2   | 2.00                     | 0.61              |
| 29:a:412:SQD:H131 | 16:t:21:ILE:HD12  | 1.82                     | 0.61              |
| 6:c:237:HIS:HE1   | 25:c:501:CLA:ND   | 1.98                     | 0.61              |
| 6:c:279:LEU:HD12  | 25:c:509:CLA:CED  | 2.31                     | 0.61              |
| 20:s:267:LEU:HD13 | 25:s:314:CLA:HED1 | 1.81                     | 0.61              |
| 21:g:86:SER:HB3   | 21:g:92:PHE:HD1   | 1.65                     | 0.61              |
| 21:g:199:LEU:HG   | 39:g:615:LUT:H221 | 1.83                     | 0.61              |
| 21:n:94:ARG:HG2   | 21:y:84:GLY:CA    | 2.31                     | 0.61              |
| 21:y:86:SER:HB3   | 21:y:92:PHE:HD1   | 1.65                     | 0.61              |
| 1:3:191:TYR:CE2   | 1:3:212:LYS:HE2   | 2.36                     | 0.61              |
| 4:A:81:ALA:HB2    | 4:A:175:GLY:HA3   | 1.82                     | 0.61              |
| 22:R:199:ILE:HA   | 22:R:202:ILE:HG12 | 1.83                     | 0.61              |
| 1:5:191:TYR:CE2   | 1:5:212:LYS:HE2   | 2.36                     | 0.61              |
| 3:8:157:GLU:HA    | 3:8:160:ARG:HG2   | 1.82                     | 0.61              |
| 4:a:239:PHE:HB3   | 16:t:28:LYS:HG3   | 1.83                     | 0.61              |
| 5:b:161:LEU:HD21  | 30:b:623:LMG:C2   | 2.31                     | 0.61              |
| 5:b:392:VAL:HG13  | 5:b:397:VAL:CG2   | 2.31                     | 0.61              |
| 12:k:58:VAL:O     | 12:k:58:VAL:HG12  | 1.99                     | 0.61              |
| 15:o:227:PHE:CE2  | 15:o:287:LEU:HD13 | 2.36                     | 0.61              |
| 21:n:199:LEU:HG   | 39:n:615:LUT:H221 | 1.83                     | 0.61              |
| 1:1:114:VAL:CG1   | 1:1:241:LEU:HD11  | 2.28                     | 0.60              |
| 1:1:191:TYR:CE2   | 1:1:212:LYS:HE2   | 2.36                     | 0.60              |
| 6:C:269:GLU:HG2   | 6:C:448:ALA:HB2   | 1.83                     | 0.60              |
| 11:I:34:ARG:O     | 11:I:35:GLU:HG3   | 2.01                     | 0.60              |
| 25:Y:315:CLA:HAA1 | 25:Y:315:CLA:HED2 | 1.82                     | 0.60              |
| 1:5:204:ASP:HB3   | 1:5:207:ALA:HB3   | 1.81                     | 0.60              |
| 3:8:142:PHE:CZ    | 3:8:146:LEU:HD11  | 2.36                     | 0.60              |
| 3:8:205:LEU:HB3   | 3:8:220:LYS:HZ3   | 1.64                     | 0.60              |
| 27:a:404:PHO:H41  | 29:a:412:SQD:H192 | 1.83                     | 0.60              |
| 5:b:272:ARG:NH2   | 42:b:702:HOH:O    | 2.11                     | 0.60              |
| 7:d:133:LEU:O     | 7:d:137:VAL:HG22  | 2.01                     | 0.60              |
| 21:g:112:GLY:HA3  | 25:g:604:CLA:CHC  | 2.31                     | 0.60              |
| 21:y:138:ILE:HD13 | 24:y:307:CHL:HBC3 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:58:TYR:OH     | 24:2:601:CHL:HAA2 | 2.01                     | 0.60              |
| 5:B:71:ILE:HD13   | 25:B:606:CLA:HED3 | 1.84                     | 0.60              |
| 5:B:272:ARG:HG3   | 5:B:320:ALA:HB2   | 1.83                     | 0.60              |
| 6:C:279:LEU:HD12  | 25:C:509:CLA:CED  | 2.31                     | 0.60              |
| 25:D:403:CLA:H162 | 18:X:92:SER:OG    | 2.01                     | 0.60              |
| 21:N:94:ARG:HG2   | 21:Y:84:GLY:CA    | 2.31                     | 0.60              |
| 21:Y:191:TYR:CE2  | 21:Y:212:LYS:HE2  | 2.36                     | 0.60              |
| 21:Y:208:PHE:CE2  | 21:Y:212:LYS:HE3  | 2.36                     | 0.60              |
| 22:R:85:LYS:CG    | 22:R:86:PRO:HD2   | 2.31                     | 0.60              |
| 22:R:220:GLY:HA2  | 22:R:224:ASP:H    | 1.65                     | 0.60              |
| 22:R:220:GLY:HA3  | 22:R:224:ASP:HB3  | 1.83                     | 0.60              |
| 2:6:172:LEU:O     | 2:6:176:PHE:HD2   | 1.84                     | 0.60              |
| 1:7:86:SER:HB3    | 1:7:92:PHE:HD1    | 1.65                     | 0.60              |
| 3:8:84:ASP:OD2    | 3:8:87:GLY:HA2    | 2.02                     | 0.60              |
| 5:b:327:ALA:HB1   | 30:b:620:LMG:HC8  | 1.83                     | 0.60              |
| 20:s:237:LEU:O    | 20:s:241:ILE:HD12 | 2.01                     | 0.60              |
| 24:n:609:CHL:HHC  | 24:n:609:CHL:HBB1 | 1.82                     | 0.60              |
| 25:y:303:CLA:HBA1 | 39:y:317:LUT:H382 | 1.83                     | 0.60              |
| 25:r:603:CLA:C1D  | 25:r:608:CLA:H92  | 1.95                     | 0.60              |
| 2:2:208:THR:O     | 2:2:212:LEU:HG    | 2.01                     | 0.60              |
| 4:A:172:MET:CE    | 25:A:402:CLA:HBC2 | 2.30                     | 0.60              |
| 21:G:191:TYR:CE2  | 21:G:212:LYS:HE2  | 2.36                     | 0.60              |
| 25:N:603:CLA:H203 | 24:N:607:CHL:H172 | 1.82                     | 0.60              |
| 22:R:258:VAL:HB   | 25:R:612:CLA:HHD  | 1.83                     | 0.60              |
| 2:6:58:TYR:OH     | 24:6:601:CHL:HAA2 | 2.01                     | 0.60              |
| 1:7:208:PHE:CE2   | 1:7:212:LYS:HE3   | 2.36                     | 0.60              |
| 4:a:328:MET:HG2   | 7:d:326:ILE:CG1   | 2.31                     | 0.60              |
| 5:b:157:HIS:HB2   | 25:b:606:CLA:C4C  | 2.31                     | 0.60              |
| 5:b:282:GLN:NE2   | 23:u:100:ILE:HD11 | 2.15                     | 0.60              |
| 7:d:236:PHE:HD1   | 7:d:244:THR:HG21  | 1.66                     | 0.60              |
| 24:g:606:CHL:CBA  | 40:g:617:NEX:H403 | 2.31                     | 0.60              |
| 21:n:208:PHE:CE2  | 21:n:212:LYS:HE3  | 2.36                     | 0.60              |
| 21:y:90:GLU:OE1   | 21:y:90:GLU:HA    | 2.00                     | 0.60              |
| 22:r:247:ARG:HD3  | 25:r:602:CLA:CHD  | 2.31                     | 0.60              |
| 2:2:107:MET:HG2   | 2:2:111:PHE:HE2   | 1.67                     | 0.60              |
| 2:2:172:LEU:O     | 2:2:176:PHE:HD2   | 1.84                     | 0.60              |
| 1:3:90:GLU:OE1    | 1:3:90:GLU:HA     | 2.00                     | 0.60              |
| 6:C:251:HIS:CE1   | 25:C:506:CLA:HMA3 | 2.35                     | 0.60              |
| 25:C:512:CLA:H192 | 26:S:301:LHG:H222 | 1.83                     | 0.60              |
| 7:D:305:ARG:HD3   | 14:M:1:MET:HE1    | 1.82                     | 0.60              |
| 15:O:232:LEU:O    | 15:O:234:PRO:HD3  | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:N:603:CLA:H203 | 24:N:607:CHL:H193 | 1.84                     | 0.60              |
| 22:R:100:ASN:OD1  | 22:R:101:LEU:N    | 2.34                     | 0.60              |
| 22:R:103:LYS:HG2  | 22:R:105:LEU:CD1  | 2.32                     | 0.60              |
| 22:R:185:PRO:HB3  | 21:y:151:SER:OG   | 2.01                     | 0.60              |
| 3:8:222:GLU:HG2   | 3:8:225:LYS:CD    | 2.27                     | 0.60              |
| 4:a:129:ARG:NH2   | 7:d:257:ILE:O     | 2.34                     | 0.60              |
| 6:c:163:ILE:O     | 6:c:167:LEU:HD23  | 2.00                     | 0.60              |
| 6:c:269:GLU:HG2   | 6:c:448:ALA:HB2   | 1.83                     | 0.60              |
| 7:d:127:MET:SD    | 7:d:151:ILE:HD12  | 2.41                     | 0.60              |
| 7:d:280:LEU:HD21  | 25:d:402:CLA:HBA2 | 1.83                     | 0.60              |
| 7:d:305:ARG:HH11  | 14:m:1:MET:HE2    | 1.65                     | 0.60              |
| 4:A:239:PHE:HB3   | 16:T:28:LYS:HG3   | 1.83                     | 0.60              |
| 4:A:259:ILE:HG23  | 4:A:259:ILE:O     | 2.02                     | 0.60              |
| 27:A:403:PHO:H41  | 29:A:411:SQD:H192 | 1.83                     | 0.60              |
| 21:Y:97:GLU:CG    | 21:Y:190:LEU:HD21 | 2.20                     | 0.60              |
| 2:6:139:ILE:O     | 2:6:139:ILE:HG22  | 2.01                     | 0.60              |
| 5:b:153:PHE:O     | 5:b:158:VAL:HG23  | 2.00                     | 0.60              |
| 21:n:158:ILE:CD1  | 21:y:257:TRP:HE3  | 2.11                     | 0.60              |
| 21:y:208:PHE:CE2  | 21:y:212:LYS:HE3  | 2.36                     | 0.60              |
| 25:y:315:CLA:HED2 | 25:y:315:CLA:HAA1 | 1.82                     | 0.60              |
| 22:r:100:ASN:OD1  | 22:r:101:LEU:N    | 2.34                     | 0.60              |
| 22:r:258:VAL:HB   | 25:r:612:CLA:HHD  | 1.83                     | 0.60              |
| 2:2:139:ILE:O     | 2:2:139:ILE:HG22  | 2.01                     | 0.60              |
| 2:2:224:MET:HG2   | 25:2:602:CLA:HMC3 | 1.82                     | 0.60              |
| 1:3:208:PHE:CE2   | 1:3:212:LYS:HE3   | 2.36                     | 0.60              |
| 3:4:157:GLU:HA    | 3:4:160:ARG:HG2   | 1.82                     | 0.60              |
| 5:B:392:VAL:HG13  | 5:B:397:VAL:CG2   | 2.31                     | 0.60              |
| 16:T:7:THR:HG21   | 28:T:101:BCR:H363 | 1.84                     | 0.60              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:CHB  | 2.31                     | 0.60              |
| 21:Y:224:PHE:HE2  | 25:Y:314:CLA:HAB  | 1.65                     | 0.60              |
| 22:R:247:ARG:HD3  | 25:R:602:CLA:CHD  | 2.31                     | 0.60              |
| 1:7:97:GLU:CG     | 1:7:190:LEU:HD21  | 2.20                     | 0.60              |
| 11:i:24:LEU:HD13  | 28:i:101:BCR:HC41 | 1.83                     | 0.60              |
| 15:o:232:LEU:O    | 15:o:234:PRO:HD3  | 2.02                     | 0.60              |
| 20:s:182:LEU:HD23 | 24:s:306:CHL:HMA1 | 1.83                     | 0.60              |
| 21:g:90:GLU:OE1   | 21:g:90:GLU:HA    | 2.00                     | 0.60              |
| 21:n:191:TYR:CE2  | 21:n:212:LYS:HE2  | 2.36                     | 0.60              |
| 22:r:103:LYS:HG2  | 22:r:105:LEU:CD1  | 2.32                     | 0.60              |
| 2:2:145:LEU:CD2   | 2:2:154:VAL:HG22  | 2.26                     | 0.60              |
| 5:B:47:PRO:HG3    | 5:B:78:TRP:CE2    | 2.36                     | 0.60              |
| 5:B:327:ALA:HB1   | 30:B:620:LMG:HC8  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:C:507:CLA:H142 | 28:I:101:BCR:H362 | 1.81                     | 0.60              |
| 9:F:21:ALA:HB1    | 38:F:101:HEM:HAC  | 1.84                     | 0.60              |
| 21:Y:172:VAL:HG21 | 40:Y:318:NEX:H34  | 1.84                     | 0.60              |
| 4:a:259:ILE:HG23  | 4:a:259:ILE:O     | 2.02                     | 0.60              |
| 7:d:157:VAL:HG12  | 7:d:172:PRO:HG2   | 1.84                     | 0.60              |
| 20:s:113:PHE:HE1  | 25:s:304:CLA:HBD  | 1.66                     | 0.60              |
| 21:y:231:VAL:CG1  | 25:y:314:CLA:HHD  | 2.31                     | 0.60              |
| 22:r:220:GLY:HA2  | 22:r:224:ASP:H    | 1.65                     | 0.60              |
| 2:2:179:ASN:ND2   | 2:2:188:ASN:O     | 2.35                     | 0.60              |
| 2:2:193:GLY:HA2   | 2:2:197:PHE:CD2   | 2.34                     | 0.60              |
| 3:4:84:ASP:OD2    | 3:4:87:GLY:HA2    | 2.02                     | 0.60              |
| 3:4:174:TRP:HE3   | 3:4:180:LYS:HD2   | 1.63                     | 0.60              |
| 29:A:411:SQD:H131 | 16:T:21:ILE:HD12  | 1.82                     | 0.60              |
| 6:C:215:LYS:CG    | 6:C:221:GLU:HB3   | 2.31                     | 0.60              |
| 6:C:225:VAL:HG22  | 6:C:289:PHE:CD1   | 2.37                     | 0.60              |
| 6:C:285:ILE:HG22  | 6:C:289:PHE:CZ    | 2.37                     | 0.60              |
| 15:O:143:PHE:CD2  | 17:W:81:VAL:HG11  | 2.36                     | 0.60              |
| 20:S:237:LEU:O    | 20:S:241:ILE:HD12 | 2.01                     | 0.60              |
| 24:G:606:CHL:CBA  | 40:G:617:NEX:H403 | 2.31                     | 0.60              |
| 22:R:144:GLY:O    | 22:R:148:MET:HG3  | 2.02                     | 0.60              |
| 22:R:253:PHE:CZ   | 41:R:616:XAT:H10  | 2.37                     | 0.60              |
| 2:6:179:ASN:ND2   | 2:6:188:ASN:O     | 2.35                     | 0.60              |
| 4:a:77:ILE:HD13   | 13:l:30:VAL:HG13  | 1.84                     | 0.60              |
| 4:a:219:VAL:HG13  | 4:a:246:TYR:CD1   | 2.36                     | 0.60              |
| 5:b:47:PRO:HG3    | 5:b:78:TRP:CE2    | 2.36                     | 0.60              |
| 5:b:388:SER:HA    | 7:d:345:GLU:CD    | 2.26                     | 0.60              |
| 21:g:100:VAL:HG21 | 21:g:190:LEU:HD13 | 1.84                     | 0.60              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:CHB  | 2.31                     | 0.60              |
| 21:n:169:MET:HG3  | 24:n:609:CHL:CMC  | 2.32                     | 0.60              |
| 22:r:178:SER:OG   | 22:r:183:PRO:HA   | 2.00                     | 0.60              |
| 1:1:138:ILE:HD11  | 24:1:302:CHL:HMD3 | 1.83                     | 0.60              |
| 1:3:100:VAL:HG21  | 1:3:190:LEU:HD13  | 1.84                     | 0.60              |
| 4:A:222:SER:OG    | 4:A:246:TYR:HB2   | 2.02                     | 0.60              |
| 4:A:248:ILE:HD13  | 4:A:268:SER:OG    | 2.02                     | 0.60              |
| 4:A:328:MET:HG2   | 7:D:326:ILE:CG1   | 2.31                     | 0.60              |
| 6:C:175:LEU:HD22  | 25:C:501:CLA:C3D  | 2.32                     | 0.60              |
| 19:Z:3:ILE:O      | 19:Z:7:LEU:HD23   | 2.02                     | 0.60              |
| 21:Y:151:SER:OG   | 22:r:185:PRO:HB3  | 2.01                     | 0.60              |
| 4:a:248:ILE:HD13  | 4:a:268:SER:OG    | 2.02                     | 0.60              |
| 6:c:87:ILE:HD13   | 25:c:504:CLA:HMB2 | 1.84                     | 0.60              |
| 6:c:91:HIS:O      | 6:c:95:LEU:HD13   | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:t:7:THR:HG21   | 28:t:101:BCR:H363 | 1.84                     | 0.60              |
| 2:2:111:PHE:O     | 2:2:115:THR:HG23  | 2.02                     | 0.60              |
| 4:A:235:GLU:OE1   | 7:D:264:ASN:ND2   | 2.35                     | 0.60              |
| 30:A:408:LMG:HC61 | 6:C:221:GLU:OE2   | 2.02                     | 0.60              |
| 5:B:333:GLY:O     | 5:B:441:GLY:N     | 2.34                     | 0.60              |
| 21:G:112:GLY:HA3  | 25:G:604:CLA:CHC  | 2.31                     | 0.60              |
| 21:N:67:PRO:CG    | 21:N:70:LEU:HD12  | 2.29                     | 0.60              |
| 24:N:606:CHL:HBC2 | 24:N:607:CHL:HHD  | 1.82                     | 0.60              |
| 25:N:613:CLA:HMC1 | 25:N:613:CLA:HBC3 | 1.83                     | 0.60              |
| 2:6:107:MET:HG2   | 2:6:111:PHE:HE2   | 1.67                     | 0.60              |
| 3:8:138:ALA:HB3   | 3:8:140:PHE:CD2   | 2.37                     | 0.60              |
| 6:c:215:LYS:CG    | 6:c:221:GLU:HB3   | 2.31                     | 0.60              |
| 22:r:144:GLY:O    | 22:r:148:MET:HG3  | 2.02                     | 0.60              |
| 23:u:84:ALA:HB1   | 23:u:100:ILE:CG2  | 2.31                     | 0.60              |
| 4:A:179:THR:HG21  | 25:A:402:CLA:CHD  | 2.32                     | 0.59              |
| 5:B:336:ILE:HG22  | 5:B:336:ILE:O     | 2.02                     | 0.59              |
| 6:C:327:ASN:HD22  | 6:C:330:SER:HB2   | 1.67                     | 0.59              |
| 24:N:609:CHL:HHC  | 24:N:609:CHL:HBB1 | 1.82                     | 0.59              |
| 25:N:610:CLA:CBB  | 25:N:612:CLA:H3A  | 2.32                     | 0.59              |
| 22:R:93:ASP:O     | 22:R:107:GLY:HA3  | 2.02                     | 0.59              |
| 22:R:150:ALA:HA   | 41:R:616:XAT:C18  | 2.32                     | 0.59              |
| 2:6:184:VAL:HB    | 2:6:196:TYR:CE2   | 2.33                     | 0.59              |
| 4:a:235:GLU:OE1   | 7:d:264:ASN:ND2   | 2.35                     | 0.59              |
| 30:a:409:LMG:HC61 | 6:c:221:GLU:OE2   | 2.02                     | 0.59              |
| 29:l:102:SQD:H312 | 14:m:17:VAL:HG13  | 1.84                     | 0.59              |
| 21:n:138:ILE:HD12 | 21:n:144:LEU:CD1  | 2.33                     | 0.59              |
| 25:n:610:CLA:CBB  | 25:n:612:CLA:H3A  | 2.32                     | 0.59              |
| 24:y:307:CHL:HMB2 | 24:y:310:CHL:OMC  | 2.01                     | 0.59              |
| 22:r:274:HIS:O    | 22:r:278:PRO:HA   | 2.01                     | 0.59              |
| 6:C:87:ILE:HD13   | 25:C:504:CLA:HMB2 | 1.84                     | 0.59              |
| 15:O:100:LYS:HE3  | 15:O:105:VAL:HG22 | 1.84                     | 0.59              |
| 25:N:602:CLA:HMC1 | 39:N:616:LUT:C31  | 2.32                     | 0.59              |
| 21:Y:111:LEU:HD23 | 25:Y:305:CLA:HMC2 | 1.84                     | 0.59              |
| 21:Y:138:ILE:HD13 | 24:Y:307:CHL:HBC3 | 1.83                     | 0.59              |
| 1:5:100:VAL:HG21  | 1:5:190:LEU:HD13  | 1.84                     | 0.59              |
| 2:6:214:VAL:HA    | 2:6:217:ILE:CD1   | 2.32                     | 0.59              |
| 4:a:45:THR:HG23   | 25:a:403:CLA:H201 | 1.84                     | 0.59              |
| 5:b:467:ILE:HG21  | 7:d:127:MET:CE    | 2.32                     | 0.59              |
| 25:b:607:CLA:H171 | 25:b:613:CLA:C16  | 2.23                     | 0.59              |
| 6:c:285:ILE:HG22  | 6:c:289:PHE:CZ    | 2.37                     | 0.59              |
| 6:c:327:ASN:HD22  | 6:c:330:SER:HB2   | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:c:511:CLA:H142 | 12:k:47:PHE:CE2   | 2.37                     | 0.59              |
| 25:c:512:CLA:H192 | 26:s:301:LHG:H222 | 1.84                     | 0.59              |
| 25:d:403:CLA:H162 | 18:x:92:SER:OG    | 2.01                     | 0.59              |
| 2:2:214:VAL:HA    | 2:2:217:ILE:CD1   | 2.32                     | 0.59              |
| 4:A:328:MET:CG    | 7:D:326:ILE:HG12  | 2.33                     | 0.59              |
| 6:C:91:HIS:O      | 6:C:95:LEU:HD13   | 2.02                     | 0.59              |
| 6:C:131:TYR:CE1   | 6:C:135:LEU:HD22  | 2.38                     | 0.59              |
| 7:D:157:VAL:HG12  | 7:D:172:PRO:HG2   | 1.84                     | 0.59              |
| 7:D:236:PHE:HD1   | 7:D:244:THR:HG21  | 1.66                     | 0.59              |
| 21:N:169:MET:HG3  | 24:N:609:CHL:CMC  | 2.32                     | 0.59              |
| 3:8:78:PRO:HB2    | 3:8:229:ILE:CG2   | 2.32                     | 0.59              |
| 7:d:56:VAL:O      | 7:d:67:SER:HB3    | 2.02                     | 0.59              |
| 11:i:34:ARG:O     | 11:i:35:GLU:HG3   | 2.01                     | 0.59              |
| 20:s:119:ARG:HH11 | 25:s:310:CLA:CHD  | 2.15                     | 0.59              |
| 20:s:218:GLY:O    | 20:s:222:LYS:HG3  | 2.00                     | 0.59              |
| 21:g:244:LEU:HD22 | 39:g:615:LUT:H163 | 1.84                     | 0.59              |
| 21:n:100:VAL:HG21 | 21:n:190:LEU:HD13 | 1.84                     | 0.59              |
| 25:n:603:CLA:H191 | 24:n:607:CHL:H122 | 1.84                     | 0.59              |
| 2:2:181:LEU:HD13  | 24:2:603:CHL:CAB  | 2.30                     | 0.59              |
| 1:3:229:PHE:CD2   | 1:3:240:PRO:HB3   | 2.38                     | 0.59              |
| 25:C:510:CLA:HHD  | 25:C:510:CLA:HBC3 | 1.84                     | 0.59              |
| 20:S:119:ARG:HH11 | 25:S:310:CLA:CHD  | 2.15                     | 0.59              |
| 21:G:244:LEU:HD22 | 39:G:615:LUT:H163 | 1.84                     | 0.59              |
| 2:6:127:PHE:O     | 2:6:128:LYS:HG3   | 2.03                     | 0.59              |
| 2:6:155:HIS:HE1   | 2:6:158:SER:HA    | 1.67                     | 0.59              |
| 5:b:241:SER:O     | 5:b:245:VAL:HG23  | 2.02                     | 0.59              |
| 5:b:272:ARG:HG3   | 5:b:320:ALA:HB2   | 1.83                     | 0.59              |
| 21:y:97:GLU:CG    | 21:y:190:LEU:HD21 | 2.20                     | 0.59              |
| 21:y:153:VAL:HG13 | 24:y:306:CHL:CHD  | 2.32                     | 0.59              |
| 22:r:150:ALA:HA   | 41:r:616:XAT:C18  | 2.32                     | 0.59              |
| 22:r:199:ILE:HA   | 22:r:202:ILE:HG12 | 1.83                     | 0.59              |
| 20:S:169:ILE:HG13 | 24:S:306:CHL:OBD  | 2.03                     | 0.59              |
| 20:S:223:VAL:O    | 20:S:226:ILE:HG22 | 2.03                     | 0.59              |
| 21:Y:67:PRO:CG    | 21:Y:70:LEU:HD12  | 2.29                     | 0.59              |
| 4:a:19:ASN:O      | 4:a:23:SER:HB2    | 2.03                     | 0.59              |
| 5:b:71:ILE:HD13   | 25:b:606:CLA:HED3 | 1.84                     | 0.59              |
| 25:n:603:CLA:H203 | 24:n:607:CHL:H193 | 1.84                     | 0.59              |
| 21:y:111:LEU:HD23 | 25:y:305:CLA:HMC2 | 1.84                     | 0.59              |
| 22:r:93:ASP:O     | 22:r:107:GLY:HA3  | 2.02                     | 0.59              |
| 22:r:253:PHE:CZ   | 41:r:616:XAT:H10  | 2.37                     | 0.59              |
| 1:1:229:PHE:CD2   | 1:1:240:PRO:HB3   | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:121:LYS:NZ    | 2:2:241:PRO:HB2   | 2.17                     | 0.59              |
| 3:4:78:PRO:HB2    | 3:4:229:ILE:CG2   | 2.32                     | 0.59              |
| 3:4:138:ALA:HB3   | 3:4:140:PHE:CD2   | 2.37                     | 0.59              |
| 4:A:331:MET:HE2   | 7:D:321:LEU:HB3   | 1.83                     | 0.59              |
| 5:B:241:SER:O     | 5:B:245:VAL:HG23  | 2.02                     | 0.59              |
| 5:B:388:SER:HA    | 7:D:345:GLU:CD    | 2.26                     | 0.59              |
| 6:C:227:VAL:HG21  | 28:I:101:BCR:H292 | 1.82                     | 0.59              |
| 6:C:449:ARG:HH12  | 11:I:28:PRO:CG    | 2.16                     | 0.59              |
| 25:C:511:CLA:H102 | 19:Z:24:PRO:HB3   | 1.83                     | 0.59              |
| 20:S:83:GLU:OE2   | 20:S:96:ASP:HB3   | 2.03                     | 0.59              |
| 25:N:603:CLA:H191 | 24:N:607:CHL:H122 | 1.84                     | 0.59              |
| 21:Y:100:VAL:HG21 | 21:Y:190:LEU:HD13 | 1.84                     | 0.59              |
| 4:a:222:SER:OG    | 4:a:246:TYR:HB2   | 2.02                     | 0.59              |
| 6:c:225:VAL:HG22  | 6:c:289:PHE:CD1   | 2.37                     | 0.59              |
| 15:o:158:PHE:CE2  | 15:o:322:LYS:HB2  | 2.36                     | 0.59              |
| 18:x:97:LEU:O     | 18:x:101:ILE:HG12 | 2.01                     | 0.59              |
| 25:y:304:CLA:H2A  | 25:y:304:CLA:O2A  | 1.99                     | 0.59              |
| 22:r:220:GLY:HA3  | 22:r:224:ASP:HB3  | 1.83                     | 0.59              |
| 2:2:121:LYS:HZ2   | 2:2:241:PRO:HB2   | 1.68                     | 0.59              |
| 2:2:127:PHE:O     | 2:2:128:LYS:HG3   | 2.03                     | 0.59              |
| 3:4:146:LEU:O     | 3:4:150:LEU:HG    | 2.03                     | 0.59              |
| 4:A:129:ARG:NH2   | 7:D:257:ILE:O     | 2.34                     | 0.59              |
| 4:A:158:PHE:O     | 4:A:162:PRO:HG2   | 2.03                     | 0.59              |
| 4:A:192:ILE:HD13  | 25:A:401:CLA:C1D  | 2.32                     | 0.59              |
| 25:C:511:CLA:H142 | 12:K:47:PHE:CE2   | 2.37                     | 0.59              |
| 15:O:158:PHE:CE2  | 15:O:322:LYS:HB2  | 2.36                     | 0.59              |
| 18:X:97:LEU:O     | 18:X:101:ILE:HG12 | 2.01                     | 0.59              |
| 20:S:141:CYS:C    | 20:S:143:PRO:HA   | 2.28                     | 0.59              |
| 21:G:67:PRO:CG    | 21:G:70:LEU:HD12  | 2.29                     | 0.59              |
| 21:Y:153:VAL:HG13 | 24:Y:306:CHL:CHD  | 2.32                     | 0.59              |
| 2:6:112:GLY:O     | 2:6:116:PRO:HD3   | 2.03                     | 0.59              |
| 1:7:229:PHE:CD2   | 1:7:240:PRO:HB3   | 2.38                     | 0.59              |
| 4:a:192:ILE:HD13  | 25:a:402:CLA:C1D  | 2.33                     | 0.59              |
| 6:c:175:LEU:HD22  | 25:c:501:CLA:C3D  | 2.32                     | 0.59              |
| 25:c:511:CLA:H102 | 19:z:24:PRO:HB3   | 1.83                     | 0.59              |
| 20:s:141:CYS:C    | 20:s:143:PRO:HA   | 2.28                     | 0.59              |
| 20:s:169:ILE:HG13 | 24:s:306:CHL:OBD  | 2.03                     | 0.59              |
| 20:s:223:VAL:O    | 20:s:226:ILE:HG22 | 2.03                     | 0.59              |
| 22:r:240:LEU:O    | 22:r:243:ILE:HG22 | 2.03                     | 0.59              |
| 3:4:221:LEU:HA    | 3:4:224:LEU:HD21  | 1.82                     | 0.59              |
| 4:A:127:MET:HG3   | 4:A:144:ALA:HB1   | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:C:28:GLN:OE1    | 7:D:231:ASN:ND2   | 2.35                     | 0.59              |
| 6:C:66:ALA:N      | 6:C:119:LEU:HD21  | 2.18                     | 0.59              |
| 6:C:154:ARG:HB3   | 6:C:256:PRO:HG2   | 1.85                     | 0.59              |
| 6:C:369:LEU:CD2   | 6:C:380:LEU:HD23  | 2.33                     | 0.59              |
| 28:T:101:BCR:H292 | 28:T:101:BCR:C36  | 2.29                     | 0.59              |
| 21:Y:104:ARG:HD3  | 25:Y:311:CLA:CHD  | 2.33                     | 0.59              |
| 22:R:240:LEU:O    | 22:R:243:ILE:HG22 | 2.03                     | 0.59              |
| 3:8:146:LEU:O     | 3:8:150:LEU:HG    | 2.03                     | 0.59              |
| 5:b:41:GLU:OE1    | 5:b:63:ILE:HG13   | 2.03                     | 0.59              |
| 6:c:154:ARG:HB3   | 6:c:256:PRO:HG2   | 1.85                     | 0.59              |
| 25:c:511:CLA:C16  | 19:z:20:LEU:HD12  | 2.31                     | 0.59              |
| 20:s:83:GLU:OE2   | 20:s:96:ASP:HB3   | 2.03                     | 0.59              |
| 24:s:307:CHL:HBC3 | 24:s:307:CHL:HMC  | 1.85                     | 0.59              |
| 25:y:311:CLA:HMC1 | 39:y:316:LUT:C31  | 2.33                     | 0.59              |
| 2:2:184:VAL:HB    | 2:2:196:TYR:CE2   | 2.33                     | 0.59              |
| 7:D:153:VAL:HG21  | 7:D:280:LEU:HD22  | 1.85                     | 0.59              |
| 25:N:613:CLA:HMC1 | 25:N:613:CLA:CBC  | 2.32                     | 0.59              |
| 25:Y:303:CLA:HBB1 | 25:Y:303:CLA:HMB3 | 1.83                     | 0.59              |
| 25:Y:311:CLA:HMC1 | 39:Y:316:LUT:C31  | 2.33                     | 0.59              |
| 2:6:121:LYS:NZ    | 2:6:241:PRO:HB2   | 2.17                     | 0.59              |
| 2:6:127:PHE:HB3   | 2:6:140:PHE:CD2   | 2.38                     | 0.59              |
| 2:6:145:LEU:CD2   | 2:6:154:VAL:HG22  | 2.26                     | 0.59              |
| 2:6:193:GLY:HA2   | 2:6:197:PHE:CD2   | 2.34                     | 0.59              |
| 6:c:28:GLN:OE1    | 7:d:231:ASN:ND2   | 2.35                     | 0.59              |
| 6:c:272:LEU:CD2   | 25:c:508:CLA:HHB  | 2.33                     | 0.59              |
| 8:e:27:ILE:HG23   | 8:e:28:PRO:CD     | 2.32                     | 0.59              |
| 9:f:21:ALA:HB1    | 38:f:101:HEM:HAC  | 1.84                     | 0.59              |
| 21:g:146:TYR:HE2  | 25:g:604:CLA:H2   | 1.65                     | 0.59              |
| 21:n:229:PHE:CD2  | 21:n:240:PRO:HB3  | 2.38                     | 0.59              |
| 4:A:19:ASN:O      | 4:A:23:SER:HB2    | 2.03                     | 0.59              |
| 25:B:601:CLA:C1B  | 25:B:602:CLA:HBB2 | 2.32                     | 0.59              |
| 7:D:56:VAL:O      | 7:D:67:SER:HB3    | 2.02                     | 0.59              |
| 20:S:146:VAL:HG11 | 20:S:149:LYS:NZ   | 2.17                     | 0.59              |
| 21:N:98:LEU:HD22  | 25:N:603:CLA:HAA2 | 1.85                     | 0.59              |
| 21:N:111:LEU:HD23 | 25:N:604:CLA:HMC2 | 1.85                     | 0.59              |
| 3:8:125:VAL:HB    | 3:8:127:TRP:CD1   | 2.38                     | 0.59              |
| 4:a:133:LEU:CD2   | 7:d:257:ILE:HG12  | 2.33                     | 0.59              |
| 4:a:202:VAL:HG22  | 25:a:402:CLA:CHB  | 2.32                     | 0.59              |
| 5:b:357:ARG:CZ    | 23:u:96:PRO:HD2   | 2.33                     | 0.59              |
| 21:n:67:PRO:CG    | 21:n:70:LEU:HD12  | 2.29                     | 0.59              |
| 21:n:221:LEU:HD12 | 26:n:618:LHG:H272 | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:178:ALA:HA    | 2:2:64:VAL:CG2    | 2.07                     | 0.58              |
| 4:A:149:ALA:HB3   | 4:A:150:PRO:HD3   | 1.85                     | 0.58              |
| 26:B:625:LHG:HC5  | 7:D:270:PHE:HZ    | 1.68                     | 0.58              |
| 7:D:280:LEU:HD21  | 25:D:402:CLA:HBA2 | 1.83                     | 0.58              |
| 8:E:27:ILE:HG23   | 8:E:28:PRO:CD     | 2.32                     | 0.58              |
| 15:O:92:LEU:HA    | 15:O:96:GLU:OE2   | 2.04                     | 0.58              |
| 21:G:226:MET:HG2  | 39:G:616:LUT:H12  | 1.85                     | 0.58              |
| 22:R:91:GLN:NE2   | 22:R:113:ARG:HD2  | 2.18                     | 0.58              |
| 24:R:605:CHL:HBB1 | 41:R:616:XAT:H162 | 1.85                     | 0.58              |
| 4:a:224:ILE:HD13  | 5:b:482:ILE:CG1   | 2.32                     | 0.58              |
| 5:b:191:ASP:OD1   | 10:h:70:ILE:HD13  | 2.03                     | 0.58              |
| 25:b:601:CLA:C1B  | 25:b:602:CLA:HBB2 | 2.32                     | 0.58              |
| 25:c:510:CLA:HBC3 | 25:c:510:CLA:HHD  | 1.85                     | 0.58              |
| 25:n:613:CLA:HMC3 | 25:n:613:CLA:CBC  | 2.33                     | 0.58              |
| 4:A:133:LEU:CD2   | 7:D:257:ILE:HG12  | 2.33                     | 0.58              |
| 4:A:329:GLU:HA    | 4:A:332:HIS:CD2   | 2.38                     | 0.58              |
| 5:B:357:ARG:CZ    | 23:U:96:PRO:HD2   | 2.33                     | 0.58              |
| 5:B:451:PHE:CE2   | 25:B:604:CLA:HMA3 | 2.36                     | 0.58              |
| 5:B:467:ILE:HG21  | 7:D:127:MET:CE    | 2.32                     | 0.58              |
| 6:C:67:MET:HE3    | 6:C:71:GLU:HG3    | 1.84                     | 0.58              |
| 11:I:24:LEU:CD1   | 28:I:101:BCR:HC41 | 2.33                     | 0.58              |
| 25:G:614:CLA:HAA1 | 25:G:614:CLA:CBD  | 2.33                     | 0.58              |
| 21:Y:138:ILE:HD12 | 21:Y:144:LEU:CD1  | 2.32                     | 0.58              |
| 3:8:157:GLU:HG3   | 3:8:161:TRP:HE1   | 1.66                     | 0.58              |
| 3:8:177:PRO:HD2   | 3:8:178:TRP:CZ3   | 2.38                     | 0.58              |
| 4:a:131:TRP:HZ2   | 6:c:449:ARG:HD2   | 1.67                     | 0.58              |
| 4:a:179:THR:HG21  | 25:a:403:CLA:CHD  | 2.32                     | 0.58              |
| 6:c:66:ALA:N      | 6:c:119:LEU:HD21  | 2.18                     | 0.58              |
| 6:c:308:GLU:HA    | 6:c:361:LEU:CD2   | 2.34                     | 0.58              |
| 20:s:146:VAL:HG11 | 20:s:149:LYS:NZ   | 2.17                     | 0.58              |
| 21:g:62:PHE:CZ    | 21:y:175:TYR:HE1  | 2.21                     | 0.58              |
| 21:n:97:GLU:CG    | 21:n:190:LEU:HD21 | 2.20                     | 0.58              |
| 21:n:138:ILE:HD13 | 24:n:606:CHL:CBC  | 2.33                     | 0.58              |
| 21:y:104:ARG:HD3  | 25:y:311:CLA:CHD  | 2.33                     | 0.58              |
| 25:y:303:CLA:HBB1 | 25:y:303:CLA:HMB3 | 1.83                     | 0.58              |
| 1:1:100:VAL:HG21  | 1:1:190:LEU:HD13  | 1.84                     | 0.58              |
| 3:4:147:GLY:O     | 3:4:151:LEU:HD23  | 2.03                     | 0.58              |
| 4:A:77:ILE:HD13   | 13:L:30:VAL:HG13  | 1.84                     | 0.58              |
| 5:B:191:ASP:OD1   | 10:H:70:ILE:HD13  | 2.03                     | 0.58              |
| 6:C:289:PHE:CD2   | 25:C:501:CLA:H12  | 2.39                     | 0.58              |
| 15:O:306:LEU:HD21 | 15:O:322:LYS:CE   | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:S:190:ILE:HG13 | 20:S:191:THR:N    | 2.19                     | 0.58              |
| 21:G:62:PHE:CZ    | 21:Y:175:TYR:HE1  | 2.21                     | 0.58              |
| 21:G:78:TYR:OH    | 21:G:217:LYS:NZ   | 2.20                     | 0.58              |
| 21:G:229:PHE:CD2  | 21:G:240:PRO:HB3  | 2.38                     | 0.58              |
| 25:G:610:CLA:HMC1 | 39:G:615:LUT:C32  | 2.33                     | 0.58              |
| 21:N:221:LEU:HD12 | 26:N:618:LHG:H272 | 1.85                     | 0.58              |
| 21:N:232:GLN:NE2  | 25:N:613:CLA:C4D  | 2.40                     | 0.58              |
| 22:R:274:HIS:ND1  | 25:R:612:CLA:HAA2 | 2.18                     | 0.58              |
| 4:a:158:PHE:O     | 4:a:162:PRO:HG2   | 2.03                     | 0.58              |
| 25:a:403:CLA:C1B  | 27:a:404:PHO:H192 | 2.34                     | 0.58              |
| 5:b:244:ALA:CB    | 25:b:610:CLA:HMA1 | 2.33                     | 0.58              |
| 21:n:231:VAL:HG21 | 25:n:613:CLA:CAC  | 2.30                     | 0.58              |
| 22:r:85:LYS:CG    | 22:r:86:PRO:HD2   | 2.31                     | 0.58              |
| 2:2:112:GLY:O     | 2:2:116:PRO:HD3   | 2.03                     | 0.58              |
| 5:B:41:GLU:OE1    | 5:B:63:ILE:HG13   | 2.03                     | 0.58              |
| 6:C:272:LEU:CD2   | 25:C:508:CLA:HHB  | 2.33                     | 0.58              |
| 6:C:308:GLU:HA    | 6:C:361:LEU:CD2   | 2.34                     | 0.58              |
| 7:D:190:HIS:HA    | 7:D:295:ARG:HD3   | 1.86                     | 0.58              |
| 21:N:97:GLU:CG    | 21:N:190:LEU:HD21 | 2.20                     | 0.58              |
| 2:6:111:PHE:O     | 2:6:115:THR:HG23  | 2.02                     | 0.58              |
| 1:7:138:ILE:HD12  | 1:7:144:LEU:CD1   | 2.33                     | 0.58              |
| 26:b:625:LHG:HC5  | 7:d:270:PHE:HZ    | 1.68                     | 0.58              |
| 6:c:272:LEU:HD21  | 25:c:508:CLA:C1B  | 2.34                     | 0.58              |
| 25:c:506:CLA:H52  | 26:c:517:LHG:H261 | 1.86                     | 0.58              |
| 25:c:512:CLA:HMA2 | 25:c:513:CLA:H203 | 1.85                     | 0.58              |
| 19:z:3:ILE:O      | 19:z:7:LEU:HD23   | 2.02                     | 0.58              |
| 25:g:610:CLA:HMC1 | 39:g:615:LUT:C32  | 2.33                     | 0.58              |
| 21:n:98:LEU:HD22  | 25:n:603:CLA:HAA2 | 1.85                     | 0.58              |
| 21:y:172:VAL:HG21 | 40:y:318:NEX:H34  | 1.84                     | 0.58              |
| 21:y:229:PHE:CD2  | 21:y:240:PRO:HB3  | 2.38                     | 0.58              |
| 1:3:138:ILE:HD12  | 1:3:144:LEU:CD1   | 2.33                     | 0.58              |
| 3:4:78:PRO:HB2    | 3:4:229:ILE:HG21  | 1.86                     | 0.58              |
| 4:A:224:ILE:HD13  | 5:B:482:ILE:CG1   | 2.32                     | 0.58              |
| 4:A:283:ILE:O     | 4:A:286:THR:HG22  | 2.03                     | 0.58              |
| 6:C:457:LYS:HE2   | 7:D:230:ALA:CA    | 2.34                     | 0.58              |
| 25:C:511:CLA:C16  | 19:Z:20:LEU:HD12  | 2.31                     | 0.58              |
| 29:L:101:SQD:H312 | 14:M:17:VAL:HG13  | 1.84                     | 0.58              |
| 15:O:190:GLU:OE1  | 15:O:215:VAL:HG13 | 2.04                     | 0.58              |
| 20:S:266:LEU:HD13 | 25:S:313:CLA:CMD  | 2.34                     | 0.58              |
| 21:G:100:VAL:HG21 | 21:G:190:LEU:HD13 | 1.84                     | 0.58              |
| 21:Y:122:ASN:CB   | 32:Y:320:AJP:C80  | 2.79                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:89:GLY:HA3    | 3:8:95:LEU:HD21   | 1.85                     | 0.58              |
| 3:8:147:GLY:O     | 3:8:151:LEU:HD23  | 2.03                     | 0.58              |
| 13:l:3:GLN:HG3    | 13:l:4:SER:H      | 1.68                     | 0.58              |
| 21:y:100:VAL:HG21 | 21:y:190:LEU:HD13 | 1.84                     | 0.58              |
| 25:y:304:CLA:HAB  | 39:y:317:LUT:C35  | 2.33                     | 0.58              |
| 22:r:91:GLN:NE2   | 22:r:113:ARG:HD2  | 2.18                     | 0.58              |
| 3:4:125:VAL:HB    | 3:4:127:TRP:CD1   | 2.38                     | 0.58              |
| 6:C:272:LEU:HD21  | 25:C:508:CLA:C1B  | 2.34                     | 0.58              |
| 25:C:512:CLA:HMA2 | 25:C:513:CLA:H203 | 1.85                     | 0.58              |
| 10:H:59:GLU:OE1   | 18:X:84:LYS:HD2   | 2.04                     | 0.58              |
| 2:6:105:TRP:CD1   | 24:6:603:CHL:HED1 | 2.39                     | 0.58              |
| 5:b:346:PHE:O     | 5:b:354:LEU:N     | 2.32                     | 0.58              |
| 7:d:30:PHE:O      | 7:d:129:ARG:NH1   | 2.33                     | 0.58              |
| 15:o:100:LYS:HE3  | 15:o:105:VAL:HG22 | 1.84                     | 0.58              |
| 15:o:190:GLU:OE1  | 15:o:215:VAL:HG13 | 2.04                     | 0.58              |
| 21:g:107:MET:HE3  | 25:g:610:CLA:HMC2 | 1.86                     | 0.58              |
| 21:g:115:PHE:CD2  | 25:g:604:CLA:HHD  | 2.38                     | 0.58              |
| 25:n:602:CLA:HMC1 | 39:n:616:LUT:C31  | 2.32                     | 0.58              |
| 21:y:138:ILE:HD12 | 21:y:144:LEU:CD1  | 2.33                     | 0.58              |
| 2:2:145:LEU:HD13  | 2:2:150:ASN:N     | 2.19                     | 0.58              |
| 4:A:131:TRP:HZ2   | 6:C:449:ARG:HD2   | 1.67                     | 0.58              |
| 25:A:402:CLA:C1B  | 27:A:403:PHO:H192 | 2.34                     | 0.58              |
| 5:B:464:PHE:HB2   | 7:D:281:TRP:CZ2   | 2.38                     | 0.58              |
| 25:D:403:CLA:H52  | 18:X:91:ALA:HB3   | 1.84                     | 0.58              |
| 21:N:100:VAL:HG21 | 21:N:190:LEU:HD13 | 1.84                     | 0.58              |
| 25:N:603:CLA:H191 | 24:N:607:CHL:C12  | 2.34                     | 0.58              |
| 2:6:104:ARG:NH2   | 24:6:603:CHL:HBD  | 2.19                     | 0.58              |
| 2:6:129:GLU:HB2   | 2:6:239:LYS:HE2   | 1.86                     | 0.58              |
| 1:7:100:VAL:HG21  | 1:7:190:LEU:HD13  | 1.84                     | 0.58              |
| 5:b:464:PHE:HB2   | 7:d:281:TRP:CZ2   | 2.38                     | 0.58              |
| 25:b:607:CLA:H151 | 26:b:625:LHG:C19  | 2.33                     | 0.58              |
| 25:b:608:CLA:HAB  | 7:d:124:ILE:HG12  | 1.85                     | 0.58              |
| 6:c:67:MET:HE3    | 6:c:71:GLU:HG3    | 1.84                     | 0.58              |
| 7:d:153:VAL:HG21  | 7:d:280:LEU:HD22  | 1.85                     | 0.58              |
| 7:d:173:SER:HB2   | 7:d:178:ALA:CB    | 2.28                     | 0.58              |
| 10:h:22:LEU:HG    | 22:r:124:PHE:HE2  | 1.69                     | 0.58              |
| 20:s:130:ILE:HD12 | 25:s:305:CLA:HAC1 | 1.86                     | 0.58              |
| 21:g:229:PHE:CD2  | 21:g:240:PRO:HB3  | 2.38                     | 0.58              |
| 25:n:610:CLA:H52  | 39:n:615:LUT:C28  | 2.32                     | 0.58              |
| 21:y:103:SER:HB2  | 21:y:219:GLY:CA   | 2.34                     | 0.58              |
| 22:r:274:HIS:ND1  | 25:r:612:CLA:HAA2 | 2.18                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:155:HIS:HE1   | 2:2:158:SER:HA    | 1.67                     | 0.58              |
| 1:3:67:PRO:CG     | 1:3:70:LEU:HD12   | 2.29                     | 0.58              |
| 5:B:477:ASP:HA    | 22:R:104:ASN:O    | 2.04                     | 0.58              |
| 29:L:101:SQD:H282 | 29:L:101:SQD:H121 | 1.86                     | 0.58              |
| 21:N:165:GLN:HE21 | 24:N:607:CHL:HMC  | 1.69                     | 0.58              |
| 25:Y:304:CLA:HAB  | 39:Y:317:LUT:C35  | 2.33                     | 0.58              |
| 4:a:232:SER:HG    | 5:b:7:ARG:HD2     | 1.69                     | 0.58              |
| 4:a:331:MET:HE2   | 7:d:321:LEU:HB3   | 1.83                     | 0.58              |
| 6:c:131:TYR:CE1   | 6:c:135:LEU:HD22  | 2.38                     | 0.58              |
| 25:d:403:CLA:H52  | 18:x:91:ALA:HB3   | 1.84                     | 0.58              |
| 21:g:138:ILE:HD12 | 21:g:144:LEU:CD1  | 2.33                     | 0.58              |
| 22:r:158:GLU:CB   | 22:r:268:LEU:HD12 | 2.31                     | 0.58              |
| 4:A:45:THR:HG23   | 25:A:402:CLA:H201 | 1.84                     | 0.58              |
| 4:A:202:VAL:HG22  | 25:A:401:CLA:CHB  | 2.32                     | 0.58              |
| 29:A:407:SQD:H151 | 26:C:519:LHG:H342 | 1.86                     | 0.58              |
| 5:B:155:ALA:O     | 5:B:159:THR:OG1   | 2.19                     | 0.58              |
| 25:B:607:CLA:H151 | 26:B:625:LHG:C19  | 2.33                     | 0.58              |
| 25:B:612:CLA:H171 | 25:B:613:CLA:HBB2 | 1.86                     | 0.58              |
| 35:B:626:DGD:O5D  | 35:B:626:DGD:O4D  | 2.18                     | 0.58              |
| 7:D:181:ARG:HD2   | 7:D:334:ASP:OD1   | 2.04                     | 0.58              |
| 14:M:24:ILE:HG23  | 14:m:27:VAL:HG21  | 1.86                     | 0.58              |
| 15:O:130:LYS:CE   | 15:O:177:PRO:HB2  | 2.25                     | 0.58              |
| 21:G:115:PHE:CD2  | 25:G:604:CLA:HHD  | 2.38                     | 0.58              |
| 22:R:158:GLU:CB   | 22:R:268:LEU:HD12 | 2.31                     | 0.58              |
| 2:6:145:LEU:HD13  | 2:6:150:ASN:N     | 2.19                     | 0.58              |
| 4:a:140:ARG:NH1   | 26:c:519:LHG:O5   | 2.33                     | 0.58              |
| 5:b:75:TRP:CD1    | 5:b:92:SER:HG     | 2.21                     | 0.58              |
| 7:d:190:HIS:HA    | 7:d:295:ARG:HD3   | 1.86                     | 0.58              |
| 9:f:13:ARG:O      | 9:f:17:VAL:HG22   | 2.03                     | 0.58              |
| 21:g:139:PHE:HD2  | 24:g:607:CHL:OBD  | 1.87                     | 0.58              |
| 3:4:177:PRO:HD2   | 3:4:178:TRP:CZ3   | 2.38                     | 0.58              |
| 4:A:139:MET:HE3   | 7:D:222:THR:HG23  | 1.86                     | 0.58              |
| 21:Y:103:SER:HB2  | 21:Y:219:GLY:CA   | 2.34                     | 0.58              |
| 21:Y:229:PHE:CD2  | 21:Y:240:PRO:HB3  | 2.38                     | 0.58              |
| 1:5:229:PHE:CD2   | 1:5:240:PRO:HB3   | 2.38                     | 0.58              |
| 2:6:107:MET:HG2   | 2:6:111:PHE:CE2   | 2.39                     | 0.58              |
| 3:8:156:VAL:HG22  | 3:8:160:ARG:HE    | 1.69                     | 0.58              |
| 4:a:329:GLU:HA    | 4:a:332:HIS:CD2   | 2.38                     | 0.58              |
| 25:b:615:CLA:C19  | 25:b:616:CLA:HBC3 | 2.33                     | 0.58              |
| 6:c:369:LEU:CD2   | 6:c:380:LEU:HD23  | 2.33                     | 0.58              |
| 7:d:350:GLY:O     | 7:d:353:LEU:HD23  | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:i:24:LEU:CD1   | 28:i:101:BCR:HC41 | 2.33                     | 0.58              |
| 15:o:117:ILE:HG12 | 15:o:300:ILE:HG21 | 1.85                     | 0.58              |
| 20:s:63:TYR:HE2   | 20:s:219:ALA:HB1  | 1.66                     | 0.58              |
| 20:s:266:LEU:HD13 | 25:s:313:CLA:CMD  | 2.34                     | 0.58              |
| 21:n:78:TYR:OH    | 21:n:217:LYS:NZ   | 2.20                     | 0.58              |
| 25:r:603:CLA:HMD1 | 25:r:608:CLA:C1   | 2.34                     | 0.58              |
| 1:3:81:ASP:OD2    | 1:3:84:GLY:HA2    | 2.04                     | 0.57              |
| 1:3:133:LYS:O     | 1:3:136:SER:OG    | 2.20                     | 0.57              |
| 25:B:608:CLA:HAB  | 7:D:124:ILE:HG12  | 1.85                     | 0.57              |
| 25:D:403:CLA:H18  | 18:X:92:SER:HB3   | 1.86                     | 0.57              |
| 15:O:117:ILE:HG12 | 15:O:300:ILE:HG21 | 1.85                     | 0.57              |
| 25:S:304:CLA:HMC2 | 39:S:316:LUT:C12  | 2.34                     | 0.57              |
| 21:G:97:GLU:CG    | 21:G:190:LEU:HD21 | 2.20                     | 0.57              |
| 21:N:229:PHE:CD2  | 21:N:240:PRO:HB3  | 2.38                     | 0.57              |
| 1:7:164:THR:CG2   | 1:7:168:LEU:HD12  | 2.34                     | 0.57              |
| 25:a:406:CLA:HMC1 | 11:i:11:VAL:CG1   | 2.30                     | 0.57              |
| 6:c:291:TRP:O     | 6:c:305:THR:HG23  | 2.04                     | 0.57              |
| 25:c:508:CLA:HAB  | 25:c:510:CLA:H3A  | 1.86                     | 0.57              |
| 29:l:102:SQD:H282 | 29:l:102:SQD:H121 | 1.86                     | 0.57              |
| 20:s:111:GLN:HA   | 25:s:303:CLA:HMA1 | 1.86                     | 0.57              |
| 20:s:190:ILE:HG13 | 20:s:191:THR:N    | 2.19                     | 0.57              |
| 24:s:306:CHL:HHC  | 24:s:306:CHL:HBB1 | 1.86                     | 0.57              |
| 21:g:82:THR:O     | 21:y:94:ARG:HG3   | 2.04                     | 0.57              |
| 21:g:98:LEU:CD2   | 25:g:603:CLA:CAA  | 2.78                     | 0.57              |
| 1:1:81:ASP:OD2    | 1:1:84:GLY:HA2    | 2.05                     | 0.57              |
| 1:1:97:GLU:CG     | 1:1:190:LEU:HD21  | 2.20                     | 0.57              |
| 1:1:152:LEU:HD23  | 24:1:301:CHL:HED3 | 1.86                     | 0.57              |
| 2:2:127:PHE:CD2   | 2:2:148:LEU:HD23  | 2.39                     | 0.57              |
| 1:3:164:THR:CG2   | 1:3:168:LEU:HD12  | 2.34                     | 0.57              |
| 3:4:156:VAL:HG22  | 3:4:160:ARG:HE    | 1.69                     | 0.57              |
| 5:B:222:PRO:HB3   | 10:H:38:GLY:H     | 1.69                     | 0.57              |
| 25:C:506:CLA:H52  | 26:C:517:LHG:H261 | 1.86                     | 0.57              |
| 25:C:508:CLA:HAB  | 25:C:510:CLA:H3A  | 1.86                     | 0.57              |
| 7:D:237:ASN:OD1   | 7:D:238:PRO:HD2   | 2.05                     | 0.57              |
| 9:F:13:ARG:O      | 9:F:17:VAL:HG22   | 2.03                     | 0.57              |
| 24:S:307:CHL:HBC3 | 24:S:307:CHL:HMC  | 1.85                     | 0.57              |
| 21:G:62:PHE:O     | 21:Y:178:ALA:HB2  | 2.04                     | 0.57              |
| 21:N:182:PRO:HG3  | 40:N:617:NEX:H161 | 1.86                     | 0.57              |
| 21:Y:164:THR:CG2  | 21:Y:168:LEU:HD12 | 2.34                     | 0.57              |
| 22:R:207:ASN:OD1  | 22:R:215:ARG:NH2  | 2.37                     | 0.57              |
| 25:6:604:CLA:HBC3 | 26:6:606:LHG:C38  | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:a:127:MET:HG3   | 4:a:144:ALA:HB1   | 1.85                     | 0.57              |
| 5:b:281:GLN:OE1   | 23:u:91:VAL:HG13  | 2.04                     | 0.57              |
| 6:c:319:VAL:O     | 6:c:322:GLN:HG2   | 2.04                     | 0.57              |
| 25:d:403:CLA:H18  | 18:x:92:SER:HB3   | 1.86                     | 0.57              |
| 1:1:133:LYS:O     | 1:1:136:SER:OG    | 2.20                     | 0.57              |
| 2:2:121:LYS:HD3   | 2:2:245:LEU:HD12  | 1.87                     | 0.57              |
| 3:4:131:GLY:O     | 3:4:134:PRO:HD2   | 2.04                     | 0.57              |
| 4:A:283:ILE:HA    | 4:A:286:THR:HG22  | 1.86                     | 0.57              |
| 30:A:410:LMG:H301 | 35:A:415:DGD:HB22 | 1.87                     | 0.57              |
| 6:C:237:HIS:HD2   | 28:I:101:BCR:H272 | 1.69                     | 0.57              |
| 6:C:319:VAL:O     | 6:C:322:GLN:HG2   | 2.04                     | 0.57              |
| 16:T:11:VAL:HG13  | 28:T:101:BCR:H331 | 1.86                     | 0.57              |
| 21:G:164:THR:CG2  | 21:G:168:LEU:HD12 | 2.34                     | 0.57              |
| 21:N:228:GLY:O    | 21:N:232:GLN:OE1  | 2.23                     | 0.57              |
| 21:Y:228:GLY:O    | 21:Y:232:GLN:OE1  | 2.23                     | 0.57              |
| 22:R:283:ILE:HA   | 25:R:612:CLA:CAD  | 2.34                     | 0.57              |
| 1:7:103:SER:HB2   | 1:7:219:GLY:CA    | 2.34                     | 0.57              |
| 5:b:336:ILE:HG22  | 5:b:336:ILE:O     | 2.02                     | 0.57              |
| 6:c:289:PHE:CD2   | 25:c:501:CLA:H12  | 2.39                     | 0.57              |
| 13:l:26:PHE:O     | 13:l:30:VAL:HG23  | 2.05                     | 0.57              |
| 21:g:62:PHE:O     | 21:y:178:ALA:HB2  | 2.04                     | 0.57              |
| 25:n:603:CLA:H191 | 24:n:607:CHL:C12  | 2.34                     | 0.57              |
| 22:r:207:ASN:OD1  | 22:r:215:ARG:NH2  | 2.37                     | 0.57              |
| 24:r:605:CHL:HBB1 | 41:r:616:XAT:H162 | 1.85                     | 0.57              |
| 1:1:164:THR:CG2   | 1:1:168:LEU:HD12  | 2.34                     | 0.57              |
| 1:1:228:GLY:O     | 1:1:232:GLN:OE1   | 2.23                     | 0.57              |
| 2:2:129:GLU:HB2   | 2:2:239:LYS:HE2   | 1.86                     | 0.57              |
| 5:B:281:GLN:OE1   | 23:U:91:VAL:HG13  | 2.04                     | 0.57              |
| 6:C:363:ALA:O     | 6:C:367:GLU:HG2   | 2.04                     | 0.57              |
| 7:D:236:PHE:CD1   | 7:D:244:THR:HG21  | 2.38                     | 0.57              |
| 9:F:13:ARG:NE     | 38:F:101:HEM:O2D  | 2.32                     | 0.57              |
| 14:M:28:LYS:HB2   | 14:m:27:VAL:HG11  | 1.87                     | 0.57              |
| 21:N:81:ASP:OD2   | 21:N:84:GLY:HA2   | 2.04                     | 0.57              |
| 21:N:138:ILE:HD12 | 21:N:144:LEU:CD1  | 2.33                     | 0.57              |
| 40:Y:318:NEX:H361 | 40:Y:318:NEX:C28  | 2.25                     | 0.57              |
| 25:R:610:CLA:C2B  | 26:R:618:LHG:HC2  | 2.34                     | 0.57              |
| 23:U:81:THR:OG1   | 23:U:103:TYR:O    | 2.23                     | 0.57              |
| 1:5:103:SER:HB2   | 1:5:219:GLY:CA    | 2.34                     | 0.57              |
| 1:7:81:ASP:OD2    | 1:7:84:GLY:HA2    | 2.05                     | 0.57              |
| 4:a:149:ALA:HB3   | 4:a:150:PRO:HD3   | 1.85                     | 0.57              |
| 4:a:328:MET:CG    | 7:d:326:ILE:HG12  | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:222:PRO:HB3   | 10:h:38:GLY:H     | 1.70                     | 0.57              |
| 5:b:477:ASP:HA    | 22:r:104:ASN:O    | 2.04                     | 0.57              |
| 25:b:612:CLA:H171 | 25:b:613:CLA:HBB2 | 1.86                     | 0.57              |
| 7:d:247:MET:HE3   | 31:d:405:PL9:H522 | 1.85                     | 0.57              |
| 10:h:29:GLU:HA    | 22:r:113:ARG:HH12 | 1.69                     | 0.57              |
| 10:h:59:GLU:OE1   | 18:x:84:LYS:HD2   | 2.04                     | 0.57              |
| 21:n:94:ARG:HG2   | 21:y:84:GLY:HA3   | 1.86                     | 0.57              |
| 21:y:81:ASP:OD2   | 21:y:84:GLY:HA2   | 2.05                     | 0.57              |
| 21:y:228:GLY:O    | 21:y:232:GLN:OE1  | 2.23                     | 0.57              |
| 2:2:127:PHE:HB3   | 2:2:140:PHE:CD2   | 2.38                     | 0.57              |
| 25:2:604:CLA:HBC3 | 26:2:606:LHG:C38  | 2.35                     | 0.57              |
| 6:C:199:ILE:CG2   | 6:C:231:GLU:HG3   | 2.35                     | 0.57              |
| 10:H:29:GLU:HA    | 22:R:113:ARG:HH12 | 1.69                     | 0.57              |
| 12:K:58:VAL:O     | 12:K:61:ARG:HG3   | 2.04                     | 0.57              |
| 18:X:96:VAL:O     | 18:X:100:ILE:HG12 | 2.05                     | 0.57              |
| 21:G:228:GLY:O    | 21:G:232:GLN:OE1  | 2.23                     | 0.57              |
| 21:N:164:THR:CG2  | 21:N:168:LEU:HD12 | 2.34                     | 0.57              |
| 21:Y:132:PHE:CB   | 24:Y:308:CHL:HMA3 | 2.34                     | 0.57              |
| 22:R:93:ASP:OD1   | 22:R:110:ILE:HD11 | 2.05                     | 0.57              |
| 1:5:164:THR:CG2   | 1:5:168:LEU:HD12  | 2.34                     | 0.57              |
| 2:6:121:LYS:HD3   | 2:6:245:LEU:HD12  | 1.87                     | 0.57              |
| 4:a:84:PRO:HA     | 4:a:112:TYR:CG    | 2.39                     | 0.57              |
| 4:a:283:ILE:HA    | 4:a:286:THR:HG22  | 1.86                     | 0.57              |
| 5:b:451:PHE:CE2   | 25:b:604:CLA:HMA3 | 2.36                     | 0.57              |
| 7:d:236:PHE:CD1   | 7:d:244:THR:HG21  | 2.38                     | 0.57              |
| 20:s:153:LEU:HB3  | 20:s:159:THR:HG22 | 1.87                     | 0.57              |
| 21:n:215:GLU:HG3  | 25:n:610:CLA:C1B  | 2.35                     | 0.57              |
| 26:n:618:LHG:H291 | 26:n:618:LHG:H121 | 1.86                     | 0.57              |
| 5:B:388:SER:HB3   | 7:D:345:GLU:OE2   | 2.04                     | 0.57              |
| 21:N:103:SER:HB2  | 21:N:219:GLY:CA   | 2.34                     | 0.57              |
| 21:N:138:ILE:HD13 | 24:N:606:CHL:CBC  | 2.33                     | 0.57              |
| 25:N:610:CLA:H52  | 39:N:615:LUT:H30  | 1.87                     | 0.57              |
| 26:N:618:LHG:H291 | 26:N:618:LHG:H121 | 1.86                     | 0.57              |
| 3:8:221:LEU:O     | 3:8:224:LEU:HD23  | 2.05                     | 0.57              |
| 25:b:604:CLA:H171 | 26:b:622:LHG:H311 | 1.85                     | 0.57              |
| 6:c:154:ARG:HH22  | 17:w:128:GLU:HA   | 1.70                     | 0.57              |
| 15:o:307:GLN:O    | 15:o:321:VAL:HG12 | 2.05                     | 0.57              |
| 21:y:164:THR:CG2  | 21:y:168:LEU:HD12 | 2.34                     | 0.57              |
| 22:r:220:GLY:HA2  | 22:r:224:ASP:HB3  | 1.87                     | 0.57              |
| 24:r:607:CHL:H93  | 24:r:607:CHL:HMB3 | 1.85                     | 0.57              |
| 1:1:138:ILE:HD12  | 1:1:144:LEU:CD1   | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:129:GLU:HB2   | 2:2:239:LYS:NZ    | 2.19                     | 0.57              |
| 4:A:46:SER:OG     | 35:A:415:DGD:HBH2 | 2.05                     | 0.57              |
| 5:B:244:ALA:CB    | 25:B:610:CLA:HMA1 | 2.33                     | 0.57              |
| 6:C:304:PRO:O     | 6:C:305:THR:CB    | 2.53                     | 0.57              |
| 7:D:350:GLY:O     | 7:D:353:LEU:HD23  | 2.04                     | 0.57              |
| 13:L:26:PHE:O     | 13:L:30:VAL:HG23  | 2.05                     | 0.57              |
| 20:S:173:LEU:HA   | 20:S:176:VAL:HG22 | 1.87                     | 0.57              |
| 21:G:82:THR:O     | 21:Y:94:ARG:HG3   | 2.04                     | 0.57              |
| 21:G:107:MET:HE3  | 25:G:610:CLA:HMC2 | 1.85                     | 0.57              |
| 22:R:206:ARG:NH2  | 25:R:608:CLA:HMA3 | 2.20                     | 0.57              |
| 24:R:607:CHL:H93  | 24:R:607:CHL:HMB3 | 1.85                     | 0.57              |
| 1:5:133:LYS:O     | 1:5:136:SER:OG    | 2.20                     | 0.57              |
| 2:6:50:TRP:CG     | 2:6:213:LYS:HD3   | 2.40                     | 0.57              |
| 1:7:228:GLY:O     | 1:7:232:GLN:OE1   | 2.23                     | 0.57              |
| 3:8:136:ALA:HB1   | 3:8:140:PHE:CZ    | 2.40                     | 0.57              |
| 4:a:255:PHE:CD2   | 4:a:264:SER:HB3   | 2.40                     | 0.57              |
| 4:a:283:ILE:O     | 4:a:286:THR:HG22  | 2.03                     | 0.57              |
| 29:a:408:SQD:H151 | 26:c:519:LHG:H342 | 1.86                     | 0.57              |
| 6:c:50:LEU:O      | 6:c:54:VAL:HG23   | 2.05                     | 0.57              |
| 7:d:94:TRP:NE1    | 18:x:87:LEU:HD22  | 2.20                     | 0.57              |
| 15:o:218:LEU:HA   | 15:o:231:PHE:HB3  | 1.87                     | 0.57              |
| 15:o:306:LEU:HD21 | 15:o:322:LYS:CE   | 2.33                     | 0.57              |
| 18:x:96:VAL:O     | 18:x:100:ILE:HG12 | 2.05                     | 0.57              |
| 21:g:228:GLY:O    | 21:g:232:GLN:OE1  | 2.23                     | 0.57              |
| 21:n:111:LEU:HD23 | 25:n:604:CLA:HMC2 | 1.85                     | 0.57              |
| 21:n:165:GLN:HE21 | 24:n:607:CHL:HMC  | 1.69                     | 0.57              |
| 23:u:81:THR:OG1   | 23:u:103:TYR:O    | 2.23                     | 0.57              |
| 1:1:117:GLU:O     | 1:1:121:ARG:HG3   | 2.05                     | 0.57              |
| 2:2:104:ARG:NH2   | 24:2:603:CHL:HBD  | 2.19                     | 0.57              |
| 2:2:105:TRP:CD1   | 24:2:603:CHL:HED1 | 2.39                     | 0.57              |
| 3:4:205:LEU:HB3   | 3:4:220:LYS:HZ3   | 1.70                     | 0.57              |
| 4:A:255:PHE:CD2   | 4:A:264:SER:HB3   | 2.40                     | 0.57              |
| 4:A:256:GLY:O     | 4:A:261:GLN:HA    | 2.05                     | 0.57              |
| 10:H:22:LEU:HG    | 22:R:124:PHE:HE2  | 1.69                     | 0.57              |
| 21:N:76:GLY:HA3   | 21:N:216:LEU:CD2  | 2.24                     | 0.57              |
| 21:N:215:GLU:HG3  | 25:N:610:CLA:C1B  | 2.35                     | 0.57              |
| 25:R:603:CLA:HMD1 | 25:R:608:CLA:C1   | 2.34                     | 0.57              |
| 1:5:117:GLU:O     | 1:5:121:ARG:HG3   | 2.05                     | 0.57              |
| 1:5:138:ILE:HD12  | 1:5:144:LEU:CD1   | 2.33                     | 0.57              |
| 1:7:78:TYR:OH     | 1:7:217:LYS:NZ    | 2.20                     | 0.57              |
| 5:b:144:PHE:CE1   | 5:b:210:ILE:HG23  | 2.40                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:c:87:ILE:HD13   | 25:c:504:CLA:C2B  | 2.35                     | 0.57              |
| 6:c:457:LYS:HE2   | 7:d:230:ALA:CA    | 2.34                     | 0.57              |
| 7:d:67:SER:OG     | 7:d:70:GLU:HG3    | 2.04                     | 0.57              |
| 7:d:181:ARG:HD2   | 7:d:334:ASP:OD1   | 2.04                     | 0.57              |
| 9:f:13:ARG:NE     | 38:f:101:HEM:O2D  | 2.32                     | 0.57              |
| 12:k:58:VAL:O     | 12:k:61:ARG:HG3   | 2.04                     | 0.57              |
| 15:o:92:LEU:HA    | 15:o:96:GLU:OE2   | 2.04                     | 0.57              |
| 21:g:218:ASN:OD1  | 25:g:611:CLA:CMD  | 2.52                     | 0.57              |
| 1:1:67:PRO:CG     | 1:1:70:LEU:HD12   | 2.29                     | 0.57              |
| 2:2:172:LEU:HD22  | 24:2:603:CHL:HMB3 | 1.87                     | 0.57              |
| 2:2:210:ALA:HA    | 2:2:213:LYS:HZ2   | 1.69                     | 0.57              |
| 3:4:89:GLY:HA3    | 3:4:95:LEU:HD21   | 1.85                     | 0.57              |
| 3:4:221:LEU:O     | 3:4:224:LEU:HD23  | 2.05                     | 0.57              |
| 5:B:329:SER:O     | 5:B:444:ARG:HD3   | 2.05                     | 0.57              |
| 6:C:237:HIS:CD2   | 28:I:101:BCR:H272 | 2.39                     | 0.57              |
| 25:C:501:CLA:HMB3 | 28:I:101:BCR:C26  | 2.34                     | 0.57              |
| 7:D:67:SER:OG     | 7:D:70:GLU:HG3    | 2.04                     | 0.57              |
| 14:M:27:VAL:HG21  | 14:m:24:ILE:HG23  | 1.86                     | 0.57              |
| 15:O:227:PHE:CZ   | 15:O:287:LEU:HB2  | 2.40                     | 0.57              |
| 15:O:307:GLN:O    | 15:O:321:VAL:HG12 | 2.05                     | 0.57              |
| 21:G:146:TYR:HE2  | 25:G:604:CLA:H2   | 1.65                     | 0.57              |
| 21:G:218:ASN:OD1  | 25:G:611:CLA:CMD  | 2.52                     | 0.57              |
| 21:Y:117:GLU:O    | 21:Y:121:ARG:HG3  | 2.05                     | 0.57              |
| 1:5:78:TYR:OH     | 1:5:217:LYS:NZ    | 2.20                     | 0.57              |
| 1:5:228:GLY:O     | 1:5:232:GLN:OE1   | 2.23                     | 0.57              |
| 4:a:139:MET:HE3   | 7:d:222:THR:HG23  | 1.86                     | 0.57              |
| 4:a:274:PHE:HD1   | 29:a:408:SQD:H132 | 1.70                     | 0.57              |
| 5:b:341:LEU:HD21  | 5:b:431:GLU:HB2   | 1.87                     | 0.57              |
| 5:b:388:SER:HB3   | 7:d:345:GLU:OE2   | 2.04                     | 0.57              |
| 6:c:363:ALA:O     | 6:c:367:GLU:HG2   | 2.04                     | 0.57              |
| 6:c:449:ARG:HH12  | 11:i:28:PRO:CG    | 2.16                     | 0.57              |
| 21:g:81:ASP:OD2   | 21:g:84:GLY:HA2   | 2.05                     | 0.57              |
| 21:g:226:MET:HG2  | 39:g:616:LUT:H12  | 1.85                     | 0.57              |
| 21:n:164:THR:CG2  | 21:n:168:LEU:HD12 | 2.34                     | 0.57              |
| 4:A:84:PRO:HA     | 4:A:112:TYR:CG    | 2.39                     | 0.57              |
| 13:L:3:GLN:HG3    | 13:L:4:SER:H      | 1.68                     | 0.57              |
| 20:S:130:ILE:HD12 | 25:S:305:CLA:HAC1 | 1.86                     | 0.57              |
| 21:G:98:LEU:CD2   | 25:G:603:CLA:CAA  | 2.78                     | 0.57              |
| 21:G:139:PHE:HD2  | 24:G:607:CHL:OBD  | 1.87                     | 0.57              |
| 24:G:601:CHL:CMB  | 26:Y:301:LHG:H161 | 2.35                     | 0.57              |
| 22:R:158:GLU:OE2  | 22:R:164:THR:HA   | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:6:129:GLU:OE1   | 2:6:239:LYS:NZ    | 2.27                     | 0.57              |
| 1:7:117:GLU:O     | 1:7:121:ARG:HG3   | 2.05                     | 0.57              |
| 3:8:181:THR:O     | 3:8:182:ALA:HB2   | 2.05                     | 0.57              |
| 4:a:64:ARG:HG2    | 6:c:337:LEU:HD21  | 1.87                     | 0.57              |
| 5:b:333:GLY:O     | 5:b:441:GLY:N     | 2.34                     | 0.57              |
| 25:c:513:CLA:HMD3 | 20:s:75:LEU:HD11  | 1.85                     | 0.57              |
| 7:d:237:ASN:OD1   | 7:d:238:PRO:HD2   | 2.05                     | 0.57              |
| 8:e:19:TYR:N      | 8:e:22:ILE:HG22   | 2.20                     | 0.57              |
| 21:g:103:SER:HB2  | 21:g:219:GLY:CA   | 2.34                     | 0.57              |
| 21:n:182:PRO:HG3  | 40:n:617:NEX:H161 | 1.86                     | 0.57              |
| 21:y:78:TYR:OH    | 21:y:217:LYS:NZ   | 2.20                     | 0.57              |
| 21:y:132:PHE:CB   | 24:y:308:CHL:HMA3 | 2.34                     | 0.57              |
| 2:2:50:TRP:CG     | 2:2:213:LYS:HD3   | 2.40                     | 0.56              |
| 6:C:291:TRP:O     | 6:C:305:THR:HG23  | 2.04                     | 0.56              |
| 21:G:84:GLY:HA3   | 21:Y:94:ARG:HG2   | 1.87                     | 0.56              |
| 21:N:188:ASP:OD2  | 21:N:191:TYR:HB2  | 2.05                     | 0.56              |
| 1:5:188:ASP:OD2   | 1:5:191:TYR:HB2   | 2.05                     | 0.56              |
| 3:8:142:PHE:O     | 3:8:146:LEU:HD13  | 2.05                     | 0.56              |
| 35:a:401:DGD:HB22 | 30:a:411:LMG:H301 | 1.87                     | 0.56              |
| 6:c:237:HIS:HD2   | 28:i:101:BCR:H272 | 1.69                     | 0.56              |
| 16:t:11:VAL:HG13  | 28:t:101:BCR:H331 | 1.86                     | 0.56              |
| 20:s:146:VAL:HG21 | 20:s:149:LYS:HZ1  | 1.70                     | 0.56              |
| 21:g:117:GLU:O    | 21:g:121:ARG:HG3  | 2.05                     | 0.56              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:HHB  | 1.87                     | 0.56              |
| 24:g:601:CHL:CMB  | 26:y:301:LHG:H161 | 2.35                     | 0.56              |
| 21:y:188:ASP:OD2  | 21:y:191:TYR:HB2  | 2.05                     | 0.56              |
| 21:y:251:PRO:HB2  | 25:y:315:CLA:CMA  | 2.30                     | 0.56              |
| 1:1:138:ILE:HG21  | 24:1:302:CHL:HBC1 | 1.87                     | 0.56              |
| 2:2:175:GLY:O     | 2:2:179:ASN:N     | 2.38                     | 0.56              |
| 3:4:218:PHE:HB3   | 3:4:219:GLU:OE1   | 2.05                     | 0.56              |
| 25:B:604:CLA:H171 | 26:B:622:LHG:H311 | 1.86                     | 0.56              |
| 6:C:163:ILE:CG2   | 25:C:512:CLA:HAB  | 2.32                     | 0.56              |
| 7:D:247:MET:HE3   | 31:D:405:PL9:H522 | 1.85                     | 0.56              |
| 13:L:21:GLY:O     | 13:L:25:ILE:HG12  | 2.04                     | 0.56              |
| 20:S:202:PRO:CG   | 24:S:308:CHL:HBC2 | 2.35                     | 0.56              |
| 21:G:81:ASP:OD2   | 21:G:84:GLY:HA2   | 2.04                     | 0.56              |
| 21:G:103:SER:HB2  | 21:G:219:GLY:CA   | 2.34                     | 0.56              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:HHB  | 1.87                     | 0.56              |
| 21:N:131:TRP:HB2  | 39:N:616:LUT:H21  | 1.87                     | 0.56              |
| 25:c:501:CLA:HMB3 | 28:i:101:BCR:C26  | 2.34                     | 0.56              |
| 15:o:220:ALA:HA   | 15:o:229:GLY:HA3  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:81:ASP:OD2   | 21:n:84:GLY:HA2   | 2.04                     | 0.56              |
| 25:y:315:CLA:HBC3 | 25:y:315:CLA:HHD  | 1.87                     | 0.56              |
| 22:r:158:GLU:OE2  | 22:r:164:THR:HA   | 2.05                     | 0.56              |
| 25:r:610:CLA:C2B  | 26:r:618:LHG:HC2  | 2.34                     | 0.56              |
| 1:3:103:SER:HB2   | 1:3:219:GLY:CA    | 2.34                     | 0.56              |
| 3:4:89:GLY:O      | 3:4:95:LEU:HD11   | 2.05                     | 0.56              |
| 3:4:123:SER:HA    | 3:4:133:GLN:OE1   | 2.06                     | 0.56              |
| 5:B:341:LEU:HD21  | 5:B:431:GLU:HB2   | 1.87                     | 0.56              |
| 5:B:347:ARG:O     | 5:B:397:VAL:HA    | 2.05                     | 0.56              |
| 6:C:50:LEU:O      | 6:C:54:VAL:HG23   | 2.05                     | 0.56              |
| 6:C:87:ILE:HD13   | 25:C:504:CLA:C2B  | 2.35                     | 0.56              |
| 25:D:403:CLA:H101 | 18:X:92:SER:OG    | 2.06                     | 0.56              |
| 8:E:19:TYR:N      | 8:E:22:ILE:HG22   | 2.20                     | 0.56              |
| 15:O:117:ILE:HG12 | 15:O:300:ILE:CG2  | 2.36                     | 0.56              |
| 19:Z:14:ILE:HG23  | 19:Z:18:ILE:CD1   | 2.36                     | 0.56              |
| 21:G:69:TYR:CE2   | 21:G:87:ALA:HA    | 2.41                     | 0.56              |
| 21:G:126:PHE:CE1  | 21:G:147:LEU:HA   | 2.41                     | 0.56              |
| 21:G:227:PHE:CD2  | 25:G:602:CLA:H161 | 2.40                     | 0.56              |
| 21:N:94:ARG:HG2   | 21:Y:84:GLY:HA3   | 1.86                     | 0.56              |
| 24:N:606:CHL:HHC  | 24:N:606:CHL:HBB1 | 1.87                     | 0.56              |
| 22:R:58:TRP:CH2   | 22:R:80:PRO:HG3   | 2.41                     | 0.56              |
| 22:R:253:PHE:CD2  | 41:R:616:XAT:H12  | 2.41                     | 0.56              |
| 1:5:138:ILE:HG21  | 24:5:302:CHL:HBC1 | 1.87                     | 0.56              |
| 2:6:55:ARG:NH1    | 2:6:77:ASP:OD1    | 2.38                     | 0.56              |
| 2:6:97:ALA:HB2    | 2:6:190:LEU:HD11  | 1.87                     | 0.56              |
| 2:6:127:PHE:CD2   | 2:6:148:LEU:HD23  | 2.39                     | 0.56              |
| 2:6:128:LYS:HD2   | 2:6:133:PHE:O     | 2.05                     | 0.56              |
| 2:6:130:PRO:O     | 2:6:134:LYS:HG3   | 2.05                     | 0.56              |
| 2:6:179:ASN:CA    | 24:6:603:CHL:HMC  | 2.28                     | 0.56              |
| 2:6:211:GLU:HA    | 2:6:214:VAL:CG1   | 2.33                     | 0.56              |
| 3:8:131:GLY:O     | 3:8:134:PRO:HD2   | 2.04                     | 0.56              |
| 4:a:256:GLY:O     | 4:a:261:GLN:HA    | 2.05                     | 0.56              |
| 5:b:3:LEU:HD11    | 13:l:9:GLN:HB3    | 1.88                     | 0.56              |
| 5:b:347:ARG:O     | 5:b:397:VAL:HA    | 2.05                     | 0.56              |
| 6:c:199:ILE:CG2   | 6:c:231:GLU:HG3   | 2.35                     | 0.56              |
| 6:c:237:HIS:CD2   | 28:i:101:BCR:H272 | 2.39                     | 0.56              |
| 13:l:21:GLY:O     | 13:l:25:ILE:HG12  | 2.04                     | 0.56              |
| 15:o:312:ASP:OD1  | 15:o:313:LEU:N    | 2.38                     | 0.56              |
| 25:s:304:CLA:HMC2 | 39:s:316:LUT:C12  | 2.34                     | 0.56              |
| 21:g:164:THR:CG2  | 21:g:168:LEU:HD12 | 2.34                     | 0.56              |
| 22:r:58:TRP:CH2   | 22:r:80:PRO:HG3   | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:206:ARG:NH2  | 25:r:608:CLA:HMA3 | 2.20                     | 0.56              |
| 22:r:283:ILE:HA   | 25:r:612:CLA:CAD  | 2.35                     | 0.56              |
| 1:1:103:SER:HB2   | 1:1:219:GLY:CA    | 2.34                     | 0.56              |
| 5:B:3:LEU:CD1     | 13:L:9:GLN:HB3    | 2.35                     | 0.56              |
| 5:B:3:LEU:HD11    | 13:L:9:GLN:HB3    | 1.88                     | 0.56              |
| 6:C:60:ILE:HG23   | 25:C:510:CLA:HMC1 | 1.87                     | 0.56              |
| 7:D:94:TRP:NE1    | 18:X:87:LEU:HD22  | 2.20                     | 0.56              |
| 14:M:27:VAL:HG11  | 14:m:28:LYS:HB2   | 1.87                     | 0.56              |
| 20:S:153:LEU:HB3  | 20:S:159:THR:HG22 | 1.87                     | 0.56              |
| 25:R:601:CLA:CHA  | 26:R:618:LHG:H121 | 2.35                     | 0.56              |
| 4:a:218:LEU:HD12  | 31:a:410:PL9:O1   | 2.05                     | 0.56              |
| 4:a:223:LEU:HB2   | 7:d:140:ARG:NH2   | 2.18                     | 0.56              |
| 5:b:471:ALA:HB2   | 7:d:131:PHE:HE1   | 1.71                     | 0.56              |
| 6:c:161:LEU:HD11  | 25:c:506:CLA:HBB1 | 1.88                     | 0.56              |
| 6:c:304:PRO:O     | 6:c:305:THR:CB    | 2.53                     | 0.56              |
| 25:c:501:CLA:CHB  | 28:i:101:BCR:H271 | 2.33                     | 0.56              |
| 13:l:13:LEU:O     | 14:m:29:THR:HG21  | 2.05                     | 0.56              |
| 21:n:228:GLY:O    | 21:n:232:GLN:OE1  | 2.23                     | 0.56              |
| 22:r:144:GLY:HA3  | 22:r:246:ALA:CB   | 2.20                     | 0.56              |
| 25:r:601:CLA:CHB  | 26:r:618:LHG:H112 | 2.35                     | 0.56              |
| 1:1:146:TYR:HB3   | 1:1:152:LEU:CD1   | 2.36                     | 0.56              |
| 2:2:130:PRO:O     | 2:2:134:LYS:HG3   | 2.05                     | 0.56              |
| 1:3:228:GLY:O     | 1:3:232:GLN:OE1   | 2.23                     | 0.56              |
| 4:A:14:TRP:HB3    | 17:W:119:TYR:HB2  | 1.88                     | 0.56              |
| 5:B:454:GLY:HA2   | 30:B:620:LMG:H211 | 1.87                     | 0.56              |
| 15:O:220:ALA:HA   | 15:O:229:GLY:HA3  | 1.86                     | 0.56              |
| 20:S:111:GLN:HA   | 25:S:303:CLA:HMA1 | 1.86                     | 0.56              |
| 24:S:306:CHL:HHC  | 24:S:306:CHL:HBB1 | 1.86                     | 0.56              |
| 25:G:614:CLA:HBC3 | 25:G:614:CLA:CMC  | 2.35                     | 0.56              |
| 24:N:607:CHL:H161 | 24:Y:302:CHL:H142 | 1.88                     | 0.56              |
| 22:R:220:GLY:HA2  | 22:R:224:ASP:HB3  | 1.87                     | 0.56              |
| 1:5:146:TYR:HB3   | 1:5:152:LEU:CD1   | 2.36                     | 0.56              |
| 1:5:152:LEU:HD23  | 24:5:301:CHL:HED3 | 1.86                     | 0.56              |
| 2:6:129:GLU:HB2   | 2:6:239:LYS:NZ    | 2.19                     | 0.56              |
| 3:8:78:PRO:HB2    | 3:8:229:ILE:HG21  | 1.86                     | 0.56              |
| 25:y:315:CLA:HBD  | 25:y:315:CLA:HBA2 | 1.88                     | 0.56              |
| 22:r:124:PHE:HD1  | 25:r:614:CLA:HHC  | 1.70                     | 0.56              |
| 22:r:146:TRP:CH2  | 25:r:608:CLA:HBC3 | 2.40                     | 0.56              |
| 2:2:246:LEU:HA    | 2:2:249:LEU:CD2   | 2.36                     | 0.56              |
| 5:B:482:ILE:HG21  | 7:D:139:LEU:CD2   | 2.33                     | 0.56              |
| 21:G:146:TYR:HB3  | 21:G:152:LEU:CD1  | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:69:TYR:CE2   | 21:N:87:ALA:HA    | 2.41                     | 0.56              |
| 25:Y:315:CLA:HBA2 | 25:Y:315:CLA:HBD  | 1.88                     | 0.56              |
| 22:R:152:LEU:HD13 | 25:R:611:CLA:HBB2 | 1.88                     | 0.56              |
| 23:U:84:ALA:HB1   | 23:U:100:ILE:CG2  | 2.31                     | 0.56              |
| 2:6:172:LEU:HD22  | 24:6:603:CHL:HMB3 | 1.87                     | 0.56              |
| 3:8:184:ASN:O     | 3:8:195:PRO:HA    | 2.05                     | 0.56              |
| 5:b:3:LEU:CD1     | 13:l:9:GLN:HB3    | 2.35                     | 0.56              |
| 25:b:601:CLA:H101 | 25:b:601:CLA:CGA  | 2.35                     | 0.56              |
| 22:r:67:TRP:CZ2   | 22:r:85:LYS:HG3   | 2.41                     | 0.56              |
| 22:r:152:LEU:HD13 | 25:r:611:CLA:HBB2 | 1.87                     | 0.56              |
| 22:r:253:PHE:CD2  | 41:r:616:XAT:H12  | 2.41                     | 0.56              |
| 25:r:601:CLA:CHA  | 26:r:618:LHG:H121 | 2.35                     | 0.56              |
| 1:3:188:ASP:OD2   | 1:3:191:TYR:HB2   | 2.06                     | 0.56              |
| 3:4:142:PHE:O     | 3:4:146:LEU:HD13  | 2.05                     | 0.56              |
| 5:B:26:HIS:O      | 5:B:30:VAL:HG23   | 2.05                     | 0.56              |
| 5:B:41:GLU:HB3    | 5:B:60:MET:SD     | 2.46                     | 0.56              |
| 25:B:601:CLA:H101 | 25:B:601:CLA:CGA  | 2.35                     | 0.56              |
| 6:C:161:LEU:HD11  | 25:C:506:CLA:HBB1 | 1.88                     | 0.56              |
| 6:C:272:LEU:HD21  | 25:C:508:CLA:HHB  | 1.87                     | 0.56              |
| 13:L:13:LEU:O     | 14:M:29:THR:HG21  | 2.05                     | 0.56              |
| 21:G:188:ASP:OD2  | 21:G:191:TYR:HB2  | 2.05                     | 0.56              |
| 21:G:224:PHE:HE2  | 25:G:613:CLA:HAB  | 1.71                     | 0.56              |
| 21:N:133:LYS:O    | 21:N:136:SER:OG   | 2.20                     | 0.56              |
| 21:Y:227:PHE:HE2  | 25:Y:303:CLA:H162 | 1.71                     | 0.56              |
| 1:5:126:PHE:CE1   | 1:5:147:LEU:HA    | 2.41                     | 0.56              |
| 3:8:123:SER:HA    | 3:8:133:GLN:OE1   | 2.06                     | 0.56              |
| 4:a:46:SER:OG     | 35:a:401:DGD:HBH2 | 2.05                     | 0.56              |
| 6:c:272:LEU:HD21  | 25:c:508:CLA:HHB  | 1.87                     | 0.56              |
| 6:c:393:ALA:O     | 6:c:396:MET:HG2   | 2.06                     | 0.56              |
| 38:f:101:HEM:O1D  | 38:f:101:HEM:HHA  | 2.06                     | 0.56              |
| 21:n:117:GLU:O    | 21:n:121:ARG:HG3  | 2.05                     | 0.56              |
| 25:n:610:CLA:H52  | 39:n:615:LUT:H30  | 1.87                     | 0.56              |
| 21:y:69:TYR:CE2   | 21:y:87:ALA:HA    | 2.41                     | 0.56              |
| 21:y:126:PHE:CE1  | 21:y:147:LEU:HA   | 2.41                     | 0.56              |
| 2:2:107:MET:HG2   | 2:2:111:PHE:CE2   | 2.39                     | 0.56              |
| 2:2:128:LYS:HD2   | 2:2:133:PHE:O     | 2.05                     | 0.56              |
| 3:4:184:ASN:O     | 3:4:195:PRO:HA    | 2.05                     | 0.56              |
| 4:A:224:ILE:HD11  | 4:A:247:ASN:OD1   | 2.05                     | 0.56              |
| 20:S:63:TYR:HE2   | 20:S:219:ALA:HB1  | 1.66                     | 0.56              |
| 20:S:170:ASN:OD1  | 20:S:171:LEU:N    | 2.36                     | 0.56              |
| 21:N:117:GLU:O    | 21:N:121:ARG:HG3  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:132:PHE:CB   | 24:N:607:CHL:HMA3 | 2.36                     | 0.56              |
| 21:Y:81:ASP:OD2   | 21:Y:84:GLY:HA2   | 2.04                     | 0.56              |
| 21:Y:126:PHE:CE1  | 21:Y:147:LEU:HA   | 2.41                     | 0.56              |
| 1:5:138:ILE:HG13  | 1:5:144:LEU:CB    | 2.31                     | 0.56              |
| 2:6:90:GLU:O      | 2:6:94:LYS:HG2    | 2.06                     | 0.56              |
| 5:b:72:THR:HG23   | 5:b:80:ILE:CG2    | 2.23                     | 0.56              |
| 5:b:155:ALA:O     | 5:b:159:THR:OG1   | 2.19                     | 0.56              |
| 18:x:87:LEU:HD12  | 18:x:88:LEU:HD22  | 1.88                     | 0.56              |
| 20:s:146:VAL:HG11 | 20:s:149:LYS:HZ3  | 1.71                     | 0.56              |
| 20:s:262:PHE:HD2  | 25:s:314:CLA:HMA1 | 1.71                     | 0.56              |
| 21:n:133:LYS:O    | 21:n:136:SER:OG   | 2.20                     | 0.56              |
| 2:2:55:ARG:NH1    | 2:2:77:ASP:OD1    | 2.38                     | 0.56              |
| 2:2:217:ILE:CD1   | 25:2:604:CLA:CAD  | 2.84                     | 0.56              |
| 1:3:117:GLU:O     | 1:3:121:ARG:HG3   | 2.05                     | 0.56              |
| 3:4:155:TRP:CD1   | 3:4:159:LYS:NZ    | 2.74                     | 0.56              |
| 3:4:181:THR:O     | 3:4:182:ALA:HB2   | 2.05                     | 0.56              |
| 4:A:64:ARG:HG2    | 6:C:337:LEU:HD21  | 1.87                     | 0.56              |
| 4:A:218:LEU:HD12  | 31:A:409:PL9:O1   | 2.05                     | 0.56              |
| 5:B:237:VAL:CG2   | 25:B:610:CLA:HBC2 | 2.36                     | 0.56              |
| 6:C:160:ILE:HG12  | 25:C:512:CLA:HMC3 | 1.88                     | 0.56              |
| 6:C:393:ALA:O     | 6:C:396:MET:HG2   | 2.06                     | 0.56              |
| 25:C:511:CLA:H102 | 19:Z:24:PRO:CB    | 2.35                     | 0.56              |
| 15:O:136:PHE:HB2  | 15:O:174:ILE:O    | 2.05                     | 0.56              |
| 21:G:117:GLU:O    | 21:G:121:ARG:HG3  | 2.05                     | 0.56              |
| 21:N:96:ARG:O     | 21:N:100:VAL:HG23 | 2.06                     | 0.56              |
| 25:N:602:CLA:HBC1 | 26:N:618:LHG:H251 | 1.88                     | 0.56              |
| 22:R:67:TRP:CZ2   | 22:R:85:LYS:HG3   | 2.41                     | 0.56              |
| 22:R:146:TRP:CH2  | 25:R:608:CLA:HBC3 | 2.40                     | 0.56              |
| 25:R:601:CLA:CHB  | 26:R:618:LHG:H112 | 2.35                     | 0.56              |
| 1:5:67:PRO:CG     | 1:5:70:LEU:HD12   | 2.29                     | 0.56              |
| 2:6:100:VAL:CB    | 2:6:190:LEU:HD23  | 2.36                     | 0.56              |
| 1:7:76:GLY:HA3    | 1:7:216:LEU:CD2   | 2.24                     | 0.56              |
| 6:c:26:ARG:NH2    | 6:c:41:ARG:HB3    | 2.20                     | 0.56              |
| 25:c:511:CLA:H162 | 19:z:20:LEU:CD1   | 2.32                     | 0.56              |
| 7:d:22:TRP:CD1    | 7:d:25:ARG:HH12   | 2.24                     | 0.56              |
| 25:d:403:CLA:H101 | 18:x:92:SER:OG    | 2.06                     | 0.56              |
| 28:d:404:BCR:H382 | 28:d:404:BCR:H23C | 1.87                     | 0.56              |
| 14:m:26:TYR:O     | 14:m:29:THR:HG22  | 2.06                     | 0.56              |
| 20:s:173:LEU:HA   | 20:s:176:VAL:HG22 | 1.87                     | 0.56              |
| 21:g:146:TYR:HB3  | 21:g:152:LEU:CD1  | 2.36                     | 0.56              |
| 21:g:224:PHE:HE2  | 25:g:613:CLA:HAB  | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:50:TRP:C     | 21:n:55:ARG:HD2   | 2.31                     | 0.56              |
| 21:n:103:SER:HB2  | 21:n:219:GLY:CA   | 2.34                     | 0.56              |
| 21:n:126:PHE:CE1  | 21:n:147:LEU:HA   | 2.41                     | 0.56              |
| 25:n:610:CLA:H71  | 25:n:612:CLA:H102 | 1.88                     | 0.56              |
| 2:2:211:GLU:HA    | 2:2:214:VAL:CG1   | 2.33                     | 0.56              |
| 5:B:37:MET:HE2    | 5:B:37:MET:HA     | 1.88                     | 0.56              |
| 6:C:26:ARG:NH2    | 6:C:41:ARG:HB3    | 2.20                     | 0.56              |
| 6:C:154:ARG:HH22  | 17:W:128:GLU:HA   | 1.70                     | 0.56              |
| 25:S:305:CLA:HBB1 | 39:S:316:LUT:H181 | 1.87                     | 0.56              |
| 25:S:312:CLA:HBB1 | 39:S:315:LUT:H14  | 1.87                     | 0.56              |
| 21:G:95:ASN:C     | 25:G:602:CLA:HMA1 | 2.31                     | 0.56              |
| 25:Y:303:CLA:H72  | 25:Y:303:CLA:H122 | 1.88                     | 0.56              |
| 2:6:217:ILE:CD1   | 25:6:604:CLA:CAD  | 2.84                     | 0.56              |
| 2:6:246:LEU:HA    | 2:6:249:LEU:CD2   | 2.36                     | 0.56              |
| 3:8:162:VAL:O     | 3:8:166:ASN:N     | 2.33                     | 0.56              |
| 4:a:224:ILE:HD11  | 4:a:247:ASN:OD1   | 2.05                     | 0.56              |
| 5:b:41:GLU:HB3    | 5:b:60:MET:SD     | 2.46                     | 0.56              |
| 5:b:355:PHE:HB3   | 23:u:94:THR:HG22  | 1.88                     | 0.56              |
| 10:h:56:ILE:CD1   | 18:x:84:LYS:HE3   | 2.16                     | 0.56              |
| 20:s:202:PRO:CG   | 24:s:308:CHL:HBC2 | 2.35                     | 0.56              |
| 25:s:312:CLA:HBB1 | 39:s:315:LUT:H14  | 1.87                     | 0.56              |
| 21:g:69:TYR:CE2   | 21:g:87:ALA:HA    | 2.41                     | 0.56              |
| 21:n:132:PHE:HB3  | 24:n:607:CHL:HMA3 | 1.88                     | 0.56              |
| 21:y:50:TRP:C     | 21:y:55:ARG:HD2   | 2.31                     | 0.56              |
| 21:y:146:TYR:HB3  | 21:y:152:LEU:CD1  | 2.36                     | 0.56              |
| 3:4:166:ASN:ND2   | 22:R:61:GLY:O     | 2.39                     | 0.55              |
| 5:B:144:PHE:CE1   | 5:B:210:ILE:HG23  | 2.40                     | 0.55              |
| 25:B:606:CLA:CAD  | 26:B:622:LHG:HC62 | 2.36                     | 0.55              |
| 6:C:175:LEU:HD23  | 6:C:237:HIS:ND1   | 2.22                     | 0.55              |
| 25:C:511:CLA:H162 | 19:Z:20:LEU:CD1   | 2.33                     | 0.55              |
| 38:F:101:HEM:O1D  | 38:F:101:HEM:HHA  | 2.06                     | 0.55              |
| 13:L:13:LEU:HB2   | 14:M:25:ILE:CG2   | 2.36                     | 0.55              |
| 15:O:218:LEU:HA   | 15:O:231:PHE:HB3  | 1.86                     | 0.55              |
| 17:W:108:VAL:O    | 17:W:112:ILE:HD12 | 2.06                     | 0.55              |
| 21:N:231:VAL:HG21 | 25:N:613:CLA:CAC  | 2.30                     | 0.55              |
| 24:N:607:CHL:H201 | 24:N:609:CHL:H62  | 1.88                     | 0.55              |
| 21:Y:128:GLU:OE1  | 21:Y:133:LYS:HB3  | 2.06                     | 0.55              |
| 2:6:121:LYS:HZ2   | 2:6:241:PRO:HB2   | 1.71                     | 0.55              |
| 3:8:89:GLY:O      | 3:8:95:LEU:HD11   | 2.05                     | 0.55              |
| 21:n:69:TYR:CE2   | 21:n:87:ALA:HA    | 2.41                     | 0.55              |
| 21:n:138:ILE:HG13 | 21:n:144:LEU:CB   | 2.31                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:n:606:CHL:HHC  | 24:n:606:CHL:HBB1 | 1.87                     | 0.55              |
| 25:y:303:CLA:HBB1 | 25:y:303:CLA:CMB  | 2.36                     | 0.55              |
| 25:y:303:CLA:H72  | 25:y:303:CLA:H122 | 1.88                     | 0.55              |
| 1:1:126:PHE:CE1   | 1:1:147:LEU:HA    | 2.41                     | 0.55              |
| 1:3:126:PHE:CE1   | 1:3:147:LEU:HA    | 2.41                     | 0.55              |
| 1:3:146:TYR:HB3   | 1:3:152:LEU:CD1   | 2.36                     | 0.55              |
| 3:4:183:GLU:CD    | 3:4:185:PHE:HE1   | 2.15                     | 0.55              |
| 4:A:274:PHE:HD1   | 29:A:407:SQD:H132 | 1.70                     | 0.55              |
| 6:C:369:LEU:CD2   | 6:C:384:ILE:HG12  | 2.36                     | 0.55              |
| 16:T:20:ALA:O     | 16:T:24:ARG:HB3   | 2.06                     | 0.55              |
| 20:S:178:GLU:OE1  | 24:S:307:CHL:HMC  | 2.06                     | 0.55              |
| 21:G:138:ILE:HD12 | 21:G:144:LEU:CD1  | 2.32                     | 0.55              |
| 21:N:138:ILE:HD13 | 24:N:606:CHL:HBC3 | 1.87                     | 0.55              |
| 21:N:224:PHE:HZ   | 25:N:613:CLA:H93  | 1.71                     | 0.55              |
| 25:N:604:CLA:HBA2 | 40:N:617:NEX:H241 | 1.88                     | 0.55              |
| 21:Y:116:PRO:HB2  | 21:Y:129:ALA:O    | 2.07                     | 0.55              |
| 21:Y:133:LYS:O    | 21:Y:136:SER:OG   | 2.20                     | 0.55              |
| 1:7:126:PHE:CE1   | 1:7:147:LEU:HA    | 2.41                     | 0.55              |
| 1:7:146:TYR:HB3   | 1:7:152:LEU:CD1   | 2.36                     | 0.55              |
| 3:8:218:PHE:HB3   | 3:8:219:GLU:OE1   | 2.05                     | 0.55              |
| 5:b:329:SER:O     | 5:b:444:ARG:HD3   | 2.05                     | 0.55              |
| 6:c:437:LEU:HD22  | 25:c:502:CLA:CBC  | 2.37                     | 0.55              |
| 7:d:147:PHE:O     | 7:d:150:PRO:HD2   | 2.06                     | 0.55              |
| 15:o:227:PHE:CZ   | 15:o:287:LEU:HB2  | 2.40                     | 0.55              |
| 20:s:135:ASN:HD21 | 20:s:141:CYS:HB2  | 1.72                     | 0.55              |
| 21:g:126:PHE:CE1  | 21:g:147:LEU:HA   | 2.41                     | 0.55              |
| 21:g:188:ASP:OD2  | 21:g:191:TYR:HB2  | 2.05                     | 0.55              |
| 21:g:218:ASN:ND2  | 25:g:612:CLA:C4A  | 2.62                     | 0.55              |
| 21:g:227:PHE:CD2  | 25:g:602:CLA:H161 | 2.40                     | 0.55              |
| 21:n:116:PRO:HB2  | 21:n:129:ALA:O    | 2.07                     | 0.55              |
| 21:n:127:GLY:CA   | 21:n:137:GLN:HG3  | 2.37                     | 0.55              |
| 21:n:188:ASP:OD2  | 21:n:191:TYR:HB2  | 2.05                     | 0.55              |
| 21:n:224:PHE:HZ   | 25:n:613:CLA:H93  | 1.71                     | 0.55              |
| 21:y:117:GLU:O    | 21:y:121:ARG:HG3  | 2.05                     | 0.55              |
| 21:y:227:PHE:HE2  | 25:y:303:CLA:H162 | 1.71                     | 0.55              |
| 23:u:97:THR:CA    | 23:u:102:ARG:HH21 | 2.09                     | 0.55              |
| 2:2:97:ALA:HB2    | 2:2:190:LEU:HD11  | 1.87                     | 0.55              |
| 1:3:58:TYR:CD1    | 1:3:80:TRP:HB2    | 2.42                     | 0.55              |
| 3:4:159:LYS:HZ2   | 25:R:601:CLA:HMB2 | 1.69                     | 0.55              |
| 3:4:164:PHE:HB2   | 3:4:192:GLN:OE1   | 2.06                     | 0.55              |
| 28:D:404:BCR:H382 | 28:D:404:BCR:H23C | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:S:69:ILE:HG13  | 20:S:71:LEU:O     | 2.07                     | 0.55              |
| 21:G:50:TRP:C     | 21:G:55:ARG:HD2   | 2.31                     | 0.55              |
| 25:G:613:CLA:C3B  | 39:G:615:LUT:H183 | 2.37                     | 0.55              |
| 21:N:128:GLU:OE1  | 21:N:133:LYS:HB3  | 2.06                     | 0.55              |
| 21:Y:50:TRP:C     | 21:Y:55:ARG:HD2   | 2.31                     | 0.55              |
| 21:Y:188:ASP:OD2  | 21:Y:191:TYR:HB2  | 2.05                     | 0.55              |
| 1:5:69:TYR:CE2    | 1:5:87:ALA:HA     | 2.41                     | 0.55              |
| 1:5:72:GLY:HA2    | 1:5:77:ASP:OD2    | 2.07                     | 0.55              |
| 4:a:14:TRP:HB3    | 17:w:119:TYR:HB2  | 1.88                     | 0.55              |
| 5:b:170:ASP:HB2   | 5:b:171:PRO:HD2   | 1.87                     | 0.55              |
| 5:b:454:GLY:HA2   | 30:b:620:LMG:H211 | 1.87                     | 0.55              |
| 25:s:312:CLA:HHC  | 39:s:315:LUT:C13  | 2.36                     | 0.55              |
| 25:g:613:CLA:C3B  | 39:g:615:LUT:H183 | 2.37                     | 0.55              |
| 22:r:93:ASP:OD1   | 22:r:110:ILE:HD11 | 2.05                     | 0.55              |
| 2:2:158:SER:O     | 2:2:161:ALA:HB3   | 2.07                     | 0.55              |
| 2:2:242:LEU:O     | 2:2:246:LEU:HG    | 2.06                     | 0.55              |
| 1:3:69:TYR:CE2    | 1:3:87:ALA:HA     | 2.41                     | 0.55              |
| 1:3:76:GLY:HA3    | 1:3:216:LEU:CD2   | 2.24                     | 0.55              |
| 8:E:57:THR:HG23   | 8:E:60:ARG:H      | 1.72                     | 0.55              |
| 25:S:305:CLA:C2B  | 39:S:316:LUT:H183 | 2.37                     | 0.55              |
| 21:G:127:GLY:CA   | 21:G:137:GLN:HG3  | 2.37                     | 0.55              |
| 21:N:56:VAL:HG21  | 26:N:618:LHG:O2   | 2.07                     | 0.55              |
| 21:N:58:TYR:CD1   | 21:N:80:TRP:HB2   | 2.42                     | 0.55              |
| 21:Y:69:TYR:CE2   | 21:Y:87:ALA:HA    | 2.41                     | 0.55              |
| 21:Y:96:ARG:O     | 21:Y:100:VAL:HG23 | 2.06                     | 0.55              |
| 1:5:50:TRP:C      | 1:5:55:ARG:HD2    | 2.31                     | 0.55              |
| 1:5:81:ASP:OD2    | 1:5:84:GLY:HA2    | 2.05                     | 0.55              |
| 1:7:127:GLY:CA    | 1:7:137:GLN:HG3   | 2.37                     | 0.55              |
| 3:8:94:PHE:O      | 3:8:98:TYR:CD2    | 2.60                     | 0.55              |
| 4:a:140:ARG:NH2   | 7:d:220:GLU:HG2   | 2.22                     | 0.55              |
| 4:a:238:ARG:NH2   | 4:a:241:GLN:HB2   | 2.22                     | 0.55              |
| 25:c:511:CLA:H102 | 19:z:24:PRO:CB    | 2.35                     | 0.55              |
| 17:w:108:VAL:O    | 17:w:112:ILE:HD12 | 2.06                     | 0.55              |
| 21:g:67:PRO:CG    | 21:g:70:LEU:HD12  | 2.29                     | 0.55              |
| 21:g:127:GLY:CA   | 21:g:137:GLN:HG3  | 2.37                     | 0.55              |
| 21:n:132:PHE:CB   | 24:n:607:CHL:HMA3 | 2.36                     | 0.55              |
| 21:y:67:PRO:CG    | 21:y:70:LEU:HD12  | 2.29                     | 0.55              |
| 21:y:72:GLY:HA2   | 21:y:77:ASP:OD2   | 2.07                     | 0.55              |
| 21:y:128:GLU:OE1  | 21:y:133:LYS:HB3  | 2.06                     | 0.55              |
| 25:y:313:CLA:HAC2 | 25:y:314:CLA:H191 | 1.87                     | 0.55              |
| 25:r:612:CLA:C1B  | 39:r:615:LUT:H183 | 2.37                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:90:GLU:O      | 2:2:94:LYS:HG2    | 2.06                     | 0.55              |
| 2:2:100:VAL:CB    | 2:2:190:LEU:HD23  | 2.36                     | 0.55              |
| 1:3:50:TRP:C      | 1:3:55:ARG:HD2    | 2.31                     | 0.55              |
| 7:D:147:PHE:O     | 7:D:150:PRO:HD2   | 2.06                     | 0.55              |
| 20:S:85:LEU:HD23  | 20:S:94:GLY:HA2   | 1.88                     | 0.55              |
| 20:S:110:TYR:CD2  | 25:S:303:CLA:H12  | 2.42                     | 0.55              |
| 20:S:122:MET:HB3  | 39:S:315:LUT:C34  | 2.37                     | 0.55              |
| 21:N:98:LEU:HD11  | 21:Y:83:ALA:HA    | 1.88                     | 0.55              |
| 21:N:226:MET:HG2  | 39:N:616:LUT:H12  | 1.89                     | 0.55              |
| 25:N:611:CLA:HBC2 | 25:N:612:CLA:HAC1 | 1.87                     | 0.55              |
| 22:R:130:VAL:HG23 | 22:R:131:PHE:CD1  | 2.42                     | 0.55              |
| 1:5:116:PRO:HB2   | 1:5:129:ALA:O     | 2.07                     | 0.55              |
| 1:7:58:TYR:CD1    | 1:7:80:TRP:HB2    | 2.42                     | 0.55              |
| 1:7:69:TYR:CE2    | 1:7:87:ALA:HA     | 2.41                     | 0.55              |
| 5:b:26:HIS:O      | 5:b:30:VAL:HG23   | 2.05                     | 0.55              |
| 5:b:237:VAL:HG22  | 25:b:610:CLA:HBC2 | 1.89                     | 0.55              |
| 5:b:272:ARG:O     | 5:b:272:ARG:HD3   | 2.06                     | 0.55              |
| 6:c:60:ILE:HG23   | 25:c:510:CLA:HMC1 | 1.87                     | 0.55              |
| 25:c:511:CLA:HBA2 | 12:k:54:TRP:CH2   | 2.42                     | 0.55              |
| 19:z:13:ILE:HD12  | 28:z:101:BCR:HC31 | 1.89                     | 0.55              |
| 20:s:69:ILE:HG13  | 20:s:71:LEU:O     | 2.07                     | 0.55              |
| 20:s:122:MET:HB3  | 39:s:315:LUT:C34  | 2.37                     | 0.55              |
| 21:g:116:PRO:HB2  | 21:g:129:ALA:O    | 2.07                     | 0.55              |
| 21:g:128:GLU:OE1  | 21:g:133:LYS:HB3  | 2.06                     | 0.55              |
| 21:y:96:ARG:O     | 21:y:100:VAL:HG23 | 2.06                     | 0.55              |
| 26:y:319:LHG:H271 | 26:y:319:LHG:HC82 | 1.89                     | 0.55              |
| 1:3:127:GLY:CA    | 1:3:137:GLN:HG3   | 2.37                     | 0.55              |
| 5:B:237:VAL:HG22  | 25:B:610:CLA:HBC2 | 1.89                     | 0.55              |
| 6:C:187:ASP:OD2   | 6:C:197:ARG:NH2   | 2.40                     | 0.55              |
| 20:S:262:PHE:HD2  | 25:S:314:CLA:HMA1 | 1.71                     | 0.55              |
| 21:G:58:TYR:CD1   | 21:G:80:TRP:HB2   | 2.42                     | 0.55              |
| 24:G:609:CHL:O2D  | 24:G:609:CHL:H2A  | 2.07                     | 0.55              |
| 21:N:60:GLY:HA3   | 24:N:601:CHL:HMC  | 1.89                     | 0.55              |
| 21:N:132:PHE:HB3  | 24:N:607:CHL:HMA3 | 1.88                     | 0.55              |
| 25:N:610:CLA:H51  | 25:N:612:CLA:CMA  | 2.37                     | 0.55              |
| 21:Y:165:GLN:OE1  | 24:Y:307:CHL:CHB  | 2.55                     | 0.55              |
| 25:Y:313:CLA:HAC2 | 25:Y:314:CLA:H191 | 1.87                     | 0.55              |
| 25:Y:315:CLA:HBC3 | 25:Y:315:CLA:HHD  | 1.87                     | 0.55              |
| 24:R:607:CHL:H112 | 24:R:607:CHL:CAB  | 2.31                     | 0.55              |
| 25:R:612:CLA:C1B  | 39:R:615:LUT:H183 | 2.37                     | 0.55              |
| 2:6:69:TYR:HE1    | 2:6:70:LEU:HG     | 1.70                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:188:ASP:OD2   | 1:7:191:TYR:HB2   | 2.06                     | 0.55              |
| 3:8:166:ASN:ND2   | 22:r:61:GLY:O     | 2.39                     | 0.55              |
| 6:c:79:LYS:HG2    | 6:c:80:PRO:HD2    | 1.89                     | 0.55              |
| 16:t:20:ALA:O     | 16:t:24:ARG:HB3   | 2.06                     | 0.55              |
| 19:z:14:ILE:HG23  | 19:z:18:ILE:CD1   | 2.36                     | 0.55              |
| 25:s:305:CLA:HBB1 | 39:s:316:LUT:H181 | 1.87                     | 0.55              |
| 25:g:614:CLA:HBC3 | 25:g:614:CLA:CMC  | 2.35                     | 0.55              |
| 21:n:138:ILE:HD13 | 24:n:606:CHL:HBC3 | 1.87                     | 0.55              |
| 23:u:85:LYS:HE2   | 23:u:101:CYS:HB2  | 1.88                     | 0.55              |
| 1:1:50:TRP:C      | 1:1:55:ARG:HD2    | 2.31                     | 0.55              |
| 1:1:69:TYR:CE2    | 1:1:87:ALA:HA     | 2.41                     | 0.55              |
| 1:1:90:GLU:OE1    | 1:1:90:GLU:CA     | 2.55                     | 0.55              |
| 1:3:96:ARG:O      | 1:3:100:VAL:HG23  | 2.06                     | 0.55              |
| 3:4:110:MET:SD    | 3:4:111:ALA:N     | 2.80                     | 0.55              |
| 3:4:169:SER:O     | 3:4:183:GLU:HG2   | 2.07                     | 0.55              |
| 6:C:79:LYS:HG2    | 6:C:80:PRO:HD2    | 1.89                     | 0.55              |
| 18:X:87:LEU:HD12  | 18:X:88:LEU:HD22  | 1.88                     | 0.55              |
| 21:G:128:GLU:OE1  | 21:G:133:LYS:HB3  | 2.06                     | 0.55              |
| 21:N:230:PHE:O    | 21:N:234:ILE:HG13 | 2.07                     | 0.55              |
| 21:Y:60:GLY:CA    | 24:Y:302:CHL:HMC  | 2.27                     | 0.55              |
| 26:Y:319:LHG:HC82 | 26:Y:319:LHG:H271 | 1.89                     | 0.55              |
| 2:6:174:GLU:HB3   | 1:7:62:PHE:HB2    | 1.88                     | 0.55              |
| 2:6:210:ALA:HA    | 2:6:213:LYS:HZ3   | 1.69                     | 0.55              |
| 1:7:138:ILE:HG13  | 1:7:144:LEU:CB    | 2.31                     | 0.55              |
| 5:b:237:VAL:CG2   | 25:b:610:CLA:HBC2 | 2.36                     | 0.55              |
| 25:b:606:CLA:CAD  | 26:b:622:LHG:HC62 | 2.36                     | 0.55              |
| 6:c:369:LEU:CD2   | 6:c:384:ILE:HG12  | 2.36                     | 0.55              |
| 21:g:50:TRP:C     | 21:g:55:ARG:HD2   | 2.31                     | 0.55              |
| 21:g:58:TYR:CD1   | 21:g:80:TRP:HB2   | 2.42                     | 0.55              |
| 21:n:72:GLY:HA2   | 21:n:77:ASP:OD2   | 2.07                     | 0.55              |
| 21:n:95:ASN:C     | 25:n:602:CLA:HMA1 | 2.32                     | 0.55              |
| 24:n:601:CHL:HBC3 | 24:n:601:CHL:CMC  | 2.37                     | 0.55              |
| 1:1:116:PRO:HB2   | 1:1:129:ALA:O     | 2.07                     | 0.55              |
| 1:1:128:GLU:OE1   | 1:1:133:LYS:HB3   | 2.06                     | 0.55              |
| 2:2:145:LEU:HB3   | 2:2:149:GLY:O     | 2.07                     | 0.55              |
| 1:3:128:GLU:OE1   | 1:3:133:LYS:HB3   | 2.07                     | 0.55              |
| 3:4:221:LEU:CD1   | 3:4:222:GLU:HG3   | 2.37                     | 0.55              |
| 5:B:224:ARG:HG2   | 10:H:37:TRP:CH2   | 2.42                     | 0.55              |
| 5:B:272:ARG:O     | 5:B:272:ARG:HD3   | 2.06                     | 0.55              |
| 25:B:607:CLA:H152 | 25:B:613:CLA:H152 | 1.89                     | 0.55              |
| 25:B:615:CLA:C19  | 25:B:616:CLA:HBC3 | 2.33                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:C:437:LEU:HD22  | 25:C:502:CLA:CBC  | 2.37                     | 0.55              |
| 21:G:90:GLU:OE1   | 21:G:90:GLU:CA    | 2.55                     | 0.55              |
| 21:N:162:TRP:CE3  | 21:Y:257:TRP:CH2  | 2.95                     | 0.55              |
| 25:N:603:CLA:O1A  | 21:Y:83:ALA:HB1   | 2.07                     | 0.55              |
| 25:N:610:CLA:H52  | 39:N:615:LUT:C28  | 2.32                     | 0.55              |
| 25:Y:315:CLA:HBA2 | 25:Y:315:CLA:CHA  | 2.37                     | 0.55              |
| 22:R:124:PHE:HD1  | 25:R:614:CLA:HHC  | 1.70                     | 0.55              |
| 1:7:116:PRO:HB2   | 1:7:129:ALA:O     | 2.07                     | 0.55              |
| 6:c:81:MET:HE2    | 6:c:89:LEU:HB3    | 1.89                     | 0.55              |
| 6:c:160:ILE:HG12  | 25:c:512:CLA:HMC3 | 1.88                     | 0.55              |
| 15:o:136:PHE:HB2  | 15:o:174:ILE:O    | 2.05                     | 0.55              |
| 21:y:86:SER:OG    | 25:y:303:CLA:HAA2 | 2.06                     | 0.55              |
| 21:y:116:PRO:HB2  | 21:y:129:ALA:O    | 2.07                     | 0.55              |
| 22:r:130:VAL:HG23 | 22:r:131:PHE:CD1  | 2.42                     | 0.55              |
| 27:A:404:PHO:H42  | 27:A:404:PHO:O1A  | 2.07                     | 0.55              |
| 5:B:355:PHE:HB3   | 23:U:94:THR:HG22  | 1.88                     | 0.55              |
| 7:D:81:THR:HG22   | 7:D:112:TRP:CE2   | 2.42                     | 0.55              |
| 7:D:96:PRO:HG2    | 10:H:63:SER:OG    | 2.07                     | 0.55              |
| 15:O:296:THR:HB   | 15:O:298:GLU:HG2  | 1.89                     | 0.55              |
| 20:S:153:LEU:CB   | 20:S:159:THR:HG22 | 2.37                     | 0.55              |
| 20:S:266:LEU:HA   | 25:S:313:CLA:OBD  | 2.07                     | 0.55              |
| 21:G:72:GLY:HA2   | 21:G:77:ASP:OD2   | 2.07                     | 0.55              |
| 21:G:107:MET:HE3  | 25:G:610:CLA:CMC  | 2.37                     | 0.55              |
| 21:G:138:ILE:HD12 | 24:G:606:CHL:HAC1 | 1.89                     | 0.55              |
| 21:N:104:ARG:HD3  | 25:N:610:CLA:CHD  | 2.36                     | 0.55              |
| 21:N:126:PHE:CE1  | 21:N:147:LEU:HA   | 2.41                     | 0.55              |
| 21:N:146:TYR:HB3  | 21:N:152:LEU:CD1  | 2.36                     | 0.55              |
| 21:Y:86:SER:OG    | 25:Y:303:CLA:HAA2 | 2.06                     | 0.55              |
| 21:Y:90:GLU:OE1   | 21:Y:90:GLU:CA    | 2.55                     | 0.55              |
| 21:Y:213:VAL:HG12 | 25:Y:312:CLA:HED2 | 1.89                     | 0.55              |
| 22:R:59:TYR:N     | 22:R:60:PRO:HD3   | 2.22                     | 0.55              |
| 2:6:158:SER:O     | 2:6:161:ALA:HB3   | 2.07                     | 0.55              |
| 2:6:242:LEU:O     | 2:6:246:LEU:HG    | 2.06                     | 0.55              |
| 1:7:50:TRP:C      | 1:7:55:ARG:HD2    | 2.31                     | 0.55              |
| 1:7:72:GLY:HA2    | 1:7:77:ASP:OD2    | 2.07                     | 0.55              |
| 1:7:90:GLU:OE1    | 1:7:90:GLU:CA     | 2.55                     | 0.55              |
| 1:7:133:LYS:O     | 1:7:136:SER:OG    | 2.20                     | 0.55              |
| 4:a:140:ARG:HH21  | 7:d:220:GLU:HG2   | 1.72                     | 0.55              |
| 29:l:101:SQD:H251 | 42:l:203:HOH:O    | 2.07                     | 0.55              |
| 20:s:153:LEU:CB   | 20:s:159:THR:HG22 | 2.37                     | 0.55              |
| 21:n:60:GLY:HA3   | 24:n:601:CHL:HMC  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:104:ARG:HD3  | 25:n:610:CLA:CHD  | 2.36                     | 0.55              |
| 21:n:131:TRP:HB2  | 39:n:616:LUT:H21  | 1.87                     | 0.55              |
| 21:y:230:PHE:O    | 21:y:234:ILE:HG13 | 2.07                     | 0.55              |
| 25:y:315:CLA:HBA2 | 25:y:315:CLA:CHA  | 2.37                     | 0.55              |
| 22:r:59:TYR:N     | 22:r:60:PRO:HD3   | 2.22                     | 0.55              |
| 1:1:188:ASP:OD2   | 1:1:191:TYR:HB2   | 2.05                     | 0.55              |
| 4:A:140:ARG:NH2   | 7:D:220:GLU:HG2   | 2.22                     | 0.55              |
| 4:A:140:ARG:NH1   | 26:C:519:LHG:O5   | 2.33                     | 0.55              |
| 15:O:134:LYS:HE2  | 15:O:175:GLU:HB2  | 1.89                     | 0.55              |
| 21:G:116:PRO:HB2  | 21:G:129:ALA:O    | 2.07                     | 0.55              |
| 1:5:128:GLU:OE1   | 1:5:133:LYS:HB3   | 2.06                     | 0.55              |
| 20:s:110:TYR:CD2  | 25:s:303:CLA:H12  | 2.42                     | 0.55              |
| 25:s:304:CLA:CHC  | 39:s:316:LUT:H15  | 2.36                     | 0.55              |
| 25:s:305:CLA:C2B  | 39:s:316:LUT:H183 | 2.37                     | 0.55              |
| 21:g:133:LYS:O    | 21:g:136:SER:OG   | 2.20                     | 0.55              |
| 25:g:604:CLA:NC   | 40:g:617:NEX:O23  | 2.41                     | 0.55              |
| 21:y:132:PHE:HB2  | 24:y:308:CHL:HMA3 | 1.89                     | 0.55              |
| 21:y:165:GLN:OE1  | 24:y:307:CHL:CHB  | 2.55                     | 0.55              |
| 1:1:72:GLY:HA2    | 1:1:77:ASP:OD2    | 2.07                     | 0.54              |
| 2:2:202:LEU:H     | 2:2:202:LEU:HD23  | 1.73                     | 0.54              |
| 1:3:72:GLY:HA2    | 1:3:77:ASP:OD2    | 2.07                     | 0.54              |
| 4:A:140:ARG:HH21  | 7:D:220:GLU:HG2   | 1.72                     | 0.54              |
| 7:D:22:TRP:CD1    | 7:D:25:ARG:HH12   | 2.24                     | 0.54              |
| 15:O:285:ILE:HG12 | 15:O:287:LEU:CD1  | 2.37                     | 0.54              |
| 15:O:290:THR:HG22 | 15:O:291:LYS:N    | 2.19                     | 0.54              |
| 25:S:304:CLA:CHC  | 39:S:316:LUT:H15  | 2.36                     | 0.54              |
| 21:Y:176:ARG:HG3  | 24:Y:309:CHL:CHD  | 2.37                     | 0.54              |
| 1:5:230:PHE:O     | 1:5:234:ILE:HG13  | 2.07                     | 0.54              |
| 5:b:224:ARG:HG2   | 10:h:37:TRP:CH2   | 2.42                     | 0.54              |
| 6:c:60:ILE:HG12   | 25:c:510:CLA:CMC  | 2.37                     | 0.54              |
| 6:c:175:LEU:HD23  | 6:c:237:HIS:ND1   | 2.21                     | 0.54              |
| 25:c:505:CLA:C19  | 35:c:515:DGD:HA81 | 2.37                     | 0.54              |
| 28:h:101:BCR:C23  | 28:h:101:BCR:H392 | 2.36                     | 0.54              |
| 15:o:117:ILE:HG12 | 15:o:300:ILE:CG2  | 2.36                     | 0.54              |
| 15:o:296:THR:HB   | 15:o:298:GLU:HG2  | 1.89                     | 0.54              |
| 20:s:85:LEU:HD23  | 20:s:94:GLY:HA2   | 1.88                     | 0.54              |
| 20:s:130:ILE:HD12 | 25:s:305:CLA:CAC  | 2.38                     | 0.54              |
| 20:s:142:GLY:N    | 20:s:143:PRO:HA   | 2.22                     | 0.54              |
| 21:g:90:GLU:OE1   | 21:g:90:GLU:CA    | 2.55                     | 0.54              |
| 21:n:230:PHE:O    | 21:n:234:ILE:HG13 | 2.07                     | 0.54              |
| 25:n:611:CLA:HBC2 | 25:n:612:CLA:HAC1 | 1.87                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:59:LEU:O     | 21:y:63:SER:OG    | 2.22                     | 0.54              |
| 1:1:59:LEU:O      | 1:1:63:SER:OG     | 2.22                     | 0.54              |
| 1:1:96:ARG:O      | 1:1:100:VAL:HG23  | 2.07                     | 0.54              |
| 2:2:174:GLU:HB3   | 1:3:62:PHE:CG     | 2.42                     | 0.54              |
| 3:4:220:LYS:O     | 3:4:224:LEU:HD23  | 2.07                     | 0.54              |
| 4:A:269:ARG:HH11  | 7:D:232:THR:HB    | 1.72                     | 0.54              |
| 29:A:407:SQD:H302 | 12:K:52:PHE:CZ    | 2.42                     | 0.54              |
| 5:B:170:ASP:HB2   | 5:B:171:PRO:HD2   | 1.87                     | 0.54              |
| 5:B:471:ALA:HB2   | 7:D:131:PHE:HE1   | 1.71                     | 0.54              |
| 6:C:60:ILE:HG12   | 25:C:510:CLA:HMC1 | 1.89                     | 0.54              |
| 7:D:305:ARG:HD3   | 14:M:1:MET:CE     | 2.37                     | 0.54              |
| 12:K:58:VAL:CG1   | 12:K:61:ARG:HD2   | 2.37                     | 0.54              |
| 14:M:26:TYR:O     | 14:M:29:THR:HG22  | 2.06                     | 0.54              |
| 15:O:174:ILE:HG21 | 15:O:190:GLU:OE1  | 2.08                     | 0.54              |
| 16:T:14:LEU:CD1   | 28:T:101:BCR:H343 | 2.37                     | 0.54              |
| 21:N:72:GLY:HA2   | 21:N:77:ASP:OD2   | 2.07                     | 0.54              |
| 21:N:116:PRO:HB2  | 21:N:129:ALA:O    | 2.07                     | 0.54              |
| 21:N:127:GLY:CA   | 21:N:137:GLN:HG3  | 2.37                     | 0.54              |
| 2:6:88:ASP:HB3    | 2:6:91:ALA:HB2    | 1.89                     | 0.54              |
| 2:6:122:TRP:O     | 2:6:123:VAL:CG2   | 2.54                     | 0.54              |
| 2:6:211:GLU:CA    | 2:6:214:VAL:HG12  | 2.37                     | 0.54              |
| 1:7:88:ASP:OD2    | 1:7:90:GLU:HB2    | 2.08                     | 0.54              |
| 1:7:96:ARG:O      | 1:7:100:VAL:HG23  | 2.06                     | 0.54              |
| 3:8:164:PHE:HB2   | 3:8:192:GLN:OE1   | 2.06                     | 0.54              |
| 4:a:269:ARG:HH11  | 7:d:232:THR:HB    | 1.72                     | 0.54              |
| 29:a:408:SQD:H302 | 12:k:52:PHE:CZ    | 2.42                     | 0.54              |
| 5:b:144:PHE:O     | 5:b:148:VAL:HG23  | 2.07                     | 0.54              |
| 5:b:223:GLN:HA    | 10:h:33:VAL:CG1   | 2.38                     | 0.54              |
| 7:d:81:THR:HG22   | 7:d:112:TRP:CE2   | 2.42                     | 0.54              |
| 7:d:88:HIS:CD2    | 7:d:167:GLY:HA2   | 2.43                     | 0.54              |
| 14:m:2:GLU:O      | 14:m:3:VAL:HG22   | 2.07                     | 0.54              |
| 21:n:128:GLU:OE1  | 21:n:133:LYS:HB3  | 2.06                     | 0.54              |
| 21:n:219:GLY:C    | 21:n:223:MET:HE2  | 2.33                     | 0.54              |
| 2:2:155:HIS:CE1   | 2:2:158:SER:HA    | 2.42                     | 0.54              |
| 2:2:179:ASN:CA    | 24:2:603:CHL:HMC  | 2.28                     | 0.54              |
| 3:4:136:ALA:HB1   | 3:4:140:PHE:CZ    | 2.40                     | 0.54              |
| 6:C:293:ASN:ND2   | 6:C:296:ALA:H     | 2.05                     | 0.54              |
| 6:C:338:GLY:HA2   | 15:O:196:TYR:OH   | 2.07                     | 0.54              |
| 6:C:452:ALA:HB1   | 17:W:131:LEU:HB3  | 1.90                     | 0.54              |
| 6:C:462:ASP:OD1   | 6:C:463:PHE:N     | 2.41                     | 0.54              |
| 25:C:505:CLA:C19  | 35:C:515:DGD:HA81 | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:H:101:BCR:C23  | 28:H:101:BCR:H392 | 2.36                     | 0.54              |
| 20:S:142:GLY:N    | 20:S:143:PRO:HA   | 2.22                     | 0.54              |
| 21:G:182:PRO:HG2  | 24:G:608:CHL:HBB2 | 1.89                     | 0.54              |
| 24:G:609:CHL:HBB1 | 24:G:609:CHL:HHC  | 1.90                     | 0.54              |
| 21:N:219:GLY:O    | 21:N:223:MET:HE2  | 2.08                     | 0.54              |
| 24:N:605:CHL:HHC  | 24:N:605:CHL:HBB1 | 1.88                     | 0.54              |
| 21:Y:58:TYR:CD1   | 21:Y:80:TRP:HB2   | 2.42                     | 0.54              |
| 1:5:88:ASP:OD2    | 1:5:90:GLU:HB2    | 2.08                     | 0.54              |
| 1:5:127:GLY:CA    | 1:5:137:GLN:HG3   | 2.37                     | 0.54              |
| 2:6:145:LEU:HB3   | 2:6:149:GLY:O     | 2.07                     | 0.54              |
| 1:7:128:GLU:OE1   | 1:7:133:LYS:HB3   | 2.06                     | 0.54              |
| 3:8:221:LEU:CD1   | 3:8:222:GLU:HG3   | 2.37                     | 0.54              |
| 27:a:405:PHO:O1A  | 27:a:405:PHO:H42  | 2.07                     | 0.54              |
| 6:c:293:ASN:ND2   | 6:c:296:ALA:H     | 2.05                     | 0.54              |
| 25:c:510:CLA:HMA2 | 25:c:510:CLA:C2   | 2.37                     | 0.54              |
| 21:g:219:GLY:C    | 21:g:223:MET:HE2  | 2.33                     | 0.54              |
| 21:g:230:PHE:O    | 21:g:234:ILE:HG13 | 2.07                     | 0.54              |
| 21:n:58:TYR:CD1   | 21:n:80:TRP:HB2   | 2.42                     | 0.54              |
| 21:n:162:TRP:CE3  | 21:y:257:TRP:CH2  | 2.95                     | 0.54              |
| 21:n:219:GLY:O    | 21:n:223:MET:HE2  | 2.08                     | 0.54              |
| 25:n:603:CLA:O1A  | 21:y:83:ALA:HB1   | 2.07                     | 0.54              |
| 25:r:601:CLA:HMA2 | 25:r:601:CLA:O2A  | 2.08                     | 0.54              |
| 1:1:58:TYR:CD1    | 1:1:80:TRP:HB2    | 2.42                     | 0.54              |
| 1:1:127:GLY:CA    | 1:1:137:GLN:HG3   | 2.37                     | 0.54              |
| 1:1:219:GLY:O     | 1:1:223:MET:HE2   | 2.08                     | 0.54              |
| 1:1:230:PHE:O     | 1:1:234:ILE:HG13  | 2.07                     | 0.54              |
| 20:S:128:PHE:CE1  | 39:S:316:LUT:H173 | 2.42                     | 0.54              |
| 20:S:134:LEU:HD23 | 24:N:605:CHL:HAA2 | 1.90                     | 0.54              |
| 25:S:312:CLA:HHC  | 39:S:315:LUT:C13  | 2.36                     | 0.54              |
| 21:G:219:GLY:C    | 21:G:223:MET:HE2  | 2.33                     | 0.54              |
| 21:G:229:PHE:CE2  | 21:G:240:PRO:HB3  | 2.43                     | 0.54              |
| 21:G:230:PHE:O    | 21:G:234:ILE:HG13 | 2.07                     | 0.54              |
| 21:N:50:TRP:C     | 21:N:55:ARG:HD2   | 2.31                     | 0.54              |
| 21:N:131:TRP:CE3  | 21:N:132:PHE:HB3  | 2.43                     | 0.54              |
| 21:N:233:ALA:HB1  | 32:N:619:AJP:C18  | 2.38                     | 0.54              |
| 24:N:601:CHL:CMC  | 24:N:601:CHL:HBC3 | 2.37                     | 0.54              |
| 21:Y:219:GLY:C    | 21:Y:223:MET:HE2  | 2.33                     | 0.54              |
| 22:R:189:SER:O    | 22:R:192:ILE:HG22 | 2.08                     | 0.54              |
| 22:R:258:VAL:HG21 | 25:R:612:CLA:HAC2 | 1.89                     | 0.54              |
| 1:5:59:LEU:O      | 1:5:63:SER:OG     | 2.22                     | 0.54              |
| 1:5:229:PHE:CE2   | 1:5:240:PRO:HB3   | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:6:55:ARG:NE     | 2:6:72:GLY:HA3    | 2.23                     | 0.54              |
| 1:7:229:PHE:CE2   | 1:7:240:PRO:HB3   | 2.43                     | 0.54              |
| 3:8:110:MET:SD    | 3:8:111:ALA:N     | 2.80                     | 0.54              |
| 3:8:169:SER:O     | 3:8:183:GLU:HG2   | 2.07                     | 0.54              |
| 25:c:504:CLA:HBC1 | 12:k:42:VAL:HA    | 1.89                     | 0.54              |
| 7:d:96:PRO:HG2    | 10:h:63:SER:OG    | 2.07                     | 0.54              |
| 13:l:13:LEU:HB2   | 14:m:25:ILE:CG2   | 2.36                     | 0.54              |
| 21:g:88:ASP:OD2   | 21:g:90:GLU:HB2   | 2.08                     | 0.54              |
| 21:g:96:ARG:O     | 21:g:100:VAL:HG23 | 2.07                     | 0.54              |
| 21:n:59:LEU:O     | 21:n:63:SER:OG    | 2.22                     | 0.54              |
| 25:n:602:CLA:HBC1 | 26:n:618:LHG:H251 | 1.88                     | 0.54              |
| 2:2:211:GLU:CA    | 2:2:214:VAL:HG12  | 2.37                     | 0.54              |
| 3:4:94:PHE:O      | 3:4:98:TYR:CD2    | 2.60                     | 0.54              |
| 6:C:81:MET:HE2    | 6:C:89:LEU:HB3    | 1.89                     | 0.54              |
| 25:C:510:CLA:H192 | 25:C:510:CLA:CHD  | 2.38                     | 0.54              |
| 7:D:57:THR:CB     | 7:D:70:GLU:OE1    | 2.55                     | 0.54              |
| 19:Z:13:ILE:HD12  | 28:Z:101:BCR:HC31 | 1.89                     | 0.54              |
| 20:S:135:ASN:HD21 | 20:S:141:CYS:HB2  | 1.72                     | 0.54              |
| 21:G:96:ARG:O     | 21:G:100:VAL:HG23 | 2.07                     | 0.54              |
| 21:N:95:ASN:C     | 25:N:602:CLA:HMA1 | 2.32                     | 0.54              |
| 25:N:610:CLA:H71  | 25:N:612:CLA:H102 | 1.88                     | 0.54              |
| 21:Y:72:GLY:HA2   | 21:Y:77:ASP:OD2   | 2.07                     | 0.54              |
| 21:Y:127:GLY:CA   | 21:Y:137:GLN:HG3  | 2.37                     | 0.54              |
| 23:U:85:LYS:HE2   | 23:U:101:CYS:HB2  | 1.88                     | 0.54              |
| 1:5:131:TRP:CE3   | 1:5:132:PHE:HB3   | 2.43                     | 0.54              |
| 2:6:50:TRP:HB2    | 2:6:213:LYS:CE    | 2.38                     | 0.54              |
| 2:6:202:LEU:HD23  | 2:6:202:LEU:H     | 1.73                     | 0.54              |
| 3:8:181:THR:HG21  | 3:8:198:ARG:HH21  | 1.72                     | 0.54              |
| 30:a:409:LMG:H292 | 6:c:216:SER:HA    | 1.89                     | 0.54              |
| 6:c:187:ASP:OD2   | 6:c:197:ARG:NH2   | 2.40                     | 0.54              |
| 7:d:57:THR:OG1    | 7:d:70:GLU:OE1    | 2.25                     | 0.54              |
| 7:d:89:SER:O      | 7:d:91:LEU:HD12   | 2.08                     | 0.54              |
| 29:l:102:SQD:H292 | 29:l:102:SQD:H152 | 1.90                     | 0.54              |
| 20:s:178:GLU:OE1  | 24:s:307:CHL:HMC  | 2.06                     | 0.54              |
| 20:s:186:GLU:HG3  | 25:s:309:CLA:C4B  | 2.38                     | 0.54              |
| 21:g:78:TYR:OH    | 21:g:217:LYS:NZ   | 2.20                     | 0.54              |
| 21:g:95:ASN:C     | 25:g:602:CLA:HMA1 | 2.31                     | 0.54              |
| 21:g:218:ASN:HD22 | 25:g:612:CLA:C4A  | 2.21                     | 0.54              |
| 21:g:229:PHE:CE2  | 21:g:240:PRO:HB3  | 2.43                     | 0.54              |
| 21:n:105:TRP:CZ3  | 24:n:609:CHL:HAC2 | 2.43                     | 0.54              |
| 21:n:130:VAL:HB   | 21:n:133:LYS:HB2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:n:607:CHL:H201 | 24:n:609:CHL:H62  | 1.88                     | 0.54              |
| 24:n:607:CHL:H161 | 24:y:302:CHL:H142 | 1.88                     | 0.54              |
| 25:n:610:CLA:H8   | 39:n:615:LUT:C30  | 2.38                     | 0.54              |
| 25:n:613:CLA:HAA1 | 25:n:613:CLA:HBD  | 1.90                     | 0.54              |
| 21:y:58:TYR:CD1   | 21:y:80:TRP:HB2   | 2.42                     | 0.54              |
| 21:y:88:ASP:OD2   | 21:y:90:GLU:HB2   | 2.08                     | 0.54              |
| 25:r:608:CLA:HBC2 | 25:r:608:CLA:CMC  | 2.38                     | 0.54              |
| 1:1:88:ASP:OD2    | 1:1:90:GLU:HB2    | 2.08                     | 0.54              |
| 3:4:181:THR:HG21  | 3:4:198:ARG:HH21  | 1.72                     | 0.54              |
| 4:A:131:TRP:HZ2   | 6:C:449:ARG:CD    | 2.21                     | 0.54              |
| 25:C:511:CLA:HBA2 | 12:K:54:TRP:CH2   | 2.42                     | 0.54              |
| 21:N:105:TRP:CZ3  | 24:N:609:CHL:HAC2 | 2.43                     | 0.54              |
| 21:Y:229:PHE:CE2  | 21:Y:240:PRO:HB3  | 2.43                     | 0.54              |
| 25:Y:303:CLA:HBB1 | 25:Y:303:CLA:CMB  | 2.36                     | 0.54              |
| 1:5:58:TYR:CD1    | 1:5:80:TRP:HB2    | 2.42                     | 0.54              |
| 1:5:219:GLY:C     | 1:5:223:MET:HE2   | 2.33                     | 0.54              |
| 2:6:50:TRP:HB2    | 2:6:213:LYS:HE2   | 1.90                     | 0.54              |
| 1:7:67:PRO:CG     | 1:7:70:LEU:HD12   | 2.29                     | 0.54              |
| 4:a:254:TYR:CE1   | 7:d:133:LEU:HB3   | 2.42                     | 0.54              |
| 7:d:57:THR:CB     | 7:d:70:GLU:OE1    | 2.55                     | 0.54              |
| 8:e:57:THR:HG23   | 8:e:60:ARG:H      | 1.72                     | 0.54              |
| 15:o:291:LYS:O    | 15:o:300:ILE:HG12 | 2.07                     | 0.54              |
| 21:n:96:ARG:O     | 21:n:100:VAL:HG23 | 2.07                     | 0.54              |
| 21:n:98:LEU:HD11  | 21:y:83:ALA:HA    | 1.88                     | 0.54              |
| 21:n:229:PHE:CE2  | 21:n:240:PRO:HB3  | 2.43                     | 0.54              |
| 1:1:105:TRP:HZ3   | 24:1:302:CHL:CMB  | 2.20                     | 0.54              |
| 24:2:601:CHL:O1D  | 26:2:606:LHG:H142 | 2.08                     | 0.54              |
| 1:3:116:PRO:HB2   | 1:3:129:ALA:O     | 2.07                     | 0.54              |
| 4:A:324:ALA:O     | 4:A:328:MET:HG3   | 2.08                     | 0.54              |
| 25:C:502:CLA:CMC  | 25:C:510:CLA:HBB1 | 2.38                     | 0.54              |
| 15:O:291:LYS:O    | 15:O:300:ILE:HG12 | 2.07                     | 0.54              |
| 20:S:186:GLU:HG3  | 25:S:309:CLA:C4B  | 2.38                     | 0.54              |
| 24:G:608:CHL:H152 | 40:G:617:NEX:H402 | 1.90                     | 0.54              |
| 21:Y:131:TRP:CE3  | 21:Y:132:PHE:HB3  | 2.43                     | 0.54              |
| 25:R:608:CLA:CMC  | 25:R:608:CLA:HBC2 | 2.38                     | 0.54              |
| 2:6:155:HIS:CE1   | 2:6:158:SER:HA    | 2.42                     | 0.54              |
| 1:7:59:LEU:O      | 1:7:63:SER:OG     | 2.22                     | 0.54              |
| 7:d:147:PHE:C     | 7:d:150:PRO:HD2   | 2.33                     | 0.54              |
| 15:o:117:ILE:HG21 | 15:o:298:GLU:HB3  | 1.89                     | 0.54              |
| 21:g:72:GLY:HA2   | 21:g:77:ASP:OD2   | 2.07                     | 0.54              |
| 21:y:213:VAL:HG12 | 25:y:312:CLA:HED2 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:221:LYS:HD2  | 22:r:222:PHE:CD2  | 2.43                     | 0.54              |
| 25:2:602:CLA:HBC1 | 26:2:606:LHG:H251 | 1.89                     | 0.54              |
| 1:3:90:GLU:OE1    | 1:3:90:GLU:CA     | 2.55                     | 0.54              |
| 4:A:254:TYR:CE1   | 7:D:133:LEU:HB3   | 2.42                     | 0.54              |
| 5:B:36:SER:OG     | 28:B:618:BCR:H362 | 2.08                     | 0.54              |
| 25:C:504:CLA:HBC1 | 12:K:42:VAL:HA    | 1.89                     | 0.54              |
| 7:D:89:SER:O      | 7:D:91:LEU:HD12   | 2.08                     | 0.54              |
| 25:S:304:CLA:HBD  | 25:S:304:CLA:HAA2 | 1.89                     | 0.54              |
| 21:G:219:GLY:O    | 21:G:223:MET:HE2  | 2.08                     | 0.54              |
| 21:N:225:SER:OG   | 39:N:615:LUT:H192 | 2.08                     | 0.54              |
| 25:N:603:CLA:HMC1 | 39:N:616:LUT:C13  | 2.38                     | 0.54              |
| 21:Y:104:ARG:HD3  | 25:Y:311:CLA:C4C  | 2.38                     | 0.54              |
| 1:5:90:GLU:OE1    | 1:5:90:GLU:CA     | 2.55                     | 0.54              |
| 1:7:230:PHE:O     | 1:7:234:ILE:HG13  | 2.07                     | 0.54              |
| 3:8:173:GLU:HB3   | 22:r:59:TYR:CZ    | 2.43                     | 0.54              |
| 4:a:27:ARG:NH2    | 7:d:259:GLY:O     | 2.36                     | 0.54              |
| 15:o:172:ASP:OD1  | 15:o:173:GLU:N    | 2.41                     | 0.54              |
| 15:o:233:VAL:HB   | 15:o:281:SER:O    | 2.08                     | 0.54              |
| 20:s:119:ARG:HD2  | 24:s:308:CHL:OBD  | 2.07                     | 0.54              |
| 20:s:170:ASN:H    | 20:s:173:LEU:HB2  | 1.73                     | 0.54              |
| 21:g:219:GLY:O    | 21:g:223:MET:HE2  | 2.08                     | 0.54              |
| 21:n:56:VAL:HG11  | 24:n:601:CHL:HBC1 | 1.90                     | 0.54              |
| 21:n:172:VAL:HG13 | 24:n:608:CHL:C1B  | 2.38                     | 0.54              |
| 21:n:233:ALA:HB1  | 32:n:619:AJP:C18  | 2.37                     | 0.54              |
| 24:n:608:CHL:H42  | 39:n:615:LUT:H362 | 1.90                     | 0.54              |
| 22:r:255:GLY:O    | 22:r:259:GLN:HG3  | 2.07                     | 0.54              |
| 3:4:173:GLU:HB3   | 22:R:59:TYR:CZ    | 2.43                     | 0.54              |
| 4:A:238:ARG:NH2   | 4:A:241:GLN:HB2   | 2.22                     | 0.54              |
| 6:C:60:ILE:HG12   | 25:C:510:CLA:CMC  | 2.37                     | 0.54              |
| 25:C:501:CLA:CHB  | 28:I:101:BCR:H271 | 2.33                     | 0.54              |
| 25:C:510:CLA:HMA2 | 25:C:510:CLA:C2   | 2.37                     | 0.54              |
| 8:E:19:TYR:HB3    | 8:E:20:TRP:CE3    | 2.43                     | 0.54              |
| 29:L:103:SQD:H251 | 42:L:203:HOH:O    | 2.07                     | 0.54              |
| 15:O:172:ASP:OD1  | 15:O:173:GLU:N    | 2.41                     | 0.54              |
| 20:S:122:MET:HE3  | 20:S:229:GLY:CA   | 2.38                     | 0.54              |
| 21:G:131:TRP:CE3  | 21:G:132:PHE:HB3  | 2.43                     | 0.54              |
| 25:G:603:CLA:HAC1 | 24:G:607:CHL:HBB2 | 1.90                     | 0.54              |
| 21:N:172:VAL:HG13 | 24:N:608:CHL:C1B  | 2.38                     | 0.54              |
| 21:Y:230:PHE:O    | 21:Y:234:ILE:HG13 | 2.07                     | 0.54              |
| 22:R:184:LEU:HD13 | 24:R:605:CHL:OBD  | 2.08                     | 0.54              |
| 25:R:601:CLA:HMA2 | 25:R:601:CLA:O2A  | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:608:CLA:HBC2 | 25:R:608:CLA:HMC3 | 1.90                     | 0.54              |
| 2:6:175:GLY:O     | 2:6:179:ASN:N     | 2.38                     | 0.54              |
| 1:7:219:GLY:C     | 1:7:223:MET:HE2   | 2.33                     | 0.54              |
| 25:b:607:CLA:H152 | 25:b:613:CLA:H152 | 1.89                     | 0.54              |
| 35:b:626:DGD:O5D  | 35:b:626:DGD:O4D  | 2.18                     | 0.54              |
| 15:o:117:ILE:HG22 | 15:o:298:GLU:HB3  | 1.89                     | 0.54              |
| 15:o:174:ILE:HG21 | 15:o:190:GLU:OE1  | 2.08                     | 0.54              |
| 20:s:266:LEU:HA   | 25:s:313:CLA:OBD  | 2.07                     | 0.54              |
| 25:g:614:CLA:HAA1 | 25:g:614:CLA:CBD  | 2.33                     | 0.54              |
| 21:n:56:VAL:HG21  | 26:n:618:LHG:O2   | 2.07                     | 0.54              |
| 21:n:226:MET:HG2  | 39:n:616:LUT:H12  | 1.89                     | 0.54              |
| 25:n:603:CLA:HMC1 | 39:n:616:LUT:C13  | 2.38                     | 0.54              |
| 21:y:127:GLY:CA   | 21:y:137:GLN:HG3  | 2.37                     | 0.54              |
| 1:1:78:TYR:OH     | 1:1:217:LYS:NZ    | 2.20                     | 0.54              |
| 1:1:165:GLN:O     | 1:1:169:MET:HB2   | 2.08                     | 0.54              |
| 1:3:130:VAL:HB    | 1:3:133:LYS:HB2   | 1.90                     | 0.54              |
| 4:A:27:ARG:NH2    | 7:D:259:GLY:O     | 2.36                     | 0.54              |
| 4:A:184:ILE:HG23  | 4:A:328:MET:SD    | 2.48                     | 0.54              |
| 7:D:88:HIS:CD2    | 7:D:167:GLY:HA2   | 2.43                     | 0.54              |
| 7:D:222:THR:HG21  | 7:D:250:ALA:HB2   | 1.90                     | 0.54              |
| 21:N:90:GLU:OE1   | 21:N:90:GLU:CA    | 2.55                     | 0.54              |
| 1:5:96:ARG:O      | 1:5:100:VAL:HG23  | 2.06                     | 0.54              |
| 2:6:174:GLU:HB3   | 1:7:62:PHE:CG     | 2.42                     | 0.54              |
| 1:7:165:GLN:O     | 1:7:169:MET:HB2   | 2.08                     | 0.54              |
| 5:b:37:MET:HA     | 5:b:37:MET:HE2    | 1.88                     | 0.54              |
| 6:c:365:TRP:O     | 6:c:368:PRO:HD2   | 2.08                     | 0.54              |
| 6:c:452:ALA:HB1   | 17:w:131:LEU:HB3  | 1.90                     | 0.54              |
| 15:o:285:ILE:HG12 | 15:o:287:LEU:CD1  | 2.37                     | 0.54              |
| 21:n:90:GLU:OE1   | 21:n:90:GLU:CA    | 2.55                     | 0.54              |
| 2:2:55:ARG:NE     | 2:2:72:GLY:HA3    | 2.23                     | 0.53              |
| 25:B:607:CLA:HBB1 | 25:B:607:CLA:HMB1 | 1.91                     | 0.53              |
| 14:M:2:GLU:O      | 14:M:3:VAL:HG22   | 2.07                     | 0.53              |
| 15:O:158:PHE:CD2  | 15:O:322:LYS:HB2  | 2.43                     | 0.53              |
| 25:S:311:CLA:HAA1 | 25:S:311:CLA:HBD  | 1.90                     | 0.53              |
| 21:N:165:GLN:O    | 21:N:169:MET:HB2  | 2.08                     | 0.53              |
| 21:Y:219:GLY:O    | 21:Y:223:MET:HE2  | 2.08                     | 0.53              |
| 24:Y:302:CHL:CMB  | 26:Y:319:LHG:H161 | 2.38                     | 0.53              |
| 24:6:601:CHL:O1D  | 26:6:606:LHG:H142 | 2.08                     | 0.53              |
| 25:6:602:CLA:HBC1 | 26:6:606:LHG:H251 | 1.89                     | 0.53              |
| 5:b:314:TYR:CE2   | 5:b:316:GLY:HA3   | 2.43                     | 0.53              |
| 6:c:338:GLY:HA2   | 15:o:196:TYR:OH   | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:c:462:ASP:OD1   | 6:c:463:PHE:N     | 2.41                     | 0.53              |
| 12:k:58:VAL:CG1   | 12:k:61:ARG:HD2   | 2.37                     | 0.53              |
| 15:o:158:PHE:CD2  | 15:o:322:LYS:HB2  | 2.43                     | 0.53              |
| 25:s:304:CLA:HAB  | 39:s:316:LUT:C15  | 2.39                     | 0.53              |
| 21:g:59:LEU:O     | 21:g:63:SER:OG    | 2.22                     | 0.53              |
| 21:g:87:ALA:HB1   | 21:y:90:GLU:HB3   | 1.90                     | 0.53              |
| 21:g:182:PRO:HG2  | 24:g:608:CHL:HBB2 | 1.89                     | 0.53              |
| 21:n:165:GLN:O    | 21:n:169:MET:HB2  | 2.08                     | 0.53              |
| 21:n:210:GLU:OE1  | 21:n:214:LYS:NZ   | 2.38                     | 0.53              |
| 21:n:231:VAL:CG2  | 25:n:613:CLA:HAC1 | 2.35                     | 0.53              |
| 25:n:604:CLA:HBA2 | 40:n:617:NEX:H241 | 1.89                     | 0.53              |
| 21:y:90:GLU:OE1   | 21:y:90:GLU:CA    | 2.55                     | 0.53              |
| 21:y:122:ASN:CB   | 32:y:320:AJP:C80  | 2.79                     | 0.53              |
| 21:y:131:TRP:CE3  | 21:y:132:PHE:HB3  | 2.43                     | 0.53              |
| 24:y:302:CHL:CMB  | 26:y:319:LHG:H161 | 2.38                     | 0.53              |
| 1:1:219:GLY:C     | 1:1:223:MET:HE2   | 2.33                     | 0.53              |
| 1:3:165:GLN:O     | 1:3:169:MET:HB2   | 2.08                     | 0.53              |
| 1:3:230:PHE:O     | 1:3:234:ILE:HG13  | 2.07                     | 0.53              |
| 3:4:69:ASP:N      | 3:4:70:PRO:HD2    | 2.23                     | 0.53              |
| 4:A:51:ALA:HB3    | 4:A:82:ILE:HD12   | 1.90                     | 0.53              |
| 5:B:16:PRO:HB3    | 5:B:133:LEU:HD11  | 1.91                     | 0.53              |
| 5:B:144:PHE:O     | 5:B:148:VAL:HG23  | 2.07                     | 0.53              |
| 5:B:368:VAL:HB    | 5:B:381:VAL:HB    | 1.90                     | 0.53              |
| 25:S:304:CLA:HAB  | 39:S:316:LUT:C15  | 2.39                     | 0.53              |
| 21:G:88:ASP:OD2   | 21:G:90:GLU:HB2   | 2.08                     | 0.53              |
| 21:Y:132:PHE:HB2  | 24:Y:308:CHL:HMA3 | 1.90                     | 0.53              |
| 22:R:255:GLY:O    | 22:R:259:GLN:HG3  | 2.07                     | 0.53              |
| 3:8:69:ASP:N      | 3:8:70:PRO:HD2    | 2.23                     | 0.53              |
| 3:8:220:LYS:O     | 3:8:224:LEU:HD23  | 2.07                     | 0.53              |
| 4:a:131:TRP:HZ2   | 6:c:449:ARG:CD    | 2.21                     | 0.53              |
| 4:a:286:THR:OG1   | 25:a:402:CLA:O1D  | 2.25                     | 0.53              |
| 6:c:60:ILE:HG12   | 25:c:510:CLA:HMC1 | 1.89                     | 0.53              |
| 15:o:134:LYS:HE2  | 15:o:175:GLU:HB2  | 1.89                     | 0.53              |
| 20:s:170:ASN:OD1  | 20:s:171:LEU:N    | 2.36                     | 0.53              |
| 25:s:304:CLA:HBD  | 25:s:304:CLA:HAA2 | 1.89                     | 0.53              |
| 21:g:84:GLY:HA3   | 21:y:94:ARG:HG2   | 1.88                     | 0.53              |
| 21:g:131:TRP:CE3  | 21:g:132:PHE:HB3  | 2.43                     | 0.53              |
| 24:g:609:CHL:O2D  | 24:g:609:CHL:H2A  | 2.07                     | 0.53              |
| 24:n:605:CHL:HHC  | 24:n:605:CHL:HBB1 | 1.88                     | 0.53              |
| 25:n:610:CLA:H71  | 25:n:612:CLA:C10  | 2.38                     | 0.53              |
| 21:y:176:ARG:HG3  | 24:y:309:CHL:CHD  | 2.37                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:219:GLY:C    | 21:y:223:MET:HE2  | 2.33                     | 0.53              |
| 22:r:258:VAL:HG21 | 25:r:612:CLA:HAC2 | 1.89                     | 0.53              |
| 1:1:69:TYR:OH     | 1:1:81:ASP:OD2    | 2.20                     | 0.53              |
| 2:2:174:GLU:HB3   | 1:3:62:PHE:HB2    | 1.88                     | 0.53              |
| 27:A:404:PHO:HBB1 | 27:A:404:PHO:CMB  | 2.38                     | 0.53              |
| 5:B:331:ASP:HA    | 5:B:335:GLY:O     | 2.08                     | 0.53              |
| 7:D:147:PHE:C     | 7:D:150:PRO:HD2   | 2.33                     | 0.53              |
| 20:S:119:ARG:HD2  | 24:S:308:CHL:OBD  | 2.07                     | 0.53              |
| 21:G:130:VAL:HB   | 21:G:133:LYS:HB2  | 1.90                     | 0.53              |
| 21:N:130:VAL:HB   | 21:N:133:LYS:HB2  | 1.90                     | 0.53              |
| 21:N:229:PHE:CE2  | 21:N:240:PRO:HB3  | 2.43                     | 0.53              |
| 2:6:126:ASP:HA    | 2:6:148:LEU:CG    | 2.37                     | 0.53              |
| 3:8:221:LEU:HD12  | 3:8:222:GLU:HG3   | 1.91                     | 0.53              |
| 5:b:368:VAL:HB    | 5:b:381:VAL:HB    | 1.90                     | 0.53              |
| 7:d:299:PHE:O     | 7:d:303:GLU:HG2   | 2.09                     | 0.53              |
| 7:d:305:ARG:HD3   | 14:m:1:MET:CE     | 2.37                     | 0.53              |
| 20:s:122:MET:HE3  | 20:s:229:GLY:CA   | 2.38                     | 0.53              |
| 20:s:266:LEU:O    | 20:s:270:ILE:HG23 | 2.09                     | 0.53              |
| 21:n:76:GLY:HA3   | 21:n:216:LEU:CD2  | 2.24                     | 0.53              |
| 21:n:159:LEU:HD11 | 21:y:257:TRP:HB3  | 1.88                     | 0.53              |
| 1:1:130:VAL:HB    | 1:1:133:LYS:HB2   | 1.90                     | 0.53              |
| 1:1:131:TRP:CE3   | 1:1:132:PHE:HB3   | 2.43                     | 0.53              |
| 2:2:126:ASP:HA    | 2:2:148:LEU:CG    | 2.37                     | 0.53              |
| 1:3:219:GLY:C     | 1:3:223:MET:HE2   | 2.33                     | 0.53              |
| 1:3:219:GLY:O     | 1:3:223:MET:HE2   | 2.08                     | 0.53              |
| 3:4:118:VAL:HG23  | 3:4:122:TRP:CE2   | 2.44                     | 0.53              |
| 3:4:173:GLU:OE1   | 22:R:59:TYR:HA    | 2.08                     | 0.53              |
| 5:B:274:GLN:HB3   | 5:B:279:TYR:HB3   | 1.90                     | 0.53              |
| 6:C:365:TRP:O     | 6:C:368:PRO:HD2   | 2.07                     | 0.53              |
| 6:C:461:ARG:NH1   | 7:D:242:GLU:HG3   | 2.23                     | 0.53              |
| 8:E:19:TYR:CA     | 8:E:22:ILE:HG22   | 2.39                     | 0.53              |
| 10:H:65:VAL:HG22  | 18:X:80:SER:OG    | 2.09                     | 0.53              |
| 21:G:138:ILE:HG13 | 21:G:144:LEU:CB   | 2.31                     | 0.53              |
| 21:G:172:VAL:CG1  | 24:G:608:CHL:C1B  | 2.86                     | 0.53              |
| 21:N:78:TYR:OH    | 21:N:217:LYS:NZ   | 2.20                     | 0.53              |
| 21:N:88:ASP:OD2   | 21:N:90:GLU:HB2   | 2.08                     | 0.53              |
| 25:N:603:CLA:HBC1 | 24:N:609:CHL:HBC2 | 1.91                     | 0.53              |
| 1:5:105:TRP:HZ3   | 24:5:302:CHL:CMB  | 2.20                     | 0.53              |
| 3:8:94:PHE:O      | 3:8:98:TYR:HD2    | 1.92                     | 0.53              |
| 25:c:510:CLA:H192 | 25:c:510:CLA:CHD  | 2.38                     | 0.53              |
| 15:o:144:THR:OG1  | 15:o:322:LYS:HB3  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:s:177:ALA:CB   | 24:s:306:CHL:HED2 | 2.38                     | 0.53              |
| 20:s:266:LEU:HD13 | 25:s:313:CLA:HMD2 | 1.91                     | 0.53              |
| 21:g:172:VAL:CG1  | 24:g:608:CHL:C1B  | 2.86                     | 0.53              |
| 24:g:609:CHL:HHC  | 24:g:609:CHL:HBB1 | 1.90                     | 0.53              |
| 21:n:88:ASP:OD2   | 21:n:90:GLU:HB2   | 2.08                     | 0.53              |
| 25:n:611:CLA:HMC2 | 26:n:618:LHG:H341 | 1.91                     | 0.53              |
| 21:y:219:GLY:O    | 21:y:223:MET:HE2  | 2.08                     | 0.53              |
| 1:1:229:PHE:CE2   | 1:1:240:PRO:HB3   | 2.43                     | 0.53              |
| 2:2:104:ARG:HG3   | 24:2:603:CHL:CED  | 2.39                     | 0.53              |
| 2:2:122:TRP:O     | 2:2:123:VAL:CG2   | 2.54                     | 0.53              |
| 1:3:88:ASP:OD2    | 1:3:90:GLU:HB2    | 2.08                     | 0.53              |
| 3:4:221:LEU:HD12  | 3:4:222:GLU:HG3   | 1.90                     | 0.53              |
| 4:A:133:LEU:HD21  | 7:D:256:GLN:HB2   | 1.90                     | 0.53              |
| 5:B:161:LEU:HD21  | 30:B:623:LMG:O2   | 2.08                     | 0.53              |
| 6:C:209:ILE:HG13  | 6:C:239:TRP:NE1   | 2.23                     | 0.53              |
| 7:D:57:THR:OG1    | 7:D:70:GLU:OE1    | 2.25                     | 0.53              |
| 7:D:173:SER:HB2   | 7:D:178:ALA:CB    | 2.28                     | 0.53              |
| 10:H:56:ILE:HA    | 18:X:84:LYS:CE    | 2.37                     | 0.53              |
| 29:L:101:SQD:H152 | 29:L:101:SQD:H292 | 1.90                     | 0.53              |
| 15:O:140:PRO:HD2  | 15:O:169:TYR:HD2  | 1.71                     | 0.53              |
| 21:N:115:PHE:CD2  | 25:N:604:CLA:HHD  | 2.44                     | 0.53              |
| 21:N:219:GLY:C    | 21:N:223:MET:HE2  | 2.33                     | 0.53              |
| 25:N:610:CLA:H8   | 39:N:615:LUT:C30  | 2.38                     | 0.53              |
| 21:Y:59:LEU:O     | 21:Y:63:SER:OG    | 2.22                     | 0.53              |
| 2:6:97:ALA:HB1    | 2:6:190:LEU:HD11  | 1.91                     | 0.53              |
| 2:6:104:ARG:HH21  | 24:6:603:CHL:HBA2 | 1.73                     | 0.53              |
| 1:7:131:TRP:CE3   | 1:7:132:PHE:HB3   | 2.43                     | 0.53              |
| 3:8:118:VAL:HG23  | 3:8:122:TRP:CE2   | 2.44                     | 0.53              |
| 3:8:183:GLU:CD    | 3:8:185:PHE:HE1   | 2.15                     | 0.53              |
| 4:a:133:LEU:HD21  | 7:d:256:GLN:HB2   | 1.90                     | 0.53              |
| 7:d:350:GLY:HA2   | 7:d:353:LEU:CD2   | 2.39                     | 0.53              |
| 20:s:223:VAL:HG12 | 25:s:311:CLA:HED1 | 1.91                     | 0.53              |
| 21:g:231:VAL:CG1  | 25:g:613:CLA:HHD  | 2.39                     | 0.53              |
| 24:g:608:CHL:H152 | 40:g:617:NEX:H402 | 1.89                     | 0.53              |
| 26:n:618:LHG:H321 | 26:n:618:LHG:H122 | 1.90                     | 0.53              |
| 21:y:138:ILE:HG13 | 21:y:144:LEU:CB   | 2.31                     | 0.53              |
| 21:y:165:GLN:O    | 21:y:169:MET:HB2  | 2.08                     | 0.53              |
| 2:2:50:TRP:HB2    | 2:2:213:LYS:HE2   | 1.90                     | 0.53              |
| 2:2:104:ARG:HH21  | 24:2:603:CHL:HBA2 | 1.73                     | 0.53              |
| 1:3:59:LEU:O      | 1:3:63:SER:OG     | 2.22                     | 0.53              |
| 4:A:56:PRO:HB2    | 15:O:208:ARG:NH2  | 2.24                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:A:408:LMG:H292 | 6:C:216:SER:HA    | 1.89                     | 0.53              |
| 25:B:608:CLA:C15  | 25:B:609:CLA:H203 | 2.39                     | 0.53              |
| 7:D:220:GLU:HA    | 7:D:223:LEU:HG    | 1.91                     | 0.53              |
| 7:D:299:PHE:O     | 7:D:303:GLU:HG2   | 2.09                     | 0.53              |
| 15:O:117:ILE:HG21 | 15:O:298:GLU:HB3  | 1.89                     | 0.53              |
| 20:S:196:PHE:HB2  | 24:S:308:CHL:CBC  | 2.39                     | 0.53              |
| 21:N:159:LEU:HD11 | 21:Y:257:TRP:HB3  | 1.88                     | 0.53              |
| 25:N:613:CLA:HBD  | 25:N:613:CLA:HAA1 | 1.90                     | 0.53              |
| 21:Y:130:VAL:HB   | 21:Y:133:LYS:HB2  | 1.90                     | 0.53              |
| 1:5:219:GLY:O     | 1:5:223:MET:HE2   | 2.08                     | 0.53              |
| 2:6:130:PRO:HG2   | 2:6:133:PHE:CB    | 2.37                     | 0.53              |
| 2:6:178:ILE:HG12  | 1:7:64:GLY:CA     | 2.39                     | 0.53              |
| 4:a:184:ILE:HG23  | 4:a:328:MET:SD    | 2.48                     | 0.53              |
| 27:a:405:PHO:CMB  | 27:a:405:PHO:HBB1 | 2.38                     | 0.53              |
| 5:b:36:SER:OG     | 28:b:618:BCR:H362 | 2.08                     | 0.53              |
| 5:b:110:ALA:HB1   | 25:b:616:CLA:HBB  | 1.91                     | 0.53              |
| 6:c:209:ILE:HG13  | 6:c:239:TRP:NE1   | 2.23                     | 0.53              |
| 6:c:461:ARG:NH1   | 7:d:242:GLU:HG3   | 2.23                     | 0.53              |
| 8:e:19:TYR:HB3    | 8:e:20:TRP:CE3    | 2.43                     | 0.53              |
| 15:o:177:PRO:CG   | 15:o:189:LYS:HE3  | 2.39                     | 0.53              |
| 21:g:138:ILE:HD12 | 24:g:606:CHL:HAC1 | 1.89                     | 0.53              |
| 21:g:165:GLN:O    | 21:g:169:MET:HB2  | 2.08                     | 0.53              |
| 21:n:225:SER:OG   | 39:n:615:LUT:H192 | 2.08                     | 0.53              |
| 21:y:130:VAL:HB   | 21:y:133:LYS:HB2  | 1.90                     | 0.53              |
| 22:r:85:LYS:HG2   | 22:r:86:PRO:CD    | 2.38                     | 0.53              |
| 22:r:184:LEU:HD13 | 24:r:605:CHL:OBD  | 2.08                     | 0.53              |
| 25:2:604:CLA:HHC  | 26:2:606:LHG:HC41 | 1.90                     | 0.53              |
| 3:4:110:MET:O     | 3:4:113:VAL:HG12  | 2.09                     | 0.53              |
| 5:B:320:ALA:HB1   | 7:D:293:ASN:HD22  | 1.73                     | 0.53              |
| 20:S:177:ALA:CB   | 24:S:306:CHL:HED2 | 2.38                     | 0.53              |
| 21:G:115:PHE:HB3  | 21:G:116:PRO:HD3  | 1.91                     | 0.53              |
| 21:N:56:VAL:HG11  | 24:N:601:CHL:HBC1 | 1.90                     | 0.53              |
| 21:N:144:LEU:HD22 | 24:N:606:CHL:HMD2 | 1.91                     | 0.53              |
| 21:N:227:PHE:CD2  | 25:N:602:CLA:H171 | 2.44                     | 0.53              |
| 21:Y:88:ASP:OD2   | 21:Y:90:GLU:HB2   | 2.08                     | 0.53              |
| 21:Y:108:LEU:HD11 | 25:Y:311:CLA:CBC  | 2.39                     | 0.53              |
| 21:Y:131:TRP:CZ3  | 21:Y:132:PHE:HB3  | 2.44                     | 0.53              |
| 1:7:130:VAL:HB    | 1:7:133:LYS:HB2   | 1.90                     | 0.53              |
| 1:7:219:GLY:O     | 1:7:223:MET:HE2   | 2.08                     | 0.53              |
| 4:a:51:ALA:HB3    | 4:a:82:ILE:HD12   | 1.90                     | 0.53              |
| 7:d:287:VAL:HG21  | 25:d:402:CLA:HED2 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:s:188:TYR:OH   | 40:s:317:NEX:H162 | 2.08                     | 0.53              |
| 25:g:603:CLA:HAC1 | 24:g:607:CHL:HBB2 | 1.90                     | 0.53              |
| 21:n:131:TRP:CZ3  | 21:n:132:PHE:HB3  | 2.44                     | 0.53              |
| 21:y:229:PHE:CE2  | 21:y:240:PRO:HB3  | 2.43                     | 0.53              |
| 22:r:238:LEU:HD22 | 25:r:609:CLA:O1A  | 2.09                     | 0.53              |
| 2:2:50:TRP:HB2    | 2:2:213:LYS:CE    | 2.38                     | 0.53              |
| 4:A:49:ILE:HA     | 31:D:405:PL9:H503 | 1.91                     | 0.53              |
| 4:A:335:ASN:HB3   | 6:C:334:PRO:HB3   | 1.91                     | 0.53              |
| 5:B:110:ALA:HB1   | 25:B:616:CLA:HBB  | 1.91                     | 0.53              |
| 6:C:451:ALA:HB2   | 6:C:456:GLU:OE1   | 2.08                     | 0.53              |
| 25:C:501:CLA:C1C  | 25:C:503:CLA:H71  | 2.39                     | 0.53              |
| 25:C:505:CLA:H191 | 35:C:515:DGD:HA81 | 1.91                     | 0.53              |
| 7:D:237:ASN:HB3   | 7:D:240:GLN:HB2   | 1.90                     | 0.53              |
| 13:L:5:ASN:HD22   | 13:L:8:GLU:HB2    | 1.74                     | 0.53              |
| 15:O:188:PHE:HD2  | 15:O:218:LEU:HD11 | 1.74                     | 0.53              |
| 15:O:233:VAL:HB   | 15:O:281:SER:O    | 2.08                     | 0.53              |
| 15:O:312:ASP:OD1  | 15:O:313:LEU:N    | 2.38                     | 0.53              |
| 20:S:188:TYR:OH   | 40:S:317:NEX:H162 | 2.08                     | 0.53              |
| 20:S:223:VAL:HG12 | 25:S:311:CLA:HED1 | 1.91                     | 0.53              |
| 21:G:179:GLY:HA2  | 24:G:608:CHL:HAC1 | 1.91                     | 0.53              |
| 24:G:606:CHL:CBB  | 39:G:616:LUT:H161 | 2.39                     | 0.53              |
| 24:N:607:CHL:HBA2 | 24:Y:302:CHL:H201 | 1.90                     | 0.53              |
| 1:5:115:PHE:HB3   | 1:5:116:PRO:HD3   | 1.91                     | 0.53              |
| 2:6:191:TYR:CZ    | 2:6:212:LEU:HD22  | 2.44                     | 0.53              |
| 1:7:100:VAL:CG2   | 1:7:190:LEU:HD13  | 2.39                     | 0.53              |
| 1:7:131:TRP:CZ3   | 1:7:132:PHE:HB3   | 2.44                     | 0.53              |
| 7:d:220:GLU:HA    | 7:d:223:LEU:HG    | 1.91                     | 0.53              |
| 22:r:67:TRP:CZ3   | 22:r:82:GLY:HA2   | 2.44                     | 0.53              |
| 22:r:189:SER:O    | 22:r:192:ILE:HG22 | 2.08                     | 0.53              |
| 2:2:191:TYR:CZ    | 2:2:212:LEU:HD22  | 2.44                     | 0.53              |
| 3:4:162:VAL:O     | 3:4:166:ASN:N     | 2.33                     | 0.53              |
| 4:A:56:PRO:HD2    | 4:A:106:LEU:HB3   | 1.91                     | 0.53              |
| 4:A:76:ASN:ND2    | 13:L:34:ASN:HB3   | 2.24                     | 0.53              |
| 4:A:255:PHE:HE2   | 4:A:264:SER:HB3   | 1.74                     | 0.53              |
| 5:B:218:SER:O     | 22:R:130:VAL:HG21 | 2.09                     | 0.53              |
| 15:O:177:PRO:CG   | 15:O:189:LYS:HE3  | 2.39                     | 0.53              |
| 25:G:604:CLA:NC   | 40:G:617:NEX:O23  | 2.41                     | 0.53              |
| 25:N:610:CLA:H71  | 25:N:612:CLA:C10  | 2.38                     | 0.53              |
| 25:N:611:CLA:HMC2 | 26:N:618:LHG:H341 | 1.91                     | 0.53              |
| 21:Y:78:TYR:OH    | 21:Y:217:LYS:NZ   | 2.20                     | 0.53              |
| 25:Y:303:CLA:HMB1 | 25:Y:303:CLA:C2   | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:U:97:THR:CA    | 23:U:102:ARG:HH21 | 2.09                     | 0.53              |
| 1:5:131:TRP:CZ3   | 1:5:132:PHE:HB3   | 2.44                     | 0.53              |
| 1:5:165:GLN:O     | 1:5:169:MET:HB2   | 2.08                     | 0.53              |
| 4:a:324:ALA:O     | 4:a:328:MET:HG3   | 2.08                     | 0.53              |
| 5:b:19:LEU:O      | 5:b:22:VAL:HG22   | 2.08                     | 0.53              |
| 5:b:274:GLN:HB3   | 5:b:279:TYR:HB3   | 1.90                     | 0.53              |
| 6:c:225:VAL:HG22  | 6:c:289:PHE:HE1   | 1.73                     | 0.53              |
| 6:c:451:ALA:HB2   | 6:c:456:GLU:OE1   | 2.08                     | 0.53              |
| 7:d:194:LEU:HD22  | 7:d:316:TYR:CE1   | 2.42                     | 0.53              |
| 7:d:237:ASN:HB3   | 7:d:240:GLN:HB2   | 1.90                     | 0.53              |
| 14:m:5:ILE:HG13   | 14:m:6:LEU:HD12   | 1.91                     | 0.53              |
| 15:o:145:VAL:HG11 | 15:o:203:LEU:CD1  | 2.35                     | 0.53              |
| 21:g:69:TYR:OH    | 21:g:81:ASP:OD2   | 2.20                     | 0.53              |
| 21:g:107:MET:HE3  | 25:g:610:CLA:CMC  | 2.38                     | 0.53              |
| 21:g:198:PRO:HD2  | 39:g:615:LUT:H23  | 1.91                     | 0.53              |
| 24:g:606:CHL:CBB  | 39:g:616:LUT:H161 | 2.39                     | 0.53              |
| 21:y:131:TRP:CZ3  | 21:y:132:PHE:HB3  | 2.44                     | 0.53              |
| 24:r:607:CHL:H93  | 24:r:607:CHL:CMB  | 2.39                     | 0.53              |
| 25:r:608:CLA:HBC2 | 25:r:608:CLA:HMC3 | 1.90                     | 0.53              |
| 1:1:131:TRP:CZ3   | 1:1:132:PHE:HB3   | 2.44                     | 0.53              |
| 2:2:161:ALA:HB1   | 2:2:165:PHE:CE2   | 2.44                     | 0.53              |
| 1:3:100:VAL:HG11  | 1:3:190:LEU:HD13  | 1.91                     | 0.53              |
| 1:3:131:TRP:CE3   | 1:3:132:PHE:HB3   | 2.43                     | 0.53              |
| 5:B:19:LEU:O      | 5:B:22:VAL:HG22   | 2.08                     | 0.53              |
| 6:C:189:TRP:CH2   | 6:C:362:ARG:HG2   | 2.44                     | 0.53              |
| 7:D:350:GLY:HA2   | 7:D:353:LEU:CD2   | 2.39                     | 0.53              |
| 10:H:29:GLU:HA    | 22:R:113:ARG:HH22 | 1.74                     | 0.53              |
| 14:M:5:ILE:HG13   | 14:M:6:LEU:HD12   | 1.91                     | 0.53              |
| 15:O:117:ILE:HG22 | 15:O:298:GLU:HB3  | 1.89                     | 0.53              |
| 20:S:266:LEU:O    | 20:S:270:ILE:HG23 | 2.09                     | 0.53              |
| 21:G:131:TRP:CZ3  | 21:G:132:PHE:HB3  | 2.44                     | 0.53              |
| 25:G:613:CLA:C1B  | 39:G:615:LUT:H42  | 2.39                     | 0.53              |
| 21:N:131:TRP:CZ3  | 21:N:132:PHE:HB3  | 2.44                     | 0.53              |
| 21:N:176:ARG:HG3  | 24:N:608:CHL:CHD  | 2.39                     | 0.53              |
| 22:R:144:GLY:HA3  | 22:R:246:ALA:CB   | 2.20                     | 0.53              |
| 22:R:150:ALA:CB   | 41:R:616:XAT:H181 | 2.39                     | 0.53              |
| 2:6:161:ALA:HB1   | 2:6:165:PHE:CE2   | 2.44                     | 0.53              |
| 3:8:103:LEU:HD22  | 3:8:193:GLY:CA    | 2.39                     | 0.53              |
| 4:a:56:PRO:HB2    | 15:o:208:ARG:NH2  | 2.24                     | 0.53              |
| 5:b:331:ASP:HA    | 5:b:335:GLY:O     | 2.08                     | 0.53              |
| 5:b:482:ILE:HG21  | 7:d:139:LEU:CD2   | 2.33                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:c:513:CLA:CMB  | 25:c:513:CLA:HBB1 | 2.39                     | 0.53              |
| 13:l:5:ASN:HD22   | 13:l:8:GLU:HB2    | 1.74                     | 0.53              |
| 21:g:94:ARG:HG2   | 21:n:84:GLY:CA    | 2.38                     | 0.53              |
| 21:g:100:VAL:CG2  | 21:g:190:LEU:HD13 | 2.39                     | 0.53              |
| 24:g:606:CHL:HBC2 | 24:g:607:CHL:HHD  | 1.90                     | 0.53              |
| 21:y:100:VAL:CG2  | 21:y:190:LEU:HD13 | 2.39                     | 0.53              |
| 21:y:104:ARG:HD3  | 25:y:311:CLA:C4C  | 2.38                     | 0.53              |
| 22:r:94:ILE:H     | 22:r:94:ILE:HD12  | 1.74                     | 0.53              |
| 2:2:69:TYR:HE1    | 2:2:70:LEU:HG     | 1.70                     | 0.52              |
| 1:3:229:PHE:CE2   | 1:3:240:PRO:HB3   | 2.43                     | 0.52              |
| 3:4:114:LEU:O     | 3:4:118:VAL:HG12  | 2.09                     | 0.52              |
| 21:G:133:LYS:O    | 21:G:136:SER:OG   | 2.20                     | 0.52              |
| 21:N:164:THR:HG23 | 21:N:168:LEU:HD12 | 1.92                     | 0.52              |
| 21:Y:165:GLN:O    | 21:Y:169:MET:HB2  | 2.08                     | 0.52              |
| 22:R:238:LEU:HD22 | 25:R:609:CLA:O1A  | 2.09                     | 0.52              |
| 2:6:104:ARG:HG3   | 24:6:603:CHL:CED  | 2.39                     | 0.52              |
| 3:8:155:TRP:CD1   | 3:8:159:LYS:NZ    | 2.74                     | 0.52              |
| 3:8:173:GLU:OE1   | 22:r:59:TYR:HA    | 2.08                     | 0.52              |
| 5:b:320:ALA:HB1   | 7:d:293:ASN:HD22  | 1.73                     | 0.52              |
| 5:b:380:ASP:OD2   | 7:d:343:PRO:HG2   | 2.09                     | 0.52              |
| 11:i:14:PHE:CZ    | 11:i:18:LEU:HD11  | 2.44                     | 0.52              |
| 24:s:307:CHL:HBC3 | 24:s:307:CHL:CMC  | 2.39                     | 0.52              |
| 25:s:311:CLA:HAA1 | 25:s:311:CLA:HBD  | 1.90                     | 0.52              |
| 21:n:56:VAL:HB    | 24:n:601:CHL:HBC2 | 1.91                     | 0.52              |
| 40:n:617:NEX:H42  | 40:n:617:NEX:H172 | 1.91                     | 0.52              |
| 21:y:108:LEU:HD11 | 25:y:311:CLA:CBC  | 2.39                     | 0.52              |
| 22:r:245:HIS:CD2  | 25:r:610:CLA:HMD1 | 2.45                     | 0.52              |
| 25:r:604:CLA:HHC  | 40:r:617:NEX:H222 | 1.91                     | 0.52              |
| 1:1:164:THR:HG23  | 1:1:168:LEU:HD12  | 1.92                     | 0.52              |
| 2:2:117:GLU:HB3   | 2:2:121:LYS:CE    | 2.40                     | 0.52              |
| 1:3:131:TRP:CZ3   | 1:3:132:PHE:HB3   | 2.44                     | 0.52              |
| 20:S:170:ASN:H    | 20:S:173:LEU:HB2  | 1.73                     | 0.52              |
| 21:G:94:ARG:HG2   | 21:N:84:GLY:CA    | 2.38                     | 0.52              |
| 21:G:165:GLN:O    | 21:G:169:MET:HB2  | 2.08                     | 0.52              |
| 21:G:218:ASN:HD22 | 25:G:612:CLA:C4A  | 2.21                     | 0.52              |
| 24:N:608:CHL:H42  | 39:N:615:LUT:H362 | 1.90                     | 0.52              |
| 24:Y:308:CHL:H2   | 32:Y:322:AJP:O79  | 2.09                     | 0.52              |
| 22:R:143:HIS:HB3  | 22:R:250:MET:HE3  | 1.91                     | 0.52              |
| 24:R:607:CHL:H93  | 24:R:607:CHL:CMB  | 2.38                     | 0.52              |
| 1:5:100:VAL:CG2   | 1:5:190:LEU:HD13  | 2.39                     | 0.52              |
| 25:6:604:CLA:HHC  | 26:6:606:LHG:HC41 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:114:LEU:O     | 3:8:118:VAL:HG12  | 2.09                     | 0.52              |
| 25:c:505:CLA:H191 | 35:c:515:DGD:HA81 | 1.91                     | 0.52              |
| 8:e:19:TYR:CA     | 8:e:22:ILE:HG22   | 2.39                     | 0.52              |
| 8:e:55:TYR:O      | 8:e:60:ARG:NH1    | 2.35                     | 0.52              |
| 10:h:29:GLU:HA    | 22:r:113:ARG:HH22 | 1.75                     | 0.52              |
| 10:h:67:LEU:O     | 10:h:68:ASP:HB2   | 2.08                     | 0.52              |
| 21:n:131:TRP:CE3  | 21:n:132:PHE:HB3  | 2.43                     | 0.52              |
| 21:n:176:ARG:HG3  | 24:n:608:CHL:CHD  | 2.39                     | 0.52              |
| 21:n:227:PHE:CD2  | 25:n:602:CLA:H171 | 2.44                     | 0.52              |
| 25:n:610:CLA:H51  | 25:n:612:CLA:CMA  | 2.37                     | 0.52              |
| 21:y:164:THR:HG23 | 21:y:168:LEU:HD12 | 1.92                     | 0.52              |
| 22:r:143:HIS:HB3  | 22:r:250:MET:HE3  | 1.91                     | 0.52              |
| 1:1:100:VAL:HG11  | 1:1:190:LEU:HD13  | 1.92                     | 0.52              |
| 1:1:115:PHE:HB3   | 1:1:116:PRO:HD3   | 1.91                     | 0.52              |
| 2:2:116:PRO:HG3   | 2:2:134:LYS:CE    | 2.40                     | 0.52              |
| 3:4:78:PRO:C      | 3:4:229:ILE:HG21  | 2.35                     | 0.52              |
| 4:A:57:PRO:HB2    | 4:A:66:PRO:HB2    | 1.91                     | 0.52              |
| 4:A:223:LEU:HB2   | 7:D:140:ARG:NH2   | 2.18                     | 0.52              |
| 25:A:401:CLA:HMC1 | 25:D:402:CLA:CAC  | 2.40                     | 0.52              |
| 5:B:314:TYR:CE2   | 5:B:316:GLY:HA3   | 2.43                     | 0.52              |
| 25:B:615:CLA:HMA2 | 25:B:615:CLA:HBA1 | 1.91                     | 0.52              |
| 28:B:617:BCR:H322 | 30:B:620:LMG:H111 | 1.92                     | 0.52              |
| 6:C:316:THR:HA    | 6:C:319:VAL:HG12  | 1.91                     | 0.52              |
| 7:D:287:VAL:HG21  | 25:D:402:CLA:HED2 | 1.91                     | 0.52              |
| 20:S:81:ILE:O     | 20:S:81:ILE:HG22  | 2.09                     | 0.52              |
| 21:G:100:VAL:HG11 | 21:G:190:LEU:HD13 | 1.92                     | 0.52              |
| 21:G:164:THR:HG23 | 21:G:168:LEU:HD12 | 1.92                     | 0.52              |
| 21:G:232:GLN:NE2  | 25:G:613:CLA:C4D  | 2.44                     | 0.52              |
| 25:N:603:CLA:C19  | 24:N:607:CHL:H172 | 2.39                     | 0.52              |
| 21:Y:100:VAL:CG2  | 21:Y:190:LEU:HD13 | 2.39                     | 0.52              |
| 21:Y:215:GLU:HB2  | 25:Y:311:CLA:CHB  | 2.40                     | 0.52              |
| 1:7:115:PHE:HB3   | 1:7:116:PRO:HD3   | 1.91                     | 0.52              |
| 1:7:164:THR:HG23  | 1:7:168:LEU:HD12  | 1.92                     | 0.52              |
| 3:8:110:MET:O     | 3:8:113:VAL:HG12  | 2.08                     | 0.52              |
| 4:a:76:ASN:ND2    | 13:l:34:ASN:HB3   | 2.24                     | 0.52              |
| 25:a:402:CLA:HMC1 | 25:d:402:CLA:CAC  | 2.40                     | 0.52              |
| 25:a:402:CLA:H191 | 26:d:406:LHG:H161 | 1.92                     | 0.52              |
| 5:b:188:GLU:O     | 5:b:194:VAL:HG21  | 2.10                     | 0.52              |
| 25:b:608:CLA:C15  | 25:b:609:CLA:H203 | 2.39                     | 0.52              |
| 7:d:222:THR:HG21  | 7:d:250:ALA:HB2   | 1.90                     | 0.52              |
| 11:i:24:LEU:HD12  | 28:i:101:BCR:HC31 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:t:14:LEU:CD1   | 28:t:101:BCR:H343 | 2.37                     | 0.52              |
| 20:s:134:LEU:HD23 | 24:n:605:CHL:HAA2 | 1.90                     | 0.52              |
| 25:g:613:CLA:C1B  | 39:g:615:LUT:H42  | 2.39                     | 0.52              |
| 21:n:86:SER:OG    | 25:n:602:CLA:HAA2 | 2.10                     | 0.52              |
| 21:y:76:GLY:HA3   | 21:y:216:LEU:CD2  | 2.25                     | 0.52              |
| 25:y:303:CLA:C2   | 25:y:303:CLA:HMB1 | 2.39                     | 0.52              |
| 22:r:57:LEU:HB2   | 22:r:59:TYR:CD1   | 2.45                     | 0.52              |
| 22:r:150:ALA:CB   | 41:r:616:XAT:H181 | 2.39                     | 0.52              |
| 1:1:138:ILE:HG13  | 1:1:144:LEU:CB    | 2.31                     | 0.52              |
| 2:2:88:ASP:HB3    | 2:2:91:ALA:HB2    | 1.89                     | 0.52              |
| 2:2:178:ILE:HG12  | 1:3:64:GLY:CA     | 2.39                     | 0.52              |
| 1:3:115:PHE:HB3   | 1:3:116:PRO:HD3   | 1.91                     | 0.52              |
| 3:4:94:PHE:O      | 3:4:98:TYR:HD2    | 1.92                     | 0.52              |
| 4:A:161:TYR:HA    | 4:A:294:ALA:CB    | 2.39                     | 0.52              |
| 19:Z:14:ILE:HG23  | 19:Z:18:ILE:HD11  | 1.92                     | 0.52              |
| 20:S:115:LEU:O    | 20:S:119:ARG:HG3  | 2.09                     | 0.52              |
| 20:S:130:ILE:HD12 | 25:S:305:CLA:CAC  | 2.38                     | 0.52              |
| 20:S:135:ASN:ND2  | 20:S:141:CYS:HB2  | 2.25                     | 0.52              |
| 25:N:613:CLA:H142 | 25:N:613:CLA:C2   | 2.40                     | 0.52              |
| 21:Y:164:THR:HG23 | 21:Y:168:LEU:HD12 | 1.92                     | 0.52              |
| 22:R:56:PRO:C     | 22:R:57:LEU:HD22  | 2.35                     | 0.52              |
| 22:R:57:LEU:HB2   | 22:R:59:TYR:CD1   | 2.44                     | 0.52              |
| 22:R:221:LYS:HD2  | 22:R:222:PHE:CD2  | 2.43                     | 0.52              |
| 22:R:270:ASN:HB3  | 25:R:612:CLA:HED3 | 1.92                     | 0.52              |
| 2:6:116:PRO:HG3   | 2:6:134:LYS:CE    | 2.40                     | 0.52              |
| 2:6:117:GLU:HB3   | 2:6:121:LYS:CE    | 2.40                     | 0.52              |
| 2:6:184:VAL:HG12  | 2:6:185:GLY:O     | 2.09                     | 0.52              |
| 1:7:100:VAL:HG11  | 1:7:190:LEU:HD13  | 1.91                     | 0.52              |
| 5:b:161:LEU:HD21  | 30:b:623:LMG:O2   | 2.08                     | 0.52              |
| 6:c:51:GLY:HA2    | 6:c:132:HIS:HB2   | 1.91                     | 0.52              |
| 6:c:459:ILE:HG21  | 6:c:464:GLU:HG3   | 1.92                     | 0.52              |
| 20:s:196:PHE:HB2  | 24:s:308:CHL:CB   | 2.39                     | 0.52              |
| 25:s:305:CLA:O1A  | 25:s:305:CLA:H3A  | 2.09                     | 0.52              |
| 25:n:603:CLA:HBC1 | 24:n:609:CHL:HBC2 | 1.91                     | 0.52              |
| 25:r:610:CLA:CB   | 26:r:618:LHG:HC5  | 2.33                     | 0.52              |
| 25:S:305:CLA:O1A  | 25:S:305:CLA:H3A  | 2.09                     | 0.52              |
| 21:N:60:GLY:H     | 24:N:601:CHL:CHC  | 2.23                     | 0.52              |
| 40:N:617:NEX:H42  | 40:N:617:NEX:H172 | 1.91                     | 0.52              |
| 25:Y:304:CLA:HMD3 | 24:Y:310:CHL:C4D  | 2.40                     | 0.52              |
| 22:R:229:ALA:O    | 22:R:235:THR:OG1  | 2.26                     | 0.52              |
| 27:a:405:PHO:H193 | 25:d:401:CLA:HHB  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:277:GLN:OE1   | 23:u:99:LYS:NZ    | 2.33                     | 0.52              |
| 6:c:87:ILE:CD1    | 25:c:504:CLA:HMB2 | 2.40                     | 0.52              |
| 7:d:57:THR:HB     | 7:d:70:GLU:OE1    | 2.09                     | 0.52              |
| 13:l:13:LEU:CB    | 14:m:25:ILE:HG22  | 2.40                     | 0.52              |
| 24:n:607:CHL:HBA2 | 24:y:302:CHL:H201 | 1.91                     | 0.52              |
| 3:4:110:MET:O     | 3:4:114:LEU:HD13  | 2.10                     | 0.52              |
| 7:D:194:LEU:HD22  | 7:D:316:TYR:CE1   | 2.42                     | 0.52              |
| 10:H:67:LEU:O     | 10:H:68:ASP:HB2   | 2.08                     | 0.52              |
| 11:I:14:PHE:CZ    | 11:I:18:LEU:HD11  | 2.44                     | 0.52              |
| 25:S:305:CLA:C1C  | 40:S:317:NEX:H222 | 2.39                     | 0.52              |
| 21:G:100:VAL:CG2  | 21:G:190:LEU:HD13 | 2.39                     | 0.52              |
| 21:G:224:PHE:CE2  | 25:G:613:CLA:HAB  | 2.45                     | 0.52              |
| 24:G:606:CHL:HBC2 | 24:G:607:CHL:HHD  | 1.90                     | 0.52              |
| 21:N:86:SER:OG    | 25:N:602:CLA:HAA2 | 2.10                     | 0.52              |
| 21:N:115:PHE:HB3  | 21:N:116:PRO:HD3  | 1.91                     | 0.52              |
| 21:Y:115:PHE:HB3  | 21:Y:116:PRO:HD3  | 1.91                     | 0.52              |
| 1:5:100:VAL:HG11  | 1:5:190:LEU:HD13  | 1.92                     | 0.52              |
| 2:6:127:PHE:N     | 2:6:148:LEU:HD21  | 2.25                     | 0.52              |
| 5:b:16:PRO:HB3    | 5:b:133:LEU:HD11  | 1.90                     | 0.52              |
| 5:b:45:PHE:O      | 5:b:58:GLN:OE1    | 2.27                     | 0.52              |
| 9:f:17:VAL:HG23   | 9:f:18:HIS:CD2    | 2.45                     | 0.52              |
| 9:f:20:LEU:O      | 9:f:24:THR:OG1    | 2.15                     | 0.52              |
| 15:o:188:PHE:HD2  | 15:o:218:LEU:HD11 | 1.74                     | 0.52              |
| 18:x:99:VAL:O     | 18:x:103:VAL:HG23 | 2.10                     | 0.52              |
| 21:g:225:SER:O    | 21:g:229:PHE:CD1  | 2.63                     | 0.52              |
| 25:g:602:CLA:H121 | 25:g:602:CLA:C9   | 2.38                     | 0.52              |
| 21:n:100:VAL:CG2  | 21:n:190:LEU:HD13 | 2.39                     | 0.52              |
| 21:n:115:PHE:HB3  | 21:n:116:PRO:HD3  | 1.91                     | 0.52              |
| 21:y:215:GLU:HB2  | 25:y:311:CLA:CHB  | 2.40                     | 0.52              |
| 22:r:138:GLU:OE2  | 25:r:608:CLA:HED3 | 2.09                     | 0.52              |
| 22:r:202:ILE:HG13 | 22:r:203:GLU:N    | 2.25                     | 0.52              |
| 2:2:100:VAL:HG11  | 2:2:190:LEU:HD23  | 1.91                     | 0.52              |
| 4:A:297:LEU:HD11  | 6:C:425:TRP:CZ3   | 2.45                     | 0.52              |
| 30:A:408:LMG:O5   | 17:W:87:THR:O     | 2.27                     | 0.52              |
| 5:B:380:ASP:OD2   | 7:D:343:PRO:HG2   | 2.09                     | 0.52              |
| 25:B:604:CLA:H92  | 25:B:604:CLA:C4   | 2.34                     | 0.52              |
| 9:F:17:VAL:HG23   | 9:F:18:HIS:CD2    | 2.45                     | 0.52              |
| 21:N:56:VAL:HB    | 24:N:601:CHL:HBC2 | 1.91                     | 0.52              |
| 21:N:86:SER:HB3   | 21:N:92:PHE:CD1   | 2.45                     | 0.52              |
| 21:Y:100:VAL:HB   | 21:Y:190:LEU:HD13 | 1.92                     | 0.52              |
| 22:R:138:GLU:OE2  | 25:R:608:CLA:HED3 | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:R:602:CLA:O2D  | 25:R:602:CLA:H2A  | 2.10                     | 0.52              |
| 24:6:603:CHL:CMC  | 24:6:603:CHL:HBC3 | 2.40                     | 0.52              |
| 4:a:161:TYR:HA    | 4:a:294:ALA:CB    | 2.39                     | 0.52              |
| 6:c:79:LYS:HD3    | 6:c:83:GLU:HB3    | 1.92                     | 0.52              |
| 20:s:128:PHE:CE1  | 39:s:316:LUT:H173 | 2.42                     | 0.52              |
| 21:g:69:TYR:CE1   | 21:y:90:GLU:HG3   | 2.44                     | 0.52              |
| 21:g:115:PHE:HB3  | 21:g:116:PRO:HD3  | 1.91                     | 0.52              |
| 21:g:131:TRP:CZ3  | 21:g:132:PHE:HB3  | 2.44                     | 0.52              |
| 21:n:115:PHE:CD2  | 25:n:604:CLA:HHD  | 2.44                     | 0.52              |
| 24:n:609:CHL:HBC3 | 24:y:302:CHL:C9   | 2.40                     | 0.52              |
| 1:1:225:SER:O     | 1:1:229:PHE:CD1   | 2.63                     | 0.52              |
| 3:4:183:GLU:HB3   | 3:4:185:PHE:CE1   | 2.45                     | 0.52              |
| 3:4:253:LEU:HD12  | 3:4:254:GLY:N     | 2.25                     | 0.52              |
| 5:B:122:ILE:HA    | 10:H:24:LYS:CD    | 2.40                     | 0.52              |
| 5:B:341:LEU:HD12  | 5:B:429:ILE:CG2   | 2.38                     | 0.52              |
| 25:B:601:CLA:HMC1 | 28:H:101:BCR:C19  | 2.40                     | 0.52              |
| 6:C:79:LYS:HD3    | 6:C:83:GLU:HB3    | 1.92                     | 0.52              |
| 6:C:447:ARG:HD3   | 25:C:508:CLA:HED1 | 1.92                     | 0.52              |
| 7:D:12:GLU:OE1    | 7:D:12:GLU:N      | 2.43                     | 0.52              |
| 7:D:12:GLU:HG2    | 7:D:13:LYS:N      | 2.25                     | 0.52              |
| 15:O:144:THR:OG1  | 15:O:322:LYS:HB3  | 2.09                     | 0.52              |
| 28:T:101:BCR:H271 | 5:b:39:LEU:CB     | 2.39                     | 0.52              |
| 21:Y:138:ILE:HD13 | 24:Y:307:CHL:CBC  | 2.39                     | 0.52              |
| 1:5:94:ARG:HA     | 1:5:94:ARG:HE     | 1.75                     | 0.52              |
| 1:7:225:SER:O     | 1:7:229:PHE:CD1   | 2.63                     | 0.52              |
| 4:a:40:THR:HG23   | 25:a:406:CLA:HBB1 | 1.92                     | 0.52              |
| 4:a:49:ILE:HA     | 31:d:405:PL9:H503 | 1.91                     | 0.52              |
| 4:a:56:PRO:HD2    | 4:a:106:LEU:HB3   | 1.91                     | 0.52              |
| 25:b:615:CLA:HMA2 | 25:b:615:CLA:HBA1 | 1.91                     | 0.52              |
| 6:c:320:ARG:O     | 6:c:323:ARG:HB2   | 2.10                     | 0.52              |
| 7:d:12:GLU:OE1    | 7:d:12:GLU:N      | 2.43                     | 0.52              |
| 15:o:290:THR:HG22 | 15:o:291:LYS:N    | 2.19                     | 0.52              |
| 21:g:100:VAL:HG11 | 21:g:190:LEU:HD13 | 1.92                     | 0.52              |
| 21:g:224:PHE:CE2  | 25:g:613:CLA:HAB  | 2.45                     | 0.52              |
| 21:n:144:LEU:HD22 | 24:n:606:CHL:HMD2 | 1.91                     | 0.52              |
| 21:y:69:TYR:OH    | 21:y:81:ASP:OD2   | 2.20                     | 0.52              |
| 21:y:86:SER:HB3   | 21:y:92:PHE:CD1   | 2.45                     | 0.52              |
| 25:y:304:CLA:HMD3 | 24:y:310:CHL:C4D  | 2.40                     | 0.52              |
| 1:1:100:VAL:CG2   | 1:1:190:LEU:HD13  | 2.39                     | 0.52              |
| 2:2:127:PHE:N     | 2:2:148:LEU:HD21  | 2.25                     | 0.52              |
| 2:2:173:VAL:HA    | 2:2:176:PHE:CD2   | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:103:LEU:HD22  | 3:4:193:GLY:CA    | 2.39                     | 0.52              |
| 4:A:170:ASP:OD2   | 6:C:357:ARG:NH1   | 2.43                     | 0.52              |
| 5:B:154:GLY:HA3   | 5:B:202:HIS:CB    | 2.40                     | 0.52              |
| 5:B:340:TRP:O     | 5:B:405:GLU:HG3   | 2.10                     | 0.52              |
| 9:F:31:ILE:O      | 9:F:35:GLN:HG2    | 2.10                     | 0.52              |
| 13:L:13:LEU:CB    | 14:M:25:ILE:HG22  | 2.40                     | 0.52              |
| 15:O:130:LYS:CD   | 15:O:179:GLU:HB2  | 2.40                     | 0.52              |
| 20:S:58:GLU:OE1   | 20:S:61:LYS:NZ    | 2.35                     | 0.52              |
| 21:G:69:TYR:CE1   | 21:Y:90:GLU:HG3   | 2.44                     | 0.52              |
| 21:G:107:MET:HE1  | 25:G:610:CLA:CHC  | 2.40                     | 0.52              |
| 24:G:606:CHL:CBA  | 40:G:617:NEX:H30  | 2.40                     | 0.52              |
| 26:N:618:LHG:H122 | 26:N:618:LHG:H321 | 1.90                     | 0.52              |
| 21:Y:51:TYR:HE2   | 21:Y:209:ALA:HB1  | 1.75                     | 0.52              |
| 21:Y:146:TYR:HB3  | 21:Y:152:LEU:CD1  | 2.36                     | 0.52              |
| 22:R:94:ILE:H     | 22:R:94:ILE:HD12  | 1.74                     | 0.52              |
| 1:5:130:VAL:HB    | 1:5:133:LYS:HB2   | 1.90                     | 0.52              |
| 4:a:57:PRO:HB2    | 4:a:66:PRO:HB2    | 1.90                     | 0.52              |
| 4:a:223:LEU:HD12  | 7:d:140:ARG:HH22  | 1.74                     | 0.52              |
| 4:a:297:LEU:HD11  | 6:c:425:TRP:CZ3   | 2.45                     | 0.52              |
| 5:b:154:GLY:HA3   | 5:b:202:HIS:HB2   | 1.92                     | 0.52              |
| 25:b:607:CLA:HBB1 | 25:b:607:CLA:HMB1 | 1.91                     | 0.52              |
| 6:c:30:THR:HG23   | 6:c:31:THR:CG2    | 2.37                     | 0.52              |
| 6:c:189:TRP:CH2   | 6:c:362:ARG:HG2   | 2.44                     | 0.52              |
| 25:c:501:CLA:C1C  | 25:c:503:CLA:H71  | 2.39                     | 0.52              |
| 7:d:12:GLU:HG2    | 7:d:13:LYS:N      | 2.25                     | 0.52              |
| 10:h:65:VAL:HG22  | 18:x:80:SER:OG    | 2.09                     | 0.52              |
| 25:s:305:CLA:C1C  | 40:s:317:NEX:H222 | 2.39                     | 0.52              |
| 21:g:107:MET:HE1  | 25:g:610:CLA:CHC  | 2.40                     | 0.52              |
| 25:g:602:CLA:H92  | 25:g:603:CLA:H122 | 1.91                     | 0.52              |
| 24:g:606:CHL:CBA  | 40:g:617:NEX:H30  | 2.40                     | 0.52              |
| 21:n:60:GLY:H     | 24:n:601:CHL:CHC  | 2.23                     | 0.52              |
| 21:n:100:VAL:HG11 | 21:n:190:LEU:HD13 | 1.92                     | 0.52              |
| 21:n:164:THR:HG23 | 21:n:168:LEU:HD12 | 1.92                     | 0.52              |
| 1:1:100:VAL:HB    | 1:1:190:LEU:HD13  | 1.92                     | 0.52              |
| 2:2:130:PRO:HG2   | 2:2:133:PHE:CB    | 2.37                     | 0.52              |
| 2:2:211:GLU:O     | 2:2:214:VAL:HG12  | 2.09                     | 0.52              |
| 24:2:603:CHL:CMC  | 24:2:603:CHL:HBC3 | 2.40                     | 0.52              |
| 1:3:94:ARG:HA     | 1:3:94:ARG:HE     | 1.75                     | 0.52              |
| 1:3:100:VAL:CG2   | 1:3:190:LEU:HD13  | 2.39                     | 0.52              |
| 4:A:331:MET:HE1   | 7:D:321:LEU:HD22  | 1.92                     | 0.52              |
| 25:A:401:CLA:H191 | 26:D:406:LHG:H161 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:A:404:PHO:H202 | 25:D:401:CLA:C1B  | 2.40                     | 0.52              |
| 5:B:39:LEU:CB     | 28:t:101:BCR:H271 | 2.39                     | 0.52              |
| 11:I:24:LEU:HD12  | 28:I:101:BCR:HC31 | 1.92                     | 0.52              |
| 18:X:99:VAL:O     | 18:X:103:VAL:HG23 | 2.10                     | 0.52              |
| 25:S:311:CLA:CHB  | 26:S:318:LHG:HC31 | 2.40                     | 0.52              |
| 21:G:131:TRP:O    | 21:G:134:ALA:HB3  | 2.10                     | 0.52              |
| 21:G:231:VAL:CG1  | 25:G:613:CLA:HHD  | 2.39                     | 0.52              |
| 21:N:100:VAL:HB   | 21:N:190:LEU:HD13 | 1.92                     | 0.52              |
| 21:N:225:SER:O    | 21:N:229:PHE:CD1  | 2.63                     | 0.52              |
| 21:Y:131:TRP:O    | 21:Y:134:ALA:HB3  | 2.10                     | 0.52              |
| 24:Y:306:CHL:HHC  | 24:Y:306:CHL:HBB1 | 1.92                     | 0.52              |
| 25:R:603:CLA:HMC1 | 41:R:616:XAT:C13  | 2.40                     | 0.52              |
| 2:6:100:VAL:HG11  | 2:6:190:LEU:HD23  | 1.91                     | 0.52              |
| 3:8:183:GLU:HB3   | 3:8:185:PHE:CE1   | 2.45                     | 0.52              |
| 4:a:335:ASN:HB3   | 6:c:334:PRO:HB3   | 1.91                     | 0.52              |
| 5:b:478:VAL:O     | 5:b:478:VAL:HG22  | 2.10                     | 0.52              |
| 6:c:316:THR:HA    | 6:c:319:VAL:HG12  | 1.91                     | 0.52              |
| 7:d:150:PRO:HB3   | 25:d:402:CLA:H41  | 1.92                     | 0.52              |
| 21:g:164:THR:HG23 | 21:g:168:LEU:HD12 | 1.92                     | 0.52              |
| 21:y:115:PHE:HB3  | 21:y:116:PRO:HD3  | 1.91                     | 0.52              |
| 21:y:133:LYS:O    | 21:y:136:SER:OG   | 2.20                     | 0.52              |
| 25:r:602:CLA:O2D  | 25:r:602:CLA:H2A  | 2.10                     | 0.52              |
| 2:2:181:LEU:HD12  | 24:2:603:CHL:CHC  | 2.40                     | 0.51              |
| 1:3:86:SER:HB3    | 1:3:92:PHE:CD1    | 2.45                     | 0.51              |
| 5:B:154:GLY:HA3   | 5:B:202:HIS:HB2   | 1.91                     | 0.51              |
| 5:B:188:GLU:O     | 5:B:194:VAL:HG21  | 2.10                     | 0.51              |
| 26:B:625:LHG:HC5  | 7:D:270:PHE:CZ    | 2.46                     | 0.51              |
| 6:C:267:SER:CB    | 17:W:133:LEU:HD23 | 2.40                     | 0.51              |
| 25:C:513:CLA:CMB  | 25:C:513:CLA:HBB1 | 2.39                     | 0.51              |
| 20:S:266:LEU:HD13 | 25:S:313:CLA:HMD2 | 1.90                     | 0.51              |
| 25:G:602:CLA:H121 | 25:G:602:CLA:C9   | 2.38                     | 0.51              |
| 21:Y:98:LEU:HD22  | 25:Y:304:CLA:CBA  | 2.40                     | 0.51              |
| 2:6:228:PHE:O     | 2:6:232:VAL:HG23  | 2.10                     | 0.51              |
| 1:7:69:TYR:OH     | 1:7:81:ASP:OD2    | 2.20                     | 0.51              |
| 28:b:617:BCR:H322 | 30:b:620:LMG:H111 | 1.92                     | 0.51              |
| 6:c:433:LEU:HD13  | 25:c:502:CLA:CHC  | 2.41                     | 0.51              |
| 15:o:140:PRO:HD2  | 15:o:169:TYR:HD2  | 1.71                     | 0.51              |
| 20:s:135:ASN:ND2  | 20:s:141:CYS:HB2  | 2.25                     | 0.51              |
| 25:s:303:CLA:HAB  | 39:s:316:LUT:H32  | 1.91                     | 0.51              |
| 21:g:130:VAL:HB   | 21:g:133:LYS:HB2  | 1.90                     | 0.51              |
| 21:n:146:TYR:HB3  | 21:n:152:LEU:CD1  | 2.36                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:603:CLA:HMC1 | 41:r:616:XAT:C13  | 2.40                     | 0.51              |
| 2:2:101:ILE:O     | 2:2:104:ARG:HB3   | 2.11                     | 0.51              |
| 1:3:51:TYR:HE2    | 1:3:209:ALA:HB1   | 1.75                     | 0.51              |
| 6:C:30:THR:HG23   | 6:C:31:THR:CG2    | 2.37                     | 0.51              |
| 21:G:51:TYR:HE2   | 21:G:209:ALA:HB1  | 1.75                     | 0.51              |
| 21:G:59:LEU:O     | 21:G:63:SER:OG    | 2.22                     | 0.51              |
| 21:G:198:PRO:HD2  | 39:G:615:LUT:H23  | 1.91                     | 0.51              |
| 25:G:602:CLA:H92  | 25:G:603:CLA:H122 | 1.91                     | 0.51              |
| 21:N:59:LEU:O     | 21:N:63:SER:OG    | 2.22                     | 0.51              |
| 21:N:100:VAL:CG2  | 21:N:190:LEU:HD13 | 2.39                     | 0.51              |
| 21:N:172:VAL:CG1  | 24:N:608:CHL:C1B  | 2.88                     | 0.51              |
| 3:8:94:PHE:HB3    | 3:8:98:TYR:CE2    | 2.42                     | 0.51              |
| 27:a:405:PHO:H202 | 25:d:401:CLA:C1B  | 2.40                     | 0.51              |
| 7:d:94:TRP:O      | 18:x:83:LEU:HD23  | 2.10                     | 0.51              |
| 21:g:100:VAL:HB   | 21:g:190:LEU:HD13 | 1.92                     | 0.51              |
| 21:y:100:VAL:HG11 | 21:y:190:LEU:HD13 | 1.92                     | 0.51              |
| 1:3:225:SER:O     | 1:3:229:PHE:CD1   | 2.63                     | 0.51              |
| 4:A:223:LEU:HD12  | 7:D:140:ARG:HH22  | 1.74                     | 0.51              |
| 5:B:39:LEU:HB3    | 28:t:101:BCR:H381 | 1.93                     | 0.51              |
| 5:B:223:GLN:HA    | 10:H:33:VAL:CG1   | 2.38                     | 0.51              |
| 25:C:505:CLA:HAA1 | 25:C:505:CLA:CBD  | 2.39                     | 0.51              |
| 26:C:519:LHG:HC5  | 7:D:220:GLU:OE2   | 2.11                     | 0.51              |
| 7:D:57:THR:HB     | 7:D:70:GLU:OE1    | 2.09                     | 0.51              |
| 7:D:94:TRP:O      | 18:X:83:LEU:HD23  | 2.10                     | 0.51              |
| 20:S:262:PHE:CE2  | 25:S:314:CLA:H3A  | 2.43                     | 0.51              |
| 21:G:100:VAL:HB   | 21:G:190:LEU:HD13 | 1.92                     | 0.51              |
| 25:N:602:CLA:HBC2 | 25:N:602:CLA:CMC  | 2.40                     | 0.51              |
| 2:6:210:ALA:O     | 2:6:213:LYS:HG2   | 2.10                     | 0.51              |
| 3:8:78:PRO:C      | 3:8:229:ILE:HG21  | 2.35                     | 0.51              |
| 5:b:218:SER:O     | 22:r:130:VAL:HG21 | 2.09                     | 0.51              |
| 25:c:513:CLA:HMD3 | 20:s:75:LEU:CD1   | 2.41                     | 0.51              |
| 15:o:296:THR:HG22 | 15:o:296:THR:O    | 2.09                     | 0.51              |
| 20:s:115:LEU:O    | 20:s:119:ARG:HG3  | 2.09                     | 0.51              |
| 20:s:115:LEU:HB3  | 20:s:119:ARG:HH21 | 1.75                     | 0.51              |
| 21:n:69:TYR:OH    | 21:n:81:ASP:OD2   | 2.20                     | 0.51              |
| 21:n:225:SER:O    | 21:n:229:PHE:CD1  | 2.63                     | 0.51              |
| 24:y:308:CHL:H2   | 32:y:322:AJP:O79  | 2.09                     | 0.51              |
| 22:r:270:ASN:HB3  | 25:r:612:CLA:HED3 | 1.92                     | 0.51              |
| 2:2:210:ALA:O     | 2:2:213:LYS:HG2   | 2.10                     | 0.51              |
| 3:4:156:VAL:O     | 3:4:159:LYS:HB2   | 2.11                     | 0.51              |
| 4:A:58:VAL:HB     | 4:A:83:ILE:HB     | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:45:PHE:O      | 5:B:58:GLN:OE1    | 2.27                     | 0.51              |
| 24:S:307:CHL:HBC3 | 24:S:307:CHL:CMC  | 2.39                     | 0.51              |
| 21:Y:100:VAL:HG11 | 21:Y:190:LEU:HD13 | 1.92                     | 0.51              |
| 1:5:131:TRP:O     | 1:5:134:ALA:HB3   | 2.10                     | 0.51              |
| 1:5:146:TYR:CD1   | 1:5:147:LEU:HG    | 2.46                     | 0.51              |
| 2:6:173:VAL:HA    | 2:6:176:PHE:CD2   | 2.44                     | 0.51              |
| 2:6:181:LEU:HD12  | 24:6:603:CHL:CHC  | 2.40                     | 0.51              |
| 1:7:100:VAL:HB    | 1:7:190:LEU:HD13  | 1.92                     | 0.51              |
| 1:7:128:GLU:CB    | 1:7:137:GLN:HB2   | 2.41                     | 0.51              |
| 5:b:340:TRP:O     | 5:b:405:GLU:HG3   | 2.10                     | 0.51              |
| 6:c:80:PRO:HD2    | 6:c:83:GLU:OE1    | 2.10                     | 0.51              |
| 12:k:58:VAL:HG12  | 12:k:61:ARG:HD2   | 1.92                     | 0.51              |
| 25:s:311:CLA:CHB  | 26:s:318:LHG:HC31 | 2.40                     | 0.51              |
| 21:g:131:TRP:O    | 21:g:134:ALA:HB3  | 2.11                     | 0.51              |
| 21:y:225:SER:O    | 21:y:229:PHE:CD1  | 2.63                     | 0.51              |
| 24:y:306:CHL:HHC  | 24:y:306:CHL:HBB1 | 1.92                     | 0.51              |
| 1:1:210:GLU:OE1   | 1:1:214:LYS:NZ    | 2.38                     | 0.51              |
| 2:2:104:ARG:HE    | 24:2:603:CHL:CBD  | 2.13                     | 0.51              |
| 2:2:129:GLU:OE1   | 2:2:239:LYS:NZ    | 2.27                     | 0.51              |
| 2:2:210:ALA:HA    | 2:2:213:LYS:HZ3   | 1.76                     | 0.51              |
| 27:A:404:PHO:HAB  | 25:D:402:CLA:C1   | 2.41                     | 0.51              |
| 6:C:320:ARG:O     | 6:C:323:ARG:HB2   | 2.10                     | 0.51              |
| 6:C:459:ILE:HG21  | 6:C:464:GLU:HG3   | 1.92                     | 0.51              |
| 25:C:513:CLA:HMD1 | 20:S:75:LEU:CD1   | 2.39                     | 0.51              |
| 21:G:128:GLU:CB   | 21:G:137:GLN:HB2  | 2.41                     | 0.51              |
| 21:G:225:SER:O    | 21:G:229:PHE:CD1  | 2.63                     | 0.51              |
| 21:N:104:ARG:HD3  | 25:N:610:CLA:C4C  | 2.41                     | 0.51              |
| 25:N:610:CLA:H18  | 40:N:617:NEX:H372 | 1.92                     | 0.51              |
| 21:Y:227:PHE:CD2  | 25:Y:303:CLA:H202 | 2.40                     | 0.51              |
| 1:5:164:THR:HG23  | 1:5:168:LEU:HD12  | 1.92                     | 0.51              |
| 1:5:225:SER:O     | 1:5:229:PHE:CD1   | 2.63                     | 0.51              |
| 3:8:110:MET:O     | 3:8:114:LEU:HD13  | 2.10                     | 0.51              |
| 3:8:253:LEU:HD12  | 3:8:254:GLY:N     | 2.25                     | 0.51              |
| 4:a:58:VAL:HB     | 4:a:83:ILE:HB     | 1.93                     | 0.51              |
| 5:b:203:ILE:O     | 5:b:207:THR:HG23  | 2.10                     | 0.51              |
| 11:i:6:LEU:HD23   | 17:w:101:LEU:CD2  | 2.41                     | 0.51              |
| 20:s:81:ILE:O     | 20:s:81:ILE:HG22  | 2.09                     | 0.51              |
| 20:s:182:LEU:HD23 | 24:s:306:CHL:CMA  | 2.41                     | 0.51              |
| 20:s:230:ARG:HD3  | 25:s:303:CLA:CHD  | 2.40                     | 0.51              |
| 21:g:146:TYR:CD1  | 21:g:147:LEU:HG   | 2.46                     | 0.51              |
| 21:g:179:GLY:HA2  | 24:g:608:CHL:HAC1 | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:172:VAL:CG1  | 24:n:608:CHL:C1B  | 2.89                     | 0.51              |
| 25:n:603:CLA:C19  | 24:n:607:CHL:H172 | 2.39                     | 0.51              |
| 21:y:100:VAL:HB   | 21:y:190:LEU:HD13 | 1.92                     | 0.51              |
| 21:y:107:MET:HE1  | 25:y:311:CLA:CHC  | 2.40                     | 0.51              |
| 1:1:131:TRP:O     | 1:1:134:ALA:HB3   | 2.10                     | 0.51              |
| 2:2:239:LYS:HB2   | 2:2:242:LEU:HB2   | 1.92                     | 0.51              |
| 1:3:146:TYR:CD1   | 1:3:147:LEU:HG    | 2.46                     | 0.51              |
| 4:A:43:THR:O      | 4:A:47:VAL:HG23   | 2.11                     | 0.51              |
| 4:A:50:ILE:HG22   | 28:A:406:BCR:H271 | 1.92                     | 0.51              |
| 25:B:602:CLA:HBC3 | 25:B:602:CLA:HHD  | 1.93                     | 0.51              |
| 25:B:614:CLA:HBD  | 25:B:614:CLA:HAA1 | 1.93                     | 0.51              |
| 6:C:51:GLY:HA2    | 6:C:132:HIS:HB2   | 1.91                     | 0.51              |
| 6:C:80:PRO:HD2    | 6:C:83:GLU:OE1    | 2.10                     | 0.51              |
| 6:C:318:LEU:HD12  | 6:C:340:TYR:HB3   | 1.93                     | 0.51              |
| 8:E:73:LEU:O      | 8:E:77:ASP:OD2    | 2.29                     | 0.51              |
| 14:M:32:GLN:HG3   | 14:m:32:GLN:HG3   | 1.92                     | 0.51              |
| 20:S:115:LEU:HB3  | 20:S:119:ARG:HH21 | 1.75                     | 0.51              |
| 21:G:87:ALA:HB1   | 21:Y:90:GLU:HB3   | 1.90                     | 0.51              |
| 21:N:108:LEU:HD11 | 25:N:610:CLA:CBC  | 2.41                     | 0.51              |
| 24:N:609:CHL:HBC3 | 24:Y:302:CHL:C9   | 2.40                     | 0.51              |
| 21:Y:196:PHE:HZ   | 24:Y:309:CHL:C1C  | 2.24                     | 0.51              |
| 21:Y:225:SER:O    | 21:Y:229:PHE:CD1  | 2.63                     | 0.51              |
| 22:R:245:HIS:CD2  | 25:R:610:CLA:HMD1 | 2.45                     | 0.51              |
| 1:5:100:VAL:HB    | 1:5:190:LEU:HD13  | 1.92                     | 0.51              |
| 2:6:211:GLU:O     | 2:6:214:VAL:HG12  | 2.09                     | 0.51              |
| 2:6:236:VAL:O     | 2:6:237:THR:OG1   | 2.24                     | 0.51              |
| 2:6:239:LYS:HB2   | 2:6:242:LEU:HB2   | 1.92                     | 0.51              |
| 2:6:244:ASN:O     | 2:6:248:HIS:ND1   | 2.44                     | 0.51              |
| 5:b:41:GLU:HB3    | 5:b:63:ILE:CD1    | 2.41                     | 0.51              |
| 5:b:154:GLY:HA3   | 5:b:202:HIS:CB    | 2.40                     | 0.51              |
| 5:b:187:VAL:HG13  | 25:b:601:CLA:HMD2 | 1.93                     | 0.51              |
| 25:b:601:CLA:HMC1 | 28:h:101:BCR:C19  | 2.39                     | 0.51              |
| 6:c:267:SER:CB    | 17:w:133:LEU:HD23 | 2.40                     | 0.51              |
| 7:d:262:PHE:O     | 31:d:405:PL9:H522 | 2.11                     | 0.51              |
| 8:e:73:LEU:O      | 8:e:77:ASP:OD2    | 2.29                     | 0.51              |
| 15:o:215:VAL:HG22 | 15:o:218:LEU:HB3  | 1.93                     | 0.51              |
| 20:s:262:PHE:CD2  | 25:s:314:CLA:HMA1 | 2.46                     | 0.51              |
| 21:n:100:VAL:HB   | 21:n:190:LEU:HD13 | 1.92                     | 0.51              |
| 21:n:108:LEU:HD11 | 25:n:610:CLA:CBC  | 2.41                     | 0.51              |
| 21:n:131:TRP:O    | 21:n:134:ALA:HB3  | 2.10                     | 0.51              |
| 21:n:132:PHE:CD2  | 24:n:607:CHL:HED1 | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:128:GLU:CB   | 21:y:137:GLN:HB2  | 2.41                     | 0.51              |
| 21:y:138:ILE:HD13 | 24:y:307:CHL:CBC  | 2.39                     | 0.51              |
| 23:u:96:PRO:C     | 23:u:97:THR:HG1   | 2.07                     | 0.51              |
| 2:2:184:VAL:HG12  | 2:2:185:GLY:O     | 2.09                     | 0.51              |
| 3:4:225:LYS:HA    | 3:4:228:GLU:OE2   | 2.11                     | 0.51              |
| 27:A:404:PHO:HBB1 | 27:A:404:PHO:HMB3 | 1.93                     | 0.51              |
| 5:B:382:PRO:HB3   | 7:D:345:GLU:CD    | 2.35                     | 0.51              |
| 15:O:146:LYS:HB2  | 15:O:158:PHE:CE1  | 2.46                     | 0.51              |
| 20:S:105:GLU:O    | 20:S:109:LYS:HG3  | 2.11                     | 0.51              |
| 20:S:182:LEU:HD23 | 24:S:306:CHL:CMA  | 2.41                     | 0.51              |
| 21:G:104:ARG:HD3  | 25:G:610:CLA:CHD  | 2.40                     | 0.51              |
| 21:N:104:ARG:HB3  | 25:N:610:CLA:HBC2 | 1.92                     | 0.51              |
| 21:N:146:TYR:CD1  | 21:N:147:LEU:HG   | 2.46                     | 0.51              |
| 21:Y:156:GLN:HB2  | 24:Y:306:CHL:CBB  | 2.41                     | 0.51              |
| 25:R:603:CLA:CHD  | 25:R:608:CLA:H92  | 2.29                     | 0.51              |
| 2:6:125:VAL:HG13  | 2:6:148:LEU:HD11  | 1.92                     | 0.51              |
| 1:7:146:TYR:CD1   | 1:7:147:LEU:HG    | 2.46                     | 0.51              |
| 3:8:156:VAL:O     | 3:8:159:LYS:HB2   | 2.11                     | 0.51              |
| 4:a:202:VAL:HG22  | 25:a:402:CLA:HBB  | 1.92                     | 0.51              |
| 25:b:615:CLA:H51  | 25:b:616:CLA:C20  | 2.41                     | 0.51              |
| 25:c:511:CLA:HBA1 | 28:k:101:BCR:H271 | 1.93                     | 0.51              |
| 26:c:519:LHG:HC5  | 7:d:220:GLU:OE2   | 2.11                     | 0.51              |
| 15:o:130:LYS:CD   | 15:o:179:GLU:HB2  | 2.40                     | 0.51              |
| 19:z:14:ILE:HG23  | 19:z:18:ILE:HD11  | 1.92                     | 0.51              |
| 21:n:94:ARG:HA    | 21:n:94:ARG:HE    | 1.75                     | 0.51              |
| 1:1:86:SER:HB3    | 1:1:92:PHE:CD1    | 2.45                     | 0.51              |
| 2:2:244:ASN:O     | 2:2:248:HIS:ND1   | 2.44                     | 0.51              |
| 5:B:462:PHE:CE2   | 25:B:613:CLA:HMB3 | 2.46                     | 0.51              |
| 6:C:87:ILE:CD1    | 25:C:504:CLA:HMB2 | 2.40                     | 0.51              |
| 21:G:95:ASN:HA    | 21:G:98:LEU:HB2   | 1.93                     | 0.51              |
| 21:G:131:TRP:HA   | 39:G:616:LUT:O3   | 2.11                     | 0.51              |
| 21:N:131:TRP:O    | 21:N:134:ALA:HB3  | 2.10                     | 0.51              |
| 21:N:231:VAL:CG2  | 25:N:613:CLA:HAC1 | 2.35                     | 0.51              |
| 21:Y:146:TYR:CD1  | 21:Y:147:LEU:HG   | 2.46                     | 0.51              |
| 1:7:131:TRP:O     | 1:7:134:ALA:HB3   | 2.10                     | 0.51              |
| 4:a:43:THR:O      | 4:a:47:VAL:HG23   | 2.11                     | 0.51              |
| 5:b:110:ALA:CB    | 25:b:616:CLA:HBB  | 2.40                     | 0.51              |
| 5:b:360:PRO:O     | 5:b:361:THR:CG2   | 2.58                     | 0.51              |
| 6:c:447:ARG:HD3   | 25:c:508:CLA:HED1 | 1.92                     | 0.51              |
| 11:i:27:ASP:HB3   | 11:i:28:PRO:HD3   | 1.93                     | 0.51              |
| 15:o:187:ASN:OD1  | 15:o:187:ASN:O    | 2.28                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:s:83:GLU:HG3   | 20:s:83:GLU:O     | 2.10                     | 0.51              |
| 20:s:187:TYR:HA   | 20:s:190:ILE:HG12 | 1.93                     | 0.51              |
| 21:g:94:ARG:HA    | 21:g:94:ARG:HE    | 1.75                     | 0.51              |
| 21:n:128:GLU:CB   | 21:n:137:GLN:HB2  | 2.41                     | 0.51              |
| 21:y:60:GLY:HA3   | 24:y:302:CHL:CMC  | 2.28                     | 0.51              |
| 40:y:318:NEX:H361 | 40:y:318:NEX:C28  | 2.25                     | 0.51              |
| 22:r:204:PHE:CE1  | 25:r:614:CLA:HAC2 | 2.46                     | 0.51              |
| 1:1:146:TYR:CD1   | 1:1:147:LEU:HG    | 2.46                     | 0.51              |
| 2:2:228:PHE:O     | 2:2:232:VAL:HG23  | 2.10                     | 0.51              |
| 5:B:203:ILE:O     | 5:B:207:THR:HG23  | 2.10                     | 0.51              |
| 6:C:433:LEU:HD13  | 25:C:502:CLA:CHC  | 2.41                     | 0.51              |
| 20:S:230:ARG:HD3  | 25:S:303:CLA:CHD  | 2.40                     | 0.51              |
| 25:R:604:CLA:HHC  | 40:R:617:NEX:H222 | 1.91                     | 0.51              |
| 3:8:215:GLU:HB3   | 3:8:216:PRO:HD3   | 1.93                     | 0.51              |
| 5:b:7:ARG:HD3     | 25:b:611:CLA:HED1 | 1.93                     | 0.51              |
| 5:b:122:ILE:HA    | 10:h:24:LYS:CD    | 2.40                     | 0.51              |
| 6:c:163:ILE:CG2   | 25:c:512:CLA:HAB  | 2.32                     | 0.51              |
| 7:d:85:SER:OG     | 23:u:102:ARG:NH1  | 2.44                     | 0.51              |
| 15:o:140:PRO:HD2  | 15:o:169:TYR:CE2  | 2.46                     | 0.51              |
| 21:g:87:ALA:HB1   | 21:y:90:GLU:HB2   | 1.93                     | 0.51              |
| 21:g:104:ARG:HD3  | 25:g:610:CLA:CHD  | 2.40                     | 0.51              |
| 21:y:95:ASN:HA    | 21:y:98:LEU:HB2   | 1.93                     | 0.51              |
| 21:y:196:PHE:HZ   | 24:y:309:CHL:C1C  | 2.24                     | 0.51              |
| 22:r:56:PRO:C     | 22:r:57:LEU:HD22  | 2.35                     | 0.51              |
| 3:4:75:GLY:HA2    | 3:4:80:ASP:HB3    | 1.93                     | 0.51              |
| 6:C:76:VAL:O      | 6:C:76:VAL:HG13   | 2.11                     | 0.51              |
| 15:O:296:THR:HG22 | 15:O:296:THR:O    | 2.09                     | 0.51              |
| 19:Z:3:ILE:HD12   | 19:Z:3:ILE:H      | 1.76                     | 0.51              |
| 20:S:83:GLU:HG3   | 20:S:83:GLU:O     | 2.10                     | 0.51              |
| 21:G:210:GLU:OE1  | 21:G:214:LYS:NZ   | 2.38                     | 0.51              |
| 21:N:100:VAL:HG11 | 21:N:190:LEU:HD13 | 1.92                     | 0.51              |
| 21:N:132:PHE:CD2  | 24:N:607:CHL:HED1 | 2.45                     | 0.51              |
| 21:Y:107:MET:HE1  | 25:Y:311:CLA:CHC  | 2.40                     | 0.51              |
| 25:R:602:CLA:HAB  | 41:R:616:XAT:H30  | 1.93                     | 0.51              |
| 2:6:57:LYS:HD3    | 2:6:63:SER:CB     | 2.41                     | 0.51              |
| 2:6:130:PRO:HG3   | 2:6:239:LYS:HE2   | 1.93                     | 0.51              |
| 3:8:183:GLU:HB3   | 3:8:185:PHE:HD1   | 1.75                     | 0.51              |
| 3:8:225:LYS:HA    | 3:8:228:GLU:OE2   | 2.11                     | 0.51              |
| 4:a:170:ASP:OD2   | 6:c:357:ARG:NH1   | 2.43                     | 0.51              |
| 4:a:205:VAL:HG12  | 7:d:205:VAL:HG12  | 1.93                     | 0.51              |
| 6:c:203:THR:HG21  | 6:c:208:VAL:HG11  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:d:240:GLN:HE22  | 7:d:242:GLU:CG    | 2.24                     | 0.51              |
| 20:s:221:LEU:HB3  | 25:s:310:CLA:H3A  | 1.93                     | 0.51              |
| 21:n:85:LEU:HD13  | 25:n:602:CLA:H42  | 1.92                     | 0.51              |
| 24:n:609:CHL:H91  | 24:n:609:CHL:H142 | 1.93                     | 0.51              |
| 21:y:51:TYR:HE2   | 21:y:209:ALA:HB1  | 1.75                     | 0.51              |
| 2:2:57:LYS:HD3    | 2:2:63:SER:CB     | 2.41                     | 0.50              |
| 2:2:97:ALA:HB1    | 2:2:190:LEU:HD11  | 1.91                     | 0.50              |
| 1:3:100:VAL:HB    | 1:3:190:LEU:HD13  | 1.92                     | 0.50              |
| 1:3:164:THR:HG23  | 1:3:168:LEU:HD12  | 1.92                     | 0.50              |
| 4:A:40:THR:HG23   | 25:A:405:CLA:HBB1 | 1.92                     | 0.50              |
| 4:A:205:VAL:HG12  | 7:D:205:VAL:HG12  | 1.93                     | 0.50              |
| 5:B:110:ALA:CB    | 25:B:616:CLA:HHB  | 2.40                     | 0.50              |
| 26:B:625:LHG:H122 | 26:B:625:LHG:H331 | 1.92                     | 0.50              |
| 6:C:471:PRO:O     | 6:C:472:LEU:HB2   | 2.11                     | 0.50              |
| 12:K:58:VAL:HG12  | 12:K:61:ARG:HD2   | 1.92                     | 0.50              |
| 15:O:187:ASN:OD1  | 15:O:187:ASN:O    | 2.28                     | 0.50              |
| 18:X:93:GLY:O     | 18:X:96:VAL:HG22  | 2.11                     | 0.50              |
| 20:S:169:ILE:HD12 | 24:S:306:CHL:HED1 | 1.92                     | 0.50              |
| 20:S:209:LEU:O    | 21:N:195:SER:HA   | 2.11                     | 0.50              |
| 21:Y:95:ASN:HA    | 21:Y:98:LEU:HB2   | 1.93                     | 0.50              |
| 22:R:144:GLY:CA   | 22:R:246:ALA:HB1  | 2.19                     | 0.50              |
| 22:R:154:ALA:O    | 22:R:157:VAL:HG12 | 2.11                     | 0.50              |
| 22:R:202:ILE:HG13 | 22:R:203:GLU:N    | 2.25                     | 0.50              |
| 22:R:277:ASP:HB2  | 22:R:280:HIS:HD1  | 1.75                     | 0.50              |
| 24:R:607:CHL:CBB  | 40:R:617:NEX:H12  | 2.40                     | 0.50              |
| 5:b:382:PRO:HB3   | 7:d:345:GLU:CD    | 2.35                     | 0.50              |
| 5:b:458:PHE:HB3   | 25:b:604:CLA:HBC2 | 1.93                     | 0.50              |
| 21:n:146:TYR:CD1  | 21:n:147:LEU:HG   | 2.46                     | 0.50              |
| 21:y:131:TRP:O    | 21:y:134:ALA:HB3  | 2.10                     | 0.50              |
| 24:y:302:CHL:C9   | 24:y:302:CHL:H51  | 2.41                     | 0.50              |
| 25:y:312:CLA:H52  | 25:y:312:CLA:H92  | 1.92                     | 0.50              |
| 22:r:240:LEU:HG   | 22:r:244:LYS:HD2  | 1.93                     | 0.50              |
| 25:r:602:CLA:HAB  | 41:r:616:XAT:H30  | 1.93                     | 0.50              |
| 1:1:117:GLU:HB2   | 1:1:241:LEU:HD12  | 1.93                     | 0.50              |
| 2:2:127:PHE:HB3   | 2:2:140:PHE:HE2   | 1.75                     | 0.50              |
| 4:A:202:VAL:HG22  | 25:A:401:CLA:HHB  | 1.92                     | 0.50              |
| 27:A:404:PHO:H193 | 25:D:401:CLA:HHB  | 1.92                     | 0.50              |
| 25:B:616:CLA:CMC  | 25:B:616:CLA:HBC2 | 2.42                     | 0.50              |
| 25:C:503:CLA:HAA1 | 25:C:503:CLA:HBD  | 1.94                     | 0.50              |
| 25:C:513:CLA:HBB1 | 25:C:513:CLA:HMB3 | 1.93                     | 0.50              |
| 7:D:78:ALA:CB     | 7:D:175:GLY:HA3   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:E:28:PRO:O      | 8:E:32:ILE:HG12   | 2.12                     | 0.50              |
| 15:O:140:PRO:HD2  | 15:O:169:TYR:CE2  | 2.46                     | 0.50              |
| 25:S:305:CLA:H43  | 40:S:317:NEX:H23  | 1.93                     | 0.50              |
| 21:G:59:LEU:HD23  | 24:G:601:CHL:C1B  | 2.41                     | 0.50              |
| 21:N:98:LEU:HD22  | 25:N:603:CLA:CAA  | 2.40                     | 0.50              |
| 21:N:136:SER:HB3  | 24:N:607:CHL:O1D  | 2.11                     | 0.50              |
| 2:6:210:ALA:HA    | 2:6:213:LYS:HZ2   | 1.76                     | 0.50              |
| 4:a:85:THR:CG2    | 4:a:89:ILE:HD12   | 2.41                     | 0.50              |
| 4:a:89:ILE:HD13   | 4:a:94:TYR:CD2    | 2.46                     | 0.50              |
| 4:a:331:MET:HE1   | 7:d:321:LEU:HD22  | 1.92                     | 0.50              |
| 5:b:271:THR:O     | 5:b:272:ARG:HB3   | 2.12                     | 0.50              |
| 25:b:616:CLA:CMC  | 25:b:616:CLA:HBC2 | 2.42                     | 0.50              |
| 6:c:61:VAL:HG12   | 6:c:118:HIS:O     | 2.12                     | 0.50              |
| 6:c:318:LEU:HD12  | 6:c:340:TYR:HB3   | 1.93                     | 0.50              |
| 25:c:505:CLA:HAA1 | 25:c:505:CLA:CBD  | 2.39                     | 0.50              |
| 7:d:108:LEU:HD21  | 8:e:72:SER:HB2    | 1.93                     | 0.50              |
| 20:s:72:PRO:HG3   | 24:s:302:CHL:CBB  | 2.41                     | 0.50              |
| 20:s:105:GLU:O    | 20:s:109:LYS:HG3  | 2.11                     | 0.50              |
| 20:s:209:LEU:O    | 21:n:195:SER:HA   | 2.11                     | 0.50              |
| 21:g:86:SER:HB3   | 21:g:92:PHE:CD1   | 2.45                     | 0.50              |
| 21:n:98:LEU:HD22  | 25:n:603:CLA:CAA  | 2.40                     | 0.50              |
| 21:n:104:ARG:HD3  | 25:n:610:CLA:C4C  | 2.41                     | 0.50              |
| 21:y:146:TYR:CD1  | 21:y:147:LEU:HG   | 2.46                     | 0.50              |
| 24:y:308:CHL:HHD  | 24:y:308:CHL:CBC  | 2.36                     | 0.50              |
| 22:r:277:ASP:HB2  | 22:r:280:HIS:HD1  | 1.75                     | 0.50              |
| 1:1:158:ILE:O     | 1:1:161:ILE:HB    | 2.12                     | 0.50              |
| 4:A:290:ILE:HG13  | 25:A:401:CLA:CED  | 2.41                     | 0.50              |
| 5:B:59:GLY:O      | 25:B:607:CLA:HED2 | 2.12                     | 0.50              |
| 5:B:360:PRO:O     | 5:B:361:THR:CG2   | 2.58                     | 0.50              |
| 5:B:458:PHE:HB3   | 25:B:604:CLA:HBC2 | 1.93                     | 0.50              |
| 5:B:478:VAL:O     | 5:B:478:VAL:HG22  | 2.10                     | 0.50              |
| 6:C:199:ILE:HG13  | 6:C:234:ILE:HG13  | 1.93                     | 0.50              |
| 8:E:38:VAL:HG21   | 9:F:30:SER:O      | 2.11                     | 0.50              |
| 20:S:188:TYR:CD1  | 20:S:193:GLY:HA3  | 2.46                     | 0.50              |
| 21:G:154:HIS:O    | 21:G:154:HIS:ND1  | 2.43                     | 0.50              |
| 21:N:85:LEU:HD13  | 25:N:602:CLA:H42  | 1.92                     | 0.50              |
| 24:N:609:CHL:H91  | 24:N:609:CHL:H142 | 1.93                     | 0.50              |
| 22:R:85:LYS:HG2   | 22:R:86:PRO:CD    | 2.38                     | 0.50              |
| 22:R:124:PHE:CD1  | 25:R:614:CLA:HHC  | 2.46                     | 0.50              |
| 1:7:86:SER:HB3    | 1:7:92:PHE:CD1    | 2.45                     | 0.50              |
| 3:8:123:SER:OG    | 3:8:133:GLN:HB2   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:a:232:SER:OG    | 5:b:7:ARG:NH1     | 2.44                     | 0.50              |
| 5:b:462:PHE:CE2   | 25:b:613:CLA:HMB3 | 2.46                     | 0.50              |
| 15:o:296:THR:HG22 | 15:o:298:GLU:OE2  | 2.12                     | 0.50              |
| 25:s:303:CLA:CAB  | 39:s:316:LUT:H32  | 2.42                     | 0.50              |
| 22:r:150:ALA:HA   | 41:r:616:XAT:H181 | 1.94                     | 0.50              |
| 2:2:120:GLN:HB3   | 2:2:129:GLU:CG    | 2.41                     | 0.50              |
| 6:C:28:GLN:O      | 6:C:32:GLY:N      | 2.42                     | 0.50              |
| 6:C:175:LEU:HB2   | 25:C:501:CLA:CMD  | 2.41                     | 0.50              |
| 6:C:236:GLY:HA2   | 6:C:239:TRP:HD1   | 1.77                     | 0.50              |
| 26:D:406:LHG:HC42 | 13:L:16:THR:HG21  | 1.94                     | 0.50              |
| 18:X:79:ILE:H     | 18:X:79:ILE:HD12  | 1.77                     | 0.50              |
| 24:Y:302:CHL:C9   | 24:Y:302:CHL:H51  | 2.42                     | 0.50              |
| 25:Y:311:CLA:HAB  | 39:Y:316:LUT:H32  | 1.94                     | 0.50              |
| 22:R:72:LEU:HB3   | 22:R:137:ARG:CZ   | 2.41                     | 0.50              |
| 25:R:610:CLA:CBC  | 26:R:618:LHG:HC5  | 2.33                     | 0.50              |
| 5:b:377:VAL:HG11  | 7:d:343:PRO:CG    | 2.41                     | 0.50              |
| 25:b:607:CLA:H193 | 25:b:613:CLA:H141 | 1.94                     | 0.50              |
| 6:c:76:VAL:O      | 6:c:76:VAL:HG13   | 2.11                     | 0.50              |
| 6:c:290:VAL:HG21  | 25:c:502:CLA:CED  | 2.41                     | 0.50              |
| 25:c:502:CLA:CMC  | 25:c:510:CLA:HBB1 | 2.38                     | 0.50              |
| 7:d:135:ARG:NH2   | 7:d:138:GLN:OE1   | 2.42                     | 0.50              |
| 15:o:114:CYS:SG   | 15:o:139:GLU:HB2  | 2.52                     | 0.50              |
| 15:o:146:LYS:HB2  | 15:o:158:PHE:CE1  | 2.46                     | 0.50              |
| 20:s:144:GLU:HB3  | 20:s:153:LEU:CD2  | 2.41                     | 0.50              |
| 20:s:171:LEU:O    | 20:s:175:VAL:HG23 | 2.11                     | 0.50              |
| 25:s:305:CLA:H43  | 40:s:317:NEX:H23  | 1.93                     | 0.50              |
| 21:n:95:ASN:HA    | 21:n:98:LEU:HB2   | 1.93                     | 0.50              |
| 2:2:130:PRO:HG3   | 2:2:239:LYS:CE    | 2.42                     | 0.50              |
| 2:2:179:ASN:CA    | 24:2:603:CHL:CMC  | 2.85                     | 0.50              |
| 1:3:131:TRP:O     | 1:3:134:ALA:HB3   | 2.10                     | 0.50              |
| 4:A:286:THR:OG1   | 25:A:401:CLA:O1D  | 2.25                     | 0.50              |
| 5:B:41:GLU:HB3    | 5:B:63:ILE:CD1    | 2.41                     | 0.50              |
| 7:D:240:GLN:HE22  | 7:D:242:GLU:CG    | 2.24                     | 0.50              |
| 15:O:296:THR:HG22 | 15:O:298:GLU:OE2  | 2.11                     | 0.50              |
| 20:S:119:ARG:HD3  | 25:S:310:CLA:C4C  | 2.41                     | 0.50              |
| 20:S:124:GLY:HA2  | 39:S:316:LUT:H181 | 1.92                     | 0.50              |
| 21:G:158:ILE:O    | 21:G:161:ILE:HB   | 2.12                     | 0.50              |
| 21:G:215:GLU:HG3  | 25:G:610:CLA:C2B  | 2.41                     | 0.50              |
| 24:G:606:CHL:HBB1 | 39:G:616:LUT:H161 | 1.94                     | 0.50              |
| 21:N:128:GLU:CB   | 21:N:137:GLN:HB2  | 2.41                     | 0.50              |
| 21:N:204:ASP:O    | 21:N:208:PHE:N    | 2.40                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:N:611:CLA:CMC  | 26:N:618:LHG:H341 | 2.42                     | 0.50              |
| 21:Y:86:SER:HB3   | 21:Y:92:PHE:CD1   | 2.45                     | 0.50              |
| 2:6:131:VAL:HA    | 2:6:134:LYS:HD2   | 1.94                     | 0.50              |
| 3:8:177:PRO:HD2   | 3:8:178:TRP:CE3   | 2.47                     | 0.50              |
| 20:s:58:GLU:OE1   | 20:s:61:LYS:NZ    | 2.35                     | 0.50              |
| 20:s:119:ARG:HD3  | 25:s:310:CLA:C4C  | 2.41                     | 0.50              |
| 20:s:131:PRO:HG3  | 25:s:305:CLA:C1D  | 2.42                     | 0.50              |
| 21:g:131:TRP:HA   | 39:g:616:LUT:O3   | 2.11                     | 0.50              |
| 21:n:214:LYS:HG2  | 25:n:611:CLA:O2D  | 2.11                     | 0.50              |
| 21:y:214:LYS:HG2  | 25:y:312:CLA:O2D  | 2.12                     | 0.50              |
| 22:r:68:LEU:HD11  | 25:r:602:CLA:CED  | 2.42                     | 0.50              |
| 22:r:154:ALA:O    | 22:r:157:VAL:HG12 | 2.11                     | 0.50              |
| 2:2:103:GLY:HA3   | 2:2:219:ASN:HB3   | 1.93                     | 0.50              |
| 1:3:95:ASN:HA     | 1:3:98:LEU:HB2    | 1.93                     | 0.50              |
| 3:4:157:GLU:HG3   | 3:4:161:TRP:NE1   | 2.26                     | 0.50              |
| 4:A:57:PRO:HB2    | 4:A:66:PRO:CB     | 2.42                     | 0.50              |
| 4:A:220:THR:O     | 4:A:223:LEU:HG    | 2.12                     | 0.50              |
| 7:D:108:LEU:HD21  | 8:E:72:SER:HB2    | 1.93                     | 0.50              |
| 11:I:6:LEU:HD23   | 17:W:101:LEU:CD2  | 2.41                     | 0.50              |
| 20:S:146:VAL:HG21 | 20:S:149:LYS:HZ1  | 1.77                     | 0.50              |
| 25:S:310:CLA:H51  | 25:S:312:CLA:CMA  | 2.33                     | 0.50              |
| 21:G:138:ILE:CD1  | 24:G:606:CHL:HAC1 | 2.42                     | 0.50              |
| 21:G:146:TYR:CD1  | 21:G:147:LEU:HG   | 2.46                     | 0.50              |
| 21:G:215:GLU:CB   | 25:G:610:CLA:C2B  | 2.90                     | 0.50              |
| 24:N:607:CHL:H203 | 25:Y:303:CLA:C15  | 2.42                     | 0.50              |
| 21:Y:158:ILE:O    | 21:Y:161:ILE:HB   | 2.12                     | 0.50              |
| 2:6:127:PHE:HB3   | 2:6:140:PHE:HE2   | 1.75                     | 0.50              |
| 2:6:179:ASN:CA    | 24:6:603:CHL:CMC  | 2.85                     | 0.50              |
| 2:6:183:GLY:O     | 2:6:184:VAL:HG23  | 2.12                     | 0.50              |
| 4:a:50:ILE:HG22   | 28:a:407:BCR:H271 | 1.92                     | 0.50              |
| 27:a:405:PHO:HBB1 | 27:a:405:PHO:HMB3 | 1.93                     | 0.50              |
| 27:a:405:PHO:HAB  | 25:d:402:CLA:C1   | 2.41                     | 0.50              |
| 5:b:59:GLY:O      | 25:b:607:CLA:HED2 | 2.12                     | 0.50              |
| 25:b:614:CLA:HBA1 | 28:b:617:BCR:H403 | 1.94                     | 0.50              |
| 26:b:625:LHG:H331 | 26:b:625:LHG:H122 | 1.92                     | 0.50              |
| 6:c:175:LEU:HB2   | 25:c:501:CLA:CMD  | 2.41                     | 0.50              |
| 6:c:457:LYS:CD    | 7:d:230:ALA:HA    | 2.42                     | 0.50              |
| 9:f:31:ILE:O      | 9:f:35:GLN:HG2    | 2.10                     | 0.50              |
| 10:h:22:LEU:CG    | 22:r:124:PHE:HE2  | 2.25                     | 0.50              |
| 19:z:3:ILE:HD12   | 19:z:3:ILE:H      | 1.76                     | 0.50              |
| 21:g:138:ILE:HG13 | 21:g:144:LEU:CB   | 2.31                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:215:GLU:HG3  | 25:g:610:CLA:C2B  | 2.41                     | 0.50              |
| 21:y:156:GLN:HB2  | 24:y:306:CHL:CBB  | 2.41                     | 0.50              |
| 21:y:227:PHE:CD2  | 25:y:303:CLA:H171 | 2.47                     | 0.50              |
| 25:y:311:CLA:HAB  | 39:y:316:LUT:H32  | 1.94                     | 0.50              |
| 2:2:125:VAL:HG13  | 2:2:148:LEU:HD11  | 1.92                     | 0.50              |
| 4:A:64:ARG:CG     | 6:C:337:LEU:HD21  | 2.42                     | 0.50              |
| 4:A:85:THR:CG2    | 4:A:89:ILE:HD12   | 2.41                     | 0.50              |
| 5:B:214:LEU:HD13  | 25:R:603:CLA:HED1 | 1.94                     | 0.50              |
| 6:C:447:ARG:CD    | 25:C:508:CLA:HED1 | 2.42                     | 0.50              |
| 7:D:19:MET:SD     | 18:X:103:VAL:HG22 | 2.52                     | 0.50              |
| 11:I:27:ASP:HB3   | 11:I:28:PRO:HD3   | 1.93                     | 0.50              |
| 14:M:6:LEU:O      | 14:M:9:ILE:HG22   | 2.12                     | 0.50              |
| 20:S:72:PRO:HG3   | 24:S:302:CHL:CBB  | 2.41                     | 0.50              |
| 25:S:303:CLA:CAB  | 39:S:316:LUT:H32  | 2.42                     | 0.50              |
| 21:G:94:ARG:HA    | 21:G:94:ARG:HE    | 1.75                     | 0.50              |
| 21:N:158:ILE:O    | 21:N:161:ILE:HB   | 2.12                     | 0.50              |
| 21:N:210:GLU:OE1  | 21:N:214:LYS:NZ   | 2.38                     | 0.50              |
| 25:R:603:CLA:C1B  | 25:R:608:CLA:H111 | 2.42                     | 0.50              |
| 1:5:103:SER:O     | 1:5:107:MET:HG3   | 2.12                     | 0.50              |
| 1:5:158:ILE:O     | 1:5:161:ILE:HB    | 2.12                     | 0.50              |
| 2:6:69:TYR:HH     | 2:6:81:ASP:CG     | 2.19                     | 0.50              |
| 4:a:77:ILE:HB     | 13:l:34:ASN:HD21  | 1.77                     | 0.50              |
| 4:a:290:ILE:HG13  | 25:a:402:CLA:CED  | 2.41                     | 0.50              |
| 25:b:614:CLA:HBD  | 25:b:614:CLA:HAA1 | 1.93                     | 0.50              |
| 6:c:87:ILE:HD13   | 25:c:504:CLA:C1B  | 2.42                     | 0.50              |
| 10:h:56:ILE:HA    | 18:x:84:LYS:CE    | 2.37                     | 0.50              |
| 12:k:40:MET:N     | 12:k:41:PRO:HD2   | 2.27                     | 0.50              |
| 18:x:79:ILE:H     | 18:x:79:ILE:HD12  | 1.77                     | 0.50              |
| 25:n:610:CLA:H18  | 40:n:617:NEX:H372 | 1.92                     | 0.50              |
| 21:y:94:ARG:HA    | 21:y:94:ARG:HE    | 1.75                     | 0.50              |
| 2:2:121:LYS:HD3   | 2:2:242:LEU:HD23  | 1.93                     | 0.50              |
| 2:2:130:PRO:HG3   | 2:2:239:LYS:HE2   | 1.93                     | 0.50              |
| 4:A:77:ILE:HB     | 13:L:34:ASN:HD21  | 1.77                     | 0.50              |
| 4:A:89:ILE:HD13   | 4:A:94:TYR:CD2    | 2.46                     | 0.50              |
| 4:A:224:ILE:O     | 7:D:266:ARG:NH2   | 2.43                     | 0.50              |
| 5:B:121:GLU:HG2   | 10:H:15:ARG:O     | 2.12                     | 0.50              |
| 25:B:607:CLA:H193 | 25:B:613:CLA:H141 | 1.94                     | 0.50              |
| 6:C:87:ILE:HD13   | 25:C:504:CLA:C1B  | 2.41                     | 0.50              |
| 6:C:203:THR:HG21  | 6:C:208:VAL:HG11  | 1.93                     | 0.50              |
| 6:C:379:ARG:HG2   | 6:C:383:ASP:OD2   | 2.11                     | 0.50              |
| 7:D:85:SER:OG     | 23:U:102:ARG:NH1  | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:Z:12:LEU:HD13  | 19:Z:50:LEU:HB3   | 1.94                     | 0.50              |
| 25:S:303:CLA:C7   | 25:S:304:CLA:HMA1 | 2.39                     | 0.50              |
| 21:G:76:GLY:HA3   | 21:G:216:LEU:CD2  | 2.24                     | 0.50              |
| 21:G:215:GLU:HG3  | 25:G:610:CLA:C3B  | 2.42                     | 0.50              |
| 21:N:103:SER:O    | 21:N:107:MET:HG3  | 2.12                     | 0.50              |
| 25:N:604:CLA:HBB  | 39:N:616:LUT:H3   | 1.94                     | 0.50              |
| 21:Y:127:GLY:HA3  | 21:Y:137:GLN:CG   | 2.42                     | 0.50              |
| 22:R:204:PHE:CE1  | 25:R:614:CLA:HAC2 | 2.46                     | 0.50              |
| 22:R:220:GLY:HA2  | 22:R:224:ASP:CB   | 2.42                     | 0.50              |
| 2:6:101:ILE:O     | 2:6:104:ARG:HB3   | 2.11                     | 0.50              |
| 2:6:120:GLN:HB3   | 2:6:129:GLU:CG    | 2.41                     | 0.50              |
| 1:7:94:ARG:HA     | 1:7:94:ARG:HE     | 1.75                     | 0.50              |
| 1:7:154:HIS:O     | 1:7:154:HIS:ND1   | 2.44                     | 0.50              |
| 25:a:402:CLA:H51  | 27:a:404:PHO:C3B  | 2.42                     | 0.50              |
| 5:b:280:PHE:O     | 5:b:281:GLN:HB2   | 2.12                     | 0.50              |
| 30:b:623:LMG:H371 | 25:r:608:CLA:C13  | 2.42                     | 0.50              |
| 6:c:447:ARG:CD    | 25:c:508:CLA:HED1 | 2.42                     | 0.50              |
| 7:d:320:ILE:O     | 7:d:324:GLU:HG3   | 2.12                     | 0.50              |
| 20:s:124:GLY:HA2  | 39:s:316:LUT:H181 | 1.93                     | 0.50              |
| 20:s:169:ILE:HD12 | 24:s:306:CHL:HED1 | 1.92                     | 0.50              |
| 21:g:158:ILE:O    | 21:g:161:ILE:HB   | 2.12                     | 0.50              |
| 21:g:209:ALA:CA   | 21:g:212:LYS:HG3  | 2.34                     | 0.50              |
| 25:n:602:CLA:HBC2 | 25:n:602:CLA:CMC  | 2.40                     | 0.50              |
| 25:n:604:CLA:HBB  | 39:n:616:LUT:H3   | 1.94                     | 0.50              |
| 21:y:103:SER:O    | 21:y:107:MET:HG3  | 2.12                     | 0.50              |
| 21:y:127:GLY:HA3  | 21:y:137:GLN:CG   | 2.42                     | 0.50              |
| 21:y:158:ILE:O    | 21:y:161:ILE:HB   | 2.12                     | 0.50              |
| 22:r:124:PHE:CD1  | 25:r:614:CLA:HHC  | 2.46                     | 0.50              |
| 3:4:215:GLU:HB3   | 3:4:216:PRO:HD3   | 1.93                     | 0.50              |
| 6:C:435:PHE:O     | 6:C:439:VAL:HG23  | 2.12                     | 0.50              |
| 6:C:457:LYS:CD    | 7:D:230:ALA:HA    | 2.42                     | 0.50              |
| 7:D:150:PRO:HB3   | 25:D:402:CLA:H41  | 1.92                     | 0.50              |
| 28:T:101:BCR:H381 | 5:b:39:LEU:HB3    | 1.93                     | 0.50              |
| 20:S:171:LEU:O    | 20:S:175:VAL:HG23 | 2.11                     | 0.50              |
| 20:S:221:LEU:HB3  | 25:S:310:CLA:H3A  | 1.93                     | 0.50              |
| 25:S:303:CLA:HAB  | 39:S:316:LUT:H32  | 1.91                     | 0.50              |
| 21:G:69:TYR:OH    | 21:G:81:ASP:OD2   | 2.20                     | 0.50              |
| 25:N:603:CLA:C20  | 24:N:607:CHL:H172 | 2.42                     | 0.50              |
| 25:Y:312:CLA:H52  | 25:Y:312:CLA:H92  | 1.92                     | 0.50              |
| 22:R:67:TRP:CZ3   | 22:R:82:GLY:HA2   | 2.44                     | 0.50              |
| 2:6:103:GLY:HA3   | 2:6:219:ASN:HB3   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:72:THR:CG2    | 5:b:80:ILE:HG22   | 2.26                     | 0.50              |
| 5:b:341:LEU:HD12  | 5:b:429:ILE:CG2   | 2.39                     | 0.50              |
| 6:c:97:TRP:HH2    | 30:c:520:LMG:H172 | 1.75                     | 0.50              |
| 25:c:510:CLA:H2   | 25:c:510:CLA:CMA  | 2.41                     | 0.50              |
| 7:d:179:ILE:HG21  | 25:d:401:CLA:C4C  | 2.42                     | 0.50              |
| 14:m:6:LEU:O      | 14:m:9:ILE:HG22   | 2.12                     | 0.50              |
| 21:g:215:GLU:CB   | 25:g:610:CLA:C2B  | 2.90                     | 0.50              |
| 21:n:136:SER:HB3  | 24:n:607:CHL:O1D  | 2.11                     | 0.50              |
| 21:y:98:LEU:HD22  | 25:y:304:CLA:CBA  | 2.40                     | 0.50              |
| 25:r:603:CLA:C1B  | 25:r:608:CLA:H111 | 2.42                     | 0.50              |
| 40:r:617:NEX:H12  | 40:r:617:NEX:H191 | 1.93                     | 0.50              |
| 2:2:246:LEU:HA    | 2:2:249:LEU:HD23  | 1.94                     | 0.49              |
| 3:4:177:PRO:HD2   | 3:4:178:TRP:CE3   | 2.47                     | 0.49              |
| 25:A:401:CLA:H51  | 27:A:403:PHO:C3B  | 2.42                     | 0.49              |
| 5:B:7:ARG:HD3     | 25:B:611:CLA:HED1 | 1.93                     | 0.49              |
| 25:B:601:CLA:CHB  | 25:B:602:CLA:HBB2 | 2.42                     | 0.49              |
| 25:B:614:CLA:HBA1 | 28:B:617:BCR:H403 | 1.94                     | 0.49              |
| 25:B:615:CLA:H51  | 25:B:616:CLA:C20  | 2.41                     | 0.49              |
| 6:C:257:PHE:O     | 6:C:261:ARG:HG3   | 2.12                     | 0.49              |
| 6:C:378:SER:OG    | 6:C:382:LYS:HE3   | 2.12                     | 0.49              |
| 12:K:40:MET:N     | 12:K:41:PRO:HD2   | 2.27                     | 0.49              |
| 25:N:603:CLA:H192 | 24:N:607:CHL:C17  | 2.42                     | 0.49              |
| 21:Y:227:PHE:CD2  | 25:Y:303:CLA:H171 | 2.47                     | 0.49              |
| 22:R:68:LEU:HD11  | 25:R:602:CLA:CED  | 2.42                     | 0.49              |
| 40:R:617:NEX:H12  | 40:R:617:NEX:H191 | 1.93                     | 0.49              |
| 1:5:57:LYS:HD2    | 1:5:63:SER:CB     | 2.42                     | 0.49              |
| 1:5:117:GLU:HB2   | 1:5:241:LEU:HD12  | 1.93                     | 0.49              |
| 1:5:154:HIS:O     | 1:5:154:HIS:ND1   | 2.43                     | 0.49              |
| 2:6:64:VAL:HG12   | 2:6:65:GLN:N      | 2.27                     | 0.49              |
| 2:6:130:PRO:HG3   | 2:6:239:LYS:CE    | 2.42                     | 0.49              |
| 3:8:158:SER:O     | 3:8:162:VAL:HG12  | 2.12                     | 0.49              |
| 4:a:40:THR:HA     | 4:a:118:HIS:HD1   | 1.77                     | 0.49              |
| 4:a:64:ARG:CG     | 6:c:337:LEU:HD21  | 2.42                     | 0.49              |
| 4:a:255:PHE:HE2   | 4:a:264:SER:HB3   | 1.74                     | 0.49              |
| 5:b:460:LEU:HD21  | 7:d:160:ILE:CD1   | 2.42                     | 0.49              |
| 25:b:601:CLA:CHB  | 25:b:602:CLA:HBB2 | 2.42                     | 0.49              |
| 26:b:625:LHG:HC5  | 7:d:270:PHE:CZ    | 2.46                     | 0.49              |
| 7:d:78:ALA:CB     | 7:d:175:GLY:HA3   | 2.42                     | 0.49              |
| 21:g:59:LEU:HD23  | 24:g:601:CHL:C1B  | 2.41                     | 0.49              |
| 21:n:104:ARG:HB3  | 25:n:610:CLA:HBC2 | 1.92                     | 0.49              |
| 22:r:144:GLY:CA   | 22:r:246:ALA:HB1  | 2.20                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:603:CLA:CHD  | 25:r:608:CLA:H92  | 2.29                     | 0.49              |
| 3:4:213:VAL:O     | 3:4:213:VAL:HG12  | 2.12                     | 0.49              |
| 30:B:623:LMG:H371 | 25:R:608:CLA:C13  | 2.42                     | 0.49              |
| 25:C:510:CLA:H2   | 25:C:510:CLA:CMA  | 2.41                     | 0.49              |
| 25:C:511:CLA:HAA1 | 25:C:511:CLA:CBD  | 2.42                     | 0.49              |
| 10:H:22:LEU:CG    | 22:R:124:PHE:HE2  | 2.25                     | 0.49              |
| 20:S:187:TYR:HA   | 20:S:190:ILE:HG12 | 1.93                     | 0.49              |
| 21:N:214:LYS:HG2  | 25:N:611:CLA:O2D  | 2.11                     | 0.49              |
| 21:Y:196:PHE:CE2  | 24:Y:309:CHL:HBC2 | 2.48                     | 0.49              |
| 4:a:214:MET:HE1   | 27:a:405:PHO:CAD  | 2.43                     | 0.49              |
| 25:b:602:CLA:H191 | 35:b:626:DGD:HBT1 | 1.95                     | 0.49              |
| 25:b:602:CLA:HBC3 | 25:b:602:CLA:HHD  | 1.93                     | 0.49              |
| 25:b:604:CLA:H92  | 25:b:604:CLA:C4   | 2.34                     | 0.49              |
| 6:c:379:ARG:HG2   | 6:c:383:ASP:OD2   | 2.11                     | 0.49              |
| 25:c:503:CLA:HAA1 | 25:c:503:CLA:HBD  | 1.94                     | 0.49              |
| 25:c:513:CLA:HBB1 | 25:c:513:CLA:HMB3 | 1.93                     | 0.49              |
| 26:d:406:LHG:HC42 | 13:l:16:THR:HG21  | 1.94                     | 0.49              |
| 19:z:12:LEU:HD13  | 19:z:50:LEU:HB3   | 1.94                     | 0.49              |
| 20:s:188:TYR:CD1  | 20:s:193:GLY:HA3  | 2.46                     | 0.49              |
| 21:g:103:SER:O    | 21:g:107:MET:HG3  | 2.12                     | 0.49              |
| 25:n:603:CLA:H142 | 25:y:304:CLA:C14  | 2.42                     | 0.49              |
| 24:y:307:CHL:CMC  | 24:y:308:CHL:C4C  | 2.90                     | 0.49              |
| 2:2:116:PRO:CG    | 2:2:134:LYS:HE3   | 2.42                     | 0.49              |
| 2:2:183:GLY:O     | 2:2:184:VAL:HG23  | 2.12                     | 0.49              |
| 2:2:249:LEU:HD12  | 2:2:250:ASP:N     | 2.28                     | 0.49              |
| 3:4:77:LEU:HD23   | 3:4:78:PRO:O      | 2.11                     | 0.49              |
| 3:4:123:SER:OG    | 3:4:133:GLN:HB2   | 2.11                     | 0.49              |
| 27:A:404:PHO:H152 | 25:D:401:CLA:HMB2 | 1.95                     | 0.49              |
| 5:B:187:VAL:HG13  | 25:B:601:CLA:HMD2 | 1.93                     | 0.49              |
| 5:B:277:GLN:OE1   | 23:U:99:LYS:NZ    | 2.33                     | 0.49              |
| 6:C:25:GLY:O      | 6:C:26:ARG:HG3    | 2.12                     | 0.49              |
| 6:C:61:VAL:HG12   | 6:C:118:HIS:O     | 2.12                     | 0.49              |
| 15:O:145:VAL:HG11 | 15:O:203:LEU:CD1  | 2.35                     | 0.49              |
| 20:S:262:PHE:CD2  | 25:S:314:CLA:HMA1 | 2.46                     | 0.49              |
| 21:G:57:LYS:HD2   | 21:G:63:SER:CB    | 2.42                     | 0.49              |
| 21:G:90:GLU:CB    | 21:N:87:ALA:HB1   | 2.42                     | 0.49              |
| 21:Y:57:LYS:HD2   | 21:Y:63:SER:CB    | 2.42                     | 0.49              |
| 22:R:150:ALA:HB1  | 41:R:616:XAT:H181 | 1.95                     | 0.49              |
| 1:5:107:MET:HG2   | 1:5:222:ALA:HB3   | 1.94                     | 0.49              |
| 2:6:55:ARG:HE     | 2:6:72:GLY:HA3    | 1.77                     | 0.49              |
| 2:6:211:GLU:O     | 2:6:215:LYS:HG3   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:95:ASN:HA     | 1:7:98:LEU:HB2    | 1.93                     | 0.49              |
| 3:8:77:LEU:HD23   | 3:8:78:PRO:O      | 2.11                     | 0.49              |
| 3:8:157:GLU:HG3   | 3:8:161:TRP:NE1   | 2.26                     | 0.49              |
| 4:a:85:THR:O      | 4:a:169:SER:HB3   | 2.12                     | 0.49              |
| 5:b:121:GLU:HG2   | 10:h:15:ARG:O     | 2.12                     | 0.49              |
| 25:b:614:CLA:H71  | 29:l:102:SQD:C15  | 2.43                     | 0.49              |
| 6:c:257:PHE:O     | 6:c:261:ARG:HG3   | 2.12                     | 0.49              |
| 6:c:327:ASN:ND2   | 15:o:192:ASP:HB2  | 2.26                     | 0.49              |
| 21:g:57:LYS:HD2   | 21:g:63:SER:CB    | 2.42                     | 0.49              |
| 21:g:138:ILE:CD1  | 24:g:606:CHL:HAC1 | 2.42                     | 0.49              |
| 24:g:606:CHL:HBB1 | 39:g:616:LUT:H161 | 1.94                     | 0.49              |
| 21:n:51:TYR:HE2   | 21:n:209:ALA:HB1  | 1.75                     | 0.49              |
| 21:n:57:LYS:HD2   | 21:n:63:SER:CB    | 2.42                     | 0.49              |
| 21:n:172:VAL:HG22 | 40:n:617:NEX:H201 | 1.94                     | 0.49              |
| 25:n:603:CLA:CAC  | 24:y:302:CHL:H102 | 2.42                     | 0.49              |
| 21:y:56:VAL:CB    | 24:y:302:CHL:HBC1 | 2.43                     | 0.49              |
| 21:y:196:PHE:CE2  | 24:y:309:CHL:HBC2 | 2.47                     | 0.49              |
| 25:y:315:CLA:HBA2 | 25:y:315:CLA:CBD  | 2.42                     | 0.49              |
| 22:r:63:ILE:HG13  | 22:r:63:ILE:O     | 2.12                     | 0.49              |
| 22:r:158:GLU:OE2  | 22:r:266:GLY:HA3  | 2.12                     | 0.49              |
| 2:2:130:PRO:HG2   | 2:2:133:PHE:CG    | 2.47                     | 0.49              |
| 2:2:131:VAL:HA    | 2:2:134:LYS:HD2   | 1.94                     | 0.49              |
| 1:3:117:GLU:HB2   | 1:3:241:LEU:HD12  | 1.95                     | 0.49              |
| 1:3:158:ILE:O     | 1:3:161:ILE:HB    | 2.12                     | 0.49              |
| 3:4:219:GLU:HG3   | 3:4:222:GLU:CB    | 2.41                     | 0.49              |
| 4:A:85:THR:O      | 4:A:169:SER:HB3   | 2.12                     | 0.49              |
| 6:C:277:ALA:HB2   | 6:C:441:HIS:CG    | 2.47                     | 0.49              |
| 6:C:290:VAL:HG21  | 25:C:502:CLA:CED  | 2.41                     | 0.49              |
| 20:S:131:PRO:HG3  | 25:S:305:CLA:C1D  | 2.42                     | 0.49              |
| 21:N:95:ASN:HA    | 21:N:98:LEU:HB2   | 1.93                     | 0.49              |
| 24:Y:307:CHL:CMC  | 24:Y:308:CHL:C4C  | 2.90                     | 0.49              |
| 22:R:67:TRP:CE2   | 22:R:85:LYS:HA    | 2.48                     | 0.49              |
| 22:R:279:LEU:H    | 22:R:279:LEU:HD12 | 1.76                     | 0.49              |
| 25:R:603:CLA:HMB2 | 25:R:603:CLA:H143 | 1.94                     | 0.49              |
| 23:U:79:ARG:O     | 23:U:84:ALA:HB2   | 2.13                     | 0.49              |
| 2:6:121:LYS:HD3   | 2:6:242:LEU:HD23  | 1.93                     | 0.49              |
| 8:e:28:PRO:O      | 8:e:32:ILE:HG12   | 2.12                     | 0.49              |
| 20:s:262:PHE:CE2  | 25:s:314:CLA:H3A  | 2.43                     | 0.49              |
| 21:y:57:LYS:HD2   | 21:y:63:SER:CB    | 2.42                     | 0.49              |
| 24:y:310:CHL:NA   | 24:y:310:CHL:HBA1 | 2.27                     | 0.49              |
| 22:r:220:GLY:HA2  | 22:r:224:ASP:CB   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:94:ARG:HA     | 1:1:94:ARG:HE     | 1.75                     | 0.49              |
| 2:2:117:GLU:O     | 2:2:121:LYS:HB2   | 2.13                     | 0.49              |
| 2:2:145:LEU:HB3   | 2:2:149:GLY:C     | 2.37                     | 0.49              |
| 25:C:511:CLA:HBA1 | 28:K:101:BCR:H271 | 1.93                     | 0.49              |
| 7:D:135:ARG:NH2   | 7:D:138:GLN:OE1   | 2.42                     | 0.49              |
| 15:O:177:PRO:CD   | 15:O:189:LYS:HE3  | 2.43                     | 0.49              |
| 21:G:86:SER:HB3   | 21:G:92:PHE:CD1   | 2.45                     | 0.49              |
| 21:N:57:LYS:HD2   | 21:N:63:SER:CB    | 2.42                     | 0.49              |
| 21:N:154:HIS:O    | 21:N:154:HIS:ND1  | 2.44                     | 0.49              |
| 25:N:603:CLA:CAC  | 24:Y:302:CHL:H102 | 2.42                     | 0.49              |
| 25:Y:315:CLA:HBA2 | 25:Y:315:CLA:CBD  | 2.42                     | 0.49              |
| 22:R:150:ALA:HA   | 41:R:616:XAT:H181 | 1.94                     | 0.49              |
| 1:7:57:LYS:HD2    | 1:7:63:SER:CB     | 2.42                     | 0.49              |
| 27:a:405:PHO:H152 | 25:d:401:CLA:HMB2 | 1.95                     | 0.49              |
| 25:b:607:CLA:HMC2 | 28:b:618:BCR:H323 | 1.95                     | 0.49              |
| 6:c:95:LEU:HD23   | 25:c:502:CLA:H143 | 1.95                     | 0.49              |
| 18:x:93:GLY:O     | 18:x:96:VAL:HG22  | 2.12                     | 0.49              |
| 20:s:225:GLU:HB2  | 25:s:310:CLA:C2B  | 2.42                     | 0.49              |
| 21:g:144:LEU:HD11 | 25:g:604:CLA:HAA2 | 1.95                     | 0.49              |
| 21:n:176:ARG:NH2  | 24:n:609:CHL:O1D  | 2.44                     | 0.49              |
| 25:n:603:CLA:H192 | 24:n:607:CHL:C17  | 2.42                     | 0.49              |
| 24:n:607:CHL:H203 | 25:y:303:CLA:C15  | 2.42                     | 0.49              |
| 2:2:64:VAL:HG12   | 2:2:65:GLN:N      | 2.27                     | 0.49              |
| 4:A:232:SER:OG    | 5:B:7:ARG:NH1     | 2.44                     | 0.49              |
| 5:B:280:PHE:O     | 5:B:281:GLN:HB2   | 2.12                     | 0.49              |
| 5:B:453:PHE:HB2   | 7:D:292:LEU:HD12  | 1.93                     | 0.49              |
| 25:B:613:CLA:H172 | 28:B:618:BCR:H312 | 1.94                     | 0.49              |
| 10:H:32:LYS:HB2   | 22:R:113:ARG:NH1  | 2.28                     | 0.49              |
| 15:O:215:VAL:HG22 | 15:O:218:LEU:HB3  | 1.93                     | 0.49              |
| 21:G:215:GLU:CB   | 25:G:610:CLA:C1B  | 2.89                     | 0.49              |
| 22:R:158:GLU:OE2  | 22:R:266:GLY:HA3  | 2.12                     | 0.49              |
| 22:R:164:THR:HG23 | 22:R:167:ASP:H    | 1.78                     | 0.49              |
| 1:5:86:SER:HB3    | 1:5:92:PHE:CD1    | 2.45                     | 0.49              |
| 1:7:51:TYR:HE2    | 1:7:209:ALA:HB1   | 1.75                     | 0.49              |
| 1:7:103:SER:O     | 1:7:107:MET:HG3   | 2.12                     | 0.49              |
| 30:a:409:LMG:O5   | 17:w:87:THR:O     | 2.27                     | 0.49              |
| 7:d:44:PHE:HB3    | 7:d:114:PHE:CE2   | 2.48                     | 0.49              |
| 7:d:240:GLN:OE1   | 7:d:242:GLU:HG2   | 2.13                     | 0.49              |
| 21:n:132:PHE:HD2  | 24:n:607:CHL:HED1 | 1.77                     | 0.49              |
| 21:y:227:PHE:CD2  | 25:y:303:CLA:H202 | 2.40                     | 0.49              |
| 22:r:72:LEU:HB3   | 22:r:137:ARG:CZ   | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:279:LEU:H    | 22:r:279:LEU:HD12 | 1.76                     | 0.49              |
| 1:1:57:LYS:HD2    | 1:1:63:SER:CB     | 2.42                     | 0.49              |
| 1:1:116:PRO:HA    | 1:1:126:PHE:HE2   | 1.78                     | 0.49              |
| 2:2:204:ASP:C     | 2:2:208:THR:HG23  | 2.38                     | 0.49              |
| 2:2:236:VAL:O     | 2:2:237:THR:OG1   | 2.24                     | 0.49              |
| 3:4:158:SER:O     | 3:4:162:VAL:HG12  | 2.12                     | 0.49              |
| 5:B:377:VAL:HG11  | 7:D:343:PRO:CG    | 2.41                     | 0.49              |
| 25:B:609:CLA:HMA2 | 25:B:610:CLA:HMC2 | 1.94                     | 0.49              |
| 25:B:614:CLA:H71  | 29:L:101:SQD:C15  | 2.43                     | 0.49              |
| 6:C:227:VAL:HG21  | 28:I:101:BCR:C29  | 2.43                     | 0.49              |
| 7:D:262:PHE:O     | 31:D:405:PL9:H522 | 2.11                     | 0.49              |
| 7:D:320:ILE:O     | 7:D:324:GLU:HG3   | 2.12                     | 0.49              |
| 15:O:179:GLU:HB3  | 15:O:187:ASN:OD1  | 2.12                     | 0.49              |
| 20:S:135:ASN:HA   | 20:S:138:GLY:O    | 2.12                     | 0.49              |
| 21:G:103:SER:O    | 21:G:107:MET:HG3  | 2.12                     | 0.49              |
| 21:G:144:LEU:HD11 | 25:G:604:CLA:HAA2 | 1.95                     | 0.49              |
| 24:N:609:CHL:H72  | 24:Y:302:CHL:C11  | 2.40                     | 0.49              |
| 21:Y:214:LYS:HG2  | 25:Y:312:CLA:O2D  | 2.12                     | 0.49              |
| 4:a:57:PRO:HB2    | 4:a:66:PRO:CB     | 2.42                     | 0.49              |
| 4:a:131:TRP:CZ2   | 6:c:449:ARG:HD2   | 2.48                     | 0.49              |
| 4:a:162:PRO:HB3   | 4:a:168:PHE:HA    | 1.94                     | 0.49              |
| 5:b:453:PHE:HB2   | 7:d:292:LEU:HD12  | 1.93                     | 0.49              |
| 5:b:471:ALA:HB2   | 7:d:131:PHE:CE1   | 2.48                     | 0.49              |
| 6:c:135:LEU:O     | 6:c:135:LEU:HD23  | 2.13                     | 0.49              |
| 6:c:435:PHE:O     | 6:c:439:VAL:HG23  | 2.12                     | 0.49              |
| 7:d:19:MET:SD     | 18:x:103:VAL:HG22 | 2.52                     | 0.49              |
| 20:s:119:ARG:HB3  | 25:s:310:CLA:HAC1 | 1.95                     | 0.49              |
| 20:s:135:ASN:HA   | 20:s:138:GLY:O    | 2.12                     | 0.49              |
| 20:s:188:TYR:HD1  | 20:s:193:GLY:HA3  | 1.77                     | 0.49              |
| 21:g:95:ASN:HA    | 21:g:98:LEU:HB2   | 1.93                     | 0.49              |
| 25:n:611:CLA:CMC  | 26:n:618:LHG:H341 | 2.42                     | 0.49              |
| 21:y:204:ASP:O    | 21:y:208:PHE:N    | 2.40                     | 0.49              |
| 1:3:116:PRO:HA    | 1:3:126:PHE:HE2   | 1.78                     | 0.49              |
| 1:3:127:GLY:HA3   | 1:3:137:GLN:CG    | 2.42                     | 0.49              |
| 3:4:221:LEU:HA    | 3:4:224:LEU:HD23  | 1.95                     | 0.49              |
| 4:A:254:TYR:HE1   | 7:D:134:ALA:N     | 2.11                     | 0.49              |
| 5:B:164:PRO:HG3   | 25:B:606:CLA:O1D  | 2.12                     | 0.49              |
| 5:B:360:PRO:C     | 5:B:361:THR:HG22  | 2.38                     | 0.49              |
| 6:C:213:LEU:HD11  | 28:I:101:BCR:H373 | 1.95                     | 0.49              |
| 6:C:361:LEU:HD12  | 35:C:515:DGD:O3E  | 2.13                     | 0.49              |
| 21:G:127:GLY:HA3  | 21:G:137:GLN:CG   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:51:TYR:HE2   | 21:N:209:ALA:HB1  | 1.75                     | 0.49              |
| 21:N:227:PHE:CD2  | 25:N:602:CLA:H202 | 2.41                     | 0.49              |
| 21:Y:154:HIS:O    | 21:Y:154:HIS:ND1  | 2.44                     | 0.49              |
| 1:5:95:ASN:HA     | 1:5:98:LEU:HB2    | 1.93                     | 0.49              |
| 1:5:209:ALA:CA    | 1:5:212:LYS:HG3   | 2.34                     | 0.49              |
| 2:6:116:PRO:HG2   | 2:6:117:GLU:OE1   | 2.13                     | 0.49              |
| 2:6:249:LEU:HD12  | 2:6:250:ASP:N     | 2.28                     | 0.49              |
| 1:7:127:GLY:HA3   | 1:7:137:GLN:CG    | 2.42                     | 0.49              |
| 3:8:75:GLY:HA2    | 3:8:80:ASP:HB3    | 1.93                     | 0.49              |
| 5:b:245:VAL:HG21  | 25:b:612:CLA:CED  | 2.43                     | 0.49              |
| 6:c:97:TRP:HE1    | 6:c:178:LYS:CE    | 2.25                     | 0.49              |
| 6:c:321:ASP:OD2   | 6:c:340:TYR:OH    | 2.27                     | 0.49              |
| 6:c:378:SER:OG    | 6:c:382:LYS:HE3   | 2.12                     | 0.49              |
| 6:c:457:LYS:HD3   | 7:d:230:ALA:HA    | 1.94                     | 0.49              |
| 7:d:341:ILE:HG23  | 7:d:341:ILE:O     | 2.13                     | 0.49              |
| 8:e:38:VAL:HG21   | 9:f:30:SER:O      | 2.11                     | 0.49              |
| 15:o:177:PRO:CD   | 15:o:189:LYS:HE3  | 2.43                     | 0.49              |
| 21:g:90:GLU:CB    | 21:n:87:ALA:HB1   | 2.42                     | 0.49              |
| 21:n:107:MET:HE1  | 25:n:610:CLA:CHC  | 2.42                     | 0.49              |
| 22:r:218:PRO:HB2  | 22:r:223:PHE:CD2  | 2.48                     | 0.49              |
| 2:2:137:SER:HA    | 2:2:140:PHE:CE2   | 2.48                     | 0.49              |
| 1:3:138:ILE:HG13  | 1:3:144:LEU:CB    | 2.31                     | 0.49              |
| 5:B:245:VAL:HG21  | 25:B:612:CLA:CED  | 2.43                     | 0.49              |
| 5:B:271:THR:O     | 5:B:272:ARG:HB3   | 2.12                     | 0.49              |
| 7:D:44:PHE:HB3    | 7:D:114:PHE:CE2   | 2.48                     | 0.49              |
| 7:D:179:ILE:HG21  | 25:D:401:CLA:C4C  | 2.42                     | 0.49              |
| 7:D:192:TRP:CE3   | 7:D:290:LEU:HD11  | 2.48                     | 0.49              |
| 7:D:198:HIS:HE1   | 25:D:402:CLA:C1C  | 2.26                     | 0.49              |
| 7:D:240:GLN:OE1   | 7:D:242:GLU:HG2   | 2.13                     | 0.49              |
| 10:H:25:PRO:CG    | 22:R:122:THR:HB   | 2.42                     | 0.49              |
| 15:O:113:GLN:NE2  | 17:W:80:LEU:HD11  | 2.16                     | 0.49              |
| 21:G:97:GLU:HA    | 21:G:190:LEU:CD1  | 2.24                     | 0.49              |
| 25:G:612:CLA:HBD  | 25:G:612:CLA:HAA2 | 1.95                     | 0.49              |
| 21:N:107:MET:HE1  | 25:N:610:CLA:CHC  | 2.42                     | 0.49              |
| 25:N:603:CLA:H142 | 25:Y:304:CLA:C14  | 2.42                     | 0.49              |
| 21:Y:103:SER:O    | 21:Y:107:MET:HG3  | 2.12                     | 0.49              |
| 24:R:605:CHL:HAB  | 25:R:608:CLA:CBC  | 2.43                     | 0.49              |
| 23:U:97:THR:HG22  | 23:U:102:ARG:NH2  | 2.28                     | 0.49              |
| 2:6:130:PRO:HG2   | 2:6:133:PHE:CG    | 2.47                     | 0.49              |
| 1:7:117:GLU:HB2   | 1:7:241:LEU:HD12  | 1.95                     | 0.49              |
| 3:8:73:LEU:HB3    | 3:8:80:ASP:OD1    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:a:220:THR:O     | 4:a:223:LEU:HG    | 2.12                     | 0.49              |
| 29:a:408:SQD:H441 | 7:d:233:PHE:CE2   | 2.48                     | 0.49              |
| 25:b:608:CLA:H18  | 25:d:403:CLA:HBA1 | 1.95                     | 0.49              |
| 10:h:22:LEU:HB3   | 22:r:124:PHE:CE2  | 2.48                     | 0.49              |
| 14:m:26:TYR:O     | 14:m:30:VAL:HG13  | 2.13                     | 0.49              |
| 21:g:76:GLY:HA3   | 21:g:216:LEU:CD2  | 2.24                     | 0.49              |
| 25:2:604:CLA:HBD  | 25:2:604:CLA:CAA  | 2.41                     | 0.49              |
| 3:4:187:ASN:O     | 3:4:188:TYR:HB2   | 2.12                     | 0.49              |
| 4:A:40:THR:HA     | 4:A:118:HIS:HD1   | 1.77                     | 0.49              |
| 25:C:504:CLA:H101 | 35:C:516:DGD:HBH2 | 1.94                     | 0.49              |
| 19:Z:58:ASN:O     | 19:Z:61:ILE:HG12  | 2.13                     | 0.49              |
| 21:G:209:ALA:CA   | 21:G:212:LYS:HG3  | 2.34                     | 0.49              |
| 21:N:60:GLY:HA3   | 24:N:601:CHL:CMC  | 2.43                     | 0.49              |
| 21:N:116:PRO:HA   | 21:N:126:PHE:HE2  | 1.78                     | 0.49              |
| 21:N:127:GLY:HA3  | 21:N:137:GLN:CG   | 2.42                     | 0.49              |
| 21:N:138:ILE:HG13 | 21:N:144:LEU:CB   | 2.31                     | 0.49              |
| 24:N:607:CHL:H202 | 24:N:609:CHL:C3   | 2.43                     | 0.49              |
| 21:Y:251:PRO:HB2  | 25:Y:315:CLA:CMA  | 2.30                     | 0.49              |
| 24:5:301:CHL:HHD  | 24:5:301:CHL:HBC2 | 1.95                     | 0.49              |
| 3:8:213:VAL:O     | 3:8:213:VAL:HG12  | 2.12                     | 0.49              |
| 27:a:404:PHO:H42  | 26:d:406:LHG:H342 | 1.95                     | 0.49              |
| 5:b:296:GLN:NE2   | 5:b:304:LYS:HD2   | 2.22                     | 0.49              |
| 25:b:613:CLA:H172 | 28:b:618:BCR:H312 | 1.94                     | 0.49              |
| 6:c:25:GLY:O      | 6:c:26:ARG:HG3    | 2.12                     | 0.49              |
| 7:d:141:PRO:O     | 7:d:145:ILE:HD12  | 2.13                     | 0.49              |
| 7:d:194:LEU:O     | 13:l:35:TYR:OH    | 2.14                     | 0.49              |
| 14:m:15:ILE:O     | 14:m:19:THR:OG1   | 2.18                     | 0.49              |
| 15:o:113:GLN:NE2  | 17:w:80:LEU:HD11  | 2.16                     | 0.49              |
| 15:o:145:VAL:CG1  | 15:o:203:LEU:HD11 | 2.37                     | 0.49              |
| 21:g:107:MET:HG2  | 21:g:222:ALA:HB3  | 1.93                     | 0.49              |
| 21:g:116:PRO:HA   | 21:g:126:PHE:HE2  | 1.78                     | 0.49              |
| 21:g:139:PHE:CD2  | 24:g:607:CHL:OBD  | 2.66                     | 0.49              |
| 21:g:215:GLU:CB   | 25:g:610:CLA:C1B  | 2.89                     | 0.49              |
| 21:n:158:ILE:O    | 21:n:161:ILE:HB   | 2.12                     | 0.49              |
| 22:r:67:TRP:CE2   | 22:r:85:LYS:HA    | 2.48                     | 0.49              |
| 22:r:160:LEU:HD13 | 22:r:180:LEU:HD21 | 1.95                     | 0.49              |
| 2:2:55:ARG:HE     | 2:2:72:GLY:HA3    | 1.77                     | 0.48              |
| 4:A:202:VAL:HG13  | 25:A:401:CLA:HMB2 | 1.95                     | 0.48              |
| 5:B:460:LEU:HD21  | 7:D:160:ILE:CD1   | 2.42                     | 0.48              |
| 7:D:343:PRO:HD2   | 7:D:346:VAL:HG21  | 1.95                     | 0.48              |
| 20:S:132:GLU:HA   | 20:S:145:ALA:CB   | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:86:SER:OG    | 25:G:602:CLA:O1A  | 2.23                     | 0.48              |
| 21:N:132:PHE:HD2  | 24:N:607:CHL:HED1 | 1.77                     | 0.48              |
| 25:N:604:CLA:C1C  | 40:N:617:NEX:H222 | 2.42                     | 0.48              |
| 21:Y:69:TYR:OH    | 21:Y:81:ASP:OD2   | 2.20                     | 0.48              |
| 22:R:63:ILE:O     | 22:R:63:ILE:HG13  | 2.12                     | 0.48              |
| 22:R:160:LEU:HD13 | 22:R:180:LEU:HD21 | 1.95                     | 0.48              |
| 1:5:204:ASP:O     | 1:5:208:PHE:N     | 2.40                     | 0.48              |
| 2:6:116:PRO:CG    | 2:6:134:LYS:HE3   | 2.42                     | 0.48              |
| 2:6:117:GLU:O     | 2:6:121:LYS:HB2   | 2.13                     | 0.48              |
| 2:6:127:PHE:HE2   | 2:6:145:LEU:CB    | 2.24                     | 0.48              |
| 25:6:604:CLA:CHC  | 26:6:606:LHG:HC5  | 2.43                     | 0.48              |
| 4:a:202:VAL:HG13  | 25:a:402:CLA:HMB2 | 1.95                     | 0.48              |
| 5:b:164:PRO:HG3   | 25:b:606:CLA:O1D  | 2.12                     | 0.48              |
| 6:c:223:TRP:CG    | 6:c:224:ILE:H     | 2.31                     | 0.48              |
| 25:c:504:CLA:H101 | 35:c:516:DGD:HBH2 | 1.94                     | 0.48              |
| 25:c:511:CLA:H142 | 12:k:47:PHE:HE2   | 1.77                     | 0.48              |
| 7:d:343:PRO:HD2   | 7:d:346:VAL:HG21  | 1.95                     | 0.48              |
| 10:h:32:LYS:HB2   | 22:r:113:ARG:NH1  | 2.28                     | 0.48              |
| 21:g:215:GLU:HG3  | 25:g:610:CLA:C3B  | 2.42                     | 0.48              |
| 25:n:603:CLA:C20  | 24:n:607:CHL:H172 | 2.42                     | 0.48              |
| 25:n:613:CLA:H142 | 25:n:613:CLA:C2   | 2.40                     | 0.48              |
| 22:r:72:LEU:CB    | 22:r:137:ARG:HH22 | 2.26                     | 0.48              |
| 22:r:164:THR:HG23 | 22:r:167:ASP:H    | 1.78                     | 0.48              |
| 22:r:192:ILE:O    | 22:r:196:VAL:HG23 | 2.13                     | 0.48              |
| 2:2:127:PHE:HE2   | 2:2:145:LEU:CB    | 2.24                     | 0.48              |
| 1:3:57:LYS:HD2    | 1:3:63:SER:CB     | 2.42                     | 0.48              |
| 1:3:103:SER:O     | 1:3:107:MET:HG3   | 2.12                     | 0.48              |
| 25:B:608:CLA:H18  | 25:D:403:CLA:HBA1 | 1.95                     | 0.48              |
| 6:C:97:TRP:HE1    | 6:C:178:LYS:CE    | 2.25                     | 0.48              |
| 6:C:135:LEU:O     | 6:C:135:LEU:HD23  | 2.13                     | 0.48              |
| 6:C:175:LEU:HD23  | 6:C:237:HIS:CE1   | 2.48                     | 0.48              |
| 6:C:211:GLY:O     | 6:C:215:LYS:HB2   | 2.13                     | 0.48              |
| 25:C:506:CLA:H141 | 25:C:506:CLA:H162 | 1.63                     | 0.48              |
| 7:D:162:PRO:CB    | 7:D:171:ALA:HB2   | 2.42                     | 0.48              |
| 12:K:34:ASN:N     | 12:K:35:PRO:HD2   | 2.28                     | 0.48              |
| 15:O:114:CYS:SG   | 15:O:139:GLU:HB2  | 2.52                     | 0.48              |
| 21:G:224:PHE:CG   | 26:Y:301:LHG:H281 | 2.49                     | 0.48              |
| 24:G:605:CHL:H3A  | 24:G:605:CHL:HBA2 | 1.36                     | 0.48              |
| 21:N:172:VAL:HG22 | 40:N:617:NEX:H201 | 1.94                     | 0.48              |
| 21:N:176:ARG:NH2  | 24:N:609:CHL:O1D  | 2.44                     | 0.48              |
| 2:6:145:LEU:HB3   | 2:6:149:GLY:C     | 2.37                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:6:209:PHE:C     | 2:6:213:LYS:HZ2   | 2.22                     | 0.48              |
| 1:7:204:ASP:O     | 1:7:208:PHE:N     | 2.40                     | 0.48              |
| 3:8:187:ASN:O     | 3:8:188:TYR:HB2   | 2.12                     | 0.48              |
| 3:8:222:GLU:HA    | 3:8:225:LYS:HB2   | 1.95                     | 0.48              |
| 5:b:236:THR:HB    | 5:b:473:THR:HG21  | 1.95                     | 0.48              |
| 6:c:175:LEU:HD23  | 6:c:237:HIS:CE1   | 2.48                     | 0.48              |
| 6:c:199:ILE:HG13  | 6:c:234:ILE:HG13  | 1.93                     | 0.48              |
| 6:c:279:LEU:O     | 25:c:502:CLA:HBC1 | 2.13                     | 0.48              |
| 6:c:332:GLN:HG2   | 15:o:238:GLY:O    | 2.14                     | 0.48              |
| 7:d:192:TRP:CE3   | 7:d:290:LEU:HD11  | 2.48                     | 0.48              |
| 15:o:171:LEU:HD22 | 15:o:194:ILE:O    | 2.13                     | 0.48              |
| 15:o:179:GLU:HB3  | 15:o:187:ASN:OD1  | 2.12                     | 0.48              |
| 24:n:601:CHL:HBC3 | 24:n:601:CHL:HMC  | 1.94                     | 0.48              |
| 1:1:95:ASN:HA     | 1:1:98:LEU:HB2    | 1.93                     | 0.48              |
| 3:4:175:ALA:CB    | 25:R:601:CLA:HHC  | 2.43                     | 0.48              |
| 4:A:60:ILE:HB     | 4:A:83:ILE:CG2    | 2.44                     | 0.48              |
| 5:B:285:TYR:CZ    | 23:U:90:GLN:HG3   | 2.49                     | 0.48              |
| 5:B:368:VAL:HG21  | 5:B:422:ARG:HG2   | 1.95                     | 0.48              |
| 25:B:602:CLA:H191 | 35:B:626:DGD:HBT1 | 1.95                     | 0.48              |
| 25:B:607:CLA:HMC2 | 28:B:618:BCR:H323 | 1.95                     | 0.48              |
| 6:C:332:GLN:HG2   | 15:O:238:GLY:O    | 2.14                     | 0.48              |
| 6:C:457:LYS:HD3   | 7:D:230:ALA:HA    | 1.94                     | 0.48              |
| 20:S:119:ARG:HB3  | 25:S:310:CLA:HAC1 | 1.95                     | 0.48              |
| 21:G:60:GLY:H     | 24:G:601:CHL:CHC  | 2.26                     | 0.48              |
| 22:R:240:LEU:HG   | 22:R:244:LYS:HD2  | 1.93                     | 0.48              |
| 2:6:246:LEU:HA    | 2:6:249:LEU:HD23  | 1.94                     | 0.48              |
| 1:7:158:ILE:O     | 1:7:161:ILE:HB    | 2.12                     | 0.48              |
| 4:a:60:ILE:HB     | 4:a:83:ILE:HG22   | 1.96                     | 0.48              |
| 4:a:140:ARG:NH2   | 7:d:220:GLU:O     | 2.40                     | 0.48              |
| 25:a:402:CLA:H102 | 27:a:404:PHO:HAA1 | 1.95                     | 0.48              |
| 25:b:609:CLA:HMA2 | 25:b:610:CLA:HMC2 | 1.94                     | 0.48              |
| 6:c:140:LEU:HD22  | 25:c:513:CLA:CMA  | 2.44                     | 0.48              |
| 6:c:471:PRO:O     | 6:c:472:LEU:HB2   | 2.11                     | 0.48              |
| 25:c:501:CLA:HHC  | 25:c:501:CLA:HBB1 | 1.96                     | 0.48              |
| 11:i:34:ARG:C     | 11:i:35:GLU:HG3   | 2.39                     | 0.48              |
| 25:s:310:CLA:H51  | 25:s:312:CLA:CMA  | 2.34                     | 0.48              |
| 21:g:127:GLY:HA3  | 21:g:137:GLN:CG   | 2.42                     | 0.48              |
| 21:g:128:GLU:CB   | 21:g:137:GLN:HB2  | 2.41                     | 0.48              |
| 24:g:606:CHL:HAA1 | 40:g:617:NEX:H381 | 1.96                     | 0.48              |
| 21:n:103:SER:O    | 21:n:107:MET:HG3  | 2.12                     | 0.48              |
| 25:n:602:CLA:HMB1 | 25:n:602:CLA:C2   | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:164:THR:CG2  | 22:r:167:ASP:HB2  | 2.43                     | 0.48              |
| 23:u:97:THR:HG22  | 23:u:102:ARG:NH2  | 2.28                     | 0.48              |
| 1:1:58:TYR:CE1    | 1:1:80:TRP:HA     | 2.49                     | 0.48              |
| 1:1:103:SER:O     | 1:1:107:MET:HG3   | 2.12                     | 0.48              |
| 2:2:114:ILE:O     | 2:2:118:VAL:HG23  | 2.13                     | 0.48              |
| 4:A:272:HIS:CD2   | 7:D:219:VAL:HG21  | 2.48                     | 0.48              |
| 25:A:401:CLA:H102 | 27:A:403:PHO:HAA1 | 1.95                     | 0.48              |
| 5:B:236:THR:HB    | 5:B:473:THR:HG21  | 1.95                     | 0.48              |
| 7:D:141:PRO:O     | 7:D:145:ILE:HD12  | 2.13                     | 0.48              |
| 15:O:171:LEU:HD22 | 15:O:194:ILE:O    | 2.13                     | 0.48              |
| 25:G:603:CLA:ND   | 24:G:609:CHL:H8   | 2.28                     | 0.48              |
| 21:N:94:ARG:HA    | 21:N:94:ARG:HE    | 1.75                     | 0.48              |
| 25:N:602:CLA:HMB1 | 25:N:602:CLA:C2   | 2.44                     | 0.48              |
| 21:Y:210:GLU:OE1  | 21:Y:214:LYS:NZ   | 2.38                     | 0.48              |
| 22:R:185:PRO:CD   | 21:y:151:SER:HB2  | 2.43                     | 0.48              |
| 6:c:277:ALA:HB2   | 6:c:441:HIS:CG    | 2.47                     | 0.48              |
| 25:s:305:CLA:HBB1 | 25:s:305:CLA:HMB1 | 1.95                     | 0.48              |
| 25:g:610:CLA:H41  | 25:g:612:CLA:CMA  | 2.41                     | 0.48              |
| 25:n:604:CLA:C1C  | 40:n:617:NEX:H222 | 2.43                     | 0.48              |
| 22:r:58:TRP:CD2   | 22:r:78:PHE:HD1   | 2.31                     | 0.48              |
| 24:r:607:CHL:H112 | 24:r:607:CHL:CAB  | 2.31                     | 0.48              |
| 25:r:614:CLA:HHD  | 25:r:614:CLA:CBC  | 2.37                     | 0.48              |
| 1:1:107:MET:HG2   | 1:1:222:ALA:HB3   | 1.94                     | 0.48              |
| 2:2:69:TYR:HH     | 2:2:81:ASP:CG     | 2.21                     | 0.48              |
| 2:2:175:GLY:HA3   | 2:2:181:LEU:CG    | 2.44                     | 0.48              |
| 25:2:604:CLA:H41  | 25:2:604:CLA:H61  | 1.61                     | 0.48              |
| 3:4:222:GLU:HA    | 3:4:225:LYS:HB2   | 1.95                     | 0.48              |
| 3:4:225:LYS:CA    | 3:4:228:GLU:OE1   | 2.61                     | 0.48              |
| 6:C:279:LEU:O     | 25:C:502:CLA:HBC1 | 2.13                     | 0.48              |
| 10:H:22:LEU:HB3   | 22:R:124:PHE:CE2  | 2.48                     | 0.48              |
| 11:I:34:ARG:C     | 11:I:35:GLU:HG3   | 2.38                     | 0.48              |
| 20:S:67:ARG:HH11  | 20:S:87:GLY:HA2   | 1.78                     | 0.48              |
| 25:S:305:CLA:HBB1 | 25:S:305:CLA:HMB1 | 1.95                     | 0.48              |
| 21:Y:94:ARG:HA    | 21:Y:94:ARG:HE    | 1.75                     | 0.48              |
| 21:Y:116:PRO:HA   | 21:Y:126:PHE:HE2  | 1.78                     | 0.48              |
| 21:Y:151:SER:HB2  | 22:r:185:PRO:CD   | 2.43                     | 0.48              |
| 21:Y:209:ALA:CA   | 21:Y:212:LYS:HG3  | 2.34                     | 0.48              |
| 22:R:164:THR:CG2  | 22:R:167:ASP:HB2  | 2.44                     | 0.48              |
| 1:5:128:GLU:CB    | 1:5:137:GLN:HB2   | 2.41                     | 0.48              |
| 2:6:104:ARG:HE    | 24:6:603:CHL:CBD  | 2.13                     | 0.48              |
| 2:6:131:VAL:HA    | 2:6:134:LYS:HB2   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:175:ALA:CB    | 25:r:601:CLA:HHC  | 2.43                     | 0.48              |
| 4:a:51:ALA:HA     | 4:a:55:ALA:HB2    | 1.95                     | 0.48              |
| 4:a:131:TRP:CZ2   | 25:c:505:CLA:HAA2 | 2.49                     | 0.48              |
| 4:a:139:MET:SD    | 7:d:253:PHE:HB2   | 2.54                     | 0.48              |
| 19:z:56:ILE:HG23  | 20:s:270:ILE:CD1  | 2.44                     | 0.48              |
| 24:g:609:CHL:CAA  | 21:n:82:THR:HG21  | 2.43                     | 0.48              |
| 25:n:602:CLA:H142 | 25:n:602:CLA:H112 | 1.63                     | 0.48              |
| 24:y:307:CHL:HHC  | 24:y:308:CHL:CMC  | 2.44                     | 0.48              |
| 1:1:154:HIS:O     | 1:1:154:HIS:ND1   | 2.43                     | 0.48              |
| 2:2:131:VAL:HA    | 2:2:134:LYS:HB2   | 1.96                     | 0.48              |
| 1:3:107:MET:HG2   | 1:3:222:ALA:HB3   | 1.94                     | 0.48              |
| 4:A:214:MET:HE1   | 27:A:404:PHO:CAD  | 2.43                     | 0.48              |
| 29:A:407:SQD:H441 | 7:D:233:PHE:CE2   | 2.48                     | 0.48              |
| 5:B:115:TRP:CH2   | 25:B:614:CLA:HMA2 | 2.49                     | 0.48              |
| 5:B:223:GLN:HG2   | 10:H:36:GLY:N     | 2.28                     | 0.48              |
| 6:C:223:TRP:CG    | 6:C:224:ILE:H     | 2.31                     | 0.48              |
| 7:D:58:SER:OG     | 7:D:80:SER:OG     | 2.25                     | 0.48              |
| 20:S:188:TYR:HD1  | 20:S:193:GLY:HA3  | 1.77                     | 0.48              |
| 20:S:225:GLU:HB2  | 25:S:310:CLA:C2B  | 2.42                     | 0.48              |
| 21:G:58:TYR:CE1   | 21:G:80:TRP:HA    | 2.49                     | 0.48              |
| 21:G:107:MET:HG2  | 21:G:222:ALA:HB3  | 1.93                     | 0.48              |
| 21:Y:56:VAL:CB    | 24:Y:302:CHL:HBC1 | 2.43                     | 0.48              |
| 23:U:96:PRO:C     | 23:U:97:THR:HG1   | 2.09                     | 0.48              |
| 1:5:116:PRO:HA    | 1:5:126:PHE:HE2   | 1.78                     | 0.48              |
| 4:a:95:PRO:HD2    | 4:a:98:GLU:HG3    | 1.96                     | 0.48              |
| 5:b:200:SER:O     | 5:b:201:HIS:C     | 2.56                     | 0.48              |
| 5:b:280:PHE:O     | 5:b:281:GLN:CB    | 2.61                     | 0.48              |
| 5:b:422:ARG:O     | 5:b:425:GLN:HG2   | 2.13                     | 0.48              |
| 26:b:622:LHG:H201 | 26:b:622:LHG:H352 | 1.96                     | 0.48              |
| 6:c:227:VAL:HG21  | 28:i:101:BCR:C29  | 2.43                     | 0.48              |
| 25:c:504:CLA:H92  | 25:c:504:CLA:H62  | 1.52                     | 0.48              |
| 25:c:513:CLA:HMC1 | 28:c:514:BCR:H372 | 1.96                     | 0.48              |
| 7:d:198:HIS:HE1   | 25:d:402:CLA:C1C  | 2.26                     | 0.48              |
| 11:i:33:GLY:C     | 11:i:34:ARG:HG3   | 2.36                     | 0.48              |
| 25:g:602:CLA:H111 | 25:g:602:CLA:H72  | 1.45                     | 0.48              |
| 24:g:606:CHL:HBA2 | 40:g:617:NEX:H30  | 1.96                     | 0.48              |
| 21:n:86:SER:HB3   | 21:n:92:PHE:CD1   | 2.45                     | 0.48              |
| 2:2:116:PRO:HG2   | 2:2:117:GLU:OE1   | 2.13                     | 0.48              |
| 4:A:51:ALA:HA     | 4:A:55:ALA:HB2    | 1.95                     | 0.48              |
| 5:B:57:ARG:HG3    | 5:B:57:ARG:O      | 2.14                     | 0.48              |
| 5:B:296:GLN:NE2   | 5:B:304:LYS:HD2   | 2.22                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:379:ALA:HB2   | 5:B:395:VAL:HG11  | 1.95                     | 0.48              |
| 25:C:513:CLA:HMC1 | 28:C:514:BCR:H372 | 1.96                     | 0.48              |
| 8:E:27:ILE:HG22   | 8:E:28:PRO:HD3    | 1.92                     | 0.48              |
| 13:L:20:TRP:CE3   | 26:L:102:LHG:H132 | 2.49                     | 0.48              |
| 15:O:100:LYS:HE3  | 15:O:105:VAL:CG2  | 2.43                     | 0.48              |
| 15:O:143:PHE:HD1  | 15:O:323:ILE:HG13 | 1.78                     | 0.48              |
| 20:S:239:PHE:CE1  | 39:S:315:LUT:H41  | 2.49                     | 0.48              |
| 24:N:601:CHL:HMC  | 24:N:601:CHL:HBC3 | 1.95                     | 0.48              |
| 21:Y:58:TYR:CE1   | 21:Y:80:TRP:HA    | 2.49                     | 0.48              |
| 24:Y:310:CHL:NA   | 24:Y:310:CHL:HBA1 | 2.27                     | 0.48              |
| 4:a:60:ILE:HB     | 4:a:83:ILE:CG2    | 2.44                     | 0.48              |
| 5:b:191:ASP:HB3   | 5:b:194:VAL:HG13  | 1.95                     | 0.48              |
| 5:b:214:LEU:HD13  | 25:r:603:CLA:HED1 | 1.94                     | 0.48              |
| 5:b:360:PRO:C     | 5:b:361:THR:HG22  | 2.38                     | 0.48              |
| 5:b:368:VAL:HG21  | 5:b:422:ARG:HG2   | 1.95                     | 0.48              |
| 6:c:211:GLY:O     | 6:c:215:LYS:HB2   | 2.13                     | 0.48              |
| 6:c:224:ILE:CD1   | 6:c:289:PHE:HZ    | 2.27                     | 0.48              |
| 9:f:21:ALA:O      | 9:f:25:VAL:HG23   | 2.14                     | 0.48              |
| 15:o:100:LYS:HE3  | 15:o:105:VAL:CG2  | 2.43                     | 0.48              |
| 19:z:58:ASN:O     | 19:z:61:ILE:HG12  | 2.13                     | 0.48              |
| 20:s:67:ARG:HH11  | 20:s:87:GLY:HA2   | 1.78                     | 0.48              |
| 20:s:127:GLY:O    | 20:s:131:PRO:HD2  | 2.13                     | 0.48              |
| 21:g:231:VAL:CG1  | 25:g:613:CLA:HAC2 | 2.36                     | 0.48              |
| 21:n:127:GLY:HA3  | 21:n:137:GLN:CG   | 2.42                     | 0.48              |
| 24:n:607:CHL:H202 | 24:n:609:CHL:C3   | 2.43                     | 0.48              |
| 24:n:609:CHL:H72  | 24:y:302:CHL:C11  | 2.40                     | 0.48              |
| 24:y:309:CHL:H11  | 39:y:316:LUT:C38  | 2.43                     | 0.48              |
| 24:r:605:CHL:HAB  | 25:r:608:CLA:CBC  | 2.43                     | 0.48              |
| 24:r:607:CHL:CBB  | 40:r:617:NEX:H12  | 2.40                     | 0.48              |
| 25:2:604:CLA:HBA2 | 25:2:604:CLA:CHA  | 2.44                     | 0.48              |
| 25:2:605:CLA:HBD  | 25:2:605:CLA:CAA  | 2.35                     | 0.48              |
| 1:3:128:GLU:CB    | 1:3:137:GLN:HB2   | 2.41                     | 0.48              |
| 3:4:94:PHE:HB3    | 3:4:98:TYR:CE2    | 2.42                     | 0.48              |
| 3:4:222:GLU:HA    | 3:4:225:LYS:CD    | 2.44                     | 0.48              |
| 4:A:95:PRO:HD2    | 4:A:98:GLU:HG3    | 1.96                     | 0.48              |
| 4:A:139:MET:SD    | 7:D:253:PHE:HB2   | 2.54                     | 0.48              |
| 4:A:162:PRO:HB3   | 4:A:168:PHE:HA    | 1.94                     | 0.48              |
| 5:B:121:GLU:HB3   | 10:H:14:PRO:HB2   | 1.95                     | 0.48              |
| 25:D:403:CLA:H122 | 18:X:92:SER:OG    | 2.14                     | 0.48              |
| 25:S:311:CLA:CHD  | 26:S:318:LHG:HC62 | 2.43                     | 0.48              |
| 24:G:609:CHL:CAA  | 21:N:82:THR:HG21  | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:R:72:LEU:CB    | 22:R:137:ARG:HH22 | 2.26                     | 0.48              |
| 22:R:166:GLN:HG2  | 22:R:167:ASP:N    | 2.28                     | 0.48              |
| 2:6:137:SER:HA    | 2:6:140:PHE:CE2   | 2.48                     | 0.48              |
| 3:8:222:GLU:HA    | 3:8:225:LYS:CD    | 2.44                     | 0.48              |
| 4:a:135:PHE:CZ    | 11:i:31:ASN:HB3   | 2.49                     | 0.48              |
| 5:b:240:SER:HB3   | 25:b:610:CLA:NB   | 2.28                     | 0.48              |
| 25:b:607:CLA:H91  | 25:b:607:CLA:H111 | 1.62                     | 0.48              |
| 6:c:361:LEU:HD12  | 35:c:515:DGD:O3E  | 2.13                     | 0.48              |
| 7:d:350:GLY:HA2   | 7:d:353:LEU:HD23  | 1.96                     | 0.48              |
| 16:t:11:VAL:HG13  | 28:t:101:BCR:C33  | 2.43                     | 0.48              |
| 16:t:14:LEU:HD12  | 28:t:101:BCR:C34  | 2.42                     | 0.48              |
| 25:s:303:CLA:C7   | 25:s:304:CLA:HMA1 | 2.39                     | 0.48              |
| 21:g:60:GLY:H     | 24:g:601:CHL:CHC  | 2.26                     | 0.48              |
| 25:g:612:CLA:HAA2 | 25:g:612:CLA:HBD  | 1.95                     | 0.48              |
| 23:u:79:ARG:O     | 23:u:84:ALA:HB2   | 2.13                     | 0.48              |
| 2:2:204:ASP:O     | 2:2:208:THR:N     | 2.45                     | 0.48              |
| 2:2:211:GLU:O     | 2:2:215:LYS:HG3   | 2.13                     | 0.48              |
| 6:C:376:ASP:OD2   | 6:C:379:ARG:NE    | 2.47                     | 0.48              |
| 14:M:26:TYR:O     | 14:M:30:VAL:HG13  | 2.13                     | 0.48              |
| 16:T:14:LEU:HD12  | 28:T:101:BCR:C34  | 2.42                     | 0.48              |
| 20:S:127:GLY:O    | 20:S:131:PRO:HD2  | 2.13                     | 0.48              |
| 24:G:606:CHL:HAA1 | 40:G:617:NEX:H381 | 1.96                     | 0.48              |
| 25:G:613:CLA:HBB  | 39:G:615:LUT:H3   | 1.96                     | 0.48              |
| 21:N:50:TRP:O     | 21:N:55:ARG:HD2   | 2.14                     | 0.48              |
| 21:N:58:TYR:CE1   | 21:N:80:TRP:HA    | 2.49                     | 0.48              |
| 21:N:139:PHE:HD2  | 24:N:607:CHL:OBD  | 1.97                     | 0.48              |
| 21:N:196:PHE:HZ   | 24:N:608:CHL:C1C  | 2.27                     | 0.48              |
| 22:R:57:LEU:HB2   | 22:R:59:TYR:CE1   | 2.49                     | 0.48              |
| 22:R:242:GLU:HB2  | 25:R:609:CLA:CHB  | 2.44                     | 0.48              |
| 2:6:117:GLU:HG3   | 2:6:129:GLU:HB3   | 1.96                     | 0.48              |
| 2:6:175:GLY:HA3   | 2:6:181:LEU:CG    | 2.44                     | 0.48              |
| 24:6:601:CHL:H62  | 24:6:601:CHL:H102 | 1.58                     | 0.48              |
| 3:8:169:SER:OG    | 3:8:173:GLU:OE2   | 2.31                     | 0.48              |
| 4:a:272:HIS:CD2   | 7:d:219:VAL:HG21  | 2.48                     | 0.48              |
| 5:b:121:GLU:HB3   | 10:h:14:PRO:HB2   | 1.95                     | 0.48              |
| 5:b:139:PHE:HB2   | 25:b:610:CLA:CMD  | 2.44                     | 0.48              |
| 5:b:249:ALA:HA    | 5:b:252:VAL:HG22  | 1.96                     | 0.48              |
| 5:b:290:ALA:O     | 5:b:293:ALA:HB3   | 2.14                     | 0.48              |
| 6:c:106:ILE:HG13  | 6:c:107:ASP:N     | 2.28                     | 0.48              |
| 6:c:466:VAL:HG21  | 7:d:249:THR:HG23  | 1.96                     | 0.48              |
| 13:l:29:ALA:CB    | 14:m:15:ILE:HD11  | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:s:311:CLA:CHD  | 26:s:318:LHG:HC62 | 2.43                     | 0.48              |
| 21:g:51:TYR:HE2   | 21:g:209:ALA:HB1  | 1.75                     | 0.48              |
| 25:g:603:CLA:ND   | 24:g:609:CHL:H8   | 2.28                     | 0.48              |
| 21:n:134:ALA:HB1  | 25:n:604:CLA:HED2 | 1.96                     | 0.48              |
| 21:y:116:PRO:HA   | 21:y:126:PHE:HE2  | 1.78                     | 0.48              |
| 21:y:154:HIS:O    | 21:y:154:HIS:ND1  | 2.44                     | 0.48              |
| 25:y:305:CLA:HBC2 | 25:y:305:CLA:CMC  | 2.44                     | 0.48              |
| 22:r:166:GLN:HG2  | 22:r:167:ASP:N    | 2.28                     | 0.48              |
| 1:1:127:GLY:HA3   | 1:1:137:GLN:CG    | 2.42                     | 0.48              |
| 1:3:58:TYR:CE1    | 1:3:80:TRP:HA     | 2.49                     | 0.48              |
| 3:4:169:SER:HA    | 3:4:172:VAL:HG12  | 1.96                     | 0.48              |
| 3:4:231:HIS:O     | 3:4:234:LEU:HG    | 2.14                     | 0.48              |
| 4:A:131:TRP:HZ2   | 6:C:449:ARG:NE    | 2.12                     | 0.48              |
| 5:B:139:PHE:HB2   | 25:B:610:CLA:CMD  | 2.44                     | 0.48              |
| 5:B:240:SER:HB3   | 25:B:610:CLA:NB   | 2.28                     | 0.48              |
| 5:B:290:ALA:O     | 5:B:293:ALA:HB3   | 2.14                     | 0.48              |
| 25:B:614:CLA:CBA  | 28:B:617:BCR:H403 | 2.44                     | 0.48              |
| 6:C:140:LEU:HD22  | 25:C:513:CLA:CMA  | 2.44                     | 0.48              |
| 6:C:213:LEU:O     | 6:C:223:TRP:NE1   | 2.40                     | 0.48              |
| 6:C:224:ILE:CD1   | 6:C:289:PHE:HZ    | 2.27                     | 0.48              |
| 25:C:509:CLA:HBA2 | 42:C:607:HOH:O    | 2.14                     | 0.48              |
| 25:C:511:CLA:H142 | 12:K:47:PHE:HE2   | 1.77                     | 0.48              |
| 7:D:341:ILE:HG23  | 7:D:341:ILE:O     | 2.13                     | 0.48              |
| 13:L:29:ALA:CB    | 14:M:15:ILE:HD11  | 2.43                     | 0.48              |
| 29:L:103:SQD:H262 | 42:L:202:HOH:O    | 2.14                     | 0.48              |
| 25:S:310:CLA:H41  | 25:S:310:CLA:H62  | 1.68                     | 0.48              |
| 25:S:311:CLA:NC   | 26:S:318:LHG:HC41 | 2.29                     | 0.48              |
| 25:Y:304:CLA:H142 | 25:Y:304:CLA:H112 | 1.74                     | 0.48              |
| 22:R:127:TYR:CD2  | 22:R:135:ARG:CD   | 2.97                     | 0.48              |
| 22:R:192:ILE:O    | 22:R:196:VAL:HG23 | 2.13                     | 0.48              |
| 25:6:604:CLA:H61  | 25:6:604:CLA:H41  | 1.60                     | 0.48              |
| 1:7:116:PRO:HA    | 1:7:126:PHE:HE2   | 1.78                     | 0.48              |
| 4:a:104:GLU:OE2   | 15:o:166:ARG:CG   | 2.62                     | 0.48              |
| 6:c:235:GLY:O     | 6:c:239:TRP:CD1   | 2.67                     | 0.48              |
| 25:c:501:CLA:CGA  | 25:c:501:CLA:H3A  | 2.44                     | 0.48              |
| 7:d:99:GLN:OE1    | 8:e:73:LEU:HD13   | 2.14                     | 0.48              |
| 7:d:237:ASN:OD1   | 7:d:238:PRO:CD    | 2.62                     | 0.48              |
| 12:k:34:ASN:N     | 12:k:35:PRO:HD2   | 2.28                     | 0.48              |
| 20:s:186:GLU:OE1  | 20:s:189:ARG:NH2  | 2.46                     | 0.48              |
| 21:n:58:TYR:CE1   | 21:n:80:TRP:HA    | 2.49                     | 0.48              |
| 21:n:116:PRO:HA   | 21:n:126:PHE:HE2  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:139:PHE:HD2  | 24:n:607:CHL:OBD  | 1.97                     | 0.48              |
| 25:n:614:CLA:HAA1 | 25:n:614:CLA:HBD  | 1.96                     | 0.48              |
| 21:y:58:TYR:CE1   | 21:y:80:TRP:HA    | 2.49                     | 0.48              |
| 1:l:50:TRP:CB     | 1:l:213:VAL:HG21  | 2.44                     | 0.47              |
| 2:2:52:GLY:O      | 2:2:55:ARG:HG3    | 2.14                     | 0.47              |
| 25:2:604:CLA:CHC  | 26:2:606:LHG:HC5  | 2.43                     | 0.47              |
| 27:A:403:PHO:H42  | 26:D:406:LHG:H342 | 1.95                     | 0.47              |
| 25:B:604:CLA:H143 | 25:B:610:CLA:H93  | 1.96                     | 0.47              |
| 16:T:11:VAL:HG13  | 28:T:101:BCR:C33  | 2.43                     | 0.47              |
| 20:S:176:VAL:O    | 20:S:180:VAL:HG23 | 2.14                     | 0.47              |
| 20:S:262:PHE:HD2  | 25:S:314:CLA:CMA  | 2.27                     | 0.47              |
| 21:Y:173:GLU:OE2  | 24:Y:310:CHL:NA   | 2.47                     | 0.47              |
| 22:R:218:PRO:HB2  | 22:R:223:PHE:CD2  | 2.48                     | 0.47              |
| 1:5:50:TRP:CB     | 1:5:213:VAL:HG21  | 2.44                     | 0.47              |
| 5:b:223:GLN:HG2   | 10:h:36:GLY:N     | 2.28                     | 0.47              |
| 25:b:614:CLA:CBA  | 28:b:617:BCR:H403 | 2.44                     | 0.47              |
| 6:c:316:THR:O     | 6:c:319:VAL:HG12  | 2.14                     | 0.47              |
| 25:c:502:CLA:HAA1 | 25:c:502:CLA:CBD  | 2.40                     | 0.47              |
| 7:d:12:GLU:O      | 7:d:13:LYS:HB2    | 2.13                     | 0.47              |
| 13:l:20:TRP:CE3   | 26:l:103:LHG:H132 | 2.49                     | 0.47              |
| 20:s:132:GLU:OE1  | 20:s:145:ALA:HB3  | 2.14                     | 0.47              |
| 20:s:196:PHE:HB2  | 24:s:308:CHL:HBC3 | 1.96                     | 0.47              |
| 20:s:262:PHE:HD2  | 25:s:314:CLA:CMA  | 2.27                     | 0.47              |
| 25:s:304:CLA:HHC  | 39:s:316:LUT:H15  | 1.95                     | 0.47              |
| 25:s:311:CLA:NC   | 26:s:318:LHG:HC41 | 2.29                     | 0.47              |
| 21:g:86:SER:OG    | 25:g:602:CLA:O1A  | 2.23                     | 0.47              |
| 21:g:224:PHE:CG   | 26:y:301:LHG:H281 | 2.48                     | 0.47              |
| 21:n:50:TRP:O     | 21:n:55:ARG:HD2   | 2.14                     | 0.47              |
| 22:r:87:ALA:HB1   | 22:r:89:TYR:CE2   | 2.49                     | 0.47              |
| 22:r:120:LYS:HB2  | 22:r:126:PRO:O    | 2.14                     | 0.47              |
| 1:3:154:HIS:O     | 1:3:154:HIS:ND1   | 2.44                     | 0.47              |
| 4:A:77:ILE:H      | 13:L:34:ASN:ND2   | 2.12                     | 0.47              |
| 5:B:67:THR:HA     | 5:B:71:ILE:O      | 2.14                     | 0.47              |
| 6:C:316:THR:O     | 6:C:319:VAL:HG12  | 2.14                     | 0.47              |
| 25:C:501:CLA:H3A  | 25:C:501:CLA:CGA  | 2.44                     | 0.47              |
| 21:Y:164:THR:HG21 | 24:Y:307:CHL:HED3 | 1.96                     | 0.47              |
| 21:Y:224:PHE:CE2  | 25:Y:314:CLA:HAB  | 2.48                     | 0.47              |
| 24:Y:307:CHL:HHC  | 24:Y:308:CHL:CMC  | 2.44                     | 0.47              |
| 3:8:250:LYS:NZ    | 3:8:255:ALA:HA    | 2.29                     | 0.47              |
| 4:a:254:TYR:HE1   | 7:d:134:ALA:N     | 2.11                     | 0.47              |
| 5:b:283:GLU:HG3   | 5:b:287:ARG:HD2   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:c:519:LHG:H381 | 26:c:519:LHG:H222 | 1.95                     | 0.47              |
| 25:g:603:CLA:HMD3 | 24:g:609:CHL:C4D  | 2.45                     | 0.47              |
| 25:g:610:CLA:CBB  | 39:g:615:LUT:H32  | 2.43                     | 0.47              |
| 21:n:204:ASP:O    | 21:n:208:PHE:N    | 2.40                     | 0.47              |
| 24:n:607:CHL:C18  | 24:n:609:CHL:H71  | 2.38                     | 0.47              |
| 21:y:107:MET:HG2  | 21:y:222:ALA:HB3  | 1.94                     | 0.47              |
| 1:l:97:GLU:HA     | 1:l:190:LEU:CD1   | 2.24                     | 0.47              |
| 2:2:188:ASN:HB2   | 2:2:192:PRO:HA    | 1.96                     | 0.47              |
| 4:A:100:ALA:HB2   | 17:W:84:ARG:CZ    | 2.45                     | 0.47              |
| 4:A:131:TRP:CZ2   | 25:C:505:CLA:HAA2 | 2.49                     | 0.47              |
| 4:A:202:VAL:HG22  | 25:A:401:CLA:C1B  | 2.44                     | 0.47              |
| 4:A:321:ILE:HD11  | 7:D:180:PHE:HB2   | 1.96                     | 0.47              |
| 27:A:403:PHO:H141 | 27:A:403:PHO:H161 | 1.52                     | 0.47              |
| 25:B:608:CLA:H18  | 25:D:403:CLA:HMA2 | 1.96                     | 0.47              |
| 6:C:322:GLN:HE22  | 6:C:384:ILE:CD1   | 2.24                     | 0.47              |
| 25:C:504:CLA:H92  | 25:C:504:CLA:H62  | 1.52                     | 0.47              |
| 7:D:12:GLU:O      | 7:D:13:LYS:HB2    | 2.13                     | 0.47              |
| 7:D:107:GLN:HE21  | 8:E:48:GLY:HA3    | 1.79                     | 0.47              |
| 7:D:237:ASN:OD1   | 7:D:238:PRO:CD    | 2.62                     | 0.47              |
| 8:E:55:TYR:O      | 8:E:60:ARG:NH1    | 2.34                     | 0.47              |
| 20:S:179:VAL:HG22 | 32:S:319:AJP:C01  | 2.45                     | 0.47              |
| 20:S:237:LEU:HG   | 39:S:316:LUT:C40  | 2.45                     | 0.47              |
| 20:S:257:HIS:ND1  | 20:S:261:PRO:HA   | 2.29                     | 0.47              |
| 21:G:116:PRO:HA   | 21:G:126:PHE:HE2  | 1.78                     | 0.47              |
| 21:G:131:TRP:CB   | 39:G:616:LUT:H41  | 2.44                     | 0.47              |
| 21:G:139:PHE:CD2  | 24:G:607:CHL:OBD  | 2.66                     | 0.47              |
| 21:G:139:PHE:CE2  | 24:G:607:CHL:CMD  | 2.97                     | 0.47              |
| 25:G:603:CLA:HMD3 | 24:G:609:CHL:C4D  | 2.45                     | 0.47              |
| 22:R:120:LYS:HB2  | 22:R:126:PRO:O    | 2.14                     | 0.47              |
| 1:5:51:TYR:HE2    | 1:5:209:ALA:HB1   | 1.75                     | 0.47              |
| 2:6:66:THR:HG23   | 2:6:67:PRO:HD2    | 1.96                     | 0.47              |
| 25:6:605:CLA:HBC1 | 26:6:606:LHG:H362 | 1.95                     | 0.47              |
| 1:7:145:ASP:HB3   | 1:7:149:ASN:O     | 2.15                     | 0.47              |
| 5:b:67:THR:HA     | 5:b:71:ILE:O      | 2.14                     | 0.47              |
| 5:b:154:GLY:O     | 5:b:159:THR:HG23  | 2.15                     | 0.47              |
| 6:c:213:LEU:HD11  | 28:i:101:BCR:H373 | 1.95                     | 0.47              |
| 25:c:511:CLA:HAA1 | 25:c:511:CLA:CBF  | 2.42                     | 0.47              |
| 12:k:33:LEU:HD13  | 28:k:101:BCR:H312 | 1.96                     | 0.47              |
| 29:l:101:SQD:H262 | 42:l:202:HOH:O    | 2.14                     | 0.47              |
| 14:m:1:MET:HB2    | 14:m:3:VAL:CG1    | 2.43                     | 0.47              |
| 20:s:113:PHE:HD1  | 20:s:117:HIS:HE1  | 1.63                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:131:TRP:CB   | 39:g:616:LUT:H41  | 2.44                     | 0.47              |
| 24:g:601:CHL:H72  | 24:g:601:CHL:H111 | 1.62                     | 0.47              |
| 21:y:164:THR:HG21 | 24:y:307:CHL:HED3 | 1.96                     | 0.47              |
| 22:r:242:GLU:HB2  | 25:r:609:CLA:CHB  | 2.44                     | 0.47              |
| 1:3:50:TRP:O      | 1:3:55:ARG:HD2    | 2.14                     | 0.47              |
| 4:A:135:PHE:CZ    | 11:I:31:ASN:HB3   | 2.49                     | 0.47              |
| 5:B:268:PHE:HB2   | 5:B:448:ARG:NH2   | 2.30                     | 0.47              |
| 6:C:95:LEU:HD23   | 25:C:502:CLA:H143 | 1.95                     | 0.47              |
| 25:S:304:CLA:HHC  | 39:S:316:LUT:H15  | 1.95                     | 0.47              |
| 21:Y:131:TRP:HB3  | 39:Y:317:LUT:H41  | 1.97                     | 0.47              |
| 21:Y:209:ALA:HA   | 21:Y:212:LYS:CG   | 2.34                     | 0.47              |
| 26:Y:301:LHG:H301 | 26:Y:301:LHG:H271 | 1.62                     | 0.47              |
| 24:Y:309:CHL:H11  | 39:Y:316:LUT:C38  | 2.43                     | 0.47              |
| 22:R:58:TRP:CD2   | 22:R:78:PHE:HD1   | 2.31                     | 0.47              |
| 1:5:145:ASP:HB3   | 1:5:149:ASN:O     | 2.15                     | 0.47              |
| 2:6:172:LEU:O     | 2:6:176:PHE:CD2   | 2.67                     | 0.47              |
| 25:b:608:CLA:H18  | 25:d:403:CLA:HMA2 | 1.96                     | 0.47              |
| 15:o:143:PHE:HD1  | 15:o:323:ILE:HG13 | 1.78                     | 0.47              |
| 15:o:146:LYS:HG3  | 15:o:156:PRO:HB2  | 1.97                     | 0.47              |
| 17:w:104:ILE:O    | 17:w:108:VAL:HG23 | 2.14                     | 0.47              |
| 20:s:239:PHE:CE1  | 39:s:315:LUT:H41  | 2.49                     | 0.47              |
| 20:s:257:HIS:ND1  | 20:s:261:PRO:HA   | 2.29                     | 0.47              |
| 21:g:50:TRP:CB    | 21:g:213:VAL:HG21 | 2.45                     | 0.47              |
| 21:g:139:PHE:CE2  | 24:g:607:CHL:CMD  | 2.97                     | 0.47              |
| 21:g:209:ALA:HA   | 21:g:212:LYS:CG   | 2.34                     | 0.47              |
| 21:n:56:VAL:HB    | 24:n:601:CHL:CBC  | 2.45                     | 0.47              |
| 21:n:171:ALA:HB2  | 26:y:319:LHG:H211 | 1.96                     | 0.47              |
| 25:n:611:CLA:H3A  | 25:n:611:CLA:HBA2 | 1.40                     | 0.47              |
| 21:y:50:TRP:O     | 21:y:55:ARG:HD2   | 2.14                     | 0.47              |
| 25:r:610:CLA:H3A  | 25:r:610:CLA:C1   | 2.45                     | 0.47              |
| 1:1:76:GLY:HA3    | 1:1:216:LEU:CD2   | 2.25                     | 0.47              |
| 2:2:172:LEU:O     | 2:2:176:PHE:CD2   | 2.67                     | 0.47              |
| 3:4:58:ILE:O      | 3:4:58:ILE:HG22   | 2.15                     | 0.47              |
| 3:4:169:SER:OG    | 3:4:173:GLU:OE2   | 2.31                     | 0.47              |
| 3:4:250:LYS:NZ    | 3:4:255:ALA:HA    | 2.29                     | 0.47              |
| 4:A:17:PHE:O      | 4:A:18:CYS:SG     | 2.73                     | 0.47              |
| 4:A:157:VAL:CG1   | 4:A:172:MET:HE3   | 2.45                     | 0.47              |
| 25:A:402:CLA:H151 | 25:A:402:CLA:H111 | 1.59                     | 0.47              |
| 5:B:280:PHE:O     | 5:B:281:GLN:CB    | 2.61                     | 0.47              |
| 5:B:354:LEU:HD22  | 5:B:378:ARG:HG3   | 1.96                     | 0.47              |
| 5:B:422:ARG:O     | 5:B:425:GLN:HG2   | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:C:466:VAL:HG21  | 7:D:249:THR:HG23  | 1.96                     | 0.47              |
| 25:C:501:CLA:HHC  | 25:C:501:CLA:HBB1 | 1.96                     | 0.47              |
| 35:C:516:DGD:HAN2 | 35:C:516:DGD:HAW2 | 1.43                     | 0.47              |
| 7:D:350:GLY:HA2   | 7:D:353:LEU:HD23  | 1.96                     | 0.47              |
| 25:S:314:CLA:C4A  | 25:S:314:CLA:HBA2 | 2.44                     | 0.47              |
| 21:N:171:ALA:HB2  | 26:Y:319:LHG:H211 | 1.96                     | 0.47              |
| 21:Y:50:TRP:CB    | 21:Y:213:VAL:HG21 | 2.45                     | 0.47              |
| 22:R:72:LEU:HB3   | 22:R:137:ARG:NH2  | 2.29                     | 0.47              |
| 1:5:76:GLY:HA3    | 1:5:216:LEU:CD2   | 2.24                     | 0.47              |
| 2:6:114:ILE:O     | 2:6:118:VAL:HG23  | 2.13                     | 0.47              |
| 1:7:50:TRP:O      | 1:7:55:ARG:HD2    | 2.14                     | 0.47              |
| 4:a:157:VAL:CG1   | 4:a:172:MET:HE3   | 2.45                     | 0.47              |
| 5:b:28:ALA:HB2    | 5:b:107:CYS:HB3   | 1.96                     | 0.47              |
| 5:b:330:MET:HE1   | 5:b:446:SER:HB3   | 1.96                     | 0.47              |
| 26:b:621:LHG:H321 | 22:r:192:ILE:HD11 | 1.96                     | 0.47              |
| 21:g:132:PHE:HB2  | 24:g:607:CHL:CMA  | 2.43                     | 0.47              |
| 21:g:211:LEU:CB   | 25:g:610:CLA:HMA1 | 2.44                     | 0.47              |
| 21:n:60:GLY:HA3   | 24:n:601:CHL:CMC  | 2.43                     | 0.47              |
| 21:y:60:GLY:CA    | 24:y:302:CHL:HMC  | 2.27                     | 0.47              |
| 22:r:137:ARG:HH21 | 25:r:602:CLA:CED  | 2.22                     | 0.47              |
| 2:2:71:THR:HG22   | 2:2:71:THR:O      | 2.13                     | 0.47              |
| 4:A:60:ILE:HB     | 4:A:83:ILE:HG22   | 1.95                     | 0.47              |
| 4:A:291:SER:O     | 4:A:294:ALA:HB3   | 2.14                     | 0.47              |
| 5:B:154:GLY:O     | 5:B:159:THR:HG23  | 2.15                     | 0.47              |
| 7:D:273:LEU:C     | 7:D:273:LEU:HD23  | 2.40                     | 0.47              |
| 7:D:280:LEU:CD2   | 25:D:402:CLA:HBA2 | 2.45                     | 0.47              |
| 11:I:34:ARG:HD2   | 11:I:35:GLU:CG    | 2.41                     | 0.47              |
| 12:K:33:LEU:HD13  | 28:K:101:BCR:H312 | 1.96                     | 0.47              |
| 15:O:223:LYS:HE2  | 15:O:223:LYS:HA   | 1.97                     | 0.47              |
| 21:G:145:ASP:HB3  | 21:G:149:ASN:O    | 2.15                     | 0.47              |
| 21:G:172:VAL:CG1  | 24:G:608:CHL:NB   | 2.78                     | 0.47              |
| 25:Y:305:CLA:HBC2 | 25:Y:305:CLA:CMC  | 2.44                     | 0.47              |
| 22:R:87:ALA:HB1   | 22:R:89:TYR:CE2   | 2.49                     | 0.47              |
| 22:R:164:THR:OG1  | 22:R:166:GLN:OE1  | 2.31                     | 0.47              |
| 25:R:609:CLA:H61  | 25:R:609:CLA:H92  | 1.67                     | 0.47              |
| 2:6:120:GLN:HA    | 2:6:124:ARG:C     | 2.40                     | 0.47              |
| 2:6:211:GLU:C     | 2:6:214:VAL:HG12  | 2.40                     | 0.47              |
| 25:6:602:CLA:H71  | 25:6:602:CLA:H111 | 1.68                     | 0.47              |
| 25:6:605:CLA:HAA1 | 25:6:605:CLA:CBDB | 2.28                     | 0.47              |
| 3:8:231:HIS:O     | 3:8:234:LEU:HG    | 2.14                     | 0.47              |
| 4:a:202:VAL:HG22  | 25:a:402:CLA:C1B  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:268:PHE:HB2   | 5:b:448:ARG:NH2   | 2.29                     | 0.47              |
| 5:b:357:ARG:NH2   | 7:d:338:GLU:OE1   | 2.47                     | 0.47              |
| 6:c:157:MET:HE2   | 6:c:271:TYR:CE2   | 2.50                     | 0.47              |
| 6:c:311:GLN:HG3   | 6:c:361:LEU:HD23  | 1.97                     | 0.47              |
| 6:c:343:ARG:NH1   | 6:c:347:GLY:O     | 2.48                     | 0.47              |
| 6:c:376:ASP:OD2   | 6:c:379:ARG:NE    | 2.47                     | 0.47              |
| 7:d:162:PRO:CB    | 7:d:171:ALA:HB2   | 2.42                     | 0.47              |
| 20:s:176:VAL:O    | 20:s:180:VAL:HG23 | 2.14                     | 0.47              |
| 24:s:302:CHL:C1D  | 26:s:318:LHG:HC82 | 2.44                     | 0.47              |
| 21:g:154:HIS:O    | 21:g:154:HIS:ND1  | 2.43                     | 0.47              |
| 21:y:131:TRP:HB3  | 39:y:317:LUT:H41  | 1.97                     | 0.47              |
| 22:r:164:THR:OG1  | 22:r:166:GLN:OE1  | 2.31                     | 0.47              |
| 1:l:145:ASP:HB3   | 1:l:149:ASN:O     | 2.15                     | 0.47              |
| 24:l:301:CHL:HBC2 | 24:l:301:CHL:HHD  | 1.95                     | 0.47              |
| 2:2:117:GLU:HG3   | 2:2:129:GLU:HB3   | 1.95                     | 0.47              |
| 2:2:205:ASP:HA    | 2:2:208:THR:OG1   | 2.15                     | 0.47              |
| 2:2:223:ALA:O     | 2:2:226:SER:OG    | 2.32                     | 0.47              |
| 1:3:206:GLU:OE1   | 1:3:206:GLU:CA    | 2.63                     | 0.47              |
| 1:3:216:LEU:O     | 1:3:220:ARG:HG3   | 2.15                     | 0.47              |
| 3:4:75:GLY:H      | 3:4:80:ASP:CG     | 2.22                     | 0.47              |
| 4:A:43:THR:HG21   | 4:A:118:HIS:CE1   | 2.50                     | 0.47              |
| 4:A:220:THR:HA    | 4:A:223:LEU:HG    | 1.96                     | 0.47              |
| 5:B:20:LEU:O      | 5:B:24:ILE:HG13   | 2.15                     | 0.47              |
| 5:B:191:ASP:HB3   | 5:B:194:VAL:HG13  | 1.95                     | 0.47              |
| 5:B:200:SER:O     | 5:B:201:HIS:C     | 2.56                     | 0.47              |
| 5:B:382:PRO:CB    | 7:D:345:GLU:OE2   | 2.62                     | 0.47              |
| 25:B:604:CLA:H93  | 25:B:604:CLA:H61  | 1.59                     | 0.47              |
| 6:C:49:LEU:HD11   | 25:C:509:CLA:C1C  | 2.45                     | 0.47              |
| 6:C:235:GLY:O     | 6:C:239:TRP:CD1   | 2.67                     | 0.47              |
| 6:C:327:ASN:ND2   | 15:O:192:ASP:HB2  | 2.26                     | 0.47              |
| 6:C:429:SER:HB3   | 35:C:516:DGD:HB92 | 1.96                     | 0.47              |
| 25:C:507:CLA:HAA2 | 25:C:507:CLA:CGD  | 2.44                     | 0.47              |
| 26:C:519:LHG:H381 | 26:C:519:LHG:H222 | 1.95                     | 0.47              |
| 7:D:41:CYS:SG     | 25:D:403:CLA:CMB  | 3.03                     | 0.47              |
| 7:D:343:PRO:HD2   | 7:D:346:VAL:CG2   | 2.45                     | 0.47              |
| 9:F:20:LEU:O      | 9:F:24:THR:OG1    | 2.15                     | 0.47              |
| 9:F:21:ALA:O      | 9:F:25:VAL:HG23   | 2.14                     | 0.47              |
| 12:K:53:VAL:HG23  | 28:Z:101:BCR:H21C | 1.95                     | 0.47              |
| 29:L:103:SQD:H312 | 29:L:103:SQD:H352 | 1.97                     | 0.47              |
| 15:O:145:VAL:CG1  | 15:O:203:LEU:HD11 | 2.37                     | 0.47              |
| 19:Z:56:ILE:HG23  | 20:S:270:ILE:CD1  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:S:196:PHE:HB2  | 24:S:308:CHL:HBC3 | 1.96                     | 0.47              |
| 20:S:230:ARG:HD3  | 25:S:303:CLA:HHD  | 1.97                     | 0.47              |
| 21:N:227:PHE:HB2  | 39:N:616:LUT:H401 | 1.97                     | 0.47              |
| 24:N:609:CHL:HBC3 | 24:Y:302:CHL:H91  | 1.97                     | 0.47              |
| 25:N:614:CLA:HAA1 | 25:N:614:CLA:HBD  | 1.96                     | 0.47              |
| 21:Y:138:ILE:HG13 | 21:Y:144:LEU:CB   | 2.31                     | 0.47              |
| 21:Y:145:ASP:HB3  | 21:Y:149:ASN:O    | 2.15                     | 0.47              |
| 26:Y:319:LHG:H252 | 26:Y:319:LHG:H282 | 1.66                     | 0.47              |
| 22:R:247:ARG:HD3  | 25:R:602:CLA:HHD  | 1.97                     | 0.47              |
| 22:R:283:ILE:HG22 | 24:R:613:CHL:HED1 | 1.96                     | 0.47              |
| 1:5:216:LEU:O     | 1:5:220:ARG:HG3   | 2.15                     | 0.47              |
| 2:6:134:LYS:O     | 2:6:137:SER:OG    | 2.22                     | 0.47              |
| 2:6:174:GLU:HG3   | 1:7:59:LEU:HD22   | 1.93                     | 0.47              |
| 2:6:197:PHE:HB3   | 2:6:202:LEU:HD22  | 1.97                     | 0.47              |
| 25:6:604:CLA:HBD  | 25:6:604:CLA:CAA  | 2.41                     | 0.47              |
| 1:7:58:TYR:CE1    | 1:7:80:TRP:HA     | 2.49                     | 0.47              |
| 3:8:219:GLU:HG3   | 3:8:222:GLU:CB    | 2.41                     | 0.47              |
| 4:a:17:PHE:O      | 4:a:18:CYS:SG     | 2.73                     | 0.47              |
| 4:a:103:ASP:HB3   | 15:o:202:GLN:OE1  | 2.15                     | 0.47              |
| 4:a:291:SER:O     | 4:a:294:ALA:HB3   | 2.15                     | 0.47              |
| 25:a:403:CLA:H111 | 25:a:403:CLA:H151 | 1.59                     | 0.47              |
| 25:b:610:CLA:H13  | 25:b:612:CLA:H2   | 1.97                     | 0.47              |
| 6:c:236:GLY:HA2   | 6:c:239:TRP:HD1   | 1.77                     | 0.47              |
| 6:c:437:LEU:HD22  | 25:c:502:CLA:HBC1 | 1.97                     | 0.47              |
| 7:d:328:ALA:CB    | 7:d:348:PRO:HD2   | 2.45                     | 0.47              |
| 15:o:115:PRO:HB2  | 15:o:328:TYR:CE2  | 2.50                     | 0.47              |
| 17:w:125:GLU:O    | 17:w:126:ASP:HB3  | 2.15                     | 0.47              |
| 20:s:202:PRO:CB   | 24:s:308:CHL:HBC2 | 2.45                     | 0.47              |
| 20:s:237:LEU:HG   | 39:s:316:LUT:C40  | 2.45                     | 0.47              |
| 21:g:50:TRP:O     | 21:g:55:ARG:HD2   | 2.14                     | 0.47              |
| 21:g:145:ASP:HB3  | 21:g:149:ASN:O    | 2.15                     | 0.47              |
| 24:g:601:CHL:H52  | 24:g:601:CHL:H8   | 1.70                     | 0.47              |
| 21:n:108:LEU:HD11 | 25:n:610:CLA:HBC1 | 1.96                     | 0.47              |
| 21:n:206:GLU:OE1  | 21:n:206:GLU:CA   | 2.63                     | 0.47              |
| 21:y:145:ASP:HB3  | 21:y:149:ASN:O    | 2.15                     | 0.47              |
| 25:y:314:CLA:HBA2 | 25:y:314:CLA:H3A  | 1.57                     | 0.47              |
| 22:r:56:PRO:O     | 22:r:57:LEU:HD22  | 2.15                     | 0.47              |
| 22:r:141:LEU:HD21 | 22:r:145:ARG:NH2  | 2.30                     | 0.47              |
| 22:r:229:ALA:O    | 22:r:235:THR:OG1  | 2.26                     | 0.47              |
| 22:r:283:ILE:HG22 | 24:r:613:CHL:HED1 | 1.96                     | 0.47              |
| 25:r:601:CLA:H3A  | 25:r:601:CLA:HBA1 | 1.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:204:ASP:O     | 1:1:208:PHE:N     | 2.40                     | 0.47              |
| 1:3:50:TRP:CB     | 1:3:213:VAL:HG21  | 2.45                     | 0.47              |
| 1:3:204:ASP:O     | 1:3:208:PHE:N     | 2.40                     | 0.47              |
| 3:4:73:LEU:HB3    | 3:4:80:ASP:OD1    | 2.13                     | 0.47              |
| 5:B:257:TRP:CE2   | 7:D:292:LEU:HD22  | 2.49                     | 0.47              |
| 5:B:471:ALA:HB2   | 7:D:131:PHE:CE1   | 2.48                     | 0.47              |
| 25:B:610:CLA:H13  | 25:B:612:CLA:H2   | 1.97                     | 0.47              |
| 7:D:22:TRP:NE1    | 18:X:105:VAL:HG12 | 2.30                     | 0.47              |
| 28:T:101:BCR:C18  | 28:T:101:BCR:H272 | 2.44                     | 0.47              |
| 17:W:104:ILE:O    | 17:W:108:VAL:HG23 | 2.14                     | 0.47              |
| 17:W:125:GLU:O    | 17:W:126:ASP:HB3  | 2.15                     | 0.47              |
| 20:S:128:PHE:HE2  | 20:S:236:MET:CE   | 2.27                     | 0.47              |
| 20:S:186:GLU:OE1  | 20:S:189:ARG:NH2  | 2.47                     | 0.47              |
| 20:S:202:PRO:CB   | 24:S:308:CHL:HBC2 | 2.45                     | 0.47              |
| 25:G:613:CLA:H101 | 26:Y:301:LHG:H341 | 1.96                     | 0.47              |
| 21:N:50:TRP:CB    | 21:N:213:VAL:HG21 | 2.45                     | 0.47              |
| 21:N:56:VAL:HB    | 24:N:601:CHL:CBC  | 2.45                     | 0.47              |
| 40:N:617:NEX:H201 | 40:N:617:NEX:H15  | 1.55                     | 0.47              |
| 26:Y:319:LHG:HC92 | 26:Y:319:LHG:H121 | 1.60                     | 0.47              |
| 22:R:56:PRO:O     | 22:R:57:LEU:HD22  | 2.15                     | 0.47              |
| 24:R:605:CHL:HAB  | 25:R:608:CLA:HBC2 | 1.97                     | 0.47              |
| 1:5:55:ARG:HE     | 1:5:55:ARG:HB2    | 1.37                     | 0.47              |
| 1:5:58:TYR:CE1    | 1:5:80:TRP:HA     | 2.49                     | 0.47              |
| 1:5:97:GLU:HA     | 1:5:190:LEU:CD1   | 2.24                     | 0.47              |
| 4:a:84:PRO:HB2    | 4:a:169:SER:HA    | 1.97                     | 0.47              |
| 4:a:231:GLU:HA    | 5:b:1:MET:H2      | 1.78                     | 0.47              |
| 5:b:57:ARG:HG3    | 5:b:57:ARG:O      | 2.14                     | 0.47              |
| 5:b:224:ARG:HG2   | 10:h:37:TRP:CZ2   | 2.50                     | 0.47              |
| 5:b:257:TRP:CE2   | 7:d:292:LEU:HD22  | 2.49                     | 0.47              |
| 5:b:265:ILE:O     | 5:b:269:GLY:N     | 2.47                     | 0.47              |
| 5:b:354:LEU:HD22  | 5:b:378:ARG:HG3   | 1.96                     | 0.47              |
| 6:c:97:TRP:NE1    | 6:c:178:LYS:HE3   | 2.30                     | 0.47              |
| 25:c:507:CLA:HAA2 | 25:c:507:CLA:CGD  | 2.44                     | 0.47              |
| 8:e:27:ILE:HG22   | 8:e:28:PRO:HD3    | 1.92                     | 0.47              |
| 25:g:613:CLA:HBB  | 39:g:615:LUT:H3   | 1.96                     | 0.47              |
| 21:n:97:GLU:HA    | 21:n:190:LEU:CD1  | 2.24                     | 0.47              |
| 21:n:227:PHE:HB2  | 39:n:616:LUT:H401 | 1.97                     | 0.47              |
| 24:y:307:CHL:HAA1 | 40:y:318:NEX:H27  | 1.96                     | 0.47              |
| 1:1:216:LEU:O     | 1:1:220:ARG:HG3   | 2.15                     | 0.47              |
| 2:2:130:PRO:CG    | 2:2:239:LYS:HE2   | 2.45                     | 0.47              |
| 2:2:150:ASN:N     | 2:2:151:PRO:CD    | 2.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:2:604:CLA:CHC  | 26:2:606:LHG:HC41 | 2.45                     | 0.47              |
| 3:4:173:GLU:HB3   | 22:R:59:TYR:CE1   | 2.50                     | 0.47              |
| 5:B:249:ALA:HA    | 5:B:252:VAL:HG22  | 1.96                     | 0.47              |
| 25:B:601:CLA:HBD  | 25:B:601:CLA:HAA1 | 1.97                     | 0.47              |
| 25:B:607:CLA:H161 | 25:B:607:CLA:H141 | 1.54                     | 0.47              |
| 26:B:622:LHG:H201 | 26:B:622:LHG:H352 | 1.96                     | 0.47              |
| 6:C:97:TRP:NE1    | 6:C:178:LYS:HE3   | 2.30                     | 0.47              |
| 6:C:106:ILE:HG13  | 6:C:107:ASP:N     | 2.28                     | 0.47              |
| 6:C:157:MET:HE2   | 6:C:271:TYR:CE2   | 2.50                     | 0.47              |
| 6:C:343:ARG:NH1   | 6:C:347:GLY:O     | 2.48                     | 0.47              |
| 7:D:328:ALA:CB    | 7:D:348:PRO:HD2   | 2.45                     | 0.47              |
| 8:E:26:THR:HB     | 38:F:101:HEM:CAB  | 2.44                     | 0.47              |
| 20:S:68:ARG:NH2   | 26:S:301:LHG:HC12 | 2.23                     | 0.47              |
| 21:G:50:TRP:CB    | 21:G:213:VAL:HG21 | 2.45                     | 0.47              |
| 21:G:197:ASP:OD1  | 25:G:610:CLA:CAA  | 2.62                     | 0.47              |
| 24:G:606:CHL:HBA2 | 40:G:617:NEX:H30  | 1.96                     | 0.47              |
| 25:N:610:CLA:H92  | 25:N:610:CLA:H61  | 1.71                     | 0.47              |
| 25:Y:315:CLA:CBC  | 39:Y:316:LUT:H162 | 2.39                     | 0.47              |
| 22:R:240:LEU:O    | 22:R:244:LYS:HG3  | 2.15                     | 0.47              |
| 2:6:52:GLY:O      | 2:6:55:ARG:HG3    | 2.14                     | 0.47              |
| 3:8:222:GLU:HA    | 3:8:225:LYS:HG3   | 1.97                     | 0.47              |
| 4:a:43:THR:HG21   | 4:a:118:HIS:CE1   | 2.50                     | 0.47              |
| 4:a:329:GLU:HA    | 4:a:332:HIS:HE2   | 1.79                     | 0.47              |
| 29:a:408:SQD:O8   | 29:a:408:SQD:H4   | 2.15                     | 0.47              |
| 5:b:115:TRP:CH2   | 25:b:614:CLA:HMA2 | 2.49                     | 0.47              |
| 5:b:258:TYR:HB3   | 35:b:626:DGD:HD62 | 1.97                     | 0.47              |
| 5:b:379:ALA:HB2   | 5:b:395:VAL:HG11  | 1.96                     | 0.47              |
| 6:c:304:PRO:O     | 6:c:308:GLU:OE1   | 2.33                     | 0.47              |
| 25:c:513:CLA:CMD  | 20:s:75:LEU:HD11  | 2.45                     | 0.47              |
| 7:d:107:GLN:HE21  | 8:e:48:GLY:HA3    | 1.79                     | 0.47              |
| 8:e:26:THR:HB     | 38:f:101:HEM:CAB  | 2.44                     | 0.47              |
| 9:f:18:HIS:CE1    | 38:f:101:HEM:NB   | 2.83                     | 0.47              |
| 10:h:25:PRO:CG    | 22:r:122:THR:HB   | 2.42                     | 0.47              |
| 11:i:34:ARG:HD2   | 11:i:35:GLU:CG    | 2.41                     | 0.47              |
| 21:g:216:LEU:O    | 21:g:220:ARG:HG3  | 2.15                     | 0.47              |
| 25:g:610:CLA:H111 | 25:g:610:CLA:H142 | 1.60                     | 0.47              |
| 21:n:196:PHE:HZ   | 24:n:608:CHL:C1C  | 2.27                     | 0.47              |
| 21:y:173:GLU:OE2  | 24:y:310:CHL:NA   | 2.47                     | 0.47              |
| 21:y:224:PHE:CE2  | 25:y:314:CLA:HAB  | 2.48                     | 0.47              |
| 22:r:57:LEU:HB2   | 22:r:59:TYR:CE1   | 2.49                     | 0.47              |
| 24:r:605:CHL:CBB  | 41:r:616:XAT:H162 | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:611:CLA:H3A  | 25:r:611:CLA:HBA1 | 1.43                     | 0.47              |
| 2:2:66:THR:HG23   | 2:2:67:PRO:HD2    | 1.96                     | 0.47              |
| 2:2:127:PHE:HZ    | 2:2:145:LEU:HD12  | 1.80                     | 0.47              |
| 2:2:211:GLU:C     | 2:2:214:VAL:HG12  | 2.40                     | 0.47              |
| 3:4:144:SER:CB    | 22:R:279:LEU:O    | 2.63                     | 0.47              |
| 4:A:104:GLU:OE2   | 15:O:166:ARG:CG   | 2.62                     | 0.47              |
| 4:A:215:HIS:NE2   | 33:A:413:BCT:O2   | 2.48                     | 0.47              |
| 5:B:223:GLN:CD    | 10:H:36:GLY:H     | 2.23                     | 0.47              |
| 5:B:357:ARG:NH2   | 7:D:338:GLU:OE1   | 2.47                     | 0.47              |
| 5:B:475:PHE:O     | 5:B:478:VAL:HG12  | 2.15                     | 0.47              |
| 26:B:621:LHG:H321 | 22:R:192:ILE:HD11 | 1.96                     | 0.47              |
| 15:O:146:LYS:HG3  | 15:O:156:PRO:HB2  | 1.97                     | 0.47              |
| 20:S:113:PHE:HD1  | 20:S:117:HIS:HE1  | 1.63                     | 0.47              |
| 20:S:132:GLU:CA   | 20:S:145:ALA:HB1  | 2.40                     | 0.47              |
| 20:S:242:GLN:HE22 | 25:S:313:CLA:CHB  | 2.28                     | 0.47              |
| 21:G:100:VAL:CG1  | 21:G:190:LEU:HD13 | 2.45                     | 0.47              |
| 21:G:216:LEU:O    | 21:G:220:ARG:HG3  | 2.15                     | 0.47              |
| 24:Y:308:CHL:HHD  | 24:Y:308:CHL:CBC  | 2.36                     | 0.47              |
| 1:5:100:VAL:CG1   | 1:5:190:LEU:HD13  | 2.45                     | 0.47              |
| 1:5:127:GLY:HA3   | 1:5:137:GLN:CG    | 2.42                     | 0.47              |
| 25:6:604:CLA:HBA2 | 25:6:604:CLA:CHA  | 2.44                     | 0.47              |
| 3:8:225:LYS:CA    | 3:8:228:GLU:OE1   | 2.61                     | 0.47              |
| 4:a:77:ILE:H      | 13:l:34:ASN:ND2   | 2.12                     | 0.47              |
| 4:a:321:ILE:HD11  | 7:d:180:PHE:HB2   | 1.96                     | 0.47              |
| 5:b:5:TRP:O       | 25:b:611:CLA:H42  | 2.15                     | 0.47              |
| 5:b:37:MET:HE2    | 5:b:37:MET:CA     | 2.45                     | 0.47              |
| 5:b:214:LEU:HB3   | 25:r:603:CLA:HED1 | 1.97                     | 0.47              |
| 6:c:49:LEU:HD11   | 25:c:509:CLA:C1C  | 2.45                     | 0.47              |
| 7:d:217:ALA:O     | 7:d:221:ASN:ND2   | 2.47                     | 0.47              |
| 25:d:403:CLA:H122 | 18:x:92:SER:OG    | 2.14                     | 0.47              |
| 15:o:130:LYS:HD2  | 15:o:179:GLU:CB   | 2.45                     | 0.47              |
| 28:t:101:BCR:C18  | 28:t:101:BCR:H272 | 2.44                     | 0.47              |
| 25:s:314:CLA:C4A  | 25:s:314:CLA:HBA2 | 2.44                     | 0.47              |
| 21:g:206:GLU:OE1  | 21:g:206:GLU:CA   | 2.63                     | 0.47              |
| 21:n:50:TRP:CB    | 21:n:213:VAL:HG21 | 2.45                     | 0.47              |
| 22:r:150:ALA:HB1  | 41:r:616:XAT:H181 | 1.95                     | 0.47              |
| 1:1:50:TRP:O      | 1:1:55:ARG:HD2    | 2.14                     | 0.46              |
| 1:1:206:GLU:OE1   | 1:1:206:GLU:CA    | 2.63                     | 0.46              |
| 2:2:161:ALA:O     | 2:2:162:VAL:C     | 2.59                     | 0.46              |
| 3:4:69:ASP:N      | 3:4:70:PRO:CD     | 2.79                     | 0.46              |
| 3:4:226:LEU:CD1   | 3:4:229:ILE:HD11  | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:161:TYR:HB3   | 4:A:162:PRO:HD3   | 1.96                     | 0.46              |
| 6:C:36:TRP:O      | 25:C:508:CLA:H11  | 2.15                     | 0.46              |
| 6:C:311:GLN:HG3   | 6:C:361:LEU:HD23  | 1.97                     | 0.46              |
| 25:C:509:CLA:HMC1 | 25:C:509:CLA:HBC2 | 1.97                     | 0.46              |
| 7:D:318:LYS:HE3   | 37:D:408:CL:CL    | 2.53                     | 0.46              |
| 20:S:241:ILE:HG22 | 25:S:313:CLA:HMD3 | 1.97                     | 0.46              |
| 21:G:50:TRP:O     | 21:G:55:ARG:HD2   | 2.14                     | 0.46              |
| 21:N:131:TRP:HA   | 39:N:616:LUT:O3   | 2.15                     | 0.46              |
| 21:N:134:ALA:HB1  | 25:N:604:CLA:HED2 | 1.96                     | 0.46              |
| 21:Y:76:GLY:HA3   | 21:Y:216:LEU:CD2  | 2.24                     | 0.46              |
| 21:Y:100:VAL:CG1  | 21:Y:190:LEU:HD13 | 2.45                     | 0.46              |
| 2:6:127:PHE:HZ    | 2:6:145:LEU:HD12  | 1.80                     | 0.46              |
| 2:6:150:ASN:N     | 2:6:151:PRO:CD    | 2.78                     | 0.46              |
| 5:b:139:PHE:HB2   | 25:b:610:CLA:HMD3 | 1.97                     | 0.46              |
| 6:c:428:THR:HG22  | 35:c:516:DGD:CCB  | 2.44                     | 0.46              |
| 7:d:41:CYS:SG     | 25:d:403:CLA:CMB  | 3.03                     | 0.46              |
| 12:k:53:VAL:HG23  | 28:z:101:BCR:H21C | 1.96                     | 0.46              |
| 20:s:230:ARG:HD3  | 25:s:303:CLA:HHD  | 1.97                     | 0.46              |
| 21:g:172:VAL:CG1  | 24:g:608:CHL:NB   | 2.78                     | 0.46              |
| 25:g:611:CLA:H112 | 25:g:611:CLA:H142 | 1.59                     | 0.46              |
| 25:g:613:CLA:H101 | 26:y:301:LHG:H341 | 1.96                     | 0.46              |
| 21:y:216:LEU:O    | 21:y:220:ARG:HG3  | 2.15                     | 0.46              |
| 2:2:120:GLN:HA    | 2:2:124:ARG:C     | 2.39                     | 0.46              |
| 1:3:97:GLU:HA     | 1:3:190:LEU:CD1   | 2.24                     | 0.46              |
| 4:A:103:ASP:HB3   | 15:O:202:GLN:OE1  | 2.15                     | 0.46              |
| 5:B:37:MET:HE2    | 5:B:37:MET:CA     | 2.45                     | 0.46              |
| 5:B:224:ARG:HG2   | 10:H:37:TRP:CZ2   | 2.50                     | 0.46              |
| 9:F:18:HIS:CE1    | 38:F:101:HEM:NB   | 2.83                     | 0.46              |
| 10:H:18:THR:O     | 10:H:22:LEU:HD13  | 2.16                     | 0.46              |
| 14:M:1:MET:HB2    | 14:M:3:VAL:CG1    | 2.43                     | 0.46              |
| 20:S:132:GLU:OE1  | 20:S:145:ALA:HB3  | 2.14                     | 0.46              |
| 20:S:144:GLU:HB3  | 20:S:153:LEU:CD2  | 2.41                     | 0.46              |
| 24:S:302:CHL:C1D  | 26:S:318:LHG:HC82 | 2.44                     | 0.46              |
| 21:G:87:ALA:HB1   | 21:Y:90:GLU:HB2   | 1.93                     | 0.46              |
| 21:N:107:MET:HG2  | 21:N:222:ALA:HB3  | 1.94                     | 0.46              |
| 21:N:224:PHE:HE2  | 25:N:613:CLA:HAB  | 1.81                     | 0.46              |
| 24:R:607:CHL:HMB2 | 40:R:617:NEX:H14  | 1.97                     | 0.46              |
| 25:R:610:CLA:H3A  | 25:R:610:CLA:C1   | 2.45                     | 0.46              |
| 1:5:50:TRP:O      | 1:5:55:ARG:HD2    | 2.14                     | 0.46              |
| 2:6:204:ASP:C     | 2:6:208:THR:HG23  | 2.38                     | 0.46              |
| 25:6:604:CLA:CHC  | 26:6:606:LHG:HC41 | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:69:ASP:N      | 3:8:70:PRO:CD     | 2.79                     | 0.46              |
| 4:a:100:ALA:HB2   | 17:w:84:ARG:CZ    | 2.45                     | 0.46              |
| 4:a:131:TRP:HZ2   | 6:c:449:ARG:NE    | 2.12                     | 0.46              |
| 5:b:51:VAL:HG13   | 5:b:308:LYS:HG2   | 1.95                     | 0.46              |
| 5:b:285:TYR:CZ    | 23:u:90:GLN:HG3   | 2.49                     | 0.46              |
| 25:b:604:CLA:H143 | 25:b:610:CLA:H93  | 1.96                     | 0.46              |
| 7:d:22:TRP:NE1    | 18:x:105:VAL:HG12 | 2.30                     | 0.46              |
| 7:d:273:LEU:C     | 7:d:273:LEU:HD23  | 2.40                     | 0.46              |
| 15:o:146:LYS:HD3  | 15:o:158:PHE:HE1  | 1.80                     | 0.46              |
| 15:o:223:LYS:HE2  | 15:o:223:LYS:HA   | 1.97                     | 0.46              |
| 25:s:305:CLA:O1A  | 40:s:317:NEX:H382 | 2.15                     | 0.46              |
| 21:g:58:TYR:CE1   | 21:g:80:TRP:HA    | 2.49                     | 0.46              |
| 21:g:82:THR:N     | 39:g:616:LUT:O23  | 2.42                     | 0.46              |
| 25:g:610:CLA:H62  | 25:g:612:CLA:HMA1 | 1.97                     | 0.46              |
| 21:y:50:TRP:CB    | 21:y:213:VAL:HG21 | 2.45                     | 0.46              |
| 22:r:72:LEU:HB3   | 22:r:137:ARG:NH2  | 2.29                     | 0.46              |
| 25:r:610:CLA:HBC3 | 26:r:618:LHG:C5   | 2.37                     | 0.46              |
| 1:1:154:HIS:CE1   | 1:1:156:GLN:OE1   | 2.69                     | 0.46              |
| 2:2:197:PHE:HB3   | 2:2:202:LEU:HD22  | 1.97                     | 0.46              |
| 5:B:28:ALA:HB2    | 5:B:107:CYS:HB3   | 1.96                     | 0.46              |
| 5:B:58:GLN:HG2    | 5:B:331:ASP:OD2   | 2.16                     | 0.46              |
| 6:C:304:PRO:O     | 6:C:308:GLU:OE1   | 2.33                     | 0.46              |
| 25:S:305:CLA:O1A  | 40:S:317:NEX:H382 | 2.15                     | 0.46              |
| 21:N:56:VAL:CG1   | 24:N:601:CHL:HBC1 | 2.46                     | 0.46              |
| 21:N:216:LEU:O    | 21:N:220:ARG:HG3  | 2.15                     | 0.46              |
| 21:Y:128:GLU:CB   | 21:Y:137:GLN:HB2  | 2.41                     | 0.46              |
| 21:Y:164:THR:HG23 | 21:Y:168:LEU:CD1  | 2.46                     | 0.46              |
| 1:5:154:HIS:CE1   | 1:5:156:GLN:OE1   | 2.69                     | 0.46              |
| 1:5:164:THR:HG23  | 1:5:168:LEU:CD1   | 2.46                     | 0.46              |
| 2:6:71:THR:O      | 2:6:71:THR:HG22   | 2.14                     | 0.46              |
| 3:8:169:SER:HA    | 3:8:172:VAL:HG12  | 1.96                     | 0.46              |
| 3:8:173:GLU:HB3   | 22:r:59:TYR:CE1   | 2.50                     | 0.46              |
| 4:a:161:TYR:HB3   | 4:a:162:PRO:HD3   | 1.96                     | 0.46              |
| 4:a:214:MET:HE1   | 27:a:405:PHO:C3D  | 2.45                     | 0.46              |
| 5:b:256:MET:HG3   | 5:b:448:ARG:HG3   | 1.97                     | 0.46              |
| 6:c:429:SER:HB3   | 35:c:516:DGD:HB92 | 1.96                     | 0.46              |
| 25:c:510:CLA:H2   | 25:c:510:CLA:H61  | 1.67                     | 0.46              |
| 10:h:26:LEU:HD23  | 25:r:614:CLA:HMA1 | 1.97                     | 0.46              |
| 21:g:154:HIS:CE1  | 21:g:156:GLN:OE1  | 2.69                     | 0.46              |
| 21:g:210:GLU:OE1  | 21:g:214:LYS:NZ   | 2.38                     | 0.46              |
| 1:1:100:VAL:CG1   | 1:1:190:LEU:HD13  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:209:PHE:C     | 2:2:213:LYS:HZ2   | 2.23                     | 0.46              |
| 2:2:217:ILE:HD13  | 25:2:604:CLA:O2D  | 2.15                     | 0.46              |
| 1:3:69:TYR:OH     | 1:3:81:ASP:OD2    | 2.20                     | 0.46              |
| 4:A:221:SER:HB2   | 7:D:140:ARG:O     | 2.16                     | 0.46              |
| 5:B:5:TRP:O       | 25:B:611:CLA:H42  | 2.15                     | 0.46              |
| 21:G:55:ARG:HE    | 21:G:55:ARG:HB2   | 1.36                     | 0.46              |
| 25:G:610:CLA:H62  | 25:G:612:CLA:HMA1 | 1.97                     | 0.46              |
| 21:N:98:LEU:CD2   | 25:N:603:CLA:HAA2 | 2.46                     | 0.46              |
| 21:N:226:MET:O    | 21:N:230:PHE:CD2  | 2.69                     | 0.46              |
| 25:N:602:CLA:CBC  | 26:N:618:LHG:H251 | 2.45                     | 0.46              |
| 21:Y:108:LEU:HD11 | 25:Y:311:CLA:HBC1 | 1.97                     | 0.46              |
| 24:Y:307:CHL:HAA1 | 40:Y:318:NEX:H27  | 1.96                     | 0.46              |
| 22:R:170:LYS:HB2  | 24:R:606:CHL:O1D  | 2.15                     | 0.46              |
| 2:6:205:ASP:HA    | 2:6:208:THR:OG1   | 2.15                     | 0.46              |
| 2:6:217:ILE:HD13  | 25:6:604:CLA:O2D  | 2.15                     | 0.46              |
| 27:a:404:PHO:NB   | 7:d:210:LEU:HD12  | 2.31                     | 0.46              |
| 5:b:325:PHE:CG    | 13:l:35:TYR:HB3   | 2.51                     | 0.46              |
| 7:d:318:LYS:HE3   | 37:d:408:CL:CL    | 2.53                     | 0.46              |
| 8:e:24:SER:O      | 8:e:28:PRO:HG2    | 2.16                     | 0.46              |
| 20:s:179:VAL:HG22 | 32:s:319:AJP:C01  | 2.45                     | 0.46              |
| 21:g:87:ALA:CB    | 21:y:90:GLU:HB3   | 2.46                     | 0.46              |
| 21:g:100:VAL:CG1  | 21:g:190:LEU:HD13 | 2.45                     | 0.46              |
| 25:g:603:CLA:H3A  | 25:g:603:CLA:HBA1 | 1.58                     | 0.46              |
| 21:n:100:VAL:CG1  | 21:n:190:LEU:HD13 | 2.45                     | 0.46              |
| 21:n:216:LEU:O    | 21:n:220:ARG:HG3  | 2.15                     | 0.46              |
| 21:y:107:MET:HA   | 21:y:222:ALA:HB1  | 1.98                     | 0.46              |
| 21:y:154:HIS:CE1  | 21:y:156:GLN:OE1  | 2.69                     | 0.46              |
| 24:y:302:CHL:H51  | 24:y:302:CHL:H92  | 1.97                     | 0.46              |
| 22:r:203:GLU:OE2  | 25:r:608:CLA:C4A  | 2.63                     | 0.46              |
| 1:1:209:ALA:CA    | 1:1:212:LYS:HG3   | 2.34                     | 0.46              |
| 1:1:226:MET:O     | 1:1:230:PHE:CD2   | 2.69                     | 0.46              |
| 2:2:122:TRP:O     | 2:2:123:VAL:CB    | 2.64                     | 0.46              |
| 2:2:223:ALA:HB3   | 25:2:602:CLA:CMC  | 2.45                     | 0.46              |
| 1:3:51:TYR:C      | 1:3:55:ARG:HD3    | 2.41                     | 0.46              |
| 4:A:84:PRO:HB2    | 4:A:169:SER:HA    | 1.97                     | 0.46              |
| 4:A:231:GLU:HA    | 5:B:1:MET:H2      | 1.81                     | 0.46              |
| 29:A:407:SQD:O8   | 29:A:407:SQD:H4   | 2.15                     | 0.46              |
| 6:C:459:ILE:CG2   | 6:C:464:GLU:HG3   | 2.45                     | 0.46              |
| 8:E:71:ASP:HB3    | 23:U:103:TYR:CE1  | 2.50                     | 0.46              |
| 15:O:115:PRO:HB2  | 15:O:328:TYR:CE2  | 2.50                     | 0.46              |
| 15:O:146:LYS:HD3  | 15:O:158:PHE:HE1  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:87:ALA:CB    | 21:Y:90:GLU:HB3   | 2.46                     | 0.46              |
| 21:G:164:THR:HG23 | 21:G:168:LEU:CD1  | 2.46                     | 0.46              |
| 21:N:100:VAL:CG1  | 21:N:190:LEU:HD13 | 2.45                     | 0.46              |
| 21:N:164:THR:HG23 | 21:N:168:LEU:CD1  | 2.46                     | 0.46              |
| 24:Y:302:CHL:H51  | 24:Y:302:CHL:H92  | 1.97                     | 0.46              |
| 22:R:124:PHE:CD1  | 25:R:614:CLA:CHC  | 2.93                     | 0.46              |
| 22:R:179:TYR:HD1  | 22:R:180:LEU:N    | 2.14                     | 0.46              |
| 22:R:203:GLU:OE2  | 25:R:608:CLA:C4A  | 2.63                     | 0.46              |
| 22:R:241:ALA:O    | 22:R:245:HIS:HD2  | 1.98                     | 0.46              |
| 25:R:603:CLA:HMD1 | 25:R:608:CLA:H12  | 1.97                     | 0.46              |
| 25:R:612:CLA:HBA2 | 25:R:612:CLA:H3A  | 1.57                     | 0.46              |
| 2:6:61:PRO:HD2    | 24:6:601:CHL:HBB1 | 1.97                     | 0.46              |
| 2:6:117:GLU:HB3   | 2:6:121:LYS:HZ2   | 1.77                     | 0.46              |
| 1:7:50:TRP:CB     | 1:7:213:VAL:HG21  | 2.45                     | 0.46              |
| 1:7:107:MET:HG2   | 1:7:222:ALA:HB3   | 1.94                     | 0.46              |
| 3:8:152:LEU:O     | 3:8:155:TRP:HB3   | 2.16                     | 0.46              |
| 4:a:221:SER:HB2   | 7:d:140:ARG:O     | 2.16                     | 0.46              |
| 4:a:224:ILE:O     | 7:d:266:ARG:NH2   | 2.43                     | 0.46              |
| 5:b:413:ASP:O     | 5:b:417:VAL:HG23  | 2.16                     | 0.46              |
| 13:l:21:GLY:HA2   | 26:l:103:LHG:H261 | 1.96                     | 0.46              |
| 20:s:242:GLN:HE22 | 25:s:313:CLA:CHB  | 2.28                     | 0.46              |
| 20:s:265:ASN:OD1  | 20:s:268:THR:HG23 | 2.16                     | 0.46              |
| 26:s:301:LHG:H341 | 26:s:301:LHG:H312 | 1.76                     | 0.46              |
| 21:g:164:THR:HG23 | 21:g:168:LEU:CD1  | 2.46                     | 0.46              |
| 21:g:197:ASP:OD1  | 25:g:610:CLA:CAA  | 2.62                     | 0.46              |
| 21:n:224:PHE:HE2  | 25:n:613:CLA:HAB  | 1.81                     | 0.46              |
| 25:n:610:CLA:H62  | 25:n:610:CLA:H41  | 1.67                     | 0.46              |
| 21:y:51:TYR:C     | 21:y:55:ARG:HD3   | 2.41                     | 0.46              |
| 22:r:274:HIS:HD1  | 25:r:612:CLA:HAA2 | 1.79                     | 0.46              |
| 1:1:58:TYR:HE1    | 1:1:79:GLY:O      | 1.99                     | 0.46              |
| 1:3:208:PHE:CZ    | 1:3:212:LYS:HE3   | 2.51                     | 0.46              |
| 27:A:403:PHO:NB   | 7:D:210:LEU:HD12  | 2.31                     | 0.46              |
| 6:C:256:PRO:HA    | 25:C:506:CLA:HED2 | 1.98                     | 0.46              |
| 7:D:99:GLN:OE1    | 8:E:73:LEU:HD13   | 2.14                     | 0.46              |
| 7:D:278:THR:O     | 7:D:282:MET:HG2   | 2.16                     | 0.46              |
| 14:M:14:PHE:O     | 14:M:18:PRO:HD2   | 2.16                     | 0.46              |
| 21:N:51:TYR:C     | 21:N:55:ARG:HD3   | 2.41                     | 0.46              |
| 21:Y:51:TYR:C     | 21:Y:55:ARG:HD3   | 2.41                     | 0.46              |
| 21:Y:172:VAL:CG1  | 24:Y:309:CHL:C1B  | 2.94                     | 0.46              |
| 21:Y:226:MET:O    | 21:Y:230:PHE:CD2  | 2.69                     | 0.46              |
| 22:R:57:LEU:HD11  | 22:R:64:SER:HB2   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:R:258:VAL:HG12 | 25:R:612:CLA:CMD  | 2.45                     | 0.46              |
| 24:R:605:CHL:CBB  | 41:R:616:XAT:H162 | 2.45                     | 0.46              |
| 2:6:50:TRP:C      | 2:6:55:ARG:HG2    | 2.41                     | 0.46              |
| 1:7:154:HIS:CE1   | 1:7:156:GLN:OE1   | 2.69                     | 0.46              |
| 1:7:208:PHE:CZ    | 1:7:212:LYS:HE3   | 2.51                     | 0.46              |
| 5:b:18:ARG:O      | 5:b:22:VAL:HG13   | 2.15                     | 0.46              |
| 5:b:20:LEU:O      | 5:b:24:ILE:HG13   | 2.15                     | 0.46              |
| 5:b:475:PHE:O     | 5:b:478:VAL:HG12  | 2.16                     | 0.46              |
| 6:c:79:LYS:CG     | 6:c:80:PRO:HD2    | 2.45                     | 0.46              |
| 6:c:316:THR:HG21  | 6:c:396:MET:SD    | 2.56                     | 0.46              |
| 7:d:89:SER:HB3    | 8:e:69:ARG:HH11   | 1.80                     | 0.46              |
| 21:n:51:TYR:C     | 21:n:55:ARG:HD3   | 2.41                     | 0.46              |
| 21:n:58:TYR:HE1   | 21:n:79:GLY:O     | 1.99                     | 0.46              |
| 21:n:153:VAL:HG13 | 24:n:605:CHL:C1D  | 2.45                     | 0.46              |
| 21:y:208:PHE:CZ   | 21:y:212:LYS:HE3  | 2.51                     | 0.46              |
| 22:r:241:ALA:O    | 22:r:245:HIS:HD2  | 1.98                     | 0.46              |
| 25:r:612:CLA:H3A  | 25:r:612:CLA:HBA2 | 1.57                     | 0.46              |
| 1:1:51:TYR:HE2    | 1:1:209:ALA:HB1   | 1.75                     | 0.46              |
| 2:2:122:TRP:C     | 2:2:123:VAL:HG23  | 2.40                     | 0.46              |
| 1:3:100:VAL:CG1   | 1:3:190:LEU:HD13  | 2.45                     | 0.46              |
| 1:3:145:ASP:HB3   | 1:3:149:ASN:O     | 2.15                     | 0.46              |
| 1:3:154:HIS:CE1   | 1:3:156:GLN:OE1   | 2.69                     | 0.46              |
| 1:3:209:ALA:CA    | 1:3:212:LYS:HG3   | 2.34                     | 0.46              |
| 1:3:226:MET:O     | 1:3:230:PHE:CD2   | 2.69                     | 0.46              |
| 3:4:221:LEU:C     | 3:4:224:LEU:HD23  | 2.41                     | 0.46              |
| 4:A:331:MET:CE    | 7:D:321:LEU:HD22  | 2.46                     | 0.46              |
| 5:B:258:TYR:HB3   | 35:B:626:DGD:HD62 | 1.97                     | 0.46              |
| 5:B:330:MET:HE1   | 5:B:446:SER:HB3   | 1.96                     | 0.46              |
| 25:B:611:CLA:H112 | 25:B:611:CLA:H72  | 1.67                     | 0.46              |
| 6:C:79:LYS:CG     | 6:C:80:PRO:HD2    | 2.45                     | 0.46              |
| 28:T:101:BCR:C16  | 28:T:101:BCR:H351 | 2.45                     | 0.46              |
| 18:X:87:LEU:HD12  | 18:X:88:LEU:N     | 2.31                     | 0.46              |
| 20:S:67:ARG:HH22  | 20:S:85:LEU:HB3   | 1.81                     | 0.46              |
| 20:S:99:GLY:O     | 20:S:100:LEU:HB2  | 2.16                     | 0.46              |
| 20:S:113:PHE:C    | 20:S:117:HIS:HD1  | 2.22                     | 0.46              |
| 20:S:265:ASN:OD1  | 20:S:268:THR:HG23 | 2.16                     | 0.46              |
| 21:G:51:TYR:C     | 21:G:55:ARG:HD3   | 2.41                     | 0.46              |
| 25:G:610:CLA:H41  | 25:G:612:CLA:CMA  | 2.41                     | 0.46              |
| 21:Y:216:LEU:O    | 21:Y:220:ARG:HG3  | 2.15                     | 0.46              |
| 25:Y:303:CLA:H93  | 25:Y:303:CLA:C12  | 2.46                     | 0.46              |
| 22:R:283:ILE:HG23 | 22:R:284:ILE:N    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:226:MET:O     | 1:5:230:PHE:CD2   | 2.69                     | 0.46              |
| 2:6:188:ASN:HB2   | 2:6:192:PRO:HA    | 1.96                     | 0.46              |
| 24:6:601:CHL:HBA1 | 24:6:601:CHL:H3A  | 1.83                     | 0.46              |
| 1:7:51:TYR:C      | 1:7:55:ARG:HD3    | 2.41                     | 0.46              |
| 1:7:206:GLU:OE1   | 1:7:206:GLU:CA    | 2.63                     | 0.46              |
| 1:7:226:MET:O     | 1:7:230:PHE:CD2   | 2.69                     | 0.46              |
| 3:8:144:SER:CB    | 22:r:279:LEU:O    | 2.63                     | 0.46              |
| 6:c:189:TRP:HH2   | 6:c:362:ARG:HG2   | 1.81                     | 0.46              |
| 6:c:233:ILE:HA    | 28:i:101:BCR:H282 | 1.97                     | 0.46              |
| 6:c:459:ILE:CG2   | 6:c:464:GLU:HG3   | 2.45                     | 0.46              |
| 7:d:85:SER:CB     | 23:u:102:ARG:HD2  | 2.46                     | 0.46              |
| 7:d:247:MET:HE3   | 31:d:405:PL9:C52  | 2.46                     | 0.46              |
| 7:d:343:PRO:HD2   | 7:d:346:VAL:CG2   | 2.45                     | 0.46              |
| 12:k:35:PRO:O     | 12:k:38:ASP:HB2   | 2.16                     | 0.46              |
| 18:x:87:LEU:HD12  | 18:x:88:LEU:N     | 2.31                     | 0.46              |
| 25:s:310:CLA:H61  | 25:s:310:CLA:H92  | 1.51                     | 0.46              |
| 25:s:312:CLA:HBA1 | 25:s:312:CLA:CMA  | 2.38                     | 0.46              |
| 21:g:58:TYR:HE1   | 21:g:79:GLY:O     | 1.99                     | 0.46              |
| 21:g:204:ASP:O    | 21:g:208:PHE:N    | 2.40                     | 0.46              |
| 21:g:226:MET:O    | 21:g:230:PHE:CD2  | 2.69                     | 0.46              |
| 24:g:605:CHL:H3A  | 24:g:605:CHL:HBA2 | 1.37                     | 0.46              |
| 21:n:145:ASP:HB3  | 21:n:149:ASN:O    | 2.15                     | 0.46              |
| 21:y:105:TRP:NE1  | 24:y:309:CHL:HED2 | 2.26                     | 0.46              |
| 21:y:132:PHE:HB3  | 24:y:308:CHL:HMA3 | 1.97                     | 0.46              |
| 22:r:57:LEU:HD11  | 22:r:64:SER:HB2   | 1.98                     | 0.46              |
| 24:r:607:CHL:H3A  | 24:r:607:CHL:HBA2 | 1.60                     | 0.46              |
| 1:1:75:PRO:HG3    | 1:1:212:LYS:HB3   | 1.98                     | 0.46              |
| 4:A:54:ALA:HA     | 4:A:70:SER:OG     | 2.16                     | 0.46              |
| 25:A:402:CLA:C2B  | 27:A:403:PHO:H192 | 2.46                     | 0.46              |
| 5:B:139:PHE:HB2   | 25:B:610:CLA:HMD3 | 1.98                     | 0.46              |
| 5:B:221:PRO:HA    | 25:B:609:CLA:HED3 | 1.98                     | 0.46              |
| 25:B:605:CLA:HBD  | 25:B:605:CLA:HAA1 | 1.98                     | 0.46              |
| 25:C:502:CLA:HBA1 | 25:C:502:CLA:H3A  | 1.78                     | 0.46              |
| 28:H:101:BCR:C8   | 28:H:101:BCR:H331 | 2.46                     | 0.46              |
| 20:S:143:PRO:HD2  | 20:S:153:LEU:HD11 | 1.98                     | 0.46              |
| 21:G:58:TYR:HE1   | 21:G:79:GLY:O     | 1.99                     | 0.46              |
| 21:G:75:PRO:HG3   | 21:G:212:LYS:HB3  | 1.98                     | 0.46              |
| 21:G:154:HIS:CE1  | 21:G:156:GLN:OE1  | 2.69                     | 0.46              |
| 21:G:164:THR:HG21 | 24:G:606:CHL:CED  | 2.46                     | 0.46              |
| 21:G:206:GLU:OE1  | 21:G:206:GLU:CA   | 2.63                     | 0.46              |
| 21:N:107:MET:HA   | 21:N:222:ALA:HB1  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:145:ASP:HB3  | 21:N:149:ASN:O    | 2.15                     | 0.46              |
| 21:N:208:PHE:CZ   | 21:N:212:LYS:HE3  | 2.51                     | 0.46              |
| 21:Y:50:TRP:O     | 21:Y:55:ARG:HD2   | 2.14                     | 0.46              |
| 40:Y:318:NEX:H31  | 40:Y:318:NEX:H391 | 1.49                     | 0.46              |
| 22:R:103:LYS:CE   | 22:R:105:LEU:HD11 | 2.45                     | 0.46              |
| 25:R:612:CLA:H71  | 25:R:612:CLA:HHC  | 1.98                     | 0.46              |
| 1:5:208:PHE:CZ    | 1:5:212:LYS:HE3   | 2.51                     | 0.46              |
| 2:6:89:PRO:O      | 2:6:92:PHE:HB2    | 2.16                     | 0.46              |
| 24:6:601:CHL:H62  | 24:6:601:CHL:H41  | 1.56                     | 0.46              |
| 25:6:605:CLA:HBD  | 25:6:605:CLA:CAA  | 2.35                     | 0.46              |
| 4:a:149:ALA:HB1   | 4:a:283:ILE:HB    | 1.97                     | 0.46              |
| 4:a:220:THR:HA    | 4:a:223:LEU:HG    | 1.96                     | 0.46              |
| 5:b:58:GLN:HG2    | 5:b:331:ASP:OD2   | 2.16                     | 0.46              |
| 5:b:108:PHE:CZ    | 5:b:112:ILE:HD11  | 2.51                     | 0.46              |
| 5:b:194:VAL:HG23  | 5:b:194:VAL:O     | 2.15                     | 0.46              |
| 6:c:133:ALA:HB1   | 25:c:511:CLA:CMA  | 2.45                     | 0.46              |
| 25:c:509:CLA:HBC2 | 25:c:509:CLA:HMC1 | 1.98                     | 0.46              |
| 7:d:194:LEU:O     | 7:d:194:LEU:HG    | 2.16                     | 0.46              |
| 20:s:95:TYR:OH    | 24:s:302:CHL:O1A  | 2.30                     | 0.46              |
| 20:s:241:ILE:HG22 | 25:s:313:CLA:HMD3 | 1.97                     | 0.46              |
| 21:n:164:THR:HG23 | 21:n:168:LEU:CD1  | 2.46                     | 0.46              |
| 25:n:613:CLA:H2   | 25:n:613:CLA:H122 | 1.98                     | 0.46              |
| 25:y:304:CLA:H91  | 25:y:304:CLA:C12  | 2.46                     | 0.46              |
| 40:y:318:NEX:C36  | 40:y:318:NEX:C28  | 2.90                     | 0.46              |
| 1:3:107:MET:HA    | 1:3:222:ALA:HB1   | 1.98                     | 0.46              |
| 4:A:149:ALA:HB1   | 4:A:283:ILE:HB    | 1.97                     | 0.46              |
| 5:B:283:GLU:HG3   | 5:B:287:ARG:HD2   | 1.96                     | 0.46              |
| 5:B:413:ASP:O     | 5:B:417:VAL:HG23  | 2.16                     | 0.46              |
| 28:B:617:BCR:H15C | 28:B:617:BCR:H351 | 1.81                     | 0.46              |
| 6:C:316:THR:HG21  | 6:C:396:MET:SD    | 2.56                     | 0.46              |
| 6:C:437:LEU:HD22  | 25:C:502:CLA:HBC1 | 1.97                     | 0.46              |
| 15:O:130:LYS:HD2  | 15:O:179:GLU:CB   | 2.45                     | 0.46              |
| 15:O:228:THR:CG2  | 15:O:284:GLU:OE2  | 2.57                     | 0.46              |
| 25:N:602:CLA:H61  | 25:N:602:CLA:H93  | 1.49                     | 0.46              |
| 1:5:75:PRO:HG3    | 1:5:212:LYS:HB3   | 1.98                     | 0.46              |
| 1:5:206:GLU:OE1   | 1:5:206:GLU:CA    | 2.63                     | 0.46              |
| 1:7:75:PRO:HG3    | 1:7:212:LYS:HB3   | 1.98                     | 0.46              |
| 1:7:100:VAL:CG1   | 1:7:190:LEU:HD13  | 2.45                     | 0.46              |
| 3:8:221:LEU:C     | 3:8:224:LEU:HD23  | 2.41                     | 0.46              |
| 25:b:609:CLA:HMB1 | 25:b:610:CLA:C1B  | 2.46                     | 0.46              |
| 6:c:251:HIS:HE1   | 25:c:506:CLA:HMA3 | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:c:505:CLA:H92  | 25:c:505:CLA:H61  | 1.74                     | 0.46              |
| 29:l:101:SQD:H312 | 29:l:101:SQD:H352 | 1.97                     | 0.46              |
| 28:t:101:BCR:H351 | 28:t:101:BCR:C16  | 2.45                     | 0.46              |
| 17:w:81:VAL:HG23  | 17:w:82:ASP:OD2   | 2.16                     | 0.46              |
| 20:s:113:PHE:C    | 20:s:117:HIS:HD1  | 2.22                     | 0.46              |
| 20:s:267:LEU:HD13 | 25:s:314:CLA:CED  | 2.44                     | 0.46              |
| 21:g:208:PHE:CZ   | 21:g:212:LYS:HE3  | 2.51                     | 0.46              |
| 21:n:56:VAL:CG1   | 24:n:601:CHL:HBC1 | 2.46                     | 0.46              |
| 21:n:107:MET:HA   | 21:n:222:ALA:HB1  | 1.98                     | 0.46              |
| 21:n:215:GLU:OE1  | 25:n:610:CLA:C4A  | 2.64                     | 0.46              |
| 25:n:602:CLA:H51  | 25:n:603:CLA:HBA1 | 1.97                     | 0.46              |
| 26:y:301:LHG:H301 | 26:y:301:LHG:H271 | 1.62                     | 0.46              |
| 22:r:170:LYS:HB2  | 24:r:606:CHL:O1D  | 2.15                     | 0.46              |
| 22:r:240:LEU:O    | 22:r:244:LYS:HG3  | 2.15                     | 0.46              |
| 2:2:61:PRO:HD2    | 24:2:601:CHL:HBB1 | 1.97                     | 0.46              |
| 1:3:58:TYR:HE1    | 1:3:79:GLY:C      | 2.24                     | 0.46              |
| 3:4:152:LEU:O     | 3:4:155:TRP:HB3   | 2.16                     | 0.46              |
| 3:4:171:SER:N     | 3:4:183:GLU:OE2   | 2.48                     | 0.46              |
| 4:A:30:ILE:HD11   | 29:A:411:SQD:H442 | 1.98                     | 0.46              |
| 4:A:57:PRO:O      | 15:O:208:ARG:NH1  | 2.49                     | 0.46              |
| 4:A:131:TRP:CZ2   | 6:C:449:ARG:HD2   | 2.48                     | 0.46              |
| 4:A:214:MET:HE1   | 27:A:404:PHO:C3D  | 2.45                     | 0.46              |
| 25:A:402:CLA:O1A  | 25:A:402:CLA:H43  | 2.16                     | 0.46              |
| 5:B:18:ARG:O      | 5:B:22:VAL:HG13   | 2.15                     | 0.46              |
| 5:B:108:PHE:CZ    | 5:B:112:ILE:HD11  | 2.51                     | 0.46              |
| 5:B:194:VAL:O     | 5:B:194:VAL:HG23  | 2.15                     | 0.46              |
| 5:B:248:ALA:HB2   | 25:B:603:CLA:H52  | 1.97                     | 0.46              |
| 6:C:133:ALA:HB1   | 25:C:511:CLA:CMA  | 2.45                     | 0.46              |
| 6:C:225:VAL:HG22  | 6:C:289:PHE:HE1   | 1.73                     | 0.46              |
| 6:C:233:ILE:HA    | 28:I:101:BCR:H282 | 1.97                     | 0.46              |
| 25:C:510:CLA:HHD  | 25:C:510:CLA:H192 | 1.98                     | 0.46              |
| 7:D:97:GLU:HG3    | 8:E:69:ARG:HG3    | 1.98                     | 0.46              |
| 25:D:403:CLA:H52  | 18:X:91:ALA:HB1   | 1.98                     | 0.46              |
| 11:I:33:GLY:C     | 11:I:34:ARG:HG3   | 2.36                     | 0.46              |
| 13:L:21:GLY:HA2   | 26:L:102:LHG:H261 | 1.96                     | 0.46              |
| 20:S:67:ARG:NH2   | 20:S:85:LEU:O     | 2.49                     | 0.46              |
| 25:S:310:CLA:CBB  | 25:S:312:CLA:H3A  | 2.46                     | 0.46              |
| 21:N:154:HIS:CE1  | 21:N:156:GLN:OE1  | 2.69                     | 0.46              |
| 25:N:611:CLA:HMD2 | 25:N:612:CLA:HHD  | 1.98                     | 0.46              |
| 22:R:83:LEU:HD12  | 41:R:616:XAT:H23  | 1.98                     | 0.46              |
| 22:R:141:LEU:HD21 | 22:R:145:ARG:NH2  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:58:TYR:HE1    | 1:5:79:GLY:O      | 1.99                     | 0.46              |
| 2:6:130:PRO:CG    | 2:6:239:LYS:HE2   | 2.45                     | 0.46              |
| 25:6:605:CLA:HBA2 | 25:6:605:CLA:H3A  | 1.26                     | 0.46              |
| 3:8:97:TRP:HD1    | 3:8:164:PHE:CE2   | 2.34                     | 0.46              |
| 3:8:221:LEU:HA    | 3:8:224:LEU:HD23  | 1.95                     | 0.46              |
| 4:a:30:ILE:HD11   | 29:a:412:SQD:H442 | 1.98                     | 0.46              |
| 4:a:215:HIS:NE2   | 33:a:414:BCT:O2   | 2.48                     | 0.46              |
| 4:a:331:MET:CE    | 7:d:321:LEU:HD22  | 2.46                     | 0.46              |
| 5:b:148:VAL:HG11  | 26:b:622:LHG:H212 | 1.98                     | 0.46              |
| 5:b:330:MET:CE    | 5:b:446:SER:HB3   | 2.46                     | 0.46              |
| 28:b:618:BCR:C8   | 28:b:618:BCR:H331 | 2.46                     | 0.46              |
| 6:c:36:TRP:O      | 25:c:508:CLA:H11  | 2.15                     | 0.46              |
| 6:c:113:VAL:HG13  | 28:c:514:BCR:H313 | 1.98                     | 0.46              |
| 25:c:504:CLA:HAA1 | 35:c:516:DGD:HD61 | 1.97                     | 0.46              |
| 25:c:511:CLA:C14  | 19:z:20:LEU:HD11  | 2.45                     | 0.46              |
| 20:s:99:GLY:O     | 20:s:100:LEU:HB2  | 2.16                     | 0.46              |
| 20:s:132:GLU:HA   | 20:s:145:ALA:CB   | 2.39                     | 0.46              |
| 25:s:310:CLA:CBB  | 25:s:312:CLA:H3A  | 2.46                     | 0.46              |
| 21:n:227:PHE:CD2  | 25:n:602:CLA:H202 | 2.41                     | 0.46              |
| 21:y:131:TRP:HA   | 39:y:317:LUT:O3   | 2.16                     | 0.46              |
| 22:r:127:TYR:CD2  | 22:r:135:ARG:CD   | 2.97                     | 0.46              |
| 40:r:617:NEX:H201 | 40:r:617:NEX:H15  | 1.41                     | 0.46              |
| 1:1:55:ARG:HE     | 1:1:55:ARG:HB2    | 1.36                     | 0.45              |
| 1:1:128:GLU:CB    | 1:1:137:GLN:HB2   | 2.41                     | 0.45              |
| 1:1:153:VAL:HA    | 24:1:301:CHL:ND   | 2.30                     | 0.45              |
| 1:1:164:THR:HG23  | 1:1:168:LEU:CD1   | 2.46                     | 0.45              |
| 2:2:69:TYR:CD1    | 2:2:70:LEU:N      | 2.85                     | 0.45              |
| 24:2:601:CHL:H62  | 24:2:601:CHL:H41  | 1.56                     | 0.45              |
| 1:3:58:TYR:HE1    | 1:3:79:GLY:O      | 1.99                     | 0.45              |
| 1:3:75:PRO:HG3    | 1:3:212:LYS:HB3   | 1.98                     | 0.45              |
| 4:A:157:VAL:HG11  | 4:A:172:MET:HE3   | 1.98                     | 0.45              |
| 4:A:231:GLU:HG2   | 5:B:1:MET:CA      | 2.45                     | 0.45              |
| 5:B:285:TYR:HE2   | 23:U:87:LYS:O     | 1.99                     | 0.45              |
| 25:B:609:CLA:H3A  | 25:B:609:CLA:HBA1 | 1.47                     | 0.45              |
| 10:H:26:LEU:HD23  | 25:R:614:CLA:HMA1 | 1.97                     | 0.45              |
| 20:S:146:VAL:HG11 | 20:S:148:PHE:CZ   | 2.52                     | 0.45              |
| 21:G:183:LEU:HG   | 24:G:608:CHL:CBB  | 2.46                     | 0.45              |
| 25:G:610:CLA:CBB  | 39:G:615:LUT:H32  | 2.43                     | 0.45              |
| 21:N:50:TRP:HB3   | 21:N:213:VAL:HG21 | 1.98                     | 0.45              |
| 21:N:58:TYR:HE1   | 21:N:79:GLY:O     | 1.99                     | 0.45              |
| 21:Y:97:GLU:HA    | 21:Y:190:LEU:CD1  | 2.24                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:Y:105:TRP:NE1  | 24:Y:309:CHL:HED2 | 2.26                     | 0.45              |
| 21:Y:107:MET:HA   | 21:Y:222:ALA:HB1  | 1.98                     | 0.45              |
| 2:6:122:TRP:C     | 2:6:123:VAL:HG23  | 2.40                     | 0.45              |
| 1:7:120:ALA:HA    | 1:7:124:VAL:O     | 2.16                     | 0.45              |
| 3:8:171:SER:N     | 3:8:183:GLU:OE2   | 2.49                     | 0.45              |
| 4:a:54:ALA:HA     | 4:a:70:SER:OG     | 2.16                     | 0.45              |
| 4:a:136:ARG:NH2   | 11:i:27:ASP:OD2   | 2.48                     | 0.45              |
| 25:b:601:CLA:HBD  | 25:b:601:CLA:HAA1 | 1.97                     | 0.45              |
| 6:c:51:GLY:CA     | 6:c:132:HIS:HB2   | 2.46                     | 0.45              |
| 6:c:457:LYS:HZ3   | 7:d:228:ASP:C     | 2.22                     | 0.45              |
| 25:c:509:CLA:HBA2 | 42:c:607:HOH:O    | 2.14                     | 0.45              |
| 10:h:18:THR:O     | 10:h:22:LEU:HD13  | 2.16                     | 0.45              |
| 14:m:14:PHE:O     | 14:m:18:PRO:HD2   | 2.16                     | 0.45              |
| 15:o:228:THR:CG2  | 15:o:284:GLU:OE2  | 2.57                     | 0.45              |
| 15:o:311:THR:HG21 | 15:o:316:LYS:O    | 2.16                     | 0.45              |
| 20:s:146:VAL:HG11 | 20:s:148:PHE:CZ   | 2.51                     | 0.45              |
| 24:s:306:CHL:CBB  | 39:s:316:LUT:H161 | 2.46                     | 0.45              |
| 21:g:75:PRO:HG3   | 21:g:212:LYS:HB3  | 1.98                     | 0.45              |
| 25:g:602:CLA:C2   | 25:g:602:CLA:HMB1 | 2.47                     | 0.45              |
| 21:y:100:VAL:CG1  | 21:y:190:LEU:HD13 | 2.45                     | 0.45              |
| 21:y:161:ILE:HG21 | 24:y:308:CHL:HBC1 | 1.99                     | 0.45              |
| 21:y:206:GLU:OE1  | 21:y:206:GLU:CA   | 2.63                     | 0.45              |
| 24:y:306:CHL:HBC3 | 24:y:306:CHL:HMC  | 1.98                     | 0.45              |
| 40:y:318:NEX:H31  | 40:y:318:NEX:H391 | 1.49                     | 0.45              |
| 22:r:247:ARG:HD3  | 25:r:602:CLA:HHD  | 1.97                     | 0.45              |
| 22:r:258:VAL:HG12 | 25:r:612:CLA:CMD  | 2.45                     | 0.45              |
| 2:2:100:VAL:HB    | 2:2:190:LEU:HD23  | 1.98                     | 0.45              |
| 4:A:329:GLU:HA    | 4:A:332:HIS:HE2   | 1.79                     | 0.45              |
| 5:B:214:LEU:HB3   | 25:R:603:CLA:HED1 | 1.97                     | 0.45              |
| 5:B:256:MET:HG3   | 5:B:448:ARG:HG3   | 1.98                     | 0.45              |
| 5:B:257:TRP:CD2   | 7:D:292:LEU:HD22  | 2.52                     | 0.45              |
| 25:B:604:CLA:H152 | 25:B:604:CLA:H112 | 1.57                     | 0.45              |
| 6:C:51:GLY:CA     | 6:C:132:HIS:HB2   | 2.46                     | 0.45              |
| 25:C:504:CLA:HAA1 | 35:C:516:DGD:HD61 | 1.97                     | 0.45              |
| 7:D:85:SER:CB     | 23:U:102:ARG:HD2  | 2.46                     | 0.45              |
| 7:D:247:MET:HE3   | 31:D:405:PL9:C52  | 2.46                     | 0.45              |
| 18:X:92:SER:O     | 18:X:96:VAL:HG13  | 2.17                     | 0.45              |
| 21:G:226:MET:O    | 21:G:230:PHE:CD2  | 2.69                     | 0.45              |
| 24:G:606:CHL:HBB1 | 39:G:616:LUT:C16  | 2.47                     | 0.45              |
| 21:N:108:LEU:HD11 | 25:N:610:CLA:HBC1 | 1.96                     | 0.45              |
| 21:N:153:VAL:HG13 | 24:N:605:CHL:C1D  | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:N:602:CLA:H51  | 25:N:603:CLA:HBA1 | 1.98                     | 0.45              |
| 21:Y:58:TYR:HE1   | 21:Y:79:GLY:O     | 1.99                     | 0.45              |
| 25:Y:315:CLA:HED2 | 25:Y:315:CLA:HBD  | 1.82                     | 0.45              |
| 22:R:137:ARG:HH21 | 25:R:602:CLA:CED  | 2.22                     | 0.45              |
| 1:5:120:ALA:HA    | 1:5:124:VAL:O     | 2.16                     | 0.45              |
| 2:6:69:TYR:CD1    | 2:6:70:LEU:N      | 2.84                     | 0.45              |
| 2:6:122:TRP:O     | 2:6:123:VAL:CB    | 2.64                     | 0.45              |
| 2:6:161:ALA:HB1   | 2:6:165:PHE:HE2   | 1.81                     | 0.45              |
| 1:7:216:LEU:O     | 1:7:220:ARG:HG3   | 2.15                     | 0.45              |
| 30:a:411:LMG:H291 | 11:i:4:LEU:CD2    | 2.46                     | 0.45              |
| 5:b:281:GLN:CD    | 23:u:91:VAL:HG13  | 2.42                     | 0.45              |
| 5:b:285:TYR:HE2   | 23:u:87:LYS:O     | 1.99                     | 0.45              |
| 25:b:601:CLA:H192 | 25:b:601:CLA:H162 | 1.69                     | 0.45              |
| 25:b:616:CLA:H91  | 25:b:616:CLA:H111 | 1.72                     | 0.45              |
| 6:c:146:PHE:CE2   | 26:s:301:LHG:HC62 | 2.51                     | 0.45              |
| 7:d:278:THR:O     | 7:d:282:MET:HG2   | 2.16                     | 0.45              |
| 21:n:50:TRP:HB3   | 21:n:213:VAL:HG21 | 1.98                     | 0.45              |
| 21:n:107:MET:HG2  | 21:n:222:ALA:HB3  | 1.94                     | 0.45              |
| 25:n:602:CLA:CBC  | 26:n:618:LHG:H251 | 2.45                     | 0.45              |
| 40:n:617:NEX:H191 | 40:n:617:NEX:C12  | 2.30                     | 0.45              |
| 21:y:58:TYR:HE1   | 21:y:79:GLY:O     | 1.99                     | 0.45              |
| 21:y:164:THR:HG23 | 21:y:168:LEU:CD1  | 2.46                     | 0.45              |
| 22:r:274:HIS:CD2  | 24:r:613:CHL:NC   | 2.84                     | 0.45              |
| 24:r:605:CHL:HAB  | 25:r:608:CLA:HBC2 | 1.97                     | 0.45              |
| 24:r:607:CHL:HMB2 | 40:r:617:NEX:H14  | 1.97                     | 0.45              |
| 1:1:120:ALA:HA    | 1:1:124:VAL:O     | 2.16                     | 0.45              |
| 2:2:89:PRO:O      | 2:2:92:PHE:HB2    | 2.16                     | 0.45              |
| 3:4:97:TRP:HD1    | 3:4:164:PHE:CE2   | 2.34                     | 0.45              |
| 4:A:105:TRP:CZ3   | 4:A:111:PRO:HG3   | 2.51                     | 0.45              |
| 4:A:174:LEU:HD22  | 27:A:403:PHO:H143 | 1.98                     | 0.45              |
| 5:B:41:GLU:CD     | 5:B:62:VAL:HG22   | 2.41                     | 0.45              |
| 6:C:189:TRP:HH2   | 6:C:362:ARG:HG2   | 1.81                     | 0.45              |
| 6:C:311:GLN:HG3   | 6:C:361:LEU:CD2   | 2.47                     | 0.45              |
| 6:C:311:GLN:HE21  | 6:C:358:PHE:HB2   | 1.81                     | 0.45              |
| 6:C:428:THR:HG22  | 35:C:516:DGD:CCB  | 2.44                     | 0.45              |
| 25:C:511:CLA:C14  | 19:Z:20:LEU:HD11  | 2.45                     | 0.45              |
| 7:D:89:SER:HB3    | 8:E:69:ARG:HH11   | 1.80                     | 0.45              |
| 21:G:107:MET:HA   | 21:G:222:ALA:HB1  | 1.98                     | 0.45              |
| 21:G:218:ASN:ND2  | 25:G:612:CLA:C4A  | 2.62                     | 0.45              |
| 24:G:608:CHL:H18  | 40:G:617:NEX:H361 | 1.98                     | 0.45              |
| 25:N:603:CLA:HBC1 | 24:N:609:CHL:CBC  | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:Y:75:PRO:HG3   | 21:Y:212:LYS:HB3  | 1.98                     | 0.45              |
| 21:Y:132:PHE:HB3  | 24:Y:308:CHL:HMA3 | 1.97                     | 0.45              |
| 21:Y:206:GLU:OE1  | 21:Y:206:GLU:CA   | 2.63                     | 0.45              |
| 22:R:234:LYS:HA   | 22:R:234:LYS:HE2  | 1.99                     | 0.45              |
| 1:5:51:TYR:C      | 1:5:55:ARG:HD3    | 2.41                     | 0.45              |
| 3:8:120:GLN:OE1   | 3:8:253:LEU:HD23  | 2.16                     | 0.45              |
| 5:b:460:LEU:HD12  | 7:d:288:VAL:HG21  | 1.94                     | 0.45              |
| 25:c:511:CLA:C3B  | 28:k:101:BCR:H393 | 2.46                     | 0.45              |
| 7:d:97:GLU:HG3    | 8:e:69:ARG:HG3    | 1.98                     | 0.45              |
| 29:l:102:SQD:H462 | 14:m:28:LYS:HD2   | 1.98                     | 0.45              |
| 25:s:305:CLA:H3A  | 25:s:305:CLA:CGA  | 2.46                     | 0.45              |
| 21:g:164:THR:HG21 | 24:g:606:CHL:CED  | 2.46                     | 0.45              |
| 21:y:120:ALA:HA   | 21:y:124:VAL:O    | 2.16                     | 0.45              |
| 21:y:226:MET:O    | 21:y:230:PHE:CD2  | 2.69                     | 0.45              |
| 25:y:303:CLA:C12  | 25:y:303:CLA:H93  | 2.46                     | 0.45              |
| 25:r:603:CLA:HMD1 | 25:r:608:CLA:H12  | 1.98                     | 0.45              |
| 2:2:121:LYS:HD3   | 2:2:245:LEU:CD1   | 2.46                     | 0.45              |
| 2:2:174:GLU:HG3   | 1:3:59:LEU:HD22   | 1.93                     | 0.45              |
| 2:2:218:LYS:HA    | 2:2:221:ARG:HE    | 1.81                     | 0.45              |
| 1:3:164:THR:HG23  | 1:3:168:LEU:CD1   | 2.46                     | 0.45              |
| 3:4:120:GLN:OE1   | 3:4:253:LEU:HD23  | 2.16                     | 0.45              |
| 30:A:410:LMG:H351 | 30:A:410:LMG:H382 | 1.83                     | 0.45              |
| 30:A:410:LMG:H291 | 11:I:4:LEU:CD2    | 2.46                     | 0.45              |
| 5:B:245:VAL:HG21  | 25:B:612:CLA:HED3 | 1.99                     | 0.45              |
| 25:B:608:CLA:HBC3 | 25:B:608:CLA:HHD  | 1.98                     | 0.45              |
| 25:B:609:CLA:HMB1 | 25:B:610:CLA:C1B  | 2.46                     | 0.45              |
| 25:B:611:CLA:HAB  | 25:B:613:CLA:H3A  | 1.98                     | 0.45              |
| 6:C:146:PHE:CE2   | 26:S:301:LHG:HC62 | 2.51                     | 0.45              |
| 7:D:81:THR:HG22   | 7:D:112:TRP:NE1   | 2.32                     | 0.45              |
| 12:K:35:PRO:O     | 12:K:38:ASP:HB2   | 2.16                     | 0.45              |
| 15:O:290:THR:HB   | 15:O:300:ILE:HG13 | 1.98                     | 0.45              |
| 15:O:290:THR:O    | 15:O:291:LYS:C    | 2.59                     | 0.45              |
| 15:O:311:THR:HG21 | 15:O:316:LYS:O    | 2.16                     | 0.45              |
| 28:T:101:BCR:H271 | 5:b:39:LEU:HD13   | 1.98                     | 0.45              |
| 25:S:312:CLA:HBB1 | 39:S:315:LUT:C14  | 2.47                     | 0.45              |
| 21:G:82:THR:N     | 39:G:616:LUT:O23  | 2.42                     | 0.45              |
| 25:G:603:CLA:H3A  | 25:G:603:CLA:HBA1 | 1.58                     | 0.45              |
| 21:N:59:LEU:HD23  | 24:N:601:CHL:C1B  | 2.46                     | 0.45              |
| 25:N:613:CLA:H2   | 25:N:613:CLA:H122 | 1.98                     | 0.45              |
| 21:Y:154:HIS:CE1  | 21:Y:156:GLN:OE1  | 2.69                     | 0.45              |
| 25:Y:304:CLA:H161 | 25:Y:304:CLA:H192 | 1.74                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Y:304:CLA:H91  | 25:Y:304:CLA:C12  | 2.46                     | 0.45              |
| 24:Y:309:CHL:H91  | 24:Y:309:CHL:H112 | 1.60                     | 0.45              |
| 1:5:153:VAL:HA    | 24:5:301:CHL:ND   | 2.30                     | 0.45              |
| 2:6:161:ALA:O     | 2:6:162:VAL:C     | 2.58                     | 0.45              |
| 4:a:210:LEU:HD12  | 27:a:405:PHO:NB   | 2.31                     | 0.45              |
| 5:b:223:GLN:CD    | 10:h:36:GLY:H     | 2.23                     | 0.45              |
| 5:b:355:PHE:O     | 5:b:371:VAL:HG22  | 2.16                     | 0.45              |
| 6:c:185:VAL:HG23  | 6:c:230:LEU:CD1   | 2.47                     | 0.45              |
| 6:c:372:PRO:O     | 6:c:373:ASN:HB2   | 2.16                     | 0.45              |
| 8:e:71:ASP:HB3    | 23:u:103:TYR:CE1  | 2.50                     | 0.45              |
| 20:s:67:ARG:NH2   | 20:s:85:LEU:O     | 2.49                     | 0.45              |
| 21:g:107:MET:HA   | 21:g:222:ALA:HB1  | 1.98                     | 0.45              |
| 25:g:612:CLA:H111 | 25:g:612:CLA:H142 | 1.51                     | 0.45              |
| 21:n:58:TYR:HE1   | 21:n:79:GLY:C     | 2.24                     | 0.45              |
| 21:n:131:TRP:HA   | 39:n:616:LUT:O3   | 2.15                     | 0.45              |
| 21:n:226:MET:O    | 21:n:230:PHE:CD2  | 2.69                     | 0.45              |
| 24:n:609:CHL:HBC3 | 24:y:302:CHL:H91  | 1.97                     | 0.45              |
| 21:y:172:VAL:CG1  | 24:y:309:CHL:C1B  | 2.94                     | 0.45              |
| 24:y:309:CHL:H141 | 24:y:309:CHL:H162 | 1.86                     | 0.45              |
| 22:r:83:LEU:HD12  | 41:r:616:XAT:H23  | 1.98                     | 0.45              |
| 2:2:192:PRO:HB3   | 24:2:603:CHL:HBC2 | 1.99                     | 0.45              |
| 2:2:197:PHE:HB3   | 2:2:202:LEU:CD2   | 2.47                     | 0.45              |
| 25:2:605:CLA:HBC1 | 26:2:606:LHG:H362 | 1.95                     | 0.45              |
| 5:B:39:LEU:HD13   | 28:t:101:BCR:H271 | 1.98                     | 0.45              |
| 25:B:613:CLA:H111 | 25:B:613:CLA:H142 | 1.67                     | 0.45              |
| 6:C:376:ASP:OD1   | 6:C:379:ARG:HB2   | 2.17                     | 0.45              |
| 25:C:511:CLA:C3B  | 28:K:101:BCR:H393 | 2.46                     | 0.45              |
| 29:L:101:SQD:H92  | 29:L:101:SQD:O10  | 2.16                     | 0.45              |
| 20:S:267:LEU:HD13 | 25:S:314:CLA:CED  | 2.44                     | 0.45              |
| 24:S:306:CHL:CBB  | 39:S:316:LUT:H161 | 2.46                     | 0.45              |
| 24:S:306:CHL:HBC2 | 24:S:307:CHL:CHD  | 2.46                     | 0.45              |
| 21:G:132:PHE:CB   | 24:G:607:CHL:HMA3 | 2.41                     | 0.45              |
| 21:N:206:GLU:OE1  | 21:N:206:GLU:CA   | 2.63                     | 0.45              |
| 25:N:612:CLA:H62  | 25:N:612:CLA:H2   | 1.71                     | 0.45              |
| 25:Y:312:CLA:H142 | 25:Y:312:CLA:H111 | 1.54                     | 0.45              |
| 1:5:58:TYR:HE1    | 1:5:79:GLY:C      | 2.24                     | 0.45              |
| 1:5:107:MET:HA    | 1:5:222:ALA:HB1   | 1.98                     | 0.45              |
| 2:6:69:TYR:CG     | 2:6:92:PHE:CZ     | 3.05                     | 0.45              |
| 2:6:197:PHE:HB3   | 2:6:202:LEU:CD2   | 2.47                     | 0.45              |
| 1:7:164:THR:HG23  | 1:7:168:LEU:CD1   | 2.46                     | 0.45              |
| 4:a:205:VAL:CG1   | 7:d:205:VAL:HG12  | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:28:ALA:HB2    | 5:b:107:CYS:CB    | 2.47                     | 0.45              |
| 28:d:404:BCR:H403 | 30:d:407:LMG:H141 | 1.99                     | 0.45              |
| 20:s:143:PRO:HD2  | 20:s:153:LEU:HD11 | 1.98                     | 0.45              |
| 21:g:83:ALA:HA    | 21:y:98:LEU:HD11  | 1.98                     | 0.45              |
| 21:n:75:PRO:HG3   | 21:n:212:LYS:HB3  | 1.98                     | 0.45              |
| 21:n:98:LEU:CD2   | 25:n:603:CLA:HAA2 | 2.46                     | 0.45              |
| 21:n:120:ALA:HA   | 21:n:124:VAL:O    | 2.16                     | 0.45              |
| 1:1:51:TYR:C      | 1:1:55:ARG:HD3    | 2.41                     | 0.45              |
| 25:2:604:CLA:H52  | 25:2:604:CLA:H12  | 1.77                     | 0.45              |
| 3:4:222:GLU:HA    | 3:4:225:LYS:HG3   | 1.97                     | 0.45              |
| 4:A:205:VAL:CG1   | 7:D:205:VAL:HG12  | 2.47                     | 0.45              |
| 5:B:220:ARG:HG3   | 10:H:32:LYS:HE3   | 1.99                     | 0.45              |
| 5:B:325:PHE:CG    | 13:L:35:TYR:HB3   | 2.51                     | 0.45              |
| 25:B:602:CLA:H62  | 25:B:602:CLA:H41  | 1.79                     | 0.45              |
| 15:O:196:TYR:CB   | 15:O:212:LEU:HD21 | 2.16                     | 0.45              |
| 19:Z:57:LEU:HD23  | 19:Z:60:LEU:HD12  | 1.98                     | 0.45              |
| 20:S:190:ILE:HG13 | 20:S:191:THR:H    | 1.81                     | 0.45              |
| 21:N:58:TYR:HE1   | 21:N:79:GLY:C     | 2.24                     | 0.45              |
| 21:N:128:GLU:CB   | 21:N:133:LYS:O    | 2.65                     | 0.45              |
| 21:N:215:GLU:OE1  | 25:N:610:CLA:C4A  | 2.64                     | 0.45              |
| 21:N:224:PHE:HD1  | 25:N:602:CLA:H201 | 1.81                     | 0.45              |
| 24:N:607:CHL:C18  | 24:N:609:CHL:H71  | 2.38                     | 0.45              |
| 21:Y:114:VAL:HG13 | 21:Y:241:ILE:HD11 | 1.98                     | 0.45              |
| 21:Y:208:PHE:CZ   | 21:Y:212:LYS:HE3  | 2.51                     | 0.45              |
| 2:6:218:LYS:HA    | 2:6:221:ARG:HE    | 1.81                     | 0.45              |
| 2:6:232:VAL:CG1   | 2:6:243:GLU:OE1   | 2.65                     | 0.45              |
| 25:6:604:CLA:HBC3 | 26:6:606:LHG:H372 | 1.98                     | 0.45              |
| 1:7:50:TRP:HB3    | 1:7:213:VAL:HG21  | 1.99                     | 0.45              |
| 1:7:107:MET:HA    | 1:7:222:ALA:HB1   | 1.98                     | 0.45              |
| 3:8:170:GLN:HB2   | 3:8:183:GLU:CG    | 2.42                     | 0.45              |
| 4:a:51:ALA:CB     | 4:a:82:ILE:HD12   | 2.47                     | 0.45              |
| 4:a:105:TRP:CZ3   | 4:a:111:PRO:HG3   | 2.51                     | 0.45              |
| 27:a:405:PHO:HAB  | 25:d:402:CLA:H11  | 1.98                     | 0.45              |
| 5:b:41:GLU:CD     | 5:b:62:VAL:HG22   | 2.41                     | 0.45              |
| 25:b:605:CLA:HBD  | 25:b:605:CLA:HAA1 | 1.98                     | 0.45              |
| 25:c:504:CLA:C4   | 35:c:516:DGD:HB32 | 2.45                     | 0.45              |
| 25:c:510:CLA:HHD  | 25:c:510:CLA:H192 | 1.98                     | 0.45              |
| 28:h:101:BCR:H331 | 28:h:101:BCR:C8   | 2.46                     | 0.45              |
| 15:o:290:THR:HB   | 15:o:300:ILE:HG13 | 1.98                     | 0.45              |
| 15:o:290:THR:O    | 15:o:291:LYS:C    | 2.59                     | 0.45              |
| 20:s:67:ARG:HH22  | 20:s:85:LEU:HB3   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:s:306:CHL:HBC2 | 24:s:307:CHL:CHD  | 2.46                     | 0.45              |
| 21:g:51:TYR:C     | 21:g:55:ARG:HD3   | 2.41                     | 0.45              |
| 21:g:183:LEU:HG   | 24:g:608:CHL:CBB  | 2.46                     | 0.45              |
| 21:n:208:PHE:CZ   | 21:n:212:LYS:HE3  | 2.51                     | 0.45              |
| 25:y:315:CLA:CBC  | 39:y:316:LUT:H162 | 2.39                     | 0.45              |
| 22:r:234:LYS:HE2  | 22:r:234:LYS:HA   | 1.99                     | 0.45              |
| 2:2:50:TRP:C      | 2:2:55:ARG:HG2    | 2.41                     | 0.45              |
| 2:2:69:TYR:CG     | 2:2:92:PHE:CZ     | 3.05                     | 0.45              |
| 2:2:232:VAL:CG1   | 2:2:243:GLU:OE1   | 2.65                     | 0.45              |
| 3:4:183:GLU:HB3   | 3:4:185:PHE:HD1   | 1.75                     | 0.45              |
| 5:B:355:PHE:O     | 5:B:371:VAL:HG22  | 2.16                     | 0.45              |
| 6:C:236:GLY:HA2   | 6:C:239:TRP:CD1   | 2.52                     | 0.45              |
| 6:C:372:PRO:O     | 6:C:373:ASN:HB2   | 2.16                     | 0.45              |
| 7:D:172:PRO:HG3   | 7:D:182:PHE:CE2   | 2.52                     | 0.45              |
| 7:D:309:ASP:OD1   | 7:D:311:GLU:HG3   | 2.17                     | 0.45              |
| 8:E:24:SER:O      | 8:E:28:PRO:HG2    | 2.16                     | 0.45              |
| 15:O:130:LYS:HE2  | 15:O:177:PRO:CB   | 2.30                     | 0.45              |
| 25:S:305:CLA:H3A  | 25:S:305:CLA:CGA  | 2.46                     | 0.45              |
| 21:G:80:TRP:CE3   | 39:G:616:LUT:H383 | 2.52                     | 0.45              |
| 21:G:120:ALA:HA   | 21:G:124:VAL:O    | 2.16                     | 0.45              |
| 21:G:204:ASP:O    | 21:G:208:PHE:N    | 2.40                     | 0.45              |
| 25:G:613:CLA:H3A  | 25:G:613:CLA:HBA2 | 1.59                     | 0.45              |
| 25:G:613:CLA:H91  | 26:Y:301:LHG:H322 | 1.99                     | 0.45              |
| 21:N:227:PHE:HB2  | 39:N:616:LUT:C40  | 2.47                     | 0.45              |
| 25:N:602:CLA:H93  | 25:N:602:CLA:H111 | 1.52                     | 0.45              |
| 25:Y:304:CLA:HMD1 | 24:Y:310:CHL:C1D  | 2.47                     | 0.45              |
| 25:Y:313:CLA:H142 | 25:Y:313:CLA:H111 | 1.50                     | 0.45              |
| 26:Y:319:LHG:H171 | 26:Y:319:LHG:H202 | 1.70                     | 0.45              |
| 22:R:155:LEU:HD22 | 22:R:268:LEU:HD21 | 1.99                     | 0.45              |
| 1:5:50:TRP:HB3    | 1:5:213:VAL:HG21  | 1.98                     | 0.45              |
| 1:5:128:GLU:CB    | 1:5:133:LYS:O     | 2.65                     | 0.45              |
| 2:6:174:GLU:CD    | 1:7:59:LEU:HD22   | 2.42                     | 0.45              |
| 1:7:163:ALA:O     | 1:7:167:ILE:HG13  | 2.17                     | 0.45              |
| 3:8:58:ILE:O      | 3:8:58:ILE:HG22   | 2.15                     | 0.45              |
| 27:a:404:PHO:H141 | 27:a:404:PHO:H161 | 1.52                     | 0.45              |
| 29:a:412:SQD:H132 | 29:a:412:SQD:H162 | 1.70                     | 0.45              |
| 5:b:248:ALA:HB2   | 25:b:603:CLA:H52  | 1.97                     | 0.45              |
| 5:b:377:VAL:O     | 5:b:378:ARG:HB2   | 2.17                     | 0.45              |
| 25:b:607:CLA:H161 | 25:b:607:CLA:H141 | 1.55                     | 0.45              |
| 26:b:625:LHG:H351 | 26:b:625:LHG:H101 | 1.99                     | 0.45              |
| 6:c:225:VAL:HG13  | 6:c:289:PHE:HA    | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:c:256:PRO:HA    | 25:c:506:CLA:HED2 | 1.98                     | 0.45              |
| 7:d:172:PRO:HG3   | 7:d:182:PHE:CE2   | 2.52                     | 0.45              |
| 7:d:280:LEU:CD2   | 25:d:402:CLA:HBA2 | 2.45                     | 0.45              |
| 25:s:310:CLA:H62  | 25:s:310:CLA:H41  | 1.68                     | 0.45              |
| 21:g:58:TYR:HE1   | 21:g:79:GLY:C     | 2.24                     | 0.45              |
| 24:g:608:CHL:H18  | 40:g:617:NEX:H361 | 1.98                     | 0.45              |
| 21:n:163:ALA:O    | 21:n:167:ILE:HG13 | 2.17                     | 0.45              |
| 21:n:227:PHE:HB2  | 39:n:616:LUT:C40  | 2.47                     | 0.45              |
| 24:n:601:CHL:H3A  | 24:n:601:CHL:HBA1 | 1.63                     | 0.45              |
| 21:y:104:ARG:HB3  | 25:y:311:CLA:HBC2 | 1.96                     | 0.45              |
| 22:r:103:LYS:CD   | 22:r:105:LEU:HD11 | 2.47                     | 0.45              |
| 22:r:179:TYR:HD1  | 22:r:180:LEU:N    | 2.14                     | 0.45              |
| 25:r:611:CLA:HAA2 | 25:r:611:CLA:H12  | 1.98                     | 0.45              |
| 3:4:122:TRP:HA    | 3:4:127:TRP:CD1   | 2.40                     | 0.45              |
| 3:4:169:SER:O     | 3:4:170:GLN:HB2   | 2.17                     | 0.45              |
| 3:4:236:MET:HA    | 3:4:239:MET:HE3   | 1.98                     | 0.45              |
| 5:B:296:GLN:HE21  | 5:B:300:GLU:HB3   | 1.82                     | 0.45              |
| 5:B:330:MET:CE    | 5:B:446:SER:HB3   | 2.46                     | 0.45              |
| 5:B:372:ASP:OD1   | 5:B:376:ILE:N     | 2.49                     | 0.45              |
| 25:B:616:CLA:HMD3 | 10:H:17:THR:HG21  | 1.98                     | 0.45              |
| 6:C:113:VAL:HG13  | 28:C:514:BCR:H313 | 1.98                     | 0.45              |
| 7:D:161:TYR:HA    | 7:D:291:ALA:HB2   | 1.99                     | 0.45              |
| 15:O:146:LYS:HD3  | 15:O:158:PHE:CE1  | 2.52                     | 0.45              |
| 25:S:311:CLA:HBA1 | 25:S:311:CLA:H3A  | 1.69                     | 0.45              |
| 21:N:164:THR:HG21 | 24:N:606:CHL:O1D  | 2.16                     | 0.45              |
| 25:Y:303:CLA:H111 | 25:Y:303:CLA:H143 | 1.61                     | 0.45              |
| 22:R:141:LEU:CD2  | 22:R:216:LEU:HB3  | 2.47                     | 0.45              |
| 25:R:601:CLA:H3A  | 25:R:601:CLA:HBA1 | 1.45                     | 0.45              |
| 1:5:163:ALA:O     | 1:5:167:ILE:HG13  | 2.17                     | 0.45              |
| 1:7:97:GLU:HA     | 1:7:190:LEU:CD1   | 2.24                     | 0.45              |
| 3:8:144:SER:HB3   | 22:r:279:LEU:O    | 2.17                     | 0.45              |
| 3:8:169:SER:O     | 3:8:170:GLN:HB2   | 2.17                     | 0.45              |
| 4:a:30:ILE:HD11   | 29:a:412:SQD:C44  | 2.47                     | 0.45              |
| 5:b:110:ALA:HB1   | 25:b:616:CLA:CHB  | 2.47                     | 0.45              |
| 25:b:602:CLA:H62  | 25:b:602:CLA:H41  | 1.79                     | 0.45              |
| 6:c:364:PRO:O     | 6:c:368:PRO:HD3   | 2.17                     | 0.45              |
| 21:g:50:TRP:HB3   | 21:g:213:VAL:HG21 | 1.98                     | 0.45              |
| 21:n:154:HIS:CE1  | 21:n:156:GLN:OE1  | 2.69                     | 0.45              |
| 21:n:158:ILE:HD11 | 21:y:257:TRP:CE3  | 2.35                     | 0.45              |
| 21:y:56:VAL:HB    | 24:y:302:CHL:HBC2 | 1.98                     | 0.45              |
| 21:y:75:PRO:HG3   | 21:y:212:LYS:HB3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:128:GLU:CB   | 21:y:133:LYS:O    | 2.65                     | 0.45              |
| 25:y:304:CLA:H101 | 25:y:304:CLA:H62  | 1.40                     | 0.45              |
| 25:y:314:CLA:H141 | 25:y:314:CLA:H162 | 1.53                     | 0.45              |
| 22:r:141:LEU:CD2  | 22:r:216:LEU:HB3  | 2.47                     | 0.45              |
| 22:r:283:ILE:HG23 | 22:r:284:ILE:N    | 2.31                     | 0.45              |
| 25:r:602:CLA:H43  | 25:r:603:CLA:HBA1 | 1.99                     | 0.45              |
| 1:1:58:TYR:HE1    | 1:1:79:GLY:C      | 2.24                     | 0.45              |
| 1:1:107:MET:HA    | 1:1:222:ALA:HB1   | 1.98                     | 0.45              |
| 4:A:30:ILE:HD11   | 29:A:411:SQD:C44  | 2.47                     | 0.45              |
| 4:A:37:MET:HB2    | 4:A:125:CYS:CB    | 2.47                     | 0.45              |
| 4:A:238:ARG:O     | 4:A:241:GLN:HB3   | 2.17                     | 0.45              |
| 6:C:227:VAL:CG2   | 28:I:101:BCR:H292 | 2.47                     | 0.45              |
| 25:C:513:CLA:CMD  | 20:S:75:LEU:HD11  | 2.45                     | 0.45              |
| 7:D:157:VAL:HG12  | 7:D:172:PRO:CG    | 2.47                     | 0.45              |
| 7:D:194:LEU:HG    | 7:D:194:LEU:O     | 2.16                     | 0.45              |
| 17:W:81:VAL:HG23  | 17:W:82:ASP:OD2   | 2.16                     | 0.45              |
| 21:G:83:ALA:HA    | 21:Y:98:LEU:HD11  | 1.98                     | 0.45              |
| 21:N:120:ALA:HA   | 21:N:124:VAL:O    | 2.16                     | 0.45              |
| 24:N:607:CHL:HHC  | 24:N:607:CHL:HBB1 | 1.98                     | 0.45              |
| 24:N:608:CHL:H13  | 40:N:617:NEX:C40  | 2.46                     | 0.45              |
| 25:N:613:CLA:H143 | 25:N:613:CLA:C8   | 2.38                     | 0.45              |
| 25:N:613:CLA:HBA1 | 25:N:614:CLA:C3D  | 2.47                     | 0.45              |
| 21:Y:115:PHE:HZ   | 32:Y:320:AJP:C83  | 2.30                     | 0.45              |
| 21:Y:131:TRP:HA   | 39:Y:317:LUT:O3   | 2.16                     | 0.45              |
| 24:Y:302:CHL:HBB1 | 24:Y:302:CHL:HHC  | 1.98                     | 0.45              |
| 22:R:67:TRP:CH2   | 22:R:85:LYS:HB2   | 2.51                     | 0.45              |
| 22:R:177:SER:HB2  | 24:R:605:CHL:CMD  | 2.47                     | 0.45              |
| 2:6:100:VAL:HB    | 2:6:190:LEU:HD23  | 1.98                     | 0.45              |
| 5:b:372:ASP:OD1   | 5:b:376:ILE:N     | 2.49                     | 0.45              |
| 25:b:613:CLA:H111 | 25:b:613:CLA:H142 | 1.67                     | 0.45              |
| 8:e:18:ARG:HB3    | 8:e:21:VAL:HB     | 1.98                     | 0.45              |
| 28:i:101:BCR:H15C | 28:i:101:BCR:H351 | 1.84                     | 0.45              |
| 12:k:58:VAL:O     | 12:k:58:VAL:CG1   | 2.65                     | 0.45              |
| 20:s:128:PHE:HE2  | 20:s:236:MET:CE   | 2.27                     | 0.45              |
| 20:s:190:ILE:HG13 | 20:s:191:THR:HG23 | 1.99                     | 0.45              |
| 20:s:224:LYS:HG2  | 25:s:311:CLA:CED  | 2.47                     | 0.45              |
| 20:s:238:GLY:O    | 20:s:242:GLN:HG3  | 2.17                     | 0.45              |
| 20:s:260:ASP:OD2  | 20:s:263:GLY:HA3  | 2.17                     | 0.45              |
| 21:g:128:GLU:CB   | 21:g:133:LYS:O    | 2.65                     | 0.45              |
| 21:n:128:GLU:CB   | 21:n:133:LYS:O    | 2.65                     | 0.45              |
| 25:n:603:CLA:H142 | 25:y:304:CLA:H143 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:n:608:CHL:H13  | 40:n:617:NEX:C40  | 2.46                     | 0.45              |
| 25:n:612:CLA:H62  | 25:n:612:CLA:H2   | 1.71                     | 0.45              |
| 21:y:50:TRP:HB3   | 21:y:213:VAL:HG21 | 1.99                     | 0.45              |
| 21:y:114:VAL:HG13 | 21:y:241:ILE:HD11 | 1.98                     | 0.45              |
| 21:y:115:PHE:CD2  | 25:y:305:CLA:HHD  | 2.52                     | 0.45              |
| 25:y:311:CLA:C2B  | 25:y:311:CLA:H2   | 2.46                     | 0.45              |
| 41:r:616:XAT:H35  | 41:r:616:XAT:H401 | 1.60                     | 0.45              |
| 2:2:86:SER:HB2    | 2:2:92:PHE:CD1    | 2.52                     | 0.45              |
| 24:2:601:CHL:H62  | 24:2:601:CHL:H102 | 1.58                     | 0.45              |
| 3:4:231:HIS:HA    | 3:4:234:LEU:HG    | 1.99                     | 0.45              |
| 4:A:94:TYR:OH     | 4:A:105:TRP:HA    | 2.17                     | 0.45              |
| 5:B:141:ILE:CG1   | 5:B:217:LEU:HD21  | 2.46                     | 0.45              |
| 6:C:281:VAL:CG1   | 6:C:285:ILE:HD11  | 2.47                     | 0.45              |
| 25:C:503:CLA:H193 | 25:C:503:CLA:H161 | 1.60                     | 0.45              |
| 30:C:520:LMG:H141 | 20:S:262:PHE:CD1  | 2.52                     | 0.45              |
| 20:S:144:GLU:OE2  | 20:S:149:LYS:HE2  | 2.17                     | 0.45              |
| 21:G:208:PHE:CZ   | 21:G:212:LYS:HE3  | 2.51                     | 0.45              |
| 21:N:78:TYR:CE1   | 24:N:601:CHL:HMD1 | 2.52                     | 0.45              |
| 21:Y:128:GLU:CB   | 21:Y:133:LYS:O    | 2.65                     | 0.45              |
| 21:Y:163:ALA:O    | 21:Y:167:ILE:HG13 | 2.17                     | 0.45              |
| 25:R:611:CLA:HAA2 | 25:R:611:CLA:H12  | 1.98                     | 0.45              |
| 3:8:103:LEU:HD13  | 3:8:193:GLY:CA    | 2.36                     | 0.45              |
| 3:8:118:VAL:HG23  | 3:8:122:TRP:CZ2   | 2.52                     | 0.45              |
| 3:8:181:THR:HG21  | 3:8:198:ARG:NH2   | 2.32                     | 0.45              |
| 3:8:236:MET:HA    | 3:8:239:MET:HE3   | 1.98                     | 0.45              |
| 25:a:403:CLA:O1A  | 25:a:403:CLA:H43  | 2.16                     | 0.45              |
| 5:b:41:GLU:HB3    | 5:b:63:ILE:HD11   | 1.99                     | 0.45              |
| 5:b:69:LEU:HD13   | 25:b:606:CLA:HHB  | 1.99                     | 0.45              |
| 5:b:388:SER:CB    | 5:b:391:SER:HB2   | 2.45                     | 0.45              |
| 25:b:611:CLA:HAB  | 25:b:613:CLA:H3A  | 1.98                     | 0.45              |
| 25:b:616:CLA:HMD3 | 10:h:17:THR:HG21  | 1.98                     | 0.45              |
| 6:c:311:GLN:HE21  | 6:c:358:PHE:HB2   | 1.81                     | 0.45              |
| 25:c:504:CLA:H111 | 25:c:504:CLA:H91  | 1.70                     | 0.45              |
| 15:o:143:PHE:CE2  | 17:w:81:VAL:HG11  | 2.52                     | 0.45              |
| 20:s:144:GLU:OE2  | 20:s:149:LYS:HE2  | 2.17                     | 0.45              |
| 21:g:120:ALA:HA   | 21:g:124:VAL:O    | 2.16                     | 0.45              |
| 1:1:128:GLU:CB    | 1:1:133:LYS:O     | 2.65                     | 0.44              |
| 1:3:50:TRP:HB3    | 1:3:213:VAL:HG21  | 1.99                     | 0.44              |
| 3:4:219:GLU:O     | 3:4:223:ARG:N     | 2.49                     | 0.44              |
| 4:A:157:VAL:CG1   | 4:A:172:MET:HB2   | 2.47                     | 0.44              |
| 4:A:233:ALA:O     | 4:A:235:GLU:HG2   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:2:GLY:H       | 13:L:12:GLU:CD    | 2.25                     | 0.44              |
| 5:B:91:TRP:NE1    | 26:B:622:LHG:HC61 | 2.29                     | 0.44              |
| 5:B:122:ILE:HA    | 10:H:24:LYS:HD3   | 1.99                     | 0.44              |
| 25:B:609:CLA:H13  | 25:B:609:CLA:H171 | 1.79                     | 0.44              |
| 26:B:625:LHG:H351 | 26:B:625:LHG:H101 | 1.99                     | 0.44              |
| 6:C:89:LEU:HD22   | 6:C:111:TYR:CD2   | 2.52                     | 0.44              |
| 6:C:267:SER:CA    | 17:W:133:LEU:HD23 | 2.47                     | 0.44              |
| 30:C:520:LMG:H362 | 25:S:314:CLA:OBD  | 2.17                     | 0.44              |
| 25:D:403:CLA:H61  | 25:D:403:CLA:H102 | 1.80                     | 0.44              |
| 19:Z:40:VAL:O     | 19:Z:41:PHE:C     | 2.61                     | 0.44              |
| 20:S:142:GLY:N    | 20:S:160:LEU:O    | 2.50                     | 0.44              |
| 21:G:58:TYR:HE1   | 21:G:79:GLY:C     | 2.24                     | 0.44              |
| 21:G:84:GLY:N     | 21:Y:94:ARG:CG    | 2.80                     | 0.44              |
| 21:G:163:ALA:O    | 21:G:167:ILE:HG13 | 2.17                     | 0.44              |
| 25:G:611:CLA:H3A  | 25:G:611:CLA:HBA2 | 1.28                     | 0.44              |
| 21:N:163:ALA:O    | 21:N:167:ILE:HG13 | 2.17                     | 0.44              |
| 25:N:603:CLA:H142 | 25:Y:304:CLA:H143 | 1.99                     | 0.44              |
| 21:Y:120:ALA:HA   | 21:Y:124:VAL:O    | 2.16                     | 0.44              |
| 25:Y:311:CLA:C2B  | 25:Y:311:CLA:H2   | 2.46                     | 0.44              |
| 25:Y:314:CLA:H92  | 25:Y:314:CLA:H61  | 1.56                     | 0.44              |
| 2:6:66:THR:CG2    | 2:6:67:PRO:HD2    | 2.48                     | 0.44              |
| 4:a:37:MET:HB2    | 4:a:125:CYS:CB    | 2.47                     | 0.44              |
| 4:a:155:THR:HG21  | 35:c:515:DGD:HBW1 | 1.99                     | 0.44              |
| 25:a:403:CLA:C2B  | 27:a:404:PHO:H192 | 2.46                     | 0.44              |
| 5:b:220:ARG:HG3   | 10:h:32:LYS:HE3   | 1.99                     | 0.44              |
| 25:b:609:CLA:H3A  | 25:b:609:CLA:HBA1 | 1.47                     | 0.44              |
| 28:b:618:BCR:H20C | 28:b:618:BCR:H361 | 1.85                     | 0.44              |
| 6:c:28:GLN:O      | 6:c:32:GLY:N      | 2.42                     | 0.44              |
| 30:c:520:LMG:H141 | 20:s:262:PHE:CD1  | 2.52                     | 0.44              |
| 30:c:520:LMG:H362 | 25:s:314:CLA:OBD  | 2.17                     | 0.44              |
| 7:d:58:SER:OG     | 7:d:80:SER:OG     | 2.25                     | 0.44              |
| 7:d:81:THR:HG22   | 7:d:112:TRP:NE1   | 2.32                     | 0.44              |
| 7:d:309:ASP:OD1   | 7:d:311:GLU:HG3   | 2.17                     | 0.44              |
| 25:d:403:CLA:H3A  | 25:d:403:CLA:HBA2 | 1.55                     | 0.44              |
| 12:k:58:VAL:HG12  | 12:k:61:ARG:CD    | 2.47                     | 0.44              |
| 29:l:102:SQD:H92  | 29:l:102:SQD:O10  | 2.16                     | 0.44              |
| 14:m:1:MET:HB3    | 14:m:3:VAL:HG13   | 1.99                     | 0.44              |
| 15:o:227:PHE:CZ   | 15:o:287:LEU:HD22 | 2.52                     | 0.44              |
| 28:t:101:BCR:H20C | 28:t:101:BCR:H361 | 1.83                     | 0.44              |
| 20:s:190:ILE:HG13 | 20:s:191:THR:H    | 1.81                     | 0.44              |
| 25:g:610:CLA:H13  | 25:g:610:CLA:H172 | 1.61                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:g:617:NEX:C28  | 40:g:617:NEX:C36  | 2.95                     | 0.44              |
| 21:n:154:HIS:O    | 21:n:154:HIS:ND1  | 2.44                     | 0.44              |
| 21:n:164:THR:HG21 | 24:n:606:CHL:O1D  | 2.16                     | 0.44              |
| 21:n:215:GLU:HB2  | 25:n:610:CLA:CHB  | 2.48                     | 0.44              |
| 24:n:607:CHL:H112 | 24:n:607:CHL:H91  | 1.71                     | 0.44              |
| 21:y:58:TYR:HE1   | 21:y:79:GLY:C     | 2.24                     | 0.44              |
| 22:r:177:SER:HB2  | 24:r:605:CHL:CMD  | 2.47                     | 0.44              |
| 25:r:612:CLA:H71  | 25:r:612:CLA:HHC  | 1.98                     | 0.44              |
| 2:2:129:GLU:N     | 2:2:130:PRO:CD    | 2.80                     | 0.44              |
| 2:2:193:GLY:CA    | 2:2:197:PHE:HD2   | 2.25                     | 0.44              |
| 1:3:163:ALA:O     | 1:3:167:ILE:HG13  | 2.17                     | 0.44              |
| 3:4:203:LEU:HB3   | 3:4:205:LEU:HD13  | 1.99                     | 0.44              |
| 4:A:210:LEU:HD12  | 27:A:404:PHO:NB   | 2.31                     | 0.44              |
| 25:B:610:CLA:CBD  | 25:B:610:CLA:HAA2 | 2.47                     | 0.44              |
| 6:C:225:VAL:HG13  | 6:C:289:PHE:HA    | 1.99                     | 0.44              |
| 6:C:364:PRO:O     | 6:C:368:PRO:HD3   | 2.17                     | 0.44              |
| 25:C:511:CLA:H91  | 25:C:511:CLA:H111 | 1.79                     | 0.44              |
| 25:C:512:CLA:CMA  | 25:C:513:CLA:H203 | 2.47                     | 0.44              |
| 7:D:135:ARG:HH21  | 7:D:138:GLN:CD    | 2.25                     | 0.44              |
| 10:H:52:VAL:HG22  | 18:X:88:LEU:CD1   | 2.45                     | 0.44              |
| 11:I:24:LEU:HD12  | 28:I:101:BCR:C3   | 2.47                     | 0.44              |
| 12:K:58:VAL:O     | 12:K:58:VAL:CG1   | 2.65                     | 0.44              |
| 15:O:189:LYS:HD2  | 15:O:189:LYS:O    | 2.18                     | 0.44              |
| 20:S:260:ASP:OD2  | 20:S:263:GLY:HA3  | 2.16                     | 0.44              |
| 25:N:602:CLA:H142 | 25:N:602:CLA:H112 | 1.63                     | 0.44              |
| 21:Y:50:TRP:HB3   | 21:Y:213:VAL:HG21 | 1.98                     | 0.44              |
| 21:Y:107:MET:HG2  | 21:Y:222:ALA:HB3  | 1.93                     | 0.44              |
| 21:Y:204:ASP:O    | 21:Y:208:PHE:N    | 2.40                     | 0.44              |
| 39:Y:317:LUT:H11  | 39:Y:317:LUT:H191 | 1.85                     | 0.44              |
| 25:R:602:CLA:HBC1 | 26:R:618:LHG:H282 | 2.00                     | 0.44              |
| 25:R:612:CLA:H112 | 25:R:612:CLA:H91  | 1.58                     | 0.44              |
| 2:6:126:ASP:OD1   | 2:6:129:GLU:HA    | 2.17                     | 0.44              |
| 2:6:192:PRO:HB3   | 24:6:603:CHL:HBC2 | 1.99                     | 0.44              |
| 2:6:221:ARG:HG3   | 2:6:222:LEU:N     | 2.32                     | 0.44              |
| 1:7:58:TYR:HE1    | 1:7:79:GLY:O      | 1.99                     | 0.44              |
| 3:8:75:GLY:H      | 3:8:80:ASP:CG     | 2.22                     | 0.44              |
| 3:8:231:HIS:HA    | 3:8:234:LEU:HG    | 1.99                     | 0.44              |
| 4:a:135:PHE:CE2   | 6:c:449:ARG:HD3   | 2.52                     | 0.44              |
| 4:a:174:LEU:HD22  | 27:a:404:PHO:H143 | 1.98                     | 0.44              |
| 5:b:157:HIS:CE1   | 25:b:606:CLA:C4A  | 2.96                     | 0.44              |
| 5:b:296:GLN:HE21  | 5:b:300:GLU:HB3   | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:608:CLA:HBC3 | 25:b:608:CLA:HHD  | 1.98                     | 0.44              |
| 6:c:281:VAL:CG1   | 6:c:285:ILE:HD11  | 2.47                     | 0.44              |
| 6:c:294:ASN:OD1   | 35:c:515:DGD:HE4  | 2.17                     | 0.44              |
| 6:c:376:ASP:OD1   | 6:c:379:ARG:HB2   | 2.17                     | 0.44              |
| 28:d:404:BCR:H20C | 28:d:404:BCR:H361 | 1.84                     | 0.44              |
| 26:d:406:LHG:H302 | 16:t:21:ILE:HD11  | 1.99                     | 0.44              |
| 10:h:25:PRO:HG3   | 22:r:122:THR:CB   | 2.47                     | 0.44              |
| 10:h:52:VAL:HG22  | 18:x:88:LEU:CD1   | 2.45                     | 0.44              |
| 29:l:101:SQD:H102 | 29:l:101:SQD:H131 | 1.47                     | 0.44              |
| 15:o:146:LYS:HD3  | 15:o:158:PHE:CE1  | 2.52                     | 0.44              |
| 18:x:92:SER:O     | 18:x:96:VAL:HG13  | 2.17                     | 0.44              |
| 20:s:119:ARG:HH11 | 25:s:310:CLA:C1D  | 2.30                     | 0.44              |
| 20:s:254:LEU:HD22 | 39:s:315:LUT:H163 | 1.99                     | 0.44              |
| 24:n:609:CHL:H121 | 32:n:619:AJP:C01  | 2.48                     | 0.44              |
| 22:r:141:LEU:HD23 | 22:r:216:LEU:HB3  | 1.98                     | 0.44              |
| 40:r:617:NEX:H11  | 40:r:617:NEX:H203 | 1.65                     | 0.44              |
| 1:l:208:PHE:CZ    | 1:l:212:LYS:HE3   | 2.51                     | 0.44              |
| 2:2:123:VAL:HG12  | 2:2:124:ARG:HH21  | 1.83                     | 0.44              |
| 3:4:181:THR:HG21  | 3:4:198:ARG:NH2   | 2.32                     | 0.44              |
| 4:A:40:THR:CG2    | 25:A:405:CLA:HBB1 | 2.48                     | 0.44              |
| 4:A:120:LEU:O     | 4:A:123:VAL:HG22  | 2.18                     | 0.44              |
| 4:A:155:THR:HG21  | 35:C:515:DGD:HBW1 | 1.99                     | 0.44              |
| 27:A:404:PHO:HAB  | 25:D:402:CLA:H11  | 1.98                     | 0.44              |
| 5:B:69:LEU:HD13   | 25:B:606:CLA:HHB  | 1.99                     | 0.44              |
| 5:B:330:MET:HE3   | 5:B:446:SER:N     | 2.32                     | 0.44              |
| 28:B:618:BCR:C8   | 28:B:618:BCR:H331 | 2.46                     | 0.44              |
| 7:D:201:GLY:O     | 7:D:205:VAL:HG23  | 2.18                     | 0.44              |
| 20:S:114:GLU:HB2  | 25:S:303:CLA:CHB  | 2.47                     | 0.44              |
| 20:S:254:LEU:HD22 | 39:S:315:LUT:H163 | 1.99                     | 0.44              |
| 21:G:128:GLU:CB   | 21:G:133:LYS:O    | 2.65                     | 0.44              |
| 21:G:181:GLY:HA3  | 24:G:608:CHL:HMC  | 2.00                     | 0.44              |
| 24:G:609:CHL:HBA1 | 24:N:601:CHL:HBA2 | 2.00                     | 0.44              |
| 25:N:603:CLA:HBC2 | 24:N:609:CHL:HMD2 | 2.00                     | 0.44              |
| 21:Y:80:TRP:HE3   | 25:Y:303:CLA:CMD  | 2.30                     | 0.44              |
| 21:Y:115:PHE:CD2  | 25:Y:305:CLA:HHD  | 2.52                     | 0.44              |
| 2:6:123:VAL:HG12  | 2:6:124:ARG:HH21  | 1.83                     | 0.44              |
| 3:8:159:LYS:HZ2   | 25:r:601:CLA:CMB  | 2.29                     | 0.44              |
| 4:a:157:VAL:HG11  | 4:a:172:MET:HE3   | 1.98                     | 0.44              |
| 5:b:330:MET:HE3   | 5:b:446:SER:N     | 2.32                     | 0.44              |
| 25:b:604:CLA:H112 | 25:b:604:CLA:H152 | 1.57                     | 0.44              |
| 25:b:610:CLA:CBD  | 25:b:610:CLA:HAA2 | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:c:275:SER:OG    | 25:c:509:CLA:OBD  | 2.30                     | 0.44              |
| 25:c:501:CLA:H193 | 25:c:506:CLA:C1B  | 2.48                     | 0.44              |
| 25:c:510:CLA:H112 | 25:c:510:CLA:H151 | 1.60                     | 0.44              |
| 7:d:161:TYR:HA    | 7:d:291:ALA:HB2   | 1.99                     | 0.44              |
| 12:k:39:VAL:O     | 12:k:42:VAL:HG22  | 2.17                     | 0.44              |
| 28:t:101:BCR:H272 | 28:t:101:BCR:C17  | 2.48                     | 0.44              |
| 25:s:312:CLA:HBB1 | 39:s:315:LUT:C14  | 2.47                     | 0.44              |
| 21:g:181:GLY:HA3  | 24:g:608:CHL:CMC  | 2.47                     | 0.44              |
| 25:g:604:CLA:HBB1 | 39:g:616:LUT:C18  | 2.47                     | 0.44              |
| 25:g:610:CLA:H92  | 25:g:610:CLA:H61  | 1.69                     | 0.44              |
| 21:n:59:LEU:HD23  | 24:n:601:CHL:C1B  | 2.46                     | 0.44              |
| 21:n:206:GLU:N    | 21:n:206:GLU:CD   | 2.76                     | 0.44              |
| 25:n:602:CLA:H93  | 25:n:602:CLA:H61  | 1.49                     | 0.44              |
| 24:n:607:CHL:HHC  | 24:n:607:CHL:HBB1 | 1.98                     | 0.44              |
| 25:n:611:CLA:HMD2 | 25:n:612:CLA:HHD  | 1.98                     | 0.44              |
| 21:y:108:LEU:HD11 | 25:y:311:CLA:HBC1 | 1.97                     | 0.44              |
| 21:y:163:ALA:O    | 21:y:167:ILE:HG13 | 2.17                     | 0.44              |
| 2:2:221:ARG:HG3   | 2:2:222:LEU:N     | 2.32                     | 0.44              |
| 1:3:120:ALA:HA    | 1:3:124:VAL:O     | 2.16                     | 0.44              |
| 1:3:128:GLU:CB    | 1:3:133:LYS:O     | 2.65                     | 0.44              |
| 3:4:231:HIS:HA    | 3:4:234:LEU:HD21  | 2.00                     | 0.44              |
| 4:A:258:LEU:HA    | 7:D:133:LEU:CD1   | 2.47                     | 0.44              |
| 5:B:281:GLN:CD    | 23:U:91:VAL:HG13  | 2.42                     | 0.44              |
| 25:B:611:CLA:HMA1 | 25:B:612:CLA:CMC  | 2.48                     | 0.44              |
| 8:E:18:ARG:HB3    | 8:E:21:VAL:HB     | 1.98                     | 0.44              |
| 15:O:227:PHE:CZ   | 15:O:287:LEU:HD22 | 2.52                     | 0.44              |
| 28:T:101:BCR:H272 | 28:T:101:BCR:C17  | 2.47                     | 0.44              |
| 20:S:238:GLY:O    | 20:S:242:GLN:HG3  | 2.17                     | 0.44              |
| 21:G:176:ARG:HG3  | 24:G:608:CHL:CHD  | 2.48                     | 0.44              |
| 21:G:181:GLY:HA3  | 24:G:608:CHL:CMC  | 2.47                     | 0.44              |
| 21:G:209:ALA:HA   | 21:G:212:LYS:CG   | 2.34                     | 0.44              |
| 25:N:603:CLA:H71  | 25:N:603:CLA:H112 | 1.74                     | 0.44              |
| 21:Y:58:TYR:HE1   | 21:Y:79:GLY:C     | 2.24                     | 0.44              |
| 25:Y:304:CLA:H2   | 25:Y:304:CLA:H61  | 1.86                     | 0.44              |
| 24:Y:306:CHL:HBC3 | 24:Y:306:CHL:HMC  | 1.98                     | 0.44              |
| 25:Y:311:CLA:C5   | 25:Y:313:CLA:HMA1 | 2.28                     | 0.44              |
| 22:R:67:TRP:CD2   | 22:R:85:LYS:HA    | 2.52                     | 0.44              |
| 22:R:274:HIS:CD2  | 24:R:613:CHL:NC   | 2.84                     | 0.44              |
| 25:R:610:CLA:H3A  | 25:R:610:CLA:HBA2 | 1.38                     | 0.44              |
| 1:7:58:TYR:HE1    | 1:7:79:GLY:C      | 2.24                     | 0.44              |
| 1:7:128:GLU:CB    | 1:7:133:LYS:O     | 2.65                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:225:SER:O     | 1:7:229:PHE:HD1   | 2.01                     | 0.44              |
| 4:a:258:LEU:HA    | 7:d:133:LEU:CD1   | 2.47                     | 0.44              |
| 5:b:217:LEU:HB3   | 25:r:614:CLA:HBA1 | 2.00                     | 0.44              |
| 5:b:257:TRP:CD2   | 7:d:292:LEU:HD22  | 2.52                     | 0.44              |
| 5:b:357:ARG:NH2   | 23:u:96:PRO:HG2   | 2.33                     | 0.44              |
| 25:b:603:CLA:H193 | 25:b:603:CLA:H162 | 1.54                     | 0.44              |
| 25:b:608:CLA:H122 | 7:d:121:PHE:CZ    | 2.53                     | 0.44              |
| 6:c:297:TYR:HB3   | 6:c:302:TYR:CD2   | 2.53                     | 0.44              |
| 7:d:343:PRO:O     | 7:d:346:VAL:HG22  | 2.17                     | 0.44              |
| 15:o:189:LYS:HD2  | 15:o:189:LYS:O    | 2.18                     | 0.44              |
| 20:s:130:ILE:HB   | 20:s:131:PRO:HD3  | 2.00                     | 0.44              |
| 21:g:115:PHE:HB2  | 25:g:604:CLA:HBC3 | 2.00                     | 0.44              |
| 21:g:176:ARG:HG3  | 24:g:608:CHL:CHD  | 2.48                     | 0.44              |
| 21:g:206:GLU:N    | 21:g:206:GLU:CD   | 2.76                     | 0.44              |
| 21:n:231:VAL:CG1  | 25:n:613:CLA:HAC1 | 2.46                     | 0.44              |
| 25:n:602:CLA:H172 | 25:n:602:CLA:H13  | 1.80                     | 0.44              |
| 25:n:603:CLA:HBC1 | 24:n:609:CHL:CBC  | 2.47                     | 0.44              |
| 21:y:115:PHE:HZ   | 32:y:320:AJP:C83  | 2.30                     | 0.44              |
| 25:y:312:CLA:HBA2 | 25:y:312:CLA:H12  | 1.90                     | 0.44              |
| 2:2:197:PHE:C     | 2:2:199:PRO:HD2   | 2.43                     | 0.44              |
| 3:4:118:VAL:HG23  | 3:4:122:TRP:CZ2   | 2.52                     | 0.44              |
| 3:4:144:SER:HB3   | 22:R:279:LEU:O    | 2.17                     | 0.44              |
| 4:A:140:ARG:NH2   | 7:D:220:GLU:O     | 2.40                     | 0.44              |
| 5:B:110:ALA:HB1   | 25:B:616:CLA:CHB  | 2.47                     | 0.44              |
| 6:C:240:LEU:HD22  | 25:C:501:CLA:CAB  | 2.47                     | 0.44              |
| 29:L:101:SQD:H121 | 29:L:101:SQD:C28  | 2.47                     | 0.44              |
| 14:M:27:VAL:HA    | 14:M:30:VAL:HG22  | 2.00                     | 0.44              |
| 15:O:143:PHE:CE2  | 17:W:81:VAL:HG11  | 2.52                     | 0.44              |
| 20:S:237:LEU:O    | 20:S:241:ILE:CD1  | 2.65                     | 0.44              |
| 21:G:115:PHE:HD2  | 25:G:604:CLA:HHD  | 1.83                     | 0.44              |
| 25:G:602:CLA:C2   | 25:G:602:CLA:HMB1 | 2.47                     | 0.44              |
| 25:G:610:CLA:H142 | 25:G:610:CLA:H111 | 1.61                     | 0.44              |
| 21:N:97:GLU:HA    | 21:N:190:LEU:CD1  | 2.24                     | 0.44              |
| 21:N:208:PHE:O    | 21:N:212:LYS:HG3  | 2.18                     | 0.44              |
| 21:N:209:ALA:CA   | 21:N:212:LYS:HG3  | 2.34                     | 0.44              |
| 21:Y:225:SER:O    | 21:Y:229:PHE:HD1  | 2.01                     | 0.44              |
| 25:Y:304:CLA:H122 | 25:Y:304:CLA:H91  | 1.99                     | 0.44              |
| 22:R:150:ALA:CA   | 41:R:616:XAT:H181 | 2.48                     | 0.44              |
| 25:R:602:CLA:H43  | 25:R:603:CLA:HBA1 | 1.99                     | 0.44              |
| 40:R:617:NEX:H401 | 40:R:617:NEX:H35  | 1.52                     | 0.44              |
| 2:6:100:VAL:CG1   | 2:6:190:LEU:HD23  | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:159:LEU:HD13  | 1:7:159:LEU:N     | 2.33                     | 0.44              |
| 3:8:222:GLU:HA    | 3:8:225:LYS:HD3   | 1.99                     | 0.44              |
| 5:b:242:ILE:HG22  | 5:b:466:HIS:HB2   | 2.00                     | 0.44              |
| 25:b:609:CLA:H171 | 25:b:609:CLA:H13  | 1.79                     | 0.44              |
| 6:c:311:GLN:HG3   | 6:c:361:LEU:CD2   | 2.47                     | 0.44              |
| 7:d:229:GLY:O     | 7:d:230:ALA:HB3   | 2.18                     | 0.44              |
| 20:s:114:GLU:HB2  | 25:s:303:CLA:CHB  | 2.47                     | 0.44              |
| 24:g:601:CHL:HBC1 | 26:y:301:LHG:O3   | 2.18                     | 0.44              |
| 21:y:177:VAL:HG21 | 24:y:310:CHL:CMA  | 2.48                     | 0.44              |
| 21:y:208:PHE:O    | 21:y:212:LYS:HG3  | 2.18                     | 0.44              |
| 22:r:67:TRP:CH2   | 22:r:85:LYS:HB2   | 2.51                     | 0.44              |
| 22:r:177:SER:O    | 22:r:184:LEU:N    | 2.35                     | 0.44              |
| 2:2:161:ALA:HB1   | 2:2:165:PHE:HE2   | 1.81                     | 0.44              |
| 2:2:174:GLU:CD    | 1:3:59:LEU:HD22   | 2.42                     | 0.44              |
| 2:2:217:ILE:HD13  | 25:2:604:CLA:CGD  | 2.48                     | 0.44              |
| 3:4:155:TRP:CZ2   | 25:R:601:CLA:HBB1 | 2.53                     | 0.44              |
| 4:A:49:ILE:HG23   | 31:D:405:PL9:H501 | 2.00                     | 0.44              |
| 4:A:51:ALA:CB     | 4:A:82:ILE:HD12   | 2.47                     | 0.44              |
| 5:B:28:ALA:HB2    | 5:B:107:CYS:CB    | 2.47                     | 0.44              |
| 5:B:148:VAL:HG11  | 26:B:622:LHG:H212 | 1.98                     | 0.44              |
| 5:B:346:PHE:O     | 5:B:353:GLU:HA    | 2.18                     | 0.44              |
| 5:B:361:THR:HG22  | 42:B:701:HOH:O    | 2.17                     | 0.44              |
| 6:C:297:TYR:HB3   | 6:C:302:TYR:CD2   | 2.53                     | 0.44              |
| 7:D:30:PHE:O      | 7:D:129:ARG:NH2   | 2.51                     | 0.44              |
| 21:N:158:ILE:CD1  | 21:Y:257:TRP:CE3  | 2.98                     | 0.44              |
| 25:N:610:CLA:H141 | 25:N:610:CLA:H162 | 1.63                     | 0.44              |
| 21:Y:161:ILE:HG21 | 24:Y:308:CHL:HBC1 | 1.98                     | 0.44              |
| 21:Y:206:GLU:N    | 21:Y:206:GLU:CD   | 2.76                     | 0.44              |
| 22:R:177:SER:HB2  | 24:R:605:CHL:HMD3 | 1.99                     | 0.44              |
| 1:5:225:SER:O     | 1:5:229:PHE:HD1   | 2.01                     | 0.44              |
| 24:5:301:CHL:CHD  | 24:5:301:CHL:HBC2 | 2.48                     | 0.44              |
| 2:6:86:SER:HB2    | 2:6:92:PHE:CD1    | 2.52                     | 0.44              |
| 2:6:126:ASP:C     | 2:6:148:LEU:HD21  | 2.42                     | 0.44              |
| 2:6:129:GLU:N     | 2:6:130:PRO:CD    | 2.80                     | 0.44              |
| 2:6:193:GLY:CA    | 2:6:197:PHE:HD2   | 2.25                     | 0.44              |
| 4:a:23:SER:OG     | 4:a:25:GLU:OE1    | 2.35                     | 0.44              |
| 4:a:49:ILE:HG23   | 31:d:405:PL9:H501 | 2.00                     | 0.44              |
| 4:a:64:ARG:NH1    | 15:o:165:THR:HG21 | 2.33                     | 0.44              |
| 4:a:94:TYR:OH     | 4:a:105:TRP:HA    | 2.17                     | 0.44              |
| 35:a:401:DGD:HA71 | 35:a:401:DGD:HAT1 | 1.64                     | 0.44              |
| 25:a:403:CLA:H91  | 31:d:405:PL9:H402 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:a:410:PL9:O1   | 31:a:410:PL9:HC8  | 2.17                     | 0.44              |
| 5:b:2:GLY:H       | 13:l:12:GLU:CD    | 2.25                     | 0.44              |
| 5:b:221:PRO:HA    | 25:b:609:CLA:HED3 | 1.98                     | 0.44              |
| 25:b:607:CLA:HMB1 | 25:b:607:CLA:CBB  | 2.47                     | 0.44              |
| 25:b:610:CLA:HMA2 | 25:b:610:CLA:HBA1 | 1.99                     | 0.44              |
| 25:b:616:CLA:H92  | 25:b:616:CLA:H62  | 1.76                     | 0.44              |
| 28:b:617:BCR:H382 | 28:b:617:BCR:H23C | 2.00                     | 0.44              |
| 6:c:89:LEU:HD22   | 6:c:111:TYR:CD2   | 2.52                     | 0.44              |
| 25:c:512:CLA:CMA  | 25:c:513:CLA:H203 | 2.47                     | 0.44              |
| 15:o:209:VAL:CG2  | 15:o:319:LYS:HD2  | 2.48                     | 0.44              |
| 19:z:57:LEU:HD23  | 19:z:60:LEU:HD12  | 1.98                     | 0.44              |
| 21:n:78:TYR:CE1   | 24:n:601:CHL:HMD1 | 2.52                     | 0.44              |
| 25:n:610:CLA:H141 | 25:n:610:CLA:H162 | 1.63                     | 0.44              |
| 25:n:613:CLA:HBA1 | 25:n:614:CLA:C3D  | 2.47                     | 0.44              |
| 24:y:310:CHL:H92  | 24:y:310:CHL:H62  | 1.86                     | 0.44              |
| 22:r:67:TRP:CD2   | 22:r:85:LYS:HA    | 2.52                     | 0.44              |
| 25:2:604:CLA:HBC3 | 26:2:606:LHG:H372 | 1.98                     | 0.44              |
| 1:3:208:PHE:O     | 1:3:212:LYS:HG3   | 2.18                     | 0.44              |
| 3:4:219:GLU:O     | 3:4:223:ARG:HB2   | 2.18                     | 0.44              |
| 4:A:64:ARG:NH1    | 15:O:165:THR:HG21 | 2.33                     | 0.44              |
| 5:B:204:ALA:CB    | 25:B:602:CLA:HAB  | 2.48                     | 0.44              |
| 5:B:462:PHE:HZ    | 25:B:613:CLA:HMB3 | 1.80                     | 0.44              |
| 25:C:501:CLA:H193 | 25:C:506:CLA:C1B  | 2.48                     | 0.44              |
| 7:D:68:TYR:O      | 30:D:407:LMG:HC61 | 2.18                     | 0.44              |
| 8:E:67:THR:C      | 23:U:102:ARG:HH11 | 2.26                     | 0.44              |
| 15:O:218:LEU:HD23 | 15:O:218:LEU:H    | 1.83                     | 0.44              |
| 20:S:130:ILE:HB   | 20:S:131:PRO:HD3  | 2.00                     | 0.44              |
| 20:S:132:GLU:O    | 20:S:136:LYS:HG2  | 2.18                     | 0.44              |
| 25:S:303:CLA:H93  | 25:S:303:CLA:H111 | 1.53                     | 0.44              |
| 25:G:610:CLA:C5   | 39:G:615:LUT:H30  | 2.41                     | 0.44              |
| 21:N:75:PRO:HG3   | 21:N:212:LYS:HB3  | 1.98                     | 0.44              |
| 21:Y:60:GLY:HA3   | 24:Y:302:CHL:CMC  | 2.28                     | 0.44              |
| 26:6:606:LHG:H152 | 26:6:606:LHG:H301 | 1.99                     | 0.44              |
| 4:a:157:VAL:CG1   | 4:a:172:MET:HB2   | 2.47                     | 0.44              |
| 13:l:18:LEU:HD11  | 14:m:23:LEU:HD23  | 1.99                     | 0.44              |
| 15:o:145:VAL:HG11 | 15:o:203:LEU:HD21 | 2.00                     | 0.44              |
| 20:s:236:MET:CE   | 39:s:316:LUT:H12  | 2.33                     | 0.44              |
| 20:s:237:LEU:O    | 20:s:241:ILE:CD1  | 2.65                     | 0.44              |
| 21:g:80:TRP:CE3   | 39:g:616:LUT:H383 | 2.52                     | 0.44              |
| 24:g:606:CHL:HBB1 | 39:g:616:LUT:C16  | 2.47                     | 0.44              |
| 21:n:209:ALA:HA   | 21:n:212:LYS:CG   | 2.34                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:n:612:CLA:HHC  | 25:n:612:CLA:CBB  | 2.44                     | 0.44              |
| 25:y:304:CLA:H122 | 25:y:304:CLA:H91  | 1.99                     | 0.44              |
| 25:y:311:CLA:C5   | 25:y:313:CLA:HMA1 | 2.28                     | 0.44              |
| 1:1:225:SER:O     | 1:1:229:PHE:HD1   | 2.01                     | 0.44              |
| 2:2:251:ASN:N     | 2:2:252:PRO:CD    | 2.81                     | 0.44              |
| 1:3:159:LEU:HD13  | 1:3:159:LEU:N     | 2.33                     | 0.44              |
| 3:4:73:LEU:HD12   | 3:4:80:ASP:OD1    | 2.18                     | 0.44              |
| 3:4:171:SER:HB3   | 3:4:183:GLU:OE2   | 2.18                     | 0.44              |
| 3:4:184:ASN:OD1   | 3:4:197:GLY:HA3   | 2.18                     | 0.44              |
| 5:B:41:GLU:HB3    | 5:B:63:ILE:HD11   | 1.99                     | 0.44              |
| 5:B:377:VAL:O     | 5:B:378:ARG:HB2   | 2.17                     | 0.44              |
| 25:B:610:CLA:HMA2 | 25:B:610:CLA:HBA1 | 1.99                     | 0.44              |
| 25:C:504:CLA:H91  | 25:C:504:CLA:H111 | 1.70                     | 0.44              |
| 7:D:181:ARG:NH1   | 7:D:334:ASP:OD1   | 2.51                     | 0.44              |
| 25:D:401:CLA:HMA2 | 30:D:407:LMG:H212 | 1.99                     | 0.44              |
| 26:D:406:LHG:H302 | 16:T:21:ILE:HD11  | 1.99                     | 0.44              |
| 12:K:39:VAL:O     | 12:K:42:VAL:HG22  | 2.17                     | 0.44              |
| 21:G:50:TRP:HB3   | 21:G:213:VAL:HG21 | 1.98                     | 0.44              |
| 21:G:226:MET:O    | 21:G:230:PHE:HD2  | 2.01                     | 0.44              |
| 21:N:113:CYS:HB3  | 21:N:131:TRP:CD1  | 2.53                     | 0.44              |
| 21:N:226:MET:O    | 21:N:230:PHE:HD2  | 2.01                     | 0.44              |
| 24:N:601:CHL:HBA1 | 24:N:601:CHL:H3A  | 1.62                     | 0.44              |
| 25:N:613:CLA:CBC  | 25:N:613:CLA:CMC  | 2.95                     | 0.44              |
| 21:Y:215:GLU:CG   | 25:Y:311:CLA:C1B  | 2.95                     | 0.44              |
| 21:Y:226:MET:O    | 21:Y:230:PHE:HD2  | 2.01                     | 0.44              |
| 22:R:103:LYS:CD   | 22:R:105:LEU:HD11 | 2.47                     | 0.44              |
| 1:5:113:CYS:HB3   | 1:5:131:TRP:CD1   | 2.53                     | 0.44              |
| 1:5:226:MET:O     | 1:5:230:PHE:HD2   | 2.01                     | 0.44              |
| 4:a:57:PRO:O      | 15:o:208:ARG:NH1  | 2.49                     | 0.44              |
| 25:c:506:CLA:H193 | 25:c:506:CLA:H161 | 1.70                     | 0.44              |
| 7:d:201:GLY:O     | 7:d:205:VAL:HG23  | 2.18                     | 0.44              |
| 11:i:24:LEU:HD12  | 28:i:101:BCR:C3   | 2.47                     | 0.44              |
| 21:y:196:PHE:HE2  | 24:y:309:CHL:HBC2 | 1.83                     | 0.44              |
| 25:y:304:CLA:HMD1 | 24:y:310:CHL:C1D  | 2.47                     | 0.44              |
| 25:y:313:CLA:HAA2 | 25:y:313:CLA:HBD  | 2.00                     | 0.44              |
| 40:y:318:NEX:H27  | 40:y:318:NEX:H381 | 1.91                     | 0.44              |
| 22:r:177:SER:HB2  | 24:r:605:CHL:HMD3 | 1.99                     | 0.44              |
| 29:A:407:SQD:H45  | 29:A:407:SQD:H81  | 1.64                     | 0.44              |
| 5:B:168:VAL:HG21  | 5:B:181:VAL:HG12  | 2.00                     | 0.44              |
| 5:B:357:ARG:NH2   | 23:U:96:PRO:HG2   | 2.33                     | 0.44              |
| 25:B:607:CLA:HMB1 | 25:B:607:CLA:CBB  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:608:CLA:H122 | 7:D:121:PHE:CZ    | 2.53                     | 0.44              |
| 28:B:619:BCR:H24C | 28:B:619:BCR:H371 | 1.79                     | 0.44              |
| 25:C:505:CLA:H3A  | 25:C:505:CLA:HBA2 | 1.74                     | 0.44              |
| 25:C:510:CLA:HMA2 | 25:C:510:CLA:C1   | 2.48                     | 0.44              |
| 7:D:229:GLY:O     | 7:D:230:ALA:HB3   | 2.18                     | 0.44              |
| 28:D:404:BCR:H403 | 30:D:407:LMG:H141 | 1.99                     | 0.44              |
| 12:K:58:VAL:HG12  | 12:K:61:ARG:CD    | 2.47                     | 0.44              |
| 15:O:114:CYS:SG   | 15:O:139:GLU:N    | 2.91                     | 0.44              |
| 20:S:95:TYR:CE1   | 24:S:302:CHL:HAA2 | 2.53                     | 0.44              |
| 40:S:317:NEX:H35  | 40:S:317:NEX:H401 | 1.77                     | 0.44              |
| 25:G:611:CLA:H142 | 25:G:611:CLA:H112 | 1.59                     | 0.44              |
| 21:N:57:LYS:HD2   | 21:N:63:SER:HB2   | 2.00                     | 0.44              |
| 21:N:69:TYR:OH    | 21:N:81:ASP:OD2   | 2.20                     | 0.44              |
| 21:N:215:GLU:HB2  | 25:N:610:CLA:CHB  | 2.48                     | 0.44              |
| 25:Y:303:CLA:HBB  | 25:Y:303:CLA:H12  | 1.99                     | 0.44              |
| 22:R:135:ARG:NE   | 25:R:614:CLA:OBD  | 2.51                     | 0.44              |
| 2:6:217:ILE:HD13  | 25:6:604:CLA:CGD  | 2.48                     | 0.44              |
| 2:6:223:ALA:O     | 2:6:226:SER:OG    | 2.32                     | 0.44              |
| 2:6:227:MET:HG3   | 2:6:231:PHE:CE2   | 2.53                     | 0.44              |
| 1:7:208:PHE:O     | 1:7:212:LYS:HG3   | 2.18                     | 0.44              |
| 1:7:226:MET:O     | 1:7:230:PHE:HD2   | 2.01                     | 0.44              |
| 4:a:11:GLU:OE2    | 4:a:15:GLY:HA3    | 2.17                     | 0.44              |
| 4:a:161:TYR:HA    | 4:a:294:ALA:HB2   | 1.99                     | 0.44              |
| 5:b:359:MET:HA    | 5:b:360:PRO:HD3   | 1.86                     | 0.44              |
| 25:c:505:CLA:H3A  | 25:c:505:CLA:HBA2 | 1.74                     | 0.44              |
| 25:c:510:CLA:H141 | 25:c:510:CLA:H161 | 1.67                     | 0.44              |
| 7:d:193:THR:HG23  | 25:d:402:CLA:HBC2 | 1.99                     | 0.44              |
| 25:d:403:CLA:H52  | 18:x:91:ALA:HB1   | 1.98                     | 0.44              |
| 10:h:54:LEU:O     | 10:h:57:ILE:HG12  | 2.18                     | 0.44              |
| 20:s:266:LEU:HD22 | 25:s:313:CLA:H43  | 2.00                     | 0.44              |
| 21:g:86:SER:OG    | 25:g:602:CLA:HAA2 | 2.18                     | 0.44              |
| 21:g:163:ALA:O    | 21:g:167:ILE:HG13 | 2.17                     | 0.44              |
| 21:n:244:LEU:HD11 | 25:n:614:CLA:HAC1 | 2.00                     | 0.44              |
| 24:n:601:CHL:CMD  | 26:n:618:LHG:HC41 | 2.48                     | 0.44              |
| 21:y:50:TRP:NE1   | 25:y:312:CLA:HED3 | 2.33                     | 0.44              |
| 21:y:226:MET:O    | 21:y:230:PHE:HD2  | 2.01                     | 0.44              |
| 21:y:244:LEU:CD1  | 25:y:315:CLA:HBC2 | 2.48                     | 0.44              |
| 25:y:314:CLA:H122 | 25:y:315:CLA:HMD2 | 2.00                     | 0.44              |
| 1:1:50:TRP:HB3    | 1:1:213:VAL:HG21  | 1.98                     | 0.43              |
| 1:1:126:PHE:HE1   | 1:1:147:LEU:HA    | 1.83                     | 0.43              |
| 2:2:100:VAL:CG1   | 2:2:190:LEU:HD23  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:217:ILE:CD1   | 25:2:604:CLA:CGD  | 2.97                     | 0.43              |
| 3:4:222:GLU:HA    | 3:4:225:LYS:HD3   | 1.99                     | 0.43              |
| 4:A:40:THR:O      | 4:A:43:THR:HG22   | 2.18                     | 0.43              |
| 25:A:402:CLA:H91  | 31:D:405:PL9:H402 | 2.00                     | 0.43              |
| 25:B:615:CLA:HMA2 | 25:B:615:CLA:CBA  | 2.48                     | 0.43              |
| 28:C:514:BCR:H15C | 28:C:514:BCR:H351 | 1.87                     | 0.43              |
| 10:H:22:LEU:HD23  | 22:R:124:PHE:CZ   | 2.53                     | 0.43              |
| 13:L:18:LEU:HD11  | 14:M:23:LEU:HD23  | 1.99                     | 0.43              |
| 29:L:101:SQD:H261 | 14:M:21:PHE:HD1   | 1.83                     | 0.43              |
| 15:O:184:GLY:O    | 15:O:224:PRO:HD3  | 2.18                     | 0.43              |
| 15:O:224:PRO:O    | 15:O:289:VAL:HB   | 2.18                     | 0.43              |
| 20:S:119:ARG:HH11 | 25:S:310:CLA:C1D  | 2.30                     | 0.43              |
| 21:G:113:CYS:HB3  | 21:G:131:TRP:CD1  | 2.53                     | 0.43              |
| 21:G:225:SER:O    | 21:G:229:PHE:HD1  | 2.01                     | 0.43              |
| 21:N:232:GLN:HE21 | 25:N:613:CLA:CHA  | 2.17                     | 0.43              |
| 21:Y:208:PHE:O    | 21:Y:212:LYS:HG3  | 2.18                     | 0.43              |
| 21:Y:244:LEU:CD1  | 25:Y:315:CLA:HBC2 | 2.48                     | 0.43              |
| 25:R:602:CLA:HBC1 | 26:R:618:LHG:C28  | 2.47                     | 0.43              |
| 24:R:607:CHL:H3A  | 24:R:607:CHL:HBA2 | 1.60                     | 0.43              |
| 2:6:87:ALA:HA     | 2:6:92:PHE:CZ     | 2.53                     | 0.43              |
| 2:6:121:LYS:HD3   | 2:6:245:LEU:CD1   | 2.46                     | 0.43              |
| 2:6:173:VAL:HA    | 2:6:176:PHE:CG    | 2.53                     | 0.43              |
| 3:8:155:TRP:CZ2   | 25:r:601:CLA:HBB1 | 2.53                     | 0.43              |
| 3:8:189:THR:O     | 3:8:189:THR:HG23  | 2.18                     | 0.43              |
| 5:b:141:ILE:CG1   | 5:b:217:LEU:HD21  | 2.46                     | 0.43              |
| 25:b:604:CLA:H141 | 25:b:604:CLA:H161 | 1.83                     | 0.43              |
| 6:c:240:LEU:HD22  | 25:c:501:CLA:CAB  | 2.47                     | 0.43              |
| 25:c:510:CLA:HMA2 | 25:c:510:CLA:C1   | 2.48                     | 0.43              |
| 7:d:22:TRP:CZ2    | 18:x:105:VAL:HG11 | 2.53                     | 0.43              |
| 25:d:401:CLA:HMA2 | 30:d:407:LMG:H212 | 1.99                     | 0.43              |
| 10:h:43:MET:HE2   | 10:h:43:MET:HB3   | 1.91                     | 0.43              |
| 11:i:31:ASN:HB2   | 11:i:32:PRO:HD2   | 2.00                     | 0.43              |
| 29:l:102:SQD:H261 | 14:m:21:PHE:HD1   | 1.83                     | 0.43              |
| 15:o:128:PRO:HA   | 15:o:180:VAL:HG13 | 1.99                     | 0.43              |
| 15:o:224:PRO:O    | 15:o:289:VAL:HB   | 2.18                     | 0.43              |
| 16:t:11:VAL:HG22  | 28:t:101:BCR:H342 | 2.00                     | 0.43              |
| 20:s:132:GLU:O    | 20:s:136:LYS:HG2  | 2.18                     | 0.43              |
| 21:g:56:VAL:HG11  | 26:y:301:LHG:HC2  | 1.99                     | 0.43              |
| 25:n:603:CLA:HAB  | 39:n:616:LUT:C15  | 2.48                     | 0.43              |
| 21:y:206:GLU:N    | 21:y:206:GLU:CD   | 2.76                     | 0.43              |
| 22:r:103:LYS:CE   | 22:r:105:LEU:HD11 | 2.45                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:155:LEU:HD22 | 22:r:268:LEU:HD21 | 1.99                     | 0.43              |
| 1:1:163:ALA:O     | 1:1:167:ILE:HG13  | 2.17                     | 0.43              |
| 2:2:104:ARG:CZ    | 24:2:603:CHL:HED3 | 2.49                     | 0.43              |
| 27:A:404:PHO:HAB  | 25:D:402:CLA:H12  | 2.01                     | 0.43              |
| 31:A:409:PL9:O1   | 31:A:409:PL9:HC8  | 2.17                     | 0.43              |
| 5:B:193:PHE:HE2   | 35:B:626:DGD:HE2  | 1.83                     | 0.43              |
| 5:B:242:ILE:HG22  | 5:B:466:HIS:HB2   | 2.00                     | 0.43              |
| 25:B:609:CLA:H2   | 25:B:609:CLA:H61  | 1.72                     | 0.43              |
| 8:E:67:THR:HA     | 23:U:102:ARG:NH1  | 2.33                     | 0.43              |
| 11:I:19:PHE:CE2   | 11:I:23:PHE:HE2   | 2.36                     | 0.43              |
| 15:O:158:PHE:HE2  | 15:O:306:LEU:HD22 | 1.83                     | 0.43              |
| 28:T:101:BCR:H271 | 5:b:39:LEU:HD12   | 1.99                     | 0.43              |
| 21:G:126:PHE:HE1  | 21:G:147:LEU:HA   | 1.83                     | 0.43              |
| 24:G:601:CHL:HBC1 | 26:Y:301:LHG:O3   | 2.18                     | 0.43              |
| 21:N:97:GLU:CB    | 21:N:190:LEU:HD11 | 2.48                     | 0.43              |
| 21:N:182:PRO:CB   | 40:N:617:NEX:H171 | 2.43                     | 0.43              |
| 21:Y:196:PHE:HE2  | 24:Y:309:CHL:HBC2 | 1.83                     | 0.43              |
| 21:Y:215:GLU:OE1  | 25:Y:311:CLA:C4A  | 2.66                     | 0.43              |
| 22:R:127:TYR:CE2  | 22:R:135:ARG:HD2  | 2.54                     | 0.43              |
| 22:R:274:HIS:HD1  | 25:R:612:CLA:HAA2 | 1.79                     | 0.43              |
| 25:R:612:CLA:H61  | 25:R:612:CLA:H92  | 1.56                     | 0.43              |
| 2:6:86:SER:O      | 2:6:88:ASP:N      | 2.51                     | 0.43              |
| 2:6:197:PHE:C     | 2:6:199:PRO:HD2   | 2.43                     | 0.43              |
| 2:6:216:GLU:O     | 2:6:219:ASN:HB2   | 2.18                     | 0.43              |
| 1:7:57:LYS:HD2    | 1:7:63:SER:HB2    | 2.00                     | 0.43              |
| 1:7:206:GLU:N     | 1:7:206:GLU:CD    | 2.76                     | 0.43              |
| 1:7:209:ALA:CA    | 1:7:212:LYS:HG3   | 2.34                     | 0.43              |
| 3:8:219:GLU:O     | 3:8:223:ARG:HB2   | 2.18                     | 0.43              |
| 4:a:106:LEU:HD11  | 28:a:407:BCR:H402 | 2.00                     | 0.43              |
| 4:a:276:ALA:O     | 4:a:280:VAL:HG23  | 2.18                     | 0.43              |
| 5:b:361:THR:HG22  | 42:b:701:HOH:O    | 2.17                     | 0.43              |
| 25:b:611:CLA:H112 | 25:b:611:CLA:H72  | 1.67                     | 0.43              |
| 25:b:611:CLA:HMA1 | 25:b:612:CLA:CMC  | 2.48                     | 0.43              |
| 6:c:236:GLY:HA2   | 6:c:239:TRP:CD1   | 2.52                     | 0.43              |
| 7:d:140:ARG:NH1   | 7:d:142:TYR:CE2   | 2.86                     | 0.43              |
| 26:d:406:LHG:H221 | 16:t:10:LEU:HD22  | 2.00                     | 0.43              |
| 8:e:67:THR:HA     | 23:u:102:ARG:NH1  | 2.33                     | 0.43              |
| 20:s:70:PHE:CG    | 20:s:95:TYR:HB2   | 2.53                     | 0.43              |
| 25:g:611:CLA:HHC  | 25:g:611:CLA:CBB  | 2.36                     | 0.43              |
| 25:g:613:CLA:H91  | 26:y:301:LHG:H322 | 1.99                     | 0.43              |
| 21:n:101:ILE:O    | 21:n:105:TRP:HD1  | 2.02                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:y:225:SER:O    | 21:y:229:PHE:HD1  | 2.01                     | 0.43              |
| 25:y:303:CLA:HBB  | 25:y:303:CLA:H12  | 2.00                     | 0.43              |
| 2:2:57:LYS:CD     | 2:2:63:SER:OG     | 2.66                     | 0.43              |
| 2:2:66:THR:CG2    | 2:2:67:PRO:HD2    | 2.48                     | 0.43              |
| 25:2:604:CLA:H3A  | 3:4:178:TRP:CB    | 2.48                     | 0.43              |
| 6:C:112:PHE:HE2   | 28:C:514:BCR:HC31 | 1.84                     | 0.43              |
| 6:C:294:ASN:OD1   | 35:C:515:DGD:HE4  | 2.17                     | 0.43              |
| 25:C:510:CLA:H91  | 25:C:510:CLA:H111 | 1.69                     | 0.43              |
| 7:D:343:PRO:O     | 7:D:346:VAL:HG22  | 2.17                     | 0.43              |
| 29:L:101:SQD:H462 | 14:M:28:LYS:HD2   | 1.98                     | 0.43              |
| 15:O:209:VAL:CG2  | 15:O:319:LYS:HD2  | 2.48                     | 0.43              |
| 20:S:224:LYS:HG2  | 25:S:311:CLA:CED  | 2.47                     | 0.43              |
| 21:N:162:TRP:CE3  | 21:Y:257:TRP:HH2  | 2.37                     | 0.43              |
| 21:N:244:LEU:HD11 | 25:N:614:CLA:HAC1 | 2.00                     | 0.43              |
| 21:Y:56:VAL:HB    | 24:Y:302:CHL:HBC2 | 1.98                     | 0.43              |
| 22:R:141:LEU:HD23 | 22:R:216:LEU:HB3  | 1.98                     | 0.43              |
| 1:5:57:LYS:HD2    | 1:5:63:SER:HB2    | 2.00                     | 0.43              |
| 2:6:217:ILE:CD1   | 25:6:604:CLA:CGD  | 2.97                     | 0.43              |
| 3:8:73:LEU:HD12   | 3:8:80:ASP:OD1    | 2.18                     | 0.43              |
| 3:8:79:GLY:N      | 3:8:229:ILE:HD13  | 2.33                     | 0.43              |
| 3:8:104:ILE:H     | 3:8:104:ILE:HD12  | 1.84                     | 0.43              |
| 3:8:140:PHE:HA    | 22:r:280:HIS:CD2  | 2.54                     | 0.43              |
| 4:a:231:GLU:HG2   | 5:b:1:MET:CA      | 2.45                     | 0.43              |
| 4:a:238:ARG:O     | 4:a:241:GLN:HB3   | 2.17                     | 0.43              |
| 5:b:122:ILE:HA    | 10:h:24:LYS:HD3   | 1.99                     | 0.43              |
| 25:b:603:CLA:C4B  | 25:b:605:CLA:H93  | 2.48                     | 0.43              |
| 25:b:609:CLA:H61  | 25:b:609:CLA:H2   | 1.72                     | 0.43              |
| 28:b:617:BCR:H15C | 28:b:617:BCR:H351 | 1.81                     | 0.43              |
| 7:d:157:VAL:HG12  | 7:d:172:PRO:CG    | 2.47                     | 0.43              |
| 11:i:19:PHE:CE2   | 11:i:23:PHE:HE2   | 2.36                     | 0.43              |
| 21:n:57:LYS:HD2   | 21:n:63:SER:HB2   | 2.00                     | 0.43              |
| 21:n:221:LEU:CD1  | 26:n:618:LHG:H272 | 2.48                     | 0.43              |
| 21:n:226:MET:O    | 21:n:230:PHE:HD2  | 2.01                     | 0.43              |
| 24:n:607:CHL:H18  | 24:n:609:CHL:C7   | 2.39                     | 0.43              |
| 25:n:613:CLA:CBC  | 25:n:613:CLA:CMC  | 2.95                     | 0.43              |
| 24:y:302:CHL:HHC  | 24:y:302:CHL:HBB1 | 1.98                     | 0.43              |
| 25:r:601:CLA:C1B  | 26:r:618:LHG:H112 | 2.49                     | 0.43              |
| 25:r:602:CLA:HBC1 | 26:r:618:LHG:H282 | 2.00                     | 0.43              |
| 1:1:101:ILE:O     | 1:1:105:TRP:HD1   | 2.02                     | 0.43              |
| 1:1:226:MET:O     | 1:1:230:PHE:HD2   | 2.01                     | 0.43              |
| 3:4:221:LEU:CA    | 3:4:224:LEU:HD23  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:135:PHE:CE2   | 6:C:449:ARG:HD3   | 2.52                     | 0.43              |
| 5:B:217:LEU:HB3   | 25:R:614:CLA:HBA1 | 2.00                     | 0.43              |
| 7:D:119:GLY:O     | 7:D:123:LEU:HG    | 2.18                     | 0.43              |
| 21:N:209:ALA:HA   | 21:N:212:LYS:CG   | 2.34                     | 0.43              |
| 21:Y:59:LEU:CD2   | 24:Y:302:CHL:C2B  | 2.94                     | 0.43              |
| 21:Y:97:GLU:CB    | 21:Y:190:LEU:HD11 | 2.48                     | 0.43              |
| 25:Y:304:CLA:H101 | 25:Y:304:CLA:H62  | 1.40                     | 0.43              |
| 24:Y:308:CHL:HBC2 | 24:Y:308:CHL:CHD  | 2.37                     | 0.43              |
| 25:R:603:CLA:CMC  | 41:R:616:XAT:H203 | 2.49                     | 0.43              |
| 41:R:616:XAT:H35  | 41:R:616:XAT:H401 | 1.60                     | 0.43              |
| 1:5:101:ILE:O     | 1:5:105:TRP:HD1   | 2.02                     | 0.43              |
| 1:5:159:LEU:HD13  | 1:5:159:LEU:N     | 2.33                     | 0.43              |
| 1:5:208:PHE:O     | 1:5:212:LYS:HG3   | 2.18                     | 0.43              |
| 2:6:57:LYS:CD     | 2:6:63:SER:OG     | 2.66                     | 0.43              |
| 2:6:174:GLU:OE2   | 1:7:59:LEU:HD22   | 2.19                     | 0.43              |
| 2:6:202:LEU:O     | 2:6:208:THR:HG22  | 2.19                     | 0.43              |
| 2:6:204:ASP:O     | 2:6:208:THR:N     | 2.45                     | 0.43              |
| 3:8:130:ALA:O     | 3:8:134:PRO:HD3   | 2.18                     | 0.43              |
| 3:8:231:HIS:HA    | 3:8:234:LEU:HD21  | 2.00                     | 0.43              |
| 4:a:74:GLY:CA     | 14:m:1:MET:HE2    | 2.49                     | 0.43              |
| 5:b:245:VAL:HG21  | 25:b:612:CLA:HED3 | 1.99                     | 0.43              |
| 5:b:346:PHE:O     | 5:b:353:GLU:HA    | 2.18                     | 0.43              |
| 5:b:387:GLU:O     | 7:d:345:GLU:CD    | 2.62                     | 0.43              |
| 25:b:607:CLA:H62  | 25:b:607:CLA:H93  | 1.51                     | 0.43              |
| 25:b:613:CLA:HMD2 | 28:b:618:BCR:H341 | 2.00                     | 0.43              |
| 25:b:615:CLA:HMA2 | 25:b:615:CLA:CBA  | 2.48                     | 0.43              |
| 6:c:204:LEU:C     | 6:c:239:TRP:HZ2   | 2.26                     | 0.43              |
| 7:d:90:LEU:O      | 7:d:92:LEU:N      | 2.49                     | 0.43              |
| 7:d:119:GLY:O     | 7:d:123:LEU:HG    | 2.18                     | 0.43              |
| 7:d:181:ARG:NH1   | 7:d:334:ASP:OD1   | 2.51                     | 0.43              |
| 15:o:114:CYS:SG   | 15:o:139:GLU:N    | 2.91                     | 0.43              |
| 21:g:159:LEU:HD13 | 21:g:159:LEU:N    | 2.33                     | 0.43              |
| 24:n:607:CHL:CBB  | 24:y:302:CHL:H91  | 2.48                     | 0.43              |
| 21:y:244:LEU:CD2  | 39:y:316:LUT:H163 | 2.47                     | 0.43              |
| 25:y:314:CLA:C4B  | 39:y:316:LUT:H183 | 2.49                     | 0.43              |
| 25:r:603:CLA:CMC  | 41:r:616:XAT:H203 | 2.49                     | 0.43              |
| 1:1:113:CYS:HB3   | 1:1:131:TRP:CD1   | 2.53                     | 0.43              |
| 1:1:137:GLN:HE22  | 1:1:144:LEU:HA    | 1.84                     | 0.43              |
| 2:2:88:ASP:O      | 2:2:92:PHE:N      | 2.50                     | 0.43              |
| 2:2:173:VAL:HA    | 2:2:176:PHE:CG    | 2.54                     | 0.43              |
| 1:3:97:GLU:CB     | 1:3:190:LEU:HD11  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:141:PRO:HG3   | 6:C:446:GLY:C     | 2.43                     | 0.43              |
| 25:A:405:CLA:H11  | 11:I:9:TYR:CZ     | 2.54                     | 0.43              |
| 6:C:274:TYR:HE1   | 25:C:505:CLA:O2D  | 2.01                     | 0.43              |
| 25:C:510:CLA:H193 | 25:C:510:CLA:H162 | 1.88                     | 0.43              |
| 7:D:65:ALA:CB     | 7:D:70:GLU:OE2    | 2.67                     | 0.43              |
| 7:D:217:ALA:O     | 7:D:221:ASN:ND2   | 2.47                     | 0.43              |
| 11:I:9:TYR:O      | 11:I:13:ILE:HG22  | 2.18                     | 0.43              |
| 14:M:1:MET:HB3    | 14:M:3:VAL:HG13   | 1.99                     | 0.43              |
| 15:O:174:ILE:HG12 | 15:O:195:ASP:OD1  | 2.19                     | 0.43              |
| 19:Z:16:SER:HB3   | 28:Z:101:BCR:H312 | 2.00                     | 0.43              |
| 25:S:313:CLA:H3A  | 25:S:313:CLA:HBA2 | 1.60                     | 0.43              |
| 21:G:56:VAL:HG11  | 26:Y:301:LHG:HC2  | 1.99                     | 0.43              |
| 21:G:57:LYS:HD2   | 21:G:63:SER:HB2   | 2.00                     | 0.43              |
| 21:G:208:PHE:O    | 21:G:212:LYS:HG3  | 2.18                     | 0.43              |
| 21:G:211:LEU:CB   | 25:G:610:CLA:HMA1 | 2.44                     | 0.43              |
| 40:G:617:NEX:C28  | 40:G:617:NEX:C36  | 2.95                     | 0.43              |
| 25:N:603:CLA:HAB  | 39:N:616:LUT:C15  | 2.48                     | 0.43              |
| 24:N:605:CHL:HHD  | 24:N:606:CHL:OBD  | 2.18                     | 0.43              |
| 21:Y:101:ILE:O    | 21:Y:105:TRP:HD1  | 2.01                     | 0.43              |
| 21:Y:126:PHE:HE1  | 21:Y:147:LEU:HA   | 1.83                     | 0.43              |
| 21:Y:177:VAL:HG21 | 24:Y:310:CHL:CMA  | 2.48                     | 0.43              |
| 22:R:72:LEU:HB3   | 22:R:137:ARG:HH22 | 1.83                     | 0.43              |
| 25:R:610:CLA:HBC3 | 26:R:618:LHG:C5   | 2.37                     | 0.43              |
| 2:6:178:ILE:HG22  | 2:6:180:GLY:H     | 1.84                     | 0.43              |
| 1:7:126:PHE:HE1   | 1:7:147:LEU:HA    | 1.84                     | 0.43              |
| 3:8:216:PRO:O     | 3:8:220:LYS:N     | 2.52                     | 0.43              |
| 4:a:141:PRO:HG3   | 6:c:446:GLY:C     | 2.43                     | 0.43              |
| 27:a:405:PHO:H193 | 25:d:401:CLA:CHB  | 2.49                     | 0.43              |
| 5:b:157:HIS:HE1   | 25:b:606:CLA:CHB  | 2.26                     | 0.43              |
| 5:b:276:ASP:OD1   | 5:b:361:THR:HG21  | 2.19                     | 0.43              |
| 5:b:382:PRO:CB    | 7:d:345:GLU:OE2   | 2.62                     | 0.43              |
| 25:b:614:CLA:H91  | 26:l:103:LHG:H372 | 2.00                     | 0.43              |
| 6:c:112:PHE:HE2   | 28:c:514:BCR:HC31 | 1.84                     | 0.43              |
| 6:c:227:VAL:CG2   | 28:i:101:BCR:H292 | 2.47                     | 0.43              |
| 9:f:18:HIS:HE1    | 38:f:101:HEM:C4A  | 2.37                     | 0.43              |
| 10:h:22:LEU:HD23  | 22:r:124:PHE:CZ   | 2.53                     | 0.43              |
| 15:o:158:PHE:HE2  | 15:o:306:LEU:HD22 | 1.83                     | 0.43              |
| 15:o:218:LEU:HD23 | 15:o:218:LEU:H    | 1.83                     | 0.43              |
| 21:g:208:PHE:O    | 21:g:212:LYS:HG3  | 2.18                     | 0.43              |
| 21:g:213:VAL:CG1  | 25:g:611:CLA:HED1 | 2.48                     | 0.43              |
| 25:g:613:CLA:H3A  | 25:g:613:CLA:HBA2 | 1.59                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:113:CYS:HB3  | 21:n:131:TRP:CD1  | 2.53                     | 0.43              |
| 24:n:605:CHL:HHD  | 24:n:606:CHL:OBD  | 2.18                     | 0.43              |
| 24:n:609:CHL:NC   | 24:y:302:CHL:H52  | 2.34                     | 0.43              |
| 21:y:80:TRP:O     | 39:y:317:LUT:H24  | 2.19                     | 0.43              |
| 21:y:101:ILE:O    | 21:y:105:TRP:HD1  | 2.01                     | 0.43              |
| 21:y:159:LEU:HD13 | 21:y:159:LEU:N    | 2.33                     | 0.43              |
| 21:y:215:GLU:OE1  | 25:y:311:CLA:C4A  | 2.66                     | 0.43              |
| 24:y:308:CHL:HBC2 | 24:y:308:CHL:CHD  | 2.36                     | 0.43              |
| 22:r:72:LEU:HB3   | 22:r:137:ARG:HH22 | 1.83                     | 0.43              |
| 26:2:606:LHG:H301 | 26:2:606:LHG:H152 | 1.99                     | 0.43              |
| 1:3:113:CYS:HB3   | 1:3:131:TRP:CD1   | 2.53                     | 0.43              |
| 1:3:206:GLU:N     | 1:3:206:GLU:CD    | 2.76                     | 0.43              |
| 3:4:79:GLY:N      | 3:4:229:ILE:HD13  | 2.33                     | 0.43              |
| 4:A:74:GLY:CA     | 14:M:1:MET:HE2    | 2.49                     | 0.43              |
| 4:A:192:ILE:HD13  | 25:A:401:CLA:C2D  | 2.49                     | 0.43              |
| 4:A:276:ALA:O     | 4:A:280:VAL:HG23  | 2.18                     | 0.43              |
| 25:B:613:CLA:HMD2 | 28:B:618:BCR:H341 | 2.00                     | 0.43              |
| 25:B:614:CLA:HMD2 | 29:L:101:SQD:H242 | 2.01                     | 0.43              |
| 25:B:616:CLA:H11  | 25:B:616:CLA:H51  | 1.75                     | 0.43              |
| 28:B:617:BCR:H382 | 28:B:617:BCR:H23C | 2.00                     | 0.43              |
| 25:C:502:CLA:H203 | 25:C:502:CLA:H161 | 1.84                     | 0.43              |
| 7:D:22:TRP:CZ2    | 18:X:105:VAL:HG11 | 2.53                     | 0.43              |
| 7:D:140:ARG:NH1   | 7:D:142:TYR:CE2   | 2.86                     | 0.43              |
| 25:D:402:CLA:HBC3 | 25:D:402:CLA:HHD  | 2.01                     | 0.43              |
| 8:E:56:PHE:HA     | 8:E:60:ARG:NH1    | 2.34                     | 0.43              |
| 10:H:43:MET:HE2   | 10:H:43:MET:HB3   | 1.91                     | 0.43              |
| 28:I:101:BCR:C8   | 28:I:101:BCR:H331 | 2.48                     | 0.43              |
| 15:O:92:LEU:HB3   | 15:O:96:GLU:CG    | 2.43                     | 0.43              |
| 20:S:189:ARG:NH2  | 25:S:309:CLA:HMA3 | 2.33                     | 0.43              |
| 20:S:236:MET:CE   | 39:S:316:LUT:H12  | 2.33                     | 0.43              |
| 20:S:266:LEU:HD22 | 25:S:313:CLA:H43  | 2.00                     | 0.43              |
| 21:G:115:PHE:HB2  | 25:G:604:CLA:HBC3 | 2.00                     | 0.43              |
| 21:G:213:VAL:CG1  | 25:G:611:CLA:HED1 | 2.48                     | 0.43              |
| 21:N:86:SER:OG    | 25:N:602:CLA:O1A  | 2.33                     | 0.43              |
| 1:5:97:GLU:CB     | 1:5:190:LEU:HD11  | 2.48                     | 0.43              |
| 2:6:118:VAL:O     | 2:6:122:TRP:HB2   | 2.19                     | 0.43              |
| 2:6:217:ILE:HG13  | 2:6:218:LYS:N     | 2.32                     | 0.43              |
| 2:6:251:ASN:N     | 2:6:252:PRO:CD    | 2.81                     | 0.43              |
| 1:7:113:CYS:HB3   | 1:7:131:TRP:CD1   | 2.53                     | 0.43              |
| 4:a:192:ILE:HD13  | 25:a:402:CLA:C2D  | 2.49                     | 0.43              |
| 5:b:168:VAL:HG21  | 5:b:181:VAL:HG12  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:b:356:VAL:O     | 5:b:356:VAL:HG13  | 2.19                     | 0.43              |
| 25:b:608:CLA:H61  | 25:b:608:CLA:H92  | 1.86                     | 0.43              |
| 25:c:502:CLA:HBA1 | 25:c:502:CLA:H3A  | 1.78                     | 0.43              |
| 8:e:67:THR:C      | 23:u:102:ARG:HH11 | 2.26                     | 0.43              |
| 20:s:95:TYR:CE1   | 24:s:302:CHL:HAA2 | 2.53                     | 0.43              |
| 21:g:57:LYS:HD2   | 21:g:63:SER:HB2   | 2.00                     | 0.43              |
| 21:g:126:PHE:HE1  | 21:g:147:LEU:HA   | 1.83                     | 0.43              |
| 21:g:231:VAL:HG21 | 25:g:613:CLA:HAC1 | 2.00                     | 0.43              |
| 21:n:132:PHE:HB2  | 24:n:607:CHL:HMA3 | 2.01                     | 0.43              |
| 21:n:165:GLN:NE2  | 24:n:606:CHL:NB   | 2.63                     | 0.43              |
| 21:y:209:ALA:CA   | 21:y:212:LYS:HG3  | 2.34                     | 0.43              |
| 21:y:215:GLU:HB2  | 25:y:311:CLA:C1B  | 2.49                     | 0.43              |
| 25:y:311:CLA:H122 | 39:y:316:LUT:H403 | 2.01                     | 0.43              |
| 22:r:135:ARG:NE   | 25:r:614:CLA:OBD  | 2.51                     | 0.43              |
| 2:2:87:ALA:HA     | 2:2:92:PHE:CZ     | 2.53                     | 0.43              |
| 2:2:202:LEU:O     | 2:2:208:THR:HG22  | 2.19                     | 0.43              |
| 2:2:227:MET:HG3   | 2:2:231:PHE:CE2   | 2.53                     | 0.43              |
| 1:3:101:ILE:O     | 1:3:105:TRP:HD1   | 2.02                     | 0.43              |
| 1:3:126:PHE:HE1   | 1:3:147:LEU:HA    | 1.84                     | 0.43              |
| 3:4:78:PRO:HB2    | 3:4:229:ILE:HG23  | 2.01                     | 0.43              |
| 4:A:136:ARG:NH2   | 11:I:27:ASP:OD2   | 2.48                     | 0.43              |
| 5:B:476:ARG:HG2   | 5:B:476:ARG:HH11  | 1.83                     | 0.43              |
| 6:C:75:PHE:O      | 12:K:25:LYS:HD3   | 2.18                     | 0.43              |
| 6:C:185:VAL:HG23  | 6:C:230:LEU:CD1   | 2.47                     | 0.43              |
| 25:C:512:CLA:C19  | 26:S:301:LHG:H222 | 2.48                     | 0.43              |
| 8:E:25:ILE:O      | 8:E:29:SER:OG     | 2.28                     | 0.43              |
| 28:I:101:BCR:H15C | 28:I:101:BCR:H351 | 1.84                     | 0.43              |
| 15:O:163:LEU:C    | 15:O:164:MET:HE2  | 2.44                     | 0.43              |
| 20:S:190:ILE:HG13 | 20:S:191:THR:HG23 | 1.99                     | 0.43              |
| 21:G:101:ILE:O    | 21:G:105:TRP:HD1  | 2.02                     | 0.43              |
| 21:G:206:GLU:N    | 21:G:206:GLU:CD   | 2.76                     | 0.43              |
| 24:N:609:CHL:H121 | 32:N:619:AJP:C01  | 2.48                     | 0.43              |
| 25:N:613:CLA:HBA1 | 25:N:614:CLA:CAD  | 2.49                     | 0.43              |
| 21:Y:113:CYS:HB3  | 21:Y:131:TRP:CD1  | 2.53                     | 0.43              |
| 25:Y:312:CLA:H92  | 25:Y:312:CLA:C5   | 2.49                     | 0.43              |
| 25:Y:313:CLA:HAA2 | 25:Y:313:CLA:HBD  | 2.00                     | 0.43              |
| 25:Y:314:CLA:H122 | 25:Y:315:CLA:HMD2 | 2.00                     | 0.43              |
| 25:Y:315:CLA:HED2 | 25:Y:315:CLA:CAA  | 2.48                     | 0.43              |
| 22:R:85:LYS:CG    | 22:R:86:PRO:CD    | 2.96                     | 0.43              |
| 25:6:604:CLA:H3A  | 3:8:178:TRP:CB    | 2.48                     | 0.43              |
| 3:8:203:LEU:HB3   | 3:8:205:LEU:HD13  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:606:CLA:H203 | 28:b:619:BCR:H363 | 2.00                     | 0.43              |
| 25:b:606:CLA:H172 | 25:b:616:CLA:H93  | 2.00                     | 0.43              |
| 25:c:512:CLA:C19  | 26:s:301:LHG:H222 | 2.48                     | 0.43              |
| 7:d:162:PRO:HG3   | 7:d:171:ALA:HB2   | 2.00                     | 0.43              |
| 11:i:9:TYR:O      | 11:i:13:ILE:HG22  | 2.18                     | 0.43              |
| 19:z:40:VAL:O     | 19:z:41:PHE:C     | 2.61                     | 0.43              |
| 20:s:91:GLY:O     | 20:s:230:ARG:NH1  | 2.37                     | 0.43              |
| 25:s:303:CLA:HAB  | 39:s:316:LUT:C30  | 2.44                     | 0.43              |
| 25:s:303:CLA:H52  | 25:s:303:CLA:H8   | 1.74                     | 0.43              |
| 21:g:97:GLU:HA    | 21:g:190:LEU:CD1  | 2.24                     | 0.43              |
| 21:g:97:GLU:CB    | 21:g:190:LEU:HD11 | 2.48                     | 0.43              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:CMB  | 2.49                     | 0.43              |
| 21:g:225:SER:O    | 21:g:229:PHE:HD1  | 2.01                     | 0.43              |
| 25:g:610:CLA:H72  | 25:g:610:CLA:H112 | 1.89                     | 0.43              |
| 21:n:208:PHE:O    | 21:n:212:LYS:HG3  | 2.18                     | 0.43              |
| 25:n:613:CLA:C14  | 25:n:613:CLA:H2   | 2.45                     | 0.43              |
| 21:y:80:TRP:HE3   | 25:y:303:CLA:CMD  | 2.30                     | 0.43              |
| 25:y:304:CLA:CMD  | 24:y:310:CHL:C4D  | 2.96                     | 0.43              |
| 22:r:150:ALA:CA   | 41:r:616:XAT:H181 | 2.48                     | 0.43              |
| 1:1:208:PHE:O     | 1:1:212:LYS:HG3   | 2.18                     | 0.43              |
| 3:4:130:ALA:O     | 3:4:134:PRO:HD3   | 2.18                     | 0.43              |
| 3:4:173:GLU:HG2   | 22:R:62:ALA:HB2   | 2.01                     | 0.43              |
| 4:A:11:GLU:OE2    | 4:A:15:GLY:HA3    | 2.17                     | 0.43              |
| 4:A:161:TYR:HA    | 4:A:294:ALA:HB2   | 1.99                     | 0.43              |
| 4:A:331:MET:HE3   | 7:D:321:LEU:HB3   | 1.99                     | 0.43              |
| 27:A:404:PHO:H193 | 25:D:401:CLA:CHB  | 2.49                     | 0.43              |
| 5:B:291:GLY:HA2   | 5:B:294:GLU:CD    | 2.44                     | 0.43              |
| 7:D:162:PRO:HG3   | 7:D:171:ALA:HB2   | 2.00                     | 0.43              |
| 7:D:193:THR:HG23  | 25:D:402:CLA:HBC2 | 1.99                     | 0.43              |
| 29:L:103:SQD:H281 | 29:L:103:SQD:C32  | 2.49                     | 0.43              |
| 20:S:135:ASN:HD21 | 20:S:141:CYS:CA   | 2.32                     | 0.43              |
| 21:G:137:GLN:HE22 | 21:G:144:LEU:HA   | 1.84                     | 0.43              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:HMB3 | 2.01                     | 0.43              |
| 21:G:215:GLU:HB2  | 25:G:610:CLA:CMB  | 2.49                     | 0.43              |
| 24:N:601:CHL:CMD  | 26:N:618:LHG:HC41 | 2.48                     | 0.43              |
| 21:Y:104:ARG:HB3  | 25:Y:311:CLA:HBC2 | 1.96                     | 0.43              |
| 24:Y:302:CHL:CMC  | 24:Y:302:CHL:HBC3 | 2.49                     | 0.43              |
| 25:Y:304:CLA:HMC3 | 25:Y:304:CLA:CBC  | 2.39                     | 0.43              |
| 25:Y:304:CLA:CMD  | 24:Y:310:CHL:C4D  | 2.96                     | 0.43              |
| 25:Y:304:CLA:H93  | 24:Y:310:CHL:H91  | 2.01                     | 0.43              |
| 24:Y:310:CHL:H92  | 24:Y:310:CHL:H62  | 1.85                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:101:ILE:O     | 1:7:105:TRP:HD1   | 2.02                     | 0.43              |
| 3:8:221:LEU:CA    | 3:8:224:LEU:HD23  | 2.48                     | 0.43              |
| 4:a:47:VAL:HG21   | 4:a:114:LEU:HD22  | 2.00                     | 0.43              |
| 4:a:142:TRP:CZ2   | 6:c:447:ARG:HG3   | 2.54                     | 0.43              |
| 5:b:204:ALA:CB    | 25:b:602:CLA:HAB  | 2.48                     | 0.43              |
| 28:b:618:BCR:H15C | 28:b:618:BCR:H351 | 1.83                     | 0.43              |
| 6:c:75:PHE:O      | 12:k:25:LYS:HD3   | 2.18                     | 0.43              |
| 6:c:319:VAL:HG23  | 6:c:322:GLN:HE21  | 1.84                     | 0.43              |
| 7:d:202:VAL:HG13  | 25:d:402:CLA:HBB1 | 2.01                     | 0.43              |
| 7:d:287:VAL:CG2   | 25:d:402:CLA:HED2 | 2.49                     | 0.43              |
| 8:e:56:PHE:HA     | 8:e:60:ARG:NH1    | 2.34                     | 0.43              |
| 29:l:101:SQD:H281 | 29:l:101:SQD:C32  | 2.49                     | 0.43              |
| 14:m:23:LEU:O     | 14:m:27:VAL:HG23  | 2.19                     | 0.43              |
| 25:s:303:CLA:H93  | 25:s:303:CLA:H111 | 1.53                     | 0.43              |
| 21:g:152:LEU:HD23 | 24:g:605:CHL:HED3 | 2.01                     | 0.43              |
| 24:n:606:CHL:HMB1 | 24:n:609:CHL:HAC1 | 2.01                     | 0.43              |
| 25:y:304:CLA:H93  | 24:y:310:CHL:H91  | 2.00                     | 0.43              |
| 25:r:603:CLA:H92  | 25:r:603:CLA:H61  | 1.72                     | 0.43              |
| 2:2:105:TRP:HD1   | 24:2:603:CHL:HED1 | 1.83                     | 0.43              |
| 2:2:126:ASP:C     | 2:2:148:LEU:HD21  | 2.42                     | 0.43              |
| 2:2:174:GLU:OE2   | 1:3:59:LEU:HD22   | 2.19                     | 0.43              |
| 2:2:216:GLU:O     | 2:2:219:ASN:HB2   | 2.19                     | 0.43              |
| 2:2:217:ILE:HG13  | 2:2:218:LYS:N     | 2.32                     | 0.43              |
| 1:3:226:MET:O     | 1:3:230:PHE:HD2   | 2.01                     | 0.43              |
| 4:A:106:LEU:HD11  | 28:A:406:BCR:H402 | 2.00                     | 0.43              |
| 5:B:51:VAL:HG13   | 5:B:308:LYS:HG2   | 1.95                     | 0.43              |
| 25:B:606:CLA:H203 | 28:B:619:BCR:H363 | 2.00                     | 0.43              |
| 25:B:608:CLA:CAB  | 7:D:124:ILE:HG12  | 2.49                     | 0.43              |
| 25:B:614:CLA:H61  | 25:B:614:CLA:H92  | 1.52                     | 0.43              |
| 28:B:618:BCR:H15C | 28:B:618:BCR:H351 | 1.83                     | 0.43              |
| 6:C:162:GLY:CA    | 6:C:248:GLY:HA2   | 2.48                     | 0.43              |
| 6:C:182:PHE:HE1   | 20:S:258:LEU:O    | 2.02                     | 0.43              |
| 6:C:298:PRO:O     | 6:C:299:SER:HB3   | 2.19                     | 0.43              |
| 6:C:399:ALA:HB1   | 6:C:400:PRO:HD2   | 2.01                     | 0.43              |
| 15:O:128:PRO:HA   | 15:O:180:VAL:HG13 | 1.99                     | 0.43              |
| 24:S:306:CHL:HBB1 | 39:S:316:LUT:C16  | 2.49                     | 0.43              |
| 24:G:601:CHL:HBA1 | 24:G:601:CHL:H3A  | 1.89                     | 0.43              |
| 21:N:159:LEU:HD13 | 21:N:159:LEU:N    | 2.33                     | 0.43              |
| 21:N:215:GLU:HB2  | 25:N:610:CLA:C1B  | 2.48                     | 0.43              |
| 25:N:613:CLA:CHB  | 39:N:615:LUT:H42  | 2.49                     | 0.43              |
| 21:Y:159:LEU:HD13 | 21:Y:159:LEU:N    | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Y:314:CLA:H141 | 25:Y:314:CLA:H162 | 1.53                     | 0.43              |
| 1:5:126:PHE:HE1   | 1:5:147:LEU:HA    | 1.84                     | 0.43              |
| 2:6:178:ILE:HD12  | 1:7:62:PHE:HA     | 1.97                     | 0.43              |
| 3:8:184:ASN:OD1   | 3:8:197:GLY:HA3   | 2.18                     | 0.43              |
| 3:8:228:GLU:O     | 3:8:229:ILE:C     | 2.61                     | 0.43              |
| 4:a:161:TYR:HA    | 4:a:294:ALA:HB1   | 2.00                     | 0.43              |
| 4:a:233:ALA:O     | 4:a:235:GLU:HG2   | 2.17                     | 0.43              |
| 25:a:406:CLA:H11  | 11:i:9:TYR:CZ     | 2.54                     | 0.43              |
| 25:b:607:CLA:C17  | 25:b:613:CLA:H161 | 2.28                     | 0.43              |
| 6:c:97:TRP:HE1    | 6:c:178:LYS:HE3   | 1.83                     | 0.43              |
| 6:c:273:SER:HB2   | 6:c:445:ALA:HB2   | 2.01                     | 0.43              |
| 25:c:510:CLA:H91  | 25:c:510:CLA:H111 | 1.69                     | 0.43              |
| 7:d:65:ALA:CB     | 7:d:70:GLU:OE2    | 2.67                     | 0.43              |
| 7:d:197:PHE:HA    | 7:d:200:MET:HE3   | 2.01                     | 0.43              |
| 7:d:268:LEU:HD23  | 7:d:268:LEU:C     | 2.44                     | 0.43              |
| 25:d:402:CLA:HBC3 | 25:d:402:CLA:HHD  | 2.01                     | 0.43              |
| 10:h:31:GLY:O     | 10:h:33:VAL:HG23  | 2.19                     | 0.43              |
| 21:g:101:ILE:O    | 21:g:105:TRP:HD1  | 2.02                     | 0.43              |
| 21:g:113:CYS:HB3  | 21:g:131:TRP:CD1  | 2.53                     | 0.43              |
| 21:g:127:GLY:C    | 21:g:137:GLN:HG3  | 2.44                     | 0.43              |
| 21:g:181:GLY:HA3  | 24:g:608:CHL:HMC  | 2.00                     | 0.43              |
| 24:g:609:CHL:HBA1 | 24:n:601:CHL:HBA2 | 2.00                     | 0.43              |
| 21:n:159:LEU:HD13 | 21:n:159:LEU:N    | 2.33                     | 0.43              |
| 25:n:610:CLA:H52  | 39:n:615:LUT:C30  | 2.49                     | 0.43              |
| 21:y:97:GLU:CB    | 21:y:190:LEU:HD11 | 2.48                     | 0.43              |
| 21:y:113:CYS:HB3  | 21:y:131:TRP:CD1  | 2.53                     | 0.43              |
| 21:y:121:ARG:HD2  | 21:y:241:ILE:HG22 | 2.01                     | 0.43              |
| 21:y:244:LEU:HD13 | 25:y:315:CLA:HBC2 | 2.00                     | 0.43              |
| 1:1:209:ALA:HA    | 1:1:212:LYS:CG    | 2.34                     | 0.43              |
| 2:2:86:SER:O      | 2:2:88:ASP:N      | 2.51                     | 0.43              |
| 4:A:279:PRO:O     | 4:A:283:ILE:HG12  | 2.19                     | 0.43              |
| 5:B:135:LEU:HD12  | 5:B:231:MET:O     | 2.19                     | 0.43              |
| 5:B:265:ILE:O     | 5:B:269:GLY:N     | 2.47                     | 0.43              |
| 25:B:603:CLA:C4B  | 25:B:605:CLA:H93  | 2.48                     | 0.43              |
| 6:C:204:LEU:C     | 6:C:239:TRP:HZ2   | 2.26                     | 0.43              |
| 6:C:319:VAL:HG23  | 6:C:322:GLN:HE21  | 1.84                     | 0.43              |
| 26:C:517:LHG:H332 | 26:C:517:LHG:H362 | 1.68                     | 0.43              |
| 9:F:18:HIS:HE1    | 38:F:101:HEM:C4A  | 2.37                     | 0.43              |
| 12:K:30:TYR:CZ    | 19:Z:5:PHE:HZ     | 2.36                     | 0.43              |
| 18:X:96:VAL:O     | 18:X:100:ILE:HG23 | 2.19                     | 0.43              |
| 25:S:303:CLA:H112 | 25:S:304:CLA:CMB  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:172:VAL:HG13 | 24:G:608:CHL:C1B  | 2.49                     | 0.43              |
| 24:G:601:CHL:H72  | 24:G:601:CHL:H111 | 1.62                     | 0.43              |
| 25:G:602:CLA:H72  | 25:G:602:CLA:H111 | 1.45                     | 0.43              |
| 24:G:609:CHL:H2   | 24:G:609:CHL:H61  | 1.73                     | 0.43              |
| 25:G:610:CLA:H62  | 25:G:612:CLA:CMA  | 2.49                     | 0.43              |
| 21:N:101:ILE:O    | 21:N:105:TRP:HD1  | 2.02                     | 0.43              |
| 21:N:215:GLU:CG   | 25:N:610:CLA:C1B  | 2.97                     | 0.43              |
| 21:Y:137:GLN:HE22 | 21:Y:144:LEU:HA   | 1.84                     | 0.43              |
| 21:Y:182:PRO:HB3  | 40:Y:318:NEX:C18  | 2.49                     | 0.43              |
| 22:R:258:VAL:HG12 | 25:R:612:CLA:HMD2 | 2.01                     | 0.43              |
| 25:R:601:CLA:C1B  | 26:R:618:LHG:H112 | 2.49                     | 0.43              |
| 25:R:611:CLA:HAB  | 39:R:615:LUT:C15  | 2.49                     | 0.43              |
| 2:6:219:ASN:O     | 2:6:220:GLY:C     | 2.61                     | 0.43              |
| 4:a:40:THR:CG2    | 25:a:406:CLA:HBB1 | 2.48                     | 0.43              |
| 29:a:408:SQD:H441 | 7:d:233:PHE:CD2   | 2.54                     | 0.43              |
| 5:b:336:ILE:O     | 5:b:336:ILE:CG2   | 2.67                     | 0.43              |
| 6:c:179:ALA:HA    | 6:c:185:VAL:HG13  | 2.01                     | 0.43              |
| 6:c:227:VAL:HG11  | 6:c:233:ILE:CG1   | 2.49                     | 0.43              |
| 28:i:101:BCR:C8   | 28:i:101:BCR:H331 | 2.48                     | 0.43              |
| 14:m:27:VAL:HA    | 14:m:30:VAL:HG22  | 2.00                     | 0.43              |
| 15:o:307:GLN:HG3  | 15:o:321:VAL:CG1  | 2.49                     | 0.43              |
| 19:z:16:SER:HB3   | 28:z:101:BCR:H312 | 2.00                     | 0.43              |
| 20:s:83:GLU:HG3   | 20:s:85:LEU:HD13  | 2.01                     | 0.43              |
| 20:s:248:GLU:CD   | 20:s:252:GLU:HG3  | 2.44                     | 0.43              |
| 21:g:132:PHE:CB   | 24:g:607:CHL:HMA3 | 2.41                     | 0.43              |
| 25:n:603:CLA:HBC2 | 24:n:609:CHL:HMD2 | 2.00                     | 0.43              |
| 21:y:126:PHE:HE1  | 21:y:147:LEU:HA   | 1.83                     | 0.43              |
| 21:y:182:PRO:HB3  | 40:y:318:NEX:C18  | 2.49                     | 0.43              |
| 22:r:103:LYS:CG   | 22:r:105:LEU:HD11 | 2.49                     | 0.43              |
| 22:r:253:PHE:CE2  | 41:r:616:XAT:H10  | 2.54                     | 0.43              |
| 25:r:602:CLA:HBC1 | 26:r:618:LHG:C28  | 2.48                     | 0.43              |
| 1:1:97:GLU:CB     | 1:1:190:LEU:HD11  | 2.48                     | 0.42              |
| 1:3:225:SER:O     | 1:3:229:PHE:HD1   | 2.01                     | 0.42              |
| 4:A:199:MET:SD    | 25:D:401:CLA:HED2 | 2.59                     | 0.42              |
| 5:B:242:ILE:O     | 5:B:246:PHE:CD1   | 2.72                     | 0.42              |
| 5:B:276:ASP:OD1   | 5:B:361:THR:HG21  | 2.19                     | 0.42              |
| 5:B:387:GLU:O     | 7:D:345:GLU:CD    | 2.62                     | 0.42              |
| 25:B:611:CLA:H61  | 25:B:611:CLA:H2   | 1.78                     | 0.42              |
| 6:C:221:GLU:CD    | 17:W:91:GLY:HA2   | 2.44                     | 0.42              |
| 6:C:321:ASP:OD2   | 6:C:340:TYR:OH    | 2.27                     | 0.42              |
| 20:S:83:GLU:HG3   | 20:S:85:LEU:HD13  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:159:LEU:HD13 | 21:G:159:LEU:N    | 2.33                     | 0.42              |
| 24:G:601:CHL:H8   | 24:G:601:CHL:H52  | 1.69                     | 0.42              |
| 40:G:617:NEX:H381 | 40:G:617:NEX:H27  | 1.63                     | 0.42              |
| 24:N:607:CHL:CBB  | 24:Y:302:CHL:H91  | 2.48                     | 0.42              |
| 24:N:608:CHL:H203 | 24:N:608:CHL:H161 | 1.84                     | 0.42              |
| 21:Y:244:LEU:HD13 | 25:Y:315:CLA:HBC2 | 2.00                     | 0.42              |
| 1:5:151:SER:O     | 24:5:301:CHL:HMA3 | 2.19                     | 0.42              |
| 3:8:173:GLU:HG2   | 22:r:62:ALA:HB2   | 2.01                     | 0.42              |
| 3:8:241:ILE:O     | 3:8:245:GLU:HG2   | 2.19                     | 0.42              |
| 4:a:199:MET:SD    | 25:d:401:CLA:HED2 | 2.59                     | 0.42              |
| 4:a:329:GLU:OE1   | 4:a:332:HIS:NE2   | 2.52                     | 0.42              |
| 27:a:405:PHO:HAB  | 25:d:402:CLA:H12  | 2.01                     | 0.42              |
| 5:b:188:GLU:OE1   | 10:h:68:ASP:HB3   | 2.19                     | 0.42              |
| 28:b:619:BCR:H20C | 28:b:619:BCR:H361 | 1.80                     | 0.42              |
| 6:c:267:SER:CA    | 17:w:133:LEU:HD23 | 2.47                     | 0.42              |
| 6:c:274:TYR:HE1   | 25:c:505:CLA:O2D  | 2.01                     | 0.42              |
| 6:c:298:PRO:O     | 6:c:299:SER:HB3   | 2.19                     | 0.42              |
| 25:c:504:CLA:H61  | 25:c:504:CLA:H41  | 1.49                     | 0.42              |
| 15:o:100:LYS:CE   | 15:o:105:VAL:HG22 | 2.48                     | 0.42              |
| 19:z:61:ILE:HG13  | 19:z:62:SER:N     | 2.34                     | 0.42              |
| 24:s:307:CHL:HBA1 | 24:s:307:CHL:H3A  | 1.26                     | 0.42              |
| 26:s:318:LHG:H372 | 26:s:318:LHG:H342 | 1.86                     | 0.42              |
| 21:n:215:GLU:HB2  | 25:n:610:CLA:C1B  | 2.48                     | 0.42              |
| 25:n:610:CLA:C5   | 39:n:615:LUT:H30  | 2.48                     | 0.42              |
| 25:y:311:CLA:H61  | 25:y:311:CLA:H92  | 1.82                     | 0.42              |
| 25:r:603:CLA:HMB2 | 25:r:603:CLA:H143 | 1.94                     | 0.42              |
| 25:r:611:CLA:HAB  | 39:r:615:LUT:C15  | 2.49                     | 0.42              |
| 1:1:145:ASP:OD2   | 1:1:150:PRO:HA    | 2.19                     | 0.42              |
| 2:2:178:ILE:HG22  | 2:2:180:GLY:H     | 1.84                     | 0.42              |
| 2:2:249:LEU:HD12  | 2:2:250:ASP:HB2   | 2.00                     | 0.42              |
| 1:3:57:LYS:HD2    | 1:3:63:SER:HB2    | 2.00                     | 0.42              |
| 1:3:210:GLU:OE1   | 1:3:214:LYS:NZ    | 2.38                     | 0.42              |
| 4:A:47:VAL:HG21   | 4:A:114:LEU:HD22  | 1.99                     | 0.42              |
| 4:A:161:TYR:HA    | 4:A:294:ALA:HB1   | 2.00                     | 0.42              |
| 29:A:407:SQD:H441 | 7:D:233:PHE:CD2   | 2.54                     | 0.42              |
| 25:B:607:CLA:H62  | 25:B:607:CLA:H93  | 1.51                     | 0.42              |
| 25:B:610:CLA:HHC  | 25:B:610:CLA:HBB1 | 2.01                     | 0.42              |
| 25:B:614:CLA:H91  | 26:L:102:LHG:H372 | 2.00                     | 0.42              |
| 6:C:251:HIS:HE1   | 25:C:506:CLA:HMA3 | 1.80                     | 0.42              |
| 7:D:268:LEU:HD23  | 7:D:268:LEU:C     | 2.44                     | 0.42              |
| 7:D:287:VAL:CG2   | 25:D:402:CLA:HED2 | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:54:LEU:O     | 10:H:57:ILE:HG12  | 2.18                     | 0.42              |
| 11:I:31:ASN:HB2   | 11:I:32:PRO:HD2   | 2.00                     | 0.42              |
| 29:L:103:SQD:H131 | 29:L:103:SQD:H102 | 1.47                     | 0.42              |
| 15:O:286:THR:O    | 15:O:286:THR:HG23 | 2.19                     | 0.42              |
| 15:O:307:GLN:HG3  | 15:O:321:VAL:CG1  | 2.49                     | 0.42              |
| 20:S:70:PHE:CG    | 20:S:95:TYR:HB2   | 2.54                     | 0.42              |
| 24:N:607:CHL:H61  | 24:N:607:CHL:H41  | 1.93                     | 0.42              |
| 21:Y:228:GLY:O    | 21:Y:231:VAL:N    | 2.53                     | 0.42              |
| 1:5:137:GLN:HE22  | 1:5:144:LEU:HA    | 1.84                     | 0.42              |
| 2:6:223:ALA:HB3   | 25:6:602:CLA:CMC  | 2.45                     | 0.42              |
| 3:8:171:SER:HB3   | 3:8:183:GLU:OE2   | 2.18                     | 0.42              |
| 4:a:327:GLY:O     | 4:a:330:VAL:HG22  | 2.19                     | 0.42              |
| 5:b:378:ARG:HA    | 5:b:378:ARG:NE    | 2.33                     | 0.42              |
| 6:c:146:PHE:CD2   | 26:s:301:LHG:HC5  | 2.54                     | 0.42              |
| 6:c:213:LEU:O     | 6:c:223:TRP:NE1   | 2.40                     | 0.42              |
| 6:c:267:SER:HA    | 17:w:133:LEU:CD2  | 2.49                     | 0.42              |
| 7:d:20:ASP:CG     | 7:d:24:ARG:HH11   | 2.25                     | 0.42              |
| 7:d:218:THR:CG2   | 7:d:250:ALA:HB1   | 2.49                     | 0.42              |
| 29:l:102:SQD:H121 | 29:l:102:SQD:C28  | 2.47                     | 0.42              |
| 15:o:158:PHE:HE2  | 15:o:322:LYS:HB2  | 1.82                     | 0.42              |
| 15:o:184:GLY:O    | 15:o:224:PRO:HD3  | 2.18                     | 0.42              |
| 20:s:135:ASN:HD21 | 20:s:141:CYS:CA   | 2.32                     | 0.42              |
| 20:s:189:ARG:NH2  | 25:s:309:CLA:HMA3 | 2.33                     | 0.42              |
| 21:g:114:VAL:HG13 | 21:g:241:ILE:HD11 | 2.01                     | 0.42              |
| 21:g:215:GLU:HB2  | 25:g:610:CLA:HMB3 | 2.01                     | 0.42              |
| 21:n:232:GLN:HE21 | 25:n:613:CLA:CHA  | 2.17                     | 0.42              |
| 40:n:617:NEX:C28  | 40:n:617:NEX:H381 | 2.48                     | 0.42              |
| 24:y:302:CHL:H18  | 32:y:321:AJP:C13  | 2.49                     | 0.42              |
| 41:r:616:XAT:H11  | 41:r:616:XAT:H191 | 1.79                     | 0.42              |
| 1:1:164:THR:HG21  | 24:1:302:CHL:O1D  | 2.20                     | 0.42              |
| 24:1:301:CHL:CHD  | 24:1:301:CHL:HBC2 | 2.48                     | 0.42              |
| 2:2:126:ASP:OD1   | 2:2:129:GLU:HA    | 2.17                     | 0.42              |
| 2:2:127:PHE:CZ    | 2:2:145:LEU:HD12  | 2.55                     | 0.42              |
| 2:2:202:LEU:O     | 2:2:202:LEU:HG    | 2.19                     | 0.42              |
| 25:2:604:CLA:HBC3 | 26:2:606:LHG:H382 | 2.00                     | 0.42              |
| 3:4:104:ILE:H     | 3:4:104:ILE:HD12  | 1.84                     | 0.42              |
| 4:A:327:GLY:O     | 4:A:330:VAL:HG22  | 2.19                     | 0.42              |
| 5:B:188:GLU:OE1   | 10:H:68:ASP:HB3   | 2.19                     | 0.42              |
| 5:B:371:VAL:HA    | 5:B:376:ILE:O     | 2.19                     | 0.42              |
| 5:B:378:ARG:HA    | 5:B:378:ARG:NE    | 2.33                     | 0.42              |
| 5:B:378:ARG:O     | 5:B:390:TYR:HB3   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:436:THR:HG23  | 5:B:437:LEU:N     | 2.34                     | 0.42              |
| 25:B:602:CLA:H143 | 25:B:602:CLA:H162 | 1.72                     | 0.42              |
| 6:C:146:PHE:CD2   | 26:S:301:LHG:HC5  | 2.54                     | 0.42              |
| 6:C:201:ASN:O     | 6:C:231:GLU:CG    | 2.68                     | 0.42              |
| 7:D:218:THR:CG2   | 7:D:250:ALA:HB1   | 2.49                     | 0.42              |
| 25:S:313:CLA:HAA1 | 25:S:313:CLA:CBD  | 2.48                     | 0.42              |
| 21:G:86:SER:OG    | 25:G:602:CLA:HAA2 | 2.18                     | 0.42              |
| 21:G:231:VAL:HG21 | 25:G:613:CLA:HAC1 | 2.00                     | 0.42              |
| 21:G:231:VAL:CG1  | 25:G:613:CLA:HAC2 | 2.36                     | 0.42              |
| 24:G:601:CHL:H61  | 24:G:601:CHL:H41  | 1.55                     | 0.42              |
| 25:N:604:CLA:HBC2 | 25:N:604:CLA:CMC  | 2.50                     | 0.42              |
| 24:N:609:CHL:HBA1 | 24:N:609:CHL:H3A  | 1.82                     | 0.42              |
| 21:Y:50:TRP:NE1   | 25:Y:312:CLA:HED3 | 2.33                     | 0.42              |
| 24:Y:306:CHL:HBA2 | 24:Y:306:CHL:H3A  | 1.66                     | 0.42              |
| 25:Y:314:CLA:C4B  | 39:Y:316:LUT:H183 | 2.49                     | 0.42              |
| 1:5:206:GLU:N     | 1:5:206:GLU:CD    | 2.76                     | 0.42              |
| 2:6:107:MET:HG3   | 2:6:222:LEU:HD12  | 2.01                     | 0.42              |
| 2:6:175:GLY:HA3   | 2:6:181:LEU:HD21  | 2.02                     | 0.42              |
| 2:6:239:LYS:HD2   | 2:6:242:LEU:HD11  | 1.99                     | 0.42              |
| 1:7:127:GLY:C     | 1:7:137:GLN:HG3   | 2.44                     | 0.42              |
| 4:a:279:PRO:O     | 4:a:283:ILE:HG12  | 2.19                     | 0.42              |
| 5:b:242:ILE:O     | 5:b:246:PHE:CD1   | 2.72                     | 0.42              |
| 5:b:243:ALA:HA    | 5:b:246:PHE:HE1   | 1.71                     | 0.42              |
| 5:b:476:ARG:HG2   | 5:b:476:ARG:HH11  | 1.83                     | 0.42              |
| 28:b:619:BCR:H24C | 28:b:619:BCR:H371 | 1.79                     | 0.42              |
| 25:c:506:CLA:H92  | 25:c:506:CLA:H61  | 1.62                     | 0.42              |
| 26:c:517:LHG:H332 | 26:c:517:LHG:H362 | 1.68                     | 0.42              |
| 7:d:160:ILE:HG21  | 7:d:288:VAL:HG22  | 2.02                     | 0.42              |
| 12:k:30:TYR:CZ    | 19:z:5:PHE:HZ     | 2.36                     | 0.42              |
| 12:k:58:VAL:O     | 12:k:59:SER:HB2   | 2.19                     | 0.42              |
| 18:x:96:VAL:O     | 18:x:100:ILE:HG23 | 2.19                     | 0.42              |
| 19:z:19:LEU:HD21  | 19:z:43:GLY:CA    | 2.41                     | 0.42              |
| 20:s:142:GLY:N    | 20:s:160:LEU:O    | 2.50                     | 0.42              |
| 21:g:50:TRP:NE1   | 25:g:611:CLA:HED2 | 2.34                     | 0.42              |
| 21:g:84:GLY:N     | 21:y:94:ARG:CG    | 2.80                     | 0.42              |
| 21:g:137:GLN:HE22 | 21:g:144:LEU:HA   | 1.84                     | 0.42              |
| 21:n:127:GLY:C    | 21:n:137:GLN:HG3  | 2.44                     | 0.42              |
| 25:n:613:CLA:HBA1 | 25:n:614:CLA:CAD  | 2.49                     | 0.42              |
| 21:y:57:LYS:HD2   | 21:y:63:SER:HB2   | 2.00                     | 0.42              |
| 25:y:312:CLA:H92  | 25:y:312:CLA:C5   | 2.49                     | 0.42              |
| 22:r:258:VAL:HG12 | 25:r:612:CLA:HMD2 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:609:CLA:H52  | 39:r:615:LUT:C30  | 2.49                     | 0.42              |
| 1:1:206:GLU:N     | 1:1:206:GLU:CD    | 2.76                     | 0.42              |
| 2:2:107:MET:HG3   | 2:2:222:LEU:HD12  | 2.01                     | 0.42              |
| 1:3:127:GLY:C     | 1:3:137:GLN:HG3   | 2.44                     | 0.42              |
| 4:A:47:VAL:HG21   | 4:A:114:LEU:CD2   | 2.49                     | 0.42              |
| 5:B:37:MET:HE1    | 25:B:607:CLA:HHD  | 2.01                     | 0.42              |
| 5:B:367:PRO:HB3   | 7:D:346:VAL:HB    | 2.02                     | 0.42              |
| 5:B:388:SER:CB    | 5:B:391:SER:HB2   | 2.45                     | 0.42              |
| 25:B:614:CLA:HMD2 | 29:L:101:SQD:C24  | 2.49                     | 0.42              |
| 6:C:109:PHE:O     | 6:C:113:VAL:HG23  | 2.19                     | 0.42              |
| 6:C:287:CYS:SG    | 6:C:427:SER:HB3   | 2.60                     | 0.42              |
| 7:D:258:PHE:CZ    | 26:D:406:LHG:H312 | 2.55                     | 0.42              |
| 28:H:101:BCR:H351 | 28:H:101:BCR:H15C | 1.90                     | 0.42              |
| 21:G:132:PHE:HB2  | 24:G:607:CHL:CMA  | 2.43                     | 0.42              |
| 21:G:228:GLY:O    | 21:G:231:VAL:N    | 2.53                     | 0.42              |
| 21:N:127:GLY:C    | 21:N:137:GLN:HG3  | 2.44                     | 0.42              |
| 21:N:221:LEU:CD1  | 26:N:618:LHG:H272 | 2.48                     | 0.42              |
| 25:N:610:CLA:C5   | 39:N:615:LUT:H30  | 2.48                     | 0.42              |
| 21:Y:132:PHE:CD1  | 21:Y:133:LYS:N    | 2.88                     | 0.42              |
| 21:Y:191:TYR:N    | 21:Y:192:PRO:CD   | 2.82                     | 0.42              |
| 21:Y:218:ASN:OD1  | 25:Y:312:CLA:CMD  | 2.67                     | 0.42              |
| 25:Y:303:CLA:H41  | 25:Y:304:CLA:O1A  | 2.20                     | 0.42              |
| 22:R:177:SER:O    | 22:R:184:LEU:N    | 2.35                     | 0.42              |
| 1:7:131:TRP:CD1   | 1:7:131:TRP:H     | 2.38                     | 0.42              |
| 3:8:89:GLY:CA     | 3:8:95:LEU:HD21   | 2.49                     | 0.42              |
| 3:8:251:THR:HG23  | 3:8:254:GLY:H     | 1.83                     | 0.42              |
| 4:a:335:ASN:HB3   | 6:c:334:PRO:CB    | 2.49                     | 0.42              |
| 5:b:52:LEU:C      | 5:b:54:PRO:HD3    | 2.44                     | 0.42              |
| 5:b:91:TRP:NE1    | 26:b:622:LHG:HC61 | 2.29                     | 0.42              |
| 5:b:160:GLY:HA3   | 5:b:180:PRO:HB3   | 2.01                     | 0.42              |
| 25:b:614:CLA:HMD2 | 29:l:102:SQD:H242 | 2.01                     | 0.42              |
| 25:c:506:CLA:H13  | 25:c:506:CLA:H91  | 2.01                     | 0.42              |
| 25:c:511:CLA:H3A  | 25:c:511:CLA:HBA1 | 1.68                     | 0.42              |
| 12:k:27:PRO:HB2   | 12:k:30:TYR:HD1   | 1.85                     | 0.42              |
| 15:o:92:LEU:HB3   | 15:o:96:GLU:CG    | 2.43                     | 0.42              |
| 24:g:607:CHL:CMB  | 24:g:607:CHL:HBB1 | 2.50                     | 0.42              |
| 25:g:610:CLA:C5   | 39:g:615:LUT:H30  | 2.41                     | 0.42              |
| 21:n:97:GLU:CB    | 21:n:190:LEU:HD11 | 2.48                     | 0.42              |
| 25:n:602:CLA:H52  | 25:n:602:CLA:CMB  | 2.41                     | 0.42              |
| 21:y:210:GLU:O    | 21:y:214:LYS:HG3  | 2.20                     | 0.42              |
| 1:1:57:LYS:HD2    | 1:1:63:SER:HB2    | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:210:GLU:O     | 1:1:214:LYS:HG3   | 2.20                     | 0.42              |
| 2:2:192:PRO:HB2   | 2:2:196:TYR:CD2   | 2.55                     | 0.42              |
| 3:4:189:THR:O     | 3:4:189:THR:HG23  | 2.18                     | 0.42              |
| 3:4:193:GLY:O     | 3:4:195:PRO:HD3   | 2.20                     | 0.42              |
| 3:4:216:PRO:O     | 3:4:220:LYS:N     | 2.52                     | 0.42              |
| 5:B:52:LEU:C      | 5:B:54:PRO:HD3    | 2.44                     | 0.42              |
| 6:C:147:PHE:CD1   | 25:C:513:CLA:HMB1 | 2.55                     | 0.42              |
| 25:C:504:CLA:C4   | 35:C:516:DGD:HB32 | 2.45                     | 0.42              |
| 26:C:517:LHG:HC82 | 17:W:113:TRP:HE1  | 1.84                     | 0.42              |
| 7:D:197:PHE:HA    | 7:D:200:MET:HE3   | 2.01                     | 0.42              |
| 7:D:243:GLU:HG2   | 7:D:245:TYR:H     | 1.83                     | 0.42              |
| 7:D:297:TYR:O     | 7:D:316:TYR:OH    | 2.30                     | 0.42              |
| 8:E:67:THR:CA     | 23:U:102:ARG:HH11 | 2.33                     | 0.42              |
| 14:M:23:LEU:O     | 14:M:27:VAL:HG23  | 2.19                     | 0.42              |
| 18:X:86:PHE:O     | 18:X:90:ILE:HG13  | 2.20                     | 0.42              |
| 20:S:135:ASN:ND2  | 20:S:141:CYS:N    | 2.66                     | 0.42              |
| 20:S:248:GLU:CD   | 20:S:252:GLU:HG3  | 2.44                     | 0.42              |
| 21:G:127:GLY:C    | 21:G:137:GLN:HG3  | 2.44                     | 0.42              |
| 21:N:228:GLY:O    | 21:N:231:VAL:N    | 2.53                     | 0.42              |
| 24:N:609:CHL:NC   | 24:Y:302:CHL:H52  | 2.34                     | 0.42              |
| 21:Y:176:ARG:HG3  | 24:Y:309:CHL:C1D  | 2.49                     | 0.42              |
| 21:Y:221:LEU:HD21 | 25:Y:313:CLA:HAC1 | 2.01                     | 0.42              |
| 25:R:603:CLA:H43  | 25:R:603:CLA:HED3 | 2.01                     | 0.42              |
| 25:R:603:CLA:H93  | 25:R:603:CLA:H111 | 1.62                     | 0.42              |
| 2:6:104:ARG:CZ    | 24:6:603:CHL:HED3 | 2.49                     | 0.42              |
| 1:7:145:ASP:OD2   | 1:7:150:PRO:HA    | 2.20                     | 0.42              |
| 1:7:191:TYR:N     | 1:7:192:PRO:CD    | 2.82                     | 0.42              |
| 4:a:40:THR:O      | 4:a:43:THR:HG22   | 2.18                     | 0.42              |
| 4:a:120:LEU:O     | 4:a:123:VAL:HG22  | 2.18                     | 0.42              |
| 5:b:193:PHE:HE2   | 35:b:626:DGD:HE2  | 1.83                     | 0.42              |
| 5:b:436:THR:HG23  | 5:b:437:LEU:N     | 2.34                     | 0.42              |
| 25:b:605:CLA:H162 | 25:b:609:CLA:HBB2 | 2.01                     | 0.42              |
| 25:b:614:CLA:HMD2 | 29:l:102:SQD:C24  | 2.49                     | 0.42              |
| 6:c:185:VAL:CG2   | 6:c:230:LEU:HD13  | 2.49                     | 0.42              |
| 6:c:221:GLU:CD    | 17:w:91:GLY:HA2   | 2.44                     | 0.42              |
| 7:d:68:TYR:O      | 30:d:407:LMG:HC61 | 2.18                     | 0.42              |
| 7:d:135:ARG:HH21  | 7:d:138:GLN:CD    | 2.25                     | 0.42              |
| 17:w:131:LEU:HD23 | 17:w:131:LEU:HA   | 1.82                     | 0.42              |
| 25:s:305:CLA:HMB1 | 25:s:305:CLA:CBB  | 2.49                     | 0.42              |
| 21:g:145:ASP:OD2  | 21:g:150:PRO:HA   | 2.20                     | 0.42              |
| 21:g:172:VAL:HG13 | 24:g:608:CHL:C4B  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:226:MET:O    | 21:g:230:PHE:HD2  | 2.01                     | 0.42              |
| 21:n:215:GLU:CG   | 25:n:610:CLA:C1B  | 2.97                     | 0.42              |
| 25:n:604:CLA:HMA2 | 24:n:606:CHL:CAC  | 2.50                     | 0.42              |
| 22:r:85:LYS:CG    | 22:r:86:PRO:CD    | 2.96                     | 0.42              |
| 25:r:603:CLA:H43  | 25:r:603:CLA:HED3 | 2.01                     | 0.42              |
| 25:r:614:CLA:HBD  | 25:r:614:CLA:HAA1 | 2.02                     | 0.42              |
| 1:1:132:PHE:CD1   | 1:1:133:LYS:N     | 2.88                     | 0.42              |
| 1:1:159:LEU:N     | 1:1:159:LEU:HD13  | 2.33                     | 0.42              |
| 2:2:174:GLU:HB3   | 1:3:62:PHE:CD2    | 2.55                     | 0.42              |
| 3:4:140:PHE:HA    | 22:R:280:HIS:CD2  | 2.54                     | 0.42              |
| 3:4:245:GLU:O     | 3:4:249:GLY:N     | 2.53                     | 0.42              |
| 28:B:617:BCR:H312 | 30:B:620:LMG:H341 | 2.02                     | 0.42              |
| 6:C:135:LEU:HD23  | 6:C:135:LEU:C     | 2.45                     | 0.42              |
| 6:C:227:VAL:HG11  | 6:C:233:ILE:CG1   | 2.49                     | 0.42              |
| 6:C:235:GLY:O     | 6:C:239:TRP:HD1   | 2.02                     | 0.42              |
| 6:C:267:SER:HA    | 17:W:133:LEU:CD2  | 2.49                     | 0.42              |
| 6:C:304:PRO:O     | 6:C:308:GLU:HB3   | 2.19                     | 0.42              |
| 25:C:512:CLA:H162 | 25:C:513:CLA:H152 | 2.02                     | 0.42              |
| 7:D:160:ILE:HG21  | 7:D:288:VAL:HG22  | 2.02                     | 0.42              |
| 15:O:145:VAL:HG11 | 15:O:203:LEU:HD21 | 2.00                     | 0.42              |
| 15:O:225:ASP:O    | 15:O:288:LYS:HA   | 2.20                     | 0.42              |
| 16:T:11:VAL:HG22  | 28:T:101:BCR:H342 | 2.00                     | 0.42              |
| 25:S:303:CLA:H61  | 25:S:303:CLA:H41  | 1.90                     | 0.42              |
| 21:G:145:ASP:OD2  | 21:G:150:PRO:HA   | 2.19                     | 0.42              |
| 21:G:172:VAL:HG13 | 24:G:608:CHL:C4B  | 2.49                     | 0.42              |
| 25:G:604:CLA:HBB1 | 39:G:616:LUT:C18  | 2.47                     | 0.42              |
| 21:N:137:GLN:HE22 | 21:N:144:LEU:HA   | 1.84                     | 0.42              |
| 21:N:210:GLU:O    | 21:N:214:LYS:HG3  | 2.20                     | 0.42              |
| 21:N:247:HIS:HD1  | 21:N:247:HIS:C    | 2.28                     | 0.42              |
| 25:N:604:CLA:HMA2 | 24:N:606:CHL:CAC  | 2.50                     | 0.42              |
| 21:Y:57:LYS:HD2   | 21:Y:63:SER:HB2   | 2.00                     | 0.42              |
| 21:Y:80:TRP:O     | 39:Y:317:LUT:H24  | 2.19                     | 0.42              |
| 21:Y:145:ASP:OD2  | 21:Y:150:PRO:HA   | 2.20                     | 0.42              |
| 21:Y:215:GLU:HB2  | 25:Y:311:CLA:C1B  | 2.49                     | 0.42              |
| 21:Y:247:HIS:HD1  | 21:Y:247:HIS:C    | 2.28                     | 0.42              |
| 24:Y:302:CHL:H18  | 32:Y:321:AJP:C13  | 2.49                     | 0.42              |
| 22:R:137:ARG:NH2  | 25:R:602:CLA:HED3 | 2.24                     | 0.42              |
| 2:6:174:GLU:HB3   | 1:7:62:PHE:CD2    | 2.55                     | 0.42              |
| 2:6:202:LEU:O     | 2:6:202:LEU:HG    | 2.19                     | 0.42              |
| 4:a:184:ILE:CG2   | 7:d:322:LEU:HD13  | 2.50                     | 0.42              |
| 5:b:135:LEU:HD12  | 5:b:231:MET:O     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:608:CLA:CAB  | 7:d:124:ILE:HG12  | 2.49                     | 0.42              |
| 25:b:609:CLA:HAA1 | 25:b:609:CLA:HBD  | 2.01                     | 0.42              |
| 6:c:182:PHE:HE1   | 20:s:258:LEU:O    | 2.02                     | 0.42              |
| 8:e:25:ILE:O      | 8:e:29:SER:OG     | 2.28                     | 0.42              |
| 15:o:180:VAL:CA   | 15:o:186:VAL:HG12 | 2.45                     | 0.42              |
| 18:x:86:PHE:O     | 18:x:90:ILE:HG13  | 2.20                     | 0.42              |
| 19:z:42:SER:O     | 19:z:43:GLY:C     | 2.63                     | 0.42              |
| 21:g:172:VAL:HG13 | 24:g:608:CHL:C1B  | 2.48                     | 0.42              |
| 21:g:191:TYR:N    | 21:g:192:PRO:CD   | 2.82                     | 0.42              |
| 21:g:228:GLY:O    | 21:g:231:VAL:N    | 2.53                     | 0.42              |
| 40:g:617:NEX:H391 | 40:g:617:NEX:H31  | 1.57                     | 0.42              |
| 21:n:137:GLN:HE22 | 21:n:144:LEU:HA   | 1.84                     | 0.42              |
| 25:n:603:CLA:H61  | 25:n:603:CLA:H92  | 1.50                     | 0.42              |
| 21:y:127:GLY:C    | 21:y:137:GLN:HG3  | 2.44                     | 0.42              |
| 21:y:215:GLU:CG   | 25:y:311:CLA:C1B  | 2.95                     | 0.42              |
| 24:y:302:CHL:CMC  | 24:y:302:CHL:HBC3 | 2.49                     | 0.42              |
| 25:y:303:CLA:H41  | 25:y:304:CLA:O1A  | 2.20                     | 0.42              |
| 25:y:304:CLA:H161 | 25:y:304:CLA:H192 | 1.74                     | 0.42              |
| 22:r:103:LYS:HE3  | 22:r:105:LEU:CD1  | 2.47                     | 0.42              |
| 22:r:171:VAL:O    | 22:r:175:ASP:HB2  | 2.19                     | 0.42              |
| 25:r:612:CLA:HBD  | 25:r:612:CLA:HAA1 | 2.02                     | 0.42              |
| 1:1:127:GLY:C     | 1:1:137:GLN:HG3   | 2.44                     | 0.42              |
| 2:2:118:VAL:O     | 2:2:122:TRP:HB2   | 2.19                     | 0.42              |
| 1:3:191:TYR:N     | 1:3:192:PRO:CD    | 2.82                     | 0.42              |
| 3:4:89:GLY:CA     | 3:4:95:LEU:HD21   | 2.49                     | 0.42              |
| 4:A:184:ILE:CG2   | 7:D:322:LEU:HD13  | 2.50                     | 0.42              |
| 4:A:223:LEU:O     | 5:B:482:ILE:HG12  | 2.19                     | 0.42              |
| 4:A:292:THR:CB    | 6:C:428:THR:HG23  | 2.50                     | 0.42              |
| 4:A:328:MET:O     | 4:A:332:HIS:CD2   | 2.73                     | 0.42              |
| 5:B:187:VAL:HG23  | 5:B:188:GLU:OE1   | 2.20                     | 0.42              |
| 6:C:97:TRP:HE1    | 6:C:178:LYS:HE3   | 1.83                     | 0.42              |
| 6:C:281:VAL:HG12  | 6:C:285:ILE:HD11  | 2.01                     | 0.42              |
| 7:D:172:PRO:HG3   | 7:D:182:PHE:CZ    | 2.55                     | 0.42              |
| 7:D:316:TYR:O     | 7:D:320:ILE:HG12  | 2.19                     | 0.42              |
| 10:H:31:GLY:O     | 10:H:33:VAL:HG23  | 2.19                     | 0.42              |
| 14:M:29:THR:HG23  | 14:M:30:VAL:N     | 2.35                     | 0.42              |
| 21:G:49:PRO:O     | 21:G:55:ARG:HA    | 2.20                     | 0.42              |
| 21:G:172:VAL:HG13 | 24:G:608:CHL:NB   | 2.35                     | 0.42              |
| 21:G:191:TYR:CE2  | 21:G:212:LYS:CE   | 3.03                     | 0.42              |
| 24:G:607:CHL:CMB  | 24:G:607:CHL:HBB1 | 2.50                     | 0.42              |
| 21:Y:49:PRO:O     | 21:Y:55:ARG:HA    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:R:171:VAL:O    | 22:R:175:ASP:HB2  | 2.19                     | 0.42              |
| 22:R:253:PHE:CE2  | 41:R:616:XAT:H10  | 2.54                     | 0.42              |
| 1:5:228:GLY:O     | 1:5:231:VAL:N     | 2.53                     | 0.42              |
| 2:6:137:SER:CA    | 2:6:140:PHE:CD2   | 3.02                     | 0.42              |
| 2:6:149:GLY:O     | 2:6:152:ASN:HB2   | 2.20                     | 0.42              |
| 2:6:192:PRO:HB2   | 2:6:196:TYR:CD2   | 2.55                     | 0.42              |
| 3:8:118:VAL:HG13  | 3:8:119:GLY:N     | 2.35                     | 0.42              |
| 3:8:164:PHE:HB2   | 3:8:192:GLN:CD    | 2.45                     | 0.42              |
| 30:a:411:LMG:H351 | 30:a:411:LMG:H382 | 1.83                     | 0.42              |
| 5:b:256:MET:O     | 5:b:448:ARG:HD3   | 2.20                     | 0.42              |
| 25:b:604:CLA:H93  | 25:b:604:CLA:H61  | 1.59                     | 0.42              |
| 6:c:147:PHE:CD1   | 25:c:513:CLA:HMB1 | 2.55                     | 0.42              |
| 6:c:299:SER:HA    | 6:c:423:ARG:HH21  | 1.85                     | 0.42              |
| 6:c:304:PRO:O     | 6:c:308:GLU:HB3   | 2.19                     | 0.42              |
| 8:e:30:LEU:HD13   | 9:f:22:VAL:HG13   | 2.02                     | 0.42              |
| 20:s:68:ARG:NH2   | 26:s:301:LHG:HC12 | 2.23                     | 0.42              |
| 21:g:173:GLU:OE2  | 24:g:609:CHL:NA   | 2.53                     | 0.42              |
| 21:n:80:TRP:HE3   | 25:n:602:CLA:CMD  | 2.32                     | 0.42              |
| 25:n:604:CLA:HBC2 | 25:n:604:CLA:CMC  | 2.50                     | 0.42              |
| 21:y:95:ASN:C     | 25:y:303:CLA:HMA1 | 2.45                     | 0.42              |
| 21:y:137:GLN:HE22 | 21:y:144:LEU:HA   | 1.84                     | 0.42              |
| 21:y:152:LEU:O    | 21:y:153:VAL:C    | 2.63                     | 0.42              |
| 22:r:103:LYS:HE3  | 22:r:105:LEU:CD2  | 2.47                     | 0.42              |
| 22:r:124:PHE:CD1  | 25:r:614:CLA:CHC  | 2.93                     | 0.42              |
| 25:r:610:CLA:HMB3 | 26:r:618:LHG:C2   | 2.45                     | 0.42              |
| 24:r:613:CHL:HBC3 | 24:r:613:CHL:OMC  | 2.20                     | 0.42              |
| 25:r:614:CLA:HBC3 | 25:r:614:CLA:CHD  | 2.37                     | 0.42              |
| 2:2:128:LYS:HB3   | 2:2:130:PRO:HD2   | 2.01                     | 0.42              |
| 1:3:132:PHE:CD1   | 1:3:133:LYS:N     | 2.88                     | 0.42              |
| 1:3:152:LEU:O     | 1:3:153:VAL:C     | 2.63                     | 0.42              |
| 25:B:601:CLA:H161 | 25:B:601:CLA:H141 | 1.84                     | 0.42              |
| 25:B:607:CLA:H192 | 25:B:607:CLA:H162 | 1.87                     | 0.42              |
| 6:C:79:LYS:HG2    | 6:C:80:PRO:CD     | 2.49                     | 0.42              |
| 12:K:30:TYR:CE2   | 19:Z:5:PHE:HZ     | 2.38                     | 0.42              |
| 20:S:186:GLU:HG3  | 25:S:309:CLA:NB   | 2.34                     | 0.42              |
| 20:S:252:GLU:O    | 20:S:256:LYS:HG2  | 2.20                     | 0.42              |
| 21:G:152:LEU:HD23 | 24:G:605:CHL:HED3 | 2.01                     | 0.42              |
| 21:N:80:TRP:HE3   | 25:N:602:CLA:CMD  | 2.32                     | 0.42              |
| 21:N:191:TYR:N    | 21:N:192:PRO:CD   | 2.82                     | 0.42              |
| 24:N:606:CHL:HMB1 | 24:N:609:CHL:HAC1 | 2.01                     | 0.42              |
| 25:R:609:CLA:H52  | 39:R:615:LUT:C30  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:R:613:CHL:HBC3 | 24:R:613:CHL:OMC  | 2.20                     | 0.42              |
| 25:6:604:CLA:HBC3 | 26:6:606:LHG:H382 | 2.00                     | 0.42              |
| 3:8:226:LEU:CD1   | 3:8:229:ILE:HD11  | 2.43                     | 0.42              |
| 4:a:47:VAL:HG21   | 4:a:114:LEU:CD2   | 2.50                     | 0.42              |
| 5:b:51:VAL:HG22   | 5:b:308:LYS:HD2   | 2.01                     | 0.42              |
| 6:c:209:ILE:HG13  | 6:c:239:TRP:CD1   | 2.55                     | 0.42              |
| 25:c:501:CLA:H151 | 25:c:507:CLA:H102 | 2.02                     | 0.42              |
| 7:d:280:LEU:HD23  | 7:d:280:LEU:HA    | 1.85                     | 0.42              |
| 28:h:101:BCR:H20C | 28:h:101:BCR:H361 | 1.79                     | 0.42              |
| 29:l:102:SQD:H251 | 29:l:102:SQD:H102 | 2.01                     | 0.42              |
| 14:m:29:THR:HG23  | 14:m:30:VAL:N     | 2.35                     | 0.42              |
| 15:o:236:TYR:CB   | 15:o:310:ASP:OD2  | 2.63                     | 0.42              |
| 20:s:132:GLU:CA   | 20:s:145:ALA:HB1  | 2.40                     | 0.42              |
| 20:s:252:GLU:O    | 20:s:256:LYS:HG2  | 2.20                     | 0.42              |
| 24:s:306:CHL:HBB1 | 39:s:316:LUT:C16  | 2.49                     | 0.42              |
| 24:g:601:CHL:H142 | 24:g:601:CHL:H112 | 1.84                     | 0.42              |
| 24:g:607:CHL:CMB  | 24:g:607:CHL:CBB  | 2.97                     | 0.42              |
| 24:n:601:CHL:H62  | 24:n:601:CHL:H41  | 1.58                     | 0.42              |
| 24:n:606:CHL:HAA1 | 40:n:617:NEX:H28  | 2.02                     | 0.42              |
| 25:n:613:CLA:CHB  | 39:n:615:LUT:H42  | 2.49                     | 0.42              |
| 21:y:131:TRP:CD1  | 21:y:131:TRP:H    | 2.38                     | 0.42              |
| 21:y:165:GLN:OE1  | 24:y:307:CHL:C4A  | 2.68                     | 0.42              |
| 21:y:221:LEU:HD21 | 25:y:313:CLA:HAC1 | 2.01                     | 0.42              |
| 25:y:313:CLA:H142 | 25:y:313:CLA:H111 | 1.50                     | 0.42              |
| 25:y:315:CLA:HBD  | 25:y:315:CLA:CBA  | 2.49                     | 0.42              |
| 26:y:319:LHG:H292 | 26:y:319:LHG:H322 | 1.79                     | 0.42              |
| 24:r:606:CHL:O2A  | 24:r:606:CHL:H2A  | 2.20                     | 0.42              |
| 1:1:151:SER:O     | 24:1:301:CHL:HMA3 | 2.19                     | 0.42              |
| 2:2:104:ARG:NH1   | 2:2:108:LEU:HD11  | 2.34                     | 0.42              |
| 2:2:175:GLY:HA3   | 2:2:181:LEU:HD21  | 2.02                     | 0.42              |
| 1:3:228:GLY:O     | 1:3:231:VAL:N     | 2.53                     | 0.42              |
| 3:4:122:TRP:HB3   | 3:4:127:TRP:HB2   | 2.02                     | 0.42              |
| 5:B:65:PHE:CE2    | 25:B:604:CLA:HMA2 | 2.55                     | 0.42              |
| 5:B:127:ARG:HH22  | 10:H:31:GLY:HA3   | 1.85                     | 0.42              |
| 25:B:601:CLA:H111 | 25:B:601:CLA:H93  | 1.71                     | 0.42              |
| 25:B:606:CLA:H172 | 25:B:616:CLA:H93  | 2.00                     | 0.42              |
| 25:B:613:CLA:H2A  | 25:B:613:CLA:O1D  | 2.20                     | 0.42              |
| 6:C:179:ALA:HA    | 6:C:185:VAL:HG13  | 2.01                     | 0.42              |
| 7:D:151:ILE:O     | 7:D:155:VAL:HG23  | 2.20                     | 0.42              |
| 8:E:40:THR:OG1    | 8:E:42:LEU:HD13   | 2.20                     | 0.42              |
| 12:K:58:VAL:O     | 12:K:59:SER:HB2   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:L:3:GLN:HG3    | 13:L:4:SER:N      | 2.34                     | 0.42              |
| 19:Z:61:ILE:HG13  | 19:Z:62:SER:N     | 2.34                     | 0.42              |
| 25:S:303:CLA:H52  | 25:S:303:CLA:H8   | 1.74                     | 0.42              |
| 21:G:160:ALA:HB3  | 24:G:605:CHL:OMC  | 2.20                     | 0.42              |
| 24:N:607:CHL:H171 | 25:Y:303:CLA:H162 | 2.02                     | 0.42              |
| 40:N:617:NEX:C28  | 40:N:617:NEX:H381 | 2.48                     | 0.42              |
| 1:5:127:GLY:C     | 1:5:137:GLN:HG3   | 2.44                     | 0.42              |
| 1:5:145:ASP:OD2   | 1:5:150:PRO:HA    | 2.19                     | 0.42              |
| 2:6:128:LYS:HB3   | 2:6:130:PRO:HD2   | 2.01                     | 0.42              |
| 2:6:249:LEU:HD12  | 2:6:250:ASP:HB2   | 2.00                     | 0.42              |
| 4:a:98:GLU:HA     | 4:a:98:GLU:OE2    | 2.20                     | 0.42              |
| 4:a:328:MET:O     | 4:a:332:HIS:CD2   | 2.73                     | 0.42              |
| 5:b:291:GLY:HA2   | 5:b:294:GLU:CD    | 2.44                     | 0.42              |
| 6:c:79:LYS:HG2    | 6:c:80:PRO:CD     | 2.49                     | 0.42              |
| 6:c:287:CYS:SG    | 6:c:427:SER:HB3   | 2.60                     | 0.42              |
| 7:d:243:GLU:HG2   | 7:d:245:TYR:H     | 1.83                     | 0.42              |
| 7:d:305:ARG:NH1   | 14:m:1:MET:HE2    | 2.34                     | 0.42              |
| 15:o:174:ILE:HG12 | 15:o:195:ASP:OD1  | 2.19                     | 0.42              |
| 15:o:214:THR:HG21 | 15:o:233:VAL:HA   | 2.01                     | 0.42              |
| 15:o:225:ASP:O    | 15:o:288:LYS:HA   | 2.20                     | 0.42              |
| 18:x:87:LEU:HD12  | 18:x:87:LEU:C     | 2.45                     | 0.42              |
| 20:s:186:GLU:HG3  | 25:s:309:CLA:NB   | 2.34                     | 0.42              |
| 21:n:114:VAL:HG13 | 21:n:241:ILE:HD11 | 2.01                     | 0.42              |
| 21:n:228:GLY:O    | 21:n:231:VAL:N    | 2.53                     | 0.42              |
| 22:r:255:GLY:HA2  | 25:r:612:CLA:C4C  | 2.50                     | 0.42              |
| 25:r:603:CLA:NB   | 25:r:608:CLA:H111 | 2.35                     | 0.42              |
| 25:r:609:CLA:H61  | 25:r:609:CLA:H92  | 1.67                     | 0.42              |
| 1:1:152:LEU:O     | 1:1:153:VAL:C     | 2.63                     | 0.42              |
| 2:2:218:LYS:HA    | 2:2:221:ARG:NE    | 2.35                     | 0.42              |
| 3:4:118:VAL:HG13  | 3:4:119:GLY:N     | 2.35                     | 0.42              |
| 3:4:194:TYR:OH    | 3:4:225:LYS:CG    | 2.68                     | 0.42              |
| 3:4:245:GLU:HB2   | 3:4:250:LYS:O     | 2.20                     | 0.42              |
| 4:A:79:SER:CB     | 7:D:302:GLN:HE22  | 2.33                     | 0.42              |
| 5:B:294:GLU:O     | 5:B:295:ASN:HB2   | 2.20                     | 0.42              |
| 5:B:336:ILE:O     | 5:B:336:ILE:CG2   | 2.67                     | 0.42              |
| 5:B:342:GLY:HA3   | 5:B:403:GLY:O     | 2.20                     | 0.42              |
| 25:B:610:CLA:HAA2 | 25:B:610:CLA:HBD  | 2.02                     | 0.42              |
| 6:C:273:SER:HB2   | 6:C:445:ALA:HB2   | 2.01                     | 0.42              |
| 10:H:24:LYS:HB3   | 10:H:25:PRO:HD3   | 2.02                     | 0.42              |
| 25:S:305:CLA:HMB1 | 25:S:305:CLA:CBB  | 2.50                     | 0.42              |
| 21:G:131:TRP:CD1  | 21:G:131:TRP:H    | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:137:GLN:O    | 21:N:140:SER:OG   | 2.30                     | 0.42              |
| 25:N:613:CLA:H8   | 25:N:613:CLA:C13  | 2.47                     | 0.42              |
| 25:R:604:CLA:HMA2 | 24:R:605:CHL:HAC2 | 2.02                     | 0.42              |
| 25:R:612:CLA:HBD  | 25:R:612:CLA:HAA1 | 2.02                     | 0.42              |
| 1:5:152:LEU:O     | 1:5:153:VAL:C     | 2.63                     | 0.42              |
| 24:6:603:CHL:HBC3 | 24:6:603:CHL:OMC  | 2.20                     | 0.42              |
| 1:7:97:GLU:CB     | 1:7:190:LEU:HD11  | 2.48                     | 0.42              |
| 1:7:137:GLN:HE22  | 1:7:144:LEU:HA    | 1.84                     | 0.42              |
| 1:7:152:LEU:O     | 1:7:153:VAL:C     | 2.63                     | 0.42              |
| 1:7:228:GLY:O     | 1:7:231:VAL:N     | 2.53                     | 0.42              |
| 3:8:148:THR:HG23  | 3:8:149:GLN:N     | 2.35                     | 0.42              |
| 5:b:130:LYS:HB3   | 5:b:131:PRO:HD2   | 2.02                     | 0.42              |
| 5:b:371:VAL:HA    | 5:b:376:ILE:O     | 2.20                     | 0.42              |
| 5:b:378:ARG:O     | 5:b:390:TYR:HB3   | 2.20                     | 0.42              |
| 6:c:281:VAL:HG12  | 6:c:285:ILE:HD11  | 2.01                     | 0.42              |
| 6:c:322:GLN:HE22  | 6:c:384:ILE:CD1   | 2.24                     | 0.42              |
| 25:c:502:CLA:H161 | 25:c:502:CLA:H203 | 1.84                     | 0.42              |
| 7:d:258:PHE:CZ    | 26:d:406:LHG:H312 | 2.55                     | 0.42              |
| 25:d:403:CLA:H102 | 25:d:403:CLA:H61  | 1.79                     | 0.42              |
| 21:g:172:VAL:HG13 | 24:g:608:CHL:NB   | 2.35                     | 0.42              |
| 21:g:210:GLU:O    | 21:g:214:LYS:HG3  | 2.20                     | 0.42              |
| 25:g:610:CLA:HBA2 | 39:g:615:LUT:O23  | 2.20                     | 0.42              |
| 25:n:602:CLA:H93  | 25:n:602:CLA:H111 | 1.52                     | 0.42              |
| 24:n:607:CHL:H142 | 24:n:607:CHL:H91  | 2.01                     | 0.42              |
| 21:y:191:TYR:N    | 21:y:192:PRO:CD   | 2.82                     | 0.42              |
| 25:y:305:CLA:HMA1 | 39:y:317:LUT:H3   | 2.01                     | 0.42              |
| 25:y:312:CLA:H62  | 25:y:312:CLA:H2   | 1.70                     | 0.42              |
| 26:y:319:LHG:HC92 | 26:y:319:LHG:H121 | 1.60                     | 0.42              |
| 41:r:616:XAT:H31  | 41:r:616:XAT:H391 | 1.76                     | 0.42              |
| 1:1:228:GLY:O     | 1:1:231:VAL:N     | 2.53                     | 0.41              |
| 2:2:149:GLY:O     | 2:2:152:ASN:HB2   | 2.20                     | 0.41              |
| 1:3:145:ASP:OD2   | 1:3:150:PRO:HA    | 2.19                     | 0.41              |
| 4:A:72:LEU:HG     | 4:A:72:LEU:O      | 2.20                     | 0.41              |
| 4:A:142:TRP:CZ2   | 6:C:447:ARG:HG3   | 2.54                     | 0.41              |
| 35:A:415:DGD:HAT1 | 35:A:415:DGD:HA71 | 1.64                     | 0.41              |
| 5:B:115:TRP:HH2   | 25:B:614:CLA:HMA2 | 1.84                     | 0.41              |
| 5:B:130:LYS:HB3   | 5:B:131:PRO:HD2   | 2.02                     | 0.41              |
| 5:B:168:VAL:HG13  | 5:B:195:PRO:HG2   | 2.02                     | 0.41              |
| 5:B:475:PHE:CD1   | 7:D:141:PRO:HG3   | 2.55                     | 0.41              |
| 25:B:606:CLA:H192 | 25:B:616:CLA:H52  | 2.02                     | 0.41              |
| 25:B:607:CLA:C17  | 25:B:613:CLA:H161 | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:B:619:BCR:H361 | 28:B:619:BCR:H20C | 1.80                     | 0.41              |
| 6:C:209:ILE:HG13  | 6:C:239:TRP:CD1   | 2.55                     | 0.41              |
| 6:C:239:TRP:CZ3   | 25:Y:315:CLA:CMB  | 3.03                     | 0.41              |
| 25:C:509:CLA:H3A  | 25:C:509:CLA:HBA1 | 1.90                     | 0.41              |
| 7:D:90:LEU:O      | 7:D:92:LEU:HG     | 2.20                     | 0.41              |
| 7:D:202:VAL:HG13  | 25:D:402:CLA:HBB1 | 2.01                     | 0.41              |
| 26:D:406:LHG:H221 | 16:T:10:LEU:HD22  | 2.00                     | 0.41              |
| 8:E:30:LEU:HD13   | 9:F:22:VAL:HG13   | 2.02                     | 0.41              |
| 13:L:15:ARG:HG2   | 13:L:19:TYR:CE1   | 2.55                     | 0.41              |
| 18:X:87:LEU:HD12  | 18:X:87:LEU:C     | 2.45                     | 0.41              |
| 19:Z:19:LEU:HD21  | 19:Z:43:GLY:CA    | 2.41                     | 0.41              |
| 25:S:312:CLA:HBA1 | 25:S:312:CLA:CMA  | 2.38                     | 0.41              |
| 25:S:313:CLA:H61  | 25:S:313:CLA:H2   | 1.83                     | 0.41              |
| 21:G:114:VAL:HG13 | 21:G:241:ILE:HD11 | 2.01                     | 0.41              |
| 21:G:152:LEU:O    | 21:G:153:VAL:C    | 2.63                     | 0.41              |
| 21:N:152:LEU:O    | 21:N:153:VAL:C    | 2.63                     | 0.41              |
| 21:N:225:SER:O    | 21:N:229:PHE:HD1  | 2.01                     | 0.41              |
| 25:N:603:CLA:H202 | 25:N:603:CLA:H162 | 1.72                     | 0.41              |
| 22:R:55:ARG:O     | 22:R:57:LEU:HD23  | 2.20                     | 0.41              |
| 22:R:103:LYS:CG   | 22:R:105:LEU:HD11 | 2.49                     | 0.41              |
| 41:R:616:XAT:H391 | 41:R:616:XAT:H31  | 1.76                     | 0.41              |
| 1:5:191:TYR:N     | 1:5:192:PRO:CD    | 2.82                     | 0.41              |
| 2:6:127:PHE:CZ    | 2:6:145:LEU:HD12  | 2.55                     | 0.41              |
| 2:6:178:ILE:HD12  | 1:7:62:PHE:CD1    | 2.45                     | 0.41              |
| 3:8:245:GLU:HB2   | 3:8:250:LYS:O     | 2.20                     | 0.41              |
| 4:a:331:MET:HE3   | 7:d:321:LEU:HB3   | 1.99                     | 0.41              |
| 5:b:37:MET:HE1    | 25:b:607:CLA:HHD  | 2.01                     | 0.41              |
| 25:b:606:CLA:H192 | 25:b:616:CLA:H52  | 2.02                     | 0.41              |
| 25:c:512:CLA:H203 | 25:c:513:CLA:H111 | 2.02                     | 0.41              |
| 25:c:512:CLA:H162 | 25:c:513:CLA:H152 | 2.02                     | 0.41              |
| 7:d:90:LEU:O      | 7:d:92:LEU:HG     | 2.20                     | 0.41              |
| 9:f:11:THR:O      | 9:f:11:THR:HG22   | 2.20                     | 0.41              |
| 13:l:15:ARG:HG2   | 13:l:19:TYR:CE1   | 2.55                     | 0.41              |
| 15:o:163:LEU:C    | 15:o:164:MET:HE2  | 2.44                     | 0.41              |
| 15:o:196:TYR:CB   | 15:o:212:LEU:HD21 | 2.16                     | 0.41              |
| 25:s:303:CLA:H112 | 25:s:304:CLA:CMB  | 2.49                     | 0.41              |
| 21:g:132:PHE:CD1  | 21:g:133:LYS:N    | 2.88                     | 0.41              |
| 21:n:159:LEU:CD1  | 21:y:257:TRP:CG   | 2.95                     | 0.41              |
| 21:n:162:TRP:CE3  | 21:y:257:TRP:HH2  | 2.37                     | 0.41              |
| 21:y:145:ASP:OD2  | 21:y:150:PRO:HA   | 2.20                     | 0.41              |
| 21:y:231:VAL:CG1  | 25:y:314:CLA:HAC2 | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:189:SER:HA   | 22:r:192:ILE:HG22 | 2.02                     | 0.41              |
| 1:1:191:TYR:N     | 1:1:192:PRO:CD    | 2.82                     | 0.41              |
| 2:2:219:ASN:O     | 2:2:220:GLY:C     | 2.61                     | 0.41              |
| 24:2:603:CHL:HBC3 | 24:2:603:CHL:OMC  | 2.20                     | 0.41              |
| 1:3:137:GLN:HE22  | 1:3:144:LEU:HA    | 1.84                     | 0.41              |
| 4:A:56:PRO:CD     | 4:A:106:LEU:HD13  | 2.49                     | 0.41              |
| 4:A:273:PHE:HB2   | 7:D:220:GLU:OE1   | 2.20                     | 0.41              |
| 4:A:335:ASN:HB3   | 6:C:334:PRO:CB    | 2.49                     | 0.41              |
| 5:B:160:GLY:HA3   | 5:B:180:PRO:HB3   | 2.01                     | 0.41              |
| 5:B:226:TYR:CD2   | 5:B:231:MET:HB2   | 2.55                     | 0.41              |
| 5:B:347:ARG:HA    | 5:B:352:ARG:O     | 2.20                     | 0.41              |
| 25:B:613:CLA:H162 | 25:B:613:CLA:H143 | 1.55                     | 0.41              |
| 6:C:449:ARG:NH1   | 11:I:28:PRO:HG3   | 2.27                     | 0.41              |
| 25:C:505:CLA:H92  | 25:C:505:CLA:H61  | 1.74                     | 0.41              |
| 25:C:510:CLA:H141 | 25:C:510:CLA:H161 | 1.67                     | 0.41              |
| 7:D:205:VAL:HG21  | 25:D:402:CLA:H3A  | 2.02                     | 0.41              |
| 12:K:27:PRO:HB2   | 12:K:30:TYR:HD1   | 1.85                     | 0.41              |
| 29:L:103:SQD:H312 | 29:L:103:SQD:C35  | 2.51                     | 0.41              |
| 15:O:100:LYS:CE   | 15:O:105:VAL:HG22 | 2.48                     | 0.41              |
| 15:O:158:PHE:HE2  | 15:O:322:LYS:HB2  | 1.82                     | 0.41              |
| 20:S:81:ILE:CG2   | 20:S:85:LEU:HD22  | 2.50                     | 0.41              |
| 21:G:50:TRP:NE1   | 25:G:611:CLA:HED2 | 2.34                     | 0.41              |
| 21:G:112:GLY:HA3  | 25:G:604:CLA:C1C  | 2.50                     | 0.41              |
| 21:G:176:ARG:HG3  | 24:G:608:CHL:C1D  | 2.50                     | 0.41              |
| 21:G:191:TYR:N    | 21:G:192:PRO:CD   | 2.82                     | 0.41              |
| 25:N:603:CLA:C16  | 24:N:607:CHL:H193 | 2.50                     | 0.41              |
| 21:Y:121:ARG:HD2  | 21:Y:241:ILE:HG22 | 2.01                     | 0.41              |
| 21:Y:127:GLY:C    | 21:Y:137:GLN:HG3  | 2.44                     | 0.41              |
| 21:Y:210:GLU:O    | 21:Y:214:LYS:HG3  | 2.20                     | 0.41              |
| 21:Y:231:VAL:CG1  | 25:Y:314:CLA:HAC2 | 2.48                     | 0.41              |
| 25:Y:315:CLA:HBD  | 25:Y:315:CLA:CBA  | 2.49                     | 0.41              |
| 1:5:210:GLU:O     | 1:5:214:LYS:HG3   | 2.20                     | 0.41              |
| 3:8:103:LEU:CD1   | 3:8:194:TYR:HD1   | 2.16                     | 0.41              |
| 3:8:131:GLY:C     | 3:8:134:PRO:HD2   | 2.46                     | 0.41              |
| 3:8:219:GLU:O     | 3:8:223:ARG:N     | 2.49                     | 0.41              |
| 4:a:223:LEU:O     | 5:b:482:ILE:HG12  | 2.19                     | 0.41              |
| 4:a:292:THR:CB    | 6:c:428:THR:HG23  | 2.50                     | 0.41              |
| 28:b:619:BCR:H11C | 28:b:619:BCR:H341 | 1.94                     | 0.41              |
| 6:c:399:ALA:HB1   | 6:c:400:PRO:HD2   | 2.01                     | 0.41              |
| 7:d:172:PRO:HG3   | 7:d:182:PHE:CZ    | 2.55                     | 0.41              |
| 8:e:40:THR:OG1    | 8:e:42:LEU:HD13   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:s:188:TYR:O    | 20:s:192:ASN:N    | 2.54                     | 0.41              |
| 25:g:610:CLA:H62  | 25:g:612:CLA:CMA  | 2.49                     | 0.41              |
| 21:n:49:PRO:O     | 21:n:55:ARG:HA    | 2.20                     | 0.41              |
| 21:y:132:PHE:CD1  | 21:y:133:LYS:N    | 2.88                     | 0.41              |
| 25:r:603:CLA:C4C  | 25:r:608:CLA:H92  | 2.49                     | 0.41              |
| 25:r:604:CLA:HMA2 | 24:r:605:CHL:HAC2 | 2.02                     | 0.41              |
| 1:l:165:GLN:NE2   | 24:l:302:CHL:C1B  | 2.79                     | 0.41              |
| 2:2:227:MET:HE3   | 2:2:231:PHE:CE2   | 2.55                     | 0.41              |
| 1:3:191:TYR:CE2   | 1:3:212:LYS:CE    | 3.03                     | 0.41              |
| 5:B:51:VAL:HG22   | 5:B:308:LYS:HD2   | 2.01                     | 0.41              |
| 5:B:125:ASP:OD2   | 5:B:127:ARG:HG2   | 2.20                     | 0.41              |
| 5:B:157:HIS:HE1   | 25:B:606:CLA:CHB  | 2.26                     | 0.41              |
| 5:B:325:PHE:CD2   | 13:L:35:TYR:HB3   | 2.56                     | 0.41              |
| 25:B:607:CLA:H91  | 25:B:607:CLA:H111 | 1.62                     | 0.41              |
| 25:B:614:CLA:H91  | 25:B:614:CLA:H112 | 1.90                     | 0.41              |
| 25:B:616:CLA:HBC2 | 25:B:616:CLA:HMC3 | 2.03                     | 0.41              |
| 6:C:60:ILE:HG23   | 25:C:510:CLA:CMC  | 2.50                     | 0.41              |
| 7:D:41:CYS:SG     | 25:D:403:CLA:HMB1 | 2.60                     | 0.41              |
| 28:D:404:BCR:H11C | 28:D:404:BCR:H341 | 1.96                     | 0.41              |
| 15:O:290:THR:OG1  | 15:O:301:GLY:HA2  | 2.21                     | 0.41              |
| 19:Z:23:VAL:HG22  | 19:Z:40:VAL:HG13  | 2.02                     | 0.41              |
| 21:G:132:PHE:CD1  | 21:G:133:LYS:N    | 2.88                     | 0.41              |
| 21:N:176:ARG:HG3  | 24:N:608:CHL:C1D  | 2.50                     | 0.41              |
| 21:Y:91:THR:HA    | 21:Y:94:ARG:HB2   | 2.02                     | 0.41              |
| 21:Y:191:TYR:CE2  | 21:Y:212:LYS:CE   | 3.03                     | 0.41              |
| 25:Y:303:CLA:H13  | 25:Y:303:CLA:H172 | 1.80                     | 0.41              |
| 25:Y:304:CLA:H93  | 24:Y:310:CHL:C9   | 2.50                     | 0.41              |
| 25:Y:305:CLA:HMA1 | 39:Y:317:LUT:H3   | 2.01                     | 0.41              |
| 2:6:227:MET:HE3   | 2:6:231:PHE:CE2   | 2.55                     | 0.41              |
| 24:6:601:CHL:H112 | 24:6:601:CHL:H152 | 1.79                     | 0.41              |
| 1:7:132:PHE:CD1   | 1:7:133:LYS:N     | 2.88                     | 0.41              |
| 3:8:245:GLU:O     | 3:8:249:GLY:N     | 2.53                     | 0.41              |
| 4:a:43:THR:HG21   | 4:a:118:HIS:ND1   | 2.36                     | 0.41              |
| 5:b:69:LEU:HD21   | 25:b:603:CLA:OBD  | 2.20                     | 0.41              |
| 5:b:475:PHE:CD1   | 7:d:141:PRO:HG3   | 2.55                     | 0.41              |
| 6:c:109:PHE:O     | 6:c:113:VAL:HG23  | 2.19                     | 0.41              |
| 6:c:135:LEU:HD23  | 6:c:135:LEU:C     | 2.45                     | 0.41              |
| 7:d:316:TYR:O     | 7:d:320:ILE:HG12  | 2.20                     | 0.41              |
| 10:h:24:LYS:HB3   | 10:h:25:PRO:HD3   | 2.02                     | 0.41              |
| 21:g:160:ALA:HB3  | 24:g:605:CHL:OMC  | 2.20                     | 0.41              |
| 21:n:57:LYS:NZ    | 21:n:66:SER:HB2   | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:145:ASP:OD2  | 21:n:150:PRO:HA   | 2.19                     | 0.41              |
| 24:n:607:CHL:HBA2 | 24:n:607:CHL:H3A  | 1.81                     | 0.41              |
| 40:n:617:NEX:H201 | 40:n:617:NEX:H15  | 1.55                     | 0.41              |
| 21:y:97:GLU:HA    | 21:y:190:LEU:CD1  | 2.24                     | 0.41              |
| 21:y:218:ASN:OD1  | 25:y:312:CLA:CMD  | 2.67                     | 0.41              |
| 22:r:55:ARG:O     | 22:r:57:LEU:HD23  | 2.20                     | 0.41              |
| 1:1:49:PRO:O      | 1:1:55:ARG:HA     | 2.20                     | 0.41              |
| 3:4:164:PHE:HB2   | 3:4:192:GLN:CD    | 2.45                     | 0.41              |
| 3:4:251:THR:HG23  | 3:4:254:GLY:H     | 1.83                     | 0.41              |
| 29:A:411:SQD:H132 | 29:A:411:SQD:H162 | 1.70                     | 0.41              |
| 5:B:460:LEU:HD12  | 7:D:288:VAL:HG21  | 1.94                     | 0.41              |
| 26:B:621:LHG:H311 | 26:B:621:LHG:H352 | 2.02                     | 0.41              |
| 6:C:299:SER:HA    | 6:C:423:ARG:HH21  | 1.85                     | 0.41              |
| 25:C:501:CLA:H151 | 25:C:507:CLA:H102 | 2.02                     | 0.41              |
| 28:C:514:BCR:H20C | 28:C:514:BCR:H361 | 1.84                     | 0.41              |
| 7:D:92:LEU:HD22   | 25:D:403:CLA:HAA2 | 2.02                     | 0.41              |
| 15:O:190:GLU:CD   | 15:O:215:VAL:HG13 | 2.45                     | 0.41              |
| 28:T:101:BCR:HC31 | 28:b:618:BCR:H382 | 2.01                     | 0.41              |
| 20:S:146:VAL:O    | 20:S:150:THR:OG1  | 2.38                     | 0.41              |
| 21:G:62:PHE:CZ    | 21:Y:175:TYR:CE1  | 3.06                     | 0.41              |
| 24:G:601:CHL:H122 | 24:Y:308:CHL:CAB  | 2.41                     | 0.41              |
| 25:G:611:CLA:H41  | 25:G:611:CLA:H62  | 1.60                     | 0.41              |
| 21:N:132:PHE:HB2  | 24:N:607:CHL:HMA3 | 2.01                     | 0.41              |
| 25:N:613:CLA:C2C  | 25:N:613:CLA:H62  | 2.50                     | 0.41              |
| 21:Y:165:GLN:OE1  | 24:Y:307:CHL:C4A  | 2.68                     | 0.41              |
| 22:R:154:ALA:HA   | 22:R:157:VAL:HG12 | 2.03                     | 0.41              |
| 22:R:255:GLY:HA2  | 25:R:612:CLA:C4C  | 2.50                     | 0.41              |
| 2:6:92:PHE:HB3    | 2:6:96:ARG:CZ     | 2.50                     | 0.41              |
| 25:6:602:CLA:HBA1 | 25:6:602:CLA:H3A  | 1.45                     | 0.41              |
| 3:8:78:PRO:HB2    | 3:8:229:ILE:HG23  | 2.01                     | 0.41              |
| 3:8:113:VAL:HG13  | 3:8:114:LEU:N     | 2.35                     | 0.41              |
| 3:8:122:TRP:HB3   | 3:8:127:TRP:HB2   | 2.02                     | 0.41              |
| 3:8:125:VAL:O     | 3:8:125:VAL:HG12  | 2.20                     | 0.41              |
| 4:a:317:TRP:CE3   | 7:d:181:ARG:HD3   | 2.55                     | 0.41              |
| 5:b:191:ASP:HB2   | 10:h:69:GLY:O     | 2.20                     | 0.41              |
| 5:b:226:TYR:CD2   | 5:b:231:MET:HB2   | 2.55                     | 0.41              |
| 6:c:47:GLY:HA3    | 6:c:137:PRO:O     | 2.21                     | 0.41              |
| 6:c:201:ASN:O     | 6:c:231:GLU:CG    | 2.68                     | 0.41              |
| 6:c:230:LEU:HD23  | 6:c:233:ILE:HD12  | 2.03                     | 0.41              |
| 6:c:369:LEU:HD22  | 6:c:380:LEU:CD2   | 2.47                     | 0.41              |
| 21:g:112:GLY:HA3  | 25:g:604:CLA:C1C  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:176:ARG:HG3  | 24:g:608:CHL:C1D  | 2.50                     | 0.41              |
| 21:n:132:PHE:CD1  | 21:n:133:LYS:N    | 2.88                     | 0.41              |
| 21:n:247:HIS:HD1  | 21:n:247:HIS:C    | 2.28                     | 0.41              |
| 25:n:611:CLA:HBD  | 25:n:611:CLA:HAA1 | 2.02                     | 0.41              |
| 40:y:318:NEX:H201 | 40:y:318:NEX:H15  | 1.71                     | 0.41              |
| 25:r:612:CLA:HHB  | 39:r:615:LUT:C4   | 2.42                     | 0.41              |
| 2:2:125:VAL:O     | 2:2:148:LEU:HD12  | 2.21                     | 0.41              |
| 1:3:49:PRO:O      | 1:3:55:ARG:HA     | 2.20                     | 0.41              |
| 4:A:194:MET:HE1   | 4:A:302:PHE:HD2   | 1.86                     | 0.41              |
| 4:A:329:GLU:OE1   | 4:A:332:HIS:NE2   | 2.52                     | 0.41              |
| 25:A:401:CLA:H142 | 25:A:401:CLA:H112 | 1.90                     | 0.41              |
| 5:B:191:ASP:CG    | 10:H:70:ILE:HD13  | 2.46                     | 0.41              |
| 5:B:356:VAL:O     | 5:B:356:VAL:HG13  | 2.19                     | 0.41              |
| 25:B:601:CLA:H192 | 25:B:601:CLA:H162 | 1.69                     | 0.41              |
| 25:B:609:CLA:HAA1 | 25:B:609:CLA:HBD  | 2.01                     | 0.41              |
| 6:C:47:GLY:HA3    | 6:C:137:PRO:O     | 2.21                     | 0.41              |
| 6:C:225:VAL:HG13  | 6:C:289:PHE:HD1   | 1.86                     | 0.41              |
| 35:C:515:DGD:HE4  | 35:C:515:DGD:HO5E | 1.68                     | 0.41              |
| 20:S:173:LEU:O    | 20:S:176:VAL:HG22 | 2.21                     | 0.41              |
| 21:G:244:LEU:HD22 | 39:G:615:LUT:H172 | 2.03                     | 0.41              |
| 24:G:601:CHL:HMB1 | 26:Y:301:LHG:H161 | 2.02                     | 0.41              |
| 40:G:617:NEX:H31  | 40:G:617:NEX:H391 | 1.57                     | 0.41              |
| 21:N:114:VAL:HG13 | 21:N:241:ILE:HD11 | 2.02                     | 0.41              |
| 21:N:132:PHE:CD1  | 21:N:133:LYS:N    | 2.88                     | 0.41              |
| 25:N:610:CLA:C5   | 39:N:615:LUT:H28  | 2.41                     | 0.41              |
| 22:R:103:LYS:HE3  | 22:R:105:LEU:CG   | 2.50                     | 0.41              |
| 22:R:241:ALA:O    | 22:R:245:HIS:CD2  | 2.73                     | 0.41              |
| 1:5:58:TYR:HD2    | 1:5:59:LEU:HG     | 1.86                     | 0.41              |
| 24:6:601:CHL:HBB1 | 24:6:601:CHL:HHC  | 2.02                     | 0.41              |
| 1:7:145:ASP:OD1   | 1:7:154:HIS:HA    | 2.21                     | 0.41              |
| 1:7:210:GLU:O     | 1:7:214:LYS:HG3   | 2.20                     | 0.41              |
| 4:a:56:PRO:CD     | 4:a:106:LEU:HD13  | 2.50                     | 0.41              |
| 4:a:194:MET:HE1   | 4:a:302:PHE:HD2   | 1.86                     | 0.41              |
| 5:b:7:ARG:HD3     | 25:b:611:CLA:CED  | 2.50                     | 0.41              |
| 5:b:45:PHE:O      | 5:b:46:ASP:HB3    | 2.20                     | 0.41              |
| 5:b:181:VAL:O     | 5:b:181:VAL:HG23  | 2.19                     | 0.41              |
| 5:b:242:ILE:O     | 5:b:246:PHE:HD1   | 2.03                     | 0.41              |
| 6:c:230:LEU:HD23  | 6:c:230:LEU:HA    | 1.85                     | 0.41              |
| 25:c:503:CLA:H61  | 25:c:503:CLA:H101 | 1.81                     | 0.41              |
| 8:e:67:THR:CA     | 23:u:102:ARG:HH11 | 2.33                     | 0.41              |
| 12:k:30:TYR:CE2   | 19:z:5:PHE:HZ     | 2.38                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:k:43:ILE:O     | 12:k:46:PHE:HB2   | 2.21                     | 0.41              |
| 28:k:101:BCR:H15C | 28:k:101:BCR:H351 | 1.84                     | 0.41              |
| 19:z:14:ILE:O     | 19:z:18:ILE:CD1   | 2.65                     | 0.41              |
| 25:s:311:CLA:HBA1 | 25:s:311:CLA:H3A  | 1.69                     | 0.41              |
| 21:g:152:LEU:O    | 21:g:153:VAL:C    | 2.63                     | 0.41              |
| 25:g:611:CLA:HBA2 | 25:g:611:CLA:H3A  | 1.28                     | 0.41              |
| 21:y:49:PRO:O     | 21:y:55:ARG:HA    | 2.20                     | 0.41              |
| 25:y:304:CLA:H93  | 24:y:310:CHL:C9   | 2.50                     | 0.41              |
| 22:r:103:LYS:HE3  | 22:r:105:LEU:CG   | 2.50                     | 0.41              |
| 22:r:154:ALA:HA   | 22:r:157:VAL:HG12 | 2.02                     | 0.41              |
| 22:r:241:ALA:O    | 22:r:245:HIS:CD2  | 2.73                     | 0.41              |
| 25:r:612:CLA:H91  | 25:r:612:CLA:H112 | 1.58                     | 0.41              |
| 40:r:617:NEX:H35  | 40:r:617:NEX:H401 | 1.52                     | 0.41              |
| 2:2:118:VAL:O     | 2:2:122:TRP:CB    | 2.69                     | 0.41              |
| 3:4:113:VAL:HG13  | 3:4:114:LEU:N     | 2.35                     | 0.41              |
| 3:4:125:VAL:O     | 3:4:125:VAL:HG12  | 2.20                     | 0.41              |
| 5:B:53:ASP:N      | 5:B:54:PRO:HD3    | 2.36                     | 0.41              |
| 5:B:72:THR:CG2    | 5:B:80:ILE:HG22   | 2.26                     | 0.41              |
| 5:B:191:ASP:HB2   | 10:H:69:GLY:O     | 2.20                     | 0.41              |
| 6:C:30:THR:CG2    | 6:C:31:THR:HG23   | 2.46                     | 0.41              |
| 6:C:130:ILE:HD11  | 25:C:511:CLA:H13  | 2.03                     | 0.41              |
| 6:C:175:LEU:HD13  | 25:C:501:CLA:HMD1 | 2.03                     | 0.41              |
| 7:D:240:GLN:NE2   | 7:D:242:GLU:HG2   | 2.36                     | 0.41              |
| 25:D:403:CLA:H162 | 25:D:403:CLA:H122 | 1.57                     | 0.41              |
| 15:O:220:ALA:CA   | 15:O:229:GLY:HA3  | 2.50                     | 0.41              |
| 20:S:66:ASP:HA    | 20:S:78:ARG:NH2   | 2.36                     | 0.41              |
| 21:G:97:GLU:CB    | 21:G:190:LEU:HD11 | 2.48                     | 0.41              |
| 24:G:607:CHL:CMB  | 24:G:607:CHL:CBB  | 2.97                     | 0.41              |
| 25:G:610:CLA:H92  | 25:G:610:CLA:H61  | 1.69                     | 0.41              |
| 21:N:59:LEU:HD23  | 24:N:601:CHL:C2B  | 2.51                     | 0.41              |
| 21:N:131:TRP:CD1  | 21:N:131:TRP:H    | 2.38                     | 0.41              |
| 21:N:145:ASP:OD1  | 21:N:154:HIS:HA   | 2.21                     | 0.41              |
| 21:N:191:TYR:CE2  | 21:N:212:LYS:CE   | 3.03                     | 0.41              |
| 25:N:611:CLA:HBA2 | 25:N:611:CLA:H3A  | 1.40                     | 0.41              |
| 21:Y:145:ASP:OD1  | 21:Y:154:HIS:HA   | 2.21                     | 0.41              |
| 25:Y:303:CLA:HMC2 | 39:Y:317:LUT:C31  | 2.51                     | 0.41              |
| 24:R:606:CHL:O2A  | 24:R:606:CHL:H2A  | 2.20                     | 0.41              |
| 1:5:49:PRO:O      | 1:5:55:ARG:HA     | 2.20                     | 0.41              |
| 1:5:164:THR:HG21  | 24:5:302:CHL:O1D  | 2.20                     | 0.41              |
| 2:6:116:PRO:HG3   | 2:6:134:LYS:NZ    | 2.36                     | 0.41              |
| 25:6:604:CLA:H52  | 25:6:604:CLA:H12  | 1.77                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:8:122:TRP:HA    | 3:8:127:TRP:CD1   | 2.40                     | 0.41              |
| 3:8:194:TYR:OH    | 3:8:225:LYS:CG    | 2.68                     | 0.41              |
| 4:a:72:LEU:O      | 4:a:72:LEU:HG     | 2.20                     | 0.41              |
| 5:b:30:VAL:HG12   | 25:b:605:CLA:HMD3 | 2.02                     | 0.41              |
| 5:b:65:PHE:CE2    | 25:b:604:CLA:HMA2 | 2.55                     | 0.41              |
| 5:b:115:TRP:HH2   | 25:b:614:CLA:HMA2 | 1.84                     | 0.41              |
| 5:b:125:ASP:OD2   | 5:b:127:ARG:HG2   | 2.20                     | 0.41              |
| 5:b:367:PRO:HB3   | 7:d:346:VAL:HB    | 2.02                     | 0.41              |
| 25:b:610:CLA:HAA2 | 25:b:610:CLA:HBD  | 2.02                     | 0.41              |
| 25:b:610:CLA:HBB1 | 25:b:610:CLA:HHC  | 2.01                     | 0.41              |
| 25:b:615:CLA:H61  | 25:b:615:CLA:H2   | 1.87                     | 0.41              |
| 6:c:162:GLY:CA    | 6:c:248:GLY:HA2   | 2.48                     | 0.41              |
| 15:o:146:LYS:CG   | 15:o:156:PRO:HB2  | 2.51                     | 0.41              |
| 16:t:7:THR:CG2    | 28:t:101:BCR:H363 | 2.50                     | 0.41              |
| 18:x:104:VAL:O    | 18:x:107:VAL:HG22 | 2.20                     | 0.41              |
| 19:z:23:VAL:HG22  | 19:z:40:VAL:HG13  | 2.03                     | 0.41              |
| 20:s:135:ASN:HD21 | 20:s:141:CYS:N    | 2.18                     | 0.41              |
| 21:n:145:ASP:OD1  | 21:n:154:HIS:HA   | 2.21                     | 0.41              |
| 21:n:210:GLU:O    | 21:n:214:LYS:HG3  | 2.20                     | 0.41              |
| 25:y:303:CLA:HMC2 | 39:y:317:LUT:C31  | 2.51                     | 0.41              |
| 25:y:314:CLA:H92  | 25:y:314:CLA:H61  | 1.56                     | 0.41              |
| 2:2:100:VAL:HG21  | 2:2:190:LEU:HD23  | 2.02                     | 0.41              |
| 1:3:145:ASP:OD1   | 1:3:154:HIS:HA    | 2.21                     | 0.41              |
| 3:4:219:GLU:CG    | 3:4:219:GLU:O     | 2.66                     | 0.41              |
| 3:4:231:HIS:HA    | 3:4:234:LEU:CD2   | 2.51                     | 0.41              |
| 4:A:120:LEU:HA    | 4:A:123:VAL:HG22  | 2.03                     | 0.41              |
| 5:B:45:PHE:O      | 5:B:46:ASP:HB3    | 2.20                     | 0.41              |
| 5:B:217:LEU:HB3   | 25:R:614:CLA:CBA  | 2.50                     | 0.41              |
| 5:B:290:ALA:O     | 5:B:294:GLU:OE1   | 2.39                     | 0.41              |
| 6:C:75:PHE:CD1    | 6:C:86:LEU:HD11   | 2.56                     | 0.41              |
| 9:F:11:THR:O      | 9:F:11:THR:HG22   | 2.20                     | 0.41              |
| 10:H:59:GLU:HA    | 10:H:62:ASN:OD1   | 2.20                     | 0.41              |
| 29:L:101:SQD:H251 | 29:L:101:SQD:H92  | 2.03                     | 0.41              |
| 20:S:175:VAL:HG22 | 24:S:307:CHL:HBC1 | 2.02                     | 0.41              |
| 21:G:109:GLY:HA2  | 39:G:616:LUT:H181 | 2.03                     | 0.41              |
| 21:G:210:GLU:O    | 21:G:214:LYS:HG3  | 2.20                     | 0.41              |
| 25:G:603:CLA:HED3 | 39:N:616:LUT:H372 | 2.02                     | 0.41              |
| 25:G:610:CLA:HBA2 | 39:G:615:LUT:O23  | 2.20                     | 0.41              |
| 25:G:614:CLA:HBA2 | 25:G:614:CLA:H3A  | 1.15                     | 0.41              |
| 21:N:57:LYS:NZ    | 21:N:66:SER:HB2   | 2.35                     | 0.41              |
| 21:N:139:PHE:CD2  | 24:N:607:CHL:OBD  | 2.74                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:145:ASP:OD2  | 21:N:150:PRO:HA   | 2.19                     | 0.41              |
| 21:N:165:GLN:NE2  | 24:N:606:CHL:NB   | 2.63                     | 0.41              |
| 25:N:612:CLA:HHC  | 25:N:612:CLA:CBB  | 2.44                     | 0.41              |
| 21:Y:58:TYR:HD2   | 21:Y:59:LEU:HG    | 1.86                     | 0.41              |
| 21:Y:95:ASN:C     | 25:Y:303:CLA:HMA1 | 2.45                     | 0.41              |
| 25:R:602:CLA:H41  | 25:R:602:CLA:H62  | 1.89                     | 0.41              |
| 25:R:614:CLA:HAA1 | 25:R:614:CLA:HBD  | 2.02                     | 0.41              |
| 1:5:145:ASP:OD1   | 1:5:154:HIS:HA    | 2.21                     | 0.41              |
| 2:6:205:ASP:O     | 2:6:209:PHE:CD1   | 2.74                     | 0.41              |
| 2:6:218:LYS:HA    | 2:6:221:ARG:NE    | 2.35                     | 0.41              |
| 1:7:58:TYR:CE2    | 1:7:59:LEU:HD12   | 2.56                     | 0.41              |
| 4:a:79:SER:CB     | 7:d:302:GLN:HE22  | 2.33                     | 0.41              |
| 5:b:127:ARG:HH22  | 10:h:31:GLY:HA3   | 1.85                     | 0.41              |
| 5:b:187:VAL:HG23  | 5:b:188:GLU:OE1   | 2.20                     | 0.41              |
| 5:b:342:GLY:HA3   | 5:b:403:GLY:O     | 2.20                     | 0.41              |
| 25:b:613:CLA:O1D  | 25:b:613:CLA:H2A  | 2.20                     | 0.41              |
| 6:c:75:PHE:CD1    | 6:c:86:LEU:HD11   | 2.56                     | 0.41              |
| 6:c:215:LYS:CD    | 6:c:221:GLU:HB3   | 2.51                     | 0.41              |
| 6:c:239:TRP:CZ3   | 25:y:315:CLA:CMB  | 3.03                     | 0.41              |
| 25:c:510:CLA:H172 | 25:c:510:CLA:C1D  | 2.51                     | 0.41              |
| 7:d:151:ILE:O     | 7:d:155:VAL:HG23  | 2.20                     | 0.41              |
| 7:d:297:TYR:O     | 7:d:316:TYR:OH    | 2.30                     | 0.41              |
| 15:o:286:THR:HG23 | 15:o:286:THR:O    | 2.19                     | 0.41              |
| 20:s:135:ASN:ND2  | 20:s:141:CYS:N    | 2.66                     | 0.41              |
| 25:s:305:CLA:HBB1 | 39:s:316:LUT:C18  | 2.51                     | 0.41              |
| 21:g:49:PRO:O     | 21:g:55:ARG:HA    | 2.20                     | 0.41              |
| 21:g:58:TYR:HD2   | 21:g:59:LEU:HG    | 1.86                     | 0.41              |
| 21:g:215:GLU:CG   | 25:g:610:CLA:NB   | 2.78                     | 0.41              |
| 24:g:601:CHL:HHC  | 24:g:601:CHL:HBB1 | 2.03                     | 0.41              |
| 25:g:602:CLA:HAB  | 39:g:616:LUT:H32  | 2.03                     | 0.41              |
| 24:g:609:CHL:H2   | 24:g:609:CHL:H61  | 1.73                     | 0.41              |
| 40:g:617:NEX:H30  | 40:g:617:NEX:C40  | 2.51                     | 0.41              |
| 21:n:131:TRP:CD1  | 21:n:131:TRP:H    | 2.38                     | 0.41              |
| 21:n:244:LEU:HD12 | 21:n:244:LEU:HA   | 1.90                     | 0.41              |
| 24:n:607:CHL:H171 | 25:y:303:CLA:H162 | 2.01                     | 0.41              |
| 24:n:609:CHL:H143 | 24:n:609:CHL:H111 | 1.91                     | 0.41              |
| 2:2:120:GLN:HB3   | 2:2:129:GLU:HG2   | 2.03                     | 0.41              |
| 1:3:229:PHE:CE2   | 1:3:240:PRO:CB    | 3.04                     | 0.41              |
| 3:4:103:LEU:HD22  | 3:4:193:GLY:HA2   | 2.02                     | 0.41              |
| 3:4:131:GLY:C     | 3:4:134:PRO:HD2   | 2.46                     | 0.41              |
| 4:A:43:THR:HG21   | 4:A:118:HIS:ND1   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:265:PHE:HE2   | 29:A:407:SQD:H92  | 1.86                     | 0.41              |
| 5:B:7:ARG:HD3     | 25:B:611:CLA:CED  | 2.50                     | 0.41              |
| 5:B:256:MET:O     | 5:B:448:ARG:HD3   | 2.20                     | 0.41              |
| 28:B:618:BCR:H382 | 28:t:101:BCR:HC31 | 2.01                     | 0.41              |
| 28:B:619:BCR:H15C | 28:B:619:BCR:H351 | 1.87                     | 0.41              |
| 11:I:28:PRO:HB3   | 17:W:131:LEU:CD1  | 2.51                     | 0.41              |
| 15:O:214:THR:HG21 | 15:O:233:VAL:HA   | 2.01                     | 0.41              |
| 19:Z:58:ASN:C     | 19:Z:58:ASN:HD22  | 2.27                     | 0.41              |
| 25:S:312:CLA:HAA2 | 25:S:312:CLA:HBD  | 2.03                     | 0.41              |
| 21:G:58:TYR:CE2   | 21:G:59:LEU:HD12  | 2.56                     | 0.41              |
| 21:G:229:PHE:CE2  | 21:G:240:PRO:CB   | 3.04                     | 0.41              |
| 21:N:49:PRO:O     | 21:N:55:ARG:HA    | 2.20                     | 0.41              |
| 21:N:91:THR:HA    | 21:N:94:ARG:HB2   | 2.02                     | 0.41              |
| 21:N:206:GLU:N    | 21:N:206:GLU:CD   | 2.76                     | 0.41              |
| 25:N:613:CLA:C14  | 25:N:613:CLA:H2   | 2.45                     | 0.41              |
| 21:Y:58:TYR:CE2   | 21:Y:59:LEU:HD12  | 2.56                     | 0.41              |
| 21:Y:107:MET:CE   | 25:Y:311:CLA:CHC  | 2.97                     | 0.41              |
| 25:Y:311:CLA:H122 | 39:Y:316:LUT:H403 | 2.01                     | 0.41              |
| 22:R:155:LEU:HD23 | 22:R:155:LEU:HA   | 1.90                     | 0.41              |
| 1:5:131:TRP:CD1   | 1:5:131:TRP:H     | 2.38                     | 0.41              |
| 2:6:104:ARG:NH1   | 2:6:108:LEU:HD11  | 2.34                     | 0.41              |
| 2:6:125:VAL:O     | 2:6:148:LEU:HD12  | 2.21                     | 0.41              |
| 2:6:139:ILE:O     | 2:6:139:ILE:CG2   | 2.68                     | 0.41              |
| 3:8:103:LEU:HD22  | 3:8:193:GLY:HA2   | 2.02                     | 0.41              |
| 4:a:273:PHE:HB2   | 7:d:220:GLU:OE1   | 2.20                     | 0.41              |
| 29:a:412:SQD:H131 | 16:t:21:ILE:CD1   | 2.51                     | 0.41              |
| 5:b:157:HIS:HE2   | 5:b:164:PRO:HD2   | 1.85                     | 0.41              |
| 5:b:207:THR:HG21  | 30:b:623:LMG:H332 | 2.02                     | 0.41              |
| 5:b:223:GLN:HG2   | 10:h:36:GLY:H     | 1.86                     | 0.41              |
| 6:c:130:ILE:HD11  | 25:c:511:CLA:H13  | 2.03                     | 0.41              |
| 6:c:166:ILE:O     | 6:c:170:VAL:HG23  | 2.21                     | 0.41              |
| 6:c:322:GLN:NE2   | 6:c:384:ILE:HD12  | 2.27                     | 0.41              |
| 10:h:59:GLU:HA    | 10:h:62:ASN:OD1   | 2.20                     | 0.41              |
| 20:s:175:VAL:HG22 | 24:s:307:CHL:HBC1 | 2.02                     | 0.41              |
| 20:s:220:LEU:O    | 20:s:224:LYS:HG3  | 2.20                     | 0.41              |
| 20:s:242:GLN:HG2  | 25:s:313:CLA:ND   | 2.36                     | 0.41              |
| 24:s:306:CHL:HBB1 | 39:s:316:LUT:H161 | 2.03                     | 0.41              |
| 21:g:191:TYR:CE2  | 21:g:212:LYS:CE   | 3.03                     | 0.41              |
| 25:g:604:CLA:CHC  | 40:g:617:NEX:H222 | 2.51                     | 0.41              |
| 24:g:608:CHL:H93  | 24:g:608:CHL:H62  | 1.82                     | 0.41              |
| 21:n:55:ARG:HE    | 21:n:55:ARG:HB2   | 1.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:n:86:SER:OG    | 25:n:602:CLA:O1A  | 2.33                     | 0.41              |
| 21:n:176:ARG:HG3  | 24:n:608:CHL:C1D  | 2.50                     | 0.41              |
| 25:n:610:CLA:HMC1 | 39:n:615:LUT:H31  | 2.00                     | 0.41              |
| 25:n:613:CLA:C2C  | 25:n:613:CLA:H62  | 2.51                     | 0.41              |
| 21:y:58:TYR:HD2   | 21:y:59:LEU:HG    | 1.86                     | 0.41              |
| 21:y:176:ARG:HG3  | 24:y:309:CHL:C1D  | 2.50                     | 0.41              |
| 21:y:228:GLY:O    | 21:y:231:VAL:N    | 2.53                     | 0.41              |
| 21:y:231:VAL:CG2  | 25:y:314:CLA:HAC2 | 2.43                     | 0.41              |
| 21:y:247:HIS:HD1  | 21:y:247:HIS:C    | 2.28                     | 0.41              |
| 26:y:319:LHG:H181 | 26:y:319:LHG:H152 | 1.91                     | 0.41              |
| 22:r:127:TYR:CE2  | 22:r:135:ARG:HD2  | 2.54                     | 0.41              |
| 25:r:602:CLA:H62  | 25:r:602:CLA:H41  | 1.89                     | 0.41              |
| 1:1:58:TYR:CE2    | 1:1:59:LEU:HD12   | 2.56                     | 0.41              |
| 2:2:116:PRO:HG3   | 2:2:134:LYS:NZ    | 2.36                     | 0.41              |
| 1:3:58:TYR:HD2    | 1:3:59:LEU:HG     | 1.86                     | 0.41              |
| 1:3:209:ALA:HA    | 1:3:212:LYS:CG    | 2.34                     | 0.41              |
| 3:4:148:THR:O     | 3:4:152:LEU:HD13  | 2.21                     | 0.41              |
| 3:4:157:GLU:O     | 3:4:161:TRP:CD1   | 2.65                     | 0.41              |
| 3:4:241:ILE:O     | 3:4:245:GLU:HG2   | 2.19                     | 0.41              |
| 4:A:21:ILE:O      | 4:A:30:ILE:O      | 2.39                     | 0.41              |
| 5:B:39:LEU:HD12   | 28:t:101:BCR:H271 | 1.99                     | 0.41              |
| 5:B:84:THR:HG21   | 15:o:204:PRO:CG   | 2.51                     | 0.41              |
| 5:B:181:VAL:O     | 5:B:181:VAL:HG23  | 2.19                     | 0.41              |
| 5:B:242:ILE:O     | 5:B:246:PHE:HD1   | 2.03                     | 0.41              |
| 5:B:285:TYR:HD2   | 23:U:88:TYR:CD2   | 2.39                     | 0.41              |
| 25:B:605:CLA:H162 | 25:B:609:CLA:HBB2 | 2.01                     | 0.41              |
| 6:C:261:ARG:HA    | 6:C:266:TRP:HE1   | 1.86                     | 0.41              |
| 6:C:322:GLN:NE2   | 6:C:384:ILE:HD12  | 2.27                     | 0.41              |
| 25:C:506:CLA:H13  | 25:C:506:CLA:H91  | 2.01                     | 0.41              |
| 25:C:512:CLA:H203 | 25:C:513:CLA:H111 | 2.02                     | 0.41              |
| 26:D:406:LHG:H302 | 16:T:17:ILE:HG23  | 2.03                     | 0.41              |
| 15:O:204:PRO:CG   | 5:b:84:THR:HG21   | 2.51                     | 0.41              |
| 18:X:78:GLY:O     | 18:X:81:PRO:HG2   | 2.21                     | 0.41              |
| 19:Z:18:ILE:HD12  | 19:Z:18:ILE:H     | 1.86                     | 0.41              |
| 20:S:67:ARG:NH1   | 20:S:87:GLY:HA2   | 2.35                     | 0.41              |
| 20:S:129:ILE:HD11 | 20:S:239:PHE:CE1  | 2.56                     | 0.41              |
| 20:S:135:ASN:HD21 | 20:S:141:CYS:N    | 2.18                     | 0.41              |
| 20:S:242:GLN:HG2  | 25:S:313:CLA:ND   | 2.36                     | 0.41              |
| 24:S:306:CHL:HBB1 | 39:S:316:LUT:H161 | 2.03                     | 0.41              |
| 21:G:58:TYR:HD2   | 21:G:59:LEU:HG    | 1.85                     | 0.41              |
| 21:G:78:TYR:CE1   | 24:G:601:CHL:HMD2 | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:G:145:ASP:OD1  | 21:G:154:HIS:HA   | 2.21                     | 0.41              |
| 21:G:173:GLU:OE2  | 24:G:609:CHL:NA   | 2.53                     | 0.41              |
| 25:G:604:CLA:CHC  | 40:G:617:NEX:H222 | 2.51                     | 0.41              |
| 21:N:121:ARG:HD2  | 21:N:241:ILE:HG22 | 2.03                     | 0.41              |
| 24:N:601:CHL:HMD2 | 26:N:618:LHG:HC41 | 2.03                     | 0.41              |
| 25:N:604:CLA:HBA1 | 25:N:604:CLA:H3A  | 1.79                     | 0.41              |
| 24:N:607:CHL:H112 | 24:N:607:CHL:H91  | 1.71                     | 0.41              |
| 25:N:611:CLA:HAA1 | 25:N:611:CLA:HBD  | 2.03                     | 0.41              |
| 21:Y:57:LYS:NZ    | 21:Y:66:SER:HB3   | 2.36                     | 0.41              |
| 21:Y:152:LEU:O    | 21:Y:153:VAL:C    | 2.63                     | 0.41              |
| 21:Y:229:PHE:CD2  | 21:Y:240:PRO:CB   | 3.04                     | 0.41              |
| 21:Y:229:PHE:CE2  | 21:Y:240:PRO:CB   | 3.04                     | 0.41              |
| 21:Y:252:VAL:O    | 21:Y:255:ASN:ND2  | 2.54                     | 0.41              |
| 24:Y:302:CHL:H202 | 24:Y:302:CHL:H161 | 1.75                     | 0.41              |
| 25:Y:303:CLA:H101 | 39:Y:317:LUT:H371 | 2.02                     | 0.41              |
| 22:R:103:LYS:HE3  | 22:R:105:LEU:CD2  | 2.47                     | 0.41              |
| 22:R:167:ASP:O    | 22:R:171:VAL:HG23 | 2.21                     | 0.41              |
| 25:R:603:CLA:NB   | 25:R:608:CLA:H111 | 2.35                     | 0.41              |
| 25:R:603:CLA:C4C  | 25:R:608:CLA:H92  | 2.49                     | 0.41              |
| 1:5:132:PHE:CD1   | 1:5:133:LYS:N     | 2.88                     | 0.41              |
| 1:7:91:THR:HA     | 1:7:94:ARG:HB2    | 2.02                     | 0.41              |
| 1:7:229:PHE:CD2   | 1:7:240:PRO:CB    | 3.04                     | 0.41              |
| 3:8:193:GLY:O     | 3:8:195:PRO:HD3   | 2.20                     | 0.41              |
| 4:a:201:GLY:HA3   | 4:a:286:THR:HB    | 2.03                     | 0.41              |
| 4:a:214:MET:HE2   | 4:a:214:MET:HB2   | 1.91                     | 0.41              |
| 28:a:407:BCR:H371 | 28:a:407:BCR:H24C | 1.77                     | 0.41              |
| 5:b:200:SER:OG    | 25:b:602:CLA:HMB1 | 2.21                     | 0.41              |
| 5:b:324:LEU:HD11  | 5:b:453:PHE:CZ    | 2.56                     | 0.41              |
| 5:b:391:SER:HB3   | 5:b:394:GLN:CD    | 2.46                     | 0.41              |
| 25:b:602:CLA:H93  | 25:b:602:CLA:H61  | 1.67                     | 0.41              |
| 6:c:235:GLY:O     | 6:c:239:TRP:HD1   | 2.02                     | 0.41              |
| 6:c:327:ASN:ND2   | 6:c:330:SER:HB2   | 2.34                     | 0.41              |
| 25:c:503:CLA:H193 | 25:c:503:CLA:H161 | 1.60                     | 0.41              |
| 25:c:506:CLA:H141 | 25:c:506:CLA:H162 | 1.63                     | 0.41              |
| 35:c:516:DGD:HAN2 | 35:c:516:DGD:HAW2 | 1.43                     | 0.41              |
| 7:d:240:GLN:NE2   | 7:d:242:GLU:HG2   | 2.36                     | 0.41              |
| 29:l:102:SQD:H271 | 29:l:102:SQD:C13  | 2.35                     | 0.41              |
| 19:z:16:SER:HB3   | 28:z:101:BCR:C31  | 2.51                     | 0.41              |
| 20:s:81:ILE:CG2   | 20:s:85:LEU:HD22  | 2.50                     | 0.41              |
| 20:s:177:ALA:HB1  | 24:s:306:CHL:HED2 | 2.02                     | 0.41              |
| 25:s:312:CLA:HAA2 | 25:s:312:CLA:HBD  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:g:115:PHE:HD2  | 25:g:604:CLA:HHD  | 1.83                     | 0.41              |
| 21:g:131:TRP:CD1  | 21:g:131:TRP:H    | 2.38                     | 0.41              |
| 21:g:145:ASP:OD1  | 21:g:154:HIS:HA   | 2.21                     | 0.41              |
| 21:g:244:LEU:HD22 | 39:g:615:LUT:H172 | 2.03                     | 0.41              |
| 24:g:608:CHL:CMC  | 24:g:608:CHL:HBC3 | 2.51                     | 0.41              |
| 25:g:611:CLA:H62  | 25:g:611:CLA:H41  | 1.60                     | 0.41              |
| 25:g:611:CLA:HBC2 | 25:g:611:CLA:CMC  | 2.51                     | 0.41              |
| 21:n:58:TYR:HD2   | 21:n:59:LEU:HG    | 1.86                     | 0.41              |
| 21:n:152:LEU:O    | 21:n:153:VAL:C    | 2.63                     | 0.41              |
| 21:n:191:TYR:N    | 21:n:192:PRO:CD   | 2.82                     | 0.41              |
| 21:n:225:SER:O    | 21:n:229:PHE:HD1  | 2.01                     | 0.41              |
| 21:n:227:PHE:HD2  | 25:n:602:CLA:C20  | 2.29                     | 0.41              |
| 25:n:603:CLA:C16  | 24:n:607:CHL:H193 | 2.50                     | 0.41              |
| 21:y:55:ARG:HE    | 21:y:55:ARG:HB2   | 1.36                     | 0.41              |
| 21:y:59:LEU:CD2   | 24:y:302:CHL:C2B  | 2.94                     | 0.41              |
| 21:y:145:ASP:OD1  | 21:y:154:HIS:HA   | 2.21                     | 0.41              |
| 24:y:307:CHL:H12  | 24:y:307:CHL:HED1 | 2.03                     | 0.41              |
| 24:y:309:CHL:H91  | 24:y:309:CHL:H112 | 1.60                     | 0.41              |
| 25:y:315:CLA:HED2 | 25:y:315:CLA:HBD  | 1.82                     | 0.41              |
| 26:y:319:LHG:H361 | 26:y:319:LHG:H331 | 1.71                     | 0.41              |
| 25:r:603:CLA:H111 | 25:r:603:CLA:H93  | 1.62                     | 0.41              |
| 25:r:604:CLA:HMA2 | 24:r:605:CHL:C3C  | 2.51                     | 0.41              |
| 1:1:91:THR:HA     | 1:1:94:ARG:HB2    | 2.03                     | 0.41              |
| 2:2:92:PHE:HB3    | 2:2:96:ARG:CZ     | 2.50                     | 0.41              |
| 2:2:134:LYS:O     | 2:2:137:SER:OG    | 2.22                     | 0.41              |
| 2:2:205:ASP:O     | 2:2:209:PHE:CD1   | 2.74                     | 0.41              |
| 25:2:605:CLA:HAA1 | 25:2:605:CLA:CBD  | 2.28                     | 0.41              |
| 1:3:131:TRP:CD1   | 1:3:131:TRP:H     | 2.38                     | 0.41              |
| 4:A:98:GLU:HA     | 4:A:98:GLU:OE2    | 2.20                     | 0.41              |
| 25:A:405:CLA:H112 | 25:A:405:CLA:H93  | 1.81                     | 0.41              |
| 25:B:604:CLA:H161 | 25:B:604:CLA:H141 | 1.83                     | 0.41              |
| 6:C:56:HIS:O      | 6:C:60:ILE:HG13   | 2.21                     | 0.41              |
| 6:C:67:MET:HB3    | 6:C:88:LEU:CD1    | 2.51                     | 0.41              |
| 25:C:508:CLA:O2A  | 25:C:510:CLA:H43  | 2.20                     | 0.41              |
| 25:C:513:CLA:H11  | 28:C:514:BCR:H381 | 2.02                     | 0.41              |
| 7:D:347:LEU:HD23  | 7:D:347:LEU:HA    | 1.92                     | 0.41              |
| 21:G:91:THR:HA    | 21:G:94:ARG:HB2   | 2.03                     | 0.41              |
| 25:G:611:CLA:HBC3 | 26:Y:301:LHG:H252 | 2.03                     | 0.41              |
| 22:R:113:ARG:HG2  | 22:R:115:GLU:OE2  | 2.21                     | 0.41              |
| 2:6:57:LYS:HD3    | 2:6:63:SER:OG     | 2.21                     | 0.41              |
| 2:6:118:VAL:O     | 2:6:122:TRP:CB    | 2.69                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:7:49:PRO:O      | 1:7:55:ARG:HA     | 2.20                     | 0.41              |
| 3:8:231:HIS:HA    | 3:8:234:LEU:CD2   | 2.51                     | 0.41              |
| 3:8:240:LEU:HG    | 3:8:244:PHE:CE2   | 2.56                     | 0.41              |
| 4:a:96:ILE:HG22   | 25:a:406:CLA:OBD  | 2.21                     | 0.41              |
| 4:a:104:GLU:OE2   | 15:o:166:ARG:HD2  | 2.21                     | 0.41              |
| 4:a:141:PRO:HB3   | 42:a:513:HOH:O    | 2.21                     | 0.41              |
| 4:a:147:TYR:C     | 4:a:150:PRO:HD2   | 2.46                     | 0.41              |
| 25:a:402:CLA:HBD  | 25:a:403:CLA:HAC2 | 2.03                     | 0.41              |
| 5:b:168:VAL:HG13  | 5:b:195:PRO:HG2   | 2.03                     | 0.41              |
| 5:b:217:LEU:HB3   | 25:r:614:CLA:CBA  | 2.50                     | 0.41              |
| 5:b:290:ALA:O     | 5:b:294:GLU:OE1   | 2.39                     | 0.41              |
| 25:b:601:CLA:H92  | 28:h:101:BCR:H402 | 2.03                     | 0.41              |
| 25:b:611:CLA:H122 | 25:b:611:CLA:H162 | 1.73                     | 0.41              |
| 28:b:617:BCR:H312 | 30:b:620:LMG:H341 | 2.02                     | 0.41              |
| 26:b:621:LHG:H311 | 26:b:621:LHG:H352 | 2.02                     | 0.41              |
| 6:c:175:LEU:HD13  | 25:c:501:CLA:HMD1 | 2.03                     | 0.41              |
| 25:c:513:CLA:H11  | 28:c:514:BCR:H381 | 2.02                     | 0.41              |
| 25:c:513:CLA:H93  | 28:c:514:BCR:H393 | 2.03                     | 0.41              |
| 25:c:513:CLA:H43  | 24:s:302:CHL:CBB  | 2.51                     | 0.41              |
| 10:h:47:MET:HE2   | 10:h:47:MET:HB3   | 1.91                     | 0.41              |
| 29:l:102:SQD:H251 | 29:l:102:SQD:H92  | 2.03                     | 0.41              |
| 20:s:67:ARG:HH12  | 20:s:92:ASP:CG    | 2.29                     | 0.41              |
| 26:s:301:LHG:HC91 | 24:s:302:CHL:OMC  | 2.21                     | 0.41              |
| 21:n:59:LEU:HD23  | 24:n:601:CHL:C2B  | 2.51                     | 0.41              |
| 21:n:91:THR:HA    | 21:n:94:ARG:HB2   | 2.03                     | 0.41              |
| 24:n:607:CHL:H51  | 24:n:607:CHL:H8   | 1.66                     | 0.41              |
| 21:y:58:TYR:CE2   | 21:y:59:LEU:HD12  | 2.56                     | 0.41              |
| 25:y:303:CLA:H101 | 39:y:317:LUT:H371 | 2.02                     | 0.41              |
| 40:r:617:NEX:H191 | 40:r:617:NEX:C12  | 2.51                     | 0.41              |
| 2:2:86:SER:HG     | 2:2:92:PHE:HE1    | 1.65                     | 0.40              |
| 1:3:58:TYR:CE2    | 1:3:59:LEU:HD12   | 2.56                     | 0.40              |
| 1:3:91:THR:HA     | 1:3:94:ARG:HB2    | 2.02                     | 0.40              |
| 1:3:210:GLU:O     | 1:3:214:LYS:HG3   | 2.20                     | 0.40              |
| 25:A:401:CLA:HBD  | 25:A:402:CLA:HAC2 | 2.03                     | 0.40              |
| 5:B:73:ASN:O      | 5:B:92:SER:HB2    | 2.21                     | 0.40              |
| 5:B:207:THR:HG21  | 30:B:623:LMG:H332 | 2.02                     | 0.40              |
| 6:C:185:VAL:CG2   | 6:C:230:LEU:HD13  | 2.49                     | 0.40              |
| 25:C:510:CLA:H2   | 25:C:510:CLA:H61  | 1.67                     | 0.40              |
| 7:D:20:ASP:CG     | 7:D:24:ARG:HH11   | 2.25                     | 0.40              |
| 7:D:65:ALA:HB1    | 7:D:70:GLU:OE2    | 2.21                     | 0.40              |
| 7:D:201:GLY:C     | 25:D:402:CLA:HMA1 | 2.47                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:E:67:THR:HA     | 23:U:102:ARG:HH11 | 1.86                     | 0.40              |
| 9:F:38:GLN:O      | 9:F:39:ARG:HB2    | 2.21                     | 0.40              |
| 12:K:43:ILE:O     | 12:K:46:PHE:HB2   | 2.21                     | 0.40              |
| 20:S:68:ARG:NH2   | 26:S:301:LHG:O3   | 2.53                     | 0.40              |
| 20:S:220:LEU:O    | 20:S:224:LYS:HG3  | 2.20                     | 0.40              |
| 21:G:121:ARG:HD2  | 21:G:241:ILE:HG22 | 2.02                     | 0.40              |
| 21:N:58:TYR:CE2   | 21:N:59:LEU:HD12  | 2.56                     | 0.40              |
| 24:N:606:CHL:HMB2 | 40:N:617:NEX:C39  | 2.51                     | 0.40              |
| 24:N:606:CHL:HAA1 | 40:N:617:NEX:H28  | 2.02                     | 0.40              |
| 25:N:610:CLA:H52  | 39:N:615:LUT:C30  | 2.49                     | 0.40              |
| 24:Y:309:CHL:C1   | 39:Y:316:LUT:H383 | 2.47                     | 0.40              |
| 1:7:191:TYR:CE2   | 1:7:212:LYS:CE    | 3.03                     | 0.40              |
| 5:b:42:LEU:HD11   | 5:b:93:TYR:HB3    | 2.04                     | 0.40              |
| 5:b:73:ASN:O      | 5:b:92:SER:HB2    | 2.21                     | 0.40              |
| 6:c:225:VAL:HG13  | 6:c:289:PHE:HD1   | 1.86                     | 0.40              |
| 26:c:517:LHG:HC82 | 17:w:113:TRP:HE1  | 1.84                     | 0.40              |
| 7:d:341:ILE:O     | 7:d:341:ILE:CG2   | 2.69                     | 0.40              |
| 11:i:28:PRO:HB3   | 17:w:131:LEU:CD1  | 2.51                     | 0.40              |
| 20:s:129:ILE:HD11 | 20:s:239:PHE:CE1  | 2.56                     | 0.40              |
| 21:g:62:PHE:CZ    | 21:y:175:TYR:CE1  | 3.06                     | 0.40              |
| 21:g:214:LYS:HG2  | 25:g:611:CLA:O2D  | 2.21                     | 0.40              |
| 25:g:603:CLA:HED3 | 39:n:616:LUT:H372 | 2.02                     | 0.40              |
| 21:n:139:PHE:CD2  | 24:n:607:CHL:OBD  | 2.74                     | 0.40              |
| 21:n:152:LEU:HD23 | 21:n:152:LEU:HA   | 1.92                     | 0.40              |
| 21:n:158:ILE:CD1  | 21:y:257:TRP:CE3  | 2.98                     | 0.40              |
| 21:n:229:PHE:CE2  | 21:n:240:PRO:CB   | 3.04                     | 0.40              |
| 25:y:315:CLA:HED2 | 25:y:315:CLA:CAA  | 2.48                     | 0.40              |
| 1:1:131:TRP:CD1   | 1:1:131:TRP:H     | 2.38                     | 0.40              |
| 4:A:196:PRO:HG3   | 4:A:300:PHE:CZ    | 2.57                     | 0.40              |
| 4:A:215:HIS:CE1   | 33:A:413:BCT:O2   | 2.75                     | 0.40              |
| 5:B:13:LEU:HD23   | 5:B:13:LEU:C      | 2.47                     | 0.40              |
| 5:B:42:LEU:HD11   | 5:B:93:TYR:HB3    | 2.04                     | 0.40              |
| 5:B:391:SER:HB3   | 5:B:394:GLN:OE1   | 2.21                     | 0.40              |
| 5:B:467:ILE:HG21  | 7:D:127:MET:HE2   | 2.03                     | 0.40              |
| 25:B:615:CLA:H121 | 25:B:616:CLA:HMA3 | 2.02                     | 0.40              |
| 6:C:369:LEU:HD21  | 6:C:384:ILE:CG1   | 2.46                     | 0.40              |
| 25:C:502:CLA:HAA1 | 25:C:502:CLA:CBD  | 2.40                     | 0.40              |
| 19:Z:42:SER:O     | 19:Z:43:GLY:C     | 2.63                     | 0.40              |
| 24:G:608:CHL:CMC  | 24:G:608:CHL:HBC3 | 2.51                     | 0.40              |
| 25:G:611:CLA:CMC  | 25:G:611:CLA:HBC2 | 2.51                     | 0.40              |
| 21:N:196:PHE:CE2  | 24:N:608:CHL:HBC2 | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:229:PHE:CE2  | 21:N:240:PRO:CB   | 3.04                     | 0.40              |
| 21:N:231:VAL:CG1  | 25:N:613:CLA:HAC1 | 2.46                     | 0.40              |
| 25:N:610:CLA:H62  | 25:N:610:CLA:H41  | 1.67                     | 0.40              |
| 21:Y:161:ILE:CG2  | 24:Y:308:CHL:HBC1 | 2.52                     | 0.40              |
| 22:R:189:SER:HA   | 22:R:192:ILE:HG22 | 2.02                     | 0.40              |
| 1:5:229:PHE:CE2   | 1:5:240:PRO:CB    | 3.04                     | 0.40              |
| 1:7:209:ALA:HA    | 1:7:212:LYS:CG    | 2.34                     | 0.40              |
| 4:a:223:LEU:HD12  | 7:d:140:ARG:NH2   | 2.36                     | 0.40              |
| 5:b:53:ASP:N      | 5:b:54:PRO:HD3    | 2.36                     | 0.40              |
| 5:b:347:ARG:HA    | 5:b:352:ARG:O     | 2.20                     | 0.40              |
| 25:b:605:CLA:H141 | 25:b:605:CLA:H161 | 1.73                     | 0.40              |
| 35:b:626:DGD:HA81 | 35:b:626:DGD:HA52 | 1.83                     | 0.40              |
| 6:c:56:HIS:O      | 6:c:60:ILE:HG13   | 2.21                     | 0.40              |
| 6:c:319:VAL:HG13  | 6:c:320:ARG:N     | 2.36                     | 0.40              |
| 25:c:501:CLA:H162 | 25:c:501:CLA:H143 | 1.81                     | 0.40              |
| 25:c:505:CLA:H142 | 25:c:505:CLA:H111 | 1.90                     | 0.40              |
| 25:c:508:CLA:CBB  | 25:c:509:CLA:HMA3 | 2.51                     | 0.40              |
| 25:c:508:CLA:O2A  | 25:c:510:CLA:H43  | 2.20                     | 0.40              |
| 25:c:508:CLA:CAB  | 25:c:510:CLA:H3A  | 2.50                     | 0.40              |
| 7:d:41:CYS:SG     | 25:d:403:CLA:HMB1 | 2.60                     | 0.40              |
| 7:d:179:ILE:HG21  | 25:d:401:CLA:CHD  | 2.52                     | 0.40              |
| 26:d:406:LHG:H302 | 16:t:17:ILE:HG23  | 2.03                     | 0.40              |
| 9:f:38:GLN:O      | 9:f:39:ARG:HB2    | 2.20                     | 0.40              |
| 28:h:101:BCR:H403 | 28:h:101:BCR:C23  | 2.42                     | 0.40              |
| 11:i:21:PHE:O     | 11:i:25:SER:OG    | 2.37                     | 0.40              |
| 19:z:18:ILE:HD12  | 19:z:18:ILE:H     | 1.86                     | 0.40              |
| 25:s:311:CLA:HHC  | 25:s:311:CLA:HBB1 | 2.03                     | 0.40              |
| 21:g:82:THR:HG21  | 24:y:310:CHL:CAA  | 2.49                     | 0.40              |
| 21:g:229:PHE:CE2  | 21:g:240:PRO:CB   | 3.04                     | 0.40              |
| 21:y:57:LYS:NZ    | 21:y:66:SER:HB3   | 2.36                     | 0.40              |
| 21:y:191:TYR:CE2  | 21:y:212:LYS:CE   | 3.03                     | 0.40              |
| 22:r:167:ASP:O    | 22:r:171:VAL:HG23 | 2.21                     | 0.40              |
| 22:r:174:VAL:HG23 | 22:r:175:ASP:N    | 2.36                     | 0.40              |
| 25:r:609:CLA:HAB  | 39:r:615:LUT:H32  | 2.03                     | 0.40              |
| 25:r:609:CLA:O1D  | 25:r:609:CLA:H2A  | 2.21                     | 0.40              |
| 4:A:81:ALA:CB     | 4:A:175:GLY:HA3   | 2.49                     | 0.40              |
| 4:A:110:GLY:N     | 4:A:111:PRO:CD    | 2.85                     | 0.40              |
| 5:B:198:ILE:O     | 5:B:201:HIS:HB3   | 2.21                     | 0.40              |
| 5:B:223:GLN:HG2   | 10:H:36:GLY:H     | 1.86                     | 0.40              |
| 5:B:288:VAL:O     | 5:B:292:LEU:HG    | 2.22                     | 0.40              |
| 5:B:324:LEU:HD11  | 5:B:453:PHE:CZ    | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:603:CLA:H193 | 25:B:603:CLA:H162 | 1.54                     | 0.40              |
| 6:C:118:HIS:CE1   | 30:C:520:LMG:H212 | 2.57                     | 0.40              |
| 7:D:341:ILE:O     | 7:D:341:ILE:CG2   | 2.69                     | 0.40              |
| 15:O:131:TYR:O    | 15:O:177:PRO:HA   | 2.21                     | 0.40              |
| 15:O:217:GLN:OE1  | 15:O:232:LEU:HD12 | 2.21                     | 0.40              |
| 16:T:7:THR:CG2    | 28:T:101:BCR:H363 | 2.50                     | 0.40              |
| 17:W:101:LEU:O    | 17:W:105:LEU:HD13 | 2.22                     | 0.40              |
| 18:X:104:VAL:O    | 18:X:107:VAL:HG22 | 2.20                     | 0.40              |
| 20:S:188:TYR:O    | 20:S:192:ASN:N    | 2.54                     | 0.40              |
| 20:S:213:LYS:HE3  | 20:S:213:LYS:HB3  | 1.91                     | 0.40              |
| 24:G:601:CHL:HMB3 | 26:Y:301:LHG:H161 | 2.03                     | 0.40              |
| 25:G:602:CLA:H51  | 25:G:602:CLA:HMB3 | 2.04                     | 0.40              |
| 21:Y:107:MET:HE3  | 25:Y:311:CLA:HHC  | 2.03                     | 0.40              |
| 24:Y:308:CHL:CBC  | 24:Y:308:CHL:CHD  | 2.98                     | 0.40              |
| 22:R:174:VAL:HG23 | 22:R:175:ASP:N    | 2.36                     | 0.40              |
| 2:6:100:VAL:HG21  | 2:6:190:LEU:HD23  | 2.02                     | 0.40              |
| 2:6:120:GLN:HB3   | 2:6:129:GLU:HG2   | 2.03                     | 0.40              |
| 25:6:604:CLA:HAA2 | 3:8:178:TRP:O     | 2.22                     | 0.40              |
| 1:7:229:PHE:CE2   | 1:7:240:PRO:CB    | 3.04                     | 0.40              |
| 4:a:95:PRO:HB2    | 4:a:97:TRP:CE2    | 2.56                     | 0.40              |
| 5:b:191:ASP:CG    | 10:h:70:ILE:HD13  | 2.46                     | 0.40              |
| 5:b:294:GLU:O     | 5:b:295:ASN:HB2   | 2.20                     | 0.40              |
| 5:b:324:LEU:O     | 5:b:450:TRP:HH2   | 2.04                     | 0.40              |
| 25:b:616:CLA:HBC2 | 25:b:616:CLA:HMC3 | 2.03                     | 0.40              |
| 6:c:30:THR:CG2    | 6:c:31:THR:HG23   | 2.46                     | 0.40              |
| 6:c:67:MET:HB3    | 6:c:88:LEU:CD1    | 2.51                     | 0.40              |
| 25:c:509:CLA:H161 | 25:c:509:CLA:H141 | 1.75                     | 0.40              |
| 7:d:92:LEU:HD22   | 25:d:403:CLA:HAA2 | 2.02                     | 0.40              |
| 28:k:101:BCR:H24C | 28:k:101:BCR:H371 | 1.83                     | 0.40              |
| 13:l:3:GLN:HG3    | 13:l:4:SER:N      | 2.34                     | 0.40              |
| 15:o:190:GLU:CD   | 15:o:215:VAL:HG13 | 2.45                     | 0.40              |
| 15:o:290:THR:OG1  | 15:o:301:GLY:HA2  | 2.21                     | 0.40              |
| 19:z:58:ASN:HD22  | 19:z:58:ASN:C     | 2.27                     | 0.40              |
| 25:s:312:CLA:HAA2 | 25:s:312:CLA:CBD  | 2.52                     | 0.40              |
| 24:g:601:CHL:HMB1 | 26:y:301:LHG:H161 | 2.02                     | 0.40              |
| 25:g:611:CLA:HBC2 | 26:y:301:LHG:H312 | 2.03                     | 0.40              |
| 21:n:80:TRP:CZ3   | 39:n:616:LUT:H383 | 2.57                     | 0.40              |
| 21:y:56:VAL:CG1   | 24:y:302:CHL:HBC1 | 2.51                     | 0.40              |
| 21:y:60:GLY:H     | 24:y:302:CHL:CHC  | 2.35                     | 0.40              |
| 21:y:229:PHE:CE2  | 21:y:240:PRO:CB   | 3.04                     | 0.40              |
| 25:y:313:CLA:HBB1 | 39:y:316:LUT:H14  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:r:153:GLY:HA2  | 25:r:604:CLA:C3C  | 2.51                     | 0.40              |
| 1:1:145:ASP:OD1   | 1:1:154:HIS:HA    | 2.21                     | 0.40              |
| 1:3:229:PHE:HD2   | 1:3:240:PRO:CG    | 2.35                     | 0.40              |
| 4:A:74:GLY:HA3    | 14:M:1:MET:HE2    | 2.04                     | 0.40              |
| 5:B:223:GLN:CA    | 10:H:33:VAL:HG11  | 2.45                     | 0.40              |
| 5:B:391:SER:HB3   | 5:B:394:GLN:CD    | 2.46                     | 0.40              |
| 25:C:510:CLA:CHB  | 25:C:510:CLA:H13  | 2.52                     | 0.40              |
| 7:D:54:THR:HG22   | 9:F:34:MET:HE1    | 2.04                     | 0.40              |
| 29:L:101:SQD:H292 | 29:L:101:SQD:C15  | 2.52                     | 0.40              |
| 15:O:146:LYS:CG   | 15:O:156:PRO:HB2  | 2.51                     | 0.40              |
| 19:Z:16:SER:HB3   | 28:Z:101:BCR:C31  | 2.51                     | 0.40              |
| 24:G:609:CHL:H43  | 24:N:601:CHL:H12  | 2.03                     | 0.40              |
| 21:N:58:TYR:HD2   | 21:N:59:LEU:HG    | 1.86                     | 0.40              |
| 25:N:602:CLA:HAB  | 39:N:616:LUT:H30  | 2.02                     | 0.40              |
| 25:Y:313:CLA:HBA1 | 25:Y:313:CLA:HMA2 | 2.04                     | 0.40              |
| 22:R:103:LYS:HE3  | 22:R:105:LEU:CD1  | 2.47                     | 0.40              |
| 22:R:127:TYR:OH   | 22:R:138:GLU:OE2  | 2.38                     | 0.40              |
| 25:R:603:CLA:C1D  | 25:R:608:CLA:H61  | 2.52                     | 0.40              |
| 1:5:91:THR:HA     | 1:5:94:ARG:HB2    | 2.02                     | 0.40              |
| 2:6:251:ASN:HB3   | 25:6:605:CLA:CHB  | 2.50                     | 0.40              |
| 1:7:58:TYR:HD2    | 1:7:59:LEU:HG     | 1.86                     | 0.40              |
| 3:8:155:TRP:O     | 3:8:159:LYS:HG3   | 2.21                     | 0.40              |
| 4:a:275:LEU:O     | 4:a:279:PRO:HD2   | 2.21                     | 0.40              |
| 25:a:402:CLA:H112 | 25:a:402:CLA:H142 | 1.90                     | 0.40              |
| 5:b:325:PHE:CD2   | 13:l:35:TYR:HB3   | 2.56                     | 0.40              |
| 25:b:615:CLA:H121 | 25:b:616:CLA:HMA3 | 2.02                     | 0.40              |
| 6:c:60:ILE:HG23   | 25:c:510:CLA:CMC  | 2.50                     | 0.40              |
| 6:c:75:PHE:CZ     | 6:c:77:PRO:HA     | 2.56                     | 0.40              |
| 25:c:507:CLA:H62  | 25:c:507:CLA:H41  | 1.80                     | 0.40              |
| 9:f:16:ALA:O      | 9:f:20:LEU:HD13   | 2.22                     | 0.40              |
| 38:f:101:HEM:HHC  | 38:f:101:HEM:CBB  | 2.46                     | 0.40              |
| 10:h:54:LEU:HA    | 10:h:57:ILE:HG12  | 2.03                     | 0.40              |
| 20:s:66:ASP:HA    | 20:s:78:ARG:NH2   | 2.36                     | 0.40              |
| 20:s:173:LEU:O    | 20:s:176:VAL:HG22 | 2.21                     | 0.40              |
| 21:g:58:TYR:CE2   | 21:g:59:LEU:HD12  | 2.56                     | 0.40              |
| 25:g:603:CLA:C1C  | 24:g:609:CHL:H111 | 2.52                     | 0.40              |
| 25:g:603:CLA:H102 | 25:g:603:CLA:H62  | 1.94                     | 0.40              |
| 21:n:126:PHE:HE1  | 21:n:147:LEU:HA   | 1.84                     | 0.40              |
| 21:n:229:PHE:HD2  | 21:n:240:PRO:CG   | 2.35                     | 0.40              |
| 22:r:253:PHE:CE1  | 41:r:616:XAT:H10  | 2.57                     | 0.40              |
| 24:2:601:CHL:HBA1 | 24:2:601:CHL:H3A  | 1.83                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:2:604:CLA:HAA2 | 3:4:178:TRP:O     | 2.22                     | 0.40              |
| 3:4:148:THR:HG23  | 3:4:149:GLN:N     | 2.35                     | 0.40              |
| 3:4:176:THR:OG1   | 3:4:180:LYS:CA    | 2.67                     | 0.40              |
| 3:4:240:LEU:HG    | 3:4:244:PHE:CE2   | 2.56                     | 0.40              |
| 5:B:69:LEU:HD21   | 25:B:603:CLA:OBD  | 2.20                     | 0.40              |
| 6:C:319:VAL:HG13  | 6:C:320:ARG:N     | 2.36                     | 0.40              |
| 25:C:505:CLA:CMB  | 25:C:505:CLA:HBB1 | 2.52                     | 0.40              |
| 7:D:298:ASP:CA    | 7:D:316:TYR:OH    | 2.66                     | 0.40              |
| 15:O:140:PRO:HG3  | 15:O:213:PHE:CE2  | 2.57                     | 0.40              |
| 20:S:262:PHE:CD2  | 25:S:314:CLA:CMA  | 3.04                     | 0.40              |
| 21:G:229:PHE:CD2  | 21:G:240:PRO:CB   | 3.04                     | 0.40              |
| 25:G:602:CLA:H161 | 25:G:602:CLA:H202 | 1.88                     | 0.40              |
| 24:N:601:CHL:H62  | 24:N:601:CHL:H41  | 1.58                     | 0.40              |
| 24:N:607:CHL:H51  | 24:N:607:CHL:H8   | 1.66                     | 0.40              |
| 40:R:617:NEX:H191 | 40:R:617:NEX:C12  | 2.51                     | 0.40              |
| 1:5:209:ALA:HA    | 1:5:212:LYS:CG    | 2.34                     | 0.40              |
| 3:8:142:PHE:O     | 3:8:146:LEU:CD1   | 2.70                     | 0.40              |
| 27:a:404:PHO:H13  | 27:a:404:PHO:H102 | 1.86                     | 0.40              |
| 5:b:285:TYR:HD2   | 23:u:88:TYR:CD2   | 2.39                     | 0.40              |
| 25:b:612:CLA:H193 | 25:b:612:CLA:H162 | 1.75                     | 0.40              |
| 6:c:182:PHE:CZ    | 25:s:314:CLA:HBB1 | 2.57                     | 0.40              |
| 25:c:511:CLA:H143 | 19:z:20:LEU:CD1   | 2.49                     | 0.40              |
| 28:c:514:BCR:H20C | 28:c:514:BCR:H361 | 1.84                     | 0.40              |
| 7:d:65:ALA:HB1    | 7:d:70:GLU:OE2    | 2.21                     | 0.40              |
| 7:d:201:GLY:C     | 25:d:402:CLA:HMA1 | 2.47                     | 0.40              |
| 7:d:205:VAL:HG21  | 25:d:402:CLA:H3A  | 2.02                     | 0.40              |
| 7:d:331:ALA:HB1   | 7:d:340:LEU:HD12  | 2.04                     | 0.40              |
| 17:w:108:VAL:O    | 17:w:112:ILE:CD1  | 2.70                     | 0.40              |
| 18:x:78:GLY:O     | 18:x:81:PRO:HG2   | 2.21                     | 0.40              |
| 20:s:92:ASP:HB2   | 25:s:303:CLA:HED3 | 2.04                     | 0.40              |
| 20:s:194:LEU:HB2  | 20:s:196:PHE:CE2  | 2.57                     | 0.40              |
| 20:s:213:LYS:HE3  | 20:s:213:LYS:HB3  | 1.91                     | 0.40              |
| 21:g:78:TYR:CE1   | 24:g:601:CHL:HMD2 | 2.56                     | 0.40              |
| 21:g:121:ARG:HD2  | 21:g:241:ILE:HG22 | 2.02                     | 0.40              |
| 21:n:105:TRP:CG   | 24:n:609:CHL:HMD3 | 2.57                     | 0.40              |
| 25:n:603:CLA:C1B  | 24:n:609:CHL:H122 | 2.52                     | 0.40              |
| 21:y:91:THR:HA    | 21:y:94:ARG:HB2   | 2.02                     | 0.40              |
| 25:r:601:CLA:HED3 | 26:r:618:LHG:H162 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | 1     | 200/266 (75%) | 188 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 1   | 3     | 200/266 (75%) | 188 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 1   | 5     | 200/266 (75%) | 188 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 1   | 7     | 200/266 (75%) | 188 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 2   | 2     | 203/243 (84%) | 181 (89%) | 20 (10%) | 2 (1%)   | 13          | 39  |
| 2   | 6     | 203/243 (84%) | 181 (89%) | 20 (10%) | 2 (1%)   | 13          | 39  |
| 3   | 4     | 202/212 (95%) | 183 (91%) | 18 (9%)  | 1 (0%)   | 25          | 56  |
| 3   | 8     | 202/212 (95%) | 183 (91%) | 18 (9%)  | 1 (0%)   | 25          | 56  |
| 4   | A     | 324/352 (92%) | 309 (95%) | 14 (4%)  | 1 (0%)   | 37          | 67  |
| 4   | a     | 324/352 (92%) | 308 (95%) | 15 (5%)  | 1 (0%)   | 37          | 67  |
| 5   | B     | 485/508 (96%) | 466 (96%) | 18 (4%)  | 1 (0%)   | 44          | 73  |
| 5   | b     | 485/508 (96%) | 466 (96%) | 18 (4%)  | 1 (0%)   | 44          | 73  |
| 6   | C     | 429/459 (94%) | 417 (97%) | 11 (3%)  | 1 (0%)   | 44          | 73  |
| 6   | c     | 429/459 (94%) | 417 (97%) | 11 (3%)  | 1 (0%)   | 44          | 73  |
| 7   | D     | 340/352 (97%) | 330 (97%) | 10 (3%)  | 0        | 100         | 100 |
| 7   | d     | 340/352 (97%) | 330 (97%) | 10 (3%)  | 0        | 100         | 100 |
| 8   | E     | 64/83 (77%)   | 61 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 8   | e     | 64/83 (77%)   | 61 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 9   | F     | 27/39 (69%)   | 27 (100%) | 0        | 0        | 100         | 100 |
| 9   | f     | 27/39 (69%)   | 27 (100%) | 0        | 0        | 100         | 100 |
| 10  | H     | 58/72 (81%)   | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 10  | h     | 58/72 (81%)   | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 11  | I     | 33/36 (92%)   | 28 (85%)  | 5 (15%)  | 0        | 100         | 100 |
| 11  | i     | 33/36 (92%)   | 28 (85%)  | 5 (15%)  | 0        | 100         | 100 |
| 12  | K     | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12  | k     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 13  | L     | 34/38 (90%)     | 32 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 13  | l     | 34/38 (90%)     | 32 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 14  | M     | 30/34 (88%)     | 28 (93%)   | 1 (3%)   | 1 (3%)   | 3           | 11  |
| 14  | m     | 30/34 (88%)     | 28 (93%)   | 1 (3%)   | 1 (3%)   | 3           | 11  |
| 15  | O     | 191/247 (77%)   | 183 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 15  | o     | 191/247 (77%)   | 183 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 16  | T     | 27/33 (82%)     | 25 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 16  | t     | 27/33 (82%)     | 25 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 17  | W     | 52/54 (96%)     | 50 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 17  | w     | 52/54 (96%)     | 50 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 18  | X     | 34/42 (81%)     | 33 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 18  | x     | 34/42 (81%)     | 33 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 19  | Z     | 60/62 (97%)     | 54 (90%)   | 6 (10%)  | 0        | 100         | 100 |
| 19  | z     | 60/62 (97%)     | 54 (90%)   | 6 (10%)  | 0        | 100         | 100 |
| 20  | S     | 214/232 (92%)   | 204 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 20  | s     | 214/232 (92%)   | 203 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 21  | G     | 204/232 (88%)   | 192 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 21  | N     | 200/232 (86%)   | 189 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 21  | Y     | 211/232 (91%)   | 200 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 21  | g     | 204/232 (88%)   | 192 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 21  | n     | 200/232 (86%)   | 189 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 21  | y     | 211/232 (91%)   | 200 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 22  | R     | 233/250 (93%)   | 223 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 22  | r     | 233/250 (93%)   | 223 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 23  | U     | 23/28 (82%)     | 19 (83%)   | 4 (17%)  | 0        | 100         | 100 |
| 23  | u     | 23/28 (82%)     | 19 (83%)   | 4 (17%)  | 0        | 100         | 100 |
| All | All   | 8226/9282 (89%) | 7790 (95%) | 422 (5%) | 14 (0%)  | 45          | 73  |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 123 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4     | 182 | ALA  |
| 4   | A     | 18  | CYS  |
| 14  | M     | 3   | VAL  |
| 2   | 6     | 123 | VAL  |
| 3   | 8     | 182 | ALA  |
| 4   | a     | 18  | CYS  |
| 14  | m     | 3   | VAL  |
| 2   | 2     | 64  | VAL  |
| 5   | B     | 281 | GLN  |
| 2   | 6     | 64  | VAL  |
| 5   | b     | 281 | GLN  |
| 6   | C     | 305 | THR  |
| 6   | c     | 305 | THR  |

### 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   | 1     | 154/201 (77%) | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 1   | 3     | 154/201 (77%) | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 1   | 5     | 154/201 (77%) | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 1   | 7     | 154/201 (77%) | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 2   | 2     | 164/192 (85%) | 164 (100%) | 0        | 100         | 100 |
| 2   | 6     | 164/192 (85%) | 164 (100%) | 0        | 100         | 100 |
| 3   | 4     | 156/159 (98%) | 156 (100%) | 0        | 100         | 100 |
| 3   | 8     | 156/159 (98%) | 156 (100%) | 0        | 100         | 100 |
| 4   | A     | 263/284 (93%) | 263 (100%) | 0        | 100         | 100 |
| 4   | a     | 263/284 (93%) | 263 (100%) | 0        | 100         | 100 |
| 5   | B     | 384/402 (96%) | 384 (100%) | 0        | 100         | 100 |
| 5   | b     | 384/402 (96%) | 384 (100%) | 0        | 100         | 100 |
| 6   | C     | 340/359 (95%) | 340 (100%) | 0        | 100         | 100 |
| 6   | c     | 340/359 (95%) | 340 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 7   | D     | 274/282 (97%) | 274 (100%) | 0        | 100         | 100 |
| 7   | d     | 274/282 (97%) | 274 (100%) | 0        | 100         | 100 |
| 8   | E     | 59/73 (81%)   | 59 (100%)  | 0        | 100         | 100 |
| 8   | e     | 59/73 (81%)   | 59 (100%)  | 0        | 100         | 100 |
| 9   | F     | 24/34 (71%)   | 24 (100%)  | 0        | 100         | 100 |
| 9   | f     | 24/34 (71%)   | 24 (100%)  | 0        | 100         | 100 |
| 10  | H     | 50/60 (83%)   | 50 (100%)  | 0        | 100         | 100 |
| 10  | h     | 50/60 (83%)   | 50 (100%)  | 0        | 100         | 100 |
| 11  | I     | 32/33 (97%)   | 32 (100%)  | 0        | 100         | 100 |
| 11  | i     | 32/33 (97%)   | 32 (100%)  | 0        | 100         | 100 |
| 12  | K     | 32/32 (100%)  | 32 (100%)  | 0        | 100         | 100 |
| 12  | k     | 32/32 (100%)  | 32 (100%)  | 0        | 100         | 100 |
| 13  | L     | 34/36 (94%)   | 34 (100%)  | 0        | 100         | 100 |
| 13  | l     | 34/36 (94%)   | 34 (100%)  | 0        | 100         | 100 |
| 14  | M     | 28/30 (93%)   | 28 (100%)  | 0        | 100         | 100 |
| 14  | m     | 28/30 (93%)   | 28 (100%)  | 0        | 100         | 100 |
| 15  | O     | 167/204 (82%) | 167 (100%) | 0        | 100         | 100 |
| 15  | o     | 167/204 (82%) | 167 (100%) | 0        | 100         | 100 |
| 16  | T     | 26/30 (87%)   | 26 (100%)  | 0        | 100         | 100 |
| 16  | t     | 26/30 (87%)   | 26 (100%)  | 0        | 100         | 100 |
| 17  | W     | 47/47 (100%)  | 47 (100%)  | 0        | 100         | 100 |
| 17  | w     | 47/47 (100%)  | 47 (100%)  | 0        | 100         | 100 |
| 18  | X     | 29/34 (85%)   | 29 (100%)  | 0        | 100         | 100 |
| 18  | x     | 29/34 (85%)   | 29 (100%)  | 0        | 100         | 100 |
| 19  | Z     | 54/54 (100%)  | 54 (100%)  | 0        | 100         | 100 |
| 19  | z     | 54/54 (100%)  | 54 (100%)  | 0        | 100         | 100 |
| 20  | S     | 167/180 (93%) | 167 (100%) | 0        | 100         | 100 |
| 20  | s     | 167/180 (93%) | 167 (100%) | 0        | 100         | 100 |
| 21  | G     | 157/177 (89%) | 145 (92%)  | 12 (8%)  | 11          | 32  |
| 21  | N     | 154/177 (87%) | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 21  | Y     | 162/177 (92%) | 150 (93%)  | 12 (7%)  | 11          | 33  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 21  | g     | 157/177 (89%)   | 145 (92%)  | 12 (8%)  | 11          | 32  |
| 21  | n     | 154/177 (87%)   | 142 (92%)  | 12 (8%)  | 10          | 31  |
| 21  | y     | 162/177 (92%)   | 150 (93%)  | 12 (7%)  | 11          | 33  |
| 22  | R     | 189/201 (94%)   | 189 (100%) | 0        | 100         | 100 |
| 22  | r     | 189/201 (94%)   | 189 (100%) | 0        | 100         | 100 |
| 23  | U     | 20/23 (87%)     | 20 (100%)  | 0        | 100         | 100 |
| 23  | u     | 20/23 (87%)     | 20 (100%)  | 0        | 100         | 100 |
| All | All   | 6640/7364 (90%) | 6520 (98%) | 120 (2%) | 54          | 83  |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 48  | SER  |
| 1   | 1     | 56  | VAL  |
| 1   | 1     | 68  | SER  |
| 1   | 1     | 69  | TYR  |
| 1   | 1     | 82  | THR  |
| 1   | 1     | 90  | GLU  |
| 1   | 1     | 94  | ARG  |
| 1   | 1     | 98  | LEU  |
| 1   | 1     | 159 | LEU  |
| 1   | 1     | 165 | GLN  |
| 1   | 1     | 199 | LEU  |
| 1   | 1     | 206 | GLU  |
| 1   | 3     | 48  | SER  |
| 1   | 3     | 56  | VAL  |
| 1   | 3     | 68  | SER  |
| 1   | 3     | 69  | TYR  |
| 1   | 3     | 82  | THR  |
| 1   | 3     | 90  | GLU  |
| 1   | 3     | 94  | ARG  |
| 1   | 3     | 98  | LEU  |
| 1   | 3     | 159 | LEU  |
| 1   | 3     | 165 | GLN  |
| 1   | 3     | 199 | LEU  |
| 1   | 3     | 206 | GLU  |
| 21  | G     | 48  | SER  |
| 21  | G     | 56  | VAL  |
| 21  | G     | 68  | SER  |
| 21  | G     | 69  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | G     | 82  | THR  |
| 21  | G     | 90  | GLU  |
| 21  | G     | 94  | ARG  |
| 21  | G     | 98  | LEU  |
| 21  | G     | 159 | LEU  |
| 21  | G     | 165 | GLN  |
| 21  | G     | 199 | LEU  |
| 21  | G     | 206 | GLU  |
| 21  | N     | 48  | SER  |
| 21  | N     | 56  | VAL  |
| 21  | N     | 68  | SER  |
| 21  | N     | 69  | TYR  |
| 21  | N     | 82  | THR  |
| 21  | N     | 90  | GLU  |
| 21  | N     | 94  | ARG  |
| 21  | N     | 98  | LEU  |
| 21  | N     | 159 | LEU  |
| 21  | N     | 165 | GLN  |
| 21  | N     | 199 | LEU  |
| 21  | N     | 206 | GLU  |
| 21  | Y     | 48  | SER  |
| 21  | Y     | 56  | VAL  |
| 21  | Y     | 68  | SER  |
| 21  | Y     | 69  | TYR  |
| 21  | Y     | 82  | THR  |
| 21  | Y     | 90  | GLU  |
| 21  | Y     | 94  | ARG  |
| 21  | Y     | 98  | LEU  |
| 21  | Y     | 159 | LEU  |
| 21  | Y     | 165 | GLN  |
| 21  | Y     | 199 | LEU  |
| 21  | Y     | 206 | GLU  |
| 1   | 5     | 48  | SER  |
| 1   | 5     | 56  | VAL  |
| 1   | 5     | 68  | SER  |
| 1   | 5     | 69  | TYR  |
| 1   | 5     | 82  | THR  |
| 1   | 5     | 90  | GLU  |
| 1   | 5     | 94  | ARG  |
| 1   | 5     | 98  | LEU  |
| 1   | 5     | 159 | LEU  |
| 1   | 5     | 165 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 199 | LEU  |
| 1   | 5     | 206 | GLU  |
| 1   | 7     | 48  | SER  |
| 1   | 7     | 56  | VAL  |
| 1   | 7     | 68  | SER  |
| 1   | 7     | 69  | TYR  |
| 1   | 7     | 82  | THR  |
| 1   | 7     | 90  | GLU  |
| 1   | 7     | 94  | ARG  |
| 1   | 7     | 98  | LEU  |
| 1   | 7     | 159 | LEU  |
| 1   | 7     | 165 | GLN  |
| 1   | 7     | 199 | LEU  |
| 1   | 7     | 206 | GLU  |
| 21  | g     | 48  | SER  |
| 21  | g     | 56  | VAL  |
| 21  | g     | 68  | SER  |
| 21  | g     | 69  | TYR  |
| 21  | g     | 82  | THR  |
| 21  | g     | 90  | GLU  |
| 21  | g     | 94  | ARG  |
| 21  | g     | 98  | LEU  |
| 21  | g     | 159 | LEU  |
| 21  | g     | 165 | GLN  |
| 21  | g     | 199 | LEU  |
| 21  | g     | 206 | GLU  |
| 21  | n     | 48  | SER  |
| 21  | n     | 56  | VAL  |
| 21  | n     | 68  | SER  |
| 21  | n     | 69  | TYR  |
| 21  | n     | 82  | THR  |
| 21  | n     | 90  | GLU  |
| 21  | n     | 94  | ARG  |
| 21  | n     | 98  | LEU  |
| 21  | n     | 159 | LEU  |
| 21  | n     | 165 | GLN  |
| 21  | n     | 199 | LEU  |
| 21  | n     | 206 | GLU  |
| 21  | y     | 48  | SER  |
| 21  | y     | 56  | VAL  |
| 21  | y     | 68  | SER  |
| 21  | y     | 69  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | y     | 82  | THR  |
| 21  | y     | 90  | GLU  |
| 21  | y     | 94  | ARG  |
| 21  | y     | 98  | LEU  |
| 21  | y     | 159 | LEU  |
| 21  | y     | 165 | GLN  |
| 21  | y     | 199 | LEU  |
| 21  | y     | 206 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 102 | HIS  |
| 2   | 2     | 150 | ASN  |
| 2   | 2     | 155 | HIS  |
| 5   | B     | 73  | ASN  |
| 5   | B     | 157 | HIS  |
| 5   | B     | 282 | GLN  |
| 5   | B     | 296 | GLN  |
| 5   | B     | 332 | ASN  |
| 6   | C     | 44  | ASN  |
| 6   | C     | 237 | HIS  |
| 6   | C     | 311 | GLN  |
| 6   | C     | 322 | GLN  |
| 6   | C     | 327 | ASN  |
| 7   | D     | 339 | ASN  |
| 7   | D     | 351 | ASN  |
| 9   | F     | 38  | GLN  |
| 10  | H     | 73  | ASN  |
| 11  | I     | 26  | ASN  |
| 13  | L     | 5   | ASN  |
| 13  | L     | 34  | ASN  |
| 15  | O     | 113 | GLN  |
| 15  | O     | 202 | GLN  |
| 20  | S     | 111 | GLN  |
| 20  | S     | 135 | ASN  |
| 21  | N     | 165 | GLN  |
| 21  | Y     | 243 | ASN  |
| 22  | R     | 125 | GLN  |
| 22  | R     | 245 | HIS  |
| 2   | 6     | 150 | ASN  |
| 5   | b     | 73  | ASN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | b     | 157 | HIS  |
| 5   | b     | 282 | GLN  |
| 5   | b     | 296 | GLN  |
| 5   | b     | 332 | ASN  |
| 6   | c     | 44  | ASN  |
| 6   | c     | 237 | HIS  |
| 6   | c     | 311 | GLN  |
| 6   | c     | 322 | GLN  |
| 6   | c     | 327 | ASN  |
| 7   | d     | 339 | ASN  |
| 7   | d     | 351 | ASN  |
| 9   | f     | 38  | GLN  |
| 10  | h     | 73  | ASN  |
| 11  | i     | 26  | ASN  |
| 13  | l     | 5   | ASN  |
| 13  | l     | 34  | ASN  |
| 15  | o     | 113 | GLN  |
| 15  | o     | 202 | GLN  |
| 20  | s     | 111 | GLN  |
| 20  | s     | 135 | ASN  |
| 21  | n     | 165 | GLN  |
| 21  | y     | 243 | ASN  |
| 22  | r     | 125 | GLN  |
| 22  | r     | 245 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 374 ligands modelled in this entry, 8 are monoatomic - leaving 366 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$ |
| 25  | CLA  | a     | 403 | -    | 65,73,73     | 1.59 | 10 (15%)    | 76,113,113  | 1.80 | 16 (21%)    |
| 39  | LUT  | r     | 615 | -    | 42,43,43     | 0.95 | 3 (7%)      | 51,60,60    | 1.68 | 9 (17%)     |
| 25  | CLA  | R     | 602 | 22   | 60,68,73     | 1.72 | 9 (15%)     | 70,107,113  | 1.89 | 18 (25%)    |
| 25  | CLA  | C     | 510 | -    | 65,73,73     | 1.58 | 10 (15%)    | 76,113,113  | 1.75 | 15 (19%)    |
| 32  | AJP  | y     | 322 | -    | 48,48,95     | 0.72 | 0           | 71,78,149   | 4.10 | 30 (42%)    |
| 25  | CLA  | S     | 303 | 20   | 61,69,73     | 1.71 | 10 (16%)    | 71,108,113  | 1.74 | 14 (19%)    |
| 25  | CLA  | G     | 603 | -    | 60,68,73     | 1.67 | 9 (15%)     | 70,107,113  | 1.81 | 14 (20%)    |
| 25  | CLA  | B     | 612 | 5    | 65,73,73     | 1.63 | 10 (15%)    | 76,113,113  | 1.78 | 15 (19%)    |
| 32  | AJP  | n     | 619 | -    | 48,48,95     | 0.71 | 0           | 71,78,149   | 4.14 | 33 (46%)    |
| 32  | AJP  | a     | 413 | -    | 95,95,95     | 0.63 | 0           | 143,149,149 | 3.67 | 64 (44%)    |
| 26  | LHG  | b     | 622 | -    | 48,48,48     | 0.45 | 0           | 51,54,54    | 1.15 | 4 (7%)      |
| 39  | LUT  | N     | 616 | -    | 42,43,43     | 0.91 | 3 (7%)      | 51,60,60    | 1.53 | 6 (11%)     |
| 25  | CLA  | R     | 604 | -    | 48,56,73     | 1.80 | 10 (20%)    | 55,92,113   | 1.95 | 16 (29%)    |
| 40  | NEX  | g     | 617 | 25   | 38,46,46     | 1.61 | 8 (21%)     | 50,70,70    | 2.77 | 15 (30%)    |
| 25  | CLA  | c     | 511 | 6    | 65,73,73     | 1.59 | 9 (13%)     | 76,113,113  | 2.20 | 16 (21%)    |
| 25  | CLA  | s     | 303 | 20   | 61,69,73     | 1.71 | 9 (14%)     | 71,108,113  | 1.74 | 15 (21%)    |
| 35  | DGD  | B     | 626 | -    | 63,63,67     | 0.49 | 0           | 77,77,81    | 1.29 | 6 (7%)      |
| 32  | AJP  | Y     | 320 | -    | 48,48,95     | 0.80 | 1 (2%)      | 71,78,149   | 4.20 | 33 (46%)    |
| 25  | CLA  | n     | 614 | 21   | 48,56,73     | 1.81 | 9 (18%)     | 55,92,113   | 2.02 | 12 (21%)    |
| 30  | LMG  | A     | 410 | -    | 40,40,55     | 0.48 | 0           | 48,48,63    | 1.28 | 4 (8%)      |
| 25  | CLA  | Y     | 313 | 21   | 60,68,73     | 1.79 | 10 (16%)    | 70,107,113  | 1.75 | 15 (21%)    |
| 32  | AJP  | y     | 324 | -    | 48,48,95     | 0.71 | 0           | 71,78,149   | 4.32 | 32 (45%)    |
| 26  | LHG  | B     | 622 | -    | 48,48,48     | 0.45 | 0           | 51,54,54    | 1.15 | 4 (7%)      |
| 40  | NEX  | S     | 317 | -    | 38,46,46     | 1.61 | 8 (21%)     | 50,70,70    | 2.23 | 11 (22%)    |
| 25  | CLA  | B     | 610 | -    | 65,73,73     | 1.70 | 9 (13%)     | 76,113,113  | 1.64 | 13 (17%)    |
| 25  | CLA  | n     | 612 | 21   | 60,68,73     | 1.77 | 9 (15%)     | 70,107,113  | 1.88 | 15 (21%)    |
| 26  | LHG  | S     | 318 | 25   | 48,48,48     | 0.42 | 0           | 51,54,54    | 1.19 | 4 (7%)      |
| 25  | CLA  | C     | 507 | -    | 65,73,73     | 1.65 | 9 (13%)     | 76,113,113  | 1.66 | 14 (18%)    |
| 25  | CLA  | N     | 604 | -    | 50,58,73     | 1.81 | 10 (20%)    | 58,95,113   | 2.12 | 15 (25%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | PHO  | A     | 404 | -    | 51,69,69     | 0.52 | 0        | 47,99,99    | 1.71 | 7 (14%)  |
| 25  | CLA  | B     | 611 | 5    | 65,73,73     | 1.60 | 9 (13%)  | 76,113,113  | 1.80 | 16 (21%) |
| 25  | CLA  | g     | 612 | 21   | 60,68,73     | 1.77 | 8 (13%)  | 70,107,113  | 1.71 | 12 (17%) |
| 25  | CLA  | R     | 612 | 22   | 60,68,73     | 1.64 | 10 (16%) | 70,107,113  | 2.06 | 16 (22%) |
| 25  | CLA  | r     | 608 | 22   | 58,66,73     | 1.78 | 9 (15%)  | 67,104,113  | 1.86 | 16 (23%) |
| 25  | CLA  | 2     | 602 | 2    | 60,68,73     | 1.71 | 9 (15%)  | 70,107,113  | 2.47 | 26 (37%) |
| 25  | CLA  | S     | 313 | 20   | 55,63,73     | 1.72 | 10 (18%) | 64,101,113  | 2.39 | 15 (23%) |
| 25  | CLA  | n     | 602 | 21   | 65,73,73     | 1.70 | 10 (15%) | 76,113,113  | 1.72 | 17 (22%) |
| 25  | CLA  | 2     | 604 | 26   | 55,63,73     | 1.75 | 8 (14%)  | 64,101,113  | 2.08 | 19 (29%) |
| 30  | LMG  | a     | 411 | -    | 40,40,55     | 0.48 | 0        | 48,48,63    | 1.28 | 4 (8%)   |
| 30  | LMG  | d     | 407 | -    | 46,46,55     | 0.44 | 0        | 54,54,63    | 1.21 | 4 (7%)   |
| 24  | CHL  | n     | 608 | -    | 66,74,74     | 1.48 | 10 (15%) | 73,114,114  | 1.77 | 9 (12%)  |
| 32  | AJP  | N     | 619 | -    | 48,48,95     | 0.70 | 0        | 71,78,149   | 4.14 | 33 (46%) |
| 24  | CHL  | R     | 605 | -    | 46,54,74     | 1.74 | 11 (23%) | 49,90,114   | 2.19 | 13 (26%) |
| 24  | CHL  | 2     | 601 | 2    | 64,72,74     | 1.50 | 10 (15%) | 70,111,114  | 2.05 | 14 (20%) |
| 24  | CHL  | n     | 606 | -    | 46,54,74     | 1.73 | 12 (26%) | 49,90,114   | 2.13 | 14 (28%) |
| 35  | DGD  | A     | 415 | -    | 60,60,67     | 0.49 | 0        | 74,74,81    | 1.22 | 5 (6%)   |
| 39  | LUT  | g     | 615 | -    | 42,43,43     | 0.86 | 2 (4%)   | 51,60,60    | 1.65 | 8 (15%)  |
| 24  | CHL  | N     | 609 | 21   | 66,74,74     | 1.48 | 9 (13%)  | 73,114,114  | 1.69 | 13 (17%) |
| 40  | NEX  | R     | 617 | -    | 38,46,46     | 1.68 | 7 (18%)  | 50,70,70    | 3.06 | 17 (34%) |
| 25  | CLA  | s     | 314 | 20   | 49,57,73     | 1.93 | 10 (20%) | 55,93,113   | 1.82 | 13 (23%) |
| 24  | CHL  | N     | 608 | -    | 66,74,74     | 1.48 | 10 (15%) | 73,114,114  | 1.77 | 9 (12%)  |
| 26  | LHG  | s     | 301 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.16 | 4 (7%)   |
| 25  | CLA  | n     | 604 | -    | 50,58,73     | 1.81 | 10 (20%) | 58,95,113   | 2.12 | 15 (25%) |
| 30  | LMG  | A     | 408 | -    | 48,48,55     | 0.44 | 0        | 56,56,63    | 1.20 | 5 (8%)   |
| 39  | LUT  | S     | 316 | -    | 42,43,43     | 0.89 | 4 (9%)   | 51,60,60    | 1.65 | 8 (15%)  |
| 25  | CLA  | g     | 610 | -    | 64,72,73     | 1.61 | 8 (12%)  | 74,111,113  | 2.00 | 16 (21%) |
| 31  | PL9  | a     | 410 | -    | 13,13,55     | 0.96 | 0        | 17,17,69    | 0.72 | 0        |
| 24  | CHL  | N     | 605 | 21   | 48,56,74     | 1.67 | 10 (20%) | 51,92,114   | 2.07 | 12 (23%) |
| 28  | BCR  | B     | 617 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 29  | SQD  | L     | 101 | -    | 41,42,54     | 0.88 | 1 (2%)   | 50,53,65    | 1.11 | 3 (6%)   |
| 40  | NEX  | y     | 318 | -    | 38,46,46     | 1.73 | 9 (23%)  | 50,70,70    | 2.21 | 18 (36%) |
| 25  | CLA  | Y     | 315 | 21   | 45,53,73     | 2.00 | 10 (22%) | 52,89,113   | 1.83 | 13 (25%) |
| 26  | LHG  | d     | 406 | -    | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 24  | CHL  | s     | 308 | -    | 46,54,74     | 1.75 | 12 (26%) | 49,90,114   | 2.18 | 12 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | LHG  | l     | 103 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.17 | 4 (7%)   |
| 24  | CHL  | Y     | 307 | 21   | 50,58,74     | 1.70 | 10 (20%) | 52,94,114   | 1.88 | 14 (26%) |
| 24  | CHL  | n     | 609 | 21   | 66,74,74     | 1.48 | 10 (15%) | 73,114,114  | 1.69 | 13 (17%) |
| 26  | LHG  | c     | 519 | -    | 48,48,48     | 0.45 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 25  | CLA  | R     | 614 | 22   | 45,53,73     | 2.06 | 8 (17%)  | 52,89,113   | 1.75 | 14 (26%) |
| 24  | CHL  | n     | 605 | 21   | 48,56,74     | 1.66 | 9 (18%)  | 51,92,114   | 2.06 | 12 (23%) |
| 25  | CLA  | G     | 602 | 21   | 65,73,73     | 1.70 | 10 (15%) | 76,113,113  | 1.77 | 16 (21%) |
| 24  | CHL  | Y     | 302 | 21   | 66,74,74     | 1.46 | 11 (16%) | 73,114,114  | 1.79 | 15 (20%) |
| 30  | LMG  | C     | 520 | -    | 51,51,55     | 0.45 | 0        | 59,59,63    | 1.23 | 4 (6%)   |
| 30  | LMG  | b     | 623 | -    | 55,55,55     | 0.43 | 0        | 63,63,63    | 1.23 | 4 (6%)   |
| 32  | AJP  | G     | 618 | -    | 48,48,95     | 0.88 | 1 (2%)   | 71,78,149   | 5.33 | 38 (53%) |
| 25  | CLA  | C     | 508 | 6    | 65,73,73     | 1.58 | 9 (13%)  | 76,113,113  | 1.88 | 17 (22%) |
| 26  | LHG  | 6     | 606 | 25   | 46,46,48     | 0.44 | 0        | 49,52,54    | 1.19 | 4 (8%)   |
| 28  | BCR  | b     | 618 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.27 | 10 (17%) |
| 25  | CLA  | b     | 611 | 5    | 65,73,73     | 1.60 | 9 (13%)  | 76,113,113  | 1.80 | 16 (21%) |
| 25  | CLA  | c     | 505 | 6    | 65,73,73     | 1.64 | 9 (13%)  | 76,113,113  | 1.77 | 15 (19%) |
| 25  | CLA  | C     | 511 | 6    | 65,73,73     | 1.60 | 9 (13%)  | 76,113,113  | 2.21 | 17 (22%) |
| 25  | CLA  | B     | 609 | 5    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.81 | 17 (22%) |
| 25  | CLA  | n     | 603 | -    | 65,73,73     | 1.61 | 10 (15%) | 76,113,113  | 1.73 | 16 (21%) |
| 24  | CHL  | S     | 307 | -    | 46,54,74     | 1.74 | 10 (21%) | 49,90,114   | 2.14 | 10 (20%) |
| 25  | CLA  | y     | 313 | 21   | 60,68,73     | 1.79 | 10 (16%) | 70,107,113  | 1.75 | 15 (21%) |
| 35  | DGD  | a     | 401 | -    | 60,60,67     | 0.48 | 0        | 74,74,81    | 1.22 | 5 (6%)   |
| 24  | CHL  | l     | 302 | 1    | 46,54,74     | 1.74 | 11 (23%) | 49,90,114   | 2.12 | 10 (20%) |
| 25  | CLA  | B     | 608 | 5    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.78 | 15 (19%) |
| 25  | CLA  | D     | 402 | 7    | 65,73,73     | 1.69 | 10 (15%) | 76,113,113  | 1.82 | 17 (22%) |
| 26  | LHG  | L     | 102 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.17 | 4 (7%)   |
| 28  | BCR  | Z     | 101 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 28  | BCR  | b     | 619 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.24 | 8 (14%)  |
| 25  | CLA  | 2     | 605 | -    | 48,56,73     | 1.87 | 9 (18%)  | 55,92,113   | 1.94 | 12 (21%) |
| 25  | CLA  | b     | 616 | 5    | 65,73,73     | 1.64 | 9 (13%)  | 76,113,113  | 1.69 | 13 (17%) |
| 28  | BCR  | a     | 407 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.34 | 10 (17%) |
| 29  | SQD  | A     | 411 | -    | 53,54,54     | 0.80 | 1 (1%)   | 62,65,65    | 0.97 | 2 (3%)   |
| 25  | CLA  | c     | 502 | 6    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.81 | 15 (19%) |
| 25  | CLA  | y     | 304 | -    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.76 | 15 (19%) |
| 33  | BCT  | a     | 414 | 34   | 2,3,3        | 1.20 | 0        | 2,3,3       | 4.33 | 2 (100%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | R     | 609 | 22   | 65,73,73     | 1.68 | 9 (13%)  | 76,113,113  | 1.72 | 17 (22%) |
| 26  | LHG  | R     | 618 | 25   | 41,41,48     | 0.45 | 0        | 44,47,54    | 1.23 | 4 (9%)   |
| 24  | CHL  | N     | 606 | -    | 46,54,74     | 1.73 | 12 (26%) | 49,90,114   | 2.11 | 13 (26%) |
| 24  | CHL  | G     | 607 | -    | 46,54,74     | 1.71 | 10 (21%) | 49,90,114   | 2.02 | 12 (24%) |
| 25  | CLA  | A     | 402 | -    | 65,73,73     | 1.59 | 10 (15%) | 76,113,113  | 1.80 | 16 (21%) |
| 32  | AJP  | B     | 624 | -    | 95,95,95     | 0.61 | 0        | 143,149,149 | 3.44 | 56 (39%) |
| 32  | AJP  | y     | 323 | -    | 48,48,95     | 0.74 | 0        | 71,78,149   | 4.38 | 30 (42%) |
| 25  | CLA  | c     | 509 | 6    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.79 | 12 (15%) |
| 27  | PHO  | a     | 404 | -    | 51,69,69     | 0.52 | 0        | 47,99,99    | 1.72 | 5 (10%)  |
| 32  | AJP  | y     | 321 | -    | 48,48,95     | 0.76 | 0        | 71,78,149   | 4.21 | 27 (38%) |
| 31  | PL9  | D     | 405 | -    | 55,55,55     | 0.50 | 0        | 68,69,69    | 0.79 | 0        |
| 25  | CLA  | b     | 613 | 5    | 65,73,73     | 1.63 | 9 (13%)  | 76,113,113  | 1.63 | 14 (18%) |
| 25  | CLA  | D     | 401 | 42   | 50,58,73     | 1.81 | 10 (20%) | 58,95,113   | 2.07 | 14 (24%) |
| 25  | CLA  | B     | 604 | 5    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.78 | 15 (19%) |
| 28  | BCR  | t     | 101 | -    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 41  | XAT  | r     | 616 | -    | 39,47,47     | 1.16 | 6 (15%)  | 54,74,74    | 2.42 | 16 (29%) |
| 39  | LUT  | S     | 315 | -    | 42,43,43     | 0.92 | 3 (7%)   | 51,60,60    | 1.57 | 8 (15%)  |
| 31  | PL9  | A     | 409 | -    | 13,13,55     | 0.96 | 0        | 17,17,69    | 0.72 | 0        |
| 25  | CLA  | g     | 614 | 21   | 48,56,73     | 1.89 | 9 (18%)  | 55,92,113   | 1.80 | 13 (23%) |
| 24  | CHL  | N     | 601 | 21   | 56,64,74     | 1.60 | 11 (19%) | 61,102,114  | 1.83 | 12 (19%) |
| 26  | LHG  | B     | 625 | -    | 45,45,48     | 0.44 | 0        | 48,51,54    | 1.19 | 4 (8%)   |
| 24  | CHL  | g     | 608 | -    | 66,74,74     | 1.50 | 12 (18%) | 73,114,114  | 1.76 | 12 (16%) |
| 25  | CLA  | B     | 602 | 5    | 65,73,73     | 1.67 | 9 (13%)  | 76,113,113  | 1.75 | 17 (22%) |
| 39  | LUT  | N     | 615 | -    | 42,43,43     | 0.89 | 2 (4%)   | 51,60,60    | 1.73 | 9 (17%)  |
| 40  | NEX  | r     | 617 | -    | 38,46,46     | 1.68 | 8 (21%)  | 50,70,70    | 3.05 | 17 (34%) |
| 30  | LMG  | B     | 620 | -    | 51,51,55     | 0.44 | 0        | 59,59,63    | 1.21 | 4 (6%)   |
| 25  | CLA  | S     | 310 | 20   | 55,63,73     | 1.81 | 9 (16%)  | 64,101,113  | 1.76 | 12 (18%) |
| 29  | SQD  | l     | 102 | -    | 41,42,54     | 0.88 | 1 (2%)   | 50,53,65    | 1.11 | 3 (6%)   |
| 39  | LUT  | y     | 316 | -    | 42,43,43     | 0.83 | 2 (4%)   | 51,60,60    | 1.74 | 8 (15%)  |
| 25  | CLA  | g     | 602 | 21   | 65,73,73     | 1.70 | 10 (15%) | 76,113,113  | 1.77 | 16 (21%) |
| 24  | CHL  | Y     | 310 | 21   | 56,64,74     | 1.62 | 10 (17%) | 61,102,114  | 1.84 | 11 (18%) |
| 26  | LHG  | 2     | 606 | 25   | 46,46,48     | 0.44 | 0        | 49,52,54    | 1.19 | 4 (8%)   |
| 25  | CLA  | Y     | 305 | -    | 50,58,73     | 1.89 | 9 (18%)  | 58,95,113   | 1.85 | 14 (24%) |
| 25  | CLA  | C     | 513 | 6    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.81 | 17 (22%) |
| 25  | CLA  | r     | 609 | 22   | 65,73,73     | 1.69 | 9 (13%)  | 76,113,113  | 1.73 | 17 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | SQD  | a     | 412 | -    | 53,54,54     | 0.80 | 1 (1%)   | 62,65,65    | 0.97 | 2 (3%)   |
| 24  | CHL  | S     | 302 | 20   | 46,54,74     | 1.72 | 10 (21%) | 49,90,114   | 2.08 | 11 (22%) |
| 25  | CLA  | A     | 405 | 4    | 60,68,73     | 1.68 | 10 (16%) | 70,107,113  | 1.83 | 15 (21%) |
| 24  | CHL  | S     | 308 | -    | 46,54,74     | 1.75 | 12 (26%) | 49,90,114   | 2.18 | 12 (24%) |
| 24  | CHL  | 6     | 603 | -    | 46,54,74     | 1.86 | 13 (28%) | 49,90,114   | 2.53 | 17 (34%) |
| 25  | CLA  | B     | 615 | 5    | 65,73,73     | 1.70 | 8 (12%)  | 76,113,113  | 1.71 | 16 (21%) |
| 41  | XAT  | R     | 616 | -    | 39,47,47     | 1.17 | 6 (15%)  | 54,74,74    | 2.41 | 16 (29%) |
| 25  | CLA  | c     | 512 | -    | 65,73,73     | 1.60 | 10 (15%) | 76,113,113  | 1.74 | 18 (23%) |
| 24  | CHL  | s     | 302 | 20   | 46,54,74     | 1.72 | 11 (23%) | 49,90,114   | 2.08 | 11 (22%) |
| 25  | CLA  | S     | 309 | 20   | 45,53,73     | 2.05 | 9 (20%)  | 52,89,113   | 2.10 | 13 (25%) |
| 25  | CLA  | S     | 314 | 20   | 49,57,73     | 1.92 | 10 (20%) | 55,93,113   | 1.82 | 13 (23%) |
| 32  | AJP  | S     | 319 | -    | 48,48,95     | 0.77 | 0        | 71,78,149   | 4.19 | 29 (40%) |
| 24  | CHL  | Y     | 306 | 21   | 48,56,74     | 1.67 | 10 (20%) | 51,92,114   | 2.05 | 11 (21%) |
| 25  | CLA  | C     | 509 | 6    | 65,73,73     | 1.62 | 10 (15%) | 76,113,113  | 1.79 | 13 (17%) |
| 24  | CHL  | g     | 607 | -    | 46,54,74     | 1.71 | 9 (19%)  | 49,90,114   | 2.02 | 12 (24%) |
| 24  | CHL  | Y     | 309 | -    | 66,74,74     | 1.49 | 11 (16%) | 73,114,114  | 1.71 | 13 (17%) |
| 24  | CHL  | G     | 601 | 21   | 66,74,74     | 1.46 | 11 (16%) | 73,114,114  | 1.75 | 14 (19%) |
| 39  | LUT  | y     | 317 | -    | 42,43,43     | 0.92 | 3 (7%)   | 51,60,60    | 1.50 | 6 (11%)  |
| 24  | CHL  | R     | 613 | 22   | 42,50,74     | 1.72 | 8 (19%)  | 44,85,114   | 2.28 | 10 (22%) |
| 25  | CLA  | Y     | 312 | 26   | 60,68,73     | 1.73 | 10 (16%) | 70,107,113  | 1.71 | 16 (22%) |
| 25  | CLA  | g     | 604 | 40   | 50,58,73     | 1.88 | 9 (18%)  | 58,95,113   | 1.97 | 14 (24%) |
| 25  | CLA  | N     | 612 | 21   | 60,68,73     | 1.76 | 9 (15%)  | 70,107,113  | 1.87 | 15 (21%) |
| 28  | BCR  | k     | 101 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.30 | 9 (16%)  |
| 24  | CHL  | g     | 605 | 21   | 46,54,74     | 1.72 | 11 (23%) | 49,90,114   | 2.04 | 9 (18%)  |
| 29  | SQD  | A     | 407 | -    | 49,50,54     | 0.82 | 1 (2%)   | 58,61,65    | 0.95 | 3 (5%)   |
| 25  | CLA  | G     | 610 | -    | 64,72,73     | 1.60 | 8 (12%)  | 74,111,113  | 2.00 | 17 (22%) |
| 25  | CLA  | Y     | 311 | 21   | 60,68,73     | 1.77 | 9 (15%)  | 70,107,113  | 1.80 | 16 (22%) |
| 31  | PL9  | d     | 405 | -    | 55,55,55     | 0.50 | 0        | 68,69,69    | 0.78 | 0        |
| 39  | LUT  | s     | 315 | -    | 42,43,43     | 0.92 | 3 (7%)   | 51,60,60    | 1.57 | 8 (15%)  |
| 40  | NEX  | n     | 617 | -    | 38,46,46     | 1.67 | 7 (18%)  | 50,70,70    | 2.43 | 18 (36%) |
| 27  | PHO  | a     | 405 | -    | 51,69,69     | 0.52 | 0        | 47,99,99    | 1.71 | 7 (14%)  |
| 28  | BCR  | d     | 404 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 25  | CLA  | B     | 606 | 5    | 65,73,73     | 1.57 | 9 (13%)  | 76,113,113  | 1.81 | 14 (18%) |
| 29  | SQD  | l     | 101 | -    | 53,54,54     | 0.80 | 1 (1%)   | 62,65,65    | 1.01 | 3 (4%)   |
| 39  | LUT  | s     | 316 | -    | 42,43,43     | 0.89 | 4 (9%)   | 51,60,60    | 1.65 | 8 (15%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | G     | 611 | -    | 60,68,73     | 1.66 | 8 (13%)  | 70,107,113  | 1.78 | 20 (28%) |
| 24  | CHL  | n     | 607 | -    | 66,74,74     | 1.50 | 11 (16%) | 73,114,114  | 1.75 | 12 (16%) |
| 25  | CLA  | c     | 507 | -    | 65,73,73     | 1.65 | 9 (13%)  | 76,113,113  | 1.66 | 14 (18%) |
| 26  | LHG  | b     | 625 | -    | 45,45,48     | 0.44 | 0        | 48,51,54    | 1.19 | 4 (8%)   |
| 30  | LMG  | D     | 407 | -    | 46,46,55     | 0.44 | 0        | 54,54,63    | 1.21 | 4 (7%)   |
| 24  | CHL  | R     | 606 | -    | 46,54,74     | 1.74 | 10 (21%) | 49,90,114   | 2.01 | 9 (18%)  |
| 40  | NEX  | N     | 617 | -    | 38,46,46     | 1.67 | 7 (18%)  | 50,70,70    | 2.43 | 18 (36%) |
| 39  | LUT  | G     | 615 | -    | 42,43,43     | 0.87 | 3 (7%)   | 51,60,60    | 1.65 | 8 (15%)  |
| 35  | DGD  | C     | 515 | -    | 56,56,67     | 0.48 | 0        | 70,70,81    | 1.23 | 6 (8%)   |
| 25  | CLA  | N     | 614 | 21   | 48,56,73     | 1.81 | 9 (18%)  | 55,92,113   | 2.03 | 12 (21%) |
| 29  | SQD  | L     | 103 | -    | 53,54,54     | 0.80 | 1 (1%)   | 62,65,65    | 1.01 | 3 (4%)   |
| 26  | LHG  | r     | 618 | 25   | 41,41,48     | 0.46 | 0        | 44,47,54    | 1.22 | 4 (9%)   |
| 24  | CHL  | S     | 306 | -    | 46,54,74     | 1.75 | 12 (26%) | 49,90,114   | 2.13 | 13 (26%) |
| 25  | CLA  | B     | 601 | -    | 65,73,73     | 1.58 | 9 (13%)  | 76,113,113  | 1.92 | 15 (19%) |
| 24  | CHL  | 6     | 601 | 2    | 64,72,74     | 1.51 | 11 (17%) | 70,111,114  | 2.05 | 14 (20%) |
| 24  | CHL  | r     | 613 | 22   | 42,50,74     | 1.71 | 9 (21%)  | 44,85,114   | 2.27 | 10 (22%) |
| 25  | CLA  | S     | 312 | 20   | 49,57,73     | 1.98 | 9 (18%)  | 55,93,113   | 1.89 | 14 (25%) |
| 25  | CLA  | B     | 616 | 5    | 65,73,73     | 1.64 | 9 (13%)  | 76,113,113  | 1.69 | 13 (17%) |
| 25  | CLA  | Y     | 304 | -    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.76 | 15 (19%) |
| 25  | CLA  | s     | 305 | -    | 50,58,73     | 1.83 | 8 (16%)  | 58,95,113   | 3.36 | 19 (32%) |
| 24  | CHL  | s     | 306 | -    | 46,54,74     | 1.74 | 12 (26%) | 49,90,114   | 2.13 | 13 (26%) |
| 24  | CHL  | y     | 308 | -    | 58,66,74     | 1.60 | 11 (18%) | 63,104,114  | 1.92 | 13 (20%) |
| 40  | NEX  | Y     | 318 | -    | 38,46,46     | 1.73 | 8 (21%)  | 50,70,70    | 2.21 | 18 (36%) |
| 25  | CLA  | g     | 603 | -    | 60,68,73     | 1.67 | 9 (15%)  | 70,107,113  | 1.81 | 14 (20%) |
| 25  | CLA  | r     | 610 | 26   | 49,57,73     | 1.85 | 8 (16%)  | 55,93,113   | 3.07 | 16 (29%) |
| 26  | LHG  | C     | 518 | -    | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 28  | BCR  | K     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.30 | 9 (16%)  |
| 30  | LMG  | B     | 623 | -    | 55,55,55     | 0.43 | 0        | 63,63,63    | 1.23 | 4 (6%)   |
| 25  | CLA  | G     | 612 | 21   | 60,68,73     | 1.77 | 9 (15%)  | 70,107,113  | 1.71 | 12 (17%) |
| 35  | DGD  | c     | 516 | -    | 63,63,67     | 0.52 | 0        | 77,77,81    | 1.23 | 6 (7%)   |
| 25  | CLA  | S     | 311 | 26   | 56,64,73     | 1.72 | 9 (16%)  | 65,102,113  | 2.18 | 13 (20%) |
| 32  | AJP  | n     | 620 | -    | 48,48,95     | 0.72 | 0        | 71,78,149   | 4.20 | 32 (45%) |
| 38  | HEM  | F     | 101 | 9    | 41,50,50     | 1.91 | 8 (19%)  | 45,82,82    | 1.71 | 6 (13%)  |
| 25  | CLA  | c     | 504 | -    | 60,68,73     | 1.65 | 8 (13%)  | 70,107,113  | 2.68 | 21 (30%) |
| 25  | CLA  | d     | 401 | 42   | 50,58,73     | 1.81 | 10 (20%) | 58,95,113   | 2.07 | 14 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | C     | 503 | 6    | 65,73,73     | 1.60 | 9 (13%)  | 76,113,113  | 1.85 | 16 (21%) |
| 25  | CLA  | b     | 610 | -    | 65,73,73     | 1.69 | 9 (13%)  | 76,113,113  | 1.64 | 13 (17%) |
| 40  | NEX  | G     | 617 | 25   | 38,46,46     | 1.52 | 8 (21%)  | 50,70,70    | 2.76 | 14 (28%) |
| 28  | BCR  | A     | 406 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.34 | 10 (17%) |
| 25  | CLA  | N     | 602 | 21   | 65,73,73     | 1.70 | 10 (15%) | 76,113,113  | 1.71 | 17 (22%) |
| 25  | CLA  | 6     | 604 | 26   | 55,63,73     | 1.75 | 8 (14%)  | 64,101,113  | 2.08 | 19 (29%) |
| 24  | CHL  | g     | 609 | 21   | 61,69,74     | 1.55 | 10 (16%) | 67,108,114  | 1.94 | 12 (17%) |
| 25  | CLA  | n     | 613 | 21   | 60,68,73     | 1.63 | 10 (16%) | 70,107,113  | 1.91 | 18 (25%) |
| 25  | CLA  | b     | 606 | 5    | 65,73,73     | 1.57 | 9 (13%)  | 76,113,113  | 1.81 | 14 (18%) |
| 25  | CLA  | B     | 614 | 5    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.82 | 13 (17%) |
| 24  | CHL  | s     | 307 | -    | 46,54,74     | 1.74 | 11 (23%) | 49,90,114   | 2.13 | 11 (22%) |
| 25  | CLA  | r     | 611 | -    | 49,57,73     | 1.95 | 10 (20%) | 55,93,113   | 3.54 | 22 (40%) |
| 29  | SQD  | a     | 408 | -    | 49,50,54     | 0.82 | 1 (2%)   | 58,61,65    | 0.95 | 3 (5%)   |
| 25  | CLA  | a     | 406 | 4    | 60,68,73     | 1.68 | 10 (16%) | 70,107,113  | 1.83 | 15 (21%) |
| 35  | DGD  | C     | 516 | -    | 63,63,67     | 0.52 | 0        | 77,77,81    | 1.23 | 6 (7%)   |
| 26  | LHG  | y     | 319 | 25   | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 30  | LMG  | c     | 520 | -    | 51,51,55     | 0.45 | 0        | 59,59,63    | 1.23 | 4 (6%)   |
| 25  | CLA  | c     | 508 | 6    | 65,73,73     | 1.58 | 9 (13%)  | 76,113,113  | 1.88 | 16 (21%) |
| 25  | CLA  | g     | 611 | -    | 60,68,73     | 1.67 | 10 (16%) | 70,107,113  | 1.79 | 20 (28%) |
| 25  | CLA  | Y     | 314 | 21   | 65,73,73     | 1.57 | 9 (13%)  | 76,113,113  | 1.89 | 14 (18%) |
| 38  | HEM  | f     | 101 | 9    | 41,50,50     | 1.91 | 9 (21%)  | 45,82,82    | 1.71 | 6 (13%)  |
| 25  | CLA  | C     | 512 | -    | 65,73,73     | 1.60 | 10 (15%) | 76,113,113  | 1.74 | 19 (25%) |
| 25  | CLA  | C     | 506 | 6    | 65,73,73     | 1.69 | 9 (13%)  | 76,113,113  | 1.70 | 16 (21%) |
| 25  | CLA  | B     | 613 | 5    | 65,73,73     | 1.64 | 9 (13%)  | 76,113,113  | 1.63 | 14 (18%) |
| 32  | AJP  | N     | 620 | -    | 48,48,95     | 0.72 | 0        | 71,78,149   | 4.20 | 32 (45%) |
| 24  | CHL  | N     | 607 | -    | 66,74,74     | 1.50 | 11 (16%) | 73,114,114  | 1.75 | 12 (16%) |
| 39  | LUT  | n     | 615 | -    | 42,43,43     | 0.88 | 2 (4%)   | 51,60,60    | 1.72 | 9 (17%)  |
| 32  | AJP  | Y     | 322 | -    | 48,48,95     | 0.72 | 0        | 71,78,149   | 4.09 | 30 (42%) |
| 26  | LHG  | D     | 406 | -    | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 25  | CLA  | S     | 304 | -    | 45,53,73     | 1.92 | 10 (22%) | 52,89,113   | 2.09 | 10 (19%) |
| 24  | CHL  | Y     | 308 | -    | 58,66,74     | 1.60 | 10 (17%) | 63,104,114  | 1.92 | 13 (20%) |
| 24  | CHL  | n     | 601 | 21   | 56,64,74     | 1.60 | 11 (19%) | 61,102,114  | 1.82 | 12 (19%) |
| 25  | CLA  | C     | 501 | -    | 65,73,73     | 1.58 | 8 (12%)  | 76,113,113  | 2.48 | 20 (26%) |
| 28  | BCR  | i     | 101 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.27 | 9 (16%)  |
| 25  | CLA  | n     | 610 | 21   | 65,73,73     | 1.71 | 9 (13%)  | 76,113,113  | 1.75 | 16 (21%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | BCR  | C     | 514 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 25  | CLA  | a     | 402 | 4    | 65,73,73     | 1.60 | 10 (15%) | 76,113,113  | 1.74 | 16 (21%) |
| 24  | CHL  | G     | 609 | 21   | 61,69,74     | 1.55 | 11 (18%) | 67,108,114  | 1.92 | 13 (19%) |
| 25  | CLA  | C     | 505 | 6    | 65,73,73     | 1.64 | 9 (13%)  | 76,113,113  | 1.76 | 15 (19%) |
| 25  | CLA  | c     | 503 | 6    | 65,73,73     | 1.61 | 9 (13%)  | 76,113,113  | 1.85 | 16 (21%) |
| 25  | CLA  | R     | 611 | -    | 49,57,73     | 1.96 | 10 (20%) | 55,93,113   | 3.54 | 22 (40%) |
| 25  | CLA  | b     | 609 | 5    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.81 | 17 (22%) |
| 25  | CLA  | b     | 603 | -    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.71 | 15 (19%) |
| 25  | CLA  | b     | 612 | 5    | 65,73,73     | 1.62 | 10 (15%) | 76,113,113  | 1.78 | 15 (19%) |
| 39  | LUT  | Y     | 316 | -    | 42,43,43     | 0.83 | 2 (4%)   | 51,60,60    | 1.73 | 9 (17%)  |
| 24  | CHL  | r     | 606 | -    | 46,54,74     | 1.73 | 9 (19%)  | 49,90,114   | 2.00 | 9 (18%)  |
| 25  | CLA  | d     | 403 | -    | 65,73,73     | 1.60 | 8 (12%)  | 76,113,113  | 2.73 | 21 (27%) |
| 25  | CLA  | n     | 611 | 26   | 60,68,73     | 1.72 | 10 (16%) | 70,107,113  | 1.69 | 16 (22%) |
| 30  | LMG  | b     | 620 | -    | 51,51,55     | 0.44 | 0        | 59,59,63    | 1.20 | 4 (6%)   |
| 25  | CLA  | s     | 313 | 20   | 55,63,73     | 1.72 | 10 (18%) | 64,101,113  | 2.40 | 15 (23%) |
| 32  | AJP  | A     | 412 | -    | 95,95,95     | 0.63 | 0        | 143,149,149 | 3.67 | 64 (44%) |
| 25  | CLA  | G     | 613 | 21   | 65,73,73     | 1.58 | 10 (15%) | 76,113,113  | 1.92 | 15 (19%) |
| 26  | LHG  | n     | 618 | 25   | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.15 | 4 (7%)   |
| 28  | BCR  | I     | 101 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.28 | 9 (16%)  |
| 25  | CLA  | r     | 601 | -    | 49,57,73     | 1.84 | 9 (18%)  | 55,93,113   | 3.32 | 18 (32%) |
| 33  | BCT  | A     | 413 | 34   | 2,3,3        | 1.20 | 0        | 2,3,3       | 4.33 | 2 (100%) |
| 25  | CLA  | y     | 315 | 21   | 45,53,73     | 2.01 | 10 (22%) | 52,89,113   | 1.82 | 13 (25%) |
| 35  | DGD  | b     | 626 | -    | 63,63,67     | 0.49 | 0        | 77,77,81    | 1.29 | 6 (7%)   |
| 25  | CLA  | N     | 611 | 26   | 60,68,73     | 1.72 | 10 (16%) | 70,107,113  | 1.69 | 16 (22%) |
| 25  | CLA  | s     | 304 | -    | 45,53,73     | 1.92 | 9 (20%)  | 52,89,113   | 2.10 | 10 (19%) |
| 32  | AJP  | Y     | 324 | -    | 48,48,95     | 0.70 | 0        | 71,78,149   | 4.32 | 32 (45%) |
| 24  | CHL  | y     | 310 | 21   | 56,64,74     | 1.62 | 11 (19%) | 61,102,114  | 1.85 | 11 (18%) |
| 26  | LHG  | y     | 301 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 28  | BCR  | B     | 619 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.24 | 8 (14%)  |
| 28  | BCR  | B     | 618 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.27 | 10 (17%) |
| 25  | CLA  | g     | 613 | 21   | 65,73,73     | 1.59 | 10 (15%) | 76,113,113  | 1.92 | 14 (18%) |
| 26  | LHG  | s     | 318 | 25   | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 24  | CHL  | r     | 607 | -    | 61,69,74     | 1.55 | 11 (18%) | 67,108,114  | 1.90 | 13 (19%) |
| 25  | CLA  | 6     | 605 | -    | 48,56,73     | 1.87 | 9 (18%)  | 55,92,113   | 1.94 | 11 (20%) |
| 25  | CLA  | y     | 314 | 21   | 65,73,73     | 1.58 | 9 (13%)  | 76,113,113  | 1.90 | 14 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | y     | 305 | -    | 50,58,73     | 1.89 | 9 (18%)  | 58,95,113   | 1.85 | 14 (24%) |
| 25  | CLA  | C     | 502 | 6    | 65,73,73     | 1.63 | 9 (13%)  | 76,113,113  | 1.81 | 15 (19%) |
| 24  | CHL  | r     | 605 | -    | 46,54,74     | 1.74 | 10 (21%) | 49,90,114   | 2.19 | 13 (26%) |
| 28  | BCR  | T     | 101 | -    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 25  | CLA  | B     | 605 | 5    | 65,73,73     | 1.60 | 9 (13%)  | 76,113,113  | 1.90 | 14 (18%) |
| 26  | LHG  | C     | 517 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 25  | CLA  | c     | 510 | -    | 65,73,73     | 1.58 | 10 (15%) | 76,113,113  | 1.75 | 15 (19%) |
| 25  | CLA  | N     | 603 | -    | 65,73,73     | 1.61 | 10 (15%) | 76,113,113  | 1.73 | 16 (21%) |
| 39  | LUT  | R     | 615 | -    | 42,43,43     | 0.96 | 3 (7%)   | 51,60,60    | 1.67 | 9 (17%)  |
| 25  | CLA  | c     | 506 | 6    | 65,73,73     | 1.69 | 9 (13%)  | 76,113,113  | 1.70 | 16 (21%) |
| 24  | CHL  | l     | 301 | 1    | 46,54,74     | 1.74 | 11 (23%) | 49,90,114   | 2.02 | 11 (22%) |
| 24  | CHL  | 5     | 301 | 1    | 46,54,74     | 1.74 | 10 (21%) | 49,90,114   | 2.02 | 11 (22%) |
| 25  | CLA  | d     | 402 | 7    | 65,73,73     | 1.69 | 10 (15%) | 76,113,113  | 1.82 | 17 (22%) |
| 26  | LHG  | c     | 518 | -    | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 25  | CLA  | b     | 601 | -    | 65,73,73     | 1.57 | 9 (13%)  | 76,113,113  | 1.92 | 15 (19%) |
| 24  | CHL  | y     | 302 | 21   | 66,74,74     | 1.47 | 11 (16%) | 73,114,114  | 1.79 | 15 (20%) |
| 25  | CLA  | R     | 610 | 26   | 49,57,73     | 1.85 | 8 (16%)  | 55,93,113   | 3.07 | 16 (29%) |
| 24  | CHL  | y     | 306 | 21   | 48,56,74     | 1.67 | 10 (20%) | 51,92,114   | 2.05 | 11 (21%) |
| 25  | CLA  | r     | 603 | 22   | 60,68,73     | 1.65 | 8 (13%)  | 70,107,113  | 2.75 | 19 (27%) |
| 25  | CLA  | c     | 501 | -    | 65,73,73     | 1.58 | 8 (12%)  | 76,113,113  | 2.48 | 20 (26%) |
| 25  | CLA  | s     | 309 | 20   | 45,53,73     | 2.05 | 9 (20%)  | 52,89,113   | 2.09 | 13 (25%) |
| 32  | AJP  | s     | 319 | -    | 48,48,95     | 0.77 | 0        | 71,78,149   | 4.19 | 29 (40%) |
| 25  | CLA  | A     | 401 | 4    | 65,73,73     | 1.60 | 10 (15%) | 76,113,113  | 1.74 | 16 (21%) |
| 28  | BCR  | b     | 617 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 25  | CLA  | D     | 403 | -    | 65,73,73     | 1.60 | 8 (12%)  | 76,113,113  | 2.73 | 21 (27%) |
| 25  | CLA  | c     | 513 | 6    | 65,73,73     | 1.63 | 10 (15%) | 76,113,113  | 1.81 | 17 (22%) |
| 24  | CHL  | y     | 309 | -    | 66,74,74     | 1.49 | 11 (16%) | 73,114,114  | 1.70 | 13 (17%) |
| 28  | BCR  | c     | 514 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 24  | CHL  | R     | 607 | -    | 61,69,74     | 1.55 | 11 (18%) | 67,108,114  | 1.91 | 13 (19%) |
| 26  | LHG  | B     | 621 | -    | 46,46,48     | 0.45 | 0        | 49,52,54    | 1.18 | 4 (8%)   |
| 25  | CLA  | y     | 311 | 21   | 60,68,73     | 1.77 | 9 (15%)  | 70,107,113  | 1.80 | 16 (22%) |
| 25  | CLA  | s     | 310 | 20   | 55,63,73     | 1.80 | 9 (16%)  | 64,101,113  | 1.76 | 11 (17%) |
| 25  | CLA  | y     | 303 | 21   | 65,73,73     | 1.69 | 10 (15%) | 76,113,113  | 1.75 | 15 (19%) |
| 32  | AJP  | g     | 618 | -    | 48,48,95     | 0.88 | 1 (2%)   | 71,78,149   | 5.33 | 38 (53%) |
| 39  | LUT  | Y     | 317 | -    | 42,43,43     | 0.92 | 4 (9%)   | 51,60,60    | 1.50 | 6 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | b     | 615 | 5    | 65,73,73     | 1.70 | 8 (12%)  | 76,113,113  | 1.70 | 16 (21%) |
| 24  | CHL  | G     | 606 | -    | 50,58,74     | 1.65 | 9 (18%)  | 52,94,114   | 2.13 | 12 (23%) |
| 25  | CLA  | N     | 610 | 21   | 65,73,73     | 1.71 | 9 (13%)  | 76,113,113  | 1.74 | 16 (21%) |
| 24  | CHL  | g     | 606 | -    | 50,58,74     | 1.65 | 9 (18%)  | 52,94,114   | 2.14 | 11 (21%) |
| 24  | CHL  | 5     | 302 | 1    | 46,54,74     | 1.74 | 11 (23%) | 49,90,114   | 2.11 | 9 (18%)  |
| 35  | DGD  | c     | 515 | -    | 56,56,67     | 0.48 | 0        | 70,70,81    | 1.23 | 6 (8%)   |
| 26  | LHG  | C     | 519 | -    | 48,48,48     | 0.45 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 26  | LHG  | Y     | 319 | 25   | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 25  | CLA  | G     | 614 | 21   | 48,56,73     | 1.89 | 9 (18%)  | 55,92,113   | 1.80 | 13 (23%) |
| 25  | CLA  | R     | 601 | -    | 49,57,73     | 1.84 | 9 (18%)  | 55,93,113   | 3.30 | 18 (32%) |
| 25  | CLA  | B     | 607 | -    | 65,73,73     | 1.61 | 9 (13%)  | 76,113,113  | 1.77 | 15 (19%) |
| 39  | LUT  | n     | 616 | -    | 42,43,43     | 0.91 | 3 (7%)   | 51,60,60    | 1.53 | 6 (11%)  |
| 32  | AJP  | y     | 320 | -    | 48,48,95     | 0.80 | 1 (2%)   | 71,78,149   | 4.19 | 33 (46%) |
| 40  | NEX  | s     | 317 | -    | 38,46,46     | 1.62 | 8 (21%)  | 50,70,70    | 2.23 | 11 (22%) |
| 28  | BCR  | D     | 404 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 26  | LHG  | N     | 618 | 25   | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.15 | 4 (7%)   |
| 25  | CLA  | C     | 504 | -    | 60,68,73     | 1.66 | 8 (13%)  | 70,107,113  | 2.67 | 21 (30%) |
| 32  | AJP  | Y     | 323 | -    | 48,48,95     | 0.74 | 0        | 71,78,149   | 4.38 | 30 (42%) |
| 24  | CHL  | G     | 608 | -    | 66,74,74     | 1.50 | 12 (18%) | 73,114,114  | 1.77 | 12 (16%) |
| 24  | CHL  | g     | 601 | 21   | 66,74,74     | 1.46 | 10 (15%) | 73,114,114  | 1.74 | 13 (17%) |
| 28  | BCR  | z     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 24  | CHL  | y     | 307 | 21   | 50,58,74     | 1.70 | 10 (20%) | 52,94,114   | 1.89 | 14 (26%) |
| 25  | CLA  | r     | 612 | 22   | 60,68,73     | 1.64 | 10 (16%) | 70,107,113  | 2.06 | 16 (22%) |
| 25  | CLA  | b     | 608 | 5    | 65,73,73     | 1.62 | 10 (15%) | 76,113,113  | 1.78 | 15 (19%) |
| 28  | BCR  | h     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.30 | 9 (16%)  |
| 25  | CLA  | b     | 614 | 5    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.82 | 13 (17%) |
| 24  | CHL  | G     | 605 | 21   | 46,54,74     | 1.73 | 10 (21%) | 49,90,114   | 2.03 | 9 (18%)  |
| 28  | BCR  | H     | 101 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.30 | 9 (16%)  |
| 39  | LUT  | G     | 616 | -    | 42,43,43     | 0.91 | 3 (7%)   | 51,60,60    | 1.44 | 4 (7%)   |
| 26  | LHG  | c     | 517 | -    | 48,48,48     | 0.43 | 0        | 51,54,54    | 1.18 | 4 (7%)   |
| 25  | CLA  | s     | 311 | 26   | 56,64,73     | 1.71 | 9 (16%)  | 65,102,113  | 2.18 | 13 (20%) |
| 25  | CLA  | r     | 602 | 22   | 60,68,73     | 1.72 | 9 (15%)  | 70,107,113  | 1.88 | 18 (25%) |
| 39  | LUT  | g     | 616 | -    | 42,43,43     | 0.91 | 3 (7%)   | 51,60,60    | 1.44 | 4 (7%)   |
| 26  | LHG  | b     | 621 | -    | 46,46,48     | 0.45 | 0        | 49,52,54    | 1.18 | 4 (8%)   |
| 25  | CLA  | s     | 312 | 20   | 49,57,73     | 1.98 | 9 (18%)  | 55,93,113   | 1.89 | 14 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | Y     | 303 | 21   | 65,73,73     | 1.69 | 10 (15%) | 76,113,113  | 1.75 | 15 (19%) |
| 25  | CLA  | 6     | 602 | 2    | 60,68,73     | 1.71 | 9 (15%)  | 70,107,113  | 2.47 | 26 (37%) |
| 24  | CHL  | 2     | 603 | -    | 46,54,74     | 1.86 | 13 (28%) | 49,90,114   | 2.53 | 17 (34%) |
| 25  | CLA  | N     | 613 | 21   | 60,68,73     | 1.63 | 10 (16%) | 70,107,113  | 1.91 | 18 (25%) |
| 25  | CLA  | b     | 602 | 5    | 65,73,73     | 1.67 | 9 (13%)  | 76,113,113  | 1.75 | 16 (21%) |
| 32  | AJP  | b     | 624 | -    | 95,95,95     | 0.61 | 0        | 143,149,149 | 3.44 | 56 (39%) |
| 25  | CLA  | r     | 604 | -    | 48,56,73     | 1.79 | 9 (18%)  | 55,92,113   | 1.95 | 16 (29%) |
| 26  | LHG  | Y     | 301 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 25  | CLA  | R     | 603 | 22   | 60,68,73     | 1.66 | 8 (13%)  | 70,107,113  | 2.74 | 19 (27%) |
| 25  | CLA  | B     | 603 | -    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.70 | 15 (19%) |
| 30  | LMG  | a     | 409 | -    | 48,48,55     | 0.44 | 0        | 56,56,63    | 1.19 | 5 (8%)   |
| 25  | CLA  | R     | 608 | 22   | 58,66,73     | 1.77 | 9 (15%)  | 67,104,113  | 1.86 | 16 (23%) |
| 25  | CLA  | S     | 305 | -    | 50,58,73     | 1.83 | 8 (16%)  | 58,95,113   | 3.36 | 19 (32%) |
| 25  | CLA  | r     | 614 | 22   | 45,53,73     | 2.06 | 8 (17%)  | 52,89,113   | 1.75 | 14 (26%) |
| 25  | CLA  | G     | 604 | 40   | 50,58,73     | 1.87 | 9 (18%)  | 58,95,113   | 1.98 | 14 (24%) |
| 25  | CLA  | b     | 604 | 5    | 65,73,73     | 1.63 | 9 (13%)  | 76,113,113  | 1.79 | 16 (21%) |
| 25  | CLA  | b     | 607 | -    | 65,73,73     | 1.62 | 9 (13%)  | 76,113,113  | 1.77 | 15 (19%) |
| 25  | CLA  | y     | 312 | 26   | 60,68,73     | 1.73 | 10 (16%) | 70,107,113  | 1.71 | 16 (22%) |
| 26  | LHG  | S     | 301 | -    | 48,48,48     | 0.44 | 0        | 51,54,54    | 1.16 | 4 (7%)   |
| 27  | PHO  | A     | 403 | -    | 51,69,69     | 0.52 | 0        | 47,99,99    | 1.72 | 5 (10%)  |
| 32  | AJP  | Y     | 321 | -    | 48,48,95     | 0.76 | 0        | 71,78,149   | 4.21 | 27 (38%) |
| 25  | CLA  | b     | 605 | 5    | 65,73,73     | 1.59 | 9 (13%)  | 76,113,113  | 1.90 | 14 (18%) |

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

| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 25  | CLA  | a     | 403 | -    | 1/1/15/20   | 7/37/115/115  | -        |
| 39  | LUT  | r     | 615 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 25  | CLA  | R     | 602 | 22   | 1/1/14/20   | 10/31/109/115 | -        |
| 25  | CLA  | C     | 510 | -    | 1/1/15/20   | 14/37/115/115 | -        |
| 32  | AJP  | y     | 322 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 25  | CLA  | S     | 303 | 20   | 1/1/14/20   | 16/33/111/115 | -        |
| 25  | CLA  | G     | 603 | -    | 1/1/14/20   | 12/31/109/115 | -        |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings      |
|-----|------|-------|-----|------|-------------|---------------|------------|
| 25  | CLA  | B     | 612 | 5    | 1/1/15/20   | 8/37/115/115  | -          |
| 32  | AJP  | n     | 619 | -    | 15/15/19/38 | 1/6/117/220   | 0/7/7/11   |
| 32  | AJP  | a     | 413 | -    | 34/34/38/38 | 9/28/220/220  | 0/11/11/11 |
| 26  | LHG  | b     | 622 | -    | -           | 18/53/53/53   | -          |
| 39  | LUT  | N     | 616 | -    | -           | 4/29/67/67    | 0/2/2/2    |
| 25  | CLA  | R     | 604 | -    | 1/1/11/20   | 4/17/95/115   | -          |
| 40  | NEX  | g     | 617 | 25   | -           | 11/27/83/83   | 0/3/3/3    |
| 25  | CLA  | c     | 511 | 6    | 1/1/15/20   | 7/37/115/115  | -          |
| 25  | CLA  | s     | 303 | 20   | 1/1/14/20   | 16/33/111/115 | -          |
| 35  | DGD  | B     | 626 | -    | -           | 23/51/91/95   | 0/2/2/2    |
| 32  | AJP  | Y     | 320 | -    | 15/15/19/38 | 2/6/117/220   | 0/7/7/11   |
| 25  | CLA  | n     | 614 | 21   | 1/1/11/20   | 4/17/95/115   | -          |
| 30  | LMG  | A     | 410 | -    | -           | 13/35/55/70   | 0/1/1/1    |
| 25  | CLA  | Y     | 313 | 21   | 1/1/14/20   | 11/31/109/115 | -          |
| 32  | AJP  | y     | 324 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11   |
| 26  | LHG  | B     | 622 | -    | -           | 18/53/53/53   | -          |
| 40  | NEX  | S     | 317 | -    | -           | 6/27/83/83    | 0/3/3/3    |
| 25  | CLA  | B     | 610 | -    | 1/1/15/20   | 9/37/115/115  | -          |
| 25  | CLA  | n     | 612 | 21   | 1/1/14/20   | 18/31/109/115 | -          |
| 26  | LHG  | S     | 318 | 25   | -           | 20/53/53/53   | -          |
| 25  | CLA  | C     | 507 | -    | 1/1/15/20   | 15/37/115/115 | -          |
| 25  | CLA  | N     | 604 | -    | 1/1/12/20   | 6/19/97/115   | -          |
| 27  | PHO  | A     | 404 | -    | -           | 1/37/103/103  | 0/5/6/6    |
| 25  | CLA  | B     | 611 | 5    | 1/1/15/20   | 10/37/115/115 | -          |
| 25  | CLA  | g     | 612 | 21   | 1/1/14/20   | 11/31/109/115 | -          |
| 25  | CLA  | R     | 612 | 22   | 1/1/14/20   | 11/31/109/115 | -          |
| 25  | CLA  | r     | 608 | 22   | 1/1/13/20   | 15/29/107/115 | -          |
| 25  | CLA  | 2     | 602 | 2    | 1/1/14/20   | 13/31/109/115 | -          |
| 25  | CLA  | S     | 313 | 20   | 1/1/13/20   | 10/25/103/115 | -          |
| 25  | CLA  | n     | 602 | 21   | 1/1/15/20   | 13/37/115/115 | -          |
| 25  | CLA  | 2     | 604 | 26   | 1/1/13/20   | 9/25/103/115  | -          |
| 30  | LMG  | a     | 411 | -    | -           | 13/35/55/70   | 0/1/1/1    |
| 30  | LMG  | d     | 407 | -    | -           | 16/41/61/70   | 0/1/1/1    |
| 24  | CHL  | n     | 608 | -    | 3/3/20/26   | 15/39/137/137 | -          |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 32  | AJP  | N     | 619 | -    | 15/15/19/38 | 1/6/117/220   | 0/7/7/11 |
| 24  | CHL  | R     | 605 | -    | 3/3/16/26   | 3/15/113/137  | -        |
| 24  | CHL  | 2     | 601 | 2    | 3/3/19/26   | 16/37/135/137 | -        |
| 24  | CHL  | n     | 606 | -    | 2/2/16/26   | 4/15/113/137  | -        |
| 35  | DGD  | A     | 415 | -    | -           | 27/48/88/95   | 0/2/2/2  |
| 39  | LUT  | g     | 615 | -    | -           | 5/29/67/67    | 0/2/2/2  |
| 24  | CHL  | N     | 609 | 21   | 2/2/20/26   | 15/39/137/137 | -        |
| 40  | NEX  | R     | 617 | -    | -           | 6/27/83/83    | 0/3/3/3  |
| 25  | CLA  | s     | 314 | 20   | 1/1/11/20   | 3/18/96/115   | -        |
| 24  | CHL  | N     | 608 | -    | 3/3/20/26   | 15/39/137/137 | -        |
| 26  | LHG  | s     | 301 | -    | -           | 21/53/53/53   | -        |
| 25  | CLA  | n     | 604 | -    | 1/1/12/20   | 6/19/97/115   | -        |
| 30  | LMG  | A     | 408 | -    | -           | 18/43/63/70   | 0/1/1/1  |
| 39  | LUT  | S     | 316 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 25  | CLA  | g     | 610 | -    | 1/1/14/20   | 14/36/114/115 | -        |
| 31  | PL9  | a     | 410 | -    | -           | 2/5/18/73     | 0/1/1/1  |
| 24  | CHL  | N     | 605 | 21   | 3/3/16/26   | 7/18/116/137  | -        |
| 28  | BCR  | B     | 617 | -    | -           | 3/29/63/63    | 0/2/2/2  |
| 29  | SQD  | L     | 101 | -    | -           | 13/37/57/69   | 0/1/1/1  |
| 40  | NEX  | y     | 318 | -    | -           | 7/27/83/83    | 1/3/3/3  |
| 25  | CLA  | Y     | 315 | 21   | 1/1/11/20   | 8/13/91/115   | -        |
| 26  | LHG  | d     | 406 | -    | -           | 18/53/53/53   | -        |
| 24  | CHL  | s     | 308 | -    | 3/3/16/26   | 2/15/113/137  | -        |
| 26  | LHG  | l     | 103 | -    | -           | 29/53/53/53   | -        |
| 24  | CHL  | Y     | 307 | 21   | 3/3/16/26   | 3/20/118/137  | -        |
| 24  | CHL  | n     | 609 | 21   | 2/2/20/26   | 15/39/137/137 | -        |
| 26  | LHG  | c     | 519 | -    | -           | 21/53/53/53   | -        |
| 25  | CLA  | R     | 614 | 22   | 1/1/11/20   | 8/13/91/115   | -        |
| 24  | CHL  | n     | 605 | 21   | 3/3/16/26   | 7/18/116/137  | -        |
| 25  | CLA  | G     | 602 | 21   | 1/1/15/20   | 15/37/115/115 | -        |
| 24  | CHL  | Y     | 302 | 21   | 2/2/20/26   | 23/39/137/137 | -        |
| 30  | LMG  | C     | 520 | -    | -           | 18/46/66/70   | 0/1/1/1  |
| 30  | LMG  | b     | 623 | -    | -           | 28/50/70/70   | 0/1/1/1  |
| 32  | AJP  | G     | 618 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings      |
|-----|------|-------|-----|------|-------------|---------------|------------|
| 25  | CLA  | C     | 508 | 6    | 1/1/15/20   | 12/37/115/115 | -          |
| 26  | LHG  | 6     | 606 | 25   | -           | 25/51/51/53   | -          |
| 28  | BCR  | b     | 618 | -    | -           | 3/29/63/63    | 0/2/2/2    |
| 25  | CLA  | b     | 611 | 5    | 1/1/15/20   | 10/37/115/115 | -          |
| 25  | CLA  | c     | 505 | 6    | 1/1/15/20   | 12/37/115/115 | -          |
| 25  | CLA  | C     | 511 | 6    | 1/1/15/20   | 7/37/115/115  | -          |
| 25  | CLA  | B     | 609 | 5    | 1/1/15/20   | 11/37/115/115 | -          |
| 25  | CLA  | n     | 603 | -    | 1/1/15/20   | 17/37/115/115 | -          |
| 24  | CHL  | S     | 307 | -    | 3/3/16/26   | 7/15/113/137  | -          |
| 25  | CLA  | y     | 313 | 21   | 1/1/14/20   | 11/31/109/115 | -          |
| 35  | DGD  | a     | 401 | -    | -           | 27/48/88/95   | 0/2/2/2    |
| 24  | CHL  | l     | 302 | 1    | 3/3/16/26   | 5/15/113/137  | -          |
| 25  | CLA  | B     | 608 | 5    | 1/1/15/20   | 12/37/115/115 | -          |
| 25  | CLA  | D     | 402 | 7    | 1/1/15/20   | 10/37/115/115 | -          |
| 26  | LHG  | L     | 102 | -    | -           | 29/53/53/53   | -          |
| 28  | BCR  | Z     | 101 | -    | -           | 8/29/63/63    | 0/2/2/2    |
| 28  | BCR  | b     | 619 | -    | -           | 3/29/63/63    | 0/2/2/2    |
| 25  | CLA  | 2     | 605 | -    | 1/1/11/20   | 10/17/95/115  | -          |
| 25  | CLA  | b     | 616 | 5    | 1/1/15/20   | 17/37/115/115 | -          |
| 28  | BCR  | a     | 407 | -    | -           | 5/29/63/63    | 0/2/2/2    |
| 29  | SQD  | A     | 411 | -    | -           | 22/49/69/69   | 0/1/1/1    |
| 25  | CLA  | c     | 502 | 6    | 1/1/15/20   | 6/37/115/115  | -          |
| 25  | CLA  | y     | 304 | -    | 1/1/15/20   | 22/37/115/115 | -          |
| 25  | CLA  | R     | 609 | 22   | 1/1/15/20   | 14/37/115/115 | -          |
| 26  | LHG  | R     | 618 | 25   | -           | 12/46/46/53   | -          |
| 24  | CHL  | N     | 606 | -    | 2/2/16/26   | 4/15/113/137  | -          |
| 24  | CHL  | G     | 607 | -    | 2/2/16/26   | 6/15/113/137  | -          |
| 25  | CLA  | A     | 402 | -    | 1/1/15/20   | 7/37/115/115  | -          |
| 32  | AJP  | B     | 624 | -    | 34/34/38/38 | 14/28/220/220 | 0/11/11/11 |
| 32  | AJP  | y     | 323 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11   |
| 25  | CLA  | c     | 509 | 6    | 1/1/15/20   | 7/37/115/115  | -          |
| 27  | PHO  | a     | 404 | -    | -           | 12/37/103/103 | 0/5/6/6    |
| 32  | AJP  | y     | 321 | -    | 16/16/19/38 | 4/6/117/220   | 0/7/7/11   |
| 31  | PL9  | D     | 405 | -    | -           | 5/53/73/73    | 0/1/1/1    |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | b     | 613 | 5    | 1/1/15/20 | 15/37/115/115 | -       |
| 25  | CLA  | D     | 401 | 42   | 1/1/12/20 | 2/19/97/115   | -       |
| 25  | CLA  | B     | 604 | 5    | 1/1/15/20 | 15/37/115/115 | -       |
| 28  | BCR  | t     | 101 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 41  | XAT  | r     | 616 | -    | -         | 2/31/93/93    | 0/4/4/4 |
| 39  | LUT  | S     | 315 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 31  | PL9  | A     | 409 | -    | -         | 2/5/18/73     | 0/1/1/1 |
| 25  | CLA  | g     | 614 | 21   | 1/1/11/20 | 9/17/95/115   | -       |
| 24  | CHL  | N     | 601 | 21   | 2/2/18/26 | 13/27/125/137 | -       |
| 26  | LHG  | B     | 625 | -    | -         | 14/50/50/53   | -       |
| 24  | CHL  | g     | 608 | -    | 3/3/20/26 | 22/39/137/137 | -       |
| 25  | CLA  | B     | 602 | 5    | 1/1/15/20 | 14/37/115/115 | -       |
| 39  | LUT  | N     | 615 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 40  | NEX  | r     | 617 | -    | -         | 6/27/83/83    | 0/3/3/3 |
| 30  | LMG  | B     | 620 | -    | -         | 15/46/66/70   | 0/1/1/1 |
| 25  | CLA  | S     | 310 | 20   | 1/1/13/20 | 9/25/103/115  | -       |
| 29  | SQD  | l     | 102 | -    | -         | 13/37/57/69   | 0/1/1/1 |
| 39  | LUT  | y     | 316 | -    | -         | 3/29/67/67    | 0/2/2/2 |
| 25  | CLA  | g     | 602 | 21   | 1/1/15/20 | 15/37/115/115 | -       |
| 24  | CHL  | Y     | 310 | 21   | 3/3/18/26 | 11/27/125/137 | -       |
| 26  | LHG  | 2     | 606 | 25   | -         | 25/51/51/53   | -       |
| 25  | CLA  | Y     | 305 | -    | 1/1/12/20 | 7/19/97/115   | -       |
| 25  | CLA  | C     | 513 | 6    | 1/1/15/20 | 13/37/115/115 | -       |
| 25  | CLA  | r     | 609 | 22   | 1/1/15/20 | 14/37/115/115 | -       |
| 29  | SQD  | a     | 412 | -    | -         | 22/49/69/69   | 0/1/1/1 |
| 24  | CHL  | S     | 302 | 20   | 2/2/16/26 | 4/15/113/137  | -       |
| 25  | CLA  | A     | 405 | 4    | 1/1/14/20 | 9/31/109/115  | -       |
| 24  | CHL  | S     | 308 | -    | 3/3/16/26 | 2/15/113/137  | -       |
| 24  | CHL  | 6     | 603 | -    | 3/3/16/26 | 10/15/113/137 | -       |
| 25  | CLA  | B     | 615 | 5    | 1/1/15/20 | 10/37/115/115 | -       |
| 41  | XAT  | R     | 616 | -    | -         | 2/31/93/93    | 0/4/4/4 |
| 25  | CLA  | c     | 512 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 24  | CHL  | s     | 302 | 20   | 2/2/16/26 | 4/15/113/137  | -       |
| 25  | CLA  | S     | 309 | 20   | 1/1/11/20 | 5/13/91/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 25  | CLA  | S     | 314 | 20   | 1/1/11/20   | 3/18/96/115   | -        |
| 32  | AJP  | S     | 319 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 24  | CHL  | Y     | 306 | 21   | 3/3/16/26   | 9/18/116/137  | -        |
| 25  | CLA  | C     | 509 | 6    | 1/1/15/20   | 7/37/115/115  | -        |
| 24  | CHL  | g     | 607 | -    | 2/2/16/26   | 6/15/113/137  | -        |
| 24  | CHL  | Y     | 309 | -    | 3/3/20/26   | 20/39/137/137 | -        |
| 24  | CHL  | G     | 601 | 21   | 2/2/20/26   | 24/39/137/137 | -        |
| 39  | LUT  | y     | 317 | -    | -           | 3/29/67/67    | 0/2/2/2  |
| 24  | CHL  | R     | 613 | 22   | 3/3/15/26   | 6/10/108/137  | -        |
| 25  | CLA  | Y     | 312 | 26   | 1/1/14/20   | 11/31/109/115 | -        |
| 25  | CLA  | g     | 604 | 40   | 1/1/12/20   | 11/19/97/115  | -        |
| 25  | CLA  | N     | 612 | 21   | 1/1/14/20   | 18/31/109/115 | -        |
| 28  | BCR  | k     | 101 | -    | -           | 4/29/63/63    | 0/2/2/2  |
| 24  | CHL  | g     | 605 | 21   | 3/3/16/26   | 9/15/113/137  | -        |
| 29  | SQD  | A     | 407 | -    | -           | 21/45/65/69   | 0/1/1/1  |
| 25  | CLA  | G     | 610 | -    | 1/1/14/20   | 14/36/114/115 | -        |
| 25  | CLA  | Y     | 311 | 21   | 1/1/14/20   | 9/31/109/115  | -        |
| 31  | PL9  | d     | 405 | -    | -           | 5/53/73/73    | 0/1/1/1  |
| 39  | LUT  | s     | 315 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 40  | NEX  | n     | 617 | -    | -           | 10/27/83/83   | 0/3/3/3  |
| 27  | PHO  | a     | 405 | -    | -           | 1/37/103/103  | 0/5/6/6  |
| 28  | BCR  | d     | 404 | -    | -           | 5/29/63/63    | 0/2/2/2  |
| 25  | CLA  | B     | 606 | 5    | 1/1/15/20   | 11/37/115/115 | -        |
| 29  | SQD  | l     | 101 | -    | -           | 27/49/69/69   | 0/1/1/1  |
| 39  | LUT  | s     | 316 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 25  | CLA  | G     | 611 | -    | 1/1/14/20   | 16/31/109/115 | -        |
| 24  | CHL  | n     | 607 | -    | 2/2/20/26   | 18/39/137/137 | -        |
| 25  | CLA  | c     | 507 | -    | 1/1/15/20   | 15/37/115/115 | -        |
| 26  | LHG  | b     | 625 | -    | -           | 14/50/50/53   | -        |
| 30  | LMG  | D     | 407 | -    | -           | 16/41/61/70   | 0/1/1/1  |
| 24  | CHL  | R     | 606 | -    | 3/3/16/26   | 11/15/113/137 | -        |
| 40  | NEX  | N     | 617 | -    | -           | 10/27/83/83   | 0/3/3/3  |
| 39  | LUT  | G     | 615 | -    | -           | 5/29/67/67    | 0/2/2/2  |
| 35  | DGD  | C     | 515 | -    | -           | 17/44/84/95   | 0/2/2/2  |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 25  | CLA  | N     | 614 | 21   | 1/1/11/20   | 4/17/95/115   | -        |
| 29  | SQD  | L     | 103 | -    | -           | 27/49/69/69   | 0/1/1/1  |
| 26  | LHG  | r     | 618 | 25   | -           | 12/46/46/53   | -        |
| 24  | CHL  | S     | 306 | -    | 3/3/16/26   | 7/15/113/137  | -        |
| 25  | CLA  | B     | 601 | -    | 1/1/15/20   | 16/37/115/115 | -        |
| 24  | CHL  | 6     | 601 | 2    | 3/3/19/26   | 16/37/135/137 | -        |
| 24  | CHL  | r     | 613 | 22   | 3/3/15/26   | 6/10/108/137  | -        |
| 25  | CLA  | S     | 312 | 20   | 1/1/11/20   | 7/18/96/115   | -        |
| 25  | CLA  | B     | 616 | 5    | 1/1/15/20   | 17/37/115/115 | -        |
| 25  | CLA  | Y     | 304 | -    | 1/1/15/20   | 22/37/115/115 | -        |
| 25  | CLA  | s     | 305 | -    | 1/1/12/20   | 9/19/97/115   | -        |
| 24  | CHL  | s     | 306 | -    | 3/3/16/26   | 7/15/113/137  | -        |
| 24  | CHL  | y     | 308 | -    | 2/2/18/26   | 8/30/128/137  | -        |
| 40  | NEX  | Y     | 318 | -    | -           | 7/27/83/83    | 1/3/3/3  |
| 25  | CLA  | g     | 603 | -    | 1/1/14/20   | 11/31/109/115 | -        |
| 25  | CLA  | r     | 610 | 26   | 1/1/11/20   | 9/18/96/115   | -        |
| 26  | LHG  | C     | 518 | -    | -           | 12/53/53/53   | -        |
| 28  | BCR  | K     | 101 | -    | -           | 4/29/63/63    | 0/2/2/2  |
| 30  | LMG  | B     | 623 | -    | -           | 28/50/70/70   | 0/1/1/1  |
| 25  | CLA  | G     | 612 | 21   | 1/1/14/20   | 11/31/109/115 | -        |
| 35  | DGD  | c     | 516 | -    | -           | 28/51/91/95   | 0/2/2/2  |
| 25  | CLA  | S     | 311 | 26   | 1/1/13/20   | 12/27/105/115 | -        |
| 32  | AJP  | n     | 620 | -    | 16/16/19/38 | 4/6/117/220   | 0/7/7/11 |
| 38  | HEM  | F     | 101 | 9    | -           | 1/12/54/54    | -        |
| 25  | CLA  | c     | 504 | -    | 1/1/14/20   | 14/31/109/115 | -        |
| 25  | CLA  | d     | 401 | 42   | 1/1/12/20   | 2/19/97/115   | -        |
| 25  | CLA  | C     | 503 | 6    | 1/1/15/20   | 9/37/115/115  | -        |
| 25  | CLA  | b     | 610 | -    | 1/1/15/20   | 9/37/115/115  | -        |
| 40  | NEX  | G     | 617 | 25   | -           | 11/27/83/83   | 0/3/3/3  |
| 28  | BCR  | A     | 406 | -    | -           | 5/29/63/63    | 0/2/2/2  |
| 25  | CLA  | N     | 602 | 21   | 1/1/15/20   | 13/37/115/115 | -        |
| 25  | CLA  | 6     | 604 | 26   | 1/1/13/20   | 9/25/103/115  | -        |
| 24  | CHL  | g     | 609 | 21   | 3/3/19/26   | 10/33/131/137 | -        |
| 25  | CLA  | n     | 613 | 21   | 1/1/14/20   | 21/31/109/115 | -        |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 25  | CLA  | b     | 606 | 5    | 1/1/15/20   | 11/37/115/115 | -        |
| 25  | CLA  | B     | 614 | 5    | 1/1/15/20   | 13/37/115/115 | -        |
| 24  | CHL  | s     | 307 | -    | 3/3/16/26   | 7/15/113/137  | -        |
| 25  | CLA  | r     | 611 | -    | 1/1/11/20   | 11/18/96/115  | -        |
| 29  | SQD  | a     | 408 | -    | -           | 21/45/65/69   | 0/1/1/1  |
| 25  | CLA  | a     | 406 | 4    | 1/1/14/20   | 9/31/109/115  | -        |
| 35  | DGD  | C     | 516 | -    | -           | 28/51/91/95   | 0/2/2/2  |
| 26  | LHG  | y     | 319 | 25   | -           | 23/53/53/53   | -        |
| 30  | LMG  | c     | 520 | -    | -           | 18/46/66/70   | 0/1/1/1  |
| 25  | CLA  | c     | 508 | 6    | 1/1/15/20   | 12/37/115/115 | -        |
| 25  | CLA  | g     | 611 | -    | 1/1/14/20   | 16/31/109/115 | -        |
| 25  | CLA  | Y     | 314 | 21   | 1/1/15/20   | 16/37/115/115 | -        |
| 38  | HEM  | f     | 101 | 9    | -           | 1/12/54/54    | -        |
| 25  | CLA  | C     | 512 | -    | 1/1/15/20   | 12/37/115/115 | -        |
| 25  | CLA  | C     | 506 | 6    | 1/1/15/20   | 11/37/115/115 | -        |
| 25  | CLA  | B     | 613 | 5    | 1/1/15/20   | 15/37/115/115 | -        |
| 32  | AJP  | N     | 620 | -    | 16/16/19/38 | 4/6/117/220   | 0/7/7/11 |
| 24  | CHL  | N     | 607 | -    | 2/2/20/26   | 18/39/137/137 | -        |
| 39  | LUT  | n     | 615 | -    | -           | 8/29/67/67    | 0/2/2/2  |
| 32  | AJP  | Y     | 322 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 26  | LHG  | D     | 406 | -    | -           | 18/53/53/53   | -        |
| 25  | CLA  | S     | 304 | -    | 1/1/11/20   | 2/13/91/115   | -        |
| 24  | CHL  | Y     | 308 | -    | 2/2/18/26   | 8/30/128/137  | -        |
| 24  | CHL  | n     | 601 | 21   | 2/2/18/26   | 13/27/125/137 | -        |
| 25  | CLA  | C     | 501 | -    | 1/1/15/20   | 7/37/115/115  | -        |
| 28  | BCR  | i     | 101 | -    | -           | 4/29/63/63    | 0/2/2/2  |
| 25  | CLA  | n     | 610 | 21   | 1/1/15/20   | 15/37/115/115 | -        |
| 28  | BCR  | C     | 514 | -    | -           | 2/29/63/63    | 0/2/2/2  |
| 25  | CLA  | a     | 402 | 4    | 1/1/15/20   | 7/37/115/115  | -        |
| 24  | CHL  | G     | 609 | 21   | 3/3/19/26   | 10/33/131/137 | -        |
| 25  | CLA  | C     | 505 | 6    | 1/1/15/20   | 12/37/115/115 | -        |
| 25  | CLA  | c     | 503 | 6    | 1/1/15/20   | 9/37/115/115  | -        |
| 25  | CLA  | R     | 611 | -    | 1/1/11/20   | 11/18/96/115  | -        |
| 25  | CLA  | b     | 609 | 5    | 1/1/15/20   | 11/37/115/115 | -        |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings      |
|-----|------|-------|-----|------|-------------|---------------|------------|
| 25  | CLA  | b     | 603 | -    | 1/1/15/20   | 11/37/115/115 | -          |
| 25  | CLA  | b     | 612 | 5    | 1/1/15/20   | 8/37/115/115  | -          |
| 39  | LUT  | Y     | 316 | -    | -           | 3/29/67/67    | 0/2/2/2    |
| 24  | CHL  | r     | 606 | -    | 3/3/16/26   | 11/15/113/137 | -          |
| 25  | CLA  | d     | 403 | -    | 1/1/15/20   | 12/37/115/115 | -          |
| 25  | CLA  | n     | 611 | 26   | 1/1/14/20   | 12/31/109/115 | -          |
| 30  | LMG  | b     | 620 | -    | -           | 15/46/66/70   | 0/1/1/1    |
| 25  | CLA  | s     | 313 | 20   | 1/1/13/20   | 10/25/103/115 | -          |
| 32  | AJP  | A     | 412 | -    | 34/34/38/38 | 9/28/220/220  | 0/11/11/11 |
| 25  | CLA  | G     | 613 | 21   | 1/1/15/20   | 16/37/115/115 | -          |
| 26  | LHG  | n     | 618 | 25   | -           | 29/53/53/53   | -          |
| 28  | BCR  | I     | 101 | -    | -           | 5/29/63/63    | 0/2/2/2    |
| 25  | CLA  | r     | 601 | -    | 1/1/11/20   | 11/18/96/115  | -          |
| 25  | CLA  | y     | 315 | 21   | 1/1/11/20   | 8/13/91/115   | -          |
| 35  | DGD  | b     | 626 | -    | -           | 23/51/91/95   | 0/2/2/2    |
| 25  | CLA  | N     | 611 | 26   | 1/1/14/20   | 12/31/109/115 | -          |
| 25  | CLA  | s     | 304 | -    | 1/1/11/20   | 2/13/91/115   | -          |
| 32  | AJP  | Y     | 324 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11   |
| 24  | CHL  | y     | 310 | 21   | 3/3/18/26   | 11/27/125/137 | -          |
| 26  | LHG  | y     | 301 | -    | -           | 16/53/53/53   | -          |
| 28  | BCR  | B     | 619 | -    | -           | 3/29/63/63    | 0/2/2/2    |
| 28  | BCR  | B     | 618 | -    | -           | 3/29/63/63    | 0/2/2/2    |
| 25  | CLA  | g     | 613 | 21   | 1/1/15/20   | 16/37/115/115 | -          |
| 26  | LHG  | s     | 318 | 25   | -           | 21/53/53/53   | -          |
| 24  | CHL  | r     | 607 | -    | 3/3/19/26   | 13/33/131/137 | -          |
| 25  | CLA  | 6     | 605 | -    | 1/1/11/20   | 10/17/95/115  | -          |
| 25  | CLA  | y     | 314 | 21   | 1/1/15/20   | 16/37/115/115 | -          |
| 25  | CLA  | y     | 305 | -    | 1/1/12/20   | 7/19/97/115   | -          |
| 25  | CLA  | C     | 502 | 6    | 1/1/15/20   | 6/37/115/115  | -          |
| 24  | CHL  | r     | 605 | -    | 3/3/16/26   | 3/15/113/137  | -          |
| 28  | BCR  | T     | 101 | -    | -           | 17/29/63/63   | 0/2/2/2    |
| 25  | CLA  | B     | 605 | 5    | 1/1/15/20   | 7/37/115/115  | -          |
| 26  | LHG  | C     | 517 | -    | -           | 16/53/53/53   | -          |
| 25  | CLA  | c     | 510 | -    | 1/1/15/20   | 14/37/115/115 | -          |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 25  | CLA  | N     | 603 | -    | 1/1/15/20   | 17/37/115/115 | -        |
| 39  | LUT  | R     | 615 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 25  | CLA  | c     | 506 | 6    | 1/1/15/20   | 11/37/115/115 | -        |
| 24  | CHL  | 1     | 301 | 1    | 3/3/16/26   | 4/15/113/137  | -        |
| 24  | CHL  | 5     | 301 | 1    | 3/3/16/26   | 4/15/113/137  | -        |
| 25  | CLA  | d     | 402 | 7    | 1/1/15/20   | 10/37/115/115 | -        |
| 26  | LHG  | c     | 518 | -    | -           | 12/53/53/53   | -        |
| 25  | CLA  | b     | 601 | -    | 1/1/15/20   | 16/37/115/115 | -        |
| 24  | CHL  | y     | 302 | 21   | 2/2/20/26   | 23/39/137/137 | -        |
| 25  | CLA  | R     | 610 | 26   | 1/1/11/20   | 9/18/96/115   | -        |
| 24  | CHL  | y     | 306 | 21   | 3/3/16/26   | 9/18/116/137  | -        |
| 25  | CLA  | r     | 603 | 22   | 1/1/14/20   | 13/31/109/115 | -        |
| 25  | CLA  | c     | 501 | -    | 1/1/15/20   | 7/37/115/115  | -        |
| 25  | CLA  | s     | 309 | 20   | 1/1/11/20   | 5/13/91/115   | -        |
| 32  | AJP  | s     | 319 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 25  | CLA  | A     | 401 | 4    | 1/1/15/20   | 7/37/115/115  | -        |
| 28  | BCR  | b     | 617 | -    | -           | 3/29/63/63    | 0/2/2/2  |
| 25  | CLA  | D     | 403 | -    | 1/1/15/20   | 12/37/115/115 | -        |
| 25  | CLA  | c     | 513 | 6    | 1/1/15/20   | 13/37/115/115 | -        |
| 24  | CHL  | y     | 309 | -    | 3/3/20/26   | 20/39/137/137 | -        |
| 28  | BCR  | c     | 514 | -    | -           | 2/29/63/63    | 0/2/2/2  |
| 24  | CHL  | R     | 607 | -    | 3/3/19/26   | 13/33/131/137 | -        |
| 26  | LHG  | B     | 621 | -    | -           | 19/51/51/53   | -        |
| 25  | CLA  | y     | 311 | 21   | 1/1/14/20   | 10/31/109/115 | -        |
| 25  | CLA  | s     | 310 | 20   | 1/1/13/20   | 9/25/103/115  | -        |
| 25  | CLA  | y     | 303 | 21   | 1/1/15/20   | 12/37/115/115 | -        |
| 32  | AJP  | g     | 618 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 39  | LUT  | Y     | 317 | -    | -           | 3/29/67/67    | 0/2/2/2  |
| 25  | CLA  | b     | 615 | 5    | 1/1/15/20   | 10/37/115/115 | -        |
| 24  | CHL  | G     | 606 | -    | 3/3/16/26   | 3/20/118/137  | -        |
| 25  | CLA  | N     | 610 | 21   | 1/1/15/20   | 15/37/115/115 | -        |
| 24  | CHL  | g     | 606 | -    | 3/3/16/26   | 3/20/118/137  | -        |
| 24  | CHL  | 5     | 302 | 1    | 3/3/16/26   | 5/15/113/137  | -        |
| 35  | DGD  | c     | 515 | -    | -           | 17/44/84/95   | 0/2/2/2  |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings    |
|-----|------|-------|-----|------|-------------|---------------|----------|
| 26  | LHG  | C     | 519 | -    | -           | 21/53/53/53   | -        |
| 26  | LHG  | Y     | 319 | 25   | -           | 23/53/53/53   | -        |
| 25  | CLA  | G     | 614 | 21   | 1/1/11/20   | 9/17/95/115   | -        |
| 25  | CLA  | R     | 601 | -    | 1/1/11/20   | 11/18/96/115  | -        |
| 25  | CLA  | B     | 607 | -    | 1/1/15/20   | 16/37/115/115 | -        |
| 39  | LUT  | n     | 616 | -    | -           | 4/29/67/67    | 0/2/2/2  |
| 32  | AJP  | y     | 320 | -    | 15/15/19/38 | 2/6/117/220   | 0/7/7/11 |
| 40  | NEX  | s     | 317 | -    | -           | 6/27/83/83    | 0/3/3/3  |
| 28  | BCR  | D     | 404 | -    | -           | 5/29/63/63    | 0/2/2/2  |
| 26  | LHG  | N     | 618 | 25   | -           | 29/53/53/53   | -        |
| 25  | CLA  | C     | 504 | -    | 1/1/14/20   | 14/31/109/115 | -        |
| 32  | AJP  | Y     | 323 | -    | 15/15/19/38 | 3/6/117/220   | 0/7/7/11 |
| 24  | CHL  | G     | 608 | -    | 3/3/20/26   | 22/39/137/137 | -        |
| 24  | CHL  | g     | 601 | 21   | 2/2/20/26   | 24/39/137/137 | -        |
| 28  | BCR  | z     | 101 | -    | -           | 8/29/63/63    | 0/2/2/2  |
| 24  | CHL  | y     | 307 | 21   | 3/3/16/26   | 3/20/118/137  | -        |
| 25  | CLA  | r     | 612 | 22   | 1/1/14/20   | 11/31/109/115 | -        |
| 25  | CLA  | b     | 608 | 5    | 1/1/15/20   | 12/37/115/115 | -        |
| 28  | BCR  | h     | 101 | -    | -           | 6/29/63/63    | 0/2/2/2  |
| 25  | CLA  | b     | 614 | 5    | 1/1/15/20   | 13/37/115/115 | -        |
| 24  | CHL  | G     | 605 | 21   | 3/3/16/26   | 9/15/113/137  | -        |
| 28  | BCR  | H     | 101 | -    | -           | 6/29/63/63    | 0/2/2/2  |
| 39  | LUT  | G     | 616 | -    | -           | 0/29/67/67    | 0/2/2/2  |
| 26  | LHG  | c     | 517 | -    | -           | 17/53/53/53   | -        |
| 25  | CLA  | s     | 311 | 26   | 1/1/13/20   | 12/27/105/115 | -        |
| 25  | CLA  | r     | 602 | 22   | 1/1/14/20   | 10/31/109/115 | -        |
| 39  | LUT  | g     | 616 | -    | -           | 0/29/67/67    | 0/2/2/2  |
| 26  | LHG  | b     | 621 | -    | -           | 19/51/51/53   | -        |
| 25  | CLA  | s     | 312 | 20   | 1/1/11/20   | 7/18/96/115   | -        |
| 25  | CLA  | Y     | 303 | 21   | 1/1/15/20   | 12/37/115/115 | -        |
| 25  | CLA  | 6     | 602 | 2    | 1/1/14/20   | 13/31/109/115 | -        |
| 24  | CHL  | 2     | 603 | -    | 3/3/16/26   | 10/15/113/137 | -        |
| 25  | CLA  | N     | 613 | 21   | 1/1/14/20   | 21/31/109/115 | -        |
| 25  | CLA  | b     | 602 | 5    | 1/1/15/20   | 14/37/115/115 | -        |

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| Mol | Type | Chain | Res | Link | Chirals     | Torsions      | Rings      |
|-----|------|-------|-----|------|-------------|---------------|------------|
| 32  | AJP  | b     | 624 | -    | 34/34/38/38 | 14/28/220/220 | 0/11/11/11 |
| 25  | CLA  | r     | 604 | -    | 1/1/11/20   | 4/17/95/115   | -          |
| 26  | LHG  | Y     | 301 | -    | -           | 16/53/53/53   | -          |
| 25  | CLA  | R     | 603 | 22   | 1/1/14/20   | 13/31/109/115 | -          |
| 25  | CLA  | B     | 603 | -    | 1/1/15/20   | 11/37/115/115 | -          |
| 30  | LMG  | a     | 409 | -    | -           | 18/43/63/70   | 0/1/1/1    |
| 25  | CLA  | R     | 608 | 22   | 1/1/13/20   | 15/29/107/115 | -          |
| 25  | CLA  | S     | 305 | -    | 1/1/12/20   | 9/19/97/115   | -          |
| 25  | CLA  | r     | 614 | 22   | 1/1/11/20   | 8/13/91/115   | -          |
| 25  | CLA  | G     | 604 | 40   | 1/1/12/20   | 11/19/97/115  | -          |
| 25  | CLA  | b     | 604 | 5    | 1/1/15/20   | 15/37/115/115 | -          |
| 25  | CLA  | b     | 607 | -    | 1/1/15/20   | 16/37/115/115 | -          |
| 25  | CLA  | y     | 312 | 26   | 1/1/14/20   | 11/31/109/115 | -          |
| 26  | LHG  | S     | 301 | -    | -           | 21/53/53/53   | -          |
| 27  | PHO  | A     | 403 | -    | -           | 12/37/103/103 | 0/5/6/6    |
| 32  | AJP  | Y     | 321 | -    | 16/16/19/38 | 4/6/117/220   | 0/7/7/11   |
| 25  | CLA  | b     | 605 | 5    | 1/1/15/20   | 7/37/115/115  | -          |

All (2348) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 38  | F     | 101 | HEM  | FE-NB  | 8.66 | 2.39        | 1.96     |
| 38  | f     | 101 | HEM  | FE-NB  | 8.66 | 2.39        | 1.96     |
| 25  | N     | 610 | CLA  | C1B-NB | 7.29 | 1.41        | 1.35     |
| 25  | n     | 610 | CLA  | C1B-NB | 7.26 | 1.41        | 1.35     |
| 25  | y     | 311 | CLA  | C1B-NB | 7.19 | 1.41        | 1.35     |
| 25  | s     | 312 | CLA  | C1B-NB | 7.17 | 1.41        | 1.35     |
| 25  | S     | 312 | CLA  | C1B-NB | 7.11 | 1.41        | 1.35     |
| 25  | s     | 309 | CLA  | C1B-NB | 7.10 | 1.41        | 1.35     |
| 25  | Y     | 311 | CLA  | C1B-NB | 7.09 | 1.41        | 1.35     |
| 25  | r     | 614 | CLA  | C1B-NB | 7.06 | 1.41        | 1.35     |
| 25  | r     | 608 | CLA  | C1B-NB | 7.06 | 1.41        | 1.35     |
| 25  | S     | 309 | CLA  | C1B-NB | 7.02 | 1.41        | 1.35     |
| 25  | N     | 602 | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 25  | n     | 602 | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 25  | G     | 602 | CLA  | C4B-NB | 6.99 | 1.41        | 1.35     |
| 25  | g     | 602 | CLA  | C4B-NB | 6.99 | 1.41        | 1.35     |
| 25  | R     | 608 | CLA  | C1B-NB | 6.97 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | R     | 614 | CLA  | C1B-NB | 6.95  | 1.41        | 1.35     |
| 25  | g     | 612 | CLA  | C1B-NB | 6.88  | 1.41        | 1.35     |
| 25  | C     | 506 | CLA  | C1B-NB | 6.88  | 1.41        | 1.35     |
| 25  | c     | 506 | CLA  | C1B-NB | 6.88  | 1.41        | 1.35     |
| 25  | y     | 315 | CLA  | C4B-NB | 6.82  | 1.41        | 1.35     |
| 25  | G     | 612 | CLA  | C1B-NB | 6.81  | 1.41        | 1.35     |
| 25  | r     | 614 | CLA  | C4B-NB | 6.81  | 1.41        | 1.35     |
| 25  | s     | 314 | CLA  | C1B-NB | 6.80  | 1.41        | 1.35     |
| 25  | Y     | 303 | CLA  | C4B-NB | 6.80  | 1.41        | 1.35     |
| 25  | y     | 303 | CLA  | C4B-NB | 6.80  | 1.41        | 1.35     |
| 25  | b     | 602 | CLA  | C1B-NB | 6.80  | 1.41        | 1.35     |
| 25  | B     | 602 | CLA  | C1B-NB | 6.79  | 1.41        | 1.35     |
| 25  | Y     | 313 | CLA  | C1B-NB | 6.79  | 1.41        | 1.35     |
| 25  | d     | 402 | CLA  | C1B-NB | 6.79  | 1.41        | 1.35     |
| 25  | B     | 615 | CLA  | C1B-NB | 6.77  | 1.41        | 1.35     |
| 25  | b     | 615 | CLA  | C1B-NB | 6.77  | 1.41        | 1.35     |
| 25  | r     | 609 | CLA  | C1B-NB | 6.77  | 1.41        | 1.35     |
| 25  | R     | 614 | CLA  | C4B-NB | 6.77  | 1.41        | 1.35     |
| 25  | R     | 609 | CLA  | C1B-NB | 6.76  | 1.41        | 1.35     |
| 25  | R     | 611 | CLA  | MG-ND  | -6.76 | 1.92        | 2.05     |
| 25  | D     | 402 | CLA  | C1B-NB | 6.75  | 1.41        | 1.35     |
| 25  | y     | 313 | CLA  | C1B-NB | 6.74  | 1.41        | 1.35     |
| 25  | r     | 611 | CLA  | MG-ND  | -6.71 | 1.92        | 2.05     |
| 25  | Y     | 315 | CLA  | C4B-NB | 6.71  | 1.41        | 1.35     |
| 25  | S     | 314 | CLA  | C1B-NB | 6.70  | 1.41        | 1.35     |
| 25  | B     | 610 | CLA  | C1B-NB | 6.67  | 1.41        | 1.35     |
| 25  | b     | 610 | CLA  | C1B-NB | 6.67  | 1.41        | 1.35     |
| 25  | N     | 612 | CLA  | C1B-NB | 6.64  | 1.41        | 1.35     |
| 25  | n     | 612 | CLA  | C1B-NB | 6.64  | 1.41        | 1.35     |
| 25  | Y     | 303 | CLA  | C1B-NB | 6.62  | 1.41        | 1.35     |
| 25  | y     | 303 | CLA  | C1B-NB | 6.62  | 1.41        | 1.35     |
| 25  | G     | 612 | CLA  | C4B-NB | 6.61  | 1.41        | 1.35     |
| 25  | y     | 305 | CLA  | C4B-NB | 6.55  | 1.41        | 1.35     |
| 25  | Y     | 305 | CLA  | C4B-NB | 6.54  | 1.41        | 1.35     |
| 25  | b     | 602 | CLA  | C4B-NB | 6.53  | 1.41        | 1.35     |
| 25  | n     | 602 | CLA  | C1B-NB | 6.52  | 1.41        | 1.35     |
| 25  | Y     | 313 | CLA  | C4B-NB | 6.52  | 1.41        | 1.35     |
| 25  | B     | 602 | CLA  | C4B-NB | 6.52  | 1.41        | 1.35     |
| 25  | c     | 505 | CLA  | C4B-NB | 6.51  | 1.41        | 1.35     |
| 25  | g     | 612 | CLA  | C4B-NB | 6.50  | 1.41        | 1.35     |
| 25  | y     | 313 | CLA  | C4B-NB | 6.49  | 1.41        | 1.35     |
| 25  | S     | 303 | CLA  | C1B-NB | 6.49  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 25  | s     | 303 | CLA  | C1B-NB | 6.49 | 1.41        | 1.35     |
| 25  | B     | 616 | CLA  | C4B-NB | 6.47 | 1.41        | 1.35     |
| 25  | b     | 616 | CLA  | C4B-NB | 6.47 | 1.41        | 1.35     |
| 25  | y     | 305 | CLA  | C1B-NB | 6.47 | 1.41        | 1.35     |
| 25  | S     | 310 | CLA  | C1B-NB | 6.45 | 1.41        | 1.35     |
| 25  | g     | 602 | CLA  | C1B-NB | 6.44 | 1.41        | 1.35     |
| 25  | S     | 310 | CLA  | C4B-NB | 6.43 | 1.40        | 1.35     |
| 25  | s     | 310 | CLA  | C4B-NB | 6.43 | 1.40        | 1.35     |
| 25  | G     | 614 | CLA  | C4B-NB | 6.42 | 1.40        | 1.35     |
| 25  | g     | 614 | CLA  | C4B-NB | 6.42 | 1.40        | 1.35     |
| 25  | N     | 610 | CLA  | C4B-NB | 6.42 | 1.40        | 1.35     |
| 25  | n     | 610 | CLA  | C4B-NB | 6.42 | 1.40        | 1.35     |
| 25  | N     | 602 | CLA  | C1B-NB | 6.42 | 1.40        | 1.35     |
| 25  | B     | 610 | CLA  | C4B-NB | 6.41 | 1.40        | 1.35     |
| 25  | C     | 505 | CLA  | C4B-NB | 6.41 | 1.40        | 1.35     |
| 25  | C     | 506 | CLA  | C4B-NB | 6.41 | 1.40        | 1.35     |
| 25  | Y     | 305 | CLA  | C1B-NB | 6.40 | 1.40        | 1.35     |
| 25  | c     | 513 | CLA  | C4B-NB | 6.40 | 1.40        | 1.35     |
| 25  | g     | 604 | CLA  | C4B-NB | 6.40 | 1.40        | 1.35     |
| 25  | S     | 303 | CLA  | C4B-NB | 6.39 | 1.40        | 1.35     |
| 25  | s     | 303 | CLA  | C4B-NB | 6.39 | 1.40        | 1.35     |
| 25  | S     | 314 | CLA  | C4B-NB | 6.39 | 1.40        | 1.35     |
| 25  | b     | 608 | CLA  | C4B-NB | 6.39 | 1.40        | 1.35     |
| 25  | s     | 314 | CLA  | C4B-NB | 6.39 | 1.40        | 1.35     |
| 25  | n     | 611 | CLA  | C4B-NB | 6.38 | 1.40        | 1.35     |
| 25  | C     | 513 | CLA  | C4B-NB | 6.37 | 1.40        | 1.35     |
| 25  | c     | 506 | CLA  | C4B-NB | 6.37 | 1.40        | 1.35     |
| 25  | G     | 602 | CLA  | C1B-NB | 6.36 | 1.40        | 1.35     |
| 25  | s     | 312 | CLA  | C4B-NB | 6.36 | 1.40        | 1.35     |
| 25  | s     | 310 | CLA  | C1B-NB | 6.35 | 1.40        | 1.35     |
| 25  | R     | 602 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | r     | 602 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | Y     | 312 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | y     | 312 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | B     | 613 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | b     | 613 | CLA  | C4B-NB | 6.35 | 1.40        | 1.35     |
| 25  | G     | 604 | CLA  | C1B-NB | 6.34 | 1.40        | 1.35     |
| 25  | b     | 610 | CLA  | C4B-NB | 6.34 | 1.40        | 1.35     |
| 25  | g     | 604 | CLA  | C1B-NB | 6.34 | 1.40        | 1.35     |
| 25  | N     | 612 | CLA  | C4B-NB | 6.33 | 1.40        | 1.35     |
| 25  | n     | 612 | CLA  | C4B-NB | 6.33 | 1.40        | 1.35     |
| 25  | C     | 507 | CLA  | C4B-NB | 6.33 | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | c     | 507 | CLA  | C4B-NB | 6.33  | 1.40        | 1.35     |
| 25  | c     | 502 | CLA  | C4B-NB | 6.33  | 1.40        | 1.35     |
| 25  | Y     | 311 | CLA  | C4B-NB | 6.33  | 1.40        | 1.35     |
| 25  | y     | 311 | CLA  | C4B-NB | 6.33  | 1.40        | 1.35     |
| 25  | S     | 312 | CLA  | C4B-NB | 6.32  | 1.40        | 1.35     |
| 25  | Y     | 312 | CLA  | C1B-NB | 6.32  | 1.40        | 1.35     |
| 25  | y     | 312 | CLA  | C1B-NB | 6.32  | 1.40        | 1.35     |
| 25  | N     | 611 | CLA  | C4B-NB | 6.32  | 1.40        | 1.35     |
| 25  | R     | 602 | CLA  | C1B-NB | 6.31  | 1.40        | 1.35     |
| 25  | B     | 612 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | r     | 608 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | b     | 607 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | R     | 609 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | r     | 609 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | G     | 604 | CLA  | C4B-NB | 6.30  | 1.40        | 1.35     |
| 25  | R     | 610 | CLA  | MG-ND  | -6.29 | 1.93        | 2.05     |
| 25  | r     | 602 | CLA  | C1B-NB | 6.29  | 1.40        | 1.35     |
| 25  | B     | 608 | CLA  | C4B-NB | 6.29  | 1.40        | 1.35     |
| 25  | B     | 607 | CLA  | C4B-NB | 6.28  | 1.40        | 1.35     |
| 25  | Y     | 315 | CLA  | C1B-NB | 6.28  | 1.40        | 1.35     |
| 25  | y     | 315 | CLA  | C1B-NB | 6.28  | 1.40        | 1.35     |
| 25  | B     | 609 | CLA  | C4B-NB | 6.28  | 1.40        | 1.35     |
| 25  | b     | 609 | CLA  | C4B-NB | 6.28  | 1.40        | 1.35     |
| 25  | C     | 502 | CLA  | C4B-NB | 6.27  | 1.40        | 1.35     |
| 25  | C     | 505 | CLA  | C1B-NB | 6.27  | 1.40        | 1.35     |
| 25  | R     | 608 | CLA  | C4B-NB | 6.27  | 1.40        | 1.35     |
| 25  | B     | 603 | CLA  | C4B-NB | 6.26  | 1.40        | 1.35     |
| 25  | R     | 601 | CLA  | MG-ND  | -6.26 | 1.93        | 2.05     |
| 25  | r     | 610 | CLA  | MG-ND  | -6.26 | 1.93        | 2.05     |
| 25  | S     | 309 | CLA  | C4B-NB | 6.25  | 1.40        | 1.35     |
| 25  | d     | 402 | CLA  | C4B-NB | 6.25  | 1.40        | 1.35     |
| 25  | B     | 614 | CLA  | C4B-NB | 6.24  | 1.40        | 1.35     |
| 25  | b     | 614 | CLA  | C4B-NB | 6.24  | 1.40        | 1.35     |
| 25  | b     | 603 | CLA  | C4B-NB | 6.24  | 1.40        | 1.35     |
| 25  | b     | 612 | CLA  | C4B-NB | 6.23  | 1.40        | 1.35     |
| 25  | r     | 601 | CLA  | MG-ND  | -6.23 | 1.93        | 2.05     |
| 25  | N     | 611 | CLA  | C1B-NB | 6.22  | 1.40        | 1.35     |
| 25  | n     | 611 | CLA  | C1B-NB | 6.22  | 1.40        | 1.35     |
| 25  | B     | 615 | CLA  | C4B-NB | 6.22  | 1.40        | 1.35     |
| 25  | b     | 615 | CLA  | C4B-NB | 6.22  | 1.40        | 1.35     |
| 25  | s     | 309 | CLA  | C4B-NB | 6.21  | 1.40        | 1.35     |
| 25  | C     | 509 | CLA  | C4B-NB | 6.20  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | c     | 509 | CLA  | C4B-NB | 6.20  | 1.40        | 1.35     |
| 25  | D     | 402 | CLA  | C4B-NB | 6.19  | 1.40        | 1.35     |
| 25  | y     | 304 | CLA  | C4B-NB | 6.18  | 1.40        | 1.35     |
| 25  | B     | 604 | CLA  | C4B-NB | 6.17  | 1.40        | 1.35     |
| 25  | b     | 604 | CLA  | C4B-NB | 6.17  | 1.40        | 1.35     |
| 25  | 2     | 605 | CLA  | C4B-NB | 6.17  | 1.40        | 1.35     |
| 25  | 6     | 605 | CLA  | C4B-NB | 6.17  | 1.40        | 1.35     |
| 25  | B     | 608 | CLA  | C1B-NB | 6.14  | 1.40        | 1.35     |
| 25  | N     | 603 | CLA  | C4B-NB | 6.14  | 1.40        | 1.35     |
| 25  | n     | 603 | CLA  | C4B-NB | 6.14  | 1.40        | 1.35     |
| 25  | Y     | 304 | CLA  | C4B-NB | 6.13  | 1.40        | 1.35     |
| 25  | c     | 505 | CLA  | C1B-NB | 6.12  | 1.40        | 1.35     |
| 25  | R     | 603 | CLA  | MG-ND  | -6.12 | 1.93        | 2.05     |
| 25  | r     | 603 | CLA  | MG-ND  | -6.12 | 1.93        | 2.05     |
| 25  | B     | 603 | CLA  | C1B-NB | 6.11  | 1.40        | 1.35     |
| 25  | A     | 401 | CLA  | C4B-NB | 6.11  | 1.40        | 1.35     |
| 25  | a     | 402 | CLA  | C4B-NB | 6.11  | 1.40        | 1.35     |
| 25  | G     | 614 | CLA  | C1B-NB | 6.10  | 1.40        | 1.35     |
| 25  | N     | 604 | CLA  | C4B-NB | 6.09  | 1.40        | 1.35     |
| 25  | c     | 503 | CLA  | C4B-NB | 6.07  | 1.40        | 1.35     |
| 25  | B     | 611 | CLA  | C4B-NB | 6.07  | 1.40        | 1.35     |
| 25  | b     | 611 | CLA  | C4B-NB | 6.07  | 1.40        | 1.35     |
| 25  | A     | 405 | CLA  | C4B-NB | 6.07  | 1.40        | 1.35     |
| 25  | a     | 406 | CLA  | C4B-NB | 6.07  | 1.40        | 1.35     |
| 25  | S     | 305 | CLA  | MG-ND  | -6.06 | 1.93        | 2.05     |
| 25  | s     | 305 | CLA  | MG-ND  | -6.06 | 1.93        | 2.05     |
| 25  | d     | 403 | CLA  | MG-ND  | -6.06 | 1.93        | 2.05     |
| 25  | b     | 603 | CLA  | C1B-NB | 6.06  | 1.40        | 1.35     |
| 25  | n     | 604 | CLA  | C4B-NB | 6.06  | 1.40        | 1.35     |
| 25  | g     | 614 | CLA  | C1B-NB | 6.06  | 1.40        | 1.35     |
| 25  | S     | 304 | CLA  | C4B-NB | 6.06  | 1.40        | 1.35     |
| 25  | s     | 304 | CLA  | C4B-NB | 6.06  | 1.40        | 1.35     |
| 25  | B     | 613 | CLA  | C1B-NB | 6.05  | 1.40        | 1.35     |
| 25  | b     | 613 | CLA  | C1B-NB | 6.05  | 1.40        | 1.35     |
| 25  | S     | 311 | CLA  | C4B-NB | 6.05  | 1.40        | 1.35     |
| 25  | D     | 403 | CLA  | MG-ND  | -6.05 | 1.93        | 2.05     |
| 25  | B     | 604 | CLA  | C1B-NB | 6.04  | 1.40        | 1.35     |
| 25  | B     | 616 | CLA  | C1B-NB | 6.04  | 1.40        | 1.35     |
| 25  | b     | 604 | CLA  | C1B-NB | 6.04  | 1.40        | 1.35     |
| 25  | b     | 616 | CLA  | C1B-NB | 6.04  | 1.40        | 1.35     |
| 25  | Y     | 304 | CLA  | C1B-NB | 6.04  | 1.40        | 1.35     |
| 25  | C     | 507 | CLA  | C1B-NB | 6.03  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | b     | 608 | CLA  | C1B-NB | 6.03  | 1.40        | 1.35     |
| 25  | C     | 513 | CLA  | C1B-NB | 6.02  | 1.40        | 1.35     |
| 25  | c     | 513 | CLA  | C1B-NB | 6.02  | 1.40        | 1.35     |
| 25  | b     | 607 | CLA  | C1B-NB | 6.01  | 1.40        | 1.35     |
| 25  | C     | 504 | CLA  | MG-ND  | -6.01 | 1.93        | 2.05     |
| 25  | c     | 509 | CLA  | C1B-NB | 6.01  | 1.40        | 1.35     |
| 25  | y     | 304 | CLA  | C1B-NB | 6.01  | 1.40        | 1.35     |
| 25  | c     | 510 | CLA  | C4B-NB | 6.00  | 1.40        | 1.35     |
| 25  | B     | 614 | CLA  | C1B-NB | 6.00  | 1.40        | 1.35     |
| 25  | b     | 614 | CLA  | C1B-NB | 6.00  | 1.40        | 1.35     |
| 25  | s     | 311 | CLA  | C4B-NB | 5.99  | 1.40        | 1.35     |
| 25  | C     | 503 | CLA  | C4B-NB | 5.99  | 1.40        | 1.35     |
| 25  | c     | 503 | CLA  | C1B-NB | 5.99  | 1.40        | 1.35     |
| 25  | c     | 504 | CLA  | MG-ND  | -5.99 | 1.93        | 2.05     |
| 25  | A     | 405 | CLA  | C1B-NB | 5.99  | 1.40        | 1.35     |
| 25  | a     | 406 | CLA  | C1B-NB | 5.99  | 1.40        | 1.35     |
| 25  | c     | 507 | CLA  | C1B-NB | 5.99  | 1.40        | 1.35     |
| 25  | C     | 512 | CLA  | C4B-NB | 5.98  | 1.40        | 1.35     |
| 25  | c     | 512 | CLA  | C4B-NB | 5.98  | 1.40        | 1.35     |
| 25  | 2     | 602 | CLA  | MG-ND  | -5.98 | 1.93        | 2.05     |
| 25  | 6     | 602 | CLA  | MG-ND  | -5.98 | 1.93        | 2.05     |
| 25  | B     | 607 | CLA  | C1B-NB | 5.97  | 1.40        | 1.35     |
| 25  | C     | 503 | CLA  | C1B-NB | 5.97  | 1.40        | 1.35     |
| 25  | B     | 605 | CLA  | C4B-NB | 5.94  | 1.40        | 1.35     |
| 25  | G     | 603 | CLA  | C4B-NB | 5.94  | 1.40        | 1.35     |
| 25  | g     | 603 | CLA  | C4B-NB | 5.94  | 1.40        | 1.35     |
| 25  | C     | 510 | CLA  | C4B-NB | 5.93  | 1.40        | 1.35     |
| 25  | C     | 509 | CLA  | C1B-NB | 5.93  | 1.40        | 1.35     |
| 25  | 2     | 605 | CLA  | C1B-NB | 5.92  | 1.40        | 1.35     |
| 25  | 6     | 605 | CLA  | C1B-NB | 5.92  | 1.40        | 1.35     |
| 25  | C     | 512 | CLA  | C1B-NB | 5.92  | 1.40        | 1.35     |
| 25  | c     | 512 | CLA  | C1B-NB | 5.92  | 1.40        | 1.35     |
| 25  | C     | 502 | CLA  | C1B-NB | 5.91  | 1.40        | 1.35     |
| 25  | c     | 502 | CLA  | C1B-NB | 5.91  | 1.40        | 1.35     |
| 25  | d     | 401 | CLA  | C4B-NB | 5.91  | 1.40        | 1.35     |
| 25  | D     | 401 | CLA  | C4B-NB | 5.90  | 1.40        | 1.35     |
| 25  | b     | 605 | CLA  | C4B-NB | 5.90  | 1.40        | 1.35     |
| 25  | N     | 603 | CLA  | C1B-NB | 5.90  | 1.40        | 1.35     |
| 25  | B     | 611 | CLA  | C1B-NB | 5.89  | 1.40        | 1.35     |
| 25  | b     | 611 | CLA  | C1B-NB | 5.89  | 1.40        | 1.35     |
| 25  | G     | 603 | CLA  | C1B-NB | 5.89  | 1.40        | 1.35     |
| 25  | Y     | 314 | CLA  | C4B-NB | 5.89  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | y     | 314 | CLA  | C4B-NB | 5.89  | 1.40        | 1.35     |
| 25  | B     | 612 | CLA  | C1B-NB | 5.86  | 1.40        | 1.35     |
| 25  | N     | 614 | CLA  | C4B-NB | 5.86  | 1.40        | 1.35     |
| 25  | b     | 612 | CLA  | C1B-NB | 5.86  | 1.40        | 1.35     |
| 25  | C     | 508 | CLA  | C4B-NB | 5.86  | 1.40        | 1.35     |
| 25  | c     | 508 | CLA  | C4B-NB | 5.86  | 1.40        | 1.35     |
| 25  | n     | 603 | CLA  | C1B-NB | 5.86  | 1.40        | 1.35     |
| 25  | n     | 614 | CLA  | C4B-NB | 5.86  | 1.40        | 1.35     |
| 25  | S     | 304 | CLA  | C1B-NB | 5.84  | 1.40        | 1.35     |
| 25  | s     | 304 | CLA  | C1B-NB | 5.84  | 1.40        | 1.35     |
| 25  | B     | 605 | CLA  | C1B-NB | 5.83  | 1.40        | 1.35     |
| 25  | A     | 402 | CLA  | C4B-NB | 5.83  | 1.40        | 1.35     |
| 25  | a     | 403 | CLA  | C4B-NB | 5.83  | 1.40        | 1.35     |
| 25  | c     | 511 | CLA  | C4B-NB | 5.81  | 1.40        | 1.35     |
| 25  | C     | 501 | CLA  | MG-ND  | -5.81 | 1.94        | 2.05     |
| 25  | c     | 501 | CLA  | MG-ND  | -5.81 | 1.94        | 2.05     |
| 25  | B     | 606 | CLA  | C4B-NB | 5.80  | 1.40        | 1.35     |
| 25  | b     | 606 | CLA  | C4B-NB | 5.80  | 1.40        | 1.35     |
| 25  | g     | 603 | CLA  | C1B-NB | 5.79  | 1.40        | 1.35     |
| 25  | G     | 610 | CLA  | C4B-NB | 5.79  | 1.40        | 1.35     |
| 25  | g     | 610 | CLA  | C4B-NB | 5.79  | 1.40        | 1.35     |
| 25  | C     | 511 | CLA  | C4B-NB | 5.78  | 1.40        | 1.35     |
| 25  | b     | 605 | CLA  | C1B-NB | 5.76  | 1.40        | 1.35     |
| 25  | n     | 604 | CLA  | C1B-NB | 5.75  | 1.40        | 1.35     |
| 25  | C     | 511 | CLA  | C1B-NB | 5.74  | 1.40        | 1.35     |
| 25  | A     | 401 | CLA  | C1B-NB | 5.74  | 1.40        | 1.35     |
| 25  | a     | 402 | CLA  | C1B-NB | 5.74  | 1.40        | 1.35     |
| 25  | S     | 311 | CLA  | C1B-NB | 5.74  | 1.40        | 1.35     |
| 25  | B     | 606 | CLA  | C1B-NB | 5.73  | 1.40        | 1.35     |
| 25  | b     | 606 | CLA  | C1B-NB | 5.73  | 1.40        | 1.35     |
| 25  | G     | 611 | CLA  | C4B-NB | 5.73  | 1.40        | 1.35     |
| 25  | C     | 510 | CLA  | C1B-NB | 5.72  | 1.40        | 1.35     |
| 25  | g     | 611 | CLA  | C4B-NB | 5.71  | 1.40        | 1.35     |
| 25  | 2     | 604 | CLA  | MG-ND  | -5.71 | 1.94        | 2.05     |
| 25  | D     | 401 | CLA  | C1B-NB | 5.71  | 1.40        | 1.35     |
| 25  | d     | 401 | CLA  | C1B-NB | 5.71  | 1.40        | 1.35     |
| 25  | B     | 601 | CLA  | C4B-NB | 5.70  | 1.40        | 1.35     |
| 25  | B     | 609 | CLA  | C1B-NB | 5.70  | 1.40        | 1.35     |
| 25  | b     | 609 | CLA  | C1B-NB | 5.70  | 1.40        | 1.35     |
| 25  | S     | 313 | CLA  | C4B-NB | 5.69  | 1.40        | 1.35     |
| 25  | s     | 313 | CLA  | C4B-NB | 5.69  | 1.40        | 1.35     |
| 25  | A     | 402 | CLA  | C1B-NB | 5.68  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | a     | 403 | CLA  | C1B-NB  | 5.68  | 1.40        | 1.35     |
| 25  | y     | 314 | CLA  | C1B-NB  | 5.67  | 1.40        | 1.35     |
| 25  | r     | 612 | CLA  | C4B-NB  | 5.67  | 1.40        | 1.35     |
| 25  | c     | 510 | CLA  | C1B-NB  | 5.67  | 1.40        | 1.35     |
| 25  | 6     | 604 | CLA  | MG-ND   | -5.67 | 1.94        | 2.05     |
| 25  | s     | 311 | CLA  | C1B-NB  | 5.66  | 1.40        | 1.35     |
| 25  | R     | 612 | CLA  | C4B-NB  | 5.65  | 1.40        | 1.35     |
| 25  | S     | 313 | CLA  | C1B-NB  | 5.65  | 1.40        | 1.35     |
| 25  | N     | 604 | CLA  | C1B-NB  | 5.64  | 1.40        | 1.35     |
| 25  | b     | 601 | CLA  | C4B-NB  | 5.62  | 1.40        | 1.35     |
| 25  | B     | 601 | CLA  | C1B-NB  | 5.60  | 1.40        | 1.35     |
| 25  | b     | 601 | CLA  | C1B-NB  | 5.60  | 1.40        | 1.35     |
| 25  | c     | 511 | CLA  | C1B-NB  | 5.60  | 1.40        | 1.35     |
| 25  | c     | 501 | CLA  | C4B-NB  | 5.57  | 1.40        | 1.35     |
| 25  | s     | 313 | CLA  | C1B-NB  | 5.57  | 1.40        | 1.35     |
| 25  | G     | 613 | CLA  | C1B-NB  | 5.56  | 1.40        | 1.35     |
| 25  | g     | 613 | CLA  | C1B-NB  | 5.56  | 1.40        | 1.35     |
| 25  | N     | 613 | CLA  | C1B-NB  | 5.56  | 1.40        | 1.35     |
| 25  | n     | 613 | CLA  | C1B-NB  | 5.56  | 1.40        | 1.35     |
| 25  | C     | 501 | CLA  | C4B-NB  | 5.55  | 1.40        | 1.35     |
| 25  | R     | 604 | CLA  | C4B-NB  | 5.53  | 1.40        | 1.35     |
| 25  | r     | 604 | CLA  | C4B-NB  | 5.52  | 1.40        | 1.35     |
| 25  | Y     | 314 | CLA  | C1B-NB  | 5.52  | 1.40        | 1.35     |
| 24  | Y     | 308 | CHL  | CMC-C2C | 5.48  | 1.56        | 1.45     |
| 24  | y     | 308 | CHL  | CMC-C2C | 5.48  | 1.56        | 1.45     |
| 25  | N     | 613 | CLA  | C4B-NB  | 5.48  | 1.40        | 1.35     |
| 24  | 5     | 302 | CHL  | CMC-C2C | 5.47  | 1.56        | 1.45     |
| 25  | C     | 508 | CLA  | C1B-NB  | 5.45  | 1.40        | 1.35     |
| 25  | c     | 508 | CLA  | C1B-NB  | 5.45  | 1.40        | 1.35     |
| 25  | n     | 613 | CLA  | C4B-NB  | 5.45  | 1.40        | 1.35     |
| 24  | G     | 607 | CHL  | CMC-C2C | 5.45  | 1.56        | 1.45     |
| 24  | g     | 607 | CHL  | CMC-C2C | 5.45  | 1.56        | 1.45     |
| 24  | 6     | 601 | CHL  | CMC-C2C | 5.44  | 1.56        | 1.45     |
| 24  | R     | 613 | CHL  | CMC-C2C | 5.44  | 1.56        | 1.45     |
| 25  | R     | 603 | CLA  | C4B-NB  | 5.44  | 1.40        | 1.35     |
| 24  | n     | 601 | CHL  | CMC-C2C | 5.43  | 1.56        | 1.45     |
| 24  | N     | 601 | CHL  | CMC-C2C | 5.43  | 1.56        | 1.45     |
| 25  | g     | 613 | CLA  | C4B-NB  | 5.43  | 1.40        | 1.35     |
| 25  | G     | 613 | CLA  | C4B-NB  | 5.42  | 1.40        | 1.35     |
| 24  | r     | 607 | CHL  | CMC-C2C | 5.42  | 1.56        | 1.45     |
| 24  | 1     | 302 | CHL  | CMC-C2C | 5.41  | 1.56        | 1.45     |
| 24  | 1     | 301 | CHL  | CMC-C2C | 5.41  | 1.56        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | R     | 607 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 24  | 5     | 301 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 24  | g     | 609 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 24  | 2     | 601 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 24  | S     | 308 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 24  | s     | 308 | CHL  | CMC-C2C | 5.40  | 1.56        | 1.45     |
| 25  | r     | 612 | CLA  | C1B-NB  | 5.39  | 1.40        | 1.35     |
| 24  | r     | 606 | CHL  | CMC-C2C | 5.39  | 1.56        | 1.45     |
| 25  | C     | 504 | CLA  | C4B-NB  | 5.39  | 1.40        | 1.35     |
| 40  | n     | 617 | NEX  | C10-C9  | 5.39  | 1.42        | 1.35     |
| 25  | D     | 403 | CLA  | C4B-NB  | 5.39  | 1.40        | 1.35     |
| 24  | r     | 613 | CHL  | CMC-C2C | 5.39  | 1.56        | 1.45     |
| 24  | S     | 306 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 24  | S     | 307 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 24  | s     | 307 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 24  | G     | 606 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 24  | g     | 606 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 40  | N     | 617 | NEX  | C10-C9  | 5.38  | 1.42        | 1.35     |
| 24  | R     | 606 | CHL  | CMC-C2C | 5.38  | 1.56        | 1.45     |
| 24  | s     | 302 | CHL  | CMC-C2C | 5.37  | 1.56        | 1.45     |
| 24  | Y     | 309 | CHL  | CMC-C2C | 5.37  | 1.56        | 1.45     |
| 24  | N     | 605 | CHL  | CMC-C2C | 5.37  | 1.56        | 1.45     |
| 24  | n     | 605 | CHL  | CMC-C2C | 5.37  | 1.56        | 1.45     |
| 25  | c     | 504 | CLA  | C4B-NB  | 5.37  | 1.40        | 1.35     |
| 24  | G     | 609 | CHL  | CMC-C2C | 5.37  | 1.56        | 1.45     |
| 25  | R     | 612 | CLA  | C1B-NB  | 5.36  | 1.40        | 1.35     |
| 25  | r     | 603 | CLA  | C4B-NB  | 5.36  | 1.40        | 1.35     |
| 24  | n     | 608 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | N     | 609 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | n     | 609 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | Y     | 306 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | N     | 606 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | n     | 606 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | y     | 309 | CHL  | CMC-C2C | 5.36  | 1.56        | 1.45     |
| 24  | G     | 608 | CHL  | CMC-C2C | 5.35  | 1.56        | 1.45     |
| 24  | g     | 608 | CHL  | CMC-C2C | 5.35  | 1.56        | 1.45     |
| 24  | y     | 306 | CHL  | CMC-C2C | 5.35  | 1.56        | 1.45     |
| 25  | 2     | 602 | CLA  | MG-NA   | -5.35 | 1.93        | 2.06     |
| 25  | 6     | 602 | CLA  | MG-NA   | -5.35 | 1.93        | 2.06     |
| 25  | d     | 403 | CLA  | C4B-NB  | 5.35  | 1.40        | 1.35     |
| 24  | s     | 306 | CHL  | CMC-C2C | 5.35  | 1.56        | 1.45     |
| 25  | r     | 601 | CLA  | C4B-NB  | 5.35  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | N     | 608 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | Y     | 302 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | y     | 302 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | r     | 605 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | N     | 607 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | n     | 607 | CHL  | CMC-C2C | 5.34  | 1.56        | 1.45     |
| 24  | G     | 605 | CHL  | CMC-C2C | 5.33  | 1.56        | 1.45     |
| 24  | S     | 302 | CHL  | CMC-C2C | 5.33  | 1.56        | 1.45     |
| 24  | Y     | 307 | CHL  | CMC-C2C | 5.33  | 1.56        | 1.45     |
| 24  | Y     | 310 | CHL  | CMC-C2C | 5.33  | 1.56        | 1.45     |
| 24  | y     | 310 | CHL  | CMC-C2C | 5.33  | 1.56        | 1.45     |
| 25  | R     | 611 | CLA  | MG-NA   | -5.32 | 1.93        | 2.06     |
| 25  | r     | 611 | CLA  | MG-NA   | -5.32 | 1.93        | 2.06     |
| 24  | R     | 605 | CHL  | CMC-C2C | 5.32  | 1.56        | 1.45     |
| 24  | G     | 601 | CHL  | CMC-C2C | 5.32  | 1.56        | 1.45     |
| 24  | g     | 601 | CHL  | CMC-C2C | 5.32  | 1.56        | 1.45     |
| 24  | y     | 307 | CHL  | CMC-C2C | 5.32  | 1.56        | 1.45     |
| 25  | 2     | 602 | CLA  | MG-NC   | -5.31 | 1.93        | 2.06     |
| 25  | 6     | 602 | CLA  | MG-NC   | -5.31 | 1.93        | 2.06     |
| 25  | r     | 610 | CLA  | C4B-NB  | 5.30  | 1.39        | 1.35     |
| 25  | R     | 601 | CLA  | C4B-NB  | 5.29  | 1.39        | 1.35     |
| 25  | S     | 305 | CLA  | C4B-NB  | 5.29  | 1.39        | 1.35     |
| 25  | s     | 305 | CLA  | C4B-NB  | 5.29  | 1.39        | 1.35     |
| 24  | g     | 605 | CHL  | CMC-C2C | 5.28  | 1.56        | 1.45     |
| 25  | R     | 611 | CLA  | MG-NC   | -5.28 | 1.93        | 2.06     |
| 25  | r     | 611 | CLA  | MG-NC   | -5.28 | 1.93        | 2.06     |
| 40  | y     | 318 | NEX  | C10-C9  | 5.26  | 1.42        | 1.35     |
| 25  | R     | 610 | CLA  | C4B-NB  | 5.23  | 1.39        | 1.35     |
| 25  | 2     | 604 | CLA  | C4B-NB  | 5.22  | 1.39        | 1.35     |
| 25  | 6     | 604 | CLA  | C4B-NB  | 5.22  | 1.39        | 1.35     |
| 40  | Y     | 318 | NEX  | C10-C9  | 5.21  | 1.42        | 1.35     |
| 25  | G     | 611 | CLA  | MG-ND   | -5.18 | 1.95        | 2.05     |
| 25  | g     | 611 | CLA  | MG-ND   | -5.18 | 1.95        | 2.05     |
| 25  | r     | 604 | CLA  | C1B-NB  | 5.18  | 1.39        | 1.35     |
| 25  | R     | 604 | CLA  | C1B-NB  | 5.18  | 1.39        | 1.35     |
| 25  | r     | 610 | CLA  | MG-NA   | -5.17 | 1.94        | 2.06     |
| 25  | g     | 610 | CLA  | MG-ND   | -5.14 | 1.95        | 2.05     |
| 25  | R     | 610 | CLA  | MG-NA   | -5.13 | 1.94        | 2.06     |
| 24  | 2     | 603 | CHL  | CMC-C2C | 5.13  | 1.56        | 1.45     |
| 25  | g     | 610 | CLA  | C1B-NB  | 5.13  | 1.39        | 1.35     |
| 25  | G     | 610 | CLA  | MG-ND   | -5.10 | 1.95        | 2.05     |
| 25  | 2     | 604 | CLA  | C1B-NB  | 5.10  | 1.39        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 6     | 604 | CLA  | C1B-NB  | 5.10  | 1.39        | 1.35     |
| 24  | 6     | 603 | CHL  | CMC-C2C | 5.09  | 1.55        | 1.45     |
| 25  | g     | 611 | CLA  | C1B-NB  | 5.08  | 1.39        | 1.35     |
| 25  | S     | 305 | CLA  | MG-NA   | -5.06 | 1.94        | 2.06     |
| 25  | s     | 305 | CLA  | MG-NA   | -5.06 | 1.94        | 2.06     |
| 25  | G     | 610 | CLA  | C1B-NB  | 5.04  | 1.39        | 1.35     |
| 40  | R     | 617 | NEX  | C10-C9  | 5.04  | 1.42        | 1.35     |
| 40  | r     | 617 | NEX  | C10-C9  | 5.04  | 1.42        | 1.35     |
| 25  | G     | 611 | CLA  | C1B-NB  | 5.00  | 1.39        | 1.35     |
| 25  | R     | 611 | CLA  | C4B-NB  | 4.99  | 1.39        | 1.35     |
| 25  | R     | 604 | CLA  | MG-ND   | -4.99 | 1.95        | 2.05     |
| 25  | R     | 610 | CLA  | MG-NC   | -4.94 | 1.94        | 2.06     |
| 25  | r     | 604 | CLA  | MG-ND   | -4.93 | 1.96        | 2.05     |
| 25  | R     | 612 | CLA  | MG-ND   | -4.93 | 1.96        | 2.05     |
| 25  | r     | 610 | CLA  | MG-NC   | -4.92 | 1.94        | 2.06     |
| 25  | D     | 403 | CLA  | MG-NA   | -4.91 | 1.94        | 2.06     |
| 25  | c     | 504 | CLA  | MG-NA   | -4.91 | 1.94        | 2.06     |
| 25  | r     | 612 | CLA  | MG-ND   | -4.90 | 1.96        | 2.05     |
| 25  | d     | 403 | CLA  | MG-NA   | -4.90 | 1.94        | 2.06     |
| 25  | C     | 504 | CLA  | MG-NA   | -4.89 | 1.94        | 2.06     |
| 25  | s     | 305 | CLA  | MG-NC   | -4.89 | 1.94        | 2.06     |
| 25  | r     | 603 | CLA  | MG-NA   | -4.88 | 1.94        | 2.06     |
| 40  | s     | 317 | NEX  | C10-C9  | 4.88  | 1.42        | 1.35     |
| 25  | R     | 603 | CLA  | MG-NA   | -4.87 | 1.94        | 2.06     |
| 25  | r     | 611 | CLA  | C4B-NB  | 4.87  | 1.39        | 1.35     |
| 25  | S     | 305 | CLA  | MG-NC   | -4.86 | 1.94        | 2.06     |
| 40  | S     | 317 | NEX  | C10-C9  | 4.85  | 1.42        | 1.35     |
| 25  | R     | 601 | CLA  | MG-NA   | -4.85 | 1.94        | 2.06     |
| 25  | r     | 601 | CLA  | MG-NA   | -4.85 | 1.94        | 2.06     |
| 25  | d     | 403 | CLA  | MG-NC   | -4.82 | 1.94        | 2.06     |
| 25  | r     | 601 | CLA  | MG-NC   | -4.81 | 1.94        | 2.06     |
| 25  | n     | 614 | CLA  | MG-ND   | -4.81 | 1.96        | 2.05     |
| 25  | D     | 403 | CLA  | MG-NC   | -4.79 | 1.94        | 2.06     |
| 25  | N     | 614 | CLA  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 25  | s     | 313 | CLA  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 25  | R     | 601 | CLA  | MG-NC   | -4.78 | 1.94        | 2.06     |
| 40  | g     | 617 | NEX  | C10-C9  | 4.76  | 1.42        | 1.35     |
| 25  | C     | 504 | CLA  | MG-NC   | -4.76 | 1.95        | 2.06     |
| 25  | g     | 613 | CLA  | MG-NA   | -4.75 | 1.95        | 2.06     |
| 25  | c     | 504 | CLA  | MG-NC   | -4.75 | 1.95        | 2.06     |
| 25  | S     | 313 | CLA  | MG-ND   | -4.75 | 1.96        | 2.05     |
| 25  | R     | 603 | CLA  | MG-NC   | -4.75 | 1.95        | 2.06     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | r     | 603 | CLA  | MG-NC  | -4.75 | 1.95        | 2.06     |
| 25  | 6     | 602 | CLA  | C4B-NB | 4.72  | 1.39        | 1.35     |
| 25  | B     | 601 | CLA  | MG-ND  | -4.72 | 1.96        | 2.05     |
| 25  | b     | 601 | CLA  | MG-ND  | -4.72 | 1.96        | 2.05     |
| 25  | N     | 614 | CLA  | C1B-NB | 4.71  | 1.39        | 1.35     |
| 25  | G     | 613 | CLA  | MG-NA  | -4.71 | 1.95        | 2.06     |
| 25  | 2     | 602 | CLA  | C1B-NB | 4.69  | 1.39        | 1.35     |
| 25  | 6     | 602 | CLA  | C1B-NB | 4.69  | 1.39        | 1.35     |
| 25  | 2     | 602 | CLA  | C4B-NB | 4.69  | 1.39        | 1.35     |
| 25  | g     | 613 | CLA  | MG-ND  | -4.68 | 1.96        | 2.05     |
| 25  | C     | 501 | CLA  | MG-NA  | -4.67 | 1.95        | 2.06     |
| 25  | c     | 501 | CLA  | MG-NA  | -4.67 | 1.95        | 2.06     |
| 25  | G     | 613 | CLA  | MG-ND  | -4.64 | 1.96        | 2.05     |
| 25  | 2     | 604 | CLA  | MG-NC  | -4.62 | 1.95        | 2.06     |
| 25  | 6     | 604 | CLA  | MG-NC  | -4.62 | 1.95        | 2.06     |
| 25  | n     | 614 | CLA  | C1B-NB | 4.60  | 1.39        | 1.35     |
| 25  | C     | 501 | CLA  | MG-NC  | -4.59 | 1.95        | 2.06     |
| 25  | c     | 501 | CLA  | MG-NC  | -4.59 | 1.95        | 2.06     |
| 25  | c     | 507 | CLA  | MG-ND  | -4.58 | 1.96        | 2.05     |
| 25  | C     | 507 | CLA  | MG-ND  | -4.57 | 1.96        | 2.05     |
| 25  | R     | 611 | CLA  | C1B-NB | 4.56  | 1.39        | 1.35     |
| 25  | C     | 508 | CLA  | MG-ND  | -4.55 | 1.96        | 2.05     |
| 25  | c     | 508 | CLA  | MG-ND  | -4.55 | 1.96        | 2.05     |
| 25  | A     | 402 | CLA  | MG-ND  | -4.55 | 1.96        | 2.05     |
| 25  | N     | 612 | CLA  | MG-NA  | -4.54 | 1.95        | 2.06     |
| 29  | A     | 411 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 29  | a     | 412 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 29  | A     | 407 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 29  | a     | 408 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 29  | L     | 103 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 29  | l     | 101 | SQD  | O8-S   | 4.54  | 1.63        | 1.47     |
| 25  | B     | 606 | CLA  | MG-ND  | -4.53 | 1.96        | 2.05     |
| 25  | b     | 606 | CLA  | MG-ND  | -4.53 | 1.96        | 2.05     |
| 29  | l     | 102 | SQD  | O8-S   | 4.53  | 1.63        | 1.47     |
| 25  | a     | 403 | CLA  | MG-ND  | -4.52 | 1.96        | 2.05     |
| 29  | L     | 101 | SQD  | O8-S   | 4.51  | 1.63        | 1.47     |
| 25  | S     | 311 | CLA  | MG-ND  | -4.51 | 1.96        | 2.05     |
| 25  | n     | 612 | CLA  | MG-NA  | -4.51 | 1.95        | 2.06     |
| 25  | r     | 611 | CLA  | C1B-NB | 4.49  | 1.39        | 1.35     |
| 25  | C     | 512 | CLA  | MG-ND  | -4.49 | 1.96        | 2.05     |
| 25  | c     | 512 | CLA  | MG-ND  | -4.49 | 1.96        | 2.05     |
| 25  | r     | 609 | CLA  | MG-ND  | -4.49 | 1.96        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 511 | CLA  | MG-ND   | -4.49 | 1.96        | 2.05     |
| 25  | c     | 511 | CLA  | MG-ND   | -4.49 | 1.96        | 2.05     |
| 25  | 6     | 604 | CLA  | MG-NA   | -4.49 | 1.95        | 2.06     |
| 25  | c     | 510 | CLA  | MG-ND   | -4.49 | 1.96        | 2.05     |
| 25  | 2     | 604 | CLA  | MG-NA   | -4.48 | 1.95        | 2.06     |
| 25  | C     | 510 | CLA  | MG-ND   | -4.48 | 1.96        | 2.05     |
| 25  | s     | 311 | CLA  | MG-ND   | -4.47 | 1.96        | 2.05     |
| 25  | D     | 401 | CLA  | MG-ND   | -4.46 | 1.96        | 2.05     |
| 25  | d     | 401 | CLA  | MG-ND   | -4.46 | 1.96        | 2.05     |
| 25  | 6     | 605 | CLA  | MG-ND   | -4.46 | 1.97        | 2.05     |
| 40  | Y     | 318 | NEX  | C14-C13 | 4.45  | 1.41        | 1.35     |
| 25  | A     | 401 | CLA  | MG-ND   | -4.45 | 1.97        | 2.05     |
| 25  | a     | 402 | CLA  | MG-ND   | -4.45 | 1.97        | 2.05     |
| 25  | B     | 605 | CLA  | MG-ND   | -4.44 | 1.97        | 2.05     |
| 25  | b     | 605 | CLA  | MG-ND   | -4.44 | 1.97        | 2.05     |
| 25  | 2     | 605 | CLA  | MG-ND   | -4.43 | 1.97        | 2.05     |
| 40  | y     | 318 | NEX  | C14-C13 | 4.43  | 1.41        | 1.35     |
| 25  | R     | 609 | CLA  | MG-ND   | -4.43 | 1.97        | 2.05     |
| 25  | C     | 509 | CLA  | MG-ND   | -4.42 | 1.97        | 2.05     |
| 25  | s     | 304 | CLA  | MG-ND   | -4.42 | 1.97        | 2.05     |
| 25  | c     | 509 | CLA  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 25  | S     | 312 | CLA  | MG-NA   | -4.41 | 1.95        | 2.06     |
| 25  | s     | 312 | CLA  | MG-NA   | -4.41 | 1.95        | 2.06     |
| 25  | B     | 612 | CLA  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 25  | b     | 612 | CLA  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 25  | S     | 304 | CLA  | MG-ND   | -4.40 | 1.97        | 2.05     |
| 25  | B     | 604 | CLA  | MG-ND   | -4.39 | 1.97        | 2.05     |
| 25  | b     | 604 | CLA  | MG-ND   | -4.39 | 1.97        | 2.05     |
| 25  | y     | 304 | CLA  | MG-ND   | -4.36 | 1.97        | 2.05     |
| 25  | N     | 613 | CLA  | MG-NA   | -4.34 | 1.96        | 2.06     |
| 25  | n     | 613 | CLA  | MG-NA   | -4.34 | 1.96        | 2.06     |
| 25  | n     | 613 | CLA  | MG-ND   | -4.34 | 1.97        | 2.05     |
| 25  | B     | 615 | CLA  | MG-NA   | -4.32 | 1.96        | 2.06     |
| 25  | b     | 615 | CLA  | MG-NA   | -4.32 | 1.96        | 2.06     |
| 25  | D     | 402 | CLA  | MG-ND   | -4.31 | 1.97        | 2.05     |
| 25  | d     | 402 | CLA  | MG-ND   | -4.31 | 1.97        | 2.05     |
| 25  | N     | 613 | CLA  | MG-ND   | -4.31 | 1.97        | 2.05     |
| 25  | Y     | 304 | CLA  | MG-ND   | -4.30 | 1.97        | 2.05     |
| 25  | A     | 405 | CLA  | MG-ND   | -4.28 | 1.97        | 2.05     |
| 25  | a     | 406 | CLA  | MG-ND   | -4.28 | 1.97        | 2.05     |
| 25  | N     | 604 | CLA  | MG-ND   | -4.27 | 1.97        | 2.05     |
| 25  | n     | 604 | CLA  | MG-ND   | -4.27 | 1.97        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | G     | 611 | CLA  | C1D-C2D | -4.27 | 1.36        | 1.45     |
| 25  | C     | 513 | CLA  | MG-ND   | -4.27 | 1.97        | 2.05     |
| 25  | R     | 612 | CLA  | MG-NA   | -4.26 | 1.96        | 2.06     |
| 25  | g     | 611 | CLA  | C1D-C2D | -4.26 | 1.36        | 1.45     |
| 25  | b     | 602 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | C     | 503 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | c     | 503 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | N     | 603 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | n     | 603 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | S     | 310 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | s     | 310 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | R     | 608 | CLA  | MG-ND   | -4.25 | 1.97        | 2.05     |
| 25  | r     | 612 | CLA  | MG-NA   | -4.24 | 1.96        | 2.06     |
| 25  | r     | 608 | CLA  | MG-ND   | -4.24 | 1.97        | 2.05     |
| 25  | c     | 513 | CLA  | MG-ND   | -4.23 | 1.97        | 2.05     |
| 25  | B     | 611 | CLA  | MG-ND   | -4.23 | 1.97        | 2.05     |
| 25  | b     | 611 | CLA  | MG-ND   | -4.23 | 1.97        | 2.05     |
| 25  | b     | 615 | CLA  | MG-ND   | -4.22 | 1.97        | 2.05     |
| 25  | G     | 603 | CLA  | MG-ND   | -4.22 | 1.97        | 2.05     |
| 25  | B     | 602 | CLA  | MG-ND   | -4.22 | 1.97        | 2.05     |
| 25  | b     | 609 | CLA  | MG-ND   | -4.21 | 1.97        | 2.05     |
| 25  | N     | 611 | CLA  | MG-ND   | -4.20 | 1.97        | 2.05     |
| 25  | D     | 402 | CLA  | MG-NA   | -4.20 | 1.96        | 2.06     |
| 25  | S     | 309 | CLA  | MG-ND   | -4.19 | 1.97        | 2.05     |
| 25  | d     | 402 | CLA  | MG-NA   | -4.19 | 1.96        | 2.06     |
| 25  | B     | 615 | CLA  | MG-ND   | -4.18 | 1.97        | 2.05     |
| 25  | S     | 303 | CLA  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 25  | s     | 303 | CLA  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 25  | g     | 603 | CLA  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 25  | S     | 313 | CLA  | MG-NA   | -4.17 | 1.96        | 2.06     |
| 25  | n     | 611 | CLA  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 40  | n     | 617 | NEX  | C14-C13 | 4.17  | 1.41        | 1.35     |
| 25  | R     | 602 | CLA  | MG-ND   | -4.16 | 1.97        | 2.05     |
| 25  | b     | 607 | CLA  | MG-ND   | -4.16 | 1.97        | 2.05     |
| 40  | N     | 617 | NEX  | C14-C13 | 4.16  | 1.41        | 1.35     |
| 25  | S     | 312 | CLA  | MG-ND   | -4.16 | 1.97        | 2.05     |
| 25  | b     | 603 | CLA  | MG-ND   | -4.16 | 1.97        | 2.05     |
| 25  | s     | 313 | CLA  | MG-NA   | -4.15 | 1.96        | 2.06     |
| 25  | s     | 309 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | Y     | 315 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | B     | 607 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | B     | 609 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | n     | 612 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | Y     | 312 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | y     | 315 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 25  | r     | 609 | CLA  | MG-NA   | -4.13 | 1.96        | 2.06     |
| 25  | G     | 604 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 25  | g     | 604 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 25  | B     | 603 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 25  | y     | 312 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 25  | B     | 613 | CLA  | MG-ND   | -4.11 | 1.97        | 2.05     |
| 25  | s     | 312 | CLA  | MG-ND   | -4.11 | 1.97        | 2.05     |
| 25  | y     | 314 | CLA  | MG-ND   | -4.11 | 1.97        | 2.05     |
| 25  | S     | 309 | CLA  | MG-NA   | -4.11 | 1.96        | 2.06     |
| 25  | s     | 309 | CLA  | MG-NA   | -4.11 | 1.96        | 2.06     |
| 25  | B     | 608 | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 25  | r     | 602 | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 25  | C     | 502 | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 25  | c     | 502 | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 25  | R     | 609 | CLA  | MG-NA   | -4.10 | 1.96        | 2.06     |
| 25  | g     | 612 | CLA  | MG-NA   | -4.09 | 1.96        | 2.06     |
| 25  | b     | 608 | CLA  | MG-ND   | -4.09 | 1.97        | 2.05     |
| 25  | R     | 604 | CLA  | MG-NA   | -4.09 | 1.96        | 2.06     |
| 25  | r     | 604 | CLA  | MG-NA   | -4.09 | 1.96        | 2.06     |
| 40  | r     | 617 | NEX  | C14-C13 | 4.09  | 1.41        | 1.35     |
| 25  | c     | 506 | CLA  | MG-ND   | -4.08 | 1.97        | 2.05     |
| 25  | G     | 610 | CLA  | MG-NA   | -4.08 | 1.96        | 2.06     |
| 25  | N     | 612 | CLA  | MG-ND   | -4.07 | 1.97        | 2.05     |
| 25  | g     | 610 | CLA  | MG-NA   | -4.07 | 1.96        | 2.06     |
| 25  | C     | 511 | CLA  | MG-NA   | -4.07 | 1.96        | 2.06     |
| 25  | c     | 511 | CLA  | MG-NA   | -4.07 | 1.96        | 2.06     |
| 25  | Y     | 314 | CLA  | MG-ND   | -4.07 | 1.97        | 2.05     |
| 25  | b     | 613 | CLA  | MG-ND   | -4.06 | 1.97        | 2.05     |
| 40  | R     | 617 | NEX  | C14-C13 | 4.06  | 1.41        | 1.35     |
| 25  | B     | 614 | CLA  | MG-ND   | -4.06 | 1.97        | 2.05     |
| 25  | b     | 614 | CLA  | MG-ND   | -4.06 | 1.97        | 2.05     |
| 25  | B     | 601 | CLA  | MG-NA   | -4.05 | 1.96        | 2.06     |
| 25  | S     | 314 | CLA  | MG-ND   | -4.05 | 1.97        | 2.05     |
| 25  | s     | 314 | CLA  | MG-ND   | -4.05 | 1.97        | 2.05     |
| 25  | G     | 612 | CLA  | MG-NA   | -4.05 | 1.96        | 2.06     |
| 25  | B     | 610 | CLA  | MG-ND   | -4.04 | 1.97        | 2.05     |
| 25  | g     | 614 | CLA  | MG-ND   | -4.04 | 1.97        | 2.05     |
| 25  | G     | 611 | CLA  | MG-NA   | -4.03 | 1.96        | 2.06     |
| 25  | g     | 611 | CLA  | MG-NA   | -4.03 | 1.96        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 506 | CLA  | MG-ND   | -4.03 | 1.97        | 2.05     |
| 25  | b     | 616 | CLA  | MG-ND   | -4.03 | 1.97        | 2.05     |
| 25  | r     | 614 | CLA  | MG-NA   | -4.02 | 1.96        | 2.06     |
| 25  | b     | 601 | CLA  | MG-NA   | -4.02 | 1.96        | 2.06     |
| 25  | G     | 614 | CLA  | MG-ND   | -4.02 | 1.97        | 2.05     |
| 25  | R     | 614 | CLA  | MG-NA   | -4.01 | 1.96        | 2.06     |
| 25  | s     | 310 | CLA  | MG-NA   | -4.01 | 1.96        | 2.06     |
| 25  | N     | 602 | CLA  | MG-ND   | -4.01 | 1.97        | 2.05     |
| 25  | B     | 616 | CLA  | MG-ND   | -4.01 | 1.97        | 2.05     |
| 25  | b     | 610 | CLA  | MG-ND   | -4.00 | 1.97        | 2.05     |
| 25  | S     | 310 | CLA  | MG-NA   | -4.00 | 1.96        | 2.06     |
| 24  | R     | 613 | CHL  | C4B-NB  | 3.99  | 1.38        | 1.35     |
| 24  | r     | 613 | CHL  | C4B-NB  | 3.99  | 1.38        | 1.35     |
| 25  | Y     | 305 | CLA  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 25  | y     | 305 | CLA  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 25  | n     | 602 | CLA  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 24  | R     | 605 | CHL  | C4B-NB  | 3.98  | 1.38        | 1.35     |
| 25  | Y     | 311 | CLA  | MG-ND   | -3.97 | 1.97        | 2.05     |
| 25  | y     | 311 | CLA  | MG-ND   | -3.97 | 1.97        | 2.05     |
| 25  | y     | 312 | CLA  | C1D-C2D | -3.97 | 1.37        | 1.45     |
| 25  | B     | 610 | CLA  | MG-NA   | -3.96 | 1.96        | 2.06     |
| 25  | b     | 610 | CLA  | MG-NA   | -3.96 | 1.96        | 2.06     |
| 25  | Y     | 312 | CLA  | C1D-C2D | -3.96 | 1.37        | 1.45     |
| 25  | y     | 303 | CLA  | MG-NA   | -3.95 | 1.96        | 2.06     |
| 25  | N     | 610 | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 25  | n     | 610 | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 25  | Y     | 313 | CLA  | MG-ND   | -3.93 | 1.98        | 2.05     |
| 24  | s     | 306 | CHL  | C4B-NB  | 3.93  | 1.38        | 1.35     |
| 25  | Y     | 303 | CLA  | MG-NA   | -3.93 | 1.96        | 2.06     |
| 25  | c     | 507 | CLA  | MG-NA   | -3.93 | 1.96        | 2.06     |
| 25  | y     | 313 | CLA  | MG-ND   | -3.92 | 1.98        | 2.05     |
| 24  | G     | 606 | CHL  | C4B-NB  | 3.92  | 1.38        | 1.35     |
| 24  | g     | 606 | CHL  | C4B-NB  | 3.92  | 1.38        | 1.35     |
| 25  | G     | 602 | CLA  | MG-ND   | -3.91 | 1.98        | 2.05     |
| 24  | r     | 605 | CHL  | C4B-NB  | 3.91  | 1.38        | 1.35     |
| 24  | 1     | 302 | CHL  | C4B-NB  | 3.91  | 1.38        | 1.35     |
| 24  | 5     | 302 | CHL  | C4B-NB  | 3.91  | 1.38        | 1.35     |
| 25  | C     | 507 | CLA  | MG-NA   | -3.90 | 1.97        | 2.06     |
| 25  | N     | 611 | CLA  | C1D-C2D | -3.90 | 1.37        | 1.45     |
| 25  | n     | 611 | CLA  | C1D-C2D | -3.90 | 1.37        | 1.45     |
| 25  | g     | 602 | CLA  | MG-ND   | -3.90 | 1.98        | 2.05     |
| 24  | S     | 306 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | G     | 605 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | G     | 608 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | g     | 608 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | Y     | 306 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | G     | 609 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | g     | 609 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | Y     | 310 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | y     | 310 | CHL  | C4B-NB  | 3.89  | 1.38        | 1.35     |
| 24  | y     | 307 | CHL  | C3B-C2B | -3.89 | 1.35        | 1.40     |
| 25  | C     | 505 | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 25  | c     | 505 | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 25  | N     | 602 | CLA  | MG-NA   | -3.88 | 1.97        | 2.06     |
| 24  | s     | 307 | CHL  | C4B-NB  | 3.88  | 1.38        | 1.35     |
| 25  | n     | 602 | CLA  | MG-NA   | -3.87 | 1.97        | 2.06     |
| 24  | R     | 606 | CHL  | C4B-NB  | 3.87  | 1.38        | 1.35     |
| 24  | r     | 606 | CHL  | C4B-NB  | 3.87  | 1.38        | 1.35     |
| 24  | N     | 606 | CHL  | C4B-NB  | 3.87  | 1.38        | 1.35     |
| 24  | n     | 606 | CHL  | C4B-NB  | 3.87  | 1.38        | 1.35     |
| 25  | Y     | 303 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 25  | y     | 303 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 25  | S     | 312 | CLA  | MG-NC   | -3.87 | 1.97        | 2.06     |
| 25  | s     | 312 | CLA  | MG-NC   | -3.87 | 1.97        | 2.06     |
| 25  | n     | 612 | CLA  | MG-NC   | -3.86 | 1.97        | 2.06     |
| 25  | s     | 311 | CLA  | MG-NA   | -3.86 | 1.97        | 2.06     |
| 25  | N     | 612 | CLA  | MG-NC   | -3.86 | 1.97        | 2.06     |
| 25  | S     | 311 | CLA  | MG-NA   | -3.85 | 1.97        | 2.06     |
| 25  | R     | 612 | CLA  | MG-NC   | -3.85 | 1.97        | 2.06     |
| 25  | g     | 602 | CLA  | MG-NA   | -3.85 | 1.97        | 2.06     |
| 24  | S     | 308 | CHL  | C4B-NB  | 3.85  | 1.38        | 1.35     |
| 24  | s     | 308 | CHL  | C4B-NB  | 3.85  | 1.38        | 1.35     |
| 24  | S     | 307 | CHL  | C4B-NB  | 3.85  | 1.38        | 1.35     |
| 25  | s     | 313 | CLA  | MG-NC   | -3.85 | 1.97        | 2.06     |
| 28  | B     | 617 | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 28  | b     | 617 | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 24  | Y     | 307 | CHL  | C3B-C2B | -3.84 | 1.35        | 1.40     |
| 25  | c     | 508 | CLA  | MG-NA   | -3.84 | 1.97        | 2.06     |
| 24  | N     | 605 | CHL  | C4B-NB  | 3.84  | 1.38        | 1.35     |
| 24  | n     | 605 | CHL  | C4B-NB  | 3.84  | 1.38        | 1.35     |
| 25  | B     | 615 | CLA  | MG-NC   | -3.84 | 1.97        | 2.06     |
| 25  | b     | 615 | CLA  | MG-NC   | -3.84 | 1.97        | 2.06     |
| 24  | y     | 306 | CHL  | C4B-NB  | 3.84  | 1.38        | 1.35     |
| 25  | G     | 612 | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | F     | 101 | HEM  | C1B-NB  | -3.83 | 1.33        | 1.40     |
| 25  | A     | 402 | CLA  | MG-NA   | -3.83 | 1.97        | 2.06     |
| 25  | a     | 403 | CLA  | MG-NA   | -3.83 | 1.97        | 2.06     |
| 25  | g     | 610 | CLA  | MG-NC   | -3.83 | 1.97        | 2.06     |
| 24  | r     | 607 | CHL  | C4B-NB  | 3.83  | 1.38        | 1.35     |
| 25  | 6     | 605 | CLA  | MG-NA   | -3.83 | 1.97        | 2.06     |
| 25  | r     | 612 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 25  | G     | 602 | CLA  | MG-NA   | -3.82 | 1.97        | 2.06     |
| 24  | l     | 301 | CHL  | C4B-NB  | 3.82  | 1.38        | 1.35     |
| 25  | C     | 508 | CLA  | MG-NA   | -3.82 | 1.97        | 2.06     |
| 25  | S     | 313 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 25  | d     | 402 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 24  | g     | 605 | CHL  | C4B-NB  | 3.82  | 1.38        | 1.35     |
| 25  | G     | 610 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 38  | f     | 101 | HEM  | C4D-ND  | -3.82 | 1.33        | 1.40     |
| 25  | C     | 507 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 25  | R     | 604 | CLA  | MG-NC   | -3.82 | 1.97        | 2.06     |
| 25  | B     | 604 | CLA  | MG-NA   | -3.81 | 1.97        | 2.06     |
| 25  | D     | 402 | CLA  | MG-NC   | -3.81 | 1.97        | 2.06     |
| 25  | b     | 604 | CLA  | MG-NA   | -3.81 | 1.97        | 2.06     |
| 25  | N     | 614 | CLA  | MG-NA   | -3.81 | 1.97        | 2.06     |
| 25  | n     | 614 | CLA  | MG-NA   | -3.81 | 1.97        | 2.06     |
| 25  | Y     | 313 | CLA  | C1D-C2D | -3.80 | 1.37        | 1.45     |
| 25  | y     | 313 | CLA  | C1D-C2D | -3.80 | 1.37        | 1.45     |
| 40  | Y     | 318 | NEX  | C34-C33 | 3.80  | 1.40        | 1.35     |
| 28  | D     | 404 | BCR  | C1-C6   | -3.80 | 1.48        | 1.53     |
| 28  | d     | 404 | BCR  | C1-C6   | -3.80 | 1.48        | 1.53     |
| 25  | g     | 612 | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 25  | c     | 507 | CLA  | MG-NC   | -3.79 | 1.97        | 2.06     |
| 25  | r     | 604 | CLA  | MG-NC   | -3.79 | 1.97        | 2.06     |
| 25  | y     | 313 | CLA  | MG-NA   | -3.79 | 1.97        | 2.06     |
| 24  | n     | 607 | CHL  | C4B-NB  | 3.78  | 1.38        | 1.35     |
| 24  | g     | 607 | CHL  | C4B-NB  | 3.78  | 1.38        | 1.35     |
| 25  | B     | 605 | CLA  | MG-NA   | -3.78 | 1.97        | 2.06     |
| 24  | y     | 309 | CHL  | C4B-NB  | 3.77  | 1.38        | 1.35     |
| 25  | n     | 614 | CLA  | MG-NC   | -3.77 | 1.97        | 2.06     |
| 25  | N     | 614 | CLA  | MG-NC   | -3.77 | 1.97        | 2.06     |
| 38  | f     | 101 | HEM  | C1B-NB  | -3.77 | 1.33        | 1.40     |
| 24  | N     | 607 | CHL  | C4B-NB  | 3.77  | 1.38        | 1.35     |
| 25  | 2     | 605 | CLA  | MG-NA   | -3.77 | 1.97        | 2.06     |
| 25  | R     | 614 | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 25  | D     | 401 | CLA  | MG-NA   | -3.77 | 1.97        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | d     | 401 | CLA  | MG-NA   | -3.77 | 1.97        | 2.06     |
| 24  | N     | 608 | CHL  | C4B-NB  | 3.76  | 1.38        | 1.35     |
| 24  | 5     | 301 | CHL  | C4B-NB  | 3.76  | 1.38        | 1.35     |
| 24  | n     | 608 | CHL  | C4B-NB  | 3.76  | 1.38        | 1.35     |
| 25  | c     | 506 | CLA  | MG-NA   | -3.76 | 1.97        | 2.06     |
| 25  | R     | 602 | CLA  | MG-NA   | -3.76 | 1.97        | 2.06     |
| 25  | Y     | 313 | CLA  | MG-NA   | -3.76 | 1.97        | 2.06     |
| 38  | F     | 101 | HEM  | C4D-ND  | -3.75 | 1.33        | 1.40     |
| 25  | s     | 304 | CLA  | MG-NA   | -3.75 | 1.97        | 2.06     |
| 25  | r     | 614 | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 25  | R     | 609 | CLA  | MG-NC   | -3.75 | 1.97        | 2.06     |
| 25  | A     | 401 | CLA  | MG-NA   | -3.74 | 1.97        | 2.06     |
| 25  | a     | 402 | CLA  | MG-NA   | -3.74 | 1.97        | 2.06     |
| 25  | r     | 602 | CLA  | MG-NA   | -3.74 | 1.97        | 2.06     |
| 25  | S     | 304 | CLA  | MG-NA   | -3.74 | 1.97        | 2.06     |
| 25  | b     | 605 | CLA  | MG-NA   | -3.74 | 1.97        | 2.06     |
| 24  | R     | 607 | CHL  | C4B-NB  | 3.73  | 1.38        | 1.35     |
| 40  | y     | 318 | NEX  | C34-C33 | 3.73  | 1.40        | 1.35     |
| 25  | Y     | 314 | CLA  | MG-NA   | -3.73 | 1.97        | 2.06     |
| 25  | y     | 314 | CLA  | MG-NA   | -3.73 | 1.97        | 2.06     |
| 25  | C     | 506 | CLA  | MG-NA   | -3.73 | 1.97        | 2.06     |
| 25  | B     | 606 | CLA  | MG-NA   | -3.72 | 1.97        | 2.06     |
| 25  | b     | 606 | CLA  | MG-NA   | -3.72 | 1.97        | 2.06     |
| 24  | Y     | 309 | CHL  | C4B-NB  | 3.72  | 1.38        | 1.35     |
| 25  | C     | 510 | CLA  | MG-NA   | -3.71 | 1.97        | 2.06     |
| 25  | c     | 510 | CLA  | MG-NA   | -3.71 | 1.97        | 2.06     |
| 25  | S     | 305 | CLA  | C1B-NB  | 3.71  | 1.38        | 1.35     |
| 25  | s     | 305 | CLA  | C1B-NB  | 3.71  | 1.38        | 1.35     |
| 24  | G     | 607 | CHL  | C4B-NB  | 3.71  | 1.38        | 1.35     |
| 25  | r     | 609 | CLA  | MG-NC   | -3.71 | 1.97        | 2.06     |
| 25  | r     | 614 | CLA  | MG-NC   | -3.70 | 1.97        | 2.06     |
| 25  | C     | 512 | CLA  | MG-NA   | -3.70 | 1.97        | 2.06     |
| 25  | c     | 512 | CLA  | MG-NA   | -3.70 | 1.97        | 2.06     |
| 24  | 2     | 601 | CHL  | C4B-NB  | 3.69  | 1.38        | 1.35     |
| 24  | 6     | 601 | CHL  | C4B-NB  | 3.69  | 1.38        | 1.35     |
| 25  | S     | 309 | CLA  | MG-NC   | -3.69 | 1.97        | 2.06     |
| 25  | s     | 309 | CLA  | MG-NC   | -3.69 | 1.97        | 2.06     |
| 24  | 2     | 603 | CHL  | C4B-NB  | 3.68  | 1.38        | 1.35     |
| 28  | i     | 101 | BCR  | C1-C6   | -3.68 | 1.48        | 1.53     |
| 25  | R     | 614 | CLA  | MG-NC   | -3.68 | 1.97        | 2.06     |
| 25  | b     | 601 | CLA  | MG-NC   | -3.68 | 1.97        | 2.06     |
| 25  | C     | 513 | CLA  | MG-NA   | -3.67 | 1.97        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | c     | 513 | CLA  | MG-NA   | -3.67 | 1.97        | 2.06     |
| 25  | A     | 405 | CLA  | MG-NA   | -3.67 | 1.97        | 2.06     |
| 25  | a     | 406 | CLA  | MG-NA   | -3.67 | 1.97        | 2.06     |
| 25  | c     | 501 | CLA  | C1B-NB  | 3.66  | 1.38        | 1.35     |
| 24  | N     | 609 | CHL  | C4B-NB  | 3.66  | 1.38        | 1.35     |
| 24  | n     | 609 | CHL  | C4B-NB  | 3.66  | 1.38        | 1.35     |
| 25  | B     | 602 | CLA  | MG-NA   | -3.65 | 1.97        | 2.06     |
| 25  | b     | 602 | CLA  | MG-NA   | -3.65 | 1.97        | 2.06     |
| 25  | S     | 314 | CLA  | MG-NA   | -3.65 | 1.97        | 2.06     |
| 25  | s     | 314 | CLA  | MG-NA   | -3.65 | 1.97        | 2.06     |
| 24  | 2     | 603 | CHL  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 24  | 6     | 603 | CHL  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 25  | B     | 601 | CLA  | MG-NC   | -3.64 | 1.97        | 2.06     |
| 25  | B     | 610 | CLA  | MG-NC   | -3.64 | 1.97        | 2.06     |
| 25  | b     | 610 | CLA  | MG-NC   | -3.64 | 1.97        | 2.06     |
| 25  | d     | 403 | CLA  | C1B-NB  | 3.64  | 1.38        | 1.35     |
| 25  | B     | 603 | CLA  | MG-NA   | -3.64 | 1.97        | 2.06     |
| 25  | b     | 603 | CLA  | MG-NA   | -3.64 | 1.97        | 2.06     |
| 25  | g     | 603 | CLA  | MG-NA   | -3.63 | 1.97        | 2.06     |
| 25  | B     | 612 | CLA  | MG-NA   | -3.63 | 1.97        | 2.06     |
| 28  | I     | 101 | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 28  | T     | 101 | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 28  | t     | 101 | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 25  | b     | 612 | CLA  | MG-NA   | -3.63 | 1.97        | 2.06     |
| 25  | C     | 503 | CLA  | MG-NA   | -3.62 | 1.97        | 2.06     |
| 25  | c     | 503 | CLA  | MG-NA   | -3.62 | 1.97        | 2.06     |
| 25  | C     | 502 | CLA  | C1D-C2D | -3.62 | 1.38        | 1.45     |
| 25  | c     | 502 | CLA  | C1D-C2D | -3.62 | 1.38        | 1.45     |
| 25  | B     | 610 | CLA  | C1D-C2D | -3.62 | 1.38        | 1.45     |
| 25  | b     | 610 | CLA  | C1D-C2D | -3.62 | 1.38        | 1.45     |
| 25  | G     | 603 | CLA  | MG-NA   | -3.62 | 1.97        | 2.06     |
| 25  | n     | 610 | CLA  | C1D-C2D | -3.61 | 1.38        | 1.45     |
| 25  | C     | 501 | CLA  | C1B-NB  | 3.61  | 1.38        | 1.35     |
| 25  | C     | 511 | CLA  | MG-NC   | -3.61 | 1.97        | 2.06     |
| 25  | c     | 511 | CLA  | MG-NC   | -3.61 | 1.97        | 2.06     |
| 25  | n     | 604 | CLA  | MG-NA   | -3.61 | 1.97        | 2.06     |
| 25  | g     | 612 | CLA  | C1D-C2D | -3.61 | 1.38        | 1.45     |
| 25  | N     | 614 | CLA  | C1D-C2D | -3.60 | 1.38        | 1.45     |
| 25  | n     | 614 | CLA  | C1D-C2D | -3.60 | 1.38        | 1.45     |
| 25  | n     | 603 | CLA  | MG-NA   | -3.60 | 1.97        | 2.06     |
| 24  | N     | 607 | CHL  | O2D-CGD | 3.60  | 1.42        | 1.33     |
| 24  | n     | 607 | CHL  | O2D-CGD | 3.60  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | n     | 610 | CLA  | MG-NA   | -3.60 | 1.97        | 2.06     |
| 24  | 6     | 603 | CHL  | C4B-NB  | 3.60  | 1.38        | 1.35     |
| 25  | y     | 304 | CLA  | MG-NA   | -3.60 | 1.97        | 2.06     |
| 28  | C     | 514 | BCR  | C1-C6   | -3.60 | 1.48        | 1.53     |
| 28  | c     | 514 | BCR  | C1-C6   | -3.60 | 1.48        | 1.53     |
| 25  | N     | 610 | CLA  | C1D-C2D | -3.59 | 1.38        | 1.45     |
| 25  | R     | 603 | CLA  | C1B-NB  | 3.59  | 1.38        | 1.35     |
| 25  | N     | 604 | CLA  | MG-NA   | -3.59 | 1.97        | 2.06     |
| 24  | Y     | 302 | CHL  | C4B-NB  | 3.59  | 1.38        | 1.35     |
| 24  | y     | 302 | CHL  | C4B-NB  | 3.59  | 1.38        | 1.35     |
| 25  | Y     | 311 | CLA  | C1D-C2D | -3.59 | 1.38        | 1.45     |
| 24  | g     | 601 | CHL  | C4B-NB  | 3.59  | 1.38        | 1.35     |
| 25  | g     | 604 | CLA  | MG-NA   | -3.58 | 1.97        | 2.06     |
| 25  | N     | 610 | CLA  | MG-NA   | -3.58 | 1.97        | 2.06     |
| 25  | R     | 601 | CLA  | C1B-NB  | 3.58  | 1.38        | 1.35     |
| 25  | r     | 601 | CLA  | C1B-NB  | 3.58  | 1.38        | 1.35     |
| 25  | y     | 311 | CLA  | C1D-C2D | -3.58 | 1.38        | 1.45     |
| 25  | Y     | 304 | CLA  | C1D-C2D | -3.58 | 1.38        | 1.45     |
| 25  | S     | 303 | CLA  | MG-NA   | -3.58 | 1.97        | 2.06     |
| 25  | s     | 303 | CLA  | MG-NA   | -3.58 | 1.97        | 2.06     |
| 25  | Y     | 303 | CLA  | C1D-C2D | -3.57 | 1.38        | 1.45     |
| 25  | y     | 303 | CLA  | C1D-C2D | -3.57 | 1.38        | 1.45     |
| 25  | Y     | 311 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 25  | y     | 311 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 25  | Y     | 304 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 25  | c     | 509 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 25  | C     | 509 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 25  | S     | 310 | CLA  | C1D-C2D | -3.57 | 1.38        | 1.45     |
| 25  | N     | 603 | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 24  | Y     | 308 | CHL  | O2D-CGD | 3.57  | 1.41        | 1.33     |
| 24  | y     | 308 | CHL  | O2D-CGD | 3.57  | 1.41        | 1.33     |
| 25  | G     | 612 | CLA  | MG-NC   | -3.56 | 1.97        | 2.06     |
| 25  | G     | 604 | CLA  | MG-NA   | -3.56 | 1.97        | 2.06     |
| 25  | B     | 615 | CLA  | C1D-C2D | -3.56 | 1.38        | 1.45     |
| 25  | s     | 310 | CLA  | C1D-C2D | -3.55 | 1.38        | 1.45     |
| 25  | N     | 611 | CLA  | MG-NA   | -3.55 | 1.97        | 2.06     |
| 25  | n     | 611 | CLA  | MG-NA   | -3.55 | 1.97        | 2.06     |
| 25  | N     | 612 | CLA  | C1D-C2D | -3.55 | 1.38        | 1.45     |
| 25  | 2     | 605 | CLA  | MG-NC   | -3.55 | 1.97        | 2.06     |
| 25  | b     | 607 | CLA  | MG-NA   | -3.55 | 1.97        | 2.06     |
| 25  | B     | 612 | CLA  | MG-NC   | -3.55 | 1.97        | 2.06     |
| 25  | b     | 612 | CLA  | MG-NC   | -3.55 | 1.97        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | G     | 603 | CLA  | C1D-C2D | -3.55 | 1.38        | 1.45     |
| 25  | g     | 603 | CLA  | C1D-C2D | -3.55 | 1.38        | 1.45     |
| 25  | N     | 602 | CLA  | C1D-C2D | -3.55 | 1.38        | 1.45     |
| 40  | g     | 617 | NEX  | C14-C13 | 3.55  | 1.40        | 1.35     |
| 25  | B     | 606 | CLA  | MG-NC   | -3.55 | 1.97        | 2.06     |
| 25  | b     | 606 | CLA  | MG-NC   | -3.55 | 1.97        | 2.06     |
| 24  | N     | 601 | CHL  | C4B-NB  | 3.54  | 1.38        | 1.35     |
| 25  | B     | 611 | CLA  | MG-NA   | -3.54 | 1.97        | 2.06     |
| 25  | b     | 611 | CLA  | MG-NA   | -3.54 | 1.97        | 2.06     |
| 25  | B     | 613 | CLA  | C1D-C2D | -3.54 | 1.38        | 1.45     |
| 25  | b     | 613 | CLA  | C1D-C2D | -3.54 | 1.38        | 1.45     |
| 25  | C     | 508 | CLA  | MG-NC   | -3.54 | 1.97        | 2.06     |
| 25  | A     | 402 | CLA  | MG-NC   | -3.54 | 1.97        | 2.06     |
| 25  | a     | 403 | CLA  | MG-NC   | -3.54 | 1.97        | 2.06     |
| 25  | g     | 614 | CLA  | MG-NA   | -3.54 | 1.97        | 2.06     |
| 25  | y     | 304 | CLA  | C1D-C2D | -3.54 | 1.38        | 1.45     |
| 25  | G     | 614 | CLA  | MG-NA   | -3.54 | 1.97        | 2.06     |
| 24  | l     | 301 | CHL  | O2D-CGD | 3.53  | 1.41        | 1.33     |
| 24  | 5     | 301 | CHL  | O2D-CGD | 3.53  | 1.41        | 1.33     |
| 25  | D     | 403 | CLA  | C1B-NB  | 3.53  | 1.38        | 1.35     |
| 25  | G     | 602 | CLA  | C1D-C2D | -3.53 | 1.38        | 1.45     |
| 25  | g     | 602 | CLA  | C1D-C2D | -3.53 | 1.38        | 1.45     |
| 25  | g     | 612 | CLA  | MG-NC   | -3.53 | 1.97        | 2.06     |
| 24  | g     | 606 | CHL  | O2D-CGD | 3.53  | 1.41        | 1.33     |
| 28  | I     | 101 | BCR  | C30-C25 | -3.53 | 1.48        | 1.53     |
| 25  | S     | 311 | CLA  | MG-NC   | -3.53 | 1.97        | 2.06     |
| 25  | c     | 508 | CLA  | MG-NC   | -3.53 | 1.97        | 2.06     |
| 25  | b     | 616 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | B     | 616 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | n     | 602 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 24  | S     | 302 | CHL  | C4B-NB  | 3.52  | 1.38        | 1.35     |
| 24  | s     | 302 | CHL  | C4B-NB  | 3.52  | 1.38        | 1.35     |
| 25  | Y     | 315 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | y     | 315 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | s     | 311 | CLA  | MG-NC   | -3.52 | 1.97        | 2.06     |
| 24  | y     | 310 | CHL  | O2D-CGD | 3.52  | 1.41        | 1.33     |
| 25  | G     | 612 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | b     | 604 | CLA  | MG-NC   | -3.52 | 1.97        | 2.06     |
| 25  | Y     | 305 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | y     | 305 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 24  | N     | 601 | CHL  | O2D-CGD | 3.52  | 1.41        | 1.33     |
| 28  | k     | 101 | BCR  | C30-C25 | -3.52 | 1.48        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | B     | 607 | CLA  | MG-NA   | -3.52 | 1.97        | 2.06     |
| 25  | b     | 615 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | n     | 612 | CLA  | C1D-C2D | -3.52 | 1.38        | 1.45     |
| 25  | B     | 609 | CLA  | MG-NA   | -3.52 | 1.97        | 2.06     |
| 25  | C     | 509 | CLA  | MG-NC   | -3.51 | 1.97        | 2.06     |
| 24  | Y     | 310 | CHL  | O2D-CGD | 3.51  | 1.41        | 1.33     |
| 25  | c     | 510 | CLA  | MG-NC   | -3.51 | 1.97        | 2.06     |
| 24  | Y     | 309 | CHL  | O2D-CGD | 3.51  | 1.41        | 1.33     |
| 28  | B     | 619 | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 28  | b     | 619 | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 25  | C     | 504 | CLA  | C1B-NB  | 3.51  | 1.38        | 1.35     |
| 25  | c     | 504 | CLA  | C1B-NB  | 3.51  | 1.38        | 1.35     |
| 28  | i     | 101 | BCR  | C30-C25 | -3.51 | 1.48        | 1.53     |
| 25  | 6     | 605 | CLA  | MG-NC   | -3.51 | 1.97        | 2.06     |
| 24  | 6     | 601 | CHL  | O2D-CGD | 3.51  | 1.41        | 1.33     |
| 24  | n     | 601 | CHL  | C4B-NB  | 3.51  | 1.38        | 1.35     |
| 24  | G     | 606 | CHL  | O2D-CGD | 3.51  | 1.41        | 1.33     |
| 24  | y     | 309 | CHL  | O2D-CGD | 3.50  | 1.41        | 1.33     |
| 25  | Y     | 311 | CLA  | MG-NC   | -3.50 | 1.97        | 2.06     |
| 25  | C     | 505 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | c     | 505 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | C     | 502 | CLA  | MG-NA   | -3.50 | 1.98        | 2.06     |
| 25  | c     | 502 | CLA  | MG-NA   | -3.50 | 1.98        | 2.06     |
| 24  | R     | 613 | CHL  | O2D-CGD | 3.50  | 1.41        | 1.33     |
| 24  | G     | 608 | CHL  | O2D-CGD | 3.50  | 1.41        | 1.33     |
| 25  | s     | 314 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | B     | 604 | CLA  | MG-NC   | -3.50 | 1.98        | 2.06     |
| 25  | C     | 506 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | c     | 506 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | R     | 608 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | b     | 609 | CLA  | MG-NA   | -3.50 | 1.98        | 2.06     |
| 25  | B     | 608 | CLA  | C1D-C2D | -3.50 | 1.38        | 1.45     |
| 25  | A     | 405 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 25  | y     | 305 | CLA  | MG-NA   | -3.49 | 1.98        | 2.06     |
| 24  | Y     | 308 | CHL  | C4B-NB  | 3.49  | 1.38        | 1.35     |
| 24  | y     | 308 | CHL  | C4B-NB  | 3.49  | 1.38        | 1.35     |
| 24  | s     | 308 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 25  | c     | 509 | CLA  | MG-NC   | -3.49 | 1.98        | 2.06     |
| 25  | g     | 614 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 25  | S     | 314 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 25  | r     | 603 | CLA  | C1B-NB  | 3.49  | 1.38        | 1.35     |
| 24  | S     | 302 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | s     | 302 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 24  | R     | 606 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 24  | r     | 606 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 25  | G     | 614 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 25  | Y     | 305 | CLA  | MG-NA   | -3.49 | 1.98        | 2.06     |
| 25  | y     | 311 | CLA  | MG-NC   | -3.49 | 1.98        | 2.06     |
| 24  | g     | 601 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 25  | C     | 509 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 25  | c     | 509 | CLA  | C1D-C2D | -3.49 | 1.38        | 1.45     |
| 24  | l     | 302 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 24  | 5     | 302 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 24  | r     | 607 | CHL  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 25  | A     | 401 | CLA  | MG-NC   | -3.48 | 1.98        | 2.06     |
| 25  | a     | 402 | CLA  | MG-NC   | -3.48 | 1.98        | 2.06     |
| 24  | G     | 605 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 24  | g     | 605 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 24  | N     | 606 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 24  | n     | 601 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 25  | a     | 406 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 24  | y     | 307 | CHL  | MG-NA   | 3.48  | 2.14        | 2.06     |
| 25  | n     | 603 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 25  | b     | 608 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 25  | B     | 608 | CLA  | MG-NA   | -3.48 | 1.98        | 2.06     |
| 25  | C     | 510 | CLA  | MG-NC   | -3.48 | 1.98        | 2.06     |
| 28  | A     | 406 | BCR  | C30-C25 | -3.48 | 1.49        | 1.53     |
| 25  | G     | 604 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 25  | R     | 608 | CLA  | MG-NA   | -3.48 | 1.98        | 2.06     |
| 24  | Y     | 307 | CHL  | MG-NA   | 3.48  | 2.14        | 2.06     |
| 25  | S     | 309 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 25  | b     | 612 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 25  | s     | 309 | CLA  | C1D-C2D | -3.48 | 1.38        | 1.45     |
| 24  | 2     | 601 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 24  | r     | 613 | CHL  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 24  | R     | 605 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 24  | r     | 605 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 25  | Y     | 312 | CLA  | MG-NA   | -3.47 | 1.98        | 2.06     |
| 25  | y     | 312 | CLA  | MG-NA   | -3.47 | 1.98        | 2.06     |
| 24  | S     | 307 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 24  | s     | 307 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 24  | G     | 601 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 28  | H     | 101 | BCR  | C1-C6   | -3.47 | 1.49        | 1.53     |
| 28  | h     | 101 | BCR  | C1-C6   | -3.47 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | g     | 608 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 24  | Y     | 302 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 24  | y     | 302 | CHL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 25  | r     | 608 | CLA  | C1D-C2D | -3.47 | 1.38        | 1.45     |
| 25  | B     | 614 | CLA  | MG-NA   | -3.47 | 1.98        | 2.06     |
| 25  | b     | 614 | CLA  | MG-NA   | -3.47 | 1.98        | 2.06     |
| 25  | N     | 613 | CLA  | C1D-C2D | -3.46 | 1.38        | 1.45     |
| 28  | K     | 101 | BCR  | C1-C6   | -3.46 | 1.49        | 1.53     |
| 28  | k     | 101 | BCR  | C1-C6   | -3.46 | 1.49        | 1.53     |
| 24  | S     | 308 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 24  | 2     | 603 | CHL  | C3B-C2B | -3.46 | 1.35        | 1.40     |
| 24  | 6     | 603 | CHL  | C3B-C2B | -3.46 | 1.35        | 1.40     |
| 25  | C     | 513 | CLA  | C1D-C2D | -3.46 | 1.38        | 1.45     |
| 24  | Y     | 306 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 24  | y     | 306 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 24  | g     | 607 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 25  | N     | 610 | CLA  | MG-NC   | -3.46 | 1.98        | 2.06     |
| 25  | n     | 610 | CLA  | MG-NC   | -3.46 | 1.98        | 2.06     |
| 24  | Y     | 307 | CHL  | C4B-NB  | 3.46  | 1.38        | 1.35     |
| 24  | N     | 608 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 24  | n     | 608 | CHL  | O2D-CGD | 3.46  | 1.41        | 1.33     |
| 25  | n     | 613 | CLA  | C1D-C2D | -3.46 | 1.38        | 1.45     |
| 25  | C     | 511 | CLA  | C1D-C2D | -3.46 | 1.38        | 1.45     |
| 25  | c     | 511 | CLA  | C1D-C2D | -3.46 | 1.38        | 1.45     |
| 25  | B     | 609 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 28  | K     | 101 | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 28  | B     | 618 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 28  | b     | 618 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 25  | C     | 507 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | N     | 603 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 24  | R     | 607 | CHL  | O2D-CGD | 3.45  | 1.41        | 1.33     |
| 25  | D     | 402 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | d     | 402 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | g     | 604 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 24  | G     | 601 | CHL  | C4B-NB  | 3.45  | 1.38        | 1.35     |
| 25  | r     | 608 | CLA  | MG-NA   | -3.45 | 1.98        | 2.06     |
| 24  | N     | 605 | CHL  | O2D-CGD | 3.45  | 1.41        | 1.33     |
| 24  | n     | 605 | CHL  | O2D-CGD | 3.45  | 1.41        | 1.33     |
| 25  | R     | 602 | CLA  | MG-NC   | -3.45 | 1.98        | 2.06     |
| 25  | B     | 614 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | S     | 312 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | b     | 614 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | s     | 312 | CLA  | C1D-C2D | -3.45 | 1.38        | 1.45     |
| 25  | C     | 506 | CLA  | MG-NC   | -3.44 | 1.98        | 2.06     |
| 25  | c     | 506 | CLA  | MG-NC   | -3.44 | 1.98        | 2.06     |
| 28  | a     | 407 | BCR  | C30-C25 | -3.44 | 1.49        | 1.53     |
| 25  | B     | 613 | CLA  | MG-NA   | -3.44 | 1.98        | 2.06     |
| 25  | b     | 613 | CLA  | MG-NA   | -3.44 | 1.98        | 2.06     |
| 40  | s     | 317 | NEX  | C14-C13 | 3.44  | 1.40        | 1.35     |
| 24  | S     | 306 | CHL  | O2D-CGD | 3.44  | 1.41        | 1.33     |
| 25  | b     | 604 | CLA  | C1D-C2D | -3.44 | 1.38        | 1.45     |
| 25  | c     | 513 | CLA  | C1D-C2D | -3.44 | 1.38        | 1.45     |
| 25  | B     | 607 | CLA  | C1D-C2D | -3.44 | 1.38        | 1.45     |
| 25  | b     | 607 | CLA  | C1D-C2D | -3.44 | 1.38        | 1.45     |
| 24  | Y     | 307 | CHL  | O2D-CGD | 3.44  | 1.41        | 1.33     |
| 24  | n     | 606 | CHL  | O2D-CGD | 3.44  | 1.41        | 1.33     |
| 24  | y     | 307 | CHL  | O2D-CGD | 3.44  | 1.41        | 1.33     |
| 24  | n     | 609 | CHL  | O2D-CGD | 3.43  | 1.41        | 1.33     |
| 28  | A     | 406 | BCR  | C1-C6   | -3.43 | 1.49        | 1.53     |
| 28  | a     | 407 | BCR  | C1-C6   | -3.43 | 1.49        | 1.53     |
| 25  | b     | 608 | CLA  | MG-NA   | -3.43 | 1.98        | 2.06     |
| 24  | G     | 607 | CHL  | O2D-CGD | 3.43  | 1.41        | 1.33     |
| 24  | N     | 609 | CHL  | O2D-CGD | 3.43  | 1.41        | 1.33     |
| 25  | S     | 304 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | s     | 304 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | b     | 609 | CLA  | C1D-C2D | -3.43 | 1.38        | 1.45     |
| 25  | b     | 611 | CLA  | C1D-C2D | -3.43 | 1.38        | 1.45     |
| 25  | c     | 507 | CLA  | C1D-C2D | -3.43 | 1.38        | 1.45     |
| 25  | B     | 605 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | b     | 605 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | r     | 602 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | r     | 608 | CLA  | MG-NC   | -3.43 | 1.98        | 2.06     |
| 25  | B     | 612 | CLA  | C1D-C2D | -3.43 | 1.38        | 1.45     |
| 24  | s     | 306 | CHL  | O2D-CGD | 3.42  | 1.41        | 1.33     |
| 40  | R     | 617 | NEX  | C34-C33 | 3.42  | 1.40        | 1.35     |
| 24  | y     | 307 | CHL  | C4B-NB  | 3.42  | 1.38        | 1.35     |
| 25  | s     | 314 | CLA  | MG-NC   | -3.42 | 1.98        | 2.06     |
| 25  | D     | 401 | CLA  | MG-NC   | -3.42 | 1.98        | 2.06     |
| 25  | d     | 401 | CLA  | MG-NC   | -3.42 | 1.98        | 2.06     |
| 24  | G     | 609 | CHL  | O2D-CGD | 3.42  | 1.41        | 1.33     |
| 25  | 2     | 605 | CLA  | C1D-C2D | -3.42 | 1.38        | 1.45     |
| 25  | G     | 610 | CLA  | C1D-C2D | -3.42 | 1.38        | 1.45     |
| 25  | 6     | 605 | CLA  | C1D-C2D | -3.42 | 1.38        | 1.45     |
| 24  | 2     | 603 | CHL  | O2D-CGD | 3.42  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 6     | 603 | CHL  | O2D-CGD | 3.42  | 1.41        | 1.33     |
| 24  | g     | 609 | CHL  | O2D-CGD | 3.42  | 1.41        | 1.33     |
| 25  | S     | 303 | CLA  | C1D-C2D | -3.41 | 1.38        | 1.45     |
| 24  | R     | 613 | CHL  | C3B-C2B | -3.41 | 1.35        | 1.40     |
| 24  | Y     | 306 | CHL  | C3B-C2B | -3.41 | 1.35        | 1.40     |
| 25  | C     | 505 | CLA  | MG-NA   | -3.41 | 1.98        | 2.06     |
| 25  | c     | 505 | CLA  | MG-NA   | -3.41 | 1.98        | 2.06     |
| 24  | S     | 306 | CHL  | C3B-C2B | -3.41 | 1.35        | 1.40     |
| 24  | s     | 306 | CHL  | C3B-C2B | -3.41 | 1.35        | 1.40     |
| 25  | g     | 610 | CLA  | C1D-C2D | -3.41 | 1.38        | 1.45     |
| 24  | S     | 308 | CHL  | C3B-C2B | -3.41 | 1.35        | 1.40     |
| 25  | S     | 311 | CLA  | C1D-C2D | -3.40 | 1.38        | 1.45     |
| 25  | R     | 614 | CLA  | C1D-C2D | -3.40 | 1.38        | 1.45     |
| 25  | r     | 614 | CLA  | C1D-C2D | -3.40 | 1.38        | 1.45     |
| 25  | B     | 611 | CLA  | C1D-C2D | -3.40 | 1.38        | 1.45     |
| 25  | R     | 608 | CLA  | MG-NC   | -3.40 | 1.98        | 2.06     |
| 25  | b     | 603 | CLA  | C1D-C2D | -3.40 | 1.38        | 1.45     |
| 25  | Y     | 314 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 25  | y     | 314 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 25  | B     | 604 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 25  | S     | 314 | CLA  | MG-NC   | -3.39 | 1.98        | 2.06     |
| 25  | C     | 513 | CLA  | MG-NC   | -3.39 | 1.98        | 2.06     |
| 25  | c     | 513 | CLA  | MG-NC   | -3.39 | 1.98        | 2.06     |
| 25  | B     | 603 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 25  | c     | 503 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 24  | r     | 606 | CHL  | O2A-CGA | 3.39  | 1.42        | 1.30     |
| 40  | s     | 317 | NEX  | C12-C13 | -3.39 | 1.38        | 1.45     |
| 25  | g     | 613 | CLA  | C1D-C2D | -3.39 | 1.38        | 1.45     |
| 40  | S     | 317 | NEX  | C14-C13 | 3.39  | 1.40        | 1.35     |
| 24  | s     | 308 | CHL  | C3B-C2B | -3.39 | 1.35        | 1.40     |
| 25  | b     | 616 | CLA  | MG-NA   | -3.38 | 1.98        | 2.06     |
| 24  | R     | 605 | CHL  | O2A-CGA | 3.38  | 1.42        | 1.30     |
| 24  | r     | 605 | CHL  | O2A-CGA | 3.38  | 1.42        | 1.30     |
| 25  | n     | 604 | CLA  | C1D-C2D | -3.38 | 1.38        | 1.45     |
| 25  | d     | 401 | CLA  | C1D-C2D | -3.38 | 1.38        | 1.45     |
| 25  | r     | 609 | CLA  | C1D-C2D | -3.38 | 1.38        | 1.45     |
| 25  | G     | 613 | CLA  | C1D-C2D | -3.38 | 1.38        | 1.45     |
| 25  | C     | 512 | CLA  | C1D-C2D | -3.37 | 1.38        | 1.45     |
| 25  | c     | 512 | CLA  | C1D-C2D | -3.37 | 1.38        | 1.45     |
| 25  | s     | 303 | CLA  | C1D-C2D | -3.37 | 1.38        | 1.45     |
| 24  | 5     | 301 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 24  | r     | 605 | CHL  | C3B-C2B | -3.37 | 1.35        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | Z     | 101 | BCR  | C1-C6   | -3.37 | 1.49        | 1.53     |
| 25  | D     | 401 | CLA  | C1D-C2D | -3.37 | 1.38        | 1.45     |
| 24  | l     | 301 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 24  | G     | 605 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 24  | g     | 605 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 40  | r     | 617 | NEX  | C34-C33 | 3.37  | 1.40        | 1.35     |
| 24  | S     | 307 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 24  | Y     | 310 | CHL  | C3B-C2B | -3.37 | 1.35        | 1.40     |
| 24  | y     | 310 | CHL  | C3B-C2B | -3.37 | 1.35        | 1.40     |
| 25  | R     | 610 | CLA  | C1B-NB  | 3.37  | 1.38        | 1.35     |
| 25  | r     | 610 | CLA  | C1B-NB  | 3.37  | 1.38        | 1.35     |
| 24  | S     | 302 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 24  | s     | 302 | CHL  | O2A-CGA | 3.37  | 1.42        | 1.30     |
| 40  | S     | 317 | NEX  | C12-C13 | -3.37 | 1.38        | 1.45     |
| 24  | 2     | 603 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | 6     | 603 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | 1     | 302 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | 5     | 302 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | Y     | 308 | CHL  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 24  | s     | 307 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | y     | 302 | CHL  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 25  | s     | 311 | CLA  | C1D-C2D | -3.36 | 1.38        | 1.45     |
| 25  | N     | 604 | CLA  | MG-NC   | -3.36 | 1.98        | 2.06     |
| 25  | A     | 402 | CLA  | C1D-C2D | -3.36 | 1.38        | 1.45     |
| 25  | a     | 403 | CLA  | C1D-C2D | -3.36 | 1.38        | 1.45     |
| 24  | S     | 308 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | s     | 308 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 24  | N     | 605 | CHL  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 24  | n     | 605 | CHL  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 24  | R     | 606 | CHL  | O2A-CGA | 3.36  | 1.42        | 1.30     |
| 25  | R     | 609 | CLA  | C1D-C2D | -3.36 | 1.38        | 1.45     |
| 24  | N     | 606 | CHL  | O2A-CGA | 3.35  | 1.42        | 1.30     |
| 24  | S     | 306 | CHL  | O2A-CGA | 3.35  | 1.42        | 1.30     |
| 24  | s     | 306 | CHL  | O2A-CGA | 3.35  | 1.42        | 1.30     |
| 25  | r     | 602 | CLA  | C1D-C2D | -3.35 | 1.38        | 1.45     |
| 25  | B     | 616 | CLA  | MG-NA   | -3.35 | 1.98        | 2.06     |
| 25  | B     | 607 | CLA  | MG-NC   | -3.35 | 1.98        | 2.06     |
| 25  | C     | 503 | CLA  | C1D-C2D | -3.35 | 1.38        | 1.45     |
| 25  | A     | 401 | CLA  | C1D-C2D | -3.35 | 1.38        | 1.45     |
| 25  | a     | 402 | CLA  | C1D-C2D | -3.35 | 1.38        | 1.45     |
| 25  | S     | 303 | CLA  | MG-NC   | -3.34 | 1.98        | 2.06     |
| 25  | s     | 303 | CLA  | MG-NC   | -3.34 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | y     | 306 | CHL  | C3B-C2B | -3.34 | 1.35        | 1.40     |
| 25  | N     | 604 | CLA  | C1D-C2D | -3.34 | 1.38        | 1.45     |
| 24  | n     | 606 | CHL  | O2A-CGA | 3.34  | 1.42        | 1.30     |
| 25  | R     | 602 | CLA  | C1D-C2D | -3.34 | 1.38        | 1.45     |
| 25  | B     | 605 | CLA  | C1D-C2D | -3.34 | 1.38        | 1.45     |
| 25  | b     | 605 | CLA  | C1D-C2D | -3.34 | 1.38        | 1.45     |
| 25  | C     | 512 | CLA  | MG-NC   | -3.34 | 1.98        | 2.06     |
| 25  | c     | 512 | CLA  | MG-NC   | -3.34 | 1.98        | 2.06     |
| 25  | a     | 406 | CLA  | MG-NC   | -3.33 | 1.98        | 2.06     |
| 28  | z     | 101 | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 25  | n     | 604 | CLA  | MG-NC   | -3.33 | 1.98        | 2.06     |
| 25  | B     | 616 | CLA  | MG-NC   | -3.33 | 1.98        | 2.06     |
| 24  | R     | 605 | CHL  | C3B-C2B | -3.33 | 1.35        | 1.40     |
| 25  | R     | 610 | CLA  | C1D-C2D | -3.33 | 1.38        | 1.45     |
| 25  | r     | 610 | CLA  | C1D-C2D | -3.33 | 1.38        | 1.45     |
| 25  | C     | 501 | CLA  | C1D-C2D | -3.32 | 1.38        | 1.45     |
| 25  | c     | 501 | CLA  | C1D-C2D | -3.32 | 1.38        | 1.45     |
| 25  | N     | 611 | CLA  | MG-NC   | -3.32 | 1.98        | 2.06     |
| 24  | y     | 308 | CHL  | C3B-C2B | -3.32 | 1.35        | 1.40     |
| 25  | c     | 508 | CLA  | C1D-C2D | -3.32 | 1.38        | 1.45     |
| 25  | C     | 503 | CLA  | MG-NC   | -3.32 | 1.98        | 2.06     |
| 25  | c     | 503 | CLA  | MG-NC   | -3.32 | 1.98        | 2.06     |
| 40  | g     | 617 | NEX  | C12-C13 | -3.32 | 1.38        | 1.45     |
| 25  | B     | 611 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 24  | g     | 609 | CHL  | C3B-C2B | -3.31 | 1.35        | 1.40     |
| 24  | r     | 613 | CHL  | C3B-C2B | -3.31 | 1.35        | 1.40     |
| 25  | B     | 602 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 25  | b     | 602 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 25  | b     | 611 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 24  | N     | 607 | CHL  | C3B-C2B | -3.31 | 1.35        | 1.40     |
| 25  | b     | 607 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 25  | b     | 616 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 24  | G     | 609 | CHL  | C3B-C2B | -3.31 | 1.35        | 1.40     |
| 25  | n     | 611 | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 25  | c     | 510 | CLA  | C1D-C2D | -3.31 | 1.38        | 1.45     |
| 25  | B     | 606 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 25  | b     | 606 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 25  | A     | 405 | CLA  | MG-NC   | -3.30 | 1.98        | 2.06     |
| 25  | C     | 510 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 24  | G     | 607 | CHL  | O2A-CGA | 3.30  | 1.41        | 1.30     |
| 25  | B     | 603 | CLA  | MG-NC   | -3.30 | 1.98        | 2.06     |
| 25  | b     | 603 | CLA  | MG-NC   | -3.30 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | S     | 304 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 25  | s     | 304 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 25  | C     | 508 | CLA  | C1D-C2D | -3.30 | 1.38        | 1.45     |
| 40  | G     | 617 | NEX  | C14-C13 | 3.30  | 1.40        | 1.35     |
| 24  | g     | 607 | CHL  | O2A-CGA | 3.29  | 1.41        | 1.30     |
| 24  | y     | 309 | CHL  | C3B-C2B | -3.29 | 1.35        | 1.40     |
| 28  | C     | 514 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 28  | c     | 514 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 24  | R     | 607 | CHL  | C3B-C2B | -3.29 | 1.35        | 1.40     |
| 24  | r     | 607 | CHL  | C3B-C2B | -3.29 | 1.35        | 1.40     |
| 24  | n     | 607 | CHL  | C3B-C2B | -3.29 | 1.35        | 1.40     |
| 24  | g     | 601 | CHL  | C3B-C2B | -3.29 | 1.35        | 1.40     |
| 25  | G     | 604 | CLA  | MG-NC   | -3.29 | 1.98        | 2.06     |
| 25  | Y     | 305 | CLA  | MG-NC   | -3.28 | 1.98        | 2.06     |
| 25  | B     | 602 | CLA  | C1D-C2D | -3.28 | 1.38        | 1.45     |
| 25  | b     | 602 | CLA  | C1D-C2D | -3.28 | 1.38        | 1.45     |
| 24  | N     | 609 | CHL  | C3B-C2B | -3.28 | 1.35        | 1.40     |
| 24  | Y     | 302 | CHL  | C3B-C2B | -3.28 | 1.35        | 1.40     |
| 24  | n     | 609 | CHL  | C3B-C2B | -3.28 | 1.35        | 1.40     |
| 25  | B     | 601 | CLA  | C1D-C2D | -3.28 | 1.38        | 1.45     |
| 25  | b     | 601 | CLA  | C1D-C2D | -3.28 | 1.38        | 1.45     |
| 25  | S     | 310 | CLA  | MG-NC   | -3.28 | 1.98        | 2.06     |
| 25  | Y     | 314 | CLA  | MG-NC   | -3.28 | 1.98        | 2.06     |
| 25  | Y     | 315 | CLA  | MG-NA   | -3.27 | 1.98        | 2.06     |
| 25  | B     | 613 | CLA  | MG-NC   | -3.27 | 1.98        | 2.06     |
| 24  | S     | 302 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 24  | l     | 301 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 24  | 5     | 301 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 25  | c     | 505 | CLA  | MG-NC   | -3.27 | 1.98        | 2.06     |
| 25  | b     | 613 | CLA  | MG-NC   | -3.27 | 1.98        | 2.06     |
| 24  | G     | 601 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 24  | S     | 307 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 24  | s     | 307 | CHL  | C3B-C2B | -3.27 | 1.35        | 1.40     |
| 25  | y     | 305 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 25  | g     | 604 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 25  | Y     | 303 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 25  | y     | 303 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 25  | C     | 504 | CLA  | C1D-C2D | -3.26 | 1.38        | 1.45     |
| 25  | s     | 310 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 24  | g     | 608 | CHL  | C3B-C2B | -3.26 | 1.35        | 1.40     |
| 25  | B     | 614 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 25  | b     | 614 | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | G     | 605 | CHL  | C3B-C2B | -3.26 | 1.35        | 1.40     |
| 24  | Y     | 309 | CHL  | C3B-C2B | -3.25 | 1.35        | 1.40     |
| 25  | Y     | 313 | CLA  | MG-NC   | -3.25 | 1.98        | 2.06     |
| 25  | N     | 602 | CLA  | MG-NC   | -3.25 | 1.98        | 2.06     |
| 25  | C     | 505 | CLA  | MG-NC   | -3.25 | 1.98        | 2.06     |
| 25  | y     | 314 | CLA  | MG-NC   | -3.25 | 1.98        | 2.06     |
| 28  | B     | 618 | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 28  | b     | 618 | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 24  | G     | 606 | CHL  | C3B-C2B | -3.25 | 1.35        | 1.40     |
| 24  | g     | 606 | CHL  | C3B-C2B | -3.25 | 1.35        | 1.40     |
| 24  | R     | 606 | CHL  | C3B-C2B | -3.25 | 1.35        | 1.40     |
| 25  | D     | 403 | CLA  | C1D-C2D | -3.25 | 1.38        | 1.45     |
| 25  | d     | 403 | CLA  | C1D-C2D | -3.25 | 1.38        | 1.45     |
| 25  | n     | 602 | CLA  | MG-NC   | -3.24 | 1.98        | 2.06     |
| 25  | y     | 315 | CLA  | MG-NA   | -3.24 | 1.98        | 2.06     |
| 25  | R     | 603 | CLA  | C1D-C2D | -3.24 | 1.38        | 1.45     |
| 25  | b     | 608 | CLA  | MG-NC   | -3.24 | 1.98        | 2.06     |
| 25  | b     | 609 | CLA  | MG-NC   | -3.24 | 1.98        | 2.06     |
| 25  | y     | 313 | CLA  | MG-NC   | -3.23 | 1.98        | 2.06     |
| 25  | C     | 502 | CLA  | MG-NC   | -3.23 | 1.98        | 2.06     |
| 25  | c     | 502 | CLA  | MG-NC   | -3.23 | 1.98        | 2.06     |
| 24  | G     | 608 | CHL  | C3B-C2B | -3.23 | 1.35        | 1.40     |
| 24  | g     | 605 | CHL  | C3B-C2B | -3.23 | 1.35        | 1.40     |
| 25  | S     | 313 | CLA  | C1D-C2D | -3.22 | 1.39        | 1.45     |
| 25  | R     | 604 | CLA  | C1D-C2D | -3.22 | 1.39        | 1.45     |
| 25  | r     | 604 | CLA  | C1D-C2D | -3.22 | 1.39        | 1.45     |
| 25  | c     | 504 | CLA  | C1D-C2D | -3.22 | 1.39        | 1.45     |
| 28  | B     | 619 | BCR  | C30-C25 | -3.22 | 1.49        | 1.53     |
| 28  | b     | 619 | BCR  | C30-C25 | -3.22 | 1.49        | 1.53     |
| 25  | s     | 313 | CLA  | C1D-C2D | -3.21 | 1.39        | 1.45     |
| 24  | N     | 606 | CHL  | C3B-C2B | -3.21 | 1.35        | 1.40     |
| 24  | n     | 606 | CHL  | C3B-C2B | -3.21 | 1.35        | 1.40     |
| 25  | B     | 609 | CLA  | MG-NC   | -3.21 | 1.98        | 2.06     |
| 25  | Y     | 304 | CLA  | MG-NC   | -3.20 | 1.98        | 2.06     |
| 25  | y     | 304 | CLA  | MG-NC   | -3.20 | 1.98        | 2.06     |
| 24  | N     | 601 | CHL  | C3B-C2B | -3.20 | 1.35        | 1.40     |
| 24  | r     | 606 | CHL  | C3B-C2B | -3.20 | 1.35        | 1.40     |
| 25  | B     | 608 | CLA  | MG-NC   | -3.20 | 1.98        | 2.06     |
| 25  | G     | 603 | CLA  | MG-NC   | -3.20 | 1.98        | 2.06     |
| 25  | g     | 603 | CLA  | MG-NC   | -3.20 | 1.98        | 2.06     |
| 25  | r     | 603 | CLA  | C1D-C2D | -3.20 | 1.39        | 1.45     |
| 25  | G     | 611 | CLA  | MG-NC   | -3.19 | 1.98        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | g     | 611 | CLA  | MG-NC   | -3.19 | 1.98        | 2.06     |
| 25  | N     | 603 | CLA  | MG-NC   | -3.18 | 1.98        | 2.06     |
| 25  | n     | 603 | CLA  | MG-NC   | -3.18 | 1.98        | 2.06     |
| 24  | s     | 302 | CHL  | C3B-C2B | -3.18 | 1.36        | 1.40     |
| 25  | R     | 612 | CLA  | C1D-C2D | -3.17 | 1.39        | 1.45     |
| 25  | r     | 612 | CLA  | C1D-C2D | -3.17 | 1.39        | 1.45     |
| 24  | R     | 613 | CHL  | MG-NA   | 3.17  | 2.13        | 2.06     |
| 24  | N     | 608 | CHL  | C3B-C2B | -3.16 | 1.36        | 1.40     |
| 24  | n     | 601 | CHL  | C3B-C2B | -3.16 | 1.36        | 1.40     |
| 25  | G     | 614 | CLA  | MG-NC   | -3.16 | 1.98        | 2.06     |
| 25  | g     | 614 | CLA  | MG-NC   | -3.16 | 1.98        | 2.06     |
| 25  | r     | 601 | CLA  | C1D-C2D | -3.16 | 1.39        | 1.45     |
| 25  | G     | 602 | CLA  | MG-NC   | -3.15 | 1.98        | 2.06     |
| 24  | 2     | 601 | CHL  | C3B-C2B | -3.15 | 1.36        | 1.40     |
| 24  | 6     | 601 | CHL  | C3B-C2B | -3.15 | 1.36        | 1.40     |
| 24  | r     | 613 | CHL  | MG-NA   | 3.15  | 2.13        | 2.06     |
| 25  | S     | 305 | CLA  | C1D-C2D | -3.14 | 1.39        | 1.45     |
| 25  | s     | 305 | CLA  | C1D-C2D | -3.14 | 1.39        | 1.45     |
| 25  | y     | 315 | CLA  | MG-NC   | -3.14 | 1.98        | 2.06     |
| 25  | g     | 602 | CLA  | MG-NC   | -3.14 | 1.98        | 2.06     |
| 24  | n     | 608 | CHL  | C3B-C2B | -3.13 | 1.36        | 1.40     |
| 25  | Y     | 312 | CLA  | MG-NC   | -3.12 | 1.98        | 2.06     |
| 25  | y     | 312 | CLA  | MG-NC   | -3.12 | 1.98        | 2.06     |
| 40  | G     | 617 | NEX  | C10-C9  | 3.11  | 1.39        | 1.35     |
| 24  | Y     | 310 | CHL  | MG-NA   | 3.11  | 2.13        | 2.06     |
| 24  | y     | 310 | CHL  | MG-NA   | 3.11  | 2.13        | 2.06     |
| 25  | R     | 601 | CLA  | C1D-C2D | -3.11 | 1.39        | 1.45     |
| 40  | N     | 617 | NEX  | C34-C33 | 3.11  | 1.39        | 1.35     |
| 40  | G     | 617 | NEX  | C11-C12 | 3.10  | 1.42        | 1.34     |
| 40  | n     | 617 | NEX  | C34-C33 | 3.10  | 1.39        | 1.35     |
| 24  | 1     | 302 | CHL  | C3B-C2B | -3.10 | 1.36        | 1.40     |
| 24  | 5     | 302 | CHL  | C3B-C2B | -3.10 | 1.36        | 1.40     |
| 25  | 6     | 604 | CLA  | C1D-C2D | -3.10 | 1.39        | 1.45     |
| 25  | Y     | 315 | CLA  | MG-NC   | -3.09 | 1.98        | 2.06     |
| 24  | g     | 609 | CHL  | MG-NA   | 3.09  | 2.13        | 2.06     |
| 24  | R     | 606 | CHL  | MG-NA   | 3.08  | 2.13        | 2.06     |
| 24  | r     | 606 | CHL  | MG-NA   | 3.08  | 2.13        | 2.06     |
| 40  | G     | 617 | NEX  | C12-C13 | -3.08 | 1.39        | 1.45     |
| 28  | T     | 101 | BCR  | C30-C25 | -3.08 | 1.49        | 1.53     |
| 28  | t     | 101 | BCR  | C30-C25 | -3.07 | 1.49        | 1.53     |
| 24  | r     | 605 | CHL  | MG-NA   | 3.06  | 2.13        | 2.06     |
| 24  | S     | 306 | CHL  | MG-NA   | 3.06  | 2.13        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | s     | 306 | CHL  | MG-NA   | 3.06  | 2.13        | 2.06     |
| 25  | 2     | 604 | CLA  | C1D-C2D | -3.05 | 1.39        | 1.45     |
| 24  | S     | 307 | CHL  | MG-NA   | 3.05  | 2.13        | 2.06     |
| 24  | s     | 307 | CHL  | MG-NA   | 3.05  | 2.13        | 2.06     |
| 24  | R     | 605 | CHL  | MG-NA   | 3.05  | 2.13        | 2.06     |
| 24  | G     | 609 | CHL  | MG-NA   | 3.04  | 2.13        | 2.06     |
| 24  | N     | 609 | CHL  | MG-NA   | 3.04  | 2.13        | 2.06     |
| 28  | B     | 617 | BCR  | C30-C25 | -3.04 | 1.49        | 1.53     |
| 28  | b     | 617 | BCR  | C30-C25 | -3.04 | 1.49        | 1.53     |
| 24  | s     | 308 | CHL  | MG-NA   | 3.04  | 2.13        | 2.06     |
| 24  | n     | 609 | CHL  | MG-NA   | 3.03  | 2.13        | 2.06     |
| 24  | S     | 308 | CHL  | MG-NA   | 3.03  | 2.13        | 2.06     |
| 24  | Y     | 307 | CHL  | O2A-CGA | 3.02  | 1.42        | 1.33     |
| 25  | n     | 613 | CLA  | MG-NC   | -3.00 | 1.99        | 2.06     |
| 40  | r     | 617 | NEX  | C12-C13 | -3.00 | 1.39        | 1.45     |
| 24  | Y     | 306 | CHL  | MG-NA   | 3.00  | 2.13        | 2.06     |
| 24  | y     | 306 | CHL  | MG-NA   | 3.00  | 2.13        | 2.06     |
| 40  | R     | 617 | NEX  | C12-C13 | -2.99 | 1.39        | 1.45     |
| 28  | z     | 101 | BCR  | C30-C25 | -2.99 | 1.49        | 1.53     |
| 24  | N     | 605 | CHL  | MG-NA   | 2.99  | 2.13        | 2.06     |
| 24  | n     | 605 | CHL  | MG-NA   | 2.99  | 2.13        | 2.06     |
| 24  | y     | 307 | CHL  | O2A-CGA | 2.99  | 1.42        | 1.33     |
| 24  | N     | 605 | CHL  | O2A-CGA | 2.98  | 1.42        | 1.33     |
| 25  | 2     | 602 | CLA  | C1D-C2D | -2.98 | 1.39        | 1.45     |
| 25  | 6     | 602 | CLA  | C1D-C2D | -2.98 | 1.39        | 1.45     |
| 24  | R     | 607 | CHL  | MG-NA   | 2.98  | 2.13        | 2.06     |
| 24  | r     | 607 | CHL  | MG-NA   | 2.98  | 2.13        | 2.06     |
| 24  | G     | 608 | CHL  | O2A-CGA | 2.98  | 1.42        | 1.33     |
| 24  | Y     | 308 | CHL  | O2A-CGA | 2.98  | 1.42        | 1.33     |
| 24  | g     | 608 | CHL  | O2A-CGA | 2.98  | 1.42        | 1.33     |
| 25  | N     | 613 | CLA  | MG-NC   | -2.97 | 1.99        | 2.06     |
| 24  | y     | 308 | CHL  | O2A-CGA | 2.97  | 1.42        | 1.33     |
| 24  | n     | 605 | CHL  | O2A-CGA | 2.97  | 1.42        | 1.33     |
| 24  | r     | 607 | CHL  | O2A-CGA | 2.97  | 1.42        | 1.33     |
| 24  | 2     | 601 | CHL  | O2A-CGA | 2.97  | 1.42        | 1.33     |
| 24  | 6     | 601 | CHL  | O2A-CGA | 2.97  | 1.42        | 1.33     |
| 25  | g     | 613 | CLA  | MG-NC   | -2.96 | 1.99        | 2.06     |
| 24  | Y     | 306 | CHL  | O2A-CGA | 2.96  | 1.42        | 1.33     |
| 24  | Y     | 310 | CHL  | O2A-CGA | 2.96  | 1.42        | 1.33     |
| 24  | y     | 310 | CHL  | O2A-CGA | 2.96  | 1.42        | 1.33     |
| 24  | G     | 606 | CHL  | O2A-CGA | 2.96  | 1.42        | 1.33     |
| 24  | g     | 606 | CHL  | O2A-CGA | 2.96  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | G     | 605 | CHL  | MG-NA   | 2.95  | 2.13        | 2.06     |
| 24  | g     | 605 | CHL  | MG-NA   | 2.95  | 2.13        | 2.06     |
| 28  | Z     | 101 | BCR  | C30-C25 | -2.95 | 1.49        | 1.53     |
| 24  | N     | 601 | CHL  | O2A-CGA | 2.95  | 1.42        | 1.33     |
| 24  | y     | 306 | CHL  | O2A-CGA | 2.95  | 1.42        | 1.33     |
| 24  | 5     | 301 | CHL  | MG-NA   | 2.95  | 2.13        | 2.06     |
| 24  | N     | 608 | CHL  | O2A-CGA | 2.95  | 1.41        | 1.33     |
| 24  | Y     | 309 | CHL  | O2A-CGA | 2.95  | 1.41        | 1.33     |
| 24  | y     | 309 | CHL  | O2A-CGA | 2.95  | 1.41        | 1.33     |
| 24  | n     | 608 | CHL  | O2A-CGA | 2.95  | 1.41        | 1.33     |
| 24  | R     | 607 | CHL  | O2A-CGA | 2.94  | 1.41        | 1.33     |
| 24  | G     | 609 | CHL  | O2A-CGA | 2.94  | 1.41        | 1.33     |
| 24  | g     | 609 | CHL  | O2A-CGA | 2.94  | 1.41        | 1.33     |
| 25  | G     | 613 | CLA  | MG-NC   | -2.93 | 1.99        | 2.06     |
| 24  | n     | 601 | CHL  | O2A-CGA | 2.93  | 1.41        | 1.33     |
| 24  | G     | 607 | CHL  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 24  | Y     | 308 | CHL  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 24  | y     | 308 | CHL  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 24  | G     | 608 | CHL  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 24  | n     | 609 | CHL  | O2A-CGA | 2.93  | 1.41        | 1.33     |
| 24  | g     | 607 | CHL  | MG-NA   | 2.92  | 2.13        | 2.06     |
| 24  | N     | 609 | CHL  | O2A-CGA | 2.92  | 1.41        | 1.33     |
| 40  | Y     | 318 | NEX  | C11-C12 | 2.92  | 1.42        | 1.34     |
| 24  | g     | 608 | CHL  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 40  | y     | 318 | NEX  | C11-C12 | 2.91  | 1.42        | 1.34     |
| 24  | N     | 607 | CHL  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 24  | g     | 606 | CHL  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 40  | N     | 617 | NEX  | C11-C12 | 2.91  | 1.42        | 1.34     |
| 24  | l     | 301 | CHL  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 24  | n     | 607 | CHL  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 24  | Y     | 302 | CHL  | O2A-CGA | 2.91  | 1.41        | 1.33     |
| 24  | y     | 302 | CHL  | O2A-CGA | 2.91  | 1.41        | 1.33     |
| 28  | D     | 404 | BCR  | C30-C25 | -2.90 | 1.49        | 1.53     |
| 28  | d     | 404 | BCR  | C30-C25 | -2.90 | 1.49        | 1.53     |
| 24  | n     | 606 | CHL  | MG-NA   | 2.89  | 2.13        | 2.06     |
| 24  | g     | 601 | CHL  | O2A-CGA | 2.89  | 1.41        | 1.33     |
| 40  | n     | 617 | NEX  | C11-C12 | 2.89  | 1.42        | 1.34     |
| 24  | G     | 606 | CHL  | MG-NA   | 2.89  | 2.13        | 2.06     |
| 24  | n     | 608 | CHL  | MG-NA   | 2.88  | 2.13        | 2.06     |
| 24  | G     | 601 | CHL  | O2A-CGA | 2.88  | 1.41        | 1.33     |
| 24  | N     | 608 | CHL  | MG-NA   | 2.87  | 2.13        | 2.06     |
| 24  | Y     | 309 | CHL  | MG-NA   | 2.87  | 2.13        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | Y     | 313 | CLA  | C4B-CHC | -2.87 | 1.33        | 1.41     |
| 24  | 6     | 601 | CHL  | MG-NA   | 2.87  | 2.13        | 2.06     |
| 28  | H     | 101 | BCR  | C30-C25 | -2.86 | 1.49        | 1.53     |
| 28  | h     | 101 | BCR  | C30-C25 | -2.86 | 1.49        | 1.53     |
| 24  | N     | 606 | CHL  | MG-NA   | 2.86  | 2.13        | 2.06     |
| 24  | n     | 607 | CHL  | O2A-CGA | 2.86  | 1.41        | 1.33     |
| 24  | 5     | 302 | CHL  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 24  | 2     | 601 | CHL  | MG-NA   | 2.85  | 2.13        | 2.06     |
| 24  | N     | 607 | CHL  | O2A-CGA | 2.85  | 1.41        | 1.33     |
| 24  | y     | 309 | CHL  | MG-NA   | 2.84  | 2.13        | 2.06     |
| 24  | s     | 302 | CHL  | MG-NA   | 2.83  | 2.13        | 2.06     |
| 25  | y     | 313 | CLA  | C4B-CHC | -2.83 | 1.33        | 1.41     |
| 24  | l     | 302 | CHL  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 40  | g     | 617 | NEX  | C34-C33 | 2.82  | 1.39        | 1.35     |
| 24  | y     | 302 | CHL  | MG-NA   | 2.82  | 2.13        | 2.06     |
| 24  | S     | 302 | CHL  | MG-NA   | 2.81  | 2.12        | 2.06     |
| 40  | G     | 617 | NEX  | C34-C33 | 2.79  | 1.39        | 1.35     |
| 24  | G     | 601 | CHL  | MG-NA   | 2.79  | 2.12        | 2.06     |
| 24  | g     | 601 | CHL  | MG-NA   | 2.79  | 2.12        | 2.06     |
| 24  | Y     | 302 | CHL  | MG-NA   | 2.79  | 2.12        | 2.06     |
| 25  | y     | 315 | CLA  | C4B-CHC | -2.78 | 1.33        | 1.41     |
| 25  | R     | 611 | CLA  | C1D-C2D | -2.77 | 1.39        | 1.45     |
| 25  | r     | 611 | CLA  | C1D-C2D | -2.75 | 1.39        | 1.45     |
| 25  | Y     | 315 | CLA  | C4B-CHC | -2.73 | 1.33        | 1.41     |
| 24  | N     | 601 | CHL  | MG-NA   | 2.73  | 2.12        | 2.06     |
| 24  | n     | 601 | CHL  | MG-NA   | 2.73  | 2.12        | 2.06     |
| 24  | l     | 302 | CHL  | MG-NA   | 2.72  | 2.12        | 2.06     |
| 24  | 5     | 302 | CHL  | MG-NA   | 2.72  | 2.12        | 2.06     |
| 25  | B     | 609 | CLA  | C4B-CHC | -2.72 | 1.33        | 1.41     |
| 25  | b     | 609 | CLA  | C4B-CHC | -2.72 | 1.33        | 1.41     |
| 40  | R     | 617 | NEX  | C11-C12 | 2.71  | 1.41        | 1.34     |
| 40  | r     | 617 | NEX  | C11-C12 | 2.71  | 1.41        | 1.34     |
| 39  | R     | 615 | LUT  | C23-C24 | 2.71  | 1.54        | 1.50     |
| 39  | r     | 615 | LUT  | C23-C24 | 2.71  | 1.54        | 1.50     |
| 24  | G     | 607 | CHL  | C3B-C2B | -2.70 | 1.36        | 1.40     |
| 24  | g     | 607 | CHL  | C3B-C2B | -2.70 | 1.36        | 1.40     |
| 40  | N     | 617 | NEX  | O24-C25 | -2.69 | 1.42        | 1.46     |
| 24  | 2     | 603 | CHL  | CHD-C1D | 2.69  | 1.43        | 1.38     |
| 24  | 6     | 603 | CHL  | CHD-C1D | 2.69  | 1.43        | 1.38     |
| 25  | G     | 603 | CLA  | C4B-CHC | -2.68 | 1.33        | 1.41     |
| 25  | g     | 603 | CLA  | C4B-CHC | -2.68 | 1.33        | 1.41     |
| 40  | S     | 317 | NEX  | C32-C33 | -2.68 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 40  | n     | 617 | NEX  | C12-C13 | -2.67 | 1.40        | 1.45     |
| 40  | N     | 617 | NEX  | C12-C13 | -2.66 | 1.40        | 1.45     |
| 40  | n     | 617 | NEX  | O24-C25 | -2.66 | 1.42        | 1.46     |
| 40  | s     | 317 | NEX  | C32-C33 | -2.65 | 1.40        | 1.45     |
| 25  | c     | 505 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 24  | Y     | 307 | CHL  | C1B-NB  | 2.65  | 1.37        | 1.35     |
| 25  | G     | 604 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 25  | N     | 613 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 25  | n     | 613 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 25  | G     | 614 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 25  | g     | 604 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 25  | g     | 614 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 40  | y     | 318 | NEX  | C12-C13 | -2.65 | 1.40        | 1.45     |
| 25  | y     | 304 | CLA  | C4B-CHC | -2.64 | 1.33        | 1.41     |
| 40  | Y     | 318 | NEX  | C12-C13 | -2.64 | 1.40        | 1.45     |
| 40  | S     | 317 | NEX  | C34-C33 | 2.64  | 1.39        | 1.35     |
| 40  | s     | 317 | NEX  | C34-C33 | 2.64  | 1.39        | 1.35     |
| 40  | g     | 617 | NEX  | O24-C25 | -2.64 | 1.42        | 1.46     |
| 25  | b     | 608 | CLA  | C4B-CHC | -2.63 | 1.33        | 1.41     |
| 25  | B     | 614 | CLA  | C4B-CHC | -2.63 | 1.33        | 1.41     |
| 25  | b     | 614 | CLA  | C4B-CHC | -2.63 | 1.33        | 1.41     |
| 25  | Y     | 304 | CLA  | C4B-CHC | -2.63 | 1.33        | 1.41     |
| 25  | C     | 505 | CLA  | C4B-CHC | -2.62 | 1.33        | 1.41     |
| 25  | B     | 608 | CLA  | C4B-CHC | -2.62 | 1.33        | 1.41     |
| 25  | Y     | 312 | CLA  | C4B-CHC | -2.62 | 1.33        | 1.41     |
| 25  | C     | 502 | CLA  | C4B-CHC | -2.62 | 1.33        | 1.41     |
| 25  | c     | 502 | CLA  | C4B-CHC | -2.62 | 1.33        | 1.41     |
| 25  | N     | 603 | CLA  | C4B-CHC | -2.61 | 1.33        | 1.41     |
| 25  | n     | 603 | CLA  | C4B-CHC | -2.61 | 1.33        | 1.41     |
| 39  | n     | 616 | LUT  | C23-C24 | 2.61  | 1.53        | 1.50     |
| 25  | g     | 613 | CLA  | C4C-C3C | -2.61 | 1.40        | 1.45     |
| 40  | G     | 617 | NEX  | O24-C25 | -2.61 | 1.42        | 1.46     |
| 25  | B     | 613 | CLA  | C4B-CHC | -2.61 | 1.33        | 1.41     |
| 41  | R     | 616 | XAT  | O24-C25 | -2.60 | 1.42        | 1.46     |
| 25  | g     | 613 | CLA  | C4B-CHC | -2.60 | 1.33        | 1.41     |
| 25  | y     | 312 | CLA  | C4B-CHC | -2.60 | 1.33        | 1.41     |
| 40  | y     | 318 | NEX  | O24-C25 | -2.60 | 1.42        | 1.46     |
| 25  | N     | 613 | CLA  | C4C-C3C | -2.60 | 1.40        | 1.45     |
| 25  | G     | 613 | CLA  | C4B-CHC | -2.60 | 1.33        | 1.41     |
| 25  | C     | 513 | CLA  | C4C-C3C | -2.59 | 1.40        | 1.45     |
| 25  | B     | 611 | CLA  | C4B-CHC | -2.59 | 1.33        | 1.41     |
| 25  | b     | 611 | CLA  | C4B-CHC | -2.59 | 1.33        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | N     | 610 | CLA  | C4C-C3C | -2.59 | 1.40        | 1.45     |
| 25  | n     | 610 | CLA  | C4C-C3C | -2.59 | 1.40        | 1.45     |
| 40  | s     | 317 | NEX  | O24-C25 | -2.59 | 1.42        | 1.46     |
| 25  | c     | 513 | CLA  | C4C-C3C | -2.58 | 1.40        | 1.45     |
| 25  | Y     | 305 | CLA  | C4B-CHC | -2.58 | 1.33        | 1.41     |
| 25  | y     | 305 | CLA  | C4B-CHC | -2.58 | 1.33        | 1.41     |
| 25  | g     | 602 | CLA  | C4C-C3C | -2.58 | 1.40        | 1.45     |
| 25  | G     | 602 | CLA  | C4C-C3C | -2.58 | 1.40        | 1.45     |
| 25  | b     | 613 | CLA  | C4B-CHC | -2.58 | 1.33        | 1.41     |
| 24  | G     | 607 | CHL  | CHC-C1C | 2.58  | 1.41        | 1.35     |
| 25  | b     | 610 | CLA  | C4C-C3C | -2.58 | 1.40        | 1.45     |
| 25  | b     | 616 | CLA  | C4B-CHC | -2.58 | 1.33        | 1.41     |
| 24  | 6     | 603 | CHL  | MG-NA   | 2.58  | 2.12        | 2.06     |
| 25  | Y     | 314 | CLA  | C4B-CHC | -2.57 | 1.33        | 1.41     |
| 24  | g     | 607 | CHL  | CHC-C1C | 2.57  | 1.41        | 1.35     |
| 25  | G     | 613 | CLA  | C4C-C3C | -2.57 | 1.40        | 1.45     |
| 25  | A     | 405 | CLA  | C4B-CHC | -2.57 | 1.33        | 1.41     |
| 25  | a     | 406 | CLA  | C4B-CHC | -2.57 | 1.33        | 1.41     |
| 41  | r     | 616 | XAT  | O24-C25 | -2.57 | 1.42        | 1.46     |
| 24  | 2     | 603 | CHL  | MG-NA   | 2.57  | 2.12        | 2.06     |
| 25  | y     | 314 | CLA  | C4C-C3C | -2.57 | 1.40        | 1.45     |
| 40  | Y     | 318 | NEX  | O24-C25 | -2.57 | 1.42        | 1.46     |
| 25  | D     | 401 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 25  | C     | 503 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 25  | c     | 503 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 39  | N     | 616 | LUT  | C23-C24 | 2.56  | 1.53        | 1.50     |
| 24  | y     | 307 | CHL  | C1B-NB  | 2.56  | 1.37        | 1.35     |
| 24  | N     | 607 | CHL  | CHC-C1C | 2.56  | 1.41        | 1.35     |
| 24  | n     | 607 | CHL  | CHC-C1C | 2.56  | 1.41        | 1.35     |
| 25  | y     | 314 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 25  | B     | 616 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 40  | S     | 317 | NEX  | O24-C25 | -2.56 | 1.42        | 1.46     |
| 25  | A     | 405 | CLA  | C4C-C3C | -2.56 | 1.40        | 1.45     |
| 25  | a     | 406 | CLA  | C4C-C3C | -2.56 | 1.40        | 1.45     |
| 39  | Y     | 317 | LUT  | C23-C24 | 2.56  | 1.53        | 1.50     |
| 25  | C     | 502 | CLA  | C4C-C3C | -2.56 | 1.40        | 1.45     |
| 25  | c     | 502 | CLA  | C4C-C3C | -2.56 | 1.40        | 1.45     |
| 25  | y     | 305 | CLA  | C4C-C3C | -2.56 | 1.40        | 1.45     |
| 25  | B     | 607 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 25  | b     | 607 | CLA  | C4B-CHC | -2.56 | 1.33        | 1.41     |
| 41  | R     | 616 | XAT  | O4-C5   | -2.55 | 1.42        | 1.46     |
| 41  | r     | 616 | XAT  | O4-C5   | -2.55 | 1.42        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | Y     | 311 | CLA  | C4C-C3C | -2.55 | 1.40        | 1.45     |
| 24  | 2     | 601 | CHL  | CHC-C1C | 2.55  | 1.41        | 1.35     |
| 25  | n     | 613 | CLA  | C4C-C3C | -2.55 | 1.40        | 1.45     |
| 25  | Y     | 303 | CLA  | C4B-CHC | -2.55 | 1.33        | 1.41     |
| 25  | S     | 303 | CLA  | C4B-CHC | -2.55 | 1.33        | 1.41     |
| 25  | R     | 614 | CLA  | C4B-CHC | -2.55 | 1.33        | 1.41     |
| 25  | Y     | 314 | CLA  | C4C-C3C | -2.55 | 1.40        | 1.45     |
| 25  | b     | 603 | CLA  | C4C-C3C | -2.55 | 1.40        | 1.45     |
| 25  | C     | 512 | CLA  | C4B-CHC | -2.55 | 1.33        | 1.41     |
| 25  | c     | 512 | CLA  | C4B-CHC | -2.55 | 1.33        | 1.41     |
| 25  | y     | 311 | CLA  | C4C-C3C | -2.54 | 1.40        | 1.45     |
| 25  | B     | 604 | CLA  | C4C-C3C | -2.54 | 1.40        | 1.45     |
| 25  | R     | 608 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | d     | 401 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | g     | 602 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | y     | 303 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | B     | 603 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | b     | 603 | CLA  | C4B-CHC | -2.54 | 1.33        | 1.41     |
| 25  | R     | 614 | CLA  | C4C-C3C | -2.53 | 1.40        | 1.45     |
| 25  | B     | 610 | CLA  | C4C-C3C | -2.53 | 1.40        | 1.45     |
| 40  | R     | 617 | NEX  | O24-C25 | -2.53 | 1.42        | 1.46     |
| 40  | r     | 617 | NEX  | O24-C25 | -2.53 | 1.42        | 1.46     |
| 24  | R     | 607 | CHL  | C2-C3   | 2.53  | 1.39        | 1.33     |
| 25  | y     | 311 | CLA  | C4B-CHC | -2.53 | 1.34        | 1.41     |
| 25  | Y     | 303 | CLA  | C4C-C3C | -2.53 | 1.40        | 1.45     |
| 25  | r     | 614 | CLA  | C4C-C3C | -2.53 | 1.40        | 1.45     |
| 24  | y     | 308 | CHL  | C2-C3   | 2.53  | 1.39        | 1.33     |
| 25  | s     | 303 | CLA  | C4B-CHC | -2.53 | 1.34        | 1.41     |
| 24  | 6     | 601 | CHL  | CHC-C1C | 2.53  | 1.41        | 1.35     |
| 24  | n     | 601 | CHL  | C2-C3   | 2.52  | 1.39        | 1.33     |
| 25  | N     | 610 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 24  | Y     | 308 | CHL  | C2-C3   | 2.52  | 1.39        | 1.33     |
| 25  | Y     | 311 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 25  | N     | 604 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 25  | C     | 506 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 25  | r     | 608 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 25  | y     | 303 | CLA  | C4C-C3C | -2.52 | 1.40        | 1.45     |
| 25  | G     | 602 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |
| 25  | C     | 509 | CLA  | C4C-C3C | -2.52 | 1.40        | 1.45     |
| 25  | c     | 509 | CLA  | C4C-C3C | -2.52 | 1.40        | 1.45     |
| 24  | g     | 608 | CHL  | C2-C3   | 2.52  | 1.39        | 1.33     |
| 25  | r     | 614 | CLA  | C4B-CHC | -2.52 | 1.34        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | a     | 402 | CLA  | C4B-CHC | -2.51 | 1.34        | 1.41     |
| 24  | N     | 601 | CHL  | C2-C3   | 2.51  | 1.39        | 1.33     |
| 25  | s     | 314 | CLA  | C4B-CHC | -2.51 | 1.34        | 1.41     |
| 25  | B     | 616 | CLA  | C4C-C3C | -2.51 | 1.40        | 1.45     |
| 38  | F     | 101 | HEM  | C1D-ND  | -2.51 | 1.33        | 1.38     |
| 38  | f     | 101 | HEM  | C1D-ND  | -2.51 | 1.33        | 1.38     |
| 25  | n     | 604 | CLA  | C4C-C3C | -2.51 | 1.40        | 1.45     |
| 25  | b     | 605 | CLA  | C4B-CHC | -2.51 | 1.34        | 1.41     |
| 39  | y     | 317 | LUT  | C23-C24 | 2.51  | 1.53        | 1.50     |
| 25  | A     | 402 | CLA  | C4C-C3C | -2.51 | 1.40        | 1.45     |
| 39  | G     | 616 | LUT  | C23-C24 | 2.51  | 1.53        | 1.50     |
| 39  | g     | 616 | LUT  | C23-C24 | 2.51  | 1.53        | 1.50     |
| 25  | B     | 601 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 24  | G     | 608 | CHL  | C1B-NB  | 2.50  | 1.37        | 1.35     |
| 25  | B     | 605 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | b     | 604 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 24  | N     | 608 | CHL  | C2-C3   | 2.50  | 1.39        | 1.33     |
| 24  | n     | 608 | CHL  | C2-C3   | 2.50  | 1.39        | 1.33     |
| 25  | G     | 612 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | g     | 612 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | n     | 611 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | S     | 314 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 25  | S     | 304 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | s     | 304 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | n     | 610 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | N     | 611 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 25  | n     | 611 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 25  | S     | 314 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | C     | 505 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 25  | c     | 505 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 24  | G     | 608 | CHL  | C2-C3   | 2.50  | 1.39        | 1.33     |
| 25  | c     | 511 | CLA  | C4C-C3C | -2.50 | 1.40        | 1.45     |
| 25  | S     | 310 | CLA  | C4B-CHC | -2.50 | 1.34        | 1.41     |
| 25  | B     | 604 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 25  | b     | 604 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 40  | g     | 617 | NEX  | C11-C12 | 2.49  | 1.41        | 1.34     |
| 25  | N     | 602 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | n     | 602 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | B     | 609 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | Y     | 305 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | b     | 609 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 24  | r     | 607 | CHL  | C2-C3   | 2.49  | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | c     | 506 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 24  | Y     | 309 | CHL  | C2-C3   | 2.49  | 1.39        | 1.33     |
| 25  | N     | 614 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 24  | y     | 309 | CHL  | C2-C3   | 2.49  | 1.39        | 1.33     |
| 25  | R     | 602 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 25  | r     | 602 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 24  | N     | 609 | CHL  | CHC-C1C | 2.49  | 1.41        | 1.35     |
| 24  | n     | 609 | CHL  | CHC-C1C | 2.49  | 1.41        | 1.35     |
| 25  | B     | 603 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | B     | 614 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | A     | 402 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 25  | a     | 403 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 25  | B     | 607 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | n     | 604 | CLA  | C4B-CHC | -2.49 | 1.34        | 1.41     |
| 24  | l     | 301 | CHL  | CHC-C1C | 2.49  | 1.41        | 1.35     |
| 25  | G     | 603 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 25  | n     | 614 | CLA  | C4C-C3C | -2.49 | 1.40        | 1.45     |
| 24  | y     | 309 | CHL  | CHC-C1C | 2.48  | 1.41        | 1.35     |
| 24  | g     | 601 | CHL  | CHC-C1C | 2.48  | 1.41        | 1.35     |
| 25  | N     | 611 | CLA  | C4B-CHC | -2.48 | 1.34        | 1.41     |
| 24  | Y     | 310 | CHL  | C2-C3   | 2.48  | 1.38        | 1.33     |
| 24  | y     | 310 | CHL  | C2-C3   | 2.48  | 1.38        | 1.33     |
| 25  | g     | 603 | CLA  | C4C-C3C | -2.48 | 1.40        | 1.45     |
| 24  | g     | 608 | CHL  | CHC-C1C | 2.48  | 1.41        | 1.35     |
| 25  | N     | 604 | CLA  | C4C-C3C | -2.48 | 1.40        | 1.45     |
| 24  | 2     | 601 | CHL  | C2-C3   | 2.48  | 1.38        | 1.33     |
| 24  | 6     | 601 | CHL  | C2-C3   | 2.48  | 1.38        | 1.33     |
| 25  | R     | 602 | CLA  | C4C-C3C | -2.48 | 1.40        | 1.45     |
| 25  | r     | 602 | CLA  | C4C-C3C | -2.48 | 1.40        | 1.45     |
| 25  | A     | 401 | CLA  | C4B-CHC | -2.48 | 1.34        | 1.41     |
| 25  | C     | 513 | CLA  | C4B-CHC | -2.48 | 1.34        | 1.41     |
| 24  | y     | 302 | CHL  | C2-C3   | 2.48  | 1.38        | 1.33     |
| 24  | 5     | 301 | CHL  | CHC-C1C | 2.48  | 1.41        | 1.35     |
| 24  | g     | 609 | CHL  | C2-C3   | 2.47  | 1.38        | 1.33     |
| 24  | N     | 609 | CHL  | C2-C3   | 2.47  | 1.38        | 1.33     |
| 24  | n     | 609 | CHL  | C2-C3   | 2.47  | 1.38        | 1.33     |
| 25  | G     | 604 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |
| 25  | s     | 310 | CLA  | C4B-CHC | -2.47 | 1.34        | 1.41     |
| 25  | c     | 508 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |
| 24  | R     | 605 | CHL  | CHC-C1C | 2.47  | 1.41        | 1.35     |
| 24  | r     | 605 | CHL  | CHC-C1C | 2.47  | 1.41        | 1.35     |
| 25  | G     | 610 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 40  | g     | 617 | NEX  | C32-C33 | -2.47 | 1.40        | 1.45     |
| 40  | S     | 317 | NEX  | C11-C12 | 2.47  | 1.40        | 1.34     |
| 40  | s     | 317 | NEX  | C11-C12 | 2.47  | 1.40        | 1.34     |
| 25  | g     | 610 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |
| 25  | b     | 616 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |
| 25  | C     | 508 | CLA  | C4C-C3C | -2.47 | 1.40        | 1.45     |
| 25  | N     | 603 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | n     | 603 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 24  | G     | 601 | CHL  | CHC-C1C | 2.46  | 1.41        | 1.35     |
| 40  | G     | 617 | NEX  | C32-C33 | -2.46 | 1.40        | 1.45     |
| 24  | S     | 306 | CHL  | CHC-C1C | 2.46  | 1.41        | 1.35     |
| 24  | s     | 306 | CHL  | CHC-C1C | 2.46  | 1.41        | 1.35     |
| 25  | y     | 312 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | R     | 609 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | r     | 609 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | D     | 401 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | d     | 401 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 24  | S     | 308 | CHL  | CHC-C1C | 2.46  | 1.41        | 1.35     |
| 24  | s     | 308 | CHL  | CHC-C1C | 2.46  | 1.41        | 1.35     |
| 25  | B     | 615 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 25  | b     | 615 | CLA  | C4C-C3C | -2.46 | 1.40        | 1.45     |
| 24  | G     | 609 | CHL  | C2-C3   | 2.45  | 1.38        | 1.33     |
| 25  | Y     | 312 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 25  | a     | 403 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 24  | G     | 608 | CHL  | CHC-C1C | 2.45  | 1.41        | 1.35     |
| 24  | R     | 605 | CHL  | CBA-CGA | 2.45  | 1.56        | 1.50     |
| 24  | r     | 605 | CHL  | CBA-CGA | 2.45  | 1.56        | 1.50     |
| 25  | b     | 601 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 25  | s     | 314 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 24  | g     | 608 | CHL  | C1B-NB  | 2.45  | 1.37        | 1.35     |
| 25  | C     | 508 | CLA  | C4B-CHC | -2.45 | 1.34        | 1.41     |
| 25  | c     | 508 | CLA  | C4B-CHC | -2.45 | 1.34        | 1.41     |
| 25  | B     | 613 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 25  | b     | 613 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 25  | c     | 506 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 24  | n     | 608 | CHL  | CHC-C1C | 2.45  | 1.41        | 1.35     |
| 25  | c     | 513 | CLA  | C4B-CHC | -2.45 | 1.34        | 1.41     |
| 25  | b     | 614 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 25  | g     | 604 | CLA  | C4C-C3C | -2.45 | 1.40        | 1.45     |
| 24  | N     | 601 | CHL  | CHC-C1C | 2.45  | 1.41        | 1.35     |
| 24  | n     | 601 | CHL  | CHC-C1C | 2.45  | 1.41        | 1.35     |
| 25  | C     | 511 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | n     | 612 | CLA  | C4B-CHC | -2.44 | 1.34        | 1.41     |
| 24  | l     | 301 | CHL  | CBA-CGA | 2.44  | 1.56        | 1.50     |
| 25  | N     | 612 | CLA  | C4B-CHC | -2.44 | 1.34        | 1.41     |
| 25  | s     | 310 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 25  | s     | 311 | CLA  | C4B-CHC | -2.44 | 1.34        | 1.41     |
| 25  | b     | 605 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 24  | N     | 608 | CHL  | CHC-C1C | 2.44  | 1.41        | 1.35     |
| 25  | B     | 612 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 25  | b     | 612 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 24  | 5     | 301 | CHL  | CBA-CGA | 2.44  | 1.56        | 1.50     |
| 24  | Y     | 309 | CHL  | CHC-C1C | 2.44  | 1.41        | 1.35     |
| 24  | G     | 605 | CHL  | CHC-C1C | 2.44  | 1.41        | 1.35     |
| 24  | g     | 605 | CHL  | CHC-C1C | 2.44  | 1.41        | 1.35     |
| 24  | 6     | 603 | CHL  | CHD-C4C | 2.44  | 1.44        | 1.39     |
| 25  | S     | 304 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 24  | r     | 607 | CHL  | CHC-C1C | 2.44  | 1.41        | 1.35     |
| 25  | B     | 605 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 25  | b     | 612 | CLA  | C4B-CHC | -2.44 | 1.34        | 1.41     |
| 25  | S     | 311 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 25  | s     | 311 | CLA  | C4C-C3C | -2.44 | 1.40        | 1.45     |
| 25  | G     | 611 | CLA  | C4C-C3C | -2.43 | 1.40        | 1.45     |
| 25  | g     | 611 | CLA  | C4C-C3C | -2.43 | 1.40        | 1.45     |
| 24  | S     | 302 | CHL  | CBA-CGA | 2.43  | 1.56        | 1.50     |
| 24  | s     | 302 | CHL  | CBA-CGA | 2.43  | 1.56        | 1.50     |
| 24  | G     | 606 | CHL  | CHC-C1C | 2.43  | 1.41        | 1.35     |
| 24  | g     | 606 | CHL  | CHC-C1C | 2.43  | 1.41        | 1.35     |
| 25  | C     | 510 | CLA  | C4B-CHC | -2.43 | 1.34        | 1.41     |
| 25  | c     | 510 | CLA  | C4B-CHC | -2.43 | 1.34        | 1.41     |
| 24  | R     | 606 | CHL  | CBA-CGA | 2.43  | 1.56        | 1.50     |
| 25  | b     | 607 | CLA  | C4C-C3C | -2.43 | 1.40        | 1.45     |
| 39  | s     | 315 | LUT  | C23-C24 | 2.43  | 1.53        | 1.50     |
| 24  | Y     | 310 | CHL  | CHC-C1C | 2.43  | 1.41        | 1.35     |
| 24  | l     | 302 | CHL  | CBA-CGA | 2.43  | 1.56        | 1.50     |
| 25  | B     | 612 | CLA  | C4B-CHC | -2.43 | 1.34        | 1.41     |
| 25  | s     | 304 | CLA  | C4C-C3C | -2.43 | 1.40        | 1.45     |
| 25  | S     | 311 | CLA  | C4B-CHC | -2.43 | 1.34        | 1.41     |
| 25  | R     | 611 | CLA  | C3D-C4D | -2.42 | 1.38        | 1.44     |
| 24  | S     | 308 | CHL  | CBA-CGA | 2.42  | 1.56        | 1.50     |
| 25  | B     | 611 | CLA  | C4C-C3C | -2.42 | 1.40        | 1.45     |
| 25  | S     | 310 | CLA  | C4C-C3C | -2.42 | 1.40        | 1.45     |
| 25  | C     | 503 | CLA  | C4C-C3C | -2.42 | 1.40        | 1.45     |
| 25  | C     | 506 | CLA  | C4C-C3C | -2.42 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | c     | 503 | CLA  | C4C-C3C | -2.42 | 1.40        | 1.45     |
| 24  | N     | 606 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | n     | 606 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | G     | 609 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | g     | 609 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | S     | 302 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | R     | 607 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 39  | S     | 316 | LUT  | C23-C24 | 2.42  | 1.53        | 1.50     |
| 39  | s     | 316 | LUT  | C23-C24 | 2.42  | 1.53        | 1.50     |
| 24  | s     | 302 | CHL  | CHC-C1C | 2.42  | 1.41        | 1.35     |
| 24  | S     | 307 | CHL  | CBA-CGA | 2.42  | 1.56        | 1.50     |
| 40  | R     | 617 | NEX  | C32-C33 | -2.41 | 1.40        | 1.45     |
| 40  | r     | 617 | NEX  | C32-C33 | -2.41 | 1.40        | 1.45     |
| 38  | F     | 101 | HEM  | FE-ND   | -2.41 | 1.84        | 1.96     |
| 38  | f     | 101 | HEM  | FE-ND   | -2.41 | 1.84        | 1.96     |
| 24  | R     | 606 | CHL  | CHC-C1C | 2.41  | 1.41        | 1.35     |
| 25  | S     | 303 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 25  | s     | 303 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 24  | S     | 307 | CHL  | CHC-C1C | 2.41  | 1.41        | 1.35     |
| 24  | s     | 307 | CHL  | CHC-C1C | 2.41  | 1.41        | 1.35     |
| 24  | s     | 307 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | n     | 606 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | Y     | 302 | CHL  | C2-C3   | 2.41  | 1.38        | 1.33     |
| 25  | b     | 611 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 24  | S     | 306 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | s     | 306 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | Y     | 308 | CHL  | CHC-C1C | 2.41  | 1.41        | 1.35     |
| 24  | y     | 308 | CHL  | CHC-C1C | 2.41  | 1.41        | 1.35     |
| 25  | Y     | 313 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 25  | d     | 402 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 25  | y     | 313 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 24  | N     | 606 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | n     | 607 | CHL  | C2-C3   | 2.41  | 1.38        | 1.33     |
| 24  | G     | 605 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 24  | g     | 605 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 25  | c     | 501 | CLA  | C4C-C3C | -2.41 | 1.40        | 1.45     |
| 24  | G     | 601 | CHL  | C2-C3   | 2.41  | 1.38        | 1.33     |
| 24  | r     | 606 | CHL  | CBA-CGA | 2.41  | 1.56        | 1.50     |
| 39  | S     | 315 | LUT  | C23-C24 | 2.40  | 1.53        | 1.50     |
| 24  | 5     | 302 | CHL  | CBA-CGA | 2.40  | 1.56        | 1.50     |
| 25  | C     | 509 | CLA  | C4B-CHC | -2.40 | 1.34        | 1.41     |
| 25  | c     | 509 | CLA  | C4B-CHC | -2.40 | 1.34        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 2     | 603 | CHL  | CHD-C4C | 2.40  | 1.44        | 1.39     |
| 25  | G     | 611 | CLA  | C4B-CHC | -2.40 | 1.34        | 1.41     |
| 24  | N     | 607 | CHL  | C2-C3   | 2.40  | 1.38        | 1.33     |
| 24  | N     | 605 | CHL  | CHC-C1C | 2.40  | 1.41        | 1.35     |
| 24  | n     | 605 | CHL  | CHC-C1C | 2.40  | 1.41        | 1.35     |
| 25  | R     | 608 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | r     | 608 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 24  | r     | 606 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 25  | r     | 612 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | 2     | 605 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | 6     | 605 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 24  | g     | 601 | CHL  | C2-C3   | 2.39  | 1.38        | 1.33     |
| 24  | R     | 613 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 24  | r     | 613 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 25  | C     | 507 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | c     | 507 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 24  | y     | 310 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 24  | Y     | 302 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 24  | y     | 302 | CHL  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 24  | s     | 308 | CHL  | CBA-CGA | 2.39  | 1.56        | 1.50     |
| 25  | B     | 608 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | b     | 608 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | g     | 614 | CLA  | C4C-C3C | -2.39 | 1.40        | 1.45     |
| 25  | B     | 610 | CLA  | C4B-CHC | -2.39 | 1.34        | 1.41     |
| 25  | r     | 611 | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 24  | Y     | 306 | CHL  | CHC-C1C | 2.38  | 1.41        | 1.35     |
| 25  | Y     | 304 | CLA  | C4C-C3C | -2.38 | 1.40        | 1.45     |
| 25  | c     | 511 | CLA  | C4B-CHC | -2.38 | 1.34        | 1.41     |
| 25  | b     | 610 | CLA  | C4B-CHC | -2.38 | 1.34        | 1.41     |
| 25  | D     | 402 | CLA  | C4C-C3C | -2.38 | 1.40        | 1.45     |
| 25  | B     | 606 | CLA  | C4B-CHC | -2.38 | 1.34        | 1.41     |
| 25  | b     | 606 | CLA  | C4B-CHC | -2.38 | 1.34        | 1.41     |
| 24  | y     | 306 | CHL  | CHC-C1C | 2.38  | 1.41        | 1.35     |
| 25  | B     | 601 | CLA  | C4B-CHC | -2.38 | 1.34        | 1.41     |
| 25  | b     | 602 | CLA  | C4C-C3C | -2.37 | 1.40        | 1.45     |
| 25  | 2     | 605 | CLA  | C4B-CHC | -2.37 | 1.34        | 1.41     |
| 25  | R     | 612 | CLA  | C4C-C3C | -2.37 | 1.41        | 1.45     |
| 25  | C     | 507 | CLA  | C4B-CHC | -2.37 | 1.34        | 1.41     |
| 25  | c     | 507 | CLA  | C4B-CHC | -2.37 | 1.34        | 1.41     |
| 39  | N     | 615 | LUT  | C5-C6   | 2.37  | 1.38        | 1.34     |
| 24  | 2     | 603 | CHL  | CBA-CGA | 2.37  | 1.56        | 1.50     |
| 24  | 2     | 603 | CHL  | CHC-C1C | 2.37  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | G     | 607 | CHL  | CBA-CGA | 2.37  | 1.56        | 1.50     |
| 25  | C     | 501 | CLA  | C4C-C3C | -2.36 | 1.41        | 1.45     |
| 24  | 6     | 603 | CHL  | CBA-CGA | 2.36  | 1.56        | 1.50     |
| 25  | B     | 602 | CLA  | C4B-CHC | -2.36 | 1.34        | 1.41     |
| 25  | N     | 602 | CLA  | C4B-CHC | -2.36 | 1.34        | 1.41     |
| 25  | n     | 602 | CLA  | C4B-CHC | -2.36 | 1.34        | 1.41     |
| 25  | S     | 312 | CLA  | C4C-C3C | -2.36 | 1.41        | 1.45     |
| 25  | R     | 604 | CLA  | C4C-C3C | -2.36 | 1.41        | 1.45     |
| 25  | g     | 611 | CLA  | C4B-CHC | -2.36 | 1.34        | 1.41     |
| 25  | S     | 309 | CLA  | C4B-CHC | -2.35 | 1.34        | 1.41     |
| 25  | s     | 312 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | C     | 511 | CLA  | C4B-CHC | -2.35 | 1.34        | 1.41     |
| 25  | s     | 309 | CLA  | C4B-CHC | -2.35 | 1.34        | 1.41     |
| 25  | D     | 403 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | R     | 610 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | d     | 403 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | r     | 610 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 39  | N     | 615 | LUT  | C23-C24 | 2.35  | 1.53        | 1.50     |
| 39  | n     | 615 | LUT  | C23-C24 | 2.35  | 1.53        | 1.50     |
| 25  | A     | 401 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | a     | 402 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 38  | F     | 101 | HEM  | C4B-NB  | -2.35 | 1.34        | 1.38     |
| 25  | S     | 309 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | c     | 504 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | s     | 309 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | r     | 609 | CLA  | C4B-CHC | -2.35 | 1.34        | 1.41     |
| 25  | y     | 304 | CLA  | C4C-C3C | -2.35 | 1.41        | 1.45     |
| 25  | 6     | 605 | CLA  | C4B-CHC | -2.34 | 1.34        | 1.41     |
| 39  | G     | 616 | LUT  | C5-C6   | 2.34  | 1.38        | 1.34     |
| 39  | g     | 616 | LUT  | C5-C6   | 2.34  | 1.38        | 1.34     |
| 25  | C     | 504 | CLA  | C4C-C3C | -2.34 | 1.41        | 1.45     |
| 38  | f     | 101 | HEM  | C4B-NB  | -2.34 | 1.34        | 1.38     |
| 24  | S     | 302 | CHL  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 25  | Y     | 315 | CLA  | C4C-C3C | -2.34 | 1.41        | 1.45     |
| 24  | y     | 308 | CHL  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 24  | 6     | 603 | CHL  | CHC-C1C | 2.34  | 1.41        | 1.35     |
| 24  | Y     | 307 | CHL  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 39  | G     | 615 | LUT  | C23-C24 | 2.34  | 1.53        | 1.50     |
| 39  | g     | 615 | LUT  | C23-C24 | 2.34  | 1.53        | 1.50     |
| 25  | b     | 601 | CLA  | C4B-CHC | -2.33 | 1.34        | 1.41     |
| 25  | b     | 602 | CLA  | C4B-CHC | -2.33 | 1.34        | 1.41     |
| 24  | 1     | 302 | CHL  | CHC-C1C | 2.33  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 5     | 302 | CHL  | CHC-C1C | 2.33  | 1.40        | 1.35     |
| 25  | C     | 512 | CLA  | C4C-C3C | -2.33 | 1.41        | 1.45     |
| 25  | G     | 614 | CLA  | C4C-C3C | -2.33 | 1.41        | 1.45     |
| 25  | c     | 512 | CLA  | C4C-C3C | -2.33 | 1.41        | 1.45     |
| 25  | C     | 510 | CLA  | C4C-C3C | -2.32 | 1.41        | 1.45     |
| 39  | n     | 615 | LUT  | C5-C6   | 2.32  | 1.38        | 1.34     |
| 25  | c     | 510 | CLA  | C4C-C3C | -2.32 | 1.41        | 1.45     |
| 24  | s     | 302 | CHL  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 24  | y     | 307 | CHL  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 24  | n     | 608 | CHL  | C1B-NB  | 2.32  | 1.37        | 1.35     |
| 25  | R     | 609 | CLA  | C4B-CHC | -2.32 | 1.34        | 1.41     |
| 24  | Y     | 308 | CHL  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 25  | B     | 602 | CLA  | C4C-C3C | -2.32 | 1.41        | 1.45     |
| 25  | S     | 313 | CLA  | C4C-C3C | -2.31 | 1.41        | 1.45     |
| 25  | s     | 313 | CLA  | C4C-C3C | -2.31 | 1.41        | 1.45     |
| 24  | g     | 607 | CHL  | CBA-CGA | 2.31  | 1.56        | 1.50     |
| 25  | B     | 606 | CLA  | C4C-C3C | -2.31 | 1.41        | 1.45     |
| 25  | b     | 606 | CLA  | C4C-C3C | -2.31 | 1.41        | 1.45     |
| 39  | y     | 317 | LUT  | C5-C6   | 2.31  | 1.38        | 1.34     |
| 40  | N     | 617 | NEX  | C32-C33 | -2.31 | 1.41        | 1.45     |
| 25  | y     | 315 | CLA  | C4C-C3C | -2.31 | 1.41        | 1.45     |
| 40  | n     | 617 | NEX  | C32-C33 | -2.30 | 1.41        | 1.45     |
| 25  | B     | 608 | CLA  | C1C-C2C | -2.30 | 1.40        | 1.44     |
| 41  | r     | 616 | XAT  | C14-C13 | 2.29  | 1.38        | 1.35     |
| 25  | G     | 612 | CLA  | C4C-C3C | -2.29 | 1.41        | 1.45     |
| 25  | B     | 609 | CLA  | C1C-C2C | -2.29 | 1.40        | 1.44     |
| 25  | s     | 305 | CLA  | C4C-C3C | -2.29 | 1.41        | 1.45     |
| 24  | S     | 307 | CHL  | MG-NC   | 2.29  | 2.11        | 2.06     |
| 25  | C     | 502 | CLA  | C1C-C2C | -2.28 | 1.40        | 1.44     |
| 25  | b     | 609 | CLA  | C1C-C2C | -2.28 | 1.40        | 1.44     |
| 39  | S     | 315 | LUT  | C5-C6   | 2.28  | 1.38        | 1.34     |
| 39  | N     | 616 | LUT  | C5-C6   | 2.27  | 1.38        | 1.34     |
| 39  | n     | 616 | LUT  | C5-C6   | 2.27  | 1.38        | 1.34     |
| 25  | N     | 614 | CLA  | C4B-CHC | -2.27 | 1.34        | 1.41     |
| 25  | g     | 612 | CLA  | C4C-C3C | -2.27 | 1.41        | 1.45     |
| 25  | 2     | 604 | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 25  | 6     | 604 | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 41  | R     | 616 | XAT  | C32-C33 | -2.27 | 1.41        | 1.45     |
| 41  | r     | 616 | XAT  | C32-C33 | -2.27 | 1.41        | 1.45     |
| 25  | B     | 614 | CLA  | C1C-C2C | -2.27 | 1.40        | 1.44     |
| 25  | r     | 604 | CLA  | C4C-C3C | -2.27 | 1.41        | 1.45     |
| 24  | s     | 307 | CHL  | MG-NC   | 2.27  | 2.11        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | B     | 611 | CLA  | C1C-C2C | -2.27 | 1.40        | 1.44     |
| 25  | b     | 611 | CLA  | C1C-C2C | -2.27 | 1.40        | 1.44     |
| 24  | R     | 613 | CHL  | MG-NC   | 2.27  | 2.11        | 2.06     |
| 25  | n     | 614 | CLA  | C4B-CHC | -2.26 | 1.34        | 1.41     |
| 25  | R     | 604 | CLA  | C4B-CHC | -2.26 | 1.34        | 1.41     |
| 41  | R     | 616 | XAT  | C12-C13 | -2.26 | 1.41        | 1.45     |
| 41  | r     | 616 | XAT  | C12-C13 | -2.26 | 1.41        | 1.45     |
| 25  | r     | 603 | CLA  | C4C-C3C | -2.26 | 1.41        | 1.45     |
| 39  | Y     | 317 | LUT  | C5-C6   | 2.26  | 1.38        | 1.34     |
| 25  | S     | 305 | CLA  | C4C-C3C | -2.26 | 1.41        | 1.45     |
| 24  | y     | 307 | CHL  | CHC-C1C | 2.26  | 1.40        | 1.35     |
| 24  | G     | 607 | CHL  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 24  | g     | 607 | CHL  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 24  | r     | 613 | CHL  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 25  | b     | 608 | CLA  | C1C-C2C | -2.26 | 1.40        | 1.44     |
| 25  | c     | 502 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | g     | 603 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | S     | 303 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | s     | 303 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | C     | 505 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | c     | 505 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 32  | y     | 320 | AJP  | C85-C02 | 2.25  | 1.56        | 1.51     |
| 24  | l     | 301 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 25  | D     | 402 | CLA  | C4B-CHC | -2.25 | 1.34        | 1.41     |
| 24  | R     | 606 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 24  | r     | 606 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 24  | N     | 607 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 24  | n     | 607 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 25  | N     | 603 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | n     | 603 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 25  | d     | 402 | CLA  | C4B-CHC | -2.25 | 1.34        | 1.41     |
| 25  | b     | 614 | CLA  | C1C-C2C | -2.25 | 1.40        | 1.44     |
| 40  | G     | 617 | NEX  | C11-C10 | -2.25 | 1.36        | 1.43     |
| 25  | R     | 603 | CLA  | C4C-C3C | -2.25 | 1.41        | 1.45     |
| 24  | Y     | 307 | CHL  | CHC-C1C | 2.24  | 1.40        | 1.35     |
| 24  | N     | 608 | CHL  | C1B-NB  | 2.24  | 1.37        | 1.35     |
| 24  | Y     | 309 | CHL  | C1B-NB  | 2.24  | 1.37        | 1.35     |
| 24  | y     | 309 | CHL  | C1B-NB  | 2.24  | 1.37        | 1.35     |
| 41  | R     | 616 | XAT  | C14-C13 | 2.24  | 1.38        | 1.35     |
| 24  | G     | 609 | CHL  | MG-NC   | 2.24  | 2.11        | 2.06     |
| 24  | g     | 609 | CHL  | MG-NC   | 2.24  | 2.11        | 2.06     |
| 25  | c     | 503 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | G     | 603 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | c     | 512 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | r     | 604 | CLA  | C4B-CHC | -2.24 | 1.34        | 1.41     |
| 25  | Y     | 304 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | y     | 304 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 39  | R     | 615 | LUT  | C26-C27 | 2.24  | 1.53        | 1.50     |
| 25  | B     | 613 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | Y     | 313 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | b     | 613 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | y     | 313 | CLA  | C1C-C2C | -2.24 | 1.40        | 1.44     |
| 25  | N     | 613 | CLA  | CHD-C1D | -2.24 | 1.34        | 1.38     |
| 39  | r     | 615 | LUT  | C26-C27 | 2.24  | 1.53        | 1.50     |
| 39  | y     | 316 | LUT  | C23-C24 | 2.24  | 1.53        | 1.50     |
| 25  | r     | 612 | CLA  | C4B-CHC | -2.23 | 1.34        | 1.41     |
| 24  | l     | 302 | CHL  | C1B-NB  | 2.23  | 1.37        | 1.35     |
| 25  | S     | 312 | CLA  | C4B-CHC | -2.23 | 1.34        | 1.41     |
| 25  | S     | 313 | CLA  | C4B-CHC | -2.23 | 1.34        | 1.41     |
| 25  | s     | 313 | CLA  | C4B-CHC | -2.23 | 1.34        | 1.41     |
| 25  | G     | 604 | CLA  | C1C-C2C | -2.23 | 1.40        | 1.44     |
| 25  | N     | 604 | CLA  | C1C-C2C | -2.23 | 1.40        | 1.44     |
| 25  | g     | 604 | CLA  | C1C-C2C | -2.23 | 1.40        | 1.44     |
| 24  | N     | 609 | CHL  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 24  | n     | 609 | CHL  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 39  | R     | 615 | LUT  | C5-C6   | 2.22  | 1.38        | 1.34     |
| 39  | g     | 615 | LUT  | C5-C6   | 2.22  | 1.38        | 1.34     |
| 39  | S     | 316 | LUT  | C5-C6   | 2.22  | 1.38        | 1.34     |
| 39  | s     | 316 | LUT  | C5-C6   | 2.22  | 1.38        | 1.34     |
| 32  | Y     | 320 | AJP  | C85-C02 | 2.22  | 1.56        | 1.51     |
| 41  | R     | 616 | XAT  | C34-C33 | 2.22  | 1.38        | 1.35     |
| 41  | r     | 616 | XAT  | C34-C33 | 2.22  | 1.38        | 1.35     |
| 25  | G     | 602 | CLA  | CHD-C1D | -2.22 | 1.34        | 1.38     |
| 25  | g     | 602 | CLA  | CHD-C1D | -2.22 | 1.34        | 1.38     |
| 39  | G     | 615 | LUT  | C5-C6   | 2.22  | 1.38        | 1.34     |
| 25  | Y     | 315 | CLA  | C1C-C2C | -2.22 | 1.40        | 1.44     |
| 25  | a     | 403 | CLA  | C1C-C2C | -2.22 | 1.40        | 1.44     |
| 25  | y     | 315 | CLA  | C1C-C2C | -2.22 | 1.40        | 1.44     |
| 25  | C     | 503 | CLA  | C1C-C2C | -2.22 | 1.40        | 1.44     |
| 25  | s     | 312 | CLA  | C4B-CHC | -2.22 | 1.34        | 1.41     |
| 25  | G     | 610 | CLA  | C4B-CHC | -2.21 | 1.34        | 1.41     |
| 25  | g     | 610 | CLA  | C4B-CHC | -2.21 | 1.34        | 1.41     |
| 25  | A     | 401 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | a     | 402 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | G     | 602 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | g     | 602 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | d     | 401 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | C     | 508 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | c     | 508 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 24  | Y     | 306 | CHL  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 24  | Y     | 310 | CHL  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 39  | s     | 315 | LUT  | C5-C6   | 2.21  | 1.38        | 1.34     |
| 25  | R     | 612 | CLA  | C4B-CHC | -2.21 | 1.34        | 1.41     |
| 24  | R     | 605 | CHL  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 25  | n     | 613 | CLA  | CHD-C1D | -2.21 | 1.34        | 1.38     |
| 24  | S     | 306 | CHL  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 24  | s     | 306 | CHL  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 25  | G     | 614 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | g     | 614 | CLA  | C1C-C2C | -2.21 | 1.40        | 1.44     |
| 25  | A     | 402 | CLA  | C1C-C2C | -2.20 | 1.40        | 1.44     |
| 39  | r     | 615 | LUT  | C5-C6   | 2.20  | 1.38        | 1.34     |
| 25  | r     | 611 | CLA  | C4D-ND  | -2.20 | 1.34        | 1.37     |
| 25  | C     | 512 | CLA  | C1C-C2C | -2.20 | 1.40        | 1.44     |
| 25  | b     | 603 | CLA  | C1C-C2C | -2.20 | 1.40        | 1.44     |
| 24  | 5     | 302 | CHL  | C1B-NB  | 2.19  | 1.37        | 1.35     |
| 24  | y     | 310 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 24  | 5     | 301 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 25  | c     | 507 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 24  | r     | 605 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 25  | B     | 612 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 25  | b     | 612 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 25  | C     | 510 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 40  | Y     | 318 | NEX  | C31-C32 | 2.19  | 1.40        | 1.34     |
| 25  | B     | 616 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 25  | b     | 616 | CLA  | C1C-C2C | -2.19 | 1.40        | 1.44     |
| 24  | N     | 605 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 24  | n     | 605 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 24  | s     | 308 | CHL  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 24  | N     | 606 | CHL  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 24  | n     | 606 | CHL  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 39  | S     | 315 | LUT  | C26-C27 | 2.18  | 1.53        | 1.50     |
| 24  | S     | 308 | CHL  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 25  | R     | 601 | CLA  | C4C-C3C | -2.18 | 1.41        | 1.45     |
| 25  | r     | 601 | CLA  | C4C-C3C | -2.18 | 1.41        | 1.45     |
| 25  | B     | 607 | CLA  | C1C-C2C | -2.18 | 1.40        | 1.44     |
| 25  | C     | 507 | CLA  | C1C-C2C | -2.18 | 1.40        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | b     | 607 | CLA  | C1C-C2C | -2.18 | 1.40        | 1.44     |
| 24  | G     | 606 | CHL  | C1B-NB  | 2.18  | 1.37        | 1.35     |
| 25  | R     | 611 | CLA  | C4C-C3C | -2.18 | 1.41        | 1.45     |
| 25  | r     | 611 | CLA  | C4C-C3C | -2.18 | 1.41        | 1.45     |
| 25  | S     | 314 | CLA  | C1C-C2C | -2.18 | 1.40        | 1.44     |
| 24  | 2     | 603 | CHL  | C1B-NB  | 2.18  | 1.37        | 1.35     |
| 24  | 6     | 603 | CHL  | C1B-NB  | 2.18  | 1.37        | 1.35     |
| 24  | g     | 606 | CHL  | C1B-NB  | 2.18  | 1.37        | 1.35     |
| 25  | R     | 611 | CLA  | C4D-ND  | -2.18 | 1.34        | 1.37     |
| 24  | R     | 607 | CHL  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 24  | r     | 607 | CHL  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 25  | y     | 312 | CLA  | CHD-C1D | -2.17 | 1.34        | 1.38     |
| 25  | D     | 401 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 40  | Y     | 318 | NEX  | C32-C33 | -2.17 | 1.41        | 1.45     |
| 39  | Y     | 316 | LUT  | C23-C24 | 2.17  | 1.53        | 1.50     |
| 39  | s     | 315 | LUT  | C26-C27 | 2.17  | 1.53        | 1.50     |
| 25  | 2     | 602 | CLA  | C4C-C3C | -2.17 | 1.41        | 1.45     |
| 25  | 6     | 602 | CLA  | C4C-C3C | -2.17 | 1.41        | 1.45     |
| 25  | n     | 612 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 25  | c     | 506 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 24  | y     | 306 | CHL  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 25  | 2     | 602 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 25  | S     | 304 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 25  | A     | 405 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 25  | a     | 406 | CLA  | C1C-C2C | -2.17 | 1.40        | 1.44     |
| 24  | G     | 606 | CHL  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 24  | g     | 606 | CHL  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 25  | B     | 615 | CLA  | C4B-CHC | -2.17 | 1.35        | 1.41     |
| 25  | b     | 615 | CLA  | C4B-CHC | -2.17 | 1.35        | 1.41     |
| 25  | Y     | 314 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | y     | 314 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 39  | G     | 616 | LUT  | C1-C6   | 2.16  | 1.56        | 1.53     |
| 39  | g     | 616 | LUT  | C1-C6   | 2.16  | 1.56        | 1.53     |
| 25  | B     | 603 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | N     | 612 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | b     | 605 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | R     | 608 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | s     | 311 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | n     | 604 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | r     | 608 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 25  | Y     | 315 | CLA  | C1B-CHB | -2.16 | 1.35        | 1.41     |
| 25  | y     | 315 | CLA  | C1B-CHB | -2.16 | 1.35        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | c     | 510 | CLA  | C1C-C2C | -2.16 | 1.40        | 1.44     |
| 24  | N     | 601 | CHL  | MG-NC   | 2.15  | 2.11        | 2.06     |
| 24  | n     | 601 | CHL  | MG-NC   | 2.15  | 2.11        | 2.06     |
| 40  | y     | 318 | NEX  | C31-C32 | 2.15  | 1.40        | 1.34     |
| 25  | s     | 304 | CLA  | C1C-C2C | -2.15 | 1.40        | 1.44     |
| 24  | Y     | 308 | CHL  | C3B-CAB | -2.15 | 1.43        | 1.47     |
| 24  | y     | 308 | CHL  | C3B-CAB | -2.15 | 1.43        | 1.47     |
| 25  | B     | 605 | CLA  | C1C-C2C | -2.15 | 1.40        | 1.44     |
| 25  | b     | 604 | CLA  | C1C-C2C | -2.15 | 1.40        | 1.44     |
| 25  | r     | 602 | CLA  | C1C-C2C | -2.15 | 1.40        | 1.44     |
| 25  | c     | 509 | CLA  | C1C-C2C | -2.15 | 1.40        | 1.44     |
| 25  | C     | 506 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 25  | 6     | 602 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 25  | s     | 314 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 24  | G     | 605 | CHL  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 24  | g     | 605 | CHL  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 25  | Y     | 312 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 25  | y     | 312 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 24  | N     | 608 | CHL  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 24  | n     | 608 | CHL  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 25  | R     | 611 | CLA  | CHC-C1C | 2.14  | 1.40        | 1.35     |
| 25  | r     | 611 | CLA  | CHC-C1C | 2.14  | 1.40        | 1.35     |
| 25  | n     | 612 | CLA  | C4C-C3C | -2.14 | 1.41        | 1.45     |
| 25  | Y     | 312 | CLA  | CHD-C1D | -2.14 | 1.34        | 1.38     |
| 24  | Y     | 302 | CHL  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 24  | N     | 607 | CHL  | C3B-CAB | -2.14 | 1.43        | 1.47     |
| 25  | B     | 602 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 25  | S     | 311 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 25  | g     | 613 | CLA  | C1C-C2C | -2.14 | 1.40        | 1.44     |
| 24  | n     | 607 | CHL  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 39  | Y     | 316 | LUT  | C5-C6   | 2.13  | 1.38        | 1.34     |
| 40  | y     | 318 | NEX  | C32-C33 | -2.13 | 1.41        | 1.45     |
| 25  | B     | 604 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | C     | 513 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | c     | 513 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | C     | 511 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | c     | 511 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | Y     | 305 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | y     | 305 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | 2     | 605 | CLA  | C1C-C2C | -2.13 | 1.40        | 1.44     |
| 25  | S     | 305 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 38  | F     | 101 | HEM  | CHB-C1B | 2.13  | 1.40        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 509 | CLA  | C1C-C2C | -2.12 | 1.40        | 1.44     |
| 40  | S     | 317 | NEX  | C11-C10 | -2.12 | 1.36        | 1.43     |
| 40  | s     | 317 | NEX  | C11-C10 | -2.12 | 1.36        | 1.43     |
| 25  | s     | 305 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 40  | g     | 617 | NEX  | C11-C10 | -2.12 | 1.36        | 1.43     |
| 25  | n     | 614 | CLA  | C1C-C2C | -2.12 | 1.40        | 1.44     |
| 25  | D     | 403 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 24  | N     | 606 | CHL  | C1B-NB  | 2.12  | 1.37        | 1.35     |
| 24  | n     | 606 | CHL  | C1B-NB  | 2.12  | 1.37        | 1.35     |
| 25  | N     | 602 | CLA  | CHD-C1D | -2.12 | 1.34        | 1.38     |
| 25  | n     | 602 | CLA  | CHD-C1D | -2.12 | 1.34        | 1.38     |
| 24  | G     | 608 | CHL  | MG-NC   | 2.12  | 2.11        | 2.06     |
| 24  | Y     | 309 | CHL  | MG-NC   | 2.11  | 2.11        | 2.06     |
| 38  | f     | 101 | HEM  | CHB-C1B | 2.11  | 1.40        | 1.35     |
| 24  | y     | 302 | CHL  | MG-NC   | 2.11  | 2.11        | 2.06     |
| 25  | R     | 602 | CLA  | C1C-C2C | -2.11 | 1.40        | 1.44     |
| 39  | y     | 316 | LUT  | C5-C6   | 2.10  | 1.38        | 1.34     |
| 25  | S     | 309 | CLA  | C1C-C2C | -2.10 | 1.40        | 1.44     |
| 39  | S     | 316 | LUT  | C26-C27 | 2.10  | 1.53        | 1.50     |
| 39  | s     | 316 | LUT  | C26-C27 | 2.10  | 1.53        | 1.50     |
| 24  | g     | 608 | CHL  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 25  | d     | 403 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 25  | 6     | 605 | CLA  | C1C-C2C | -2.10 | 1.40        | 1.44     |
| 25  | R     | 601 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 25  | r     | 601 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 24  | y     | 309 | CHL  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 25  | S     | 313 | CLA  | C1C-C2C | -2.10 | 1.40        | 1.44     |
| 25  | Y     | 303 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | Y     | 313 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | y     | 303 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | y     | 313 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | N     | 614 | CLA  | C1C-C2C | -2.09 | 1.40        | 1.44     |
| 25  | N     | 612 | CLA  | C4C-C3C | -2.09 | 1.41        | 1.45     |
| 25  | B     | 610 | CLA  | C1C-C2C | -2.09 | 1.40        | 1.44     |
| 25  | b     | 610 | CLA  | C1C-C2C | -2.09 | 1.40        | 1.44     |
| 25  | C     | 504 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 25  | c     | 504 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 24  | G     | 601 | CHL  | MG-NC   | 2.09  | 2.11        | 2.06     |
| 24  | g     | 601 | CHL  | MG-NC   | 2.09  | 2.11        | 2.06     |
| 25  | N     | 611 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | n     | 611 | CLA  | CHD-C1D | -2.09 | 1.34        | 1.38     |
| 25  | G     | 613 | CLA  | C1C-C2C | -2.09 | 1.40        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 501 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 25  | b     | 602 | CLA  | C1C-C2C | -2.09 | 1.40        | 1.44     |
| 25  | S     | 313 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 25  | N     | 613 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | n     | 613 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | R     | 612 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 24  | 2     | 603 | CHL  | O1D-CGD | 2.08  | 1.26        | 1.21     |
| 24  | 6     | 603 | CHL  | O1D-CGD | 2.08  | 1.26        | 1.21     |
| 25  | D     | 402 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | d     | 402 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 24  | Y     | 310 | CHL  | C3B-CAB | -2.08 | 1.43        | 1.47     |
| 25  | s     | 309 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | r     | 609 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | Y     | 303 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | y     | 303 | CLA  | C1C-C2C | -2.08 | 1.40        | 1.44     |
| 25  | b     | 601 | CLA  | C1C-C2C | -2.07 | 1.40        | 1.44     |
| 25  | S     | 312 | CLA  | C1C-C2C | -2.07 | 1.40        | 1.44     |
| 38  | F     | 101 | HEM  | C3B-C4B | 2.07  | 1.49        | 1.44     |
| 38  | f     | 101 | HEM  | C3B-C4B | 2.07  | 1.49        | 1.44     |
| 25  | R     | 609 | CLA  | C1C-C2C | -2.07 | 1.40        | 1.44     |
| 25  | c     | 512 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 25  | A     | 402 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 25  | a     | 403 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 25  | N     | 602 | CLA  | C1C-C2C | -2.07 | 1.40        | 1.44     |
| 25  | n     | 602 | CLA  | C1C-C2C | -2.07 | 1.40        | 1.44     |
| 24  | 2     | 601 | CHL  | O1D-CGD | 2.06  | 1.26        | 1.21     |
| 24  | 6     | 601 | CHL  | O1D-CGD | 2.06  | 1.26        | 1.21     |
| 25  | g     | 613 | CLA  | CHD-C1D | -2.06 | 1.34        | 1.38     |
| 25  | r     | 612 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 25  | G     | 613 | CLA  | CHD-C1D | -2.06 | 1.34        | 1.38     |
| 24  | N     | 607 | CHL  | C1B-NB  | 2.06  | 1.37        | 1.35     |
| 25  | y     | 311 | CLA  | C1C-C2C | -2.06 | 1.40        | 1.44     |
| 25  | Y     | 311 | CLA  | C1C-C2C | -2.06 | 1.40        | 1.44     |
| 25  | R     | 604 | CLA  | C1C-C2C | -2.06 | 1.40        | 1.44     |
| 24  | G     | 609 | CHL  | O1D-CGD | 2.06  | 1.26        | 1.21     |
| 25  | S     | 310 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |
| 25  | s     | 310 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |
| 25  | B     | 606 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |
| 25  | b     | 606 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |
| 25  | C     | 509 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | c     | 509 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | s     | 313 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | Y     | 304 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | c     | 501 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | y     | 304 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 24  | G     | 608 | CHL  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 24  | g     | 608 | CHL  | O1D-CGD | 2.05  | 1.26        | 1.21     |
| 24  | l     | 301 | CHL  | O1D-CGD | 2.05  | 1.26        | 1.21     |
| 24  | S     | 308 | CHL  | O1D-CGD | 2.05  | 1.26        | 1.21     |
| 25  | r     | 612 | CLA  | C1C-C2C | -2.05 | 1.40        | 1.44     |
| 24  | G     | 605 | CHL  | O1D-CGD | 2.05  | 1.26        | 1.21     |
| 24  | Y     | 309 | CHL  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 25  | R     | 603 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | r     | 603 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | R     | 610 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 24  | Y     | 302 | CHL  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 24  | g     | 605 | CHL  | O1D-CGD | 2.05  | 1.26        | 1.21     |
| 24  | R     | 613 | CHL  | O1D-CGD | 2.04  | 1.26        | 1.21     |
| 24  | R     | 607 | CHL  | O1D-CGD | 2.04  | 1.26        | 1.21     |
| 24  | r     | 607 | CHL  | O1D-CGD | 2.04  | 1.26        | 1.21     |
| 24  | Y     | 306 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 24  | y     | 306 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 24  | Y     | 307 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 39  | Y     | 317 | LUT  | C1-C6   | 2.04  | 1.56        | 1.53     |
| 25  | s     | 312 | CLA  | C1C-C2C | -2.04 | 1.40        | 1.44     |
| 25  | n     | 604 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 39  | S     | 316 | LUT  | C1-C6   | 2.04  | 1.56        | 1.53     |
| 24  | g     | 601 | CHL  | O1D-CGD | 2.04  | 1.26        | 1.21     |
| 25  | b     | 612 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 24  | y     | 310 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 24  | G     | 607 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 25  | s     | 313 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 24  | g     | 605 | CHL  | C1B-NB  | 2.04  | 1.37        | 1.35     |
| 32  | g     | 618 | AJP  | C05-C06 | 2.04  | 1.57        | 1.53     |
| 24  | R     | 607 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 24  | r     | 607 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 24  | r     | 613 | CHL  | O1D-CGD | 2.04  | 1.26        | 1.21     |
| 24  | n     | 606 | CHL  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 25  | D     | 402 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 25  | d     | 402 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 25  | D     | 401 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | d     | 401 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 24  | l     | 302 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |
| 24  | 5     | 302 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | R     | 605 | CHL  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 24  | n     | 606 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |
| 25  | C     | 512 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | B     | 604 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | C     | 510 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | S     | 314 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | B     | 612 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 24  | s     | 308 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |
| 25  | G     | 612 | CLA  | C1C-C2C | -2.03 | 1.40        | 1.44     |
| 25  | A     | 405 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | a     | 406 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 24  | y     | 310 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |
| 24  | 6     | 601 | CHL  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 24  | S     | 306 | CHL  | C1B-NB  | 2.03  | 1.37        | 1.35     |
| 24  | G     | 601 | CHL  | O1D-CGD | 2.03  | 1.26        | 1.21     |
| 24  | n     | 607 | CHL  | C1B-NB  | 2.02  | 1.37        | 1.35     |
| 24  | G     | 608 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 24  | S     | 308 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | s     | 308 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 25  | B     | 601 | CLA  | C1C-C2C | -2.02 | 1.40        | 1.44     |
| 24  | R     | 605 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 24  | 5     | 301 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 24  | r     | 605 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 24  | y     | 307 | CHL  | C4C-C3C | -2.02 | 1.41        | 1.45     |
| 25  | g     | 611 | CLA  | CHD-C1D | -2.02 | 1.34        | 1.38     |
| 25  | 2     | 602 | CLA  | CHC-C1C | 2.02  | 1.40        | 1.35     |
| 25  | 6     | 602 | CLA  | CHC-C1C | 2.02  | 1.40        | 1.35     |
| 25  | c     | 510 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 24  | s     | 306 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 39  | N     | 616 | LUT  | C26-C27 | 2.02  | 1.53        | 1.50     |
| 39  | n     | 616 | LUT  | C26-C27 | 2.02  | 1.53        | 1.50     |
| 24  | n     | 601 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 39  | Y     | 317 | LUT  | C26-C27 | 2.02  | 1.53        | 1.50     |
| 25  | r     | 604 | CLA  | C1C-C2C | -2.02 | 1.40        | 1.44     |
| 25  | 2     | 604 | CLA  | C4C-C3C | -2.02 | 1.41        | 1.45     |
| 25  | 6     | 604 | CLA  | C4C-C3C | -2.02 | 1.41        | 1.45     |
| 24  | s     | 302 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | N     | 605 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 38  | f     | 101 | HEM  | CHA-C4D | 2.02  | 1.40        | 1.35     |
| 24  | S     | 307 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | s     | 307 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 25  | r     | 610 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | N     | 604 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 25  | n     | 610 | CLA  | C1C-C2C | -2.02 | 1.40        | 1.44     |
| 24  | s     | 306 | CHL  | C1B-NB  | 2.02  | 1.37        | 1.35     |
| 24  | N     | 605 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | n     | 605 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 40  | y     | 318 | NEX  | C35-C15 | 2.02  | 1.41        | 1.36     |
| 40  | r     | 617 | NEX  | C31-C32 | 2.02  | 1.39        | 1.34     |
| 24  | n     | 609 | CHL  | O1D-CGD | 2.02  | 1.26        | 1.21     |
| 24  | y     | 309 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | G     | 609 | CHL  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 24  | N     | 606 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 25  | R     | 612 | CLA  | C1C-C2C | -2.01 | 1.40        | 1.44     |
| 39  | y     | 317 | LUT  | C1-C6   | 2.01  | 1.56        | 1.53     |
| 25  | N     | 610 | CLA  | CHD-C1D | -2.01 | 1.34        | 1.38     |
| 24  | 2     | 601 | CHL  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 24  | 6     | 601 | CHL  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 28  | T     | 101 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 25  | A     | 401 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 25  | a     | 402 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 24  | S     | 306 | CHL  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 24  | N     | 601 | CHL  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 24  | s     | 306 | CHL  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 24  | S     | 306 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 24  | Y     | 306 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 24  | y     | 306 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 25  | B     | 608 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 25  | S     | 303 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 25  | b     | 608 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 28  | t     | 101 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 24  | N     | 601 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 24  | s     | 307 | CHL  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 25  | c     | 513 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 39  | G     | 615 | LUT  | C26-C27 | 2.01  | 1.53        | 1.50     |
| 25  | R     | 601 | CLA  | C1C-C2C | -2.01 | 1.40        | 1.44     |
| 25  | r     | 601 | CLA  | C1C-C2C | -2.01 | 1.40        | 1.44     |
| 24  | S     | 308 | CHL  | C1B-NB  | 2.01  | 1.37        | 1.35     |
| 24  | s     | 308 | CHL  | C1B-NB  | 2.01  | 1.37        | 1.35     |
| 39  | s     | 316 | LUT  | C1-C6   | 2.01  | 1.56        | 1.53     |
| 24  | r     | 613 | CHL  | C1B-NB  | 2.01  | 1.37        | 1.35     |
| 25  | N     | 611 | CLA  | C1C-C2C | -2.01 | 1.40        | 1.44     |
| 25  | n     | 611 | CLA  | C1C-C2C | -2.01 | 1.40        | 1.44     |
| 25  | s     | 314 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | l     | 301 | CHL  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 24  | Y     | 302 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 24  | g     | 609 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 24  | n     | 601 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 25  | g     | 611 | CLA  | C1C-C2C | -2.00 | 1.40        | 1.44     |
| 24  | G     | 601 | CHL  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 24  | g     | 608 | CHL  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 24  | S     | 302 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 24  | s     | 302 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 32  | G     | 618 | AJP  | C05-C06 | 2.00  | 1.57        | 1.53     |
| 25  | C     | 513 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 24  | y     | 308 | CHL  | C1B-NB  | 2.00  | 1.37        | 1.35     |
| 24  | y     | 302 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 25  | R     | 604 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 24  | N     | 606 | CHL  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 25  | S     | 304 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 25  | c     | 502 | CLA  | C1B-CHB | -2.00 | 1.35        | 1.41     |
| 24  | R     | 606 | CHL  | O1D-CGD | 2.00  | 1.26        | 1.21     |
| 24  | y     | 302 | CHL  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 25  | N     | 603 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 25  | n     | 603 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |

All (4837) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 25  | s     | 305 | CLA  | C4A-NA-C1A  | -18.81 | 98.25       | 106.71   |
| 25  | S     | 305 | CLA  | C4A-NA-C1A  | -18.75 | 98.28       | 106.71   |
| 25  | r     | 601 | CLA  | C4A-NA-C1A  | -17.30 | 98.93       | 106.71   |
| 32  | Y     | 320 | AJP  | O09-C08-C10 | 17.23  | 145.62      | 110.17   |
| 32  | y     | 320 | AJP  | O09-C08-C10 | 17.23  | 145.62      | 110.17   |
| 25  | R     | 601 | CLA  | C4A-NA-C1A  | -17.14 | 99.00       | 106.71   |
| 32  | N     | 620 | AJP  | O09-C08-C10 | 16.48  | 144.09      | 110.17   |
| 32  | n     | 620 | AJP  | O09-C08-C10 | 16.48  | 144.09      | 110.17   |
| 25  | R     | 610 | CLA  | C4A-NA-C1A  | -16.34 | 99.36       | 106.71   |
| 25  | r     | 610 | CLA  | C4A-NA-C1A  | -16.34 | 99.36       | 106.71   |
| 25  | D     | 403 | CLA  | C4A-NA-C1A  | -16.26 | 99.40       | 106.71   |
| 25  | d     | 403 | CLA  | C4A-NA-C1A  | -16.26 | 99.40       | 106.71   |
| 25  | R     | 611 | CLA  | C4A-NA-C1A  | -16.04 | 99.50       | 106.71   |
| 25  | r     | 611 | CLA  | C4A-NA-C1A  | -16.04 | 99.50       | 106.71   |
| 32  | G     | 618 | AJP  | O09-C08-C10 | 16.03  | 143.15      | 110.17   |
| 32  | g     | 618 | AJP  | O09-C08-C10 | 16.03  | 143.15      | 110.17   |
| 32  | S     | 319 | AJP  | O09-C08-C10 | 15.97  | 143.04      | 110.17   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 32  | s     | 319 | AJP  | O09-C08-C10 | 15.95  | 142.99      | 110.17   |
| 32  | N     | 619 | AJP  | O09-C08-C10 | 15.92  | 142.93      | 110.17   |
| 32  | n     | 619 | AJP  | O09-C08-C10 | 15.91  | 142.91      | 110.17   |
| 32  | y     | 323 | AJP  | O09-C08-C10 | 15.74  | 142.56      | 110.17   |
| 32  | Y     | 323 | AJP  | O09-C08-C10 | 15.72  | 142.53      | 110.17   |
| 32  | Y     | 323 | AJP  | O84-C05-C04 | 15.68  | 125.34      | 110.77   |
| 32  | y     | 323 | AJP  | O84-C05-C04 | 15.64  | 125.31      | 110.77   |
| 25  | r     | 603 | CLA  | C4A-NA-C1A  | -15.47 | 99.75       | 106.71   |
| 25  | R     | 603 | CLA  | C4A-NA-C1A  | -15.35 | 99.80       | 106.71   |
| 32  | Y     | 321 | AJP  | O09-C08-C10 | 15.30  | 141.66      | 110.17   |
| 32  | y     | 321 | AJP  | O09-C08-C10 | 15.28  | 141.61      | 110.17   |
| 32  | Y     | 322 | AJP  | O09-C08-C10 | 15.19  | 141.42      | 110.17   |
| 32  | y     | 322 | AJP  | O09-C08-C10 | 15.17  | 141.38      | 110.17   |
| 32  | A     | 412 | AJP  | O84-C05-C04 | 15.12  | 124.82      | 110.77   |
| 32  | a     | 413 | AJP  | O84-C05-C04 | 15.12  | 124.82      | 110.77   |
| 25  | c     | 504 | CLA  | C4A-NA-C1A  | -15.03 | 99.95       | 106.71   |
| 32  | Y     | 324 | AJP  | O09-C08-C10 | 15.01  | 141.06      | 110.17   |
| 32  | y     | 324 | AJP  | O09-C08-C10 | 15.00  | 141.03      | 110.17   |
| 25  | C     | 504 | CLA  | C4A-NA-C1A  | -14.98 | 99.97       | 106.71   |
| 32  | g     | 618 | AJP  | C80-C20-C15 | -14.94 | 90.60       | 111.18   |
| 32  | G     | 618 | AJP  | C80-C20-C15 | -14.93 | 90.61       | 111.18   |
| 32  | A     | 412 | AJP  | O09-C08-C10 | 14.68  | 140.38      | 110.17   |
| 32  | a     | 413 | AJP  | O09-C08-C10 | 14.66  | 140.34      | 110.17   |
| 32  | B     | 624 | AJP  | O09-C08-C10 | 14.58  | 140.17      | 110.17   |
| 32  | b     | 624 | AJP  | O09-C08-C10 | 14.58  | 140.17      | 110.17   |
| 32  | G     | 618 | AJP  | C80-C20-C21 | -14.47 | 87.00       | 108.97   |
| 32  | g     | 618 | AJP  | C80-C20-C21 | -14.47 | 87.00       | 108.97   |
| 32  | y     | 324 | AJP  | O84-C05-C04 | 14.39  | 124.15      | 110.77   |
| 32  | Y     | 324 | AJP  | O84-C05-C04 | 14.39  | 124.14      | 110.77   |
| 25  | C     | 501 | CLA  | C4A-NA-C1A  | -14.34 | 100.26      | 106.71   |
| 25  | c     | 501 | CLA  | C4A-NA-C1A  | -14.34 | 100.26      | 106.71   |
| 32  | Y     | 321 | AJP  | O84-C05-C04 | 13.89  | 123.68      | 110.77   |
| 32  | y     | 321 | AJP  | O84-C05-C04 | 13.89  | 123.68      | 110.77   |
| 32  | y     | 322 | AJP  | O84-C05-C04 | 13.80  | 123.60      | 110.77   |
| 32  | Y     | 322 | AJP  | O84-C05-C04 | 13.75  | 123.55      | 110.77   |
| 32  | B     | 624 | AJP  | O84-C05-C04 | 13.35  | 123.18      | 110.77   |
| 32  | b     | 624 | AJP  | O84-C05-C04 | 13.35  | 123.18      | 110.77   |
| 32  | g     | 618 | AJP  | O84-C05-C04 | 12.72  | 122.59      | 110.77   |
| 32  | G     | 618 | AJP  | O84-C05-C04 | 12.71  | 122.59      | 110.77   |
| 32  | G     | 618 | AJP  | C80-C20-C19 | -11.92 | 90.14       | 110.36   |
| 32  | g     | 618 | AJP  | C80-C20-C19 | -11.91 | 90.15       | 110.36   |
| 32  | Y     | 323 | AJP  | O09-C05-C04 | -11.89 | 81.05       | 108.60   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 32  | y     | 323 | AJP  | O09-C05-C04 | -11.89 | 81.05       | 108.60   |
| 24  | 6     | 601 | CHL  | C4A-NA-C1A  | 11.88  | 112.05      | 106.71   |
| 32  | S     | 319 | AJP  | O84-C05-C04 | 11.87  | 121.81      | 110.77   |
| 32  | s     | 319 | AJP  | O84-C05-C04 | 11.87  | 121.81      | 110.77   |
| 24  | 2     | 601 | CHL  | C4A-NA-C1A  | 11.81  | 112.02      | 106.71   |
| 32  | A     | 412 | AJP  | O09-C05-C04 | -11.66 | 81.58       | 108.60   |
| 32  | a     | 413 | AJP  | O09-C05-C04 | -11.66 | 81.58       | 108.60   |
| 32  | y     | 324 | AJP  | O09-C05-C04 | -11.60 | 81.71       | 108.60   |
| 25  | C     | 511 | CLA  | C4A-NA-C1A  | -11.60 | 101.49      | 106.71   |
| 32  | Y     | 324 | AJP  | O09-C05-C04 | -11.58 | 81.76       | 108.60   |
| 32  | y     | 321 | AJP  | C24-C23-C22 | 11.53  | 123.23      | 111.00   |
| 32  | Y     | 321 | AJP  | C24-C23-C22 | 11.51  | 123.21      | 111.00   |
| 32  | Y     | 323 | AJP  | C24-C23-C22 | 11.50  | 123.19      | 111.00   |
| 25  | c     | 511 | CLA  | C4A-NA-C1A  | -11.48 | 101.54      | 106.71   |
| 32  | y     | 323 | AJP  | C24-C23-C22 | 11.47  | 123.17      | 111.00   |
| 32  | y     | 321 | AJP  | O09-C05-C04 | -11.46 | 82.04       | 108.60   |
| 32  | Y     | 321 | AJP  | O09-C05-C04 | -11.44 | 82.08       | 108.60   |
| 32  | B     | 624 | AJP  | C24-C23-C22 | 11.34  | 123.03      | 111.00   |
| 32  | b     | 624 | AJP  | C24-C23-C22 | 11.34  | 123.03      | 111.00   |
| 32  | N     | 619 | AJP  | O84-C05-C04 | 11.27  | 121.25      | 110.77   |
| 32  | n     | 619 | AJP  | O84-C05-C04 | 11.27  | 121.25      | 110.77   |
| 32  | Y     | 322 | AJP  | O09-C05-C04 | -11.19 | 82.67       | 108.60   |
| 32  | y     | 322 | AJP  | O09-C05-C04 | -11.18 | 82.68       | 108.60   |
| 32  | n     | 619 | AJP  | O09-C05-C04 | -11.17 | 82.72       | 108.60   |
| 32  | N     | 619 | AJP  | O09-C05-C04 | -11.17 | 82.72       | 108.60   |
| 32  | S     | 319 | AJP  | O09-C05-C04 | -11.10 | 82.88       | 108.60   |
| 32  | s     | 319 | AJP  | O09-C05-C04 | -11.10 | 82.88       | 108.60   |
| 32  | N     | 620 | AJP  | O84-C05-C04 | 11.08  | 121.07      | 110.77   |
| 32  | n     | 620 | AJP  | O84-C05-C04 | 11.08  | 121.07      | 110.77   |
| 32  | G     | 618 | AJP  | C21-C20-C19 | 10.99  | 119.53      | 107.14   |
| 32  | g     | 618 | AJP  | C21-C20-C19 | 10.99  | 119.53      | 107.14   |
| 24  | r     | 605 | CHL  | C4A-NA-C1A  | 10.70  | 111.52      | 106.71   |
| 24  | s     | 308 | CHL  | C4A-NA-C1A  | 10.67  | 111.50      | 106.71   |
| 24  | R     | 605 | CHL  | C4A-NA-C1A  | 10.66  | 111.50      | 106.71   |
| 25  | S     | 313 | CLA  | C4A-NA-C1A  | -10.66 | 101.92      | 106.71   |
| 25  | s     | 313 | CLA  | C4A-NA-C1A  | -10.66 | 101.92      | 106.71   |
| 24  | S     | 308 | CHL  | C4A-NA-C1A  | 10.63  | 111.48      | 106.71   |
| 32  | B     | 624 | AJP  | O09-C05-C04 | -10.63 | 83.97       | 108.60   |
| 32  | b     | 624 | AJP  | O09-C05-C04 | -10.63 | 83.97       | 108.60   |
| 32  | A     | 412 | AJP  | C24-C23-C22 | 10.62  | 122.27      | 111.00   |
| 32  | a     | 413 | AJP  | C24-C23-C22 | 10.59  | 122.23      | 111.00   |
| 32  | Y     | 320 | AJP  | O09-C05-C04 | -10.58 | 84.07       | 108.60   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 32  | y     | 320 | AJP  | O09-C05-C04 | -10.58 | 84.07       | 108.60   |
| 32  | S     | 319 | AJP  | C24-C23-C22 | 10.51  | 122.14      | 111.00   |
| 32  | s     | 319 | AJP  | C24-C23-C22 | 10.51  | 122.14      | 111.00   |
| 24  | S     | 307 | CHL  | C4A-NA-C1A  | 10.35  | 111.36      | 106.71   |
| 32  | G     | 618 | AJP  | O09-C05-C04 | -10.33 | 84.66       | 108.60   |
| 32  | g     | 618 | AJP  | O09-C05-C04 | -10.33 | 84.66       | 108.60   |
| 24  | g     | 609 | CHL  | C4A-NA-C1A  | 10.31  | 111.34      | 106.71   |
| 24  | g     | 606 | CHL  | C4A-NA-C1A  | 10.27  | 111.32      | 106.71   |
| 24  | s     | 307 | CHL  | C4A-NA-C1A  | 10.26  | 111.32      | 106.71   |
| 25  | 2     | 602 | CLA  | C4A-NA-C1A  | 10.25  | 111.31      | 106.71   |
| 25  | 6     | 602 | CLA  | C4A-NA-C1A  | 10.25  | 111.31      | 106.71   |
| 32  | n     | 620 | AJP  | O09-C05-C04 | -10.20 | 84.96       | 108.60   |
| 24  | G     | 606 | CHL  | C4A-NA-C1A  | 10.19  | 111.29      | 106.71   |
| 24  | G     | 609 | CHL  | C4A-NA-C1A  | 10.18  | 111.28      | 106.71   |
| 32  | N     | 620 | AJP  | O09-C05-C04 | -10.18 | 85.02       | 108.60   |
| 24  | R     | 607 | CHL  | C4A-NA-C1A  | 10.16  | 111.28      | 106.71   |
| 24  | S     | 306 | CHL  | C4A-NA-C1A  | 10.11  | 111.25      | 106.71   |
| 24  | s     | 306 | CHL  | C4A-NA-C1A  | 10.11  | 111.25      | 106.71   |
| 24  | 1     | 302 | CHL  | C4A-NA-C1A  | 10.09  | 111.24      | 106.71   |
| 24  | 5     | 302 | CHL  | C4A-NA-C1A  | 10.09  | 111.24      | 106.71   |
| 24  | r     | 607 | CHL  | C4A-NA-C1A  | 10.08  | 111.24      | 106.71   |
| 25  | S     | 311 | CLA  | C4A-NA-C1A  | -10.06 | 102.18      | 106.71   |
| 25  | s     | 311 | CLA  | C4A-NA-C1A  | -10.06 | 102.18      | 106.71   |
| 24  | 6     | 603 | CHL  | C4A-NA-C1A  | 10.04  | 111.22      | 106.71   |
| 32  | A     | 412 | AJP  | O84-C05-O09 | -9.97  | 81.99       | 109.78   |
| 32  | a     | 413 | AJP  | O84-C05-O09 | -9.97  | 81.99       | 109.78   |
| 24  | 2     | 603 | CHL  | C4A-NA-C1A  | 9.97   | 111.19      | 106.71   |
| 32  | g     | 618 | AJP  | C24-C23-C22 | 9.92   | 121.52      | 111.00   |
| 24  | n     | 606 | CHL  | C4A-NA-C1A  | 9.88   | 111.15      | 106.71   |
| 32  | y     | 320 | AJP  | C03-C02-C85 | 9.88   | 122.28      | 108.56   |
| 32  | G     | 618 | AJP  | C24-C23-C22 | 9.87   | 121.47      | 111.00   |
| 32  | Y     | 320 | AJP  | C03-C02-C85 | 9.86   | 122.26      | 108.56   |
| 24  | R     | 613 | CHL  | C4A-NA-C1A  | 9.86   | 111.14      | 106.71   |
| 24  | r     | 613 | CHL  | C4A-NA-C1A  | 9.86   | 111.14      | 106.71   |
| 32  | Y     | 322 | AJP  | O84-C05-O09 | -9.83  | 82.38       | 109.78   |
| 32  | y     | 322 | AJP  | O84-C05-O09 | -9.83  | 82.39       | 109.78   |
| 32  | Y     | 324 | AJP  | O84-C05-O09 | -9.81  | 82.44       | 109.78   |
| 32  | y     | 324 | AJP  | O84-C05-O09 | -9.80  | 82.46       | 109.78   |
| 24  | N     | 606 | CHL  | C4A-NA-C1A  | 9.78   | 111.10      | 106.71   |
| 32  | B     | 624 | AJP  | O84-C05-O09 | -9.77  | 82.55       | 109.78   |
| 32  | b     | 624 | AJP  | O84-C05-O09 | -9.77  | 82.55       | 109.78   |
| 32  | g     | 618 | AJP  | O84-C05-O09 | -9.71  | 82.73       | 109.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | G     | 618 | AJP  | O84-C05-O09 | -9.70 | 82.74       | 109.78   |
| 24  | Y     | 302 | CHL  | C4A-NA-C1A  | 9.67  | 111.05      | 106.71   |
| 24  | y     | 302 | CHL  | C4A-NA-C1A  | 9.67  | 111.05      | 106.71   |
| 24  | N     | 605 | CHL  | C4A-NA-C1A  | 9.64  | 111.04      | 106.71   |
| 24  | G     | 608 | CHL  | C4A-NA-C1A  | 9.60  | 111.02      | 106.71   |
| 24  | Y     | 306 | CHL  | C4A-NA-C1A  | 9.60  | 111.02      | 106.71   |
| 40  | r     | 617 | NEX  | C15-C14-C13 | -9.59 | 113.62      | 127.31   |
| 40  | R     | 617 | NEX  | C15-C14-C13 | -9.59 | 113.63      | 127.31   |
| 24  | n     | 605 | CHL  | C4A-NA-C1A  | 9.58  | 111.01      | 106.71   |
| 24  | y     | 306 | CHL  | C4A-NA-C1A  | 9.58  | 111.01      | 106.71   |
| 24  | n     | 608 | CHL  | C4A-NA-C1A  | 9.57  | 111.01      | 106.71   |
| 24  | S     | 302 | CHL  | C4A-NA-C1A  | 9.56  | 111.00      | 106.71   |
| 24  | s     | 302 | CHL  | C4A-NA-C1A  | 9.56  | 111.00      | 106.71   |
| 24  | N     | 608 | CHL  | C4A-NA-C1A  | 9.55  | 111.00      | 106.71   |
| 32  | N     | 620 | AJP  | C26-O31-C30 | 9.55  | 123.71      | 113.13   |
| 32  | n     | 620 | AJP  | C26-O31-C30 | 9.55  | 123.71      | 113.13   |
| 25  | R     | 611 | CLA  | C4D-CHA-C1A | -9.54 | 109.64      | 121.25   |
| 25  | r     | 611 | CLA  | C4D-CHA-C1A | -9.54 | 109.64      | 121.25   |
| 24  | g     | 608 | CHL  | C4A-NA-C1A  | 9.50  | 110.97      | 106.71   |
| 32  | Y     | 323 | AJP  | C26-O31-C30 | 9.48  | 123.63      | 113.13   |
| 32  | y     | 323 | AJP  | C26-O31-C30 | 9.48  | 123.63      | 113.13   |
| 24  | 5     | 301 | CHL  | C4A-NA-C1A  | 9.47  | 110.96      | 106.71   |
| 24  | g     | 605 | CHL  | C4A-NA-C1A  | 9.46  | 110.96      | 106.71   |
| 24  | l     | 301 | CHL  | C4A-NA-C1A  | 9.38  | 110.92      | 106.71   |
| 24  | G     | 605 | CHL  | C4A-NA-C1A  | 9.37  | 110.92      | 106.71   |
| 40  | S     | 317 | NEX  | O24-C25-C24 | 9.29  | 120.36      | 113.38   |
| 40  | s     | 317 | NEX  | O24-C25-C24 | 9.27  | 120.34      | 113.38   |
| 24  | R     | 606 | CHL  | C4A-NA-C1A  | 9.21  | 110.85      | 106.71   |
| 32  | y     | 324 | AJP  | C03-C02-C85 | 9.20  | 121.33      | 108.56   |
| 32  | Y     | 324 | AJP  | C03-C02-C85 | 9.18  | 121.31      | 108.56   |
| 24  | y     | 308 | CHL  | C4A-NA-C1A  | 9.18  | 110.83      | 106.71   |
| 32  | Y     | 320 | AJP  | O31-C30-C32 | 9.17  | 121.53      | 106.83   |
| 32  | y     | 320 | AJP  | O31-C30-C32 | 9.16  | 121.53      | 106.83   |
| 25  | N     | 614 | CLA  | C4A-NA-C1A  | -9.15 | 102.59      | 106.71   |
| 24  | r     | 606 | CHL  | C4A-NA-C1A  | 9.13  | 110.81      | 106.71   |
| 24  | Y     | 308 | CHL  | C4A-NA-C1A  | 9.12  | 110.81      | 106.71   |
| 25  | g     | 610 | CLA  | C4A-NA-C1A  | -9.09 | 102.62      | 106.71   |
| 32  | Y     | 321 | AJP  | O84-C05-O09 | -9.08 | 84.48       | 109.78   |
| 32  | y     | 321 | AJP  | O84-C05-O09 | -9.07 | 84.49       | 109.78   |
| 32  | Y     | 320 | AJP  | O84-C05-C04 | 9.04  | 119.17      | 110.77   |
| 32  | y     | 320 | AJP  | O84-C05-C04 | 9.04  | 119.17      | 110.77   |
| 32  | Y     | 324 | AJP  | C24-C23-C22 | 9.03  | 120.57      | 111.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | Y     | 309 | CHL  | C4A-NA-C1A  | 9.02  | 110.76      | 106.71   |
| 32  | y     | 324 | AJP  | C24-C23-C22 | 9.01  | 120.56      | 111.00   |
| 24  | G     | 601 | CHL  | C4A-NA-C1A  | 9.00  | 110.75      | 106.71   |
| 24  | g     | 601 | CHL  | C4A-NA-C1A  | 9.00  | 110.75      | 106.71   |
| 25  | G     | 610 | CLA  | C4A-NA-C1A  | -9.00 | 102.66      | 106.71   |
| 25  | n     | 614 | CLA  | C4A-NA-C1A  | -9.00 | 102.66      | 106.71   |
| 32  | y     | 323 | AJP  | O84-C05-O09 | -9.00 | 84.71       | 109.78   |
| 32  | Y     | 323 | AJP  | O84-C05-O09 | -8.99 | 84.73       | 109.78   |
| 32  | N     | 619 | AJP  | O84-C05-O09 | -8.96 | 84.81       | 109.78   |
| 32  | n     | 619 | AJP  | O84-C05-O09 | -8.95 | 84.84       | 109.78   |
| 32  | S     | 319 | AJP  | O84-C05-O09 | -8.93 | 84.90       | 109.78   |
| 32  | s     | 319 | AJP  | O84-C05-O09 | -8.93 | 84.90       | 109.78   |
| 40  | g     | 617 | NEX  | C11-C10-C9  | -8.90 | 114.61      | 127.31   |
| 32  | n     | 620 | AJP  | O84-C05-O09 | -8.90 | 84.98       | 109.78   |
| 32  | N     | 620 | AJP  | O84-C05-O09 | -8.90 | 84.99       | 109.78   |
| 40  | n     | 617 | NEX  | O24-C25-C24 | 8.89  | 120.06      | 113.38   |
| 24  | N     | 607 | CHL  | C4A-NA-C1A  | 8.88  | 110.70      | 106.71   |
| 24  | y     | 309 | CHL  | C4A-NA-C1A  | 8.85  | 110.68      | 106.71   |
| 40  | N     | 617 | NEX  | O24-C25-C24 | 8.84  | 120.02      | 113.38   |
| 24  | n     | 607 | CHL  | C4A-NA-C1A  | 8.84  | 110.68      | 106.71   |
| 40  | G     | 617 | NEX  | O24-C25-C24 | 8.81  | 120.00      | 113.38   |
| 32  | Y     | 322 | AJP  | C24-C23-C22 | 8.77  | 120.31      | 111.00   |
| 32  | y     | 322 | AJP  | C24-C23-C22 | 8.77  | 120.31      | 111.00   |
| 40  | g     | 617 | NEX  | O24-C25-C24 | 8.77  | 119.97      | 113.38   |
| 40  | G     | 617 | NEX  | C11-C10-C9  | -8.74 | 114.84      | 127.31   |
| 32  | Y     | 324 | AJP  | C26-O31-C30 | 8.73  | 122.80      | 113.13   |
| 32  | y     | 324 | AJP  | C26-O31-C30 | 8.73  | 122.80      | 113.13   |
| 32  | N     | 620 | AJP  | C24-C23-C22 | 8.70  | 120.23      | 111.00   |
| 32  | n     | 620 | AJP  | C24-C23-C22 | 8.70  | 120.23      | 111.00   |
| 24  | y     | 310 | CHL  | C4A-NA-C1A  | 8.64  | 110.59      | 106.71   |
| 32  | g     | 618 | AJP  | C21-C20-C15 | 8.64  | 123.00      | 110.08   |
| 32  | G     | 618 | AJP  | C21-C20-C15 | 8.62  | 122.97      | 110.08   |
| 24  | Y     | 310 | CHL  | C4A-NA-C1A  | 8.62  | 110.58      | 106.71   |
| 32  | N     | 619 | AJP  | C24-C23-C22 | 8.44  | 119.95      | 111.00   |
| 32  | n     | 619 | AJP  | C24-C23-C22 | 8.44  | 119.95      | 111.00   |
| 25  | R     | 601 | CLA  | C1B-CHB-C4A | -8.42 | 113.44      | 130.12   |
| 25  | r     | 601 | CLA  | C1B-CHB-C4A | -8.38 | 113.52      | 130.12   |
| 32  | n     | 619 | AJP  | C03-C02-C85 | 8.36  | 120.17      | 108.56   |
| 32  | N     | 619 | AJP  | C03-C02-C85 | 8.35  | 120.16      | 108.56   |
| 24  | N     | 609 | CHL  | C4A-NA-C1A  | 8.16  | 110.37      | 106.71   |
| 24  | n     | 609 | CHL  | C4A-NA-C1A  | 8.14  | 110.37      | 106.71   |
| 32  | Y     | 322 | AJP  | C03-C02-C85 | 8.08  | 119.79      | 108.56   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 322 | AJP  | C03-C02-C85 | 8.06  | 119.75      | 108.56   |
| 25  | Y     | 314 | CLA  | C4A-NA-C1A  | -8.03 | 103.09      | 106.71   |
| 25  | y     | 314 | CLA  | C4A-NA-C1A  | -8.03 | 103.09      | 106.71   |
| 32  | s     | 319 | AJP  | C26-O25-C23 | 7.99  | 127.68      | 115.33   |
| 32  | S     | 319 | AJP  | C26-O25-C23 | 7.98  | 127.67      | 115.33   |
| 32  | b     | 624 | AJP  | C03-C02-C85 | 7.96  | 119.61      | 108.56   |
| 32  | s     | 319 | AJP  | C03-C02-C85 | 7.96  | 119.61      | 108.56   |
| 32  | Y     | 320 | AJP  | O84-C05-O09 | -7.94 | 87.64       | 109.78   |
| 32  | y     | 320 | AJP  | O84-C05-O09 | -7.94 | 87.64       | 109.78   |
| 32  | B     | 624 | AJP  | C03-C02-C85 | 7.94  | 119.58      | 108.56   |
| 32  | S     | 319 | AJP  | C03-C02-C85 | 7.92  | 119.57      | 108.56   |
| 25  | N     | 604 | CLA  | C4A-NA-C1A  | -7.88 | 103.16      | 106.71   |
| 24  | N     | 601 | CHL  | C4A-NA-C1A  | 7.87  | 110.24      | 106.71   |
| 40  | R     | 617 | NEX  | C35-C34-C33 | -7.86 | 116.10      | 127.31   |
| 40  | r     | 617 | NEX  | C35-C34-C33 | -7.86 | 116.10      | 127.31   |
| 25  | n     | 604 | CLA  | C4A-NA-C1A  | -7.80 | 103.20      | 106.71   |
| 24  | n     | 601 | CHL  | C4A-NA-C1A  | 7.78  | 110.20      | 106.71   |
| 32  | Y     | 321 | AJP  | C03-C02-C85 | 7.78  | 119.36      | 108.56   |
| 32  | y     | 321 | AJP  | C03-C02-C85 | 7.78  | 119.36      | 108.56   |
| 41  | R     | 616 | XAT  | O24-C25-C24 | 7.71  | 119.17      | 113.38   |
| 41  | r     | 616 | XAT  | O24-C25-C24 | 7.71  | 119.17      | 113.38   |
| 24  | G     | 607 | CHL  | C4A-NA-C1A  | 7.70  | 110.17      | 106.71   |
| 24  | g     | 607 | CHL  | C4A-NA-C1A  | 7.68  | 110.16      | 106.71   |
| 25  | g     | 613 | CLA  | C4A-NA-C1A  | -7.61 | 103.28      | 106.71   |
| 32  | n     | 620 | AJP  | O09-C05-C06 | -7.60 | 93.20       | 104.47   |
| 32  | N     | 620 | AJP  | O09-C05-C06 | -7.56 | 93.25       | 104.47   |
| 25  | S     | 305 | CLA  | C1B-CHB-C4A | -7.51 | 115.24      | 130.12   |
| 25  | B     | 606 | CLA  | CHD-C1D-ND  | -7.51 | 117.55      | 124.45   |
| 25  | b     | 606 | CLA  | CHD-C1D-ND  | -7.51 | 117.55      | 124.45   |
| 32  | a     | 413 | AJP  | O40-C39-C38 | 7.50  | 123.32      | 109.69   |
| 25  | s     | 305 | CLA  | C1B-CHB-C4A | -7.50 | 115.26      | 130.12   |
| 25  | G     | 613 | CLA  | C4A-NA-C1A  | -7.50 | 103.34      | 106.71   |
| 32  | A     | 412 | AJP  | O40-C39-C38 | 7.49  | 123.30      | 109.69   |
| 40  | R     | 617 | NEX  | O24-C25-C24 | 7.44  | 118.97      | 113.38   |
| 40  | r     | 617 | NEX  | O24-C25-C24 | 7.43  | 118.97      | 113.38   |
| 25  | r     | 612 | CLA  | CHD-C1D-ND  | -7.42 | 117.64      | 124.45   |
| 40  | y     | 318 | NEX  | C31-C30-C29 | -7.40 | 116.75      | 127.31   |
| 40  | Y     | 318 | NEX  | C31-C30-C29 | -7.40 | 116.75      | 127.31   |
| 25  | R     | 612 | CLA  | CHD-C1D-ND  | -7.36 | 117.69      | 124.45   |
| 25  | r     | 604 | CLA  | CHD-C1D-ND  | -7.36 | 117.69      | 124.45   |
| 25  | R     | 604 | CLA  | CHD-C1D-ND  | -7.35 | 117.70      | 124.45   |
| 25  | R     | 612 | CLA  | C4A-NA-C1A  | -7.29 | 103.43      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 324 | AJP  | C26-O25-C23 | 7.28  | 126.59      | 115.33   |
| 32  | y     | 324 | AJP  | C26-O25-C23 | 7.26  | 126.56      | 115.33   |
| 25  | B     | 601 | CLA  | CHD-C1D-ND  | -7.20 | 117.83      | 124.45   |
| 25  | S     | 304 | CLA  | C4A-NA-C1A  | -7.20 | 103.47      | 106.71   |
| 25  | s     | 304 | CLA  | C4A-NA-C1A  | -7.20 | 103.47      | 106.71   |
| 25  | D     | 403 | CLA  | C1B-CHB-C4A | -7.19 | 115.87      | 130.12   |
| 25  | d     | 403 | CLA  | C1B-CHB-C4A | -7.19 | 115.87      | 130.12   |
| 32  | Y     | 321 | AJP  | C12-C07-C08 | -7.19 | 97.11       | 104.88   |
| 32  | y     | 321 | AJP  | C12-C07-C08 | -7.19 | 97.11       | 104.88   |
| 25  | R     | 611 | CLA  | CHD-C1D-ND  | -7.19 | 117.85      | 124.45   |
| 25  | b     | 601 | CLA  | CHD-C1D-ND  | -7.18 | 117.86      | 124.45   |
| 25  | r     | 612 | CLA  | C4A-NA-C1A  | -7.18 | 103.48      | 106.71   |
| 25  | r     | 611 | CLA  | CHD-C1D-ND  | -7.17 | 117.86      | 124.45   |
| 40  | g     | 617 | NEX  | C27-C28-C29 | -7.13 | 114.47      | 125.53   |
| 25  | d     | 401 | CLA  | C4A-NA-C1A  | -7.11 | 103.51      | 106.71   |
| 25  | D     | 401 | CLA  | C4A-NA-C1A  | -7.10 | 103.51      | 106.71   |
| 27  | A     | 403 | PHO  | O2D-CGD-CBD | 7.10  | 119.99      | 111.00   |
| 27  | a     | 404 | PHO  | O2D-CGD-CBD | 7.10  | 119.99      | 111.00   |
| 27  | A     | 404 | PHO  | O2D-CGD-CBD | 7.10  | 119.99      | 111.00   |
| 32  | N     | 619 | AJP  | C26-O31-C30 | 7.09  | 120.98      | 113.13   |
| 32  | A     | 412 | AJP  | C03-C02-C85 | 7.09  | 118.40      | 108.56   |
| 32  | a     | 413 | AJP  | C03-C02-C85 | 7.09  | 118.40      | 108.56   |
| 40  | G     | 617 | NEX  | C27-C28-C29 | -7.06 | 114.57      | 125.53   |
| 27  | a     | 405 | PHO  | O2D-CGD-CBD | 7.06  | 119.94      | 111.00   |
| 40  | G     | 617 | NEX  | C31-C30-C29 | -7.05 | 117.25      | 127.31   |
| 32  | n     | 619 | AJP  | C26-O31-C30 | 7.03  | 120.92      | 113.13   |
| 25  | r     | 610 | CLA  | C1B-CHB-C4A | -7.01 | 116.24      | 130.12   |
| 25  | r     | 603 | CLA  | C1B-CHB-C4A | -6.99 | 116.27      | 130.12   |
| 25  | C     | 510 | CLA  | CHD-C1D-ND  | -6.99 | 118.03      | 124.45   |
| 25  | c     | 510 | CLA  | CHD-C1D-ND  | -6.99 | 118.03      | 124.45   |
| 40  | g     | 617 | NEX  | C31-C30-C29 | -6.98 | 117.34      | 127.31   |
| 25  | R     | 603 | CLA  | C1B-CHB-C4A | -6.98 | 116.30      | 130.12   |
| 25  | R     | 610 | CLA  | C1B-CHB-C4A | -6.98 | 116.31      | 130.12   |
| 32  | G     | 618 | AJP  | C03-C02-C85 | 6.96  | 118.22      | 108.56   |
| 32  | g     | 618 | AJP  | C03-C02-C85 | 6.95  | 118.21      | 108.56   |
| 32  | N     | 619 | AJP  | C26-O25-C23 | 6.93  | 126.05      | 115.33   |
| 32  | n     | 619 | AJP  | C26-O25-C23 | 6.93  | 126.05      | 115.33   |
| 32  | S     | 319 | AJP  | C29-C28-C27 | 6.90  | 120.71      | 110.69   |
| 32  | s     | 319 | AJP  | C29-C28-C27 | 6.90  | 120.71      | 110.69   |
| 25  | B     | 605 | CLA  | C4A-NA-C1A  | -6.83 | 103.63      | 106.71   |
| 25  | S     | 313 | CLA  | CHD-C1D-ND  | -6.83 | 118.18      | 124.45   |
| 25  | s     | 313 | CLA  | CHD-C1D-ND  | -6.83 | 118.18      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | c     | 508 | CLA  | CHD-C1D-ND  | -6.82 | 118.19      | 124.45   |
| 25  | C     | 508 | CLA  | CHD-C1D-ND  | -6.72 | 118.28      | 124.45   |
| 25  | c     | 507 | CLA  | CHD-C1D-ND  | -6.72 | 118.28      | 124.45   |
| 25  | b     | 605 | CLA  | C4A-NA-C1A  | -6.69 | 103.70      | 106.71   |
| 25  | C     | 507 | CLA  | CHD-C1D-ND  | -6.69 | 118.31      | 124.45   |
| 25  | A     | 401 | CLA  | CHD-C1D-ND  | -6.68 | 118.32      | 124.45   |
| 25  | a     | 402 | CLA  | CHD-C1D-ND  | -6.68 | 118.32      | 124.45   |
| 25  | B     | 605 | CLA  | CHD-C1D-ND  | -6.67 | 118.32      | 124.45   |
| 25  | b     | 605 | CLA  | CHD-C1D-ND  | -6.67 | 118.32      | 124.45   |
| 25  | S     | 310 | CLA  | CHD-C1D-ND  | -6.67 | 118.33      | 124.45   |
| 25  | s     | 310 | CLA  | CHD-C1D-ND  | -6.66 | 118.33      | 124.45   |
| 41  | r     | 616 | XAT  | O4-C5-C4    | 6.65  | 118.38      | 113.38   |
| 41  | R     | 616 | XAT  | O4-C5-C4    | 6.63  | 118.36      | 113.38   |
| 25  | c     | 509 | CLA  | C4A-NA-C1A  | -6.63 | 103.72      | 106.71   |
| 25  | N     | 612 | CLA  | CHD-C1D-ND  | -6.62 | 118.37      | 124.45   |
| 25  | s     | 304 | CLA  | CHD-C1D-ND  | -6.60 | 118.39      | 124.45   |
| 25  | n     | 612 | CLA  | CHD-C1D-ND  | -6.59 | 118.40      | 124.45   |
| 32  | B     | 624 | AJP  | O50-C45-C46 | 6.58  | 120.14      | 110.04   |
| 32  | b     | 624 | AJP  | O50-C45-C46 | 6.58  | 120.14      | 110.04   |
| 25  | b     | 604 | CLA  | CHD-C1D-ND  | -6.58 | 118.41      | 124.45   |
| 25  | C     | 509 | CLA  | C4A-NA-C1A  | -6.58 | 103.75      | 106.71   |
| 25  | g     | 604 | CLA  | C4A-NA-C1A  | -6.55 | 103.76      | 106.71   |
| 25  | R     | 609 | CLA  | CHD-C1D-ND  | -6.55 | 118.44      | 124.45   |
| 32  | N     | 620 | AJP  | C03-C02-C85 | 6.54  | 117.65      | 108.56   |
| 25  | G     | 604 | CLA  | C4A-NA-C1A  | -6.53 | 103.77      | 106.71   |
| 25  | c     | 504 | CLA  | C1B-CHB-C4A | -6.53 | 117.19      | 130.12   |
| 25  | r     | 609 | CLA  | CHD-C1D-ND  | -6.53 | 118.45      | 124.45   |
| 25  | S     | 304 | CLA  | CHD-C1D-ND  | -6.52 | 118.46      | 124.45   |
| 25  | B     | 604 | CLA  | CHD-C1D-ND  | -6.51 | 118.47      | 124.45   |
| 32  | n     | 620 | AJP  | C03-C02-C85 | 6.51  | 117.60      | 108.56   |
| 25  | C     | 504 | CLA  | C1B-CHB-C4A | -6.50 | 117.24      | 130.12   |
| 25  | B     | 601 | CLA  | C4A-NA-C1A  | -6.48 | 103.79      | 106.71   |
| 25  | A     | 402 | CLA  | CHD-C1D-ND  | -6.45 | 118.52      | 124.45   |
| 25  | C     | 502 | CLA  | C4A-NA-C1A  | -6.44 | 103.81      | 106.71   |
| 25  | c     | 502 | CLA  | C4A-NA-C1A  | -6.44 | 103.81      | 106.71   |
| 25  | R     | 602 | CLA  | C4A-NA-C1A  | -6.44 | 103.81      | 106.71   |
| 25  | r     | 602 | CLA  | C4A-NA-C1A  | -6.44 | 103.81      | 106.71   |
| 25  | a     | 403 | CLA  | CHD-C1D-ND  | -6.43 | 118.55      | 124.45   |
| 40  | N     | 617 | NEX  | C15-C14-C13 | -6.42 | 118.14      | 127.31   |
| 25  | C     | 512 | CLA  | CHD-C1D-ND  | -6.41 | 118.56      | 124.45   |
| 40  | n     | 617 | NEX  | C15-C14-C13 | -6.40 | 118.17      | 127.31   |
| 25  | c     | 512 | CLA  | CHD-C1D-ND  | -6.40 | 118.57      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 601 | CLA  | C4A-NA-C1A  | -6.39 | 103.83      | 106.71   |
| 25  | c     | 503 | CLA  | CHD-C1D-ND  | -6.39 | 118.58      | 124.45   |
| 41  | R     | 616 | XAT  | C35-C34-C33 | -6.39 | 118.20      | 127.31   |
| 41  | r     | 616 | XAT  | C35-C34-C33 | -6.39 | 118.20      | 127.31   |
| 25  | B     | 614 | CLA  | C4A-NA-C1A  | -6.37 | 103.84      | 106.71   |
| 25  | 6     | 605 | CLA  | C4A-NA-C1A  | -6.37 | 103.84      | 106.71   |
| 25  | 2     | 605 | CLA  | C4A-NA-C1A  | -6.35 | 103.85      | 106.71   |
| 25  | b     | 614 | CLA  | C4A-NA-C1A  | -6.35 | 103.85      | 106.71   |
| 25  | C     | 503 | CLA  | CHD-C1D-ND  | -6.35 | 118.62      | 124.45   |
| 25  | R     | 611 | CLA  | C2D-C1D-ND  | -6.35 | 105.43      | 110.10   |
| 25  | S     | 311 | CLA  | CHD-C1D-ND  | -6.35 | 118.62      | 124.45   |
| 25  | c     | 508 | CLA  | C4A-NA-C1A  | -6.33 | 103.86      | 106.71   |
| 32  | G     | 618 | AJP  | C15-C20-C19 | 6.31  | 117.45      | 108.58   |
| 32  | g     | 618 | AJP  | C15-C20-C19 | 6.29  | 117.42      | 108.58   |
| 25  | C     | 508 | CLA  | C4A-NA-C1A  | -6.28 | 103.88      | 106.71   |
| 25  | s     | 311 | CLA  | CHD-C1D-ND  | -6.27 | 118.69      | 124.45   |
| 25  | r     | 611 | CLA  | C2D-C1D-ND  | -6.27 | 105.48      | 110.10   |
| 25  | n     | 613 | CLA  | C4A-NA-C1A  | -6.27 | 103.89      | 106.71   |
| 25  | A     | 405 | CLA  | CHD-C1D-ND  | -6.26 | 118.70      | 124.45   |
| 25  | N     | 613 | CLA  | C4A-NA-C1A  | -6.25 | 103.90      | 106.71   |
| 32  | Y     | 322 | AJP  | O25-C23-C24 | 6.24  | 121.69      | 109.62   |
| 32  | y     | 322 | AJP  | O25-C23-C24 | 6.24  | 121.69      | 109.62   |
| 25  | a     | 406 | CLA  | CHD-C1D-ND  | -6.24 | 118.72      | 124.45   |
| 32  | A     | 412 | AJP  | O53-C46-C45 | 6.24  | 125.19      | 110.05   |
| 32  | a     | 413 | AJP  | O53-C46-C45 | 6.24  | 125.19      | 110.05   |
| 25  | B     | 609 | CLA  | C4A-NA-C1A  | -6.23 | 103.90      | 106.71   |
| 25  | b     | 609 | CLA  | C4A-NA-C1A  | -6.23 | 103.90      | 106.71   |
| 25  | G     | 613 | CLA  | CHD-C1D-ND  | -6.19 | 118.77      | 124.45   |
| 32  | N     | 619 | AJP  | O25-C23-C24 | 6.15  | 121.51      | 109.62   |
| 32  | n     | 619 | AJP  | O25-C23-C24 | 6.15  | 121.51      | 109.62   |
| 25  | g     | 613 | CLA  | CHD-C1D-ND  | -6.15 | 118.81      | 124.45   |
| 25  | s     | 313 | CLA  | C1B-CHB-C4A | -6.14 | 117.96      | 130.12   |
| 25  | S     | 309 | CLA  | C4A-NA-C1A  | -6.14 | 103.95      | 106.71   |
| 25  | s     | 309 | CLA  | C4A-NA-C1A  | -6.12 | 103.95      | 106.71   |
| 25  | b     | 607 | CLA  | CHD-C1D-ND  | -6.11 | 118.83      | 124.45   |
| 25  | c     | 503 | CLA  | C4A-NA-C1A  | -6.11 | 103.96      | 106.71   |
| 25  | S     | 313 | CLA  | C1B-CHB-C4A | -6.11 | 118.02      | 130.12   |
| 25  | 2     | 602 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 25  | 6     | 602 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 25  | B     | 607 | CLA  | CHD-C1D-ND  | -6.07 | 118.88      | 124.45   |
| 32  | A     | 412 | AJP  | O70-C69-C68 | 6.07  | 120.71      | 109.69   |
| 32  | a     | 413 | AJP  | O70-C69-C68 | 6.07  | 120.71      | 109.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 503 | CLA  | C4A-NA-C1A  | -6.04 | 103.99      | 106.71   |
| 32  | Y     | 321 | AJP  | O31-C26-C27 | 6.04  | 123.13      | 110.35   |
| 32  | y     | 321 | AJP  | O31-C26-C27 | 6.03  | 123.11      | 110.35   |
| 25  | C     | 511 | CLA  | CHD-C1D-ND  | -6.02 | 118.92      | 124.45   |
| 25  | c     | 511 | CLA  | CHD-C1D-ND  | -6.02 | 118.92      | 124.45   |
| 32  | B     | 624 | AJP  | O74-C67-C68 | 6.01  | 124.25      | 110.35   |
| 32  | b     | 624 | AJP  | O74-C67-C68 | 6.01  | 124.25      | 110.35   |
| 32  | Y     | 320 | AJP  | C05-C06-C07 | 6.01  | 113.15      | 103.37   |
| 32  | y     | 320 | AJP  | C05-C06-C07 | 6.01  | 113.15      | 103.37   |
| 25  | N     | 613 | CLA  | CHD-C1D-ND  | -6.00 | 118.94      | 124.45   |
| 25  | n     | 613 | CLA  | CHD-C1D-ND  | -6.00 | 118.94      | 124.45   |
| 32  | G     | 618 | AJP  | C29-C28-C27 | 5.99  | 119.39      | 110.69   |
| 32  | G     | 618 | AJP  | C20-C15-C16 | -5.98 | 106.14      | 112.42   |
| 32  | g     | 618 | AJP  | C29-C28-C27 | 5.98  | 119.37      | 110.69   |
| 25  | C     | 501 | CLA  | C1B-CHB-C4A | -5.97 | 118.30      | 130.12   |
| 25  | c     | 501 | CLA  | C1B-CHB-C4A | -5.97 | 118.30      | 130.12   |
| 32  | Y     | 320 | AJP  | C03-C04-C05 | -5.96 | 101.63      | 111.93   |
| 32  | y     | 320 | AJP  | C03-C04-C05 | -5.96 | 101.63      | 111.93   |
| 32  | g     | 618 | AJP  | C20-C15-C16 | -5.95 | 106.17      | 112.42   |
| 32  | y     | 324 | AJP  | O25-C23-C24 | 5.93  | 121.09      | 109.62   |
| 32  | Y     | 320 | AJP  | C12-C07-C08 | -5.93 | 98.47       | 104.88   |
| 32  | y     | 320 | AJP  | C12-C07-C08 | -5.93 | 98.47       | 104.88   |
| 25  | D     | 401 | CLA  | CHD-C1D-ND  | -5.92 | 119.01      | 124.45   |
| 25  | R     | 608 | CLA  | CHD-C1D-ND  | -5.92 | 119.01      | 124.45   |
| 25  | d     | 401 | CLA  | CHD-C1D-ND  | -5.92 | 119.01      | 124.45   |
| 32  | Y     | 324 | AJP  | C12-C07-C08 | -5.92 | 98.48       | 104.88   |
| 32  | y     | 324 | AJP  | C12-C07-C08 | -5.92 | 98.48       | 104.88   |
| 32  | A     | 412 | AJP  | O60-C59-C58 | 5.92  | 120.44      | 109.69   |
| 25  | C     | 504 | CLA  | CHD-C1D-ND  | -5.91 | 119.02      | 124.45   |
| 32  | a     | 413 | AJP  | O60-C59-C58 | 5.91  | 120.43      | 109.69   |
| 32  | Y     | 324 | AJP  | O25-C23-C24 | 5.91  | 121.04      | 109.62   |
| 25  | c     | 505 | CLA  | CHD-C1D-ND  | -5.90 | 119.03      | 124.45   |
| 25  | 2     | 604 | CLA  | CHD-C1D-ND  | -5.90 | 119.03      | 124.45   |
| 25  | 6     | 604 | CLA  | CHD-C1D-ND  | -5.90 | 119.03      | 124.45   |
| 25  | c     | 504 | CLA  | CHD-C1D-ND  | -5.90 | 119.04      | 124.45   |
| 25  | r     | 608 | CLA  | CHD-C1D-ND  | -5.90 | 119.04      | 124.45   |
| 32  | a     | 413 | AJP  | O53-C46-C47 | 5.89  | 123.97      | 110.35   |
| 32  | A     | 412 | AJP  | O53-C46-C47 | 5.89  | 123.97      | 110.35   |
| 25  | c     | 513 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 25  | B     | 611 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 25  | b     | 611 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 25  | D     | 403 | CLA  | CHD-C1D-ND  | -5.87 | 119.06      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | R     | 602 | CLA  | CHD-C1D-ND  | -5.87 | 119.06      | 124.45   |
| 25  | d     | 403 | CLA  | CHD-C1D-ND  | -5.87 | 119.06      | 124.45   |
| 32  | A     | 412 | AJP  | O44-C45-C46 | 5.87  | 123.32      | 108.10   |
| 32  | a     | 413 | AJP  | O44-C45-C46 | 5.87  | 123.30      | 108.10   |
| 32  | Y     | 320 | AJP  | C28-C29-C30 | -5.86 | 101.12      | 111.22   |
| 32  | y     | 320 | AJP  | C28-C29-C30 | -5.86 | 101.12      | 111.22   |
| 25  | C     | 513 | CLA  | CHD-C1D-ND  | -5.86 | 119.07      | 124.45   |
| 25  | r     | 602 | CLA  | CHD-C1D-ND  | -5.85 | 119.07      | 124.45   |
| 32  | Y     | 323 | AJP  | O09-C05-C06 | -5.85 | 95.78       | 104.47   |
| 32  | y     | 323 | AJP  | O09-C05-C06 | -5.85 | 95.78       | 104.47   |
| 25  | C     | 505 | CLA  | CHD-C1D-ND  | -5.84 | 119.08      | 124.45   |
| 25  | b     | 603 | CLA  | CHD-C1D-ND  | -5.83 | 119.10      | 124.45   |
| 32  | N     | 619 | AJP  | O77-C28-C27 | 5.81  | 121.78      | 110.14   |
| 32  | n     | 619 | AJP  | O77-C28-C27 | 5.81  | 121.77      | 110.14   |
| 25  | S     | 303 | CLA  | CHD-C1D-ND  | -5.81 | 119.12      | 124.45   |
| 32  | g     | 618 | AJP  | O09-C05-C06 | -5.81 | 95.85       | 104.47   |
| 32  | G     | 618 | AJP  | O09-C05-C06 | -5.80 | 95.86       | 104.47   |
| 25  | B     | 611 | CLA  | C4A-NA-C1A  | -5.79 | 104.10      | 106.71   |
| 25  | b     | 611 | CLA  | C4A-NA-C1A  | -5.79 | 104.10      | 106.71   |
| 25  | N     | 604 | CLA  | CHD-C1D-ND  | -5.79 | 119.13      | 124.45   |
| 25  | n     | 604 | CLA  | CHD-C1D-ND  | -5.78 | 119.14      | 124.45   |
| 25  | B     | 603 | CLA  | CHD-C1D-ND  | -5.78 | 119.14      | 124.45   |
| 25  | R     | 603 | CLA  | CHD-C1D-ND  | -5.77 | 119.15      | 124.45   |
| 25  | s     | 303 | CLA  | CHD-C1D-ND  | -5.76 | 119.16      | 124.45   |
| 25  | 6     | 602 | CLA  | C4D-CHA-C1A | -5.76 | 114.24      | 121.25   |
| 32  | y     | 320 | AJP  | C29-C30-C32 | 5.74  | 122.69      | 112.60   |
| 32  | B     | 624 | AJP  | O73-C68-C69 | 5.74  | 123.56      | 109.30   |
| 32  | b     | 624 | AJP  | O73-C68-C69 | 5.74  | 123.56      | 109.30   |
| 25  | 2     | 602 | CLA  | C4D-CHA-C1A | -5.74 | 114.27      | 121.25   |
| 25  | C     | 501 | CLA  | CHD-C1D-ND  | -5.73 | 119.19      | 124.45   |
| 25  | c     | 501 | CLA  | CHD-C1D-ND  | -5.73 | 119.19      | 124.45   |
| 25  | b     | 612 | CLA  | CHD-C1D-ND  | -5.73 | 119.19      | 124.45   |
| 32  | Y     | 320 | AJP  | C29-C30-C32 | 5.72  | 122.65      | 112.60   |
| 25  | R     | 610 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 25  | B     | 614 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 25  | b     | 614 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 32  | Y     | 324 | AJP  | O77-C28-C27 | 5.72  | 121.59      | 110.14   |
| 32  | y     | 324 | AJP  | O77-C28-C27 | 5.72  | 121.59      | 110.14   |
| 25  | s     | 305 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 32  | A     | 412 | AJP  | O44-C45-O50 | 5.71  | 121.79      | 109.08   |
| 32  | N     | 620 | AJP  | C26-O25-C23 | 5.71  | 124.16      | 115.33   |
| 32  | n     | 620 | AJP  | C26-O25-C23 | 5.71  | 124.16      | 115.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | S     | 305 | CLA  | CHD-C1D-ND  | -5.70 | 119.21      | 124.45   |
| 25  | r     | 603 | CLA  | CHD-C1D-ND  | -5.70 | 119.22      | 124.45   |
| 32  | Y     | 320 | AJP  | C29-C28-C27 | 5.70  | 118.96      | 110.69   |
| 32  | y     | 320 | AJP  | C29-C28-C27 | 5.70  | 118.96      | 110.69   |
| 25  | r     | 610 | CLA  | CHD-C1D-ND  | -5.69 | 119.22      | 124.45   |
| 32  | a     | 413 | AJP  | C26-O25-C23 | 5.68  | 124.12      | 115.33   |
| 32  | a     | 413 | AJP  | O44-C45-O50 | 5.67  | 121.71      | 109.08   |
| 32  | Y     | 323 | AJP  | O77-C28-C27 | 5.67  | 121.50      | 110.14   |
| 32  | y     | 323 | AJP  | O77-C28-C27 | 5.67  | 121.50      | 110.14   |
| 32  | B     | 624 | AJP  | C27-C28-C29 | 5.67  | 122.63      | 109.68   |
| 32  | b     | 624 | AJP  | C27-C28-C29 | 5.67  | 122.63      | 109.68   |
| 25  | G     | 603 | CLA  | C4A-NA-C1A  | -5.66 | 104.16      | 106.71   |
| 32  | A     | 412 | AJP  | C26-O25-C23 | 5.66  | 124.08      | 115.33   |
| 33  | A     | 413 | BCT  | O2-C-O1     | 5.66  | 134.22      | 119.55   |
| 33  | a     | 414 | BCT  | O2-C-O1     | 5.66  | 134.22      | 119.55   |
| 25  | B     | 612 | CLA  | C4A-NA-C1A  | -5.65 | 104.17      | 106.71   |
| 25  | b     | 612 | CLA  | C4A-NA-C1A  | -5.65 | 104.17      | 106.71   |
| 25  | B     | 612 | CLA  | CHD-C1D-ND  | -5.65 | 119.26      | 124.45   |
| 32  | n     | 620 | AJP  | O77-C28-C27 | 5.65  | 121.45      | 110.14   |
| 25  | g     | 603 | CLA  | C4A-NA-C1A  | -5.64 | 104.17      | 106.71   |
| 32  | N     | 620 | AJP  | O77-C28-C27 | 5.62  | 121.40      | 110.14   |
| 25  | n     | 603 | CLA  | CHD-C1D-ND  | -5.61 | 119.30      | 124.45   |
| 32  | B     | 624 | AJP  | O44-C37-C38 | 5.59  | 122.14      | 107.28   |
| 32  | b     | 624 | AJP  | O44-C37-C38 | 5.59  | 122.14      | 107.28   |
| 32  | A     | 412 | AJP  | C12-C07-C08 | -5.58 | 98.85       | 104.88   |
| 32  | B     | 624 | AJP  | O44-C45-O50 | 5.58  | 121.49      | 109.08   |
| 32  | b     | 624 | AJP  | O44-C45-O50 | 5.58  | 121.49      | 109.08   |
| 25  | N     | 603 | CLA  | CHD-C1D-ND  | -5.58 | 119.33      | 124.45   |
| 25  | y     | 314 | CLA  | CHD-C1D-ND  | -5.57 | 119.33      | 124.45   |
| 25  | B     | 608 | CLA  | CHD-C1D-ND  | -5.57 | 119.33      | 124.45   |
| 25  | b     | 608 | CLA  | CHD-C1D-ND  | -5.57 | 119.33      | 124.45   |
| 32  | a     | 413 | AJP  | C12-C07-C08 | -5.57 | 98.86       | 104.88   |
| 25  | r     | 601 | CLA  | C2A-C3A-C4A | -5.57 | 92.87       | 101.87   |
| 25  | Y     | 314 | CLA  | CHD-C1D-ND  | -5.57 | 119.34      | 124.45   |
| 25  | R     | 601 | CLA  | C2A-C3A-C4A | -5.56 | 92.88       | 101.87   |
| 25  | r     | 601 | CLA  | CHD-C1D-ND  | -5.56 | 119.35      | 124.45   |
| 32  | a     | 413 | AJP  | O74-C67-C66 | 5.55  | 123.18      | 110.35   |
| 32  | A     | 412 | AJP  | O74-C67-C66 | 5.54  | 123.17      | 110.35   |
| 32  | A     | 412 | AJP  | O31-C26-C27 | 5.54  | 122.07      | 110.35   |
| 32  | a     | 413 | AJP  | O31-C26-C27 | 5.54  | 122.07      | 110.35   |
| 25  | y     | 311 | CLA  | CHD-C1D-ND  | -5.53 | 119.37      | 124.45   |
| 25  | R     | 601 | CLA  | CHD-C1D-ND  | -5.52 | 119.38      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | Y     | 311 | CLA  | CHD-C1D-ND  | -5.51 | 119.39      | 124.45   |
| 32  | y     | 323 | AJP  | C12-C07-C08 | -5.51 | 98.93       | 104.88   |
| 25  | c     | 509 | CLA  | CHD-C1D-ND  | -5.50 | 119.40      | 124.45   |
| 32  | Y     | 321 | AJP  | O25-C23-C24 | 5.50  | 120.25      | 109.62   |
| 25  | C     | 509 | CLA  | CHD-C1D-ND  | -5.50 | 119.40      | 124.45   |
| 32  | y     | 321 | AJP  | O25-C23-C24 | 5.50  | 120.25      | 109.62   |
| 32  | Y     | 323 | AJP  | C12-C07-C08 | -5.48 | 98.96       | 104.88   |
| 25  | b     | 609 | CLA  | CHD-C1D-ND  | -5.47 | 119.42      | 124.45   |
| 25  | R     | 608 | CLA  | C4A-NA-C1A  | -5.47 | 104.25      | 106.71   |
| 25  | r     | 608 | CLA  | C4A-NA-C1A  | -5.47 | 104.25      | 106.71   |
| 25  | c     | 511 | CLA  | C1B-CHB-C4A | -5.46 | 119.31      | 130.12   |
| 25  | G     | 612 | CLA  | C1D-ND-C4D  | -5.44 | 102.47      | 106.33   |
| 25  | g     | 612 | CLA  | C1D-ND-C4D  | -5.44 | 102.47      | 106.33   |
| 25  | B     | 609 | CLA  | CHD-C1D-ND  | -5.44 | 119.46      | 124.45   |
| 25  | n     | 610 | CLA  | CHD-C1D-ND  | -5.43 | 119.47      | 124.45   |
| 25  | C     | 511 | CLA  | C1B-CHB-C4A | -5.43 | 119.37      | 130.12   |
| 32  | n     | 620 | AJP  | C01-C02-C85 | 5.43  | 120.73      | 111.18   |
| 32  | Y     | 323 | AJP  | C01-C02-C85 | 5.42  | 120.72      | 111.18   |
| 32  | y     | 323 | AJP  | C01-C02-C85 | 5.42  | 120.72      | 111.18   |
| 32  | G     | 618 | AJP  | C26-O31-C30 | 5.42  | 119.13      | 113.13   |
| 25  | b     | 602 | CLA  | CHD-C1D-ND  | -5.41 | 119.48      | 124.45   |
| 32  | N     | 620 | AJP  | C01-C02-C85 | 5.41  | 120.71      | 111.18   |
| 29  | l     | 101 | SQD  | O8-S-C6     | -5.40 | 97.13       | 105.74   |
| 32  | y     | 322 | AJP  | O77-C28-C27 | 5.40  | 120.96      | 110.14   |
| 32  | Y     | 322 | AJP  | O77-C28-C27 | 5.40  | 120.96      | 110.14   |
| 32  | N     | 620 | AJP  | O31-C26-C27 | 5.40  | 121.78      | 110.35   |
| 32  | n     | 620 | AJP  | O31-C26-C27 | 5.40  | 121.78      | 110.35   |
| 25  | N     | 610 | CLA  | CHD-C1D-ND  | -5.40 | 119.50      | 124.45   |
| 32  | y     | 324 | AJP  | O31-C26-C27 | 5.39  | 121.75      | 110.35   |
| 32  | g     | 618 | AJP  | C26-O31-C30 | 5.39  | 119.10      | 113.13   |
| 29  | L     | 103 | SQD  | O8-S-C6     | -5.39 | 97.16       | 105.74   |
| 25  | R     | 612 | CLA  | C1B-CHB-C4A | -5.38 | 119.46      | 130.12   |
| 32  | Y     | 324 | AJP  | O31-C26-C27 | 5.38  | 121.74      | 110.35   |
| 25  | B     | 602 | CLA  | CHD-C1D-ND  | -5.38 | 119.51      | 124.45   |
| 25  | r     | 612 | CLA  | C1B-CHB-C4A | -5.37 | 119.48      | 130.12   |
| 25  | G     | 610 | CLA  | CHD-C1D-ND  | -5.36 | 119.53      | 124.45   |
| 25  | y     | 313 | CLA  | C1D-ND-C4D  | -5.35 | 102.53      | 106.33   |
| 32  | y     | 321 | AJP  | C05-C06-C07 | 5.34  | 112.07      | 103.37   |
| 25  | Y     | 313 | CLA  | C1D-ND-C4D  | -5.34 | 102.54      | 106.33   |
| 32  | B     | 624 | AJP  | O40-C39-C41 | 5.33  | 119.69      | 106.44   |
| 32  | b     | 624 | AJP  | O40-C39-C41 | 5.33  | 119.69      | 106.44   |
| 32  | Y     | 321 | AJP  | C05-C06-C07 | 5.33  | 112.04      | 103.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 40  | r     | 617 | NEX  | C11-C12-C13 | -5.32 | 111.46      | 126.42   |
| 40  | R     | 617 | NEX  | C27-C28-C29 | -5.32 | 117.27      | 125.53   |
| 25  | G     | 614 | CLA  | C4A-NA-C1A  | -5.32 | 104.31      | 106.71   |
| 25  | g     | 614 | CLA  | C4A-NA-C1A  | -5.32 | 104.31      | 106.71   |
| 25  | g     | 610 | CLA  | CHD-C1D-ND  | -5.32 | 119.57      | 124.45   |
| 40  | R     | 617 | NEX  | C11-C12-C13 | -5.31 | 111.49      | 126.42   |
| 25  | b     | 608 | CLA  | C4A-NA-C1A  | -5.31 | 104.32      | 106.71   |
| 25  | r     | 611 | CLA  | C1B-CHB-C4A | -5.31 | 119.60      | 130.12   |
| 32  | S     | 319 | AJP  | O25-C23-C24 | 5.31  | 119.88      | 109.62   |
| 32  | s     | 319 | AJP  | O25-C23-C24 | 5.31  | 119.88      | 109.62   |
| 25  | R     | 611 | CLA  | C1B-CHB-C4A | -5.31 | 119.61      | 130.12   |
| 25  | R     | 614 | CLA  | CHD-C1D-ND  | -5.31 | 119.58      | 124.45   |
| 25  | r     | 614 | CLA  | CHD-C1D-ND  | -5.31 | 119.58      | 124.45   |
| 40  | r     | 617 | NEX  | C27-C28-C29 | -5.30 | 117.30      | 125.53   |
| 39  | N     | 615 | LUT  | C18-C5-C6   | 5.30  | 130.48      | 124.53   |
| 39  | n     | 615 | LUT  | C18-C5-C6   | 5.30  | 130.48      | 124.53   |
| 25  | G     | 604 | CLA  | CHD-C1D-ND  | -5.29 | 119.59      | 124.45   |
| 32  | A     | 412 | AJP  | C05-C06-C07 | 5.28  | 111.97      | 103.37   |
| 32  | a     | 413 | AJP  | C05-C06-C07 | 5.28  | 111.97      | 103.37   |
| 32  | B     | 624 | AJP  | O60-C59-C61 | 5.28  | 119.57      | 106.44   |
| 32  | b     | 624 | AJP  | O60-C59-C61 | 5.28  | 119.57      | 106.44   |
| 40  | s     | 317 | NEX  | C27-C28-C29 | -5.28 | 117.34      | 125.53   |
| 32  | y     | 324 | AJP  | C05-C06-C07 | 5.28  | 111.96      | 103.37   |
| 25  | 2     | 602 | CLA  | C2D-C1D-ND  | -5.27 | 106.22      | 110.10   |
| 25  | 6     | 602 | CLA  | C2D-C1D-ND  | -5.27 | 106.22      | 110.10   |
| 40  | S     | 317 | NEX  | C27-C28-C29 | -5.27 | 117.35      | 125.53   |
| 25  | C     | 505 | CLA  | O2D-CGD-CBD | 5.27  | 120.64      | 111.27   |
| 25  | c     | 505 | CLA  | O2D-CGD-CBD | 5.27  | 120.64      | 111.27   |
| 25  | B     | 608 | CLA  | C4A-NA-C1A  | -5.27 | 104.34      | 106.71   |
| 32  | Y     | 323 | AJP  | O31-C26-C27 | 5.27  | 121.50      | 110.35   |
| 32  | y     | 323 | AJP  | O31-C26-C27 | 5.27  | 121.50      | 110.35   |
| 32  | B     | 624 | AJP  | O74-C67-C66 | 5.27  | 122.53      | 110.35   |
| 32  | b     | 624 | AJP  | O74-C67-C66 | 5.27  | 122.53      | 110.35   |
| 32  | Y     | 324 | AJP  | C05-C06-C07 | 5.26  | 111.94      | 103.37   |
| 25  | g     | 604 | CLA  | CHD-C1D-ND  | -5.25 | 119.63      | 124.45   |
| 32  | B     | 624 | AJP  | C12-C07-C08 | -5.25 | 99.21       | 104.88   |
| 32  | b     | 624 | AJP  | C12-C07-C08 | -5.25 | 99.21       | 104.88   |
| 32  | A     | 412 | AJP  | C01-C02-C85 | 5.25  | 120.42      | 111.18   |
| 32  | a     | 413 | AJP  | C01-C02-C85 | 5.25  | 120.42      | 111.18   |
| 32  | y     | 321 | AJP  | O77-C28-C27 | 5.25  | 120.65      | 110.14   |
| 32  | Y     | 321 | AJP  | O77-C28-C27 | 5.24  | 120.64      | 110.14   |
| 25  | g     | 611 | CLA  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 603 | CLA  | CHD-C1D-ND  | -5.23 | 119.65      | 124.45   |
| 25  | b     | 605 | CLA  | O2D-CGD-CBD | 5.23  | 120.56      | 111.27   |
| 25  | R     | 611 | CLA  | CHD-C1D-C2D | 5.22  | 136.44      | 125.48   |
| 25  | Y     | 304 | CLA  | CHD-C1D-ND  | -5.22 | 119.65      | 124.45   |
| 25  | G     | 611 | CLA  | O2D-CGD-CBD | 5.21  | 120.53      | 111.27   |
| 32  | A     | 412 | AJP  | O74-C67-C68 | 5.21  | 122.40      | 110.35   |
| 32  | a     | 413 | AJP  | O74-C67-C68 | 5.21  | 122.40      | 110.35   |
| 25  | B     | 605 | CLA  | O2D-CGD-CBD | 5.21  | 120.53      | 111.27   |
| 25  | G     | 603 | CLA  | CHD-C1D-ND  | -5.21 | 119.67      | 124.45   |
| 25  | r     | 611 | CLA  | CHD-C1D-C2D | 5.19  | 136.37      | 125.48   |
| 25  | S     | 304 | CLA  | O2D-CGD-CBD | 5.19  | 120.49      | 111.27   |
| 25  | s     | 304 | CLA  | O2D-CGD-CBD | 5.19  | 120.49      | 111.27   |
| 32  | B     | 624 | AJP  | O73-C68-C67 | 5.17  | 122.30      | 110.35   |
| 32  | b     | 624 | AJP  | O73-C68-C67 | 5.17  | 122.30      | 110.35   |
| 38  | F     | 101 | HEM  | C1B-NB-C4B  | 5.17  | 110.41      | 105.07   |
| 25  | S     | 312 | CLA  | C1B-CHB-C4A | -5.16 | 119.89      | 130.12   |
| 25  | s     | 312 | CLA  | C1B-CHB-C4A | -5.16 | 119.91      | 130.12   |
| 25  | B     | 614 | CLA  | O2D-CGD-CBD | 5.16  | 120.43      | 111.27   |
| 25  | b     | 614 | CLA  | O2D-CGD-CBD | 5.16  | 120.43      | 111.27   |
| 25  | G     | 612 | CLA  | CHD-C1D-ND  | -5.15 | 119.72      | 124.45   |
| 25  | g     | 612 | CLA  | CHD-C1D-ND  | -5.15 | 119.72      | 124.45   |
| 24  | R     | 613 | CHL  | CAA-C2A-C3A | -5.15 | 104.08      | 116.10   |
| 24  | r     | 613 | CHL  | CAA-C2A-C3A | -5.15 | 104.08      | 116.10   |
| 32  | y     | 320 | AJP  | O82-C10-C08 | 5.14  | 125.77      | 111.17   |
| 32  | g     | 618 | AJP  | C01-C02-C85 | 5.14  | 120.23      | 111.18   |
| 25  | y     | 304 | CLA  | CHD-C1D-ND  | -5.14 | 119.73      | 124.45   |
| 32  | Y     | 320 | AJP  | O82-C10-C08 | 5.14  | 125.76      | 111.17   |
| 25  | N     | 612 | CLA  | C4D-CHA-C1A | -5.13 | 115.00      | 121.25   |
| 32  | G     | 618 | AJP  | C01-C02-C85 | 5.13  | 120.21      | 111.18   |
| 24  | y     | 307 | CHL  | C4A-NA-C1A  | 5.13  | 109.01      | 106.71   |
| 32  | Y     | 320 | AJP  | O31-C26-C27 | 5.13  | 121.21      | 110.35   |
| 32  | n     | 619 | AJP  | O09-C05-C06 | -5.13 | 96.86       | 104.47   |
| 32  | s     | 319 | AJP  | C12-C07-C08 | -5.12 | 99.34       | 104.88   |
| 32  | N     | 619 | AJP  | O09-C05-C06 | -5.12 | 96.88       | 104.47   |
| 32  | G     | 618 | AJP  | C05-C06-C07 | 5.12  | 111.70      | 103.37   |
| 32  | y     | 320 | AJP  | O31-C26-C27 | 5.12  | 121.18      | 110.35   |
| 32  | g     | 618 | AJP  | C05-C06-C07 | 5.12  | 111.70      | 103.37   |
| 32  | B     | 624 | AJP  | C05-C06-C07 | 5.11  | 111.69      | 103.37   |
| 32  | b     | 624 | AJP  | C05-C06-C07 | 5.11  | 111.69      | 103.37   |
| 32  | B     | 624 | AJP  | O60-C59-C58 | 5.11  | 118.98      | 109.69   |
| 32  | b     | 624 | AJP  | O60-C59-C58 | 5.11  | 118.98      | 109.69   |
| 38  | f     | 101 | HEM  | C1B-NB-C4B  | 5.11  | 110.35      | 105.07   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | n     | 612 | CLA  | C4D-CHA-C1A | -5.11 | 115.03      | 121.25   |
| 39  | G     | 616 | LUT  | C18-C5-C6   | 5.11  | 130.26      | 124.53   |
| 39  | g     | 616 | LUT  | C18-C5-C6   | 5.11  | 130.26      | 124.53   |
| 25  | c     | 506 | CLA  | CHD-C1D-ND  | -5.10 | 119.77      | 124.45   |
| 32  | y     | 321 | AJP  | C26-O31-C30 | 5.10  | 118.78      | 113.13   |
| 25  | B     | 616 | CLA  | CHD-C1D-ND  | -5.09 | 119.77      | 124.45   |
| 25  | b     | 616 | CLA  | CHD-C1D-ND  | -5.09 | 119.77      | 124.45   |
| 32  | Y     | 322 | AJP  | C26-O25-C23 | 5.09  | 123.20      | 115.33   |
| 32  | y     | 322 | AJP  | C26-O25-C23 | 5.09  | 123.20      | 115.33   |
| 25  | G     | 614 | CLA  | CHD-C1D-ND  | -5.09 | 119.78      | 124.45   |
| 25  | g     | 614 | CLA  | CHD-C1D-ND  | -5.09 | 119.78      | 124.45   |
| 32  | y     | 322 | AJP  | C05-C06-C07 | 5.09  | 111.66      | 103.37   |
| 25  | B     | 616 | CLA  | C4A-NA-C1A  | -5.09 | 104.42      | 106.71   |
| 25  | b     | 616 | CLA  | C4A-NA-C1A  | -5.09 | 104.42      | 106.71   |
| 32  | A     | 412 | AJP  | O77-C28-C27 | 5.08  | 122.10      | 110.35   |
| 32  | a     | 413 | AJP  | O77-C28-C27 | 5.08  | 122.10      | 110.35   |
| 32  | Y     | 322 | AJP  | C05-C06-C07 | 5.08  | 111.64      | 103.37   |
| 25  | Y     | 305 | CLA  | CHD-C1D-ND  | -5.08 | 119.79      | 124.45   |
| 25  | y     | 305 | CLA  | CHD-C1D-ND  | -5.08 | 119.79      | 124.45   |
| 32  | S     | 319 | AJP  | C12-C07-C08 | -5.08 | 99.39       | 104.88   |
| 32  | Y     | 321 | AJP  | C26-O31-C30 | 5.07  | 118.75      | 113.13   |
| 25  | C     | 506 | CLA  | CHD-C1D-ND  | -5.07 | 119.79      | 124.45   |
| 25  | 2     | 604 | CLA  | C4D-CHA-C1A | -5.07 | 115.08      | 121.25   |
| 25  | 6     | 604 | CLA  | C4D-CHA-C1A | -5.07 | 115.08      | 121.25   |
| 32  | B     | 624 | AJP  | O25-C26-C27 | 5.07  | 121.23      | 108.10   |
| 32  | b     | 624 | AJP  | O25-C26-C27 | 5.07  | 121.23      | 108.10   |
| 25  | A     | 405 | CLA  | C4A-NA-C1A  | -5.07 | 104.43      | 106.71   |
| 25  | a     | 406 | CLA  | C4A-NA-C1A  | -5.07 | 104.43      | 106.71   |
| 25  | S     | 305 | CLA  | C4D-CHA-C1A | -5.06 | 115.09      | 121.25   |
| 29  | A     | 411 | SQD  | O8-S-C6     | -5.05 | 97.69       | 105.74   |
| 29  | a     | 412 | SQD  | O8-S-C6     | -5.05 | 97.69       | 105.74   |
| 32  | s     | 319 | AJP  | C01-C02-C85 | 5.05  | 120.07      | 111.18   |
| 24  | Y     | 307 | CHL  | C4A-NA-C1A  | 5.04  | 108.97      | 106.71   |
| 32  | S     | 319 | AJP  | C01-C02-C85 | 5.04  | 120.05      | 111.18   |
| 25  | s     | 305 | CLA  | C4D-CHA-C1A | -5.04 | 115.11      | 121.25   |
| 32  | S     | 319 | AJP  | C05-C06-C07 | 5.04  | 111.57      | 103.37   |
| 32  | s     | 319 | AJP  | C05-C06-C07 | 5.04  | 111.57      | 103.37   |
| 32  | N     | 619 | AJP  | C05-C06-C07 | 5.03  | 111.56      | 103.37   |
| 32  | n     | 619 | AJP  | C05-C06-C07 | 5.03  | 111.56      | 103.37   |
| 25  | G     | 604 | CLA  | O2D-CGD-CBD | 5.03  | 120.21      | 111.27   |
| 25  | B     | 601 | CLA  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |
| 25  | b     | 601 | CLA  | O2D-CGD-CBD | 5.03  | 120.20      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 320 | AJP  | C26-O31-C30 | -5.02 | 107.57      | 113.13   |
| 32  | A     | 412 | AJP  | O60-C59-C61 | 5.02  | 118.93      | 106.44   |
| 25  | b     | 604 | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 25  | S     | 311 | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 25  | B     | 604 | CLA  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 25  | C     | 510 | CLA  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 25  | c     | 510 | CLA  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 25  | s     | 311 | CLA  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 25  | g     | 604 | CLA  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 32  | a     | 413 | AJP  | O60-C59-C61 | 5.00  | 118.88      | 106.44   |
| 25  | S     | 314 | CLA  | CHD-C1D-ND  | -5.00 | 119.86      | 124.45   |
| 25  | s     | 314 | CLA  | CHD-C1D-ND  | -5.00 | 119.86      | 124.45   |
| 25  | Y     | 311 | CLA  | O2D-CGD-CBD | 5.00  | 120.14      | 111.27   |
| 25  | b     | 602 | CLA  | C4A-NA-C1A  | -4.99 | 104.46      | 106.71   |
| 32  | A     | 412 | AJP  | O54-C36-C37 | 4.99  | 120.17      | 107.48   |
| 32  | y     | 320 | AJP  | C26-O31-C30 | -4.99 | 107.60      | 113.13   |
| 32  | A     | 412 | AJP  | O70-C69-C71 | 4.99  | 118.84      | 106.44   |
| 32  | a     | 413 | AJP  | O70-C69-C71 | 4.99  | 118.84      | 106.44   |
| 25  | y     | 311 | CLA  | O2D-CGD-CBD | 4.98  | 120.11      | 111.27   |
| 32  | B     | 624 | AJP  | C03-C04-C05 | -4.98 | 103.33      | 111.93   |
| 29  | l     | 102 | SQD  | O8-S-C6     | -4.97 | 97.81       | 105.74   |
| 32  | a     | 413 | AJP  | O54-C36-C37 | 4.97  | 120.11      | 107.48   |
| 25  | B     | 602 | CLA  | C4A-NA-C1A  | -4.97 | 104.47      | 106.71   |
| 32  | s     | 319 | AJP  | O31-C26-C27 | 4.97  | 120.87      | 110.35   |
| 32  | b     | 624 | AJP  | C03-C04-C05 | -4.97 | 103.35      | 111.93   |
| 32  | y     | 323 | AJP  | C03-C02-C85 | 4.97  | 115.46      | 108.56   |
| 32  | Y     | 323 | AJP  | C03-C02-C85 | 4.96  | 115.45      | 108.56   |
| 25  | b     | 616 | CLA  | C1D-ND-C4D  | -4.96 | 102.81      | 106.33   |
| 29  | L     | 101 | SQD  | O8-S-C6     | -4.96 | 97.84       | 105.74   |
| 25  | Y     | 304 | CLA  | O2D-CGD-CBD | 4.96  | 120.08      | 111.27   |
| 25  | r     | 601 | CLA  | C2D-C1D-ND  | -4.95 | 106.45      | 110.10   |
| 25  | b     | 607 | CLA  | C4A-NA-C1A  | -4.95 | 104.48      | 106.71   |
| 25  | B     | 607 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 25  | b     | 607 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 32  | S     | 319 | AJP  | O31-C26-C27 | 4.94  | 120.81      | 110.35   |
| 39  | N     | 616 | LUT  | C18-C5-C6   | 4.94  | 130.08      | 124.53   |
| 39  | n     | 616 | LUT  | C18-C5-C6   | 4.94  | 130.08      | 124.53   |
| 38  | f     | 101 | HEM  | C4D-ND-C1D  | 4.94  | 110.18      | 105.07   |
| 25  | y     | 304 | CLA  | O2D-CGD-CBD | 4.94  | 120.05      | 111.27   |
| 25  | R     | 601 | CLA  | C2D-C1D-ND  | -4.94 | 106.46      | 110.10   |
| 25  | 6     | 605 | CLA  | C4D-CHA-C1A | -4.93 | 115.25      | 121.25   |
| 25  | G     | 602 | CLA  | C1D-ND-C4D  | -4.93 | 102.83      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 602 | CLA  | C1D-ND-C4D  | -4.93 | 102.83      | 106.33   |
| 25  | B     | 602 | CLA  | O2D-CGD-CBD | 4.93  | 120.03      | 111.27   |
| 25  | b     | 602 | CLA  | O2D-CGD-CBD | 4.93  | 120.03      | 111.27   |
| 25  | B     | 616 | CLA  | C1D-ND-C4D  | -4.93 | 102.83      | 106.33   |
| 25  | c     | 505 | CLA  | C4A-NA-C1A  | -4.92 | 104.49      | 106.71   |
| 24  | N     | 607 | CHL  | O2D-CGD-CBD | 4.92  | 120.01      | 111.27   |
| 24  | n     | 607 | CHL  | O2D-CGD-CBD | 4.92  | 120.01      | 111.27   |
| 32  | A     | 412 | AJP  | C65-O70-C69 | 4.92  | 123.34      | 113.69   |
| 32  | a     | 413 | AJP  | C65-O70-C69 | 4.92  | 123.34      | 113.69   |
| 25  | 2     | 605 | CLA  | C4D-CHA-C1A | -4.91 | 115.27      | 121.25   |
| 39  | s     | 315 | LUT  | C18-C5-C6   | 4.91  | 130.04      | 124.53   |
| 39  | S     | 315 | LUT  | C18-C5-C6   | 4.91  | 130.04      | 124.53   |
| 38  | F     | 101 | HEM  | C4D-ND-C1D  | 4.90  | 110.14      | 105.07   |
| 25  | D     | 402 | CLA  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 25  | d     | 402 | CLA  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 39  | g     | 616 | LUT  | C38-C25-C24 | -4.90 | 113.08      | 123.56   |
| 39  | G     | 616 | LUT  | C38-C25-C24 | -4.90 | 113.08      | 123.56   |
| 25  | B     | 610 | CLA  | C1D-ND-C4D  | -4.89 | 102.86      | 106.33   |
| 24  | Y     | 308 | CHL  | O2D-CGD-CBD | 4.89  | 119.96      | 111.27   |
| 24  | y     | 308 | CHL  | O2D-CGD-CBD | 4.89  | 119.96      | 111.27   |
| 25  | a     | 406 | CLA  | O2D-CGD-CBD | 4.89  | 119.96      | 111.27   |
| 25  | C     | 505 | CLA  | C1D-ND-C4D  | -4.89 | 102.86      | 106.33   |
| 25  | c     | 505 | CLA  | C1D-ND-C4D  | -4.89 | 102.86      | 106.33   |
| 25  | A     | 405 | CLA  | O2D-CGD-CBD | 4.89  | 119.95      | 111.27   |
| 25  | Y     | 312 | CLA  | C1D-ND-C4D  | -4.88 | 102.87      | 106.33   |
| 32  | N     | 620 | AJP  | O25-C26-C27 | 4.88  | 120.75      | 108.10   |
| 32  | n     | 620 | AJP  | O25-C26-C27 | 4.88  | 120.75      | 108.10   |
| 40  | R     | 617 | NEX  | C35-C15-C14 | 4.88  | 133.47      | 123.47   |
| 40  | r     | 617 | NEX  | C35-C15-C14 | 4.88  | 133.47      | 123.47   |
| 25  | A     | 401 | CLA  | O2D-CGD-CBD | 4.86  | 119.91      | 111.27   |
| 25  | a     | 402 | CLA  | O2D-CGD-CBD | 4.86  | 119.91      | 111.27   |
| 25  | B     | 607 | CLA  | C4A-NA-C1A  | -4.86 | 104.52      | 106.71   |
| 39  | r     | 615 | LUT  | C18-C5-C6   | 4.86  | 129.98      | 124.53   |
| 39  | S     | 315 | LUT  | C38-C25-C24 | -4.86 | 113.17      | 123.56   |
| 39  | s     | 315 | LUT  | C38-C25-C24 | -4.85 | 113.18      | 123.56   |
| 25  | Y     | 312 | CLA  | O2D-CGD-CBD | 4.85  | 119.88      | 111.27   |
| 25  | 2     | 605 | CLA  | CHD-C1D-ND  | -4.85 | 120.00      | 124.45   |
| 32  | y     | 322 | AJP  | O25-C26-O31 | 4.84  | 124.20      | 110.67   |
| 25  | G     | 610 | CLA  | O2D-CGD-CBD | 4.84  | 119.87      | 111.27   |
| 32  | S     | 319 | AJP  | O25-C26-C27 | 4.84  | 120.64      | 108.10   |
| 32  | Y     | 322 | AJP  | O25-C26-O31 | 4.84  | 124.19      | 110.67   |
| 32  | s     | 319 | AJP  | O25-C26-C27 | 4.84  | 120.63      | 108.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 6     | 605 | CLA  | CHD-C1D-ND  | -4.83 | 120.01      | 124.45   |
| 25  | R     | 611 | CLA  | C2A-C3A-C4A | -4.83 | 94.06       | 101.87   |
| 25  | y     | 312 | CLA  | O2D-CGD-CBD | 4.83  | 119.85      | 111.27   |
| 25  | s     | 314 | CLA  | O2D-CGD-CBD | 4.83  | 119.84      | 111.27   |
| 25  | b     | 610 | CLA  | C1D-ND-C4D  | -4.82 | 102.91      | 106.33   |
| 29  | A     | 407 | SQD  | O8-S-C6     | -4.82 | 98.06       | 105.74   |
| 29  | a     | 408 | SQD  | O8-S-C6     | -4.82 | 98.06       | 105.74   |
| 39  | Y     | 316 | LUT  | C18-C5-C6   | 4.82  | 129.94      | 124.53   |
| 25  | B     | 613 | CLA  | C1D-ND-C4D  | -4.81 | 102.92      | 106.33   |
| 25  | b     | 613 | CLA  | C1D-ND-C4D  | -4.81 | 102.92      | 106.33   |
| 25  | S     | 314 | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 25  | g     | 610 | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 25  | S     | 309 | CLA  | O2D-CGD-CBD | 4.81  | 119.81      | 111.27   |
| 25  | C     | 505 | CLA  | C4A-NA-C1A  | -4.81 | 104.54      | 106.71   |
| 25  | y     | 315 | CLA  | CHD-C1D-ND  | -4.81 | 120.04      | 124.45   |
| 39  | R     | 615 | LUT  | C18-C5-C6   | 4.80  | 129.91      | 124.53   |
| 25  | s     | 309 | CLA  | O2D-CGD-CBD | 4.80  | 119.79      | 111.27   |
| 25  | Y     | 315 | CLA  | CHD-C1D-ND  | -4.79 | 120.05      | 124.45   |
| 25  | r     | 611 | CLA  | C2A-C3A-C4A | -4.79 | 94.13       | 101.87   |
| 39  | y     | 316 | LUT  | C18-C5-C6   | 4.79  | 129.91      | 124.53   |
| 25  | y     | 312 | CLA  | C1D-ND-C4D  | -4.79 | 102.93      | 106.33   |
| 39  | s     | 316 | LUT  | C38-C25-C24 | -4.79 | 113.31      | 123.56   |
| 25  | B     | 603 | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 25  | b     | 603 | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 25  | y     | 313 | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 25  | Y     | 313 | CLA  | O2D-CGD-CBD | 4.78  | 119.77      | 111.27   |
| 25  | a     | 403 | CLA  | C4A-NA-C1A  | -4.78 | 104.56      | 106.71   |
| 32  | Y     | 324 | AJP  | O77-C28-C29 | 4.77  | 121.79      | 109.94   |
| 32  | y     | 324 | AJP  | O77-C28-C29 | 4.77  | 121.79      | 109.94   |
| 39  | S     | 316 | LUT  | C38-C25-C24 | -4.77 | 113.35      | 123.56   |
| 25  | n     | 602 | CLA  | C4A-NA-C1A  | -4.77 | 104.56      | 106.71   |
| 25  | c     | 512 | CLA  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 25  | C     | 512 | CLA  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 25  | B     | 606 | CLA  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 25  | b     | 606 | CLA  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 39  | n     | 616 | LUT  | C38-C25-C24 | -4.77 | 113.36      | 123.56   |
| 25  | C     | 511 | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 25  | N     | 613 | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 25  | n     | 613 | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 25  | D     | 402 | CLA  | C1B-CHB-C4A | -4.76 | 120.69      | 130.12   |
| 25  | A     | 402 | CLA  | C4A-NA-C1A  | -4.76 | 104.57      | 106.71   |
| 25  | c     | 511 | CLA  | O2D-CGD-CBD | 4.76  | 119.72      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | y     | 305 | CLA  | C4A-NA-C1A  | -4.76 | 104.57      | 106.71   |
| 24  | G     | 609 | CHL  | O2D-CGD-CBD | 4.75  | 119.70      | 111.27   |
| 39  | N     | 616 | LUT  | C38-C25-C24 | -4.75 | 113.40      | 123.56   |
| 25  | S     | 312 | CLA  | O2D-CGD-CBD | 4.75  | 119.70      | 111.27   |
| 25  | s     | 312 | CLA  | O2D-CGD-CBD | 4.74  | 119.70      | 111.27   |
| 25  | d     | 402 | CLA  | C1B-CHB-C4A | -4.74 | 120.72      | 130.12   |
| 25  | 2     | 604 | CLA  | C4A-NA-C1A  | 4.74  | 108.84      | 106.71   |
| 25  | B     | 615 | CLA  | C1B-CHB-C4A | -4.74 | 120.73      | 130.12   |
| 24  | g     | 609 | CHL  | O2D-CGD-CBD | 4.74  | 119.69      | 111.27   |
| 25  | Y     | 305 | CLA  | C1D-ND-C4D  | -4.73 | 102.97      | 106.33   |
| 25  | y     | 305 | CLA  | C1D-ND-C4D  | -4.73 | 102.97      | 106.33   |
| 25  | C     | 502 | CLA  | CHD-C1D-ND  | -4.73 | 120.11      | 124.45   |
| 25  | c     | 502 | CLA  | CHD-C1D-ND  | -4.73 | 120.11      | 124.45   |
| 39  | G     | 615 | LUT  | C18-C5-C6   | 4.73  | 129.84      | 124.53   |
| 32  | B     | 624 | AJP  | C01-C02-C85 | 4.73  | 119.50      | 111.18   |
| 32  | b     | 624 | AJP  | C01-C02-C85 | 4.73  | 119.50      | 111.18   |
| 25  | N     | 610 | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 25  | n     | 610 | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 32  | S     | 319 | AJP  | O09-C05-C06 | -4.73 | 97.46       | 104.47   |
| 32  | s     | 319 | AJP  | O09-C05-C06 | -4.73 | 97.46       | 104.47   |
| 25  | Y     | 303 | CLA  | CHD-C1D-ND  | -4.72 | 120.11      | 124.45   |
| 25  | y     | 303 | CLA  | CHD-C1D-ND  | -4.72 | 120.11      | 124.45   |
| 40  | R     | 617 | NEX  | C12-C13-C14 | 4.72  | 126.19      | 118.94   |
| 39  | g     | 615 | LUT  | C18-C5-C6   | 4.72  | 129.83      | 124.53   |
| 25  | b     | 615 | CLA  | C1B-CHB-C4A | -4.72 | 120.78      | 130.12   |
| 25  | 6     | 604 | CLA  | C4A-NA-C1A  | 4.72  | 108.83      | 106.71   |
| 39  | R     | 615 | LUT  | C38-C25-C24 | -4.71 | 113.47      | 123.56   |
| 40  | r     | 617 | NEX  | C12-C13-C14 | 4.71  | 126.17      | 118.94   |
| 25  | G     | 602 | CLA  | CHD-C1D-ND  | -4.71 | 120.12      | 124.45   |
| 25  | g     | 602 | CLA  | CHD-C1D-ND  | -4.71 | 120.12      | 124.45   |
| 39  | g     | 615 | LUT  | C38-C25-C24 | -4.70 | 113.50      | 123.56   |
| 39  | r     | 615 | LUT  | C38-C25-C24 | -4.70 | 113.50      | 123.56   |
| 25  | N     | 611 | CLA  | C1D-ND-C4D  | -4.70 | 103.00      | 106.33   |
| 25  | Y     | 303 | CLA  | C1D-ND-C4D  | -4.70 | 103.00      | 106.33   |
| 25  | N     | 602 | CLA  | C4A-NA-C1A  | -4.69 | 104.60      | 106.71   |
| 39  | G     | 615 | LUT  | C38-C25-C24 | -4.69 | 113.52      | 123.56   |
| 32  | Y     | 320 | AJP  | O77-C28-C27 | 4.69  | 119.53      | 110.14   |
| 32  | y     | 320 | AJP  | O77-C28-C27 | 4.69  | 119.53      | 110.14   |
| 25  | C     | 506 | CLA  | O2D-CGD-CBD | 4.68  | 119.59      | 111.27   |
| 25  | c     | 506 | CLA  | O2D-CGD-CBD | 4.68  | 119.59      | 111.27   |
| 25  | y     | 303 | CLA  | C1D-ND-C4D  | -4.68 | 103.01      | 106.33   |
| 32  | G     | 618 | AJP  | O77-C28-C27 | 4.68  | 119.52      | 110.14   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | Y     | 303 | CLA  | O2D-CGD-CBD | 4.68  | 119.59      | 111.27   |
| 25  | y     | 303 | CLA  | O2D-CGD-CBD | 4.68  | 119.59      | 111.27   |
| 32  | g     | 618 | AJP  | O77-C28-C27 | 4.68  | 119.51      | 110.14   |
| 25  | y     | 311 | CLA  | C1D-ND-C4D  | -4.67 | 103.01      | 106.33   |
| 25  | r     | 604 | CLA  | O2D-CGD-CBD | 4.67  | 119.57      | 111.27   |
| 25  | n     | 610 | CLA  | C1D-ND-C4D  | -4.67 | 103.02      | 106.33   |
| 39  | N     | 615 | LUT  | C38-C25-C24 | -4.67 | 113.57      | 123.56   |
| 25  | y     | 304 | CLA  | C4A-NA-C1A  | -4.67 | 104.61      | 106.71   |
| 25  | R     | 604 | CLA  | O2D-CGD-CBD | 4.67  | 119.56      | 111.27   |
| 39  | n     | 615 | LUT  | C38-C25-C24 | -4.67 | 113.58      | 123.56   |
| 25  | N     | 610 | CLA  | C1D-ND-C4D  | -4.67 | 103.02      | 106.33   |
| 25  | S     | 313 | CLA  | C2A-C3A-C4A | -4.66 | 94.34       | 101.87   |
| 25  | s     | 313 | CLA  | C2A-C3A-C4A | -4.66 | 94.34       | 101.87   |
| 25  | S     | 310 | CLA  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 25  | s     | 310 | CLA  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 32  | G     | 618 | AJP  | C24-C19-C20 | -4.66 | 107.71      | 112.66   |
| 32  | g     | 618 | AJP  | C24-C19-C20 | -4.66 | 107.71      | 112.66   |
| 39  | y     | 317 | LUT  | C38-C25-C24 | -4.66 | 113.59      | 123.56   |
| 39  | S     | 316 | LUT  | C18-C5-C6   | 4.66  | 129.76      | 124.53   |
| 32  | g     | 618 | AJP  | O25-C26-C27 | 4.66  | 120.17      | 108.10   |
| 32  | G     | 618 | AJP  | O25-C26-C27 | 4.66  | 120.16      | 108.10   |
| 32  | B     | 624 | AJP  | C45-C46-C47 | 4.65  | 119.69      | 110.00   |
| 32  | b     | 624 | AJP  | C45-C46-C47 | 4.65  | 119.69      | 110.00   |
| 32  | a     | 413 | AJP  | O40-C39-C41 | 4.65  | 118.01      | 106.44   |
| 39  | Y     | 317 | LUT  | C38-C25-C24 | -4.65 | 113.61      | 123.56   |
| 25  | r     | 608 | CLA  | O2D-CGD-CBD | 4.65  | 119.53      | 111.27   |
| 25  | n     | 611 | CLA  | C1D-ND-C4D  | -4.65 | 103.03      | 106.33   |
| 32  | Y     | 323 | AJP  | O77-C28-C29 | 4.64  | 121.46      | 109.94   |
| 32  | y     | 323 | AJP  | O77-C28-C29 | 4.64  | 121.46      | 109.94   |
| 25  | g     | 611 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 25  | G     | 611 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 39  | s     | 316 | LUT  | C18-C5-C6   | 4.64  | 129.74      | 124.53   |
| 32  | A     | 412 | AJP  | O40-C39-C41 | 4.64  | 117.97      | 106.44   |
| 25  | n     | 611 | CLA  | O2D-CGD-CBD | 4.64  | 119.51      | 111.27   |
| 25  | S     | 309 | CLA  | CHD-C1D-ND  | -4.63 | 120.20      | 124.45   |
| 25  | B     | 615 | CLA  | O2D-CGD-CBD | 4.63  | 119.49      | 111.27   |
| 25  | D     | 402 | CLA  | CHD-C1D-ND  | -4.63 | 120.20      | 124.45   |
| 25  | d     | 402 | CLA  | CHD-C1D-ND  | -4.63 | 120.20      | 124.45   |
| 25  | b     | 610 | CLA  | O2D-CGD-CBD | 4.63  | 119.49      | 111.27   |
| 32  | N     | 620 | AJP  | C12-C07-C08 | -4.62 | 99.88       | 104.88   |
| 32  | Y     | 321 | AJP  | C29-C28-C27 | 4.62  | 117.40      | 110.69   |
| 32  | y     | 321 | AJP  | C29-C28-C27 | 4.62  | 117.40      | 110.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 413 | AJP  | C35-C36-C37 | 4.62  | 119.97      | 110.75   |
| 32  | A     | 412 | AJP  | C35-C36-C37 | 4.62  | 119.97      | 110.75   |
| 39  | Y     | 317 | LUT  | C18-C5-C6   | 4.62  | 129.71      | 124.53   |
| 24  | G     | 607 | CHL  | O2D-CGD-CBD | 4.62  | 119.47      | 111.27   |
| 25  | b     | 615 | CLA  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 39  | y     | 317 | LUT  | C18-C5-C6   | 4.61  | 129.71      | 124.53   |
| 25  | R     | 608 | CLA  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 24  | g     | 607 | CHL  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 32  | N     | 620 | AJP  | O77-C28-C29 | 4.61  | 121.37      | 109.94   |
| 25  | B     | 610 | CLA  | O2D-CGD-CBD | 4.61  | 119.45      | 111.27   |
| 25  | N     | 611 | CLA  | O2D-CGD-CBD | 4.61  | 119.45      | 111.27   |
| 25  | s     | 309 | CLA  | CHD-C1D-ND  | -4.61 | 120.22      | 124.45   |
| 25  | C     | 508 | CLA  | O2D-CGD-CBD | 4.60  | 119.45      | 111.27   |
| 25  | c     | 508 | CLA  | O2D-CGD-CBD | 4.60  | 119.45      | 111.27   |
| 32  | n     | 620 | AJP  | O77-C28-C29 | 4.60  | 121.36      | 109.94   |
| 25  | S     | 314 | CLA  | C1D-ND-C4D  | -4.60 | 103.07      | 106.33   |
| 25  | Y     | 311 | CLA  | C1D-ND-C4D  | -4.60 | 103.07      | 106.33   |
| 25  | Y     | 305 | CLA  | C4A-NA-C1A  | -4.59 | 104.64      | 106.71   |
| 25  | B     | 611 | CLA  | O2D-CGD-CBD | 4.59  | 119.43      | 111.27   |
| 25  | b     | 611 | CLA  | O2D-CGD-CBD | 4.59  | 119.43      | 111.27   |
| 25  | c     | 513 | CLA  | C4A-NA-C1A  | -4.59 | 104.64      | 106.71   |
| 25  | B     | 606 | CLA  | C1B-CHB-C4A | -4.59 | 121.03      | 130.12   |
| 25  | b     | 606 | CLA  | C1B-CHB-C4A | -4.59 | 121.03      | 130.12   |
| 25  | A     | 402 | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 25  | a     | 403 | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 25  | R     | 612 | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 25  | r     | 612 | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 25  | C     | 513 | CLA  | C4A-NA-C1A  | -4.58 | 104.64      | 106.71   |
| 32  | y     | 322 | AJP  | C12-C07-C08 | -4.58 | 99.93       | 104.88   |
| 32  | n     | 620 | AJP  | C12-C07-C08 | -4.58 | 99.93       | 104.88   |
| 25  | N     | 602 | CLA  | C1D-ND-C4D  | -4.58 | 103.08      | 106.33   |
| 39  | y     | 316 | LUT  | C38-C25-C24 | -4.58 | 113.77      | 123.56   |
| 25  | R     | 614 | CLA  | C1D-ND-C4D  | -4.57 | 103.09      | 106.33   |
| 25  | S     | 305 | CLA  | C2D-C1D-ND  | -4.57 | 106.73      | 110.10   |
| 25  | r     | 614 | CLA  | C1D-ND-C4D  | -4.57 | 103.09      | 106.33   |
| 25  | 2     | 602 | CLA  | O2D-CGD-CBD | 4.57  | 119.39      | 111.27   |
| 39  | Y     | 316 | LUT  | C38-C25-C24 | -4.57 | 113.79      | 123.56   |
| 24  | y     | 307 | CHL  | C1D-ND-C4D  | -4.56 | 103.09      | 106.33   |
| 25  | s     | 305 | CLA  | C2D-C1D-ND  | -4.56 | 106.74      | 110.10   |
| 32  | y     | 322 | AJP  | C01-C02-C85 | 4.56  | 119.21      | 111.18   |
| 25  | C     | 502 | CLA  | O2D-CGD-CBD | 4.56  | 119.37      | 111.27   |
| 25  | c     | 502 | CLA  | O2D-CGD-CBD | 4.56  | 119.37      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | s     | 314 | CLA  | C1D-ND-C4D  | -4.56 | 103.10      | 106.33   |
| 25  | n     | 602 | CLA  | C1D-ND-C4D  | -4.56 | 103.10      | 106.33   |
| 32  | Y     | 322 | AJP  | C12-C07-C08 | -4.55 | 99.96       | 104.88   |
| 25  | 6     | 602 | CLA  | O2D-CGD-CBD | 4.54  | 119.34      | 111.27   |
| 32  | n     | 619 | AJP  | O31-C26-C27 | 4.54  | 119.96      | 110.35   |
| 25  | Y     | 304 | CLA  | C4A-NA-C1A  | -4.54 | 104.67      | 106.71   |
| 32  | N     | 619 | AJP  | O31-C26-C27 | 4.53  | 119.94      | 110.35   |
| 25  | c     | 513 | CLA  | O2D-CGD-CBD | 4.53  | 119.31      | 111.27   |
| 32  | Y     | 322 | AJP  | C01-C02-C85 | 4.52  | 119.14      | 111.18   |
| 25  | N     | 603 | CLA  | O2D-CGD-CBD | 4.52  | 119.31      | 111.27   |
| 40  | y     | 318 | NEX  | C5-C6-C1    | -4.52 | 115.21      | 119.70   |
| 25  | B     | 613 | CLA  | CHD-C1D-ND  | -4.52 | 120.30      | 124.45   |
| 25  | b     | 613 | CLA  | CHD-C1D-ND  | -4.52 | 120.30      | 124.45   |
| 25  | B     | 616 | CLA  | O2D-CGD-CBD | 4.51  | 119.29      | 111.27   |
| 25  | S     | 313 | CLA  | O2D-CGD-CBD | 4.51  | 119.29      | 111.27   |
| 25  | C     | 513 | CLA  | O2D-CGD-CBD | 4.51  | 119.28      | 111.27   |
| 40  | Y     | 318 | NEX  | C5-C6-C1    | -4.51 | 115.22      | 119.70   |
| 25  | b     | 616 | CLA  | O2D-CGD-CBD | 4.51  | 119.27      | 111.27   |
| 25  | B     | 608 | CLA  | O2D-CGD-CBD | 4.50  | 119.27      | 111.27   |
| 25  | n     | 610 | CLA  | C4A-NA-C1A  | -4.50 | 104.68      | 106.71   |
| 25  | S     | 303 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 25  | b     | 608 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 25  | s     | 303 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 25  | s     | 313 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 24  | Y     | 307 | CHL  | C1D-ND-C4D  | -4.50 | 103.14      | 106.33   |
| 25  | c     | 506 | CLA  | C1D-ND-C4D  | -4.49 | 103.14      | 106.33   |
| 25  | r     | 610 | CLA  | C2D-C1D-ND  | -4.49 | 106.79      | 110.10   |
| 25  | n     | 603 | CLA  | O2D-CGD-CBD | 4.49  | 119.25      | 111.27   |
| 35  | B     | 626 | DGD  | C3G-O3G-C1D | -4.49 | 104.97      | 113.74   |
| 35  | b     | 626 | DGD  | C3G-O3G-C1D | -4.49 | 104.97      | 113.74   |
| 41  | r     | 616 | XAT  | C31-C30-C29 | -4.48 | 120.91      | 127.31   |
| 25  | S     | 312 | CLA  | CHD-C1D-ND  | -4.48 | 120.34      | 124.45   |
| 25  | Y     | 313 | CLA  | CHD-C1D-ND  | -4.48 | 120.34      | 124.45   |
| 25  | y     | 313 | CLA  | CHD-C1D-ND  | -4.48 | 120.34      | 124.45   |
| 25  | d     | 401 | CLA  | O2D-CGD-CBD | 4.48  | 119.23      | 111.27   |
| 25  | G     | 612 | CLA  | O2D-CGD-CBD | 4.48  | 119.22      | 111.27   |
| 25  | b     | 609 | CLA  | O2D-CGD-CBD | 4.48  | 119.22      | 111.27   |
| 25  | B     | 609 | CLA  | O2D-CGD-CBD | 4.47  | 119.21      | 111.27   |
| 25  | S     | 305 | CLA  | O2D-CGD-CBD | 4.46  | 119.20      | 111.27   |
| 25  | c     | 503 | CLA  | O2D-CGD-CBD | 4.46  | 119.20      | 111.27   |
| 25  | s     | 312 | CLA  | CHD-C1D-ND  | -4.46 | 120.36      | 124.45   |
| 32  | A     | 412 | AJP  | O25-C26-C27 | 4.46  | 119.65      | 108.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 413 | AJP  | O25-C26-C27 | 4.46  | 119.65      | 108.10   |
| 41  | R     | 616 | XAT  | C31-C30-C29 | -4.46 | 120.95      | 127.31   |
| 25  | R     | 610 | CLA  | C2D-C1D-ND  | -4.45 | 106.82      | 110.10   |
| 25  | g     | 602 | CLA  | O1D-CGD-CBD | -4.45 | 115.38      | 124.48   |
| 25  | s     | 305 | CLA  | O2D-CGD-CBD | 4.45  | 119.17      | 111.27   |
| 32  | Y     | 321 | AJP  | O84-C85-C02 | -4.45 | 105.77      | 112.18   |
| 32  | y     | 321 | AJP  | O84-C85-C02 | -4.45 | 105.77      | 112.18   |
| 25  | C     | 503 | CLA  | O2D-CGD-CBD | 4.45  | 119.17      | 111.27   |
| 25  | g     | 612 | CLA  | O2D-CGD-CBD | 4.44  | 119.17      | 111.27   |
| 25  | D     | 401 | CLA  | O2D-CGD-CBD | 4.44  | 119.16      | 111.27   |
| 25  | S     | 305 | CLA  | C1-C2-C3    | -4.44 | 119.57      | 126.75   |
| 32  | Y     | 323 | AJP  | C05-C06-C07 | 4.44  | 110.60      | 103.37   |
| 32  | y     | 323 | AJP  | C05-C06-C07 | 4.44  | 110.60      | 103.37   |
| 32  | Y     | 324 | AJP  | O25-C26-C27 | 4.43  | 119.59      | 108.10   |
| 25  | N     | 610 | CLA  | C4A-NA-C1A  | -4.43 | 104.71      | 106.71   |
| 24  | G     | 606 | CHL  | O2D-CGD-CBD | 4.43  | 119.14      | 111.27   |
| 25  | B     | 601 | CLA  | C1B-CHB-C4A | -4.43 | 121.34      | 130.12   |
| 39  | Y     | 316 | LUT  | C3-C4-C5    | 4.43  | 120.68      | 111.85   |
| 32  | y     | 324 | AJP  | O25-C26-C27 | 4.43  | 119.58      | 108.10   |
| 39  | G     | 615 | LUT  | C3-C4-C5    | 4.43  | 120.67      | 111.85   |
| 39  | g     | 615 | LUT  | C3-C4-C5    | 4.43  | 120.67      | 111.85   |
| 24  | g     | 606 | CHL  | O2D-CGD-CBD | 4.42  | 119.13      | 111.27   |
| 25  | n     | 614 | CLA  | CHD-C1D-ND  | -4.42 | 120.39      | 124.45   |
| 39  | y     | 316 | LUT  | C3-C4-C5    | 4.42  | 120.66      | 111.85   |
| 25  | g     | 602 | CLA  | O2D-CGD-CBD | 4.42  | 119.12      | 111.27   |
| 25  | G     | 602 | CLA  | O1D-CGD-CBD | -4.42 | 115.44      | 124.48   |
| 32  | B     | 624 | AJP  | O40-C39-C38 | 4.42  | 117.72      | 109.69   |
| 32  | b     | 624 | AJP  | O40-C39-C38 | 4.42  | 117.72      | 109.69   |
| 25  | s     | 305 | CLA  | C1-C2-C3    | -4.42 | 119.60      | 126.75   |
| 25  | B     | 610 | CLA  | CHD-C1D-ND  | -4.42 | 120.39      | 124.45   |
| 25  | g     | 614 | CLA  | O2D-CGD-CBD | 4.42  | 119.12      | 111.27   |
| 32  | N     | 619 | AJP  | O77-C28-C29 | 4.42  | 120.90      | 109.94   |
| 25  | r     | 603 | CLA  | C2D-C1D-ND  | -4.41 | 106.85      | 110.10   |
| 25  | b     | 601 | CLA  | C1B-CHB-C4A | -4.41 | 121.38      | 130.12   |
| 24  | 2     | 603 | CHL  | CHD-C1D-ND  | -4.41 | 120.40      | 124.45   |
| 24  | 6     | 603 | CHL  | CHD-C1D-ND  | -4.41 | 120.40      | 124.45   |
| 32  | Y     | 322 | AJP  | O77-C28-C29 | 4.41  | 120.88      | 109.94   |
| 32  | y     | 322 | AJP  | O77-C28-C29 | 4.41  | 120.87      | 109.94   |
| 32  | n     | 619 | AJP  | O77-C28-C29 | 4.40  | 120.87      | 109.94   |
| 25  | C     | 506 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 25  | R     | 610 | CLA  | O2D-CGD-CBD | 4.40  | 119.09      | 111.27   |
| 25  | r     | 610 | CLA  | O2D-CGD-CBD | 4.40  | 119.09      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 323 | AJP  | O84-C85-C02 | -4.40 | 105.84      | 112.18   |
| 25  | G     | 614 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 25  | g     | 614 | CLA  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 25  | N     | 614 | CLA  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 25  | b     | 610 | CLA  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 25  | R     | 603 | CLA  | C2D-C1D-ND  | -4.40 | 106.86      | 110.10   |
| 25  | r     | 611 | CLA  | C4D-C3D-CAD | -4.39 | 102.92      | 108.10   |
| 32  | Y     | 323 | AJP  | O84-C85-C02 | -4.39 | 105.85      | 112.18   |
| 25  | G     | 614 | CLA  | O2D-CGD-CBD | 4.39  | 119.07      | 111.27   |
| 32  | Y     | 321 | AJP  | O25-C26-C27 | 4.39  | 119.48      | 108.10   |
| 32  | B     | 624 | AJP  | C26-O25-C23 | 4.39  | 122.12      | 115.33   |
| 32  | b     | 624 | AJP  | C26-O25-C23 | 4.39  | 122.12      | 115.33   |
| 25  | S     | 309 | CLA  | C4D-CHA-C1A | -4.39 | 115.91      | 121.25   |
| 32  | n     | 619 | AJP  | O25-C26-C27 | 4.39  | 119.46      | 108.10   |
| 40  | S     | 317 | NEX  | C35-C34-C33 | -4.38 | 121.05      | 127.31   |
| 40  | s     | 317 | NEX  | C35-C34-C33 | -4.38 | 121.05      | 127.31   |
| 25  | G     | 602 | CLA  | O2D-CGD-CBD | 4.38  | 119.06      | 111.27   |
| 25  | s     | 309 | CLA  | C4D-CHA-C1A | -4.38 | 115.91      | 121.25   |
| 32  | N     | 619 | AJP  | O25-C26-C27 | 4.38  | 119.46      | 108.10   |
| 32  | y     | 321 | AJP  | O25-C26-C27 | 4.38  | 119.44      | 108.10   |
| 25  | 2     | 602 | CLA  | CHD-C1D-C2D | 4.37  | 134.65      | 125.48   |
| 25  | 6     | 602 | CLA  | CHD-C1D-C2D | 4.37  | 134.65      | 125.48   |
| 25  | B     | 612 | CLA  | O2D-CGD-CBD | 4.37  | 119.04      | 111.27   |
| 25  | b     | 612 | CLA  | O2D-CGD-CBD | 4.37  | 119.04      | 111.27   |
| 25  | c     | 507 | CLA  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 32  | Y     | 323 | AJP  | C01-C02-C03 | 4.37  | 121.60      | 112.09   |
| 25  | N     | 602 | CLA  | CHD-C1D-ND  | -4.37 | 120.44      | 124.45   |
| 25  | R     | 611 | CLA  | C4D-C3D-CAD | -4.37 | 102.95      | 108.10   |
| 25  | B     | 615 | CLA  | CHD-C1D-ND  | -4.36 | 120.44      | 124.45   |
| 32  | N     | 620 | AJP  | C05-C06-C07 | 4.36  | 110.47      | 103.37   |
| 25  | c     | 509 | CLA  | O2D-CGD-CBD | 4.36  | 119.02      | 111.27   |
| 32  | y     | 323 | AJP  | C01-C02-C03 | 4.36  | 121.58      | 112.09   |
| 40  | Y     | 318 | NEX  | C15-C14-C13 | -4.36 | 121.09      | 127.31   |
| 25  | C     | 509 | CLA  | O2D-CGD-CBD | 4.36  | 119.01      | 111.27   |
| 25  | 6     | 605 | CLA  | O2D-CGD-CBD | 4.36  | 119.01      | 111.27   |
| 25  | C     | 507 | CLA  | O2D-CGD-CBD | 4.35  | 119.00      | 111.27   |
| 32  | n     | 620 | AJP  | C05-C06-C07 | 4.35  | 110.46      | 103.37   |
| 39  | N     | 615 | LUT  | C3-C4-C5    | 4.35  | 120.52      | 111.85   |
| 39  | n     | 615 | LUT  | C3-C4-C5    | 4.35  | 120.52      | 111.85   |
| 25  | 6     | 604 | CLA  | O2D-CGD-CBD | 4.35  | 119.00      | 111.27   |
| 40  | r     | 617 | NEX  | C28-C29-C30 | 4.35  | 125.62      | 118.94   |
| 25  | 2     | 604 | CLA  | O2D-CGD-CBD | 4.35  | 118.99      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | n     | 602 | CLA  | CHD-C1D-ND  | -4.35 | 120.46      | 124.45   |
| 40  | R     | 617 | NEX  | C28-C29-C30 | 4.35  | 125.61      | 118.94   |
| 25  | 2     | 605 | CLA  | O2D-CGD-CBD | 4.35  | 118.99      | 111.27   |
| 32  | N     | 619 | AJP  | C12-C07-C08 | -4.34 | 100.19      | 104.88   |
| 25  | y     | 315 | CLA  | C1D-ND-C4D  | -4.34 | 103.25      | 106.33   |
| 41  | r     | 616 | XAT  | C15-C14-C13 | -4.34 | 121.12      | 127.31   |
| 25  | C     | 513 | CLA  | C4D-CHA-C1A | -4.34 | 115.97      | 121.25   |
| 25  | c     | 513 | CLA  | C4D-CHA-C1A | -4.33 | 115.97      | 121.25   |
| 32  | A     | 412 | AJP  | O77-C28-C29 | 4.33  | 121.43      | 109.94   |
| 32  | a     | 413 | AJP  | O77-C28-C29 | 4.33  | 121.43      | 109.94   |
| 25  | N     | 604 | CLA  | C1-C2-C3    | -4.33 | 119.74      | 126.75   |
| 41  | R     | 616 | XAT  | C15-C14-C13 | -4.33 | 121.13      | 127.31   |
| 25  | n     | 604 | CLA  | C1-C2-C3    | -4.33 | 119.75      | 126.75   |
| 24  | y     | 307 | CHL  | C2D-C1D-ND  | 4.32  | 113.29      | 110.10   |
| 25  | Y     | 305 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 25  | y     | 305 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 40  | y     | 318 | NEX  | C15-C14-C13 | -4.32 | 121.15      | 127.31   |
| 25  | N     | 602 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 25  | Y     | 315 | CLA  | C1D-ND-C4D  | -4.32 | 103.27      | 106.33   |
| 25  | n     | 602 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 32  | Y     | 320 | AJP  | O25-C26-C27 | 4.31  | 119.27      | 108.10   |
| 32  | y     | 320 | AJP  | O25-C26-C27 | 4.31  | 119.27      | 108.10   |
| 32  | N     | 619 | AJP  | C01-C02-C85 | 4.31  | 118.76      | 111.18   |
| 32  | n     | 619 | AJP  | C01-C02-C85 | 4.31  | 118.76      | 111.18   |
| 25  | R     | 611 | CLA  | O2D-CGD-CBD | 4.30  | 118.91      | 111.27   |
| 25  | c     | 501 | CLA  | C1-C2-C3    | -4.30 | 118.60      | 126.04   |
| 25  | 6     | 604 | CLA  | C2D-C1D-ND  | -4.30 | 106.94      | 110.10   |
| 32  | a     | 413 | AJP  | O54-C36-C35 | 4.30  | 119.36      | 108.61   |
| 32  | n     | 619 | AJP  | C12-C07-C08 | -4.30 | 100.24      | 104.88   |
| 24  | G     | 607 | CHL  | CMB-C2B-C1B | -4.29 | 121.86      | 128.46   |
| 25  | D     | 403 | CLA  | O2D-CGD-CBD | 4.29  | 118.90      | 111.27   |
| 25  | r     | 611 | CLA  | O2D-CGD-CBD | 4.29  | 118.89      | 111.27   |
| 25  | d     | 403 | CLA  | O2D-CGD-CBD | 4.29  | 118.89      | 111.27   |
| 32  | A     | 412 | AJP  | O54-C36-C35 | 4.29  | 119.33      | 108.61   |
| 25  | C     | 501 | CLA  | C1-C2-C3    | -4.29 | 118.63      | 126.04   |
| 25  | b     | 615 | CLA  | CHD-C1D-ND  | -4.28 | 120.52      | 124.45   |
| 25  | 2     | 604 | CLA  | C2D-C1D-ND  | -4.28 | 106.95      | 110.10   |
| 25  | b     | 609 | CLA  | C1D-ND-C4D  | -4.28 | 103.29      | 106.33   |
| 40  | r     | 617 | NEX  | C15-C35-C34 | 4.28  | 132.24      | 123.47   |
| 32  | s     | 319 | AJP  | O77-C28-C27 | 4.28  | 118.71      | 110.14   |
| 40  | R     | 617 | NEX  | C15-C35-C34 | 4.28  | 132.23      | 123.47   |
| 24  | g     | 607 | CHL  | CMB-C2B-C1B | -4.28 | 121.89      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | S     | 319 | AJP  | O77-C28-C27 | 4.27  | 118.69      | 110.14   |
| 39  | r     | 615 | LUT  | C3-C4-C5    | 4.27  | 120.36      | 111.85   |
| 39  | R     | 615 | LUT  | C3-C4-C5    | 4.27  | 120.36      | 111.85   |
| 25  | Y     | 303 | CLA  | O1D-CGD-CBD | -4.27 | 115.75      | 124.48   |
| 25  | y     | 303 | CLA  | O1D-CGD-CBD | -4.27 | 115.75      | 124.48   |
| 32  | G     | 618 | AJP  | O25-C23-C24 | 4.26  | 117.85      | 109.62   |
| 24  | Y     | 307 | CHL  | C2D-C1D-ND  | 4.25  | 113.24      | 110.10   |
| 25  | D     | 402 | CLA  | C4A-NA-C1A  | -4.25 | 104.79      | 106.71   |
| 40  | r     | 617 | NEX  | C20-C13-C14 | -4.24 | 116.99      | 122.92   |
| 25  | g     | 604 | CLA  | C1D-ND-C4D  | -4.23 | 103.33      | 106.33   |
| 40  | R     | 617 | NEX  | C20-C13-C14 | -4.23 | 117.00      | 122.92   |
| 25  | Y     | 311 | CLA  | C4A-NA-C1A  | -4.23 | 104.80      | 106.71   |
| 32  | g     | 618 | AJP  | O25-C23-C24 | 4.23  | 117.80      | 109.62   |
| 25  | B     | 609 | CLA  | C1D-ND-C4D  | -4.23 | 103.33      | 106.33   |
| 25  | g     | 613 | CLA  | C4D-CHA-C1A | -4.23 | 116.11      | 121.25   |
| 39  | y     | 316 | LUT  | C2-C3-C4    | 4.23  | 116.09      | 110.30   |
| 25  | B     | 614 | CLA  | C1D-ND-C4D  | -4.22 | 103.33      | 106.33   |
| 25  | b     | 614 | CLA  | C1D-ND-C4D  | -4.22 | 103.33      | 106.33   |
| 26  | R     | 618 | LHG  | O7-C7-C8    | 4.22  | 120.59      | 111.50   |
| 25  | D     | 401 | CLA  | C1-C2-C3    | -4.22 | 119.93      | 126.75   |
| 32  | B     | 624 | AJP  | O25-C26-O31 | 4.21  | 122.44      | 110.67   |
| 32  | b     | 624 | AJP  | O25-C26-O31 | 4.21  | 122.44      | 110.67   |
| 39  | Y     | 316 | LUT  | C2-C3-C4    | 4.21  | 116.07      | 110.30   |
| 25  | d     | 401 | CLA  | C1-C2-C3    | -4.21 | 119.94      | 126.75   |
| 32  | N     | 620 | AJP  | O25-C23-C24 | 4.21  | 117.76      | 109.62   |
| 32  | n     | 620 | AJP  | O25-C23-C24 | 4.21  | 117.76      | 109.62   |
| 25  | G     | 613 | CLA  | C4D-CHA-C1A | -4.20 | 116.13      | 121.25   |
| 26  | r     | 618 | LHG  | O7-C7-C8    | 4.20  | 120.56      | 111.50   |
| 25  | d     | 402 | CLA  | C4A-NA-C1A  | -4.19 | 104.82      | 106.71   |
| 25  | C     | 501 | CLA  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 25  | c     | 501 | CLA  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 25  | R     | 609 | CLA  | O2D-CGD-CBD | 4.18  | 118.70      | 111.27   |
| 25  | r     | 609 | CLA  | O2D-CGD-CBD | 4.18  | 118.69      | 111.27   |
| 25  | b     | 603 | CLA  | C1D-ND-C4D  | -4.18 | 103.37      | 106.33   |
| 25  | G     | 604 | CLA  | C1D-ND-C4D  | -4.18 | 103.37      | 106.33   |
| 32  | Y     | 320 | AJP  | O77-C28-C29 | 4.17  | 120.28      | 109.94   |
| 32  | y     | 320 | AJP  | O77-C28-C29 | 4.17  | 120.28      | 109.94   |
| 25  | y     | 311 | CLA  | C4A-NA-C1A  | -4.17 | 104.83      | 106.71   |
| 25  | D     | 403 | CLA  | C2D-C1D-ND  | -4.17 | 107.03      | 110.10   |
| 25  | d     | 403 | CLA  | C2D-C1D-ND  | -4.17 | 107.03      | 110.10   |
| 25  | B     | 608 | CLA  | C1D-ND-C4D  | -4.17 | 103.38      | 106.33   |
| 25  | b     | 608 | CLA  | C1D-ND-C4D  | -4.17 | 103.38      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | G     | 602 | CLA  | C4A-NA-C1A  | -4.16 | 104.83      | 106.71   |
| 25  | g     | 602 | CLA  | C4A-NA-C1A  | -4.16 | 104.83      | 106.71   |
| 32  | A     | 412 | AJP  | C49-C48-C47 | 4.16  | 114.78      | 109.67   |
| 25  | n     | 603 | CLA  | C4A-NA-C1A  | -4.16 | 104.84      | 106.71   |
| 25  | g     | 613 | CLA  | O2D-CGD-CBD | 4.16  | 118.66      | 111.27   |
| 32  | Y     | 321 | AJP  | O77-C28-C29 | 4.16  | 120.25      | 109.94   |
| 25  | D     | 401 | CLA  | C4D-CHA-C1A | -4.16 | 116.19      | 121.25   |
| 25  | d     | 401 | CLA  | C4D-CHA-C1A | -4.16 | 116.19      | 121.25   |
| 25  | y     | 314 | CLA  | O2D-CGD-CBD | 4.15  | 118.65      | 111.27   |
| 25  | S     | 303 | CLA  | C1D-ND-C4D  | -4.15 | 103.38      | 106.33   |
| 25  | s     | 303 | CLA  | C1D-ND-C4D  | -4.15 | 103.38      | 106.33   |
| 25  | G     | 613 | CLA  | O2D-CGD-CBD | 4.15  | 118.65      | 111.27   |
| 32  | a     | 413 | AJP  | C49-C48-C47 | 4.15  | 114.77      | 109.67   |
| 32  | y     | 321 | AJP  | O77-C28-C29 | 4.15  | 120.24      | 109.94   |
| 25  | Y     | 314 | CLA  | O2D-CGD-CBD | 4.14  | 118.62      | 111.27   |
| 25  | c     | 504 | CLA  | C2D-C1D-ND  | -4.14 | 107.06      | 110.10   |
| 26  | C     | 517 | LHG  | O7-C7-C8    | 4.13  | 120.40      | 111.50   |
| 26  | c     | 517 | LHG  | O7-C7-C8    | 4.13  | 120.40      | 111.50   |
| 25  | D     | 403 | CLA  | C2A-C3A-C4A | -4.13 | 95.20       | 101.87   |
| 25  | d     | 403 | CLA  | C2A-C3A-C4A | -4.13 | 95.20       | 101.87   |
| 25  | G     | 603 | CLA  | O2D-CGD-CBD | 4.12  | 118.59      | 111.27   |
| 25  | g     | 603 | CLA  | O2D-CGD-CBD | 4.12  | 118.59      | 111.27   |
| 24  | 2     | 603 | CHL  | C3C-C4C-NC  | -4.12 | 105.95      | 110.57   |
| 25  | r     | 601 | CLA  | O2D-CGD-CBD | 4.11  | 118.57      | 111.27   |
| 32  | n     | 619 | AJP  | O31-C30-C29 | 4.11  | 116.60      | 110.04   |
| 25  | B     | 603 | CLA  | C1D-ND-C4D  | -4.11 | 103.42      | 106.33   |
| 40  | n     | 617 | NEX  | C20-C13-C14 | -4.11 | 117.17      | 122.92   |
| 25  | s     | 314 | CLA  | C4A-NA-C1A  | -4.11 | 104.86      | 106.71   |
| 25  | B     | 604 | CLA  | C1-C2-C3    | -4.11 | 118.94      | 126.04   |
| 25  | b     | 604 | CLA  | C1-C2-C3    | -4.11 | 118.94      | 126.04   |
| 40  | n     | 617 | NEX  | C12-C13-C14 | 4.11  | 125.24      | 118.94   |
| 25  | C     | 504 | CLA  | C2D-C1D-ND  | -4.10 | 107.08      | 110.10   |
| 25  | S     | 311 | CLA  | C1B-CHB-C4A | -4.10 | 122.00      | 130.12   |
| 25  | s     | 311 | CLA  | C1B-CHB-C4A | -4.10 | 122.00      | 130.12   |
| 24  | 6     | 603 | CHL  | C3C-C4C-NC  | -4.10 | 105.98      | 110.57   |
| 30  | C     | 520 | LMG  | O7-C10-C11  | 4.09  | 120.33      | 111.50   |
| 30  | c     | 520 | LMG  | O7-C10-C11  | 4.09  | 120.33      | 111.50   |
| 25  | c     | 509 | CLA  | C1B-CHB-C4A | -4.09 | 122.01      | 130.12   |
| 25  | C     | 509 | CLA  | C1B-CHB-C4A | -4.09 | 122.01      | 130.12   |
| 40  | N     | 617 | NEX  | C20-C13-C14 | -4.09 | 117.19      | 122.92   |
| 25  | R     | 602 | CLA  | C1D-ND-C4D  | -4.09 | 103.43      | 106.33   |
| 25  | S     | 314 | CLA  | C4A-NA-C1A  | -4.09 | 104.87      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 2     | 603 | CHL  | OBD-CAD-C3D | 4.09  | 138.36      | 128.52   |
| 24  | 6     | 603 | CHL  | OBD-CAD-C3D | 4.09  | 138.36      | 128.52   |
| 25  | R     | 601 | CLA  | O2D-CGD-CBD | 4.09  | 118.53      | 111.27   |
| 32  | N     | 619 | AJP  | O31-C30-C29 | 4.09  | 116.56      | 110.04   |
| 35  | C     | 516 | DGD  | C1D-O6D-C5D | -4.08 | 105.68      | 113.69   |
| 35  | c     | 516 | DGD  | C1D-O6D-C5D | -4.08 | 105.68      | 113.69   |
| 25  | C     | 502 | CLA  | C1D-ND-C4D  | -4.08 | 103.44      | 106.33   |
| 25  | c     | 502 | CLA  | C1D-ND-C4D  | -4.08 | 103.44      | 106.33   |
| 25  | r     | 603 | CLA  | O2D-CGD-CBD | 4.07  | 118.50      | 111.27   |
| 40  | G     | 617 | NEX  | C38-C25-C26 | -4.07 | 115.44      | 122.26   |
| 25  | r     | 602 | CLA  | C1D-ND-C4D  | -4.07 | 103.44      | 106.33   |
| 26  | B     | 622 | LHG  | O7-C7-C8    | 4.07  | 120.27      | 111.50   |
| 26  | b     | 622 | LHG  | O7-C7-C8    | 4.07  | 120.27      | 111.50   |
| 39  | G     | 615 | LUT  | C2-C3-C4    | 4.07  | 115.87      | 110.30   |
| 39  | g     | 615 | LUT  | C2-C3-C4    | 4.07  | 115.87      | 110.30   |
| 25  | N     | 603 | CLA  | C4A-NA-C1A  | -4.07 | 104.88      | 106.71   |
| 40  | N     | 617 | NEX  | C12-C13-C14 | 4.07  | 125.18      | 118.94   |
| 25  | R     | 603 | CLA  | O2D-CGD-CBD | 4.06  | 118.49      | 111.27   |
| 24  | N     | 601 | CHL  | O2D-CGD-CBD | 4.06  | 118.48      | 111.27   |
| 40  | g     | 617 | NEX  | C38-C25-C26 | -4.05 | 115.47      | 122.26   |
| 25  | Y     | 312 | CLA  | CHD-C1D-ND  | -4.05 | 120.73      | 124.45   |
| 32  | Y     | 320 | AJP  | C01-C02-C85 | 4.05  | 118.31      | 111.18   |
| 25  | r     | 602 | CLA  | C1-C2-C3    | -4.05 | 119.04      | 126.04   |
| 32  | a     | 413 | AJP  | C35-O40-C39 | 4.05  | 121.63      | 113.69   |
| 40  | r     | 617 | NEX  | C39-C29-C30 | -4.04 | 117.26      | 122.92   |
| 32  | A     | 412 | AJP  | C35-O40-C39 | 4.04  | 121.63      | 113.69   |
| 25  | C     | 511 | CLA  | C2A-C3A-C4A | -4.04 | 95.34       | 101.87   |
| 26  | Y     | 301 | LHG  | O7-C7-C8    | 4.04  | 120.21      | 111.50   |
| 40  | R     | 617 | NEX  | C39-C29-C30 | -4.04 | 117.26      | 122.92   |
| 40  | y     | 318 | NEX  | O24-C25-C24 | 4.04  | 116.42      | 113.38   |
| 25  | r     | 601 | CLA  | CHD-C1D-C2D | 4.04  | 133.95      | 125.48   |
| 25  | r     | 612 | CLA  | CHD-C1D-C2D | 4.04  | 133.95      | 125.48   |
| 26  | B     | 621 | LHG  | O7-C7-C8    | 4.04  | 120.20      | 111.50   |
| 26  | b     | 621 | LHG  | O7-C7-C8    | 4.04  | 120.20      | 111.50   |
| 26  | Y     | 319 | LHG  | O7-C7-C8    | 4.03  | 120.19      | 111.50   |
| 32  | y     | 320 | AJP  | C01-C02-C85 | 4.03  | 118.28      | 111.18   |
| 32  | B     | 624 | AJP  | O53-C46-C47 | 4.03  | 119.67      | 110.35   |
| 32  | b     | 624 | AJP  | O53-C46-C47 | 4.03  | 119.67      | 110.35   |
| 32  | S     | 319 | AJP  | C03-C04-C05 | -4.03 | 104.97      | 111.93   |
| 32  | s     | 319 | AJP  | C03-C04-C05 | -4.03 | 104.97      | 111.93   |
| 26  | y     | 301 | LHG  | O7-C7-C8    | 4.03  | 120.18      | 111.50   |
| 26  | y     | 319 | LHG  | O7-C7-C8    | 4.02  | 120.17      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | r     | 601 | CLA  | C4D-CHA-C1A | -4.02 | 116.35      | 121.25   |
| 24  | l     | 302 | CHL  | O2D-CGD-CBD | 4.02  | 118.41      | 111.27   |
| 25  | R     | 601 | CLA  | CHD-C1D-C2D | 4.02  | 133.91      | 125.48   |
| 27  | A     | 403 | PHO  | C1-C2-C3    | -4.02 | 119.10      | 126.04   |
| 27  | a     | 404 | PHO  | C1-C2-C3    | -4.02 | 119.10      | 126.04   |
| 25  | R     | 602 | CLA  | C1-C2-C3    | -4.02 | 119.10      | 126.04   |
| 25  | R     | 601 | CLA  | C4D-CHA-C1A | -4.01 | 116.36      | 121.25   |
| 25  | R     | 612 | CLA  | CHD-C1D-C2D | 4.01  | 133.89      | 125.48   |
| 24  | n     | 601 | CHL  | O2D-CGD-CBD | 4.01  | 118.40      | 111.27   |
| 24  | 5     | 302 | CHL  | O2D-CGD-CBD | 4.01  | 118.39      | 111.27   |
| 25  | R     | 604 | CLA  | C1B-CHB-C4A | -4.01 | 122.18      | 130.12   |
| 25  | r     | 604 | CLA  | C1B-CHB-C4A | -4.01 | 122.18      | 130.12   |
| 25  | y     | 312 | CLA  | CHD-C1D-ND  | -4.01 | 120.77      | 124.45   |
| 25  | c     | 511 | CLA  | C2A-C3A-C4A | -4.01 | 95.40       | 101.87   |
| 25  | G     | 603 | CLA  | C1D-ND-C4D  | -4.00 | 103.49      | 106.33   |
| 25  | g     | 603 | CLA  | C1D-ND-C4D  | -4.00 | 103.49      | 106.33   |
| 25  | n     | 612 | CLA  | O2D-CGD-CBD | 4.00  | 118.38      | 111.27   |
| 25  | b     | 605 | CLA  | C1B-CHB-C4A | -4.00 | 122.20      | 130.12   |
| 32  | A     | 412 | AJP  | C04-C03-C02 | -4.00 | 103.38      | 111.81   |
| 32  | a     | 413 | AJP  | C04-C03-C02 | -4.00 | 103.38      | 111.81   |
| 32  | A     | 412 | AJP  | C26-O31-C30 | 3.99  | 121.52      | 113.69   |
| 32  | a     | 413 | AJP  | C26-O31-C30 | 3.99  | 121.52      | 113.69   |
| 25  | B     | 603 | CLA  | C4A-NA-C1A  | -3.99 | 104.91      | 106.71   |
| 25  | b     | 603 | CLA  | C4A-NA-C1A  | -3.99 | 104.91      | 106.71   |
| 32  | Y     | 324 | AJP  | C01-C02-C85 | 3.99  | 118.20      | 111.18   |
| 32  | y     | 324 | AJP  | C01-C02-C85 | 3.99  | 118.20      | 111.18   |
| 24  | y     | 310 | CHL  | O2D-CGD-CBD | 3.98  | 118.35      | 111.27   |
| 25  | y     | 305 | CLA  | C1-C2-C3    | -3.98 | 120.31      | 126.75   |
| 32  | A     | 412 | AJP  | C67-C68-C69 | -3.98 | 103.13      | 110.24   |
| 32  | a     | 413 | AJP  | C67-C68-C69 | -3.98 | 103.13      | 110.24   |
| 30  | b     | 623 | LMG  | O7-C10-C11  | 3.98  | 120.08      | 111.50   |
| 25  | r     | 604 | CLA  | CHD-C1D-C2D | 3.98  | 133.83      | 125.48   |
| 25  | S     | 305 | CLA  | CHD-C1D-C2D | 3.98  | 133.83      | 125.48   |
| 25  | s     | 305 | CLA  | CHD-C1D-C2D | 3.98  | 133.83      | 125.48   |
| 25  | N     | 604 | CLA  | C4D-CHA-C1A | -3.98 | 116.41      | 121.25   |
| 25  | N     | 612 | CLA  | O2D-CGD-CBD | 3.98  | 118.34      | 111.27   |
| 39  | n     | 615 | LUT  | C18-C5-C4   | -3.98 | 106.99      | 114.36   |
| 25  | B     | 605 | CLA  | C1B-CHB-C4A | -3.98 | 122.24      | 130.12   |
| 25  | b     | 613 | CLA  | C4A-NA-C1A  | -3.97 | 104.92      | 106.71   |
| 26  | B     | 625 | LHG  | O7-C7-C8    | 3.97  | 120.06      | 111.50   |
| 26  | b     | 625 | LHG  | O7-C7-C8    | 3.97  | 120.06      | 111.50   |
| 24  | r     | 606 | CHL  | O2D-CGD-CBD | 3.97  | 118.33      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | n     | 604 | CLA  | C4D-CHA-C1A | -3.97 | 116.42      | 121.25   |
| 24  | R     | 606 | CHL  | O2D-CGD-CBD | 3.97  | 118.33      | 111.27   |
| 25  | C     | 504 | CLA  | O2D-CGD-CBD | 3.97  | 118.32      | 111.27   |
| 39  | N     | 615 | LUT  | C18-C5-C4   | -3.97 | 107.00      | 114.36   |
| 25  | c     | 504 | CLA  | O2D-CGD-CBD | 3.97  | 118.32      | 111.27   |
| 25  | R     | 604 | CLA  | CHD-C1D-C2D | 3.97  | 133.80      | 125.48   |
| 30  | A     | 410 | LMG  | O7-C10-C11  | 3.96  | 120.04      | 111.50   |
| 30  | a     | 411 | LMG  | O7-C10-C11  | 3.96  | 120.04      | 111.50   |
| 30  | B     | 623 | LMG  | O7-C10-C11  | 3.96  | 120.04      | 111.50   |
| 24  | Y     | 310 | CHL  | O2D-CGD-CBD | 3.96  | 118.31      | 111.27   |
| 25  | Y     | 305 | CLA  | C1-C2-C3    | -3.96 | 120.35      | 126.75   |
| 25  | S     | 312 | CLA  | C1D-ND-C4D  | -3.96 | 103.53      | 106.33   |
| 32  | y     | 322 | AJP  | C29-C28-C27 | 3.95  | 116.43      | 110.69   |
| 25  | R     | 610 | CLA  | CHD-C1D-C2D | 3.95  | 133.77      | 125.48   |
| 25  | r     | 610 | CLA  | CHD-C1D-C2D | 3.95  | 133.77      | 125.48   |
| 24  | Y     | 306 | CHL  | O2D-CGD-CBD | 3.95  | 118.29      | 111.27   |
| 24  | y     | 306 | CHL  | O2D-CGD-CBD | 3.95  | 118.29      | 111.27   |
| 39  | Y     | 317 | LUT  | C18-C5-C4   | -3.95 | 107.04      | 114.36   |
| 26  | l     | 103 | LHG  | O7-C7-C8    | 3.95  | 120.00      | 111.50   |
| 25  | C     | 504 | CLA  | C1-C2-C3    | -3.94 | 119.22      | 126.04   |
| 25  | y     | 312 | CLA  | C4A-NA-C1A  | -3.94 | 104.93      | 106.71   |
| 25  | 6     | 604 | CLA  | CHD-C1D-C2D | 3.94  | 133.75      | 125.48   |
| 25  | R     | 603 | CLA  | CHD-C1D-C2D | 3.94  | 133.74      | 125.48   |
| 32  | Y     | 323 | AJP  | O25-C23-C24 | 3.94  | 117.23      | 109.62   |
| 32  | y     | 323 | AJP  | O25-C23-C24 | 3.94  | 117.23      | 109.62   |
| 39  | y     | 317 | LUT  | C18-C5-C4   | -3.94 | 107.06      | 114.36   |
| 25  | 2     | 604 | CLA  | CHD-C1D-C2D | 3.93  | 133.73      | 125.48   |
| 25  | B     | 604 | CLA  | C4A-NA-C1A  | -3.93 | 104.94      | 106.71   |
| 25  | b     | 604 | CLA  | C4A-NA-C1A  | -3.93 | 104.94      | 106.71   |
| 25  | c     | 504 | CLA  | C1-C2-C3    | -3.93 | 119.24      | 126.04   |
| 32  | Y     | 322 | AJP  | C29-C28-C27 | 3.93  | 116.40      | 110.69   |
| 25  | B     | 615 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 25  | n     | 603 | CLA  | C1D-ND-C4D  | -3.93 | 103.54      | 106.33   |
| 26  | L     | 102 | LHG  | O7-C7-C8    | 3.93  | 119.97      | 111.50   |
| 40  | Y     | 318 | NEX  | O24-C25-C24 | 3.93  | 116.33      | 113.38   |
| 32  | A     | 412 | AJP  | C26-C27-C28 | -3.93 | 101.82      | 110.00   |
| 32  | a     | 413 | AJP  | C26-C27-C28 | -3.93 | 101.82      | 110.00   |
| 25  | Y     | 313 | CLA  | C1-C2-C3    | -3.92 | 119.26      | 126.04   |
| 30  | A     | 408 | LMG  | O7-C10-C11  | 3.92  | 119.96      | 111.50   |
| 25  | B     | 612 | CLA  | C1B-CHB-C4A | -3.92 | 122.35      | 130.12   |
| 26  | d     | 406 | LHG  | O7-C7-C8    | 3.92  | 119.95      | 111.50   |
| 30  | B     | 620 | LMG  | O7-C10-C11  | 3.92  | 119.95      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 620 | LMG  | O7-C10-C11  | 3.92  | 119.95      | 111.50   |
| 39  | n     | 616 | LUT  | C18-C5-C4   | -3.92 | 107.09      | 114.36   |
| 32  | g     | 618 | AJP  | O31-C26-C27 | 3.92  | 118.64      | 110.35   |
| 26  | D     | 406 | LHG  | O7-C7-C8    | 3.92  | 119.94      | 111.50   |
| 25  | r     | 603 | CLA  | CHD-C1D-C2D | 3.91  | 133.69      | 125.48   |
| 39  | N     | 616 | LUT  | C18-C5-C4   | -3.91 | 107.11      | 114.36   |
| 25  | B     | 613 | CLA  | C4A-NA-C1A  | -3.91 | 104.95      | 106.71   |
| 32  | G     | 618 | AJP  | O31-C26-C27 | 3.91  | 118.63      | 110.35   |
| 25  | D     | 403 | CLA  | CHD-C1D-C2D | 3.91  | 133.68      | 125.48   |
| 25  | d     | 403 | CLA  | CHD-C1D-C2D | 3.91  | 133.68      | 125.48   |
| 25  | b     | 612 | CLA  | C1B-CHB-C4A | -3.91 | 122.38      | 130.12   |
| 25  | C     | 504 | CLA  | CHD-C1D-C2D | 3.90  | 133.67      | 125.48   |
| 25  | c     | 504 | CLA  | CHD-C1D-C2D | 3.90  | 133.67      | 125.48   |
| 25  | S     | 310 | CLA  | C1D-ND-C4D  | -3.90 | 103.56      | 106.33   |
| 25  | N     | 603 | CLA  | C1D-ND-C4D  | -3.90 | 103.56      | 106.33   |
| 25  | b     | 612 | CLA  | C1D-ND-C4D  | -3.90 | 103.56      | 106.33   |
| 25  | n     | 614 | CLA  | O2D-CGD-CBD | 3.90  | 118.19      | 111.27   |
| 30  | a     | 409 | LMG  | O7-C10-C11  | 3.90  | 119.90      | 111.50   |
| 39  | g     | 615 | LUT  | C18-C5-C4   | -3.90 | 107.14      | 114.36   |
| 25  | N     | 611 | CLA  | CHD-C1D-ND  | -3.90 | 120.87      | 124.45   |
| 39  | G     | 615 | LUT  | C18-C5-C4   | -3.90 | 107.14      | 114.36   |
| 25  | y     | 313 | CLA  | C1-C2-C3    | -3.90 | 119.31      | 126.04   |
| 25  | c     | 509 | CLA  | C1D-ND-C4D  | -3.90 | 103.57      | 106.33   |
| 25  | C     | 509 | CLA  | C1D-ND-C4D  | -3.89 | 103.57      | 106.33   |
| 25  | s     | 310 | CLA  | C1D-ND-C4D  | -3.89 | 103.57      | 106.33   |
| 25  | n     | 611 | CLA  | CHD-C1D-ND  | -3.89 | 120.88      | 124.45   |
| 25  | b     | 615 | CLA  | C1D-ND-C4D  | -3.89 | 103.58      | 106.33   |
| 25  | N     | 614 | CLA  | O2D-CGD-CBD | 3.88  | 118.17      | 111.27   |
| 25  | s     | 312 | CLA  | C1D-ND-C4D  | -3.88 | 103.58      | 106.33   |
| 25  | r     | 603 | CLA  | C1-C2-C3    | -3.88 | 119.34      | 126.04   |
| 32  | N     | 619 | AJP  | C03-C04-C05 | -3.88 | 105.23      | 111.93   |
| 25  | R     | 614 | CLA  | O2D-CGD-CBD | 3.87  | 118.15      | 111.27   |
| 25  | r     | 614 | CLA  | O2D-CGD-CBD | 3.87  | 118.15      | 111.27   |
| 32  | N     | 620 | AJP  | O31-C30-C29 | 3.87  | 116.22      | 110.04   |
| 32  | n     | 620 | AJP  | O31-C30-C29 | 3.87  | 116.22      | 110.04   |
| 25  | Y     | 304 | CLA  | C1D-ND-C4D  | -3.87 | 103.58      | 106.33   |
| 26  | s     | 301 | LHG  | O7-C7-C8    | 3.87  | 119.84      | 111.50   |
| 26  | c     | 518 | LHG  | O7-C7-C8    | 3.87  | 119.83      | 111.50   |
| 25  | G     | 602 | CLA  | O2D-CGD-O1D | -3.87 | 116.28      | 123.84   |
| 32  | a     | 413 | AJP  | O50-C49-C48 | 3.87  | 116.74      | 110.77   |
| 32  | Y     | 321 | AJP  | C01-C02-C85 | 3.86  | 117.98      | 111.18   |
| 32  | y     | 321 | AJP  | C01-C02-C85 | 3.86  | 117.98      | 111.18   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | S     | 301 | LHG  | O7-C7-C8    | 3.86  | 119.83      | 111.50   |
| 26  | C     | 518 | LHG  | O7-C7-C8    | 3.86  | 119.82      | 111.50   |
| 24  | 2     | 601 | CHL  | CAA-C2A-C3A | -3.86 | 102.20      | 112.78   |
| 25  | g     | 602 | CLA  | O2D-CGD-O1D | -3.86 | 116.29      | 123.84   |
| 32  | A     | 412 | AJP  | O50-C49-C48 | 3.86  | 116.73      | 110.77   |
| 25  | s     | 309 | CLA  | C1B-CHB-C4A | -3.86 | 122.48      | 130.12   |
| 35  | A     | 415 | DGD  | C6D-O5D-C1E | -3.86 | 106.21      | 113.74   |
| 35  | a     | 401 | DGD  | C6D-O5D-C1E | -3.86 | 106.21      | 113.74   |
| 32  | n     | 619 | AJP  | C03-C04-C05 | -3.86 | 105.27      | 111.93   |
| 25  | B     | 612 | CLA  | C1D-ND-C4D  | -3.85 | 103.60      | 106.33   |
| 40  | y     | 318 | NEX  | C25-C24-C23 | -3.85 | 105.13      | 112.75   |
| 25  | S     | 309 | CLA  | C1B-CHB-C4A | -3.85 | 122.49      | 130.12   |
| 39  | r     | 615 | LUT  | C18-C5-C4   | -3.85 | 107.22      | 114.36   |
| 24  | r     | 613 | CHL  | O2D-CGD-CBD | 3.85  | 118.11      | 111.27   |
| 24  | g     | 605 | CHL  | O2D-CGD-CBD | 3.85  | 118.11      | 111.27   |
| 40  | N     | 617 | NEX  | C38-C25-C26 | -3.85 | 115.81      | 122.26   |
| 39  | R     | 615 | LUT  | C2-C3-C4    | 3.85  | 115.57      | 110.30   |
| 25  | R     | 603 | CLA  | C1-C2-C3    | -3.84 | 119.39      | 126.04   |
| 39  | R     | 615 | LUT  | C18-C5-C4   | -3.84 | 107.23      | 114.36   |
| 24  | 6     | 601 | CHL  | CAA-C2A-C3A | -3.84 | 102.26      | 112.78   |
| 30  | D     | 407 | LMG  | O7-C10-C11  | 3.84  | 119.78      | 111.50   |
| 30  | d     | 407 | LMG  | O7-C10-C11  | 3.84  | 119.78      | 111.50   |
| 39  | r     | 615 | LUT  | C2-C3-C4    | 3.84  | 115.56      | 110.30   |
| 32  | Y     | 322 | AJP  | O31-C26-C27 | 3.84  | 118.47      | 110.35   |
| 24  | R     | 613 | CHL  | O2D-CGD-CBD | 3.84  | 118.09      | 111.27   |
| 40  | Y     | 318 | NEX  | C25-C24-C23 | -3.83 | 105.16      | 112.75   |
| 25  | B     | 607 | CLA  | C1D-ND-C4D  | -3.83 | 103.61      | 106.33   |
| 25  | b     | 607 | CLA  | C1D-ND-C4D  | -3.83 | 103.61      | 106.33   |
| 24  | G     | 605 | CHL  | O2D-CGD-CBD | 3.83  | 118.08      | 111.27   |
| 40  | n     | 617 | NEX  | C38-C25-C26 | -3.83 | 115.84      | 122.26   |
| 40  | n     | 617 | NEX  | C27-C28-C29 | -3.83 | 119.58      | 125.53   |
| 32  | y     | 322 | AJP  | O31-C26-C27 | 3.83  | 118.46      | 110.35   |
| 39  | y     | 316 | LUT  | C18-C5-C4   | -3.83 | 107.26      | 114.36   |
| 40  | Y     | 318 | NEX  | C38-C25-C26 | -3.83 | 115.84      | 122.26   |
| 40  | y     | 318 | NEX  | C38-C25-C26 | -3.83 | 115.84      | 122.26   |
| 25  | B     | 615 | CLA  | C1-C2-C3    | -3.83 | 119.42      | 126.04   |
| 25  | b     | 615 | CLA  | C1-C2-C3    | -3.83 | 119.42      | 126.04   |
| 25  | r     | 610 | CLA  | C4D-CHA-C1A | -3.83 | 116.59      | 121.25   |
| 24  | n     | 608 | CHL  | O2D-CGD-CBD | 3.82  | 118.06      | 111.27   |
| 25  | Y     | 312 | CLA  | C4A-NA-C1A  | -3.82 | 104.99      | 106.71   |
| 39  | Y     | 316 | LUT  | C18-C5-C4   | -3.82 | 107.27      | 114.36   |
| 25  | y     | 304 | CLA  | C1D-ND-C4D  | -3.82 | 103.62      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | n     | 611 | CLA  | C1-C2-C3    | -3.82 | 119.44      | 126.04   |
| 25  | n     | 604 | CLA  | C1D-ND-C4D  | -3.82 | 103.62      | 106.33   |
| 25  | 2     | 604 | CLA  | C1-C2-C3    | -3.81 | 119.44      | 126.04   |
| 25  | 6     | 604 | CLA  | C1-C2-C3    | -3.81 | 119.44      | 126.04   |
| 25  | B     | 613 | CLA  | O2D-CGD-CBD | 3.81  | 118.05      | 111.27   |
| 25  | b     | 613 | CLA  | O2D-CGD-CBD | 3.81  | 118.05      | 111.27   |
| 24  | N     | 608 | CHL  | O2D-CGD-CBD | 3.81  | 118.04      | 111.27   |
| 25  | N     | 611 | CLA  | C1-C2-C3    | -3.81 | 119.45      | 126.04   |
| 40  | N     | 617 | NEX  | C27-C28-C29 | -3.81 | 119.62      | 125.53   |
| 26  | 2     | 606 | LHG  | O7-C7-C8    | 3.81  | 119.70      | 111.50   |
| 25  | G     | 604 | CLA  | C4D-CHA-C1A | -3.81 | 116.62      | 121.25   |
| 24  | N     | 609 | CHL  | O2D-CGD-CBD | 3.81  | 118.03      | 111.27   |
| 26  | 6     | 606 | LHG  | O7-C7-C8    | 3.81  | 119.70      | 111.50   |
| 25  | D     | 403 | CLA  | C1-C2-C3    | -3.81 | 119.46      | 126.04   |
| 25  | d     | 403 | CLA  | C1-C2-C3    | -3.81 | 119.46      | 126.04   |
| 25  | S     | 312 | CLA  | C2A-C3A-C4A | -3.80 | 95.72       | 101.87   |
| 32  | Y     | 320 | AJP  | O82-C10-C11 | 3.80  | 127.07      | 113.75   |
| 24  | R     | 605 | CHL  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 24  | r     | 605 | CHL  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 32  | y     | 320 | AJP  | O82-C10-C11 | 3.80  | 127.06      | 113.75   |
| 24  | n     | 609 | CHL  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 35  | c     | 515 | DGD  | O2G-C1B-C2B | 3.80  | 119.69      | 111.50   |
| 25  | s     | 312 | CLA  | C2A-C3A-C4A | -3.79 | 95.74       | 101.87   |
| 25  | R     | 610 | CLA  | C4D-CHA-C1A | -3.79 | 116.63      | 121.25   |
| 24  | 6     | 603 | CHL  | CAC-C3C-C4C | 3.79  | 129.73      | 124.81   |
| 24  | 2     | 601 | CHL  | CHD-C1D-ND  | -3.79 | 120.97      | 124.45   |
| 24  | 6     | 601 | CHL  | CHD-C1D-ND  | -3.79 | 120.97      | 124.45   |
| 25  | C     | 502 | CLA  | C1-C2-C3    | -3.79 | 119.49      | 126.04   |
| 32  | A     | 412 | AJP  | C03-C04-C05 | -3.79 | 105.38      | 111.93   |
| 32  | a     | 413 | AJP  | C03-C04-C05 | -3.79 | 105.38      | 111.93   |
| 35  | C     | 515 | DGD  | O2G-C1B-C2B | 3.79  | 119.66      | 111.50   |
| 25  | C     | 501 | CLA  | C2D-C1D-ND  | -3.78 | 107.31      | 110.10   |
| 25  | c     | 501 | CLA  | C2D-C1D-ND  | -3.78 | 107.31      | 110.10   |
| 26  | s     | 318 | LHG  | O7-C7-C8    | 3.78  | 119.65      | 111.50   |
| 26  | S     | 318 | LHG  | O7-C7-C8    | 3.78  | 119.64      | 111.50   |
| 40  | S     | 317 | NEX  | C38-C25-C26 | -3.77 | 115.94      | 122.26   |
| 40  | s     | 317 | NEX  | C38-C25-C26 | -3.77 | 115.94      | 122.26   |
| 24  | 2     | 603 | CHL  | CAC-C3C-C4C | 3.77  | 129.71      | 124.81   |
| 25  | g     | 604 | CLA  | C4D-CHA-C1A | -3.77 | 116.66      | 121.25   |
| 25  | C     | 503 | CLA  | C1D-ND-C4D  | -3.77 | 103.66      | 106.33   |
| 32  | s     | 319 | AJP  | C21-C20-C19 | 3.77  | 111.38      | 107.14   |
| 25  | c     | 502 | CLA  | C1-C2-C3    | -3.77 | 119.53      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 513 | CLA  | C1-C2-C3    | -3.77 | 119.53      | 126.04   |
| 25  | c     | 513 | CLA  | C1-C2-C3    | -3.77 | 119.53      | 126.04   |
| 32  | g     | 618 | AJP  | O77-C28-C29 | 3.77  | 119.28      | 109.94   |
| 32  | G     | 618 | AJP  | O77-C28-C29 | 3.76  | 119.28      | 109.94   |
| 39  | S     | 315 | LUT  | C3-C4-C5    | 3.76  | 119.35      | 111.85   |
| 39  | s     | 315 | LUT  | C3-C4-C5    | 3.76  | 119.35      | 111.85   |
| 25  | G     | 611 | CLA  | C1B-CHB-C4A | -3.76 | 122.67      | 130.12   |
| 24  | N     | 605 | CHL  | O2D-CGD-CBD | 3.76  | 117.95      | 111.27   |
| 25  | C     | 508 | CLA  | C1B-CHB-C4A | -3.76 | 122.67      | 130.12   |
| 25  | c     | 508 | CLA  | C1B-CHB-C4A | -3.76 | 122.67      | 130.12   |
| 25  | S     | 309 | CLA  | C1D-ND-C4D  | -3.76 | 103.67      | 106.33   |
| 32  | a     | 413 | AJP  | C17-C16-C11 | -3.76 | 106.86      | 112.32   |
| 25  | y     | 304 | CLA  | C1-C2-C3    | -3.76 | 119.55      | 126.04   |
| 30  | B     | 623 | LMG  | C7-O1-C1    | -3.75 | 106.41      | 113.74   |
| 30  | b     | 623 | LMG  | C7-O1-C1    | -3.75 | 106.41      | 113.74   |
| 39  | s     | 315 | LUT  | C18-C5-C4   | -3.75 | 107.40      | 114.36   |
| 32  | B     | 624 | AJP  | C17-C16-C11 | -3.75 | 106.87      | 112.32   |
| 32  | b     | 624 | AJP  | C17-C16-C11 | -3.75 | 106.87      | 112.32   |
| 25  | C     | 503 | CLA  | C1B-CHB-C4A | -3.75 | 122.69      | 130.12   |
| 25  | c     | 503 | CLA  | C1B-CHB-C4A | -3.75 | 122.69      | 130.12   |
| 32  | S     | 319 | AJP  | C21-C20-C19 | 3.75  | 111.36      | 107.14   |
| 25  | N     | 604 | CLA  | C1D-ND-C4D  | -3.75 | 103.67      | 106.33   |
| 24  | S     | 307 | CHL  | O2D-CGD-CBD | 3.74  | 117.92      | 111.27   |
| 25  | S     | 303 | CLA  | C1-C2-C3    | -3.74 | 119.57      | 126.04   |
| 24  | s     | 307 | CHL  | O2D-CGD-CBD | 3.74  | 117.92      | 111.27   |
| 25  | g     | 611 | CLA  | C1B-CHB-C4A | -3.74 | 122.70      | 130.12   |
| 25  | r     | 608 | CLA  | C1-C2-C3    | -3.74 | 119.57      | 126.04   |
| 39  | S     | 315 | LUT  | C18-C5-C4   | -3.74 | 107.42      | 114.36   |
| 40  | S     | 317 | NEX  | C19-C9-C10  | -3.74 | 117.68      | 122.92   |
| 25  | S     | 304 | CLA  | C1B-CHB-C4A | -3.74 | 122.71      | 130.12   |
| 25  | s     | 304 | CLA  | C1B-CHB-C4A | -3.74 | 122.71      | 130.12   |
| 25  | B     | 606 | CLA  | CHD-C1D-C2D | 3.74  | 133.33      | 125.48   |
| 25  | b     | 606 | CLA  | CHD-C1D-C2D | 3.74  | 133.33      | 125.48   |
| 24  | n     | 605 | CHL  | O2D-CGD-CBD | 3.74  | 117.91      | 111.27   |
| 24  | S     | 308 | CHL  | O2D-CGD-CBD | 3.74  | 117.91      | 111.27   |
| 32  | A     | 412 | AJP  | C17-C16-C11 | -3.74 | 106.89      | 112.32   |
| 32  | B     | 624 | AJP  | O53-C46-C45 | 3.73  | 119.12      | 110.05   |
| 32  | b     | 624 | AJP  | O53-C46-C45 | 3.73  | 119.12      | 110.05   |
| 25  | R     | 608 | CLA  | C1-C2-C3    | -3.73 | 119.59      | 126.04   |
| 40  | s     | 317 | NEX  | C19-C9-C10  | -3.73 | 117.69      | 122.92   |
| 25  | C     | 506 | CLA  | C1-C2-C3    | -3.73 | 119.59      | 126.04   |
| 25  | c     | 506 | CLA  | C1-C2-C3    | -3.73 | 119.59      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | s     | 313 | CLA  | CHD-C1D-C2D | 3.73  | 133.31      | 125.48   |
| 35  | c     | 516 | DGD  | O2G-C1B-C2B | 3.73  | 119.54      | 111.50   |
| 25  | A     | 405 | CLA  | C1D-ND-C4D  | -3.73 | 103.69      | 106.33   |
| 25  | B     | 611 | CLA  | C1D-ND-C4D  | -3.73 | 103.69      | 106.33   |
| 35  | C     | 516 | DGD  | O2G-C1B-C2B | 3.72  | 119.53      | 111.50   |
| 25  | B     | 601 | CLA  | CHD-C1D-C2D | 3.72  | 133.29      | 125.48   |
| 25  | s     | 309 | CLA  | CHB-C4A-NA  | -3.72 | 119.37      | 124.51   |
| 25  | S     | 313 | CLA  | CHD-C1D-C2D | 3.72  | 133.28      | 125.48   |
| 25  | c     | 503 | CLA  | C1D-ND-C4D  | -3.72 | 103.69      | 106.33   |
| 25  | s     | 303 | CLA  | C1-C2-C3    | -3.72 | 119.61      | 126.04   |
| 25  | S     | 309 | CLA  | CHB-C4A-NA  | -3.72 | 119.37      | 124.51   |
| 25  | G     | 610 | CLA  | C4D-CHA-C1A | -3.72 | 116.72      | 121.25   |
| 25  | b     | 611 | CLA  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 32  | B     | 624 | AJP  | C65-O70-C69 | 3.71  | 120.98      | 113.69   |
| 25  | b     | 601 | CLA  | CHD-C1D-C2D | 3.71  | 133.27      | 125.48   |
| 32  | b     | 624 | AJP  | C65-O70-C69 | 3.71  | 120.97      | 113.69   |
| 25  | a     | 406 | CLA  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 25  | C     | 501 | CLA  | CHD-C1D-C2D | 3.71  | 133.25      | 125.48   |
| 25  | c     | 501 | CLA  | CHD-C1D-C2D | 3.71  | 133.25      | 125.48   |
| 25  | y     | 314 | CLA  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 32  | G     | 618 | AJP  | C12-C07-C06 | 3.70  | 133.15      | 120.56   |
| 24  | s     | 308 | CHL  | O2D-CGD-CBD | 3.70  | 117.85      | 111.27   |
| 32  | Y     | 323 | AJP  | O25-C26-O31 | 3.70  | 121.01      | 110.67   |
| 32  | y     | 323 | AJP  | O25-C26-O31 | 3.70  | 121.01      | 110.67   |
| 25  | R     | 603 | CLA  | C2A-C3A-C4A | -3.70 | 95.89       | 101.87   |
| 25  | r     | 603 | CLA  | C2A-C3A-C4A | -3.70 | 95.89       | 101.87   |
| 32  | g     | 618 | AJP  | C12-C07-C06 | 3.70  | 133.14      | 120.56   |
| 25  | Y     | 304 | CLA  | C1-C2-C3    | -3.70 | 119.65      | 126.04   |
| 32  | n     | 620 | AJP  | C03-C04-C05 | -3.70 | 105.55      | 111.93   |
| 25  | N     | 604 | CLA  | O2D-CGD-CBD | 3.69  | 117.83      | 111.27   |
| 25  | G     | 603 | CLA  | C1-C2-C3    | -3.69 | 119.66      | 126.04   |
| 41  | r     | 616 | XAT  | C18-C5-C6   | -3.69 | 116.07      | 122.26   |
| 25  | D     | 402 | CLA  | C1-C2-C3    | -3.69 | 119.66      | 126.04   |
| 24  | 2     | 603 | CHL  | O2D-CGD-O1D | -3.69 | 116.62      | 123.84   |
| 24  | 6     | 603 | CHL  | O2D-CGD-O1D | -3.69 | 116.62      | 123.84   |
| 25  | B     | 602 | CLA  | CHB-C4A-NA  | -3.69 | 119.41      | 124.51   |
| 32  | n     | 619 | AJP  | C29-C28-C27 | 3.69  | 116.04      | 110.69   |
| 25  | n     | 604 | CLA  | O2D-CGD-CBD | 3.69  | 117.82      | 111.27   |
| 25  | g     | 610 | CLA  | C4D-CHA-C1A | -3.68 | 116.77      | 121.25   |
| 25  | b     | 602 | CLA  | CHB-C4A-NA  | -3.68 | 119.42      | 124.51   |
| 25  | 6     | 602 | CLA  | C1-C2-C3    | -3.68 | 119.68      | 126.04   |
| 25  | C     | 513 | CLA  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 41  | R     | 616 | XAT  | C18-C5-C6   | -3.68 | 116.10      | 122.26   |
| 25  | s     | 309 | CLA  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 25  | 2     | 602 | CLA  | C1-C2-C3    | -3.67 | 119.69      | 126.04   |
| 32  | N     | 620 | AJP  | C03-C04-C05 | -3.67 | 105.59      | 111.93   |
| 25  | d     | 402 | CLA  | C1-C2-C3    | -3.67 | 119.69      | 126.04   |
| 32  | N     | 619 | AJP  | C29-C28-C27 | 3.67  | 116.02      | 110.69   |
| 25  | g     | 603 | CLA  | C1-C2-C3    | -3.67 | 119.70      | 126.04   |
| 32  | B     | 624 | AJP  | C38-C37-C36 | 3.67  | 120.04      | 111.66   |
| 32  | b     | 624 | AJP  | C38-C37-C36 | 3.67  | 120.04      | 111.66   |
| 24  | Y     | 302 | CHL  | O2D-CGD-CBD | 3.67  | 117.78      | 111.27   |
| 25  | g     | 610 | CLA  | C1-C2-C3    | -3.66 | 119.72      | 126.04   |
| 25  | B     | 605 | CLA  | C1-C2-C3    | -3.66 | 119.72      | 126.04   |
| 25  | c     | 513 | CLA  | C1D-ND-C4D  | -3.66 | 103.74      | 106.33   |
| 25  | S     | 309 | CLA  | C3A-C2A-C1A | -3.66 | 95.86       | 101.34   |
| 25  | s     | 313 | CLA  | C1-C2-C3    | -3.65 | 119.72      | 126.04   |
| 39  | Y     | 317 | LUT  | C11-C10-C9  | -3.65 | 122.10      | 127.31   |
| 24  | S     | 302 | CHL  | O2D-CGD-CBD | 3.65  | 117.76      | 111.27   |
| 25  | G     | 610 | CLA  | C1-C2-C3    | -3.65 | 119.73      | 126.04   |
| 39  | y     | 317 | LUT  | C11-C10-C9  | -3.65 | 122.10      | 127.31   |
| 24  | y     | 302 | CHL  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 25  | s     | 309 | CLA  | C3A-C2A-C1A | -3.65 | 95.88       | 101.34   |
| 25  | r     | 609 | CLA  | C1-C2-C3    | -3.65 | 119.73      | 126.04   |
| 25  | n     | 613 | CLA  | C1-C2-C3    | -3.65 | 119.74      | 126.04   |
| 24  | G     | 601 | CHL  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 24  | s     | 302 | CHL  | O2D-CGD-CBD | 3.64  | 117.74      | 111.27   |
| 35  | b     | 626 | DGD  | O2G-C1B-C2B | 3.64  | 119.35      | 111.50   |
| 25  | Y     | 314 | CLA  | C1D-ND-C4D  | -3.64 | 103.75      | 106.33   |
| 25  | N     | 613 | CLA  | C1-C2-C3    | -3.64 | 119.75      | 126.04   |
| 25  | S     | 313 | CLA  | C1-C2-C3    | -3.64 | 119.75      | 126.04   |
| 25  | b     | 605 | CLA  | C1-C2-C3    | -3.63 | 119.76      | 126.04   |
| 25  | R     | 609 | CLA  | C1-C2-C3    | -3.63 | 119.76      | 126.04   |
| 25  | A     | 401 | CLA  | C1-C2-C3    | -3.63 | 119.77      | 126.04   |
| 24  | R     | 607 | CHL  | O2D-CGD-CBD | 3.63  | 117.71      | 111.27   |
| 24  | 6     | 603 | CHL  | O1D-CGD-CBD | -3.63 | 117.06      | 124.48   |
| 35  | C     | 515 | DGD  | C6D-O5D-C1E | -3.63 | 106.66      | 113.74   |
| 35  | c     | 515 | DGD  | C6D-O5D-C1E | -3.63 | 106.66      | 113.74   |
| 35  | B     | 626 | DGD  | O2G-C1B-C2B | 3.62  | 119.31      | 111.50   |
| 32  | B     | 624 | AJP  | O44-C37-C36 | 3.62  | 116.68      | 107.48   |
| 32  | b     | 624 | AJP  | O44-C37-C36 | 3.62  | 116.68      | 107.48   |
| 32  | N     | 620 | AJP  | C12-C07-C06 | 3.62  | 132.87      | 120.56   |
| 25  | a     | 402 | CLA  | C1-C2-C3    | -3.62 | 119.79      | 126.04   |
| 24  | g     | 601 | CHL  | O2D-CGD-CBD | 3.62  | 117.69      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | r     | 607 | CHL  | O2D-CGD-CBD | 3.62  | 117.69      | 111.27   |
| 24  | 2     | 603 | CHL  | O1D-CGD-CBD | -3.61 | 117.09      | 124.48   |
| 32  | g     | 618 | AJP  | C12-C07-C08 | -3.61 | 100.97      | 104.88   |
| 39  | S     | 316 | LUT  | C18-C5-C4   | -3.61 | 107.66      | 114.36   |
| 39  | s     | 316 | LUT  | C18-C5-C4   | -3.61 | 107.66      | 114.36   |
| 40  | N     | 617 | NEX  | C35-C34-C33 | -3.61 | 122.16      | 127.31   |
| 32  | n     | 620 | AJP  | C12-C07-C06 | 3.61  | 132.84      | 120.56   |
| 39  | N     | 615 | LUT  | C2-C3-C4    | 3.61  | 115.24      | 110.30   |
| 25  | B     | 612 | CLA  | C1-C2-C3    | -3.61 | 119.81      | 126.04   |
| 25  | b     | 612 | CLA  | C1-C2-C3    | -3.61 | 119.81      | 126.04   |
| 25  | Y     | 311 | CLA  | C4D-CHA-C1A | -3.60 | 116.87      | 121.25   |
| 25  | y     | 311 | CLA  | C4D-CHA-C1A | -3.60 | 116.87      | 121.25   |
| 41  | r     | 616 | XAT  | C11-C10-C9  | -3.60 | 122.17      | 127.31   |
| 25  | S     | 305 | CLA  | C2A-C3A-C4A | -3.59 | 96.07       | 101.87   |
| 25  | B     | 608 | CLA  | C1-C2-C3    | -3.58 | 119.84      | 126.04   |
| 25  | b     | 608 | CLA  | C1-C2-C3    | -3.58 | 119.84      | 126.04   |
| 39  | n     | 615 | LUT  | C2-C3-C4    | 3.58  | 115.21      | 110.30   |
| 32  | G     | 618 | AJP  | C12-C07-C08 | -3.58 | 101.01      | 104.88   |
| 39  | G     | 616 | LUT  | C18-C5-C4   | -3.58 | 107.73      | 114.36   |
| 25  | B     | 606 | CLA  | C1-C2-C3    | -3.58 | 119.86      | 126.04   |
| 25  | b     | 606 | CLA  | C1-C2-C3    | -3.58 | 119.86      | 126.04   |
| 25  | b     | 609 | CLA  | C1-C2-C3    | -3.58 | 119.86      | 126.04   |
| 25  | s     | 305 | CLA  | C2A-C3A-C4A | -3.58 | 96.09       | 101.87   |
| 25  | B     | 609 | CLA  | C1-C2-C3    | -3.57 | 119.86      | 126.04   |
| 35  | A     | 415 | DGD  | O2G-C1B-C2B | 3.57  | 119.20      | 111.50   |
| 35  | a     | 401 | DGD  | O2G-C1B-C2B | 3.57  | 119.20      | 111.50   |
| 25  | Y     | 312 | CLA  | C1-C2-C3    | -3.57 | 119.86      | 126.04   |
| 25  | y     | 312 | CLA  | C1-C2-C3    | -3.57 | 119.86      | 126.04   |
| 25  | n     | 612 | CLA  | C1D-ND-C4D  | -3.57 | 103.80      | 106.33   |
| 32  | a     | 413 | AJP  | C45-O44-C37 | -3.57 | 109.13      | 117.96   |
| 30  | A     | 410 | LMG  | C7-O1-C1    | -3.57 | 106.77      | 113.74   |
| 30  | a     | 411 | LMG  | C7-O1-C1    | -3.57 | 106.77      | 113.74   |
| 32  | A     | 412 | AJP  | C45-O44-C37 | -3.57 | 109.13      | 117.96   |
| 25  | R     | 602 | CLA  | C4D-CHA-C1A | -3.56 | 116.91      | 121.25   |
| 40  | n     | 617 | NEX  | C35-C34-C33 | -3.56 | 122.23      | 127.31   |
| 41  | R     | 616 | XAT  | C11-C10-C9  | -3.56 | 122.23      | 127.31   |
| 39  | g     | 616 | LUT  | C18-C5-C4   | -3.56 | 107.76      | 114.36   |
| 27  | A     | 404 | PHO  | C1-C2-C3    | -3.56 | 119.89      | 126.04   |
| 27  | a     | 405 | PHO  | C1-C2-C3    | -3.56 | 119.89      | 126.04   |
| 30  | B     | 623 | LMG  | C1-O6-C5    | -3.55 | 106.71      | 113.69   |
| 24  | s     | 306 | CHL  | O2D-CGD-CBD | 3.55  | 117.58      | 111.27   |
| 25  | Y     | 314 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | y     | 314 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 32  | B     | 624 | AJP  | C41-C39-C38 | 3.55  | 121.32      | 113.00   |
| 32  | b     | 624 | AJP  | C41-C39-C38 | 3.55  | 121.32      | 113.00   |
| 35  | B     | 626 | DGD  | C6D-O5D-C1E | -3.55 | 106.81      | 113.74   |
| 35  | b     | 626 | DGD  | C6D-O5D-C1E | -3.55 | 106.81      | 113.74   |
| 32  | g     | 618 | AJP  | O84-C05-C06 | 3.55  | 119.82      | 107.38   |
| 26  | C     | 519 | LHG  | O7-C7-C8    | 3.55  | 119.14      | 111.50   |
| 26  | c     | 519 | LHG  | O7-C7-C8    | 3.55  | 119.14      | 111.50   |
| 32  | S     | 319 | AJP  | O77-C28-C29 | 3.55  | 118.74      | 109.94   |
| 32  | Y     | 323 | AJP  | C26-O25-C23 | 3.55  | 120.81      | 115.33   |
| 32  | y     | 323 | AJP  | C26-O25-C23 | 3.55  | 120.81      | 115.33   |
| 32  | G     | 618 | AJP  | O84-C05-C06 | 3.54  | 119.80      | 107.38   |
| 32  | s     | 319 | AJP  | O77-C28-C29 | 3.54  | 118.73      | 109.94   |
| 24  | g     | 608 | CHL  | O2D-CGD-CBD | 3.54  | 117.56      | 111.27   |
| 30  | b     | 623 | LMG  | C1-O6-C5    | -3.54 | 106.74      | 113.69   |
| 25  | B     | 611 | CLA  | C1-C2-C3    | -3.54 | 119.92      | 126.04   |
| 25  | b     | 611 | CLA  | C1-C2-C3    | -3.54 | 119.92      | 126.04   |
| 25  | r     | 602 | CLA  | C4D-CHA-C1A | -3.54 | 116.94      | 121.25   |
| 40  | g     | 617 | NEX  | C19-C9-C10  | -3.54 | 117.97      | 122.92   |
| 25  | N     | 612 | CLA  | C1-C2-C3    | -3.54 | 119.93      | 126.04   |
| 25  | n     | 612 | CLA  | C1-C2-C3    | -3.54 | 119.93      | 126.04   |
| 25  | C     | 510 | CLA  | CHD-C1D-C2D | 3.54  | 132.90      | 125.48   |
| 25  | n     | 610 | CLA  | C4D-CHA-C1A | -3.53 | 116.95      | 121.25   |
| 32  | N     | 619 | AJP  | O25-C26-O31 | 3.53  | 120.54      | 110.67   |
| 25  | R     | 611 | CLA  | CHB-C4A-NA  | -3.53 | 119.63      | 124.51   |
| 25  | r     | 611 | CLA  | CHB-C4A-NA  | -3.53 | 119.63      | 124.51   |
| 25  | n     | 602 | CLA  | C1-C2-C3    | -3.53 | 119.93      | 126.04   |
| 25  | G     | 611 | CLA  | C4A-NA-C1A  | -3.53 | 105.12      | 106.71   |
| 25  | g     | 611 | CLA  | C4A-NA-C1A  | -3.53 | 105.12      | 106.71   |
| 24  | S     | 306 | CHL  | O2D-CGD-CBD | 3.53  | 117.54      | 111.27   |
| 32  | y     | 322 | AJP  | C03-C04-C05 | -3.53 | 105.83      | 111.93   |
| 25  | c     | 510 | CLA  | CHD-C1D-C2D | 3.53  | 132.88      | 125.48   |
| 25  | Y     | 304 | CLA  | C4D-CHA-C1A | -3.53 | 116.95      | 121.25   |
| 25  | y     | 304 | CLA  | C4D-CHA-C1A | -3.53 | 116.95      | 121.25   |
| 25  | 2     | 602 | CLA  | CHC-C1C-NC  | -3.53 | 118.85      | 124.20   |
| 25  | 6     | 602 | CLA  | CHC-C1C-NC  | -3.53 | 118.85      | 124.20   |
| 32  | n     | 619 | AJP  | O25-C26-O31 | 3.52  | 120.52      | 110.67   |
| 25  | Y     | 314 | CLA  | C1-C2-C3    | -3.52 | 119.95      | 126.04   |
| 25  | s     | 311 | CLA  | C1-C2-C3    | -3.52 | 119.95      | 126.04   |
| 32  | n     | 620 | AJP  | C04-C03-C02 | -3.52 | 104.38      | 111.81   |
| 32  | Y     | 322 | AJP  | C03-C04-C05 | -3.52 | 105.85      | 111.93   |
| 24  | G     | 608 | CHL  | O2D-CGD-CBD | 3.52  | 117.53      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | Y     | 315 | CLA  | O2D-CGD-CBD | 3.52  | 117.52      | 111.27   |
| 25  | y     | 315 | CLA  | O2D-CGD-CBD | 3.52  | 117.52      | 111.27   |
| 25  | N     | 610 | CLA  | C4D-CHA-C1A | -3.52 | 116.97      | 121.25   |
| 25  | y     | 314 | CLA  | C1-C2-C3    | -3.52 | 119.96      | 126.04   |
| 25  | C     | 509 | CLA  | C1-C2-C3    | -3.52 | 119.96      | 126.04   |
| 25  | g     | 611 | CLA  | C3D-C2D-C1D | 3.52  | 110.63      | 105.83   |
| 25  | N     | 613 | CLA  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 25  | n     | 613 | CLA  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 25  | D     | 402 | CLA  | C4D-CHA-C1A | -3.51 | 116.97      | 121.25   |
| 25  | d     | 402 | CLA  | C4D-CHA-C1A | -3.51 | 116.97      | 121.25   |
| 25  | G     | 611 | CLA  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 25  | A     | 405 | CLA  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 25  | a     | 406 | CLA  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 25  | R     | 611 | CLA  | C3D-C4D-CHA | 3.51  | 120.75      | 112.72   |
| 25  | r     | 611 | CLA  | C3D-C4D-CHA | 3.51  | 120.75      | 112.72   |
| 25  | N     | 602 | CLA  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 25  | r     | 608 | CLA  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 25  | N     | 612 | CLA  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 32  | Y     | 323 | AJP  | C12-C07-C06 | 3.51  | 132.49      | 120.56   |
| 32  | N     | 620 | AJP  | C04-C03-C02 | -3.51 | 104.42      | 111.81   |
| 40  | R     | 617 | NEX  | C11-C10-C9  | 3.50  | 132.31      | 127.31   |
| 40  | r     | 617 | NEX  | C11-C10-C9  | 3.50  | 132.31      | 127.31   |
| 32  | y     | 323 | AJP  | C12-C07-C06 | 3.50  | 132.47      | 120.56   |
| 24  | 2     | 603 | CHL  | CHD-C4C-C3C | 3.50  | 129.99      | 124.84   |
| 24  | n     | 606 | CHL  | O2D-CGD-CBD | 3.50  | 117.49      | 111.27   |
| 30  | D     | 407 | LMG  | C7-O1-C1    | -3.50 | 106.90      | 113.74   |
| 30  | d     | 407 | LMG  | C7-O1-C1    | -3.50 | 106.90      | 113.74   |
| 25  | G     | 611 | CLA  | C3D-C2D-C1D | 3.50  | 110.60      | 105.83   |
| 24  | N     | 606 | CHL  | O2D-CGD-CBD | 3.49  | 117.47      | 111.27   |
| 25  | g     | 611 | CLA  | C1-C2-C3    | -3.49 | 120.00      | 126.04   |
| 32  | B     | 624 | AJP  | C12-C07-C06 | 3.49  | 132.43      | 120.56   |
| 32  | b     | 624 | AJP  | C12-C07-C06 | 3.49  | 132.43      | 120.56   |
| 25  | B     | 614 | CLA  | C1-C2-C3    | -3.49 | 120.01      | 126.04   |
| 25  | R     | 612 | CLA  | C1-C2-C3    | -3.49 | 120.01      | 126.04   |
| 25  | c     | 509 | CLA  | C1-C2-C3    | -3.49 | 120.01      | 126.04   |
| 32  | N     | 620 | AJP  | O84-C05-C06 | 3.48  | 119.60      | 107.38   |
| 24  | 6     | 603 | CHL  | CHD-C4C-C3C | 3.48  | 129.96      | 124.84   |
| 32  | n     | 620 | AJP  | O84-C05-C06 | 3.48  | 119.60      | 107.38   |
| 25  | S     | 311 | CLA  | C1-C2-C3    | -3.48 | 120.02      | 126.04   |
| 25  | C     | 512 | CLA  | C1-C2-C3    | -3.48 | 120.02      | 126.04   |
| 25  | c     | 512 | CLA  | C1-C2-C3    | -3.48 | 120.02      | 126.04   |
| 40  | Y     | 318 | NEX  | C27-C28-C29 | -3.48 | 120.13      | 125.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | r     | 612 | CLA  | C1-C2-C3    | -3.48 | 120.03      | 126.04   |
| 25  | Y     | 303 | CLA  | C4A-NA-C1A  | -3.48 | 105.14      | 106.71   |
| 25  | B     | 603 | CLA  | C1-C2-C3    | -3.48 | 120.03      | 126.04   |
| 35  | C     | 515 | DGD  | C3G-O3G-C1D | -3.48 | 106.95      | 113.74   |
| 35  | c     | 515 | DGD  | C3G-O3G-C1D | -3.48 | 106.95      | 113.74   |
| 25  | b     | 614 | CLA  | C1-C2-C3    | -3.48 | 120.03      | 126.04   |
| 32  | Y     | 320 | AJP  | C12-C07-C06 | 3.47  | 132.38      | 120.56   |
| 32  | y     | 320 | AJP  | C12-C07-C06 | 3.47  | 132.38      | 120.56   |
| 25  | y     | 303 | CLA  | C1-C2-C3    | -3.47 | 120.03      | 126.04   |
| 25  | Y     | 303 | CLA  | C1-C2-C3    | -3.47 | 120.03      | 126.04   |
| 25  | A     | 402 | CLA  | C4D-CHA-C1A | -3.47 | 117.02      | 121.25   |
| 25  | a     | 403 | CLA  | C4D-CHA-C1A | -3.47 | 117.02      | 121.25   |
| 25  | R     | 608 | CLA  | C1D-ND-C4D  | -3.47 | 103.87      | 106.33   |
| 32  | Y     | 322 | AJP  | O09-C05-C06 | -3.47 | 99.32       | 104.47   |
| 40  | y     | 318 | NEX  | C27-C28-C29 | -3.47 | 120.15      | 125.53   |
| 39  | S     | 316 | LUT  | C22-C23-C24 | 3.47  | 115.69      | 111.74   |
| 26  | n     | 618 | LHG  | O7-C7-C8    | 3.47  | 118.97      | 111.50   |
| 24  | y     | 307 | CHL  | CHD-C1D-ND  | -3.46 | 121.27      | 124.45   |
| 32  | y     | 322 | AJP  | O09-C05-C06 | -3.46 | 99.33       | 104.47   |
| 25  | b     | 603 | CLA  | C1-C2-C3    | -3.46 | 120.06      | 126.04   |
| 25  | S     | 303 | CLA  | C2A-C1A-CHA | -3.46 | 117.82      | 123.86   |
| 25  | R     | 602 | CLA  | O2D-CGD-CBD | 3.46  | 117.41      | 111.27   |
| 25  | Y     | 315 | CLA  | C4A-NA-C1A  | -3.45 | 105.15      | 106.71   |
| 25  | N     | 602 | CLA  | O1D-CGD-CBD | -3.45 | 117.42      | 124.48   |
| 25  | c     | 508 | CLA  | CHD-C1D-C2D | 3.45  | 132.72      | 125.48   |
| 25  | r     | 602 | CLA  | O2D-CGD-CBD | 3.45  | 117.40      | 111.27   |
| 39  | s     | 316 | LUT  | C22-C23-C24 | 3.45  | 115.67      | 111.74   |
| 32  | y     | 324 | AJP  | C03-C04-C05 | -3.44 | 105.98      | 111.93   |
| 25  | s     | 303 | CLA  | C2A-C1A-CHA | -3.44 | 117.84      | 123.86   |
| 32  | b     | 624 | AJP  | C04-C03-C02 | -3.44 | 104.55      | 111.81   |
| 25  | A     | 402 | CLA  | C1-C2-C3    | -3.44 | 120.09      | 126.04   |
| 25  | a     | 403 | CLA  | C1-C2-C3    | -3.44 | 120.09      | 126.04   |
| 25  | b     | 601 | CLA  | C1-C2-C3    | -3.44 | 120.09      | 126.04   |
| 32  | Y     | 323 | AJP  | O25-C26-C27 | 3.44  | 117.01      | 108.10   |
| 32  | y     | 323 | AJP  | O25-C26-C27 | 3.44  | 117.01      | 108.10   |
| 26  | N     | 618 | LHG  | O7-C7-C8    | 3.44  | 118.91      | 111.50   |
| 25  | D     | 402 | CLA  | C1D-ND-C4D  | -3.44 | 103.89      | 106.33   |
| 25  | d     | 402 | CLA  | C1D-ND-C4D  | -3.44 | 103.89      | 106.33   |
| 32  | Y     | 324 | AJP  | C03-C04-C05 | -3.43 | 106.00      | 111.93   |
| 32  | B     | 624 | AJP  | C04-C03-C02 | -3.43 | 104.57      | 111.81   |
| 25  | C     | 502 | CLA  | C4D-CHA-C1A | -3.43 | 117.07      | 121.25   |
| 32  | Y     | 320 | AJP  | O84-C05-C06 | 3.43  | 119.41      | 107.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 320 | AJP  | O84-C05-C06 | 3.43  | 119.41      | 107.38   |
| 25  | C     | 508 | CLA  | CHD-C1D-C2D | 3.43  | 132.68      | 125.48   |
| 25  | 2     | 602 | CLA  | C3D-C2D-C1D | 3.43  | 110.51      | 105.83   |
| 25  | 6     | 602 | CLA  | C3D-C2D-C1D | 3.43  | 110.51      | 105.83   |
| 25  | N     | 614 | CLA  | C2A-C1A-CHA | -3.43 | 117.87      | 123.86   |
| 25  | B     | 601 | CLA  | C1-C2-C3    | -3.43 | 120.12      | 126.04   |
| 32  | B     | 624 | AJP  | O44-C45-C46 | 3.42  | 116.97      | 108.10   |
| 32  | b     | 624 | AJP  | O44-C45-C46 | 3.42  | 116.97      | 108.10   |
| 25  | n     | 602 | CLA  | O1D-CGD-CBD | -3.42 | 117.48      | 124.48   |
| 40  | G     | 617 | NEX  | C19-C9-C10  | -3.42 | 118.13      | 122.92   |
| 25  | c     | 502 | CLA  | C4D-CHA-C1A | -3.42 | 117.09      | 121.25   |
| 41  | R     | 616 | XAT  | C6-C7-C8    | -3.42 | 118.77      | 125.99   |
| 41  | r     | 616 | XAT  | C6-C7-C8    | -3.41 | 118.77      | 125.99   |
| 25  | s     | 312 | CLA  | C4A-NA-C1A  | -3.41 | 105.17      | 106.71   |
| 25  | C     | 503 | CLA  | C1-C2-C3    | -3.41 | 120.14      | 126.04   |
| 25  | c     | 503 | CLA  | C1-C2-C3    | -3.41 | 120.14      | 126.04   |
| 25  | y     | 315 | CLA  | C4D-CHA-C1A | -3.41 | 117.09      | 121.25   |
| 40  | n     | 617 | NEX  | C39-C29-C30 | -3.41 | 118.14      | 122.92   |
| 25  | y     | 303 | CLA  | C4A-NA-C1A  | -3.41 | 105.17      | 106.71   |
| 24  | n     | 605 | CHL  | CAA-C2A-C3A | -3.41 | 103.44      | 112.78   |
| 24  | N     | 605 | CHL  | CAA-C2A-C3A | -3.41 | 103.44      | 112.78   |
| 25  | B     | 613 | CLA  | C1-C2-C3    | -3.41 | 120.15      | 126.04   |
| 25  | b     | 613 | CLA  | C1-C2-C3    | -3.41 | 120.15      | 126.04   |
| 25  | G     | 611 | CLA  | C4D-CHA-C1A | -3.41 | 117.10      | 121.25   |
| 25  | g     | 611 | CLA  | C4D-CHA-C1A | -3.41 | 117.10      | 121.25   |
| 32  | B     | 624 | AJP  | O25-C23-C24 | 3.40  | 116.19      | 109.62   |
| 32  | b     | 624 | AJP  | O25-C23-C24 | 3.40  | 116.19      | 109.62   |
| 40  | N     | 617 | NEX  | C39-C29-C30 | -3.40 | 118.16      | 122.92   |
| 25  | S     | 312 | CLA  | C4A-NA-C1A  | -3.40 | 105.18      | 106.71   |
| 25  | r     | 611 | CLA  | C1D-ND-C4D  | 3.39  | 108.75      | 106.33   |
| 25  | 2     | 604 | CLA  | C4D-C3D-CAD | -3.39 | 104.10      | 108.10   |
| 25  | 6     | 604 | CLA  | C4D-C3D-CAD | -3.39 | 104.10      | 108.10   |
| 25  | y     | 315 | CLA  | C4A-NA-C1A  | -3.39 | 105.18      | 106.71   |
| 24  | 5     | 301 | CHL  | O2D-CGD-CBD | 3.39  | 117.29      | 111.27   |
| 30  | B     | 620 | LMG  | C7-O1-C1    | -3.39 | 107.13      | 113.74   |
| 30  | b     | 620 | LMG  | C7-O1-C1    | -3.39 | 107.13      | 113.74   |
| 24  | 1     | 301 | CHL  | O2D-CGD-CBD | 3.38  | 117.28      | 111.27   |
| 25  | n     | 614 | CLA  | C2A-C1A-CHA | -3.38 | 117.94      | 123.86   |
| 24  | Y     | 307 | CHL  | CHD-C1D-ND  | -3.38 | 121.34      | 124.45   |
| 35  | A     | 415 | DGD  | C1E-O6E-C5E | -3.37 | 107.07      | 113.69   |
| 35  | a     | 401 | DGD  | C1E-O6E-C5E | -3.37 | 107.07      | 113.69   |
| 40  | n     | 617 | NEX  | C11-C12-C13 | -3.37 | 116.95      | 126.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 321 | AJP  | C01-C02-C03 | 3.37  | 119.42      | 112.09   |
| 32  | y     | 321 | AJP  | C01-C02-C03 | 3.37  | 119.42      | 112.09   |
| 40  | N     | 617 | NEX  | C11-C12-C13 | -3.37 | 116.95      | 126.42   |
| 32  | B     | 624 | AJP  | O77-C28-C27 | 3.36  | 118.12      | 110.35   |
| 32  | b     | 624 | AJP  | O77-C28-C27 | 3.36  | 118.12      | 110.35   |
| 32  | Y     | 322 | AJP  | O25-C26-C27 | 3.36  | 116.81      | 108.10   |
| 32  | y     | 322 | AJP  | O25-C26-C27 | 3.36  | 116.81      | 108.10   |
| 25  | Y     | 315 | CLA  | C4D-CHA-C1A | -3.36 | 117.17      | 121.25   |
| 41  | R     | 616 | XAT  | C38-C25-C26 | -3.35 | 116.64      | 122.26   |
| 25  | R     | 611 | CLA  | C1D-ND-C4D  | 3.35  | 108.72      | 106.33   |
| 32  | Y     | 324 | AJP  | C12-C07-C06 | 3.35  | 131.96      | 120.56   |
| 32  | Y     | 320 | AJP  | O31-C30-C29 | 3.35  | 115.38      | 110.04   |
| 39  | y     | 317 | LUT  | C3-C4-C5    | 3.35  | 118.52      | 111.85   |
| 41  | r     | 616 | XAT  | C38-C25-C26 | -3.35 | 116.65      | 122.26   |
| 39  | n     | 616 | LUT  | C3-C4-C5    | 3.35  | 118.52      | 111.85   |
| 39  | N     | 616 | LUT  | C3-C4-C5    | 3.34  | 118.52      | 111.85   |
| 32  | A     | 412 | AJP  | C12-C07-C06 | 3.34  | 131.92      | 120.56   |
| 32  | a     | 413 | AJP  | C12-C07-C06 | 3.34  | 131.92      | 120.56   |
| 39  | Y     | 317 | LUT  | C3-C4-C5    | 3.34  | 118.51      | 111.85   |
| 32  | y     | 324 | AJP  | C12-C07-C06 | 3.34  | 131.92      | 120.56   |
| 32  | y     | 322 | AJP  | C12-C07-C06 | 3.33  | 131.90      | 120.56   |
| 32  | S     | 319 | AJP  | O84-C05-C06 | 3.33  | 119.07      | 107.38   |
| 32  | s     | 319 | AJP  | O84-C05-C06 | 3.33  | 119.07      | 107.38   |
| 25  | G     | 613 | CLA  | C1-C2-C3    | -3.33 | 120.29      | 126.04   |
| 25  | g     | 613 | CLA  | C1-C2-C3    | -3.33 | 120.29      | 126.04   |
| 32  | y     | 320 | AJP  | O31-C30-C29 | 3.33  | 115.35      | 110.04   |
| 25  | d     | 401 | CLA  | C1B-CHB-C4A | -3.32 | 123.54      | 130.12   |
| 24  | R     | 607 | CHL  | C1-C2-C3    | 3.32  | 131.79      | 126.04   |
| 25  | D     | 401 | CLA  | C1B-CHB-C4A | -3.32 | 123.54      | 130.12   |
| 39  | S     | 316 | LUT  | C3-C4-C5    | 3.32  | 118.47      | 111.85   |
| 25  | s     | 304 | CLA  | C1D-ND-C4D  | -3.32 | 103.98      | 106.33   |
| 32  | G     | 618 | AJP  | O25-C26-O31 | 3.32  | 119.94      | 110.67   |
| 32  | g     | 618 | AJP  | O25-C26-O31 | 3.32  | 119.94      | 110.67   |
| 25  | N     | 604 | CLA  | C1B-CHB-C4A | -3.32 | 123.55      | 130.12   |
| 32  | N     | 619 | AJP  | O84-C05-C06 | 3.32  | 119.01      | 107.38   |
| 32  | n     | 619 | AJP  | O84-C05-C06 | 3.32  | 119.01      | 107.38   |
| 32  | Y     | 322 | AJP  | C12-C07-C06 | 3.32  | 131.84      | 120.56   |
| 25  | A     | 401 | CLA  | CHD-C1D-C2D | 3.31  | 132.43      | 125.48   |
| 25  | a     | 402 | CLA  | CHD-C1D-C2D | 3.31  | 132.43      | 125.48   |
| 25  | c     | 511 | CLA  | C1-C2-C3    | -3.31 | 120.32      | 126.04   |
| 25  | n     | 604 | CLA  | C1B-CHB-C4A | -3.31 | 123.57      | 130.12   |
| 39  | s     | 316 | LUT  | C3-C4-C5    | 3.31  | 118.44      | 111.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 2     | 602 | CLA  | C1B-CHB-C4A | -3.30 | 123.58      | 130.12   |
| 25  | 6     | 602 | CLA  | C1B-CHB-C4A | -3.30 | 123.58      | 130.12   |
| 25  | B     | 602 | CLA  | C1-C2-C3    | -3.30 | 120.34      | 126.04   |
| 25  | b     | 602 | CLA  | C1-C2-C3    | -3.30 | 120.34      | 126.04   |
| 25  | B     | 605 | CLA  | CHD-C1D-C2D | 3.30  | 132.40      | 125.48   |
| 25  | b     | 605 | CLA  | CHD-C1D-C2D | 3.30  | 132.40      | 125.48   |
| 25  | C     | 511 | CLA  | C1-C2-C3    | -3.30 | 120.34      | 126.04   |
| 25  | g     | 604 | CLA  | C1-C2-C3    | -3.30 | 121.42      | 126.75   |
| 32  | n     | 619 | AJP  | C12-C07-C06 | 3.29  | 131.76      | 120.56   |
| 30  | C     | 520 | LMG  | C1-O6-C5    | -3.29 | 107.22      | 113.69   |
| 30  | c     | 520 | LMG  | C1-O6-C5    | -3.29 | 107.22      | 113.69   |
| 25  | S     | 310 | CLA  | C1-C2-C3    | -3.29 | 120.35      | 126.04   |
| 32  | N     | 619 | AJP  | C12-C07-C06 | 3.29  | 131.76      | 120.56   |
| 40  | S     | 317 | NEX  | C39-C29-C30 | -3.29 | 118.31      | 122.92   |
| 32  | S     | 319 | AJP  | C12-C07-C06 | 3.29  | 131.76      | 120.56   |
| 32  | s     | 319 | AJP  | C12-C07-C06 | 3.29  | 131.76      | 120.56   |
| 24  | r     | 607 | CHL  | C1-C2-C3    | 3.29  | 131.74      | 126.04   |
| 24  | N     | 609 | CHL  | CAA-C2A-C3A | -3.29 | 103.77      | 112.78   |
| 24  | n     | 609 | CHL  | CAA-C2A-C3A | -3.29 | 103.77      | 112.78   |
| 40  | s     | 317 | NEX  | C39-C29-C30 | -3.29 | 118.32      | 122.92   |
| 25  | g     | 610 | CLA  | C4-C3-C5    | 3.28  | 120.80      | 115.27   |
| 30  | A     | 410 | LMG  | C1-O6-C5    | -3.28 | 107.24      | 113.69   |
| 30  | a     | 411 | LMG  | C1-O6-C5    | -3.28 | 107.24      | 113.69   |
| 24  | Y     | 310 | CHL  | CAA-C2A-C3A | -3.28 | 103.79      | 112.78   |
| 25  | Y     | 311 | CLA  | C1-C2-C3    | -3.28 | 120.37      | 126.04   |
| 25  | y     | 311 | CLA  | C1-C2-C3    | -3.28 | 120.37      | 126.04   |
| 25  | R     | 609 | CLA  | CHD-C1D-C2D | 3.28  | 132.35      | 125.48   |
| 25  | s     | 310 | CLA  | C1-C2-C3    | -3.28 | 120.38      | 126.04   |
| 25  | b     | 604 | CLA  | CHD-C1D-C2D | 3.27  | 132.35      | 125.48   |
| 24  | y     | 310 | CHL  | CAA-C2A-C3A | -3.27 | 103.81      | 112.78   |
| 32  | y     | 322 | AJP  | C29-C30-C32 | -3.27 | 106.86      | 112.60   |
| 25  | G     | 604 | CLA  | C1-C2-C3    | -3.27 | 121.47      | 126.75   |
| 25  | s     | 314 | CLA  | C4D-CHA-C1A | -3.27 | 117.27      | 121.25   |
| 25  | g     | 612 | CLA  | C1-C2-C3    | -3.26 | 120.40      | 126.04   |
| 32  | N     | 620 | AJP  | C06-C07-C08 | -3.26 | 98.40       | 104.34   |
| 25  | G     | 610 | CLA  | C4-C3-C5    | 3.26  | 120.75      | 115.27   |
| 24  | G     | 608 | CHL  | CAA-C2A-C3A | -3.26 | 103.86      | 112.78   |
| 32  | N     | 620 | AJP  | C29-C28-C27 | 3.26  | 115.42      | 110.69   |
| 25  | S     | 304 | CLA  | C1D-ND-C4D  | -3.26 | 104.02      | 106.33   |
| 32  | Y     | 322 | AJP  | C29-C30-C32 | -3.25 | 106.89      | 112.60   |
| 25  | b     | 602 | CLA  | C1D-ND-C4D  | -3.25 | 104.02      | 106.33   |
| 25  | r     | 609 | CLA  | CHD-C1D-C2D | 3.25  | 132.30      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 322 | AJP  | C21-C20-C19 | 3.25  | 110.80      | 107.14   |
| 32  | y     | 321 | AJP  | C12-C07-C06 | 3.25  | 131.61      | 120.56   |
| 25  | S     | 314 | CLA  | C4D-CHA-C1A | -3.25 | 117.29      | 121.25   |
| 25  | B     | 604 | CLA  | CHD-C1D-C2D | 3.25  | 132.29      | 125.48   |
| 32  | n     | 620 | AJP  | C06-C07-C08 | -3.25 | 98.43       | 104.34   |
| 24  | g     | 608 | CHL  | CAA-C2A-C3A | -3.25 | 103.89      | 112.78   |
| 24  | g     | 606 | CHL  | CAA-C2A-C3A | -3.24 | 103.89      | 112.78   |
| 25  | G     | 612 | CLA  | C1-C2-C3    | -3.24 | 120.43      | 126.04   |
| 25  | B     | 607 | CLA  | C1-C2-C3    | -3.24 | 120.43      | 126.04   |
| 32  | Y     | 321 | AJP  | C12-C07-C06 | 3.24  | 131.58      | 120.56   |
| 25  | R     | 611 | CLA  | C3D-C2D-C1D | 3.24  | 110.25      | 105.83   |
| 24  | G     | 606 | CHL  | CAA-C2A-C3A | -3.24 | 103.91      | 112.78   |
| 30  | C     | 520 | LMG  | C7-O1-C1    | -3.24 | 107.42      | 113.74   |
| 25  | N     | 611 | CLA  | C4A-NA-C1A  | -3.24 | 105.25      | 106.71   |
| 24  | S     | 302 | CHL  | CAA-C2A-C3A | -3.24 | 103.92      | 112.78   |
| 25  | a     | 403 | CLA  | CHD-C1D-C2D | 3.23  | 132.26      | 125.48   |
| 25  | n     | 611 | CLA  | C4A-NA-C1A  | -3.23 | 105.25      | 106.71   |
| 24  | G     | 607 | CHL  | O1D-CGD-CBD | -3.23 | 117.87      | 124.48   |
| 32  | Y     | 321 | AJP  | C04-C05-C06 | 3.23  | 122.33      | 115.69   |
| 25  | c     | 508 | CLA  | C1-C2-C3    | -3.23 | 120.46      | 126.04   |
| 25  | A     | 402 | CLA  | CHD-C1D-C2D | 3.23  | 132.25      | 125.48   |
| 25  | G     | 612 | CLA  | C1B-CHB-C4A | -3.23 | 123.73      | 130.12   |
| 35  | b     | 626 | DGD  | C1D-O6D-C5D | -3.22 | 107.36      | 113.69   |
| 24  | R     | 606 | CHL  | CAA-C2A-C3A | -3.22 | 103.95      | 112.78   |
| 25  | r     | 601 | CLA  | C3D-C2D-C1D | 3.22  | 110.23      | 105.83   |
| 25  | N     | 612 | CLA  | C1B-CHB-C4A | -3.22 | 123.73      | 130.12   |
| 32  | a     | 413 | AJP  | O50-C45-C46 | 3.22  | 114.99      | 110.04   |
| 24  | Y     | 307 | CHL  | O2D-CGD-CBD | 3.22  | 117.00      | 111.27   |
| 24  | y     | 307 | CHL  | O2D-CGD-CBD | 3.22  | 117.00      | 111.27   |
| 35  | C     | 516 | DGD  | C3G-O3G-C1D | -3.22 | 107.44      | 113.74   |
| 32  | N     | 620 | AJP  | C01-C02-C03 | 3.22  | 119.10      | 112.09   |
| 32  | n     | 620 | AJP  | C01-C02-C03 | 3.22  | 119.10      | 112.09   |
| 32  | n     | 620 | AJP  | C29-C28-C27 | 3.22  | 115.37      | 110.69   |
| 24  | S     | 307 | CHL  | CAA-C2A-C3A | -3.22 | 103.96      | 112.78   |
| 24  | s     | 307 | CHL  | CAA-C2A-C3A | -3.22 | 103.96      | 112.78   |
| 32  | N     | 620 | AJP  | C17-C16-C15 | -3.22 | 106.50      | 110.49   |
| 32  | n     | 620 | AJP  | C17-C16-C15 | -3.22 | 106.50      | 110.49   |
| 32  | y     | 322 | AJP  | C21-C20-C19 | 3.22  | 110.77      | 107.14   |
| 25  | a     | 403 | CLA  | C1B-CHB-C4A | -3.22 | 123.74      | 130.12   |
| 25  | C     | 508 | CLA  | C1-C2-C3    | -3.22 | 120.48      | 126.04   |
| 25  | b     | 607 | CLA  | C1-C2-C3    | -3.22 | 120.48      | 126.04   |
| 35  | B     | 626 | DGD  | C1D-O6D-C5D | -3.21 | 107.38      | 113.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | c     | 507 | CLA  | CHD-C1D-C2D | 3.21  | 132.22      | 125.48   |
| 24  | y     | 306 | CHL  | CAA-C2A-C3A | -3.21 | 103.98      | 112.78   |
| 32  | y     | 321 | AJP  | C04-C05-C06 | 3.21  | 122.30      | 115.69   |
| 32  | B     | 624 | AJP  | O09-C05-C06 | -3.21 | 99.70       | 104.47   |
| 32  | b     | 624 | AJP  | O09-C05-C06 | -3.21 | 99.70       | 104.47   |
| 39  | y     | 316 | LUT  | C35-C15-C14 | -3.21 | 116.90      | 123.47   |
| 25  | s     | 304 | CLA  | CHD-C1D-C2D | 3.21  | 132.21      | 125.48   |
| 24  | s     | 302 | CHL  | CAA-C2A-C3A | -3.21 | 103.99      | 112.78   |
| 25  | g     | 612 | CLA  | C1B-CHB-C4A | -3.21 | 123.77      | 130.12   |
| 24  | r     | 606 | CHL  | CAA-C2A-C3A | -3.21 | 104.00      | 112.78   |
| 30  | c     | 520 | LMG  | C7-O1-C1    | -3.21 | 107.48      | 113.74   |
| 35  | c     | 516 | DGD  | C3G-O3G-C1D | -3.20 | 107.48      | 113.74   |
| 40  | r     | 617 | NEX  | C38-C25-C26 | -3.20 | 116.89      | 122.26   |
| 25  | A     | 402 | CLA  | C1B-CHB-C4A | -3.20 | 123.77      | 130.12   |
| 25  | C     | 507 | CLA  | C1-C2-C3    | -3.20 | 120.51      | 126.04   |
| 25  | c     | 507 | CLA  | C1-C2-C3    | -3.20 | 120.51      | 126.04   |
| 40  | g     | 617 | NEX  | C40-C33-C32 | 3.20  | 123.12      | 118.08   |
| 25  | r     | 610 | CLA  | C3D-C2D-C1D | 3.20  | 110.20      | 105.83   |
| 25  | r     | 611 | CLA  | C3D-C2D-C1D | 3.20  | 110.20      | 105.83   |
| 24  | Y     | 306 | CHL  | CAA-C2A-C3A | -3.20 | 104.02      | 112.78   |
| 25  | n     | 612 | CLA  | C1B-CHB-C4A | -3.20 | 123.79      | 130.12   |
| 25  | y     | 304 | CLA  | C3D-C2D-C1D | 3.20  | 110.19      | 105.83   |
| 25  | C     | 507 | CLA  | CHD-C1D-C2D | 3.20  | 132.18      | 125.48   |
| 25  | C     | 512 | CLA  | CHD-C1D-C2D | 3.19  | 132.18      | 125.48   |
| 32  | Y     | 321 | AJP  | C28-C29-C30 | -3.19 | 105.72      | 111.22   |
| 32  | y     | 321 | AJP  | C28-C29-C30 | -3.19 | 105.72      | 111.22   |
| 25  | S     | 305 | CLA  | C3D-C2D-C1D | 3.19  | 110.19      | 105.83   |
| 25  | s     | 305 | CLA  | C3D-C2D-C1D | 3.19  | 110.19      | 105.83   |
| 24  | g     | 607 | CHL  | O1D-CGD-CBD | -3.19 | 117.95      | 124.48   |
| 25  | R     | 601 | CLA  | C3D-C2D-C1D | 3.19  | 110.18      | 105.83   |
| 39  | Y     | 316 | LUT  | C35-C15-C14 | -3.19 | 116.94      | 123.47   |
| 40  | G     | 617 | NEX  | C40-C33-C32 | 3.19  | 123.10      | 118.08   |
| 25  | c     | 512 | CLA  | CHD-C1D-C2D | 3.19  | 132.17      | 125.48   |
| 40  | R     | 617 | NEX  | C38-C25-C26 | -3.19 | 116.92      | 122.26   |
| 24  | r     | 605 | CHL  | CAA-C2A-C3A | -3.19 | 104.05      | 112.78   |
| 24  | R     | 605 | CHL  | CAA-C2A-C3A | -3.18 | 104.06      | 112.78   |
| 25  | Y     | 303 | CLA  | O2D-CGD-O1D | -3.18 | 117.61      | 123.84   |
| 25  | y     | 303 | CLA  | O2D-CGD-O1D | -3.18 | 117.61      | 123.84   |
| 25  | Y     | 304 | CLA  | C3D-C2D-C1D | 3.18  | 110.17      | 105.83   |
| 25  | S     | 304 | CLA  | CHD-C1D-C2D | 3.18  | 132.15      | 125.48   |
| 25  | S     | 311 | CLA  | CHD-C1D-C2D | 3.18  | 132.15      | 125.48   |
| 24  | G     | 601 | CHL  | CHD-C1D-ND  | -3.18 | 121.53      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | B     | 602 | CLA  | C1D-ND-C4D  | -3.18 | 104.08      | 106.33   |
| 25  | B     | 610 | CLA  | C4A-NA-C1A  | -3.18 | 105.28      | 106.71   |
| 25  | b     | 610 | CLA  | C4A-NA-C1A  | -3.18 | 105.28      | 106.71   |
| 25  | 2     | 602 | CLA  | C3C-C4C-NC  | -3.18 | 107.01      | 110.57   |
| 25  | 6     | 602 | CLA  | C3C-C4C-NC  | -3.18 | 107.01      | 110.57   |
| 25  | R     | 610 | CLA  | C3D-C2D-C1D | 3.17  | 110.16      | 105.83   |
| 25  | 2     | 605 | CLA  | C1B-CHB-C4A | -3.17 | 123.83      | 130.12   |
| 25  | R     | 603 | CLA  | C3D-C2D-C1D | 3.17  | 110.16      | 105.83   |
| 24  | S     | 306 | CHL  | CAA-C2A-C3A | -3.17 | 104.11      | 112.78   |
| 28  | A     | 406 | BCR  | C15-C14-C13 | -3.17 | 122.79      | 127.31   |
| 28  | a     | 407 | BCR  | C15-C14-C13 | -3.17 | 122.79      | 127.31   |
| 25  | Y     | 304 | CLA  | C2A-C1A-CHA | -3.16 | 118.33      | 123.86   |
| 25  | y     | 304 | CLA  | C2A-C1A-CHA | -3.16 | 118.33      | 123.86   |
| 25  | G     | 613 | CLA  | C1B-CHB-C4A | -3.16 | 123.86      | 130.12   |
| 24  | R     | 607 | CHL  | CAA-C2A-C3A | -3.16 | 104.12      | 112.78   |
| 32  | A     | 412 | AJP  | O50-C45-C46 | 3.16  | 114.89      | 110.04   |
| 25  | r     | 603 | CLA  | C3D-C2D-C1D | 3.16  | 110.14      | 105.83   |
| 24  | s     | 306 | CHL  | CAA-C2A-C3A | -3.16 | 104.13      | 112.78   |
| 32  | Y     | 323 | AJP  | C29-C28-C27 | 3.16  | 115.28      | 110.69   |
| 32  | y     | 323 | AJP  | C29-C28-C27 | 3.16  | 115.28      | 110.69   |
| 25  | s     | 312 | CLA  | C3D-C2D-C1D | 3.16  | 110.14      | 105.83   |
| 24  | Y     | 309 | CHL  | O2D-CGD-CBD | 3.16  | 116.88      | 111.27   |
| 25  | n     | 612 | CLA  | CHD-C1D-C2D | 3.16  | 132.10      | 125.48   |
| 25  | N     | 613 | CLA  | C4D-CHA-C1A | -3.15 | 117.41      | 121.25   |
| 25  | 6     | 605 | CLA  | C1B-CHB-C4A | -3.15 | 123.87      | 130.12   |
| 25  | d     | 403 | CLA  | C3D-C2D-C1D | 3.15  | 110.13      | 105.83   |
| 25  | s     | 311 | CLA  | CHD-C1D-C2D | 3.15  | 132.09      | 125.48   |
| 30  | A     | 408 | LMG  | C7-O1-C1    | -3.15 | 107.58      | 113.74   |
| 30  | a     | 409 | LMG  | C7-O1-C1    | -3.15 | 107.58      | 113.74   |
| 25  | D     | 403 | CLA  | C3D-C2D-C1D | 3.15  | 110.12      | 105.83   |
| 25  | n     | 603 | CLA  | C1-C2-C3    | -3.14 | 120.61      | 126.04   |
| 25  | n     | 613 | CLA  | C4D-CHA-C1A | -3.14 | 117.42      | 121.25   |
| 25  | N     | 612 | CLA  | CHD-C1D-C2D | 3.14  | 132.07      | 125.48   |
| 24  | y     | 307 | CHL  | O2A-CGA-CBA | 3.14  | 121.77      | 111.91   |
| 24  | S     | 308 | CHL  | CAA-C2A-C3A | -3.14 | 104.17      | 112.78   |
| 24  | s     | 308 | CHL  | CAA-C2A-C3A | -3.14 | 104.17      | 112.78   |
| 24  | r     | 607 | CHL  | CAA-C2A-C3A | -3.14 | 104.18      | 112.78   |
| 24  | Y     | 307 | CHL  | O2A-CGA-CBA | 3.14  | 121.76      | 111.91   |
| 24  | y     | 302 | CHL  | CHD-C1D-ND  | -3.14 | 121.57      | 124.45   |
| 24  | y     | 309 | CHL  | O2D-CGD-CBD | 3.14  | 116.85      | 111.27   |
| 24  | Y     | 302 | CHL  | CHD-C1D-ND  | -3.13 | 121.57      | 124.45   |
| 25  | n     | 612 | CLA  | C3D-C2D-C1D | 3.13  | 110.10      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 613 | CLA  | C1B-CHB-C4A | -3.13 | 123.92      | 130.12   |
| 25  | S     | 312 | CLA  | C3D-C2D-C1D | 3.13  | 110.10      | 105.83   |
| 24  | Y     | 309 | CHL  | CAA-C2A-C3A | -3.13 | 104.22      | 112.78   |
| 24  | N     | 608 | CHL  | CAA-C2A-C3A | -3.12 | 104.22      | 112.78   |
| 25  | b     | 615 | CLA  | C2A-C3A-C4A | -3.12 | 96.83       | 101.87   |
| 24  | n     | 606 | CHL  | CAA-C2A-C3A | -3.12 | 104.23      | 112.78   |
| 24  | g     | 608 | CHL  | C1-C2-C3    | 3.12  | 131.44      | 126.04   |
| 25  | 6     | 602 | CLA  | C4D-C3D-CAD | -3.12 | 104.42      | 108.10   |
| 32  | A     | 412 | AJP  | O34-C35-C36 | -3.12 | 102.78      | 109.10   |
| 32  | a     | 413 | AJP  | O34-C35-C36 | -3.12 | 102.78      | 109.10   |
| 24  | y     | 309 | CHL  | CAA-C2A-C3A | -3.12 | 104.24      | 112.78   |
| 25  | b     | 610 | CLA  | C1-C2-C3    | -3.12 | 120.65      | 126.04   |
| 38  | F     | 101 | HEM  | CHC-C4B-NB  | 3.12  | 127.82      | 124.43   |
| 25  | B     | 615 | CLA  | C2A-C3A-C4A | -3.12 | 96.84       | 101.87   |
| 25  | 6     | 604 | CLA  | C3D-C2D-C1D | 3.11  | 110.08      | 105.83   |
| 24  | 2     | 601 | CHL  | O2D-CGD-CBD | 3.11  | 116.80      | 111.27   |
| 24  | n     | 601 | CHL  | CHD-C1D-ND  | -3.11 | 121.60      | 124.45   |
| 25  | N     | 603 | CLA  | C1-C2-C3    | -3.11 | 120.67      | 126.04   |
| 25  | C     | 512 | CLA  | C2A-C1A-CHA | -3.11 | 118.42      | 123.86   |
| 24  | N     | 606 | CHL  | CAA-C2A-C3A | -3.11 | 104.27      | 112.78   |
| 25  | B     | 608 | CLA  | C2A-C1A-CHA | -3.11 | 118.42      | 123.86   |
| 25  | b     | 608 | CLA  | C2A-C1A-CHA | -3.11 | 118.42      | 123.86   |
| 25  | s     | 313 | CLA  | C3D-C2D-C1D | 3.11  | 110.07      | 105.83   |
| 32  | B     | 624 | AJP  | C55-O60-C59 | 3.11  | 119.78      | 113.69   |
| 32  | b     | 624 | AJP  | C55-O60-C59 | 3.11  | 119.78      | 113.69   |
| 24  | G     | 608 | CHL  | C1-C2-C3    | 3.11  | 131.41      | 126.04   |
| 24  | y     | 309 | CHL  | C1-C2-C3    | 3.10  | 131.41      | 126.04   |
| 25  | B     | 610 | CLA  | C1-C2-C3    | -3.10 | 120.67      | 126.04   |
| 24  | g     | 601 | CHL  | CHD-C1D-ND  | -3.10 | 121.60      | 124.45   |
| 35  | C     | 516 | DGD  | C6D-O5D-C1E | -3.10 | 107.68      | 113.74   |
| 24  | n     | 608 | CHL  | CAA-C2A-C3A | -3.10 | 104.28      | 112.78   |
| 25  | 2     | 604 | CLA  | C3D-C2D-C1D | 3.10  | 110.06      | 105.83   |
| 25  | c     | 504 | CLA  | C3D-C2D-C1D | 3.10  | 110.06      | 105.83   |
| 24  | 6     | 601 | CHL  | O2D-CGD-CBD | 3.10  | 116.78      | 111.27   |
| 24  | R     | 605 | CHL  | CHD-C1D-ND  | -3.10 | 121.60      | 124.45   |
| 24  | Y     | 309 | CHL  | C1-C2-C3    | 3.10  | 131.41      | 126.04   |
| 25  | C     | 504 | CLA  | C3D-C2D-C1D | 3.10  | 110.06      | 105.83   |
| 32  | Y     | 321 | AJP  | O09-C05-C06 | -3.10 | 99.87       | 104.47   |
| 25  | C     | 506 | CLA  | C1B-CHB-C4A | -3.10 | 123.99      | 130.12   |
| 25  | c     | 506 | CLA  | C1B-CHB-C4A | -3.10 | 123.99      | 130.12   |
| 35  | c     | 516 | DGD  | C6D-O5D-C1E | -3.09 | 107.69      | 113.74   |
| 32  | N     | 620 | AJP  | C17-C16-C11 | -3.09 | 107.82      | 112.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | n     | 620 | AJP  | C17-C16-C11 | -3.09 | 107.82      | 112.32   |
| 40  | G     | 617 | NEX  | C5-C4-C3    | -3.09 | 108.08      | 111.75   |
| 25  | Y     | 313 | CLA  | C3D-C2D-C1D | 3.09  | 110.05      | 105.83   |
| 25  | y     | 313 | CLA  | C3D-C2D-C1D | 3.09  | 110.05      | 105.83   |
| 25  | C     | 510 | CLA  | C1-C2-C3    | -3.09 | 120.70      | 126.04   |
| 24  | Y     | 308 | CHL  | C1-C2-C3    | 3.09  | 131.39      | 126.04   |
| 25  | C     | 501 | CLA  | C3D-C2D-C1D | 3.09  | 110.05      | 105.83   |
| 25  | N     | 612 | CLA  | C3D-C2D-C1D | 3.09  | 110.05      | 105.83   |
| 25  | c     | 501 | CLA  | C3D-C2D-C1D | 3.09  | 110.05      | 105.83   |
| 40  | R     | 617 | NEX  | C10-C11-C12 | 3.09  | 132.85      | 123.22   |
| 40  | r     | 617 | NEX  | C10-C11-C12 | 3.09  | 132.85      | 123.22   |
| 39  | S     | 315 | LUT  | C2-C3-C4    | 3.08  | 114.53      | 110.30   |
| 24  | s     | 308 | CHL  | CHD-C1D-ND  | -3.08 | 121.62      | 124.45   |
| 25  | B     | 607 | CLA  | C4-C3-C5    | 3.08  | 120.46      | 115.27   |
| 32  | A     | 412 | AJP  | O31-C30-C29 | 3.08  | 116.25      | 109.75   |
| 32  | a     | 413 | AJP  | O31-C30-C29 | 3.08  | 116.25      | 109.75   |
| 25  | c     | 512 | CLA  | C2A-C1A-CHA | -3.08 | 118.47      | 123.86   |
| 25  | N     | 614 | CLA  | C4D-CHA-C1A | -3.08 | 117.50      | 121.25   |
| 25  | c     | 501 | CLA  | C4D-CHA-C1A | -3.08 | 117.50      | 121.25   |
| 32  | y     | 321 | AJP  | O09-C05-C06 | -3.08 | 99.89       | 104.47   |
| 25  | r     | 614 | CLA  | C1B-CHB-C4A | -3.08 | 124.01      | 130.12   |
| 30  | B     | 620 | LMG  | C1-O6-C5    | -3.08 | 107.64      | 113.69   |
| 30  | b     | 620 | LMG  | C1-O6-C5    | -3.08 | 107.64      | 113.69   |
| 25  | 2     | 602 | CLA  | C4D-C3D-CAD | -3.08 | 104.47      | 108.10   |
| 25  | R     | 614 | CLA  | C1B-CHB-C4A | -3.08 | 124.02      | 130.12   |
| 25  | R     | 610 | CLA  | C4D-C3D-CAD | -3.08 | 104.47      | 108.10   |
| 24  | y     | 308 | CHL  | C1-C2-C3    | 3.08  | 131.37      | 126.04   |
| 24  | g     | 607 | CHL  | CHD-C1D-ND  | -3.08 | 121.63      | 124.45   |
| 25  | c     | 510 | CLA  | C1-C2-C3    | -3.08 | 120.72      | 126.04   |
| 39  | s     | 315 | LUT  | C2-C3-C4    | 3.08  | 114.51      | 110.30   |
| 25  | b     | 607 | CLA  | C4-C3-C5    | 3.08  | 120.44      | 115.27   |
| 32  | B     | 624 | AJP  | C61-C59-C58 | 3.07  | 120.21      | 113.00   |
| 32  | b     | 624 | AJP  | C61-C59-C58 | 3.07  | 120.21      | 113.00   |
| 25  | B     | 608 | CLA  | C4D-CHA-C1A | -3.07 | 117.51      | 121.25   |
| 25  | b     | 608 | CLA  | C4D-CHA-C1A | -3.07 | 117.51      | 121.25   |
| 25  | D     | 402 | CLA  | C3D-C2D-C1D | 3.07  | 110.03      | 105.83   |
| 25  | b     | 615 | CLA  | C3D-C2D-C1D | 3.07  | 110.03      | 105.83   |
| 25  | d     | 402 | CLA  | C3D-C2D-C1D | 3.07  | 110.03      | 105.83   |
| 25  | R     | 603 | CLA  | O1D-CGD-CBD | -3.07 | 118.19      | 124.48   |
| 24  | N     | 601 | CHL  | CHD-C1D-ND  | -3.07 | 121.63      | 124.45   |
| 25  | r     | 603 | CLA  | O1D-CGD-CBD | -3.07 | 118.19      | 124.48   |
| 40  | y     | 318 | NEX  | C20-C13-C14 | -3.07 | 118.62      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 320 | AJP  | O25-C26-O31 | 3.07  | 119.25      | 110.67   |
| 24  | r     | 605 | CHL  | CHD-C1D-ND  | -3.07 | 121.63      | 124.45   |
| 40  | Y     | 318 | NEX  | C20-C13-C14 | -3.07 | 118.63      | 122.92   |
| 24  | g     | 606 | CHL  | CHD-C1D-ND  | -3.07 | 121.64      | 124.45   |
| 25  | S     | 313 | CLA  | C3D-C2D-C1D | 3.07  | 110.02      | 105.83   |
| 25  | B     | 603 | CLA  | C2A-C1A-CHA | -3.06 | 118.50      | 123.86   |
| 25  | b     | 603 | CLA  | C2A-C1A-CHA | -3.06 | 118.50      | 123.86   |
| 35  | C     | 516 | DGD  | C1E-O6E-C5E | -3.06 | 107.68      | 113.69   |
| 35  | c     | 516 | DGD  | C1E-O6E-C5E | -3.06 | 107.68      | 113.69   |
| 25  | c     | 505 | CLA  | C2A-C1A-CHA | -3.06 | 118.51      | 123.86   |
| 32  | Y     | 324 | AJP  | C29-C28-C27 | 3.06  | 115.13      | 110.69   |
| 32  | y     | 324 | AJP  | C29-C28-C27 | 3.06  | 115.13      | 110.69   |
| 25  | C     | 501 | CLA  | C4D-CHA-C1A | -3.06 | 117.53      | 121.25   |
| 32  | B     | 624 | AJP  | O77-C28-C29 | 3.06  | 118.04      | 109.94   |
| 32  | b     | 624 | AJP  | O77-C28-C29 | 3.06  | 118.04      | 109.94   |
| 32  | Y     | 320 | AJP  | O25-C26-O31 | 3.06  | 119.21      | 110.67   |
| 25  | y     | 315 | CLA  | O1D-CGD-CBD | -3.06 | 118.23      | 124.48   |
| 24  | R     | 613 | CHL  | C2A-C3A-C4A | 3.05  | 105.68      | 101.78   |
| 25  | B     | 615 | CLA  | C3D-C2D-C1D | 3.05  | 110.00      | 105.83   |
| 24  | S     | 308 | CHL  | CHD-C1D-ND  | -3.05 | 121.65      | 124.45   |
| 38  | f     | 101 | HEM  | CHC-C4B-NB  | 3.05  | 127.75      | 124.43   |
| 41  | R     | 616 | XAT  | C26-C27-C28 | -3.05 | 119.54      | 125.99   |
| 24  | g     | 609 | CHL  | CAA-C2A-C3A | -3.05 | 104.43      | 112.78   |
| 25  | y     | 312 | CLA  | C3D-C2D-C1D | 3.05  | 109.99      | 105.83   |
| 25  | N     | 602 | CLA  | C4D-CHA-C1A | -3.05 | 117.54      | 121.25   |
| 25  | n     | 614 | CLA  | C4D-CHA-C1A | -3.05 | 117.54      | 121.25   |
| 24  | N     | 601 | CHL  | C1-C2-C3    | 3.05  | 131.31      | 126.04   |
| 24  | G     | 609 | CHL  | CAA-C2A-C3A | -3.05 | 104.44      | 112.78   |
| 25  | D     | 401 | CLA  | C1D-ND-C4D  | -3.05 | 104.17      | 106.33   |
| 25  | d     | 401 | CLA  | C1D-ND-C4D  | -3.05 | 104.17      | 106.33   |
| 25  | C     | 505 | CLA  | C2A-C1A-CHA | -3.04 | 118.54      | 123.86   |
| 24  | G     | 607 | CHL  | CHD-C1D-ND  | -3.04 | 121.66      | 124.45   |
| 25  | n     | 610 | CLA  | C1-C2-C3    | -3.04 | 120.78      | 126.04   |
| 24  | N     | 607 | CHL  | CHD-C1D-ND  | -3.04 | 121.66      | 124.45   |
| 24  | n     | 607 | CHL  | CHD-C1D-ND  | -3.04 | 121.66      | 124.45   |
| 25  | N     | 603 | CLA  | C2A-C1A-CHA | -3.04 | 118.54      | 123.86   |
| 25  | n     | 603 | CLA  | C2A-C1A-CHA | -3.04 | 118.54      | 123.86   |
| 41  | r     | 616 | XAT  | C26-C27-C28 | -3.04 | 119.57      | 125.99   |
| 25  | r     | 610 | CLA  | C4D-C3D-CAD | -3.04 | 104.52      | 108.10   |
| 25  | Y     | 315 | CLA  | O1D-CGD-CBD | -3.04 | 118.27      | 124.48   |
| 25  | s     | 309 | CLA  | C2A-C3A-C4A | -3.04 | 96.97       | 101.87   |
| 25  | c     | 504 | CLA  | O1D-CGD-CBD | -3.03 | 118.28      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 40  | R     | 617 | NEX  | C40-C33-C34 | -3.03 | 118.67      | 122.92   |
| 24  | r     | 613 | CHL  | C2A-C3A-C4A | 3.03  | 105.65      | 101.78   |
| 25  | N     | 610 | CLA  | C1-C2-C3    | -3.03 | 120.80      | 126.04   |
| 35  | B     | 626 | DGD  | C1E-O6E-C5E | -3.03 | 107.74      | 113.69   |
| 35  | b     | 626 | DGD  | C1E-O6E-C5E | -3.03 | 107.74      | 113.69   |
| 25  | G     | 613 | CLA  | CHD-C1D-C2D | 3.03  | 131.83      | 125.48   |
| 25  | c     | 503 | CLA  | CHD-C1D-C2D | 3.02  | 131.82      | 125.48   |
| 25  | n     | 602 | CLA  | C4D-CHA-C1A | -3.02 | 117.57      | 121.25   |
| 25  | n     | 614 | CLA  | C1D-ND-C4D  | -3.02 | 104.19      | 106.33   |
| 25  | R     | 601 | CLA  | C4D-C3D-CAD | -3.02 | 104.53      | 108.10   |
| 25  | C     | 511 | CLA  | CHD-C1D-C2D | 3.02  | 131.82      | 125.48   |
| 25  | c     | 511 | CLA  | CHD-C1D-C2D | 3.02  | 131.82      | 125.48   |
| 25  | S     | 309 | CLA  | C2A-C3A-C4A | -3.02 | 96.99       | 101.87   |
| 32  | y     | 322 | AJP  | O84-C05-C06 | 3.02  | 117.97      | 107.38   |
| 24  | n     | 601 | CHL  | C1-C2-C3    | 3.02  | 131.27      | 126.04   |
| 32  | S     | 319 | AJP  | C04-C03-C02 | -3.02 | 105.44      | 111.81   |
| 32  | s     | 319 | AJP  | C04-C03-C02 | -3.02 | 105.44      | 111.81   |
| 25  | r     | 601 | CLA  | C4D-C3D-CAD | -3.02 | 104.54      | 108.10   |
| 25  | C     | 504 | CLA  | O1D-CGD-CBD | -3.02 | 118.31      | 124.48   |
| 32  | Y     | 322 | AJP  | O84-C05-C06 | 3.01  | 117.95      | 107.38   |
| 32  | g     | 618 | AJP  | C01-C02-C03 | 3.01  | 118.65      | 112.09   |
| 25  | y     | 315 | CLA  | C2A-C1A-CHA | -3.01 | 118.59      | 123.86   |
| 28  | z     | 101 | BCR  | C2-C1-C6    | 3.01  | 115.12      | 110.48   |
| 25  | n     | 611 | CLA  | C3D-C2D-C1D | 3.01  | 109.94      | 105.83   |
| 32  | G     | 618 | AJP  | C01-C02-C03 | 3.01  | 118.65      | 112.09   |
| 24  | Y     | 308 | CHL  | CAA-C2A-C3A | -3.01 | 104.54      | 112.78   |
| 40  | y     | 318 | NEX  | C39-C29-C30 | -3.01 | 118.71      | 122.92   |
| 25  | r     | 609 | CLA  | C4-C3-C5    | 3.01  | 120.33      | 115.27   |
| 25  | Y     | 312 | CLA  | C3D-C2D-C1D | 3.01  | 109.93      | 105.83   |
| 25  | R     | 612 | CLA  | C3D-C2D-C1D | 3.01  | 109.93      | 105.83   |
| 25  | r     | 612 | CLA  | C3D-C2D-C1D | 3.01  | 109.93      | 105.83   |
| 28  | Z     | 101 | BCR  | C2-C1-C6    | 3.00  | 115.11      | 110.48   |
| 24  | G     | 606 | CHL  | CHD-C1D-ND  | -3.00 | 121.69      | 124.45   |
| 24  | 2     | 603 | CHL  | C4D-CHA-C1A | 3.00  | 124.90      | 121.25   |
| 25  | Y     | 311 | CLA  | C4-C3-C5    | 3.00  | 120.32      | 115.27   |
| 25  | C     | 506 | CLA  | CHB-C4A-NA  | -3.00 | 120.36      | 124.51   |
| 25  | c     | 506 | CLA  | CHB-C4A-NA  | -3.00 | 120.36      | 124.51   |
| 24  | n     | 609 | CHL  | CHD-C1D-ND  | -3.00 | 121.69      | 124.45   |
| 25  | S     | 303 | CLA  | C4A-NA-C1A  | -3.00 | 105.36      | 106.71   |
| 40  | r     | 617 | NEX  | C40-C33-C34 | -3.00 | 118.72      | 122.92   |
| 25  | y     | 311 | CLA  | C4-C3-C5    | 3.00  | 120.32      | 115.27   |
| 32  | y     | 324 | AJP  | O31-C30-C29 | 3.00  | 114.83      | 110.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 613 | CLA  | CHD-C1D-C2D | 3.00  | 131.77      | 125.48   |
| 25  | A     | 401 | CLA  | C1D-ND-C4D  | -3.00 | 104.20      | 106.33   |
| 25  | a     | 402 | CLA  | C1D-ND-C4D  | -3.00 | 104.20      | 106.33   |
| 24  | y     | 308 | CHL  | CAA-C2A-C3A | -3.00 | 104.57      | 112.78   |
| 24  | s     | 306 | CHL  | CHD-C1D-ND  | -3.00 | 121.70      | 124.45   |
| 25  | C     | 503 | CLA  | CHD-C1D-C2D | 3.00  | 131.76      | 125.48   |
| 24  | G     | 607 | CHL  | CMB-C2B-C3B | 3.00  | 130.28      | 124.68   |
| 27  | A     | 404 | PHO  | C4-C3-C5    | 2.99  | 120.31      | 115.27   |
| 27  | a     | 405 | PHO  | C4-C3-C5    | 2.99  | 120.31      | 115.27   |
| 38  | F     | 101 | HEM  | CHD-C1D-ND  | 2.99  | 127.68      | 124.43   |
| 38  | f     | 101 | HEM  | CHD-C1D-ND  | 2.99  | 127.68      | 124.43   |
| 25  | B     | 605 | CLA  | C1D-ND-C4D  | -2.99 | 104.21      | 106.33   |
| 32  | Y     | 324 | AJP  | O31-C30-C29 | 2.99  | 114.82      | 110.04   |
| 25  | N     | 603 | CLA  | C3D-C2D-C1D | 2.99  | 109.91      | 105.83   |
| 25  | N     | 611 | CLA  | C3D-C2D-C1D | 2.99  | 109.91      | 105.83   |
| 25  | 6     | 604 | CLA  | CHC-C1C-NC  | -2.99 | 119.66      | 124.20   |
| 25  | N     | 614 | CLA  | C1D-ND-C4D  | -2.99 | 104.21      | 106.33   |
| 28  | b     | 617 | BCR  | C15-C14-C13 | -2.99 | 123.04      | 127.31   |
| 24  | S     | 302 | CHL  | CHD-C1D-ND  | -2.99 | 121.71      | 124.45   |
| 25  | n     | 603 | CLA  | C3D-C2D-C1D | 2.99  | 109.91      | 105.83   |
| 24  | l     | 302 | CHL  | C1D-ND-C4D  | -2.99 | 104.21      | 106.33   |
| 25  | C     | 504 | CLA  | C4D-CHA-C1A | -2.99 | 117.61      | 121.25   |
| 25  | b     | 604 | CLA  | C1D-ND-C4D  | -2.99 | 104.21      | 106.33   |
| 25  | s     | 310 | CLA  | CHD-C1D-C2D | 2.99  | 131.74      | 125.48   |
| 32  | A     | 412 | AJP  | C01-C02-C03 | 2.99  | 118.59      | 112.09   |
| 32  | a     | 413 | AJP  | C01-C02-C03 | 2.99  | 118.59      | 112.09   |
| 24  | S     | 306 | CHL  | CHD-C1D-ND  | -2.99 | 121.71      | 124.45   |
| 28  | B     | 617 | BCR  | C15-C14-C13 | -2.98 | 123.05      | 127.31   |
| 24  | n     | 608 | CHL  | C1-C2-C3    | 2.98  | 131.20      | 126.04   |
| 25  | 2     | 604 | CLA  | CHC-C1C-NC  | -2.98 | 119.68      | 124.20   |
| 25  | S     | 311 | CLA  | C3D-C2D-C1D | 2.98  | 109.90      | 105.83   |
| 25  | b     | 604 | CLA  | C3D-C2D-C1D | 2.98  | 109.90      | 105.83   |
| 24  | G     | 605 | CHL  | CAA-C2A-C3A | -2.98 | 104.62      | 112.78   |
| 40  | Y     | 318 | NEX  | C39-C29-C30 | -2.98 | 118.75      | 122.92   |
| 24  | g     | 607 | CHL  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 24  | g     | 605 | CHL  | CAA-C2A-C3A | -2.98 | 104.62      | 112.78   |
| 32  | Y     | 323 | AJP  | C17-C16-C11 | -2.98 | 107.99      | 112.32   |
| 32  | y     | 323 | AJP  | C17-C16-C11 | -2.98 | 107.99      | 112.32   |
| 24  | N     | 606 | CHL  | CHD-C1D-ND  | -2.97 | 121.72      | 124.45   |
| 24  | n     | 606 | CHL  | CHD-C1D-ND  | -2.97 | 121.72      | 124.45   |
| 24  | 6     | 603 | CHL  | C4D-CHA-C1A | 2.97  | 124.87      | 121.25   |
| 25  | Y     | 315 | CLA  | C2A-C1A-CHA | -2.97 | 118.66      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 605 | CLA  | C1D-ND-C4D  | -2.97 | 104.22      | 106.33   |
| 24  | N     | 608 | CHL  | C1-C2-C3    | 2.97  | 131.18      | 126.04   |
| 25  | s     | 311 | CLA  | C3D-C2D-C1D | 2.97  | 109.88      | 105.83   |
| 24  | G     | 608 | CHL  | O2A-CGA-CBA | 2.97  | 121.22      | 111.91   |
| 24  | g     | 608 | CHL  | O2A-CGA-CBA | 2.97  | 121.22      | 111.91   |
| 24  | N     | 609 | CHL  | CHD-C1D-ND  | -2.97 | 121.73      | 124.45   |
| 25  | R     | 609 | CLA  | C4-C3-C5    | 2.97  | 120.26      | 115.27   |
| 25  | Y     | 311 | CLA  | C2A-C1A-CHA | -2.96 | 118.68      | 123.86   |
| 25  | y     | 311 | CLA  | C2A-C1A-CHA | -2.96 | 118.68      | 123.86   |
| 25  | G     | 610 | CLA  | C3D-C2D-C1D | 2.96  | 109.87      | 105.83   |
| 24  | 5     | 301 | CHL  | CAA-C2A-C3A | -2.96 | 104.67      | 112.78   |
| 24  | 1     | 301 | CHL  | CHD-C1D-ND  | -2.96 | 121.73      | 124.45   |
| 25  | C     | 511 | CLA  | C3D-C2D-C1D | 2.96  | 109.87      | 105.83   |
| 25  | c     | 511 | CLA  | C3D-C2D-C1D | 2.96  | 109.87      | 105.83   |
| 25  | 2     | 602 | CLA  | CHA-C1A-NA  | -2.96 | 119.62      | 126.40   |
| 25  | C     | 508 | CLA  | C3D-C2D-C1D | 2.96  | 109.87      | 105.83   |
| 24  | S     | 307 | CHL  | CHD-C1D-ND  | -2.96 | 121.74      | 124.45   |
| 24  | s     | 307 | CHL  | CHD-C1D-ND  | -2.96 | 121.74      | 124.45   |
| 28  | T     | 101 | BCR  | C15-C16-C17 | -2.96 | 117.42      | 123.47   |
| 25  | C     | 510 | CLA  | C2A-C1A-CHA | -2.96 | 118.69      | 123.86   |
| 32  | N     | 619 | AJP  | C19-C24-C23 | -2.96 | 105.57      | 112.92   |
| 32  | n     | 619 | AJP  | C19-C24-C23 | -2.96 | 105.57      | 112.92   |
| 24  | 2     | 603 | CHL  | CBC-CAC-C3C | -2.96 | 104.28      | 112.43   |
| 24  | 6     | 603 | CHL  | CBC-CAC-C3C | -2.96 | 104.28      | 112.43   |
| 25  | G     | 603 | CLA  | C3D-C2D-C1D | 2.96  | 109.86      | 105.83   |
| 25  | g     | 603 | CLA  | C3D-C2D-C1D | 2.96  | 109.86      | 105.83   |
| 25  | C     | 510 | CLA  | C3D-C2D-C1D | 2.95  | 109.86      | 105.83   |
| 25  | S     | 314 | CLA  | C2A-C1A-CHA | -2.95 | 118.69      | 123.86   |
| 25  | s     | 314 | CLA  | C2A-C1A-CHA | -2.95 | 118.69      | 123.86   |
| 24  | 5     | 301 | CHL  | CHD-C1D-ND  | -2.95 | 121.74      | 124.45   |
| 24  | G     | 609 | CHL  | O2A-CGA-CBA | 2.95  | 121.18      | 111.91   |
| 25  | c     | 504 | CLA  | C4D-CHA-C1A | -2.95 | 117.65      | 121.25   |
| 25  | 2     | 605 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.33   |
| 25  | G     | 602 | CLA  | C4-C3-C5    | 2.95  | 120.24      | 115.27   |
| 24  | 1     | 301 | CHL  | CAA-C2A-C3A | -2.95 | 104.69      | 112.78   |
| 25  | S     | 310 | CLA  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 25  | d     | 401 | CLA  | CHD-C1D-C2D | 2.95  | 131.67      | 125.48   |
| 32  | Y     | 320 | AJP  | O09-C05-C06 | -2.95 | 100.09      | 104.47   |
| 32  | y     | 320 | AJP  | O09-C05-C06 | -2.95 | 100.09      | 104.47   |
| 28  | t     | 101 | BCR  | C15-C16-C17 | -2.95 | 117.43      | 123.47   |
| 32  | Y     | 320 | AJP  | C26-O25-C23 | -2.95 | 110.77      | 115.33   |
| 25  | 6     | 602 | CLA  | CHA-C1A-NA  | -2.95 | 119.64      | 126.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 602 | CLA  | C4-C3-C5    | 2.95  | 120.23      | 115.27   |
| 25  | B     | 604 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.33   |
| 25  | s     | 303 | CLA  | C4A-NA-C1A  | -2.94 | 105.38      | 106.71   |
| 25  | G     | 610 | CLA  | CHD-C1D-C2D | 2.94  | 131.65      | 125.48   |
| 25  | N     | 604 | CLA  | O1D-CGD-CBD | -2.94 | 118.46      | 124.48   |
| 25  | c     | 510 | CLA  | C3D-C2D-C1D | 2.94  | 109.85      | 105.83   |
| 25  | n     | 611 | CLA  | O1D-CGD-CBD | -2.94 | 118.47      | 124.48   |
| 25  | D     | 401 | CLA  | CHD-C1D-C2D | 2.94  | 131.65      | 125.48   |
| 24  | g     | 609 | CHL  | O2A-CGA-CBA | 2.94  | 121.14      | 111.91   |
| 25  | g     | 614 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 25  | r     | 609 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 25  | B     | 604 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 24  | 1     | 302 | CHL  | CAA-C2A-C3A | -2.94 | 104.73      | 112.78   |
| 24  | 5     | 302 | CHL  | CAA-C2A-C3A | -2.94 | 104.73      | 112.78   |
| 25  | g     | 610 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 25  | A     | 401 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 25  | a     | 402 | CLA  | C3D-C2D-C1D | 2.94  | 109.84      | 105.83   |
| 24  | n     | 608 | CHL  | O2A-CGA-CBA | 2.93  | 121.12      | 111.91   |
| 25  | s     | 309 | CLA  | C3D-C2D-C1D | 2.93  | 109.83      | 105.83   |
| 24  | N     | 608 | CHL  | O2A-CGA-CBA | 2.93  | 121.11      | 111.91   |
| 25  | n     | 604 | CLA  | O1D-CGD-CBD | -2.93 | 118.48      | 124.48   |
| 25  | s     | 305 | CLA  | C4D-C3D-CAD | -2.93 | 104.64      | 108.10   |
| 25  | 6     | 605 | CLA  | C1D-ND-C4D  | -2.93 | 104.25      | 106.33   |
| 24  | 2     | 601 | CHL  | C1-C2-C3    | 2.93  | 131.11      | 126.04   |
| 24  | 6     | 601 | CHL  | C1-C2-C3    | 2.93  | 131.11      | 126.04   |
| 25  | B     | 601 | CLA  | C4-C3-C5    | 2.93  | 120.20      | 115.27   |
| 25  | b     | 601 | CLA  | C4-C3-C5    | 2.93  | 120.20      | 115.27   |
| 25  | C     | 513 | CLA  | C3D-C2D-C1D | 2.93  | 109.83      | 105.83   |
| 24  | 6     | 601 | CHL  | O2A-CGA-CBA | 2.93  | 121.10      | 111.91   |
| 25  | 2     | 605 | CLA  | C3D-C2D-C1D | 2.93  | 109.83      | 105.83   |
| 25  | 6     | 605 | CLA  | C3D-C2D-C1D | 2.93  | 109.83      | 105.83   |
| 25  | A     | 402 | CLA  | C1D-ND-C4D  | -2.93 | 104.25      | 106.33   |
| 25  | c     | 508 | CLA  | C3D-C2D-C1D | 2.93  | 109.83      | 105.83   |
| 32  | y     | 324 | AJP  | O09-C05-C06 | -2.93 | 100.13      | 104.47   |
| 25  | d     | 401 | CLA  | C3D-C2D-C1D | 2.93  | 109.82      | 105.83   |
| 25  | C     | 506 | CLA  | C4A-NA-C1A  | -2.92 | 105.39      | 106.71   |
| 25  | c     | 506 | CLA  | C4A-NA-C1A  | -2.92 | 105.39      | 106.71   |
| 25  | S     | 309 | CLA  | C3D-C2D-C1D | 2.92  | 109.82      | 105.83   |
| 25  | S     | 305 | CLA  | C4D-C3D-CAD | -2.92 | 104.65      | 108.10   |
| 40  | s     | 317 | NEX  | C15-C14-C13 | -2.92 | 123.14      | 127.31   |
| 24  | 2     | 601 | CHL  | O2A-CGA-CBA | 2.92  | 121.08      | 111.91   |
| 25  | N     | 611 | CLA  | O1D-CGD-CBD | -2.92 | 118.50      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | s     | 314 | CLA  | C3D-C2D-C1D | 2.92  | 109.82      | 105.83   |
| 25  | a     | 406 | CLA  | CHD-C1D-C2D | 2.92  | 131.61      | 125.48   |
| 25  | B     | 606 | CLA  | C1D-CHD-C4C | -2.92 | 119.76      | 126.06   |
| 25  | b     | 606 | CLA  | C1D-CHD-C4C | -2.92 | 119.76      | 126.06   |
| 25  | B     | 616 | CLA  | C1-C2-C3    | -2.92 | 120.99      | 126.04   |
| 25  | b     | 616 | CLA  | C1-C2-C3    | -2.92 | 120.99      | 126.04   |
| 25  | C     | 507 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.33   |
| 25  | R     | 609 | CLA  | C3D-C2D-C1D | 2.92  | 109.82      | 105.83   |
| 25  | c     | 510 | CLA  | C2A-C1A-CHA | -2.92 | 118.75      | 123.86   |
| 24  | s     | 302 | CHL  | CHD-C1D-ND  | -2.92 | 121.77      | 124.45   |
| 28  | B     | 617 | BCR  | C33-C5-C6   | -2.92 | 121.25      | 124.53   |
| 28  | b     | 617 | BCR  | C33-C5-C6   | -2.92 | 121.25      | 124.53   |
| 25  | A     | 405 | CLA  | CHD-C1D-C2D | 2.92  | 131.60      | 125.48   |
| 25  | g     | 610 | CLA  | CHD-C1D-C2D | 2.92  | 131.60      | 125.48   |
| 25  | c     | 512 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.33   |
| 25  | B     | 609 | CLA  | C3D-C2D-C1D | 2.91  | 109.81      | 105.83   |
| 25  | r     | 609 | CLA  | C1D-ND-C4D  | -2.91 | 104.27      | 106.33   |
| 32  | Y     | 324 | AJP  | O09-C05-C06 | -2.91 | 100.14      | 104.47   |
| 28  | I     | 101 | BCR  | C15-C16-C17 | -2.91 | 117.50      | 123.47   |
| 25  | A     | 402 | CLA  | C3D-C2D-C1D | 2.91  | 109.81      | 105.83   |
| 25  | a     | 403 | CLA  | C3D-C2D-C1D | 2.91  | 109.81      | 105.83   |
| 25  | g     | 613 | CLA  | C3D-C2D-C1D | 2.91  | 109.81      | 105.83   |
| 40  | S     | 317 | NEX  | C15-C14-C13 | -2.91 | 123.15      | 127.31   |
| 24  | 5     | 302 | CHL  | C1D-ND-C4D  | -2.91 | 104.27      | 106.33   |
| 32  | y     | 320 | AJP  | C26-O25-C23 | -2.91 | 110.83      | 115.33   |
| 25  | n     | 604 | CLA  | C3D-C2D-C1D | 2.91  | 109.80      | 105.83   |
| 25  | r     | 602 | CLA  | C3D-C2D-C1D | 2.91  | 109.80      | 105.83   |
| 25  | c     | 508 | CLA  | C4-C3-C5    | 2.91  | 120.16      | 115.27   |
| 24  | r     | 606 | CHL  | CHD-C1D-ND  | -2.91 | 121.78      | 124.45   |
| 25  | R     | 602 | CLA  | C3D-C2D-C1D | 2.91  | 109.80      | 105.83   |
| 28  | D     | 404 | BCR  | C33-C5-C6   | -2.91 | 121.26      | 124.53   |
| 28  | d     | 404 | BCR  | C33-C5-C6   | -2.91 | 121.26      | 124.53   |
| 28  | b     | 617 | BCR  | C15-C16-C17 | -2.91 | 117.52      | 123.47   |
| 24  | y     | 309 | CHL  | O2A-CGA-CBA | 2.90  | 121.02      | 111.91   |
| 28  | B     | 617 | BCR  | C15-C16-C17 | -2.90 | 117.53      | 123.47   |
| 25  | S     | 304 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 25  | s     | 304 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 25  | D     | 401 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 32  | g     | 618 | AJP  | O31-C30-C32 | 2.90  | 111.48      | 106.83   |
| 25  | B     | 601 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 25  | N     | 604 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 25  | b     | 601 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 323 | AJP  | O31-C30-C29 | 2.90  | 114.67      | 110.04   |
| 32  | y     | 323 | AJP  | O31-C30-C29 | 2.90  | 114.67      | 110.04   |
| 25  | B     | 610 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 25  | b     | 610 | CLA  | C3D-C2D-C1D | 2.90  | 109.79      | 105.83   |
| 24  | Y     | 309 | CHL  | O2A-CGA-CBA | 2.90  | 121.00      | 111.91   |
| 25  | A     | 405 | CLA  | C4-C3-C5    | 2.90  | 120.15      | 115.27   |
| 25  | a     | 406 | CLA  | C4-C3-C5    | 2.90  | 120.15      | 115.27   |
| 28  | i     | 101 | BCR  | C15-C16-C17 | -2.90 | 117.54      | 123.47   |
| 25  | G     | 613 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | n     | 613 | CLA  | C4-C3-C5    | 2.89  | 120.14      | 115.27   |
| 24  | l     | 302 | CHL  | C2D-C1D-ND  | 2.89  | 112.24      | 110.10   |
| 25  | y     | 312 | CLA  | C2A-C1A-CHA | -2.89 | 118.80      | 123.86   |
| 25  | B     | 614 | CLA  | C2A-C1A-CHA | -2.89 | 118.80      | 123.86   |
| 25  | b     | 614 | CLA  | C2A-C1A-CHA | -2.89 | 118.80      | 123.86   |
| 25  | S     | 311 | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.33   |
| 25  | c     | 507 | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.33   |
| 32  | S     | 319 | AJP  | C19-C24-C23 | -2.89 | 105.73      | 112.92   |
| 32  | s     | 319 | AJP  | C19-C24-C23 | -2.89 | 105.73      | 112.92   |
| 24  | n     | 601 | CHL  | CAA-C2A-C3A | -2.89 | 104.86      | 112.78   |
| 25  | B     | 605 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | B     | 608 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | b     | 605 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | b     | 614 | CLA  | C4-C3-C5    | 2.89  | 120.13      | 115.27   |
| 25  | R     | 604 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | r     | 604 | CLA  | C3D-C2D-C1D | 2.89  | 109.78      | 105.83   |
| 25  | Y     | 305 | CLA  | C2A-C1A-CHA | -2.89 | 118.81      | 123.86   |
| 25  | D     | 402 | CLA  | CHB-C4A-NA  | -2.89 | 120.52      | 124.51   |
| 25  | B     | 614 | CLA  | C4-C3-C5    | 2.89  | 120.13      | 115.27   |
| 25  | R     | 611 | CLA  | C3C-C4C-NC  | -2.89 | 107.33      | 110.57   |
| 25  | r     | 611 | CLA  | C3C-C4C-NC  | -2.89 | 107.33      | 110.57   |
| 24  | R     | 606 | CHL  | CHD-C1D-ND  | -2.89 | 121.80      | 124.45   |
| 25  | S     | 314 | CLA  | C3D-C2D-C1D | 2.89  | 109.77      | 105.83   |
| 25  | B     | 610 | CLA  | C1B-CHB-C4A | -2.89 | 124.40      | 130.12   |
| 25  | b     | 610 | CLA  | C1B-CHB-C4A | -2.89 | 124.40      | 130.12   |
| 25  | B     | 607 | CLA  | C3D-C2D-C1D | 2.89  | 109.77      | 105.83   |
| 25  | C     | 512 | CLA  | C3D-C2D-C1D | 2.89  | 109.77      | 105.83   |
| 25  | b     | 607 | CLA  | C3D-C2D-C1D | 2.89  | 109.77      | 105.83   |
| 25  | c     | 512 | CLA  | C3D-C2D-C1D | 2.89  | 109.77      | 105.83   |
| 24  | N     | 601 | CHL  | CAA-C2A-C3A | -2.89 | 104.88      | 112.78   |
| 32  | Y     | 323 | AJP  | C04-C03-C02 | -2.89 | 105.72      | 111.81   |
| 25  | B     | 615 | CLA  | C4A-NA-C1A  | -2.88 | 105.41      | 106.71   |
| 25  | b     | 615 | CLA  | C4A-NA-C1A  | -2.88 | 105.41      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | N     | 608 | CHL  | CMB-C2B-C1B | -2.88 | 124.03      | 128.46   |
| 32  | y     | 323 | AJP  | C04-C03-C02 | -2.88 | 105.73      | 111.81   |
| 25  | a     | 403 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.33   |
| 25  | Y     | 312 | CLA  | C2A-C1A-CHA | -2.88 | 118.82      | 123.86   |
| 25  | R     | 608 | CLA  | C4D-CHA-C1A | -2.88 | 117.75      | 121.25   |
| 25  | G     | 604 | CLA  | C3D-C2D-C1D | 2.88  | 109.76      | 105.83   |
| 25  | G     | 614 | CLA  | C3D-C2D-C1D | 2.88  | 109.76      | 105.83   |
| 32  | G     | 618 | AJP  | O31-C30-C32 | 2.88  | 111.45      | 106.83   |
| 25  | C     | 508 | CLA  | C4-C3-C5    | 2.88  | 120.11      | 115.27   |
| 25  | C     | 502 | CLA  | C3D-C2D-C1D | 2.88  | 109.76      | 105.83   |
| 32  | Y     | 323 | AJP  | C83-C06-C05 | -2.88 | 109.67      | 114.92   |
| 32  | y     | 323 | AJP  | C83-C06-C05 | -2.88 | 109.67      | 114.92   |
| 25  | N     | 613 | CLA  | C4-C3-C5    | 2.87  | 120.11      | 115.27   |
| 25  | C     | 505 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 24  | n     | 608 | CHL  | CMB-C2B-C1B | -2.87 | 124.05      | 128.46   |
| 24  | N     | 605 | CHL  | CHD-C1D-ND  | -2.87 | 121.81      | 124.45   |
| 24  | n     | 605 | CHL  | CHD-C1D-ND  | -2.87 | 121.81      | 124.45   |
| 25  | b     | 608 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 25  | b     | 608 | CLA  | C4-C3-C5    | 2.87  | 120.10      | 115.27   |
| 27  | A     | 403 | PHO  | O1D-CGD-CBD | -2.87 | 119.96      | 124.74   |
| 27  | a     | 404 | PHO  | O1D-CGD-CBD | -2.87 | 119.96      | 124.74   |
| 25  | S     | 303 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 24  | R     | 613 | CHL  | CHD-C1D-ND  | -2.87 | 121.81      | 124.45   |
| 24  | n     | 605 | CHL  | O2A-CGA-CBA | 2.87  | 120.92      | 111.91   |
| 25  | b     | 611 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 25  | c     | 502 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 25  | B     | 603 | CLA  | C4-C3-C5    | 2.87  | 120.10      | 115.27   |
| 25  | G     | 610 | CLA  | C1B-CHB-C4A | -2.87 | 124.44      | 130.12   |
| 24  | n     | 609 | CHL  | O2A-CGA-CBA | 2.87  | 120.91      | 111.91   |
| 25  | c     | 503 | CLA  | C3D-C2D-C1D | 2.87  | 109.75      | 105.83   |
| 25  | C     | 512 | CLA  | C1D-ND-C4D  | -2.87 | 104.30      | 106.33   |
| 24  | y     | 308 | CHL  | CHD-C1D-ND  | -2.87 | 121.82      | 124.45   |
| 25  | N     | 612 | CLA  | C4A-NA-C1A  | -2.87 | 105.42      | 106.71   |
| 25  | n     | 612 | CLA  | C4A-NA-C1A  | -2.87 | 105.42      | 106.71   |
| 25  | 6     | 604 | CLA  | CHA-C1A-NA  | -2.87 | 119.83      | 126.40   |
| 25  | B     | 608 | CLA  | C4-C3-C5    | 2.87  | 120.09      | 115.27   |
| 25  | R     | 612 | CLA  | C4-C3-C5    | 2.87  | 120.09      | 115.27   |
| 25  | B     | 602 | CLA  | C3D-C2D-C1D | 2.87  | 109.74      | 105.83   |
| 25  | b     | 609 | CLA  | C3D-C2D-C1D | 2.87  | 109.74      | 105.83   |
| 24  | N     | 605 | CHL  | O2A-CGA-CBA | 2.86  | 120.90      | 111.91   |
| 24  | y     | 307 | CHL  | CAA-C2A-C3A | -2.86 | 104.94      | 112.78   |
| 25  | B     | 611 | CLA  | C3D-C2D-C1D | 2.86  | 109.74      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | B     | 614 | CLA  | C3D-C2D-C1D | 2.86  | 109.74      | 105.83   |
| 25  | b     | 614 | CLA  | C3D-C2D-C1D | 2.86  | 109.74      | 105.83   |
| 25  | b     | 612 | CLA  | C3D-C2D-C1D | 2.86  | 109.74      | 105.83   |
| 24  | R     | 606 | CHL  | CMB-C2B-C1B | -2.86 | 124.07      | 128.46   |
| 30  | D     | 407 | LMG  | C1-O6-C5    | -2.86 | 108.07      | 113.69   |
| 30  | d     | 407 | LMG  | C1-O6-C5    | -2.86 | 108.07      | 113.69   |
| 25  | B     | 612 | CLA  | C3D-C2D-C1D | 2.86  | 109.73      | 105.83   |
| 25  | c     | 513 | CLA  | C3D-C2D-C1D | 2.86  | 109.73      | 105.83   |
| 25  | b     | 607 | CLA  | CHD-C1D-C2D | 2.86  | 131.47      | 125.48   |
| 24  | N     | 609 | CHL  | O2A-CGA-CBA | 2.86  | 120.88      | 111.91   |
| 25  | y     | 305 | CLA  | C2A-C1A-CHA | -2.86 | 118.86      | 123.86   |
| 25  | Y     | 314 | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 25  | s     | 311 | CLA  | C1D-ND-C4D  | -2.86 | 104.31      | 106.33   |
| 24  | Y     | 307 | CHL  | CAA-C2A-C3A | -2.86 | 104.96      | 112.78   |
| 25  | N     | 610 | CLA  | C2A-C1A-CHA | -2.86 | 118.87      | 123.86   |
| 25  | c     | 506 | CLA  | C3D-C2D-C1D | 2.85  | 109.73      | 105.83   |
| 25  | g     | 610 | CLA  | C1B-CHB-C4A | -2.85 | 124.46      | 130.12   |
| 25  | C     | 503 | CLA  | C3D-C2D-C1D | 2.85  | 109.72      | 105.83   |
| 25  | C     | 506 | CLA  | C3D-C2D-C1D | 2.85  | 109.72      | 105.83   |
| 25  | 2     | 604 | CLA  | CHA-C1A-NA  | -2.85 | 119.86      | 126.40   |
| 25  | b     | 602 | CLA  | C3D-C2D-C1D | 2.85  | 109.72      | 105.83   |
| 25  | d     | 402 | CLA  | CHB-C4A-NA  | -2.85 | 120.57      | 124.51   |
| 25  | c     | 505 | CLA  | C3D-C2D-C1D | 2.85  | 109.72      | 105.83   |
| 25  | s     | 303 | CLA  | C3D-C2D-C1D | 2.85  | 109.72      | 105.83   |
| 25  | b     | 610 | CLA  | C4-C3-C5    | 2.85  | 120.06      | 115.27   |
| 25  | y     | 314 | CLA  | C4-C3-C5    | 2.85  | 120.06      | 115.27   |
| 25  | n     | 610 | CLA  | C2A-C1A-CHA | -2.85 | 118.88      | 123.86   |
| 25  | R     | 603 | CLA  | C4D-C3D-CAD | -2.85 | 104.74      | 108.10   |
| 25  | r     | 603 | CLA  | C4D-C3D-CAD | -2.85 | 104.74      | 108.10   |
| 25  | C     | 508 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 25  | c     | 508 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 24  | r     | 613 | CHL  | CHD-C1D-ND  | -2.85 | 121.84      | 124.45   |
| 32  | A     | 412 | AJP  | O84-C05-C06 | 2.84  | 117.36      | 107.38   |
| 32  | a     | 413 | AJP  | O84-C05-C06 | 2.84  | 117.36      | 107.38   |
| 25  | B     | 610 | CLA  | C4-C3-C5    | 2.84  | 120.06      | 115.27   |
| 25  | C     | 508 | CLA  | O1D-CGD-CBD | -2.84 | 118.67      | 124.48   |
| 25  | c     | 508 | CLA  | O1D-CGD-CBD | -2.84 | 118.67      | 124.48   |
| 41  | R     | 616 | XAT  | C27-C28-C29 | -2.84 | 121.12      | 125.53   |
| 24  | r     | 606 | CHL  | CMB-C2B-C1B | -2.84 | 124.09      | 128.46   |
| 28  | C     | 514 | BCR  | C33-C5-C6   | -2.84 | 121.34      | 124.53   |
| 25  | N     | 611 | CLA  | C2A-C1A-CHA | -2.84 | 118.89      | 123.86   |
| 25  | n     | 611 | CLA  | C2A-C1A-CHA | -2.84 | 118.89      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | R     | 609 | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.33   |
| 25  | y     | 305 | CLA  | C4D-CHA-C1A | -2.84 | 117.79      | 121.25   |
| 25  | R     | 608 | CLA  | C3D-C2D-C1D | 2.84  | 109.71      | 105.83   |
| 25  | b     | 603 | CLA  | C3D-C2D-C1D | 2.84  | 109.71      | 105.83   |
| 25  | b     | 603 | CLA  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 32  | a     | 413 | AJP  | O25-C23-C24 | 2.84  | 115.11      | 109.62   |
| 25  | a     | 406 | CLA  | C3D-C2D-C1D | 2.84  | 109.71      | 105.83   |
| 24  | Y     | 308 | CHL  | CHD-C1D-ND  | -2.84 | 121.84      | 124.45   |
| 25  | N     | 613 | CLA  | C3D-C2D-C1D | 2.84  | 109.71      | 105.83   |
| 25  | c     | 504 | CLA  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 25  | B     | 607 | CLA  | CHD-C1D-C2D | 2.84  | 131.43      | 125.48   |
| 25  | R     | 603 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 25  | r     | 603 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 25  | n     | 602 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 25  | C     | 505 | CLA  | C1-C2-C3    | -2.84 | 121.14      | 126.04   |
| 25  | c     | 505 | CLA  | C1-C2-C3    | -2.84 | 121.14      | 126.04   |
| 25  | A     | 405 | CLA  | C3D-C2D-C1D | 2.83  | 109.70      | 105.83   |
| 25  | R     | 610 | CLA  | C3B-C4B-NB  | -2.83 | 105.55      | 109.21   |
| 28  | T     | 101 | BCR  | C11-C10-C9  | -2.83 | 123.27      | 127.31   |
| 25  | r     | 612 | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 25  | r     | 601 | CLA  | O1D-CGD-CBD | -2.83 | 118.69      | 124.48   |
| 32  | B     | 624 | AJP  | C01-C02-C03 | 2.83  | 118.25      | 112.09   |
| 27  | A     | 404 | PHO  | O1D-CGD-CBD | -2.83 | 120.03      | 124.74   |
| 25  | r     | 610 | CLA  | C3B-C4B-NB  | -2.83 | 105.55      | 109.21   |
| 25  | g     | 604 | CLA  | C3D-C2D-C1D | 2.83  | 109.69      | 105.83   |
| 24  | g     | 606 | CHL  | O1D-CGD-CBD | -2.83 | 118.70      | 124.48   |
| 25  | y     | 305 | CLA  | C3D-C2D-C1D | 2.83  | 109.69      | 105.83   |
| 25  | b     | 609 | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 25  | Y     | 305 | CLA  | C4D-CHA-C1A | -2.83 | 117.81      | 121.25   |
| 24  | N     | 601 | CHL  | O2A-CGA-CBA | 2.83  | 120.78      | 111.91   |
| 25  | g     | 612 | CLA  | C3D-C2D-C1D | 2.83  | 109.69      | 105.83   |
| 27  | a     | 405 | PHO  | O1D-CGD-CBD | -2.82 | 120.03      | 124.74   |
| 25  | g     | 613 | CLA  | O1D-CGD-CBD | -2.82 | 118.70      | 124.48   |
| 25  | Y     | 305 | CLA  | C3D-C2D-C1D | 2.82  | 109.69      | 105.83   |
| 24  | n     | 601 | CHL  | O2A-CGA-CBA | 2.82  | 120.77      | 111.91   |
| 32  | Y     | 322 | AJP  | C04-C03-C02 | -2.82 | 105.85      | 111.81   |
| 25  | C     | 509 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 25  | Y     | 314 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 25  | c     | 509 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 25  | y     | 314 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 32  | y     | 322 | AJP  | C04-C03-C02 | -2.82 | 105.86      | 111.81   |
| 25  | r     | 608 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | G     | 606 | CHL  | O1D-CGD-CBD | -2.82 | 118.71      | 124.48   |
| 25  | N     | 602 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 32  | Y     | 324 | AJP  | O25-C26-O31 | 2.82  | 118.55      | 110.67   |
| 32  | y     | 324 | AJP  | O25-C26-O31 | 2.82  | 118.55      | 110.67   |
| 24  | R     | 607 | CHL  | CHD-C1D-ND  | -2.82 | 121.86      | 124.45   |
| 25  | Y     | 315 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 24  | g     | 601 | CHL  | CAA-C2A-C3A | -2.82 | 105.06      | 112.78   |
| 24  | 5     | 302 | CHL  | C2D-C1D-ND  | 2.82  | 112.18      | 110.10   |
| 25  | C     | 504 | CLA  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 25  | G     | 613 | CLA  | O1D-CGD-CBD | -2.82 | 118.72      | 124.48   |
| 28  | c     | 514 | BCR  | C33-C5-C6   | -2.82 | 121.36      | 124.53   |
| 25  | g     | 603 | CLA  | O1D-CGD-CBD | -2.82 | 118.72      | 124.48   |
| 25  | c     | 502 | CLA  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 25  | y     | 303 | CLA  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 25  | B     | 603 | CLA  | C3D-C2D-C1D | 2.82  | 109.68      | 105.83   |
| 25  | Y     | 303 | CLA  | C4-C3-C5    | 2.82  | 120.01      | 115.27   |
| 32  | b     | 624 | AJP  | C01-C02-C03 | 2.82  | 118.22      | 112.09   |
| 25  | B     | 609 | CLA  | C4-C3-C5    | 2.81  | 120.01      | 115.27   |
| 25  | R     | 601 | CLA  | O1D-CGD-CBD | -2.81 | 118.73      | 124.48   |
| 24  | N     | 609 | CHL  | C1-C2-C3    | 2.81  | 130.91      | 126.04   |
| 24  | n     | 609 | CHL  | C1-C2-C3    | 2.81  | 130.91      | 126.04   |
| 32  | Y     | 322 | AJP  | C01-C02-C03 | 2.81  | 118.21      | 112.09   |
| 25  | g     | 612 | CLA  | C4-C3-C5    | 2.81  | 120.00      | 115.27   |
| 25  | y     | 311 | CLA  | C3D-C2D-C1D | 2.81  | 109.66      | 105.83   |
| 24  | G     | 601 | CHL  | CAA-C2A-C3A | -2.81 | 105.09      | 112.78   |
| 24  | r     | 607 | CHL  | CHD-C1D-ND  | -2.81 | 121.87      | 124.45   |
| 25  | B     | 606 | CLA  | C3D-C2D-C1D | 2.81  | 109.66      | 105.83   |
| 25  | b     | 606 | CLA  | C3D-C2D-C1D | 2.81  | 109.66      | 105.83   |
| 32  | g     | 618 | AJP  | C04-C03-C02 | -2.81 | 105.89      | 111.81   |
| 25  | C     | 502 | CLA  | C4-C3-C5    | 2.80  | 119.99      | 115.27   |
| 25  | S     | 310 | CLA  | C4-C3-C5    | 2.80  | 119.99      | 115.27   |
| 25  | G     | 603 | CLA  | C4D-CHA-C1A | -2.80 | 117.84      | 121.25   |
| 25  | g     | 603 | CLA  | C4D-CHA-C1A | -2.80 | 117.84      | 121.25   |
| 25  | B     | 604 | CLA  | C4-C3-C5    | 2.80  | 119.99      | 115.27   |
| 25  | b     | 604 | CLA  | C4-C3-C5    | 2.80  | 119.99      | 115.27   |
| 25  | r     | 608 | CLA  | C4D-CHA-C1A | -2.80 | 117.84      | 121.25   |
| 25  | B     | 616 | CLA  | C2A-C1A-CHA | -2.80 | 118.96      | 123.86   |
| 25  | b     | 616 | CLA  | C2A-C1A-CHA | -2.80 | 118.96      | 123.86   |
| 25  | B     | 611 | CLA  | C1B-CHB-C4A | -2.80 | 124.57      | 130.12   |
| 25  | b     | 611 | CLA  | C1B-CHB-C4A | -2.80 | 124.57      | 130.12   |
| 32  | G     | 618 | AJP  | C04-C03-C02 | -2.80 | 105.90      | 111.81   |
| 28  | B     | 617 | BCR  | C11-C10-C9  | -2.80 | 123.31      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | b     | 617 | BCR  | C11-C10-C9  | -2.80 | 123.31      | 127.31   |
| 25  | G     | 612 | CLA  | C3D-C2D-C1D | 2.80  | 109.65      | 105.83   |
| 25  | y     | 315 | CLA  | C3D-C2D-C1D | 2.80  | 109.65      | 105.83   |
| 41  | r     | 616 | XAT  | C27-C28-C29 | -2.80 | 121.19      | 125.53   |
| 25  | G     | 603 | CLA  | O1D-CGD-CBD | -2.80 | 118.76      | 124.48   |
| 25  | B     | 607 | CLA  | C2A-C1A-CHA | -2.80 | 118.97      | 123.86   |
| 25  | b     | 607 | CLA  | C2A-C1A-CHA | -2.80 | 118.97      | 123.86   |
| 32  | y     | 322 | AJP  | C01-C02-C03 | 2.80  | 118.18      | 112.09   |
| 25  | B     | 613 | CLA  | C3D-C2D-C1D | 2.80  | 109.65      | 105.83   |
| 32  | Y     | 322 | AJP  | C26-O31-C30 | 2.80  | 116.23      | 113.13   |
| 32  | A     | 412 | AJP  | O25-C23-C24 | 2.80  | 115.03      | 109.62   |
| 25  | d     | 403 | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 25  | r     | 608 | CLA  | CHD-C1D-C2D | 2.79  | 131.34      | 125.48   |
| 25  | Y     | 311 | CLA  | C3D-C2D-C1D | 2.79  | 109.64      | 105.83   |
| 25  | r     | 603 | CLA  | C4D-CHA-C1A | -2.79 | 117.85      | 121.25   |
| 25  | R     | 608 | CLA  | CHD-C1D-C2D | 2.79  | 131.34      | 125.48   |
| 28  | t     | 101 | BCR  | C11-C10-C9  | -2.79 | 123.32      | 127.31   |
| 25  | r     | 611 | CLA  | CHD-C4C-C3C | 2.79  | 128.94      | 124.84   |
| 32  | S     | 319 | AJP  | C20-C21-C22 | 2.79  | 118.67      | 114.09   |
| 25  | G     | 612 | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 25  | s     | 310 | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 35  | c     | 515 | DGD  | C1E-O6E-C5E | -2.79 | 108.21      | 113.69   |
| 25  | r     | 602 | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 35  | C     | 515 | DGD  | C1E-O6E-C5E | -2.79 | 108.21      | 113.69   |
| 32  | B     | 624 | AJP  | O31-C26-C27 | 2.79  | 116.25      | 110.35   |
| 32  | b     | 624 | AJP  | O31-C26-C27 | 2.79  | 116.25      | 110.35   |
| 24  | Y     | 306 | CHL  | O2A-CGA-CBA | 2.79  | 120.66      | 111.91   |
| 25  | R     | 603 | CLA  | C4D-CHA-C1A | -2.79 | 117.86      | 121.25   |
| 25  | R     | 602 | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 32  | a     | 413 | AJP  | C55-O54-C36 | -2.79 | 111.07      | 117.96   |
| 35  | A     | 415 | DGD  | C3G-O3G-C1D | -2.79 | 108.29      | 113.74   |
| 35  | a     | 401 | DGD  | C3G-O3G-C1D | -2.79 | 108.29      | 113.74   |
| 24  | n     | 608 | CHL  | CHD-C1D-ND  | -2.79 | 121.89      | 124.45   |
| 25  | C     | 513 | CLA  | CHD-C1D-C2D | 2.79  | 131.32      | 125.48   |
| 25  | B     | 613 | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 25  | b     | 613 | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 24  | Y     | 302 | CHL  | O2A-CGA-CBA | 2.78  | 120.65      | 111.91   |
| 24  | y     | 302 | CHL  | O2A-CGA-CBA | 2.78  | 120.65      | 111.91   |
| 25  | A     | 402 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 25  | a     | 403 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 32  | A     | 412 | AJP  | O09-C05-C06 | -2.78 | 100.34      | 104.47   |
| 32  | a     | 413 | AJP  | O09-C05-C06 | -2.78 | 100.34      | 104.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 41  | R     | 616 | XAT  | C40-C33-C34 | -2.78 | 119.03      | 122.92   |
| 25  | D     | 403 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 25  | n     | 610 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 40  | y     | 318 | NEX  | C12-C13-C14 | 2.78  | 123.21      | 118.94   |
| 32  | y     | 324 | AJP  | O84-C05-C06 | 2.78  | 117.13      | 107.38   |
| 25  | N     | 610 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 25  | S     | 305 | CLA  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 25  | S     | 313 | CLA  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 25  | s     | 305 | CLA  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 25  | n     | 610 | CLA  | C3D-C2D-C1D | 2.78  | 109.62      | 105.83   |
| 25  | G     | 610 | CLA  | C2A-C1A-CHA | -2.78 | 119.00      | 123.86   |
| 25  | G     | 611 | CLA  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 25  | n     | 613 | CLA  | C3D-C2D-C1D | 2.78  | 109.62      | 105.83   |
| 41  | r     | 616 | XAT  | C40-C33-C34 | -2.78 | 119.03      | 122.92   |
| 25  | Y     | 313 | CLA  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 28  | K     | 101 | BCR  | C15-C16-C17 | -2.78 | 117.79      | 123.47   |
| 24  | R     | 613 | CHL  | CMA-C3A-C2A | -2.78 | 109.62      | 116.10   |
| 24  | r     | 613 | CHL  | CMA-C3A-C2A | -2.78 | 109.62      | 116.10   |
| 25  | C     | 506 | CLA  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 25  | b     | 605 | CLA  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 25  | c     | 506 | CLA  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 40  | Y     | 318 | NEX  | C12-C13-C14 | 2.77  | 123.20      | 118.94   |
| 32  | A     | 412 | AJP  | C55-O54-C36 | -2.77 | 111.10      | 117.96   |
| 25  | g     | 603 | CLA  | C4-C3-C5    | 2.77  | 119.94      | 115.27   |
| 40  | s     | 317 | NEX  | C28-C29-C30 | 2.77  | 123.20      | 118.94   |
| 25  | R     | 610 | CLA  | C2A-C3A-C4A | -2.77 | 97.39       | 101.87   |
| 32  | Y     | 324 | AJP  | O84-C05-C06 | 2.77  | 117.11      | 107.38   |
| 25  | r     | 610 | CLA  | C2A-C3A-C4A | -2.77 | 97.39       | 101.87   |
| 25  | N     | 612 | CLA  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 25  | c     | 513 | CLA  | CHD-C1D-C2D | 2.77  | 131.29      | 125.48   |
| 25  | B     | 616 | CLA  | O2A-CGA-CBA | 2.77  | 120.60      | 111.91   |
| 25  | b     | 616 | CLA  | O2A-CGA-CBA | 2.77  | 120.60      | 111.91   |
| 25  | R     | 604 | CLA  | O2A-CGA-CBA | 2.77  | 120.60      | 111.91   |
| 25  | r     | 604 | CLA  | O2A-CGA-CBA | 2.77  | 120.60      | 111.91   |
| 25  | Y     | 314 | CLA  | C1B-CHB-C4A | -2.77 | 124.63      | 130.12   |
| 25  | D     | 403 | CLA  | C4D-CHA-C1A | -2.77 | 117.88      | 121.25   |
| 25  | c     | 507 | CLA  | C4D-CHA-C1A | -2.77 | 117.88      | 121.25   |
| 25  | d     | 403 | CLA  | C4D-CHA-C1A | -2.77 | 117.88      | 121.25   |
| 32  | s     | 319 | AJP  | C20-C21-C22 | 2.77  | 118.63      | 114.09   |
| 24  | y     | 306 | CHL  | O2A-CGA-CBA | 2.77  | 120.59      | 111.91   |
| 25  | b     | 613 | CLA  | C3D-C2D-C1D | 2.77  | 109.61      | 105.83   |
| 24  | Y     | 309 | CHL  | CHD-C1D-ND  | -2.77 | 121.91      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 40  | S     | 317 | NEX  | C28-C29-C30 | 2.77  | 123.19      | 118.94   |
| 25  | B     | 616 | CLA  | C3D-C2D-C1D | 2.77  | 109.61      | 105.83   |
| 25  | B     | 604 | CLA  | C1B-CHB-C4A | -2.77 | 124.64      | 130.12   |
| 25  | b     | 604 | CLA  | C1B-CHB-C4A | -2.77 | 124.64      | 130.12   |
| 25  | c     | 505 | CLA  | C4-C3-C5    | 2.77  | 119.92      | 115.27   |
| 32  | Y     | 320 | AJP  | C04-C05-C06 | 2.76  | 121.38      | 115.69   |
| 32  | y     | 320 | AJP  | C04-C05-C06 | 2.76  | 121.38      | 115.69   |
| 25  | s     | 313 | CLA  | O1D-CGD-CBD | -2.76 | 118.83      | 124.48   |
| 25  | 6     | 605 | CLA  | O1D-CGD-CBD | -2.76 | 118.83      | 124.48   |
| 25  | B     | 611 | CLA  | CHD-C1D-C2D | 2.76  | 131.28      | 125.48   |
| 28  | k     | 101 | BCR  | C15-C16-C17 | -2.76 | 117.81      | 123.47   |
| 25  | n     | 612 | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 25  | R     | 614 | CLA  | C3D-C2D-C1D | 2.76  | 109.60      | 105.83   |
| 25  | r     | 614 | CLA  | C3D-C2D-C1D | 2.76  | 109.60      | 105.83   |
| 25  | g     | 610 | CLA  | C2A-C1A-CHA | -2.76 | 119.03      | 123.86   |
| 25  | D     | 402 | CLA  | C2A-C3A-C4A | -2.76 | 97.41       | 101.87   |
| 25  | d     | 402 | CLA  | C2A-C3A-C4A | -2.76 | 97.41       | 101.87   |
| 25  | Y     | 312 | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 25  | g     | 611 | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 25  | 2     | 605 | CLA  | O1D-CGD-CBD | -2.76 | 118.83      | 124.48   |
| 24  | y     | 306 | CHL  | CHD-C1D-ND  | -2.76 | 121.92      | 124.45   |
| 25  | R     | 611 | CLA  | CHD-C4C-C3C | 2.76  | 128.90      | 124.84   |
| 32  | y     | 322 | AJP  | C26-O31-C30 | 2.76  | 116.19      | 113.13   |
| 24  | g     | 609 | CHL  | C1-C2-C3    | 2.76  | 130.82      | 126.04   |
| 25  | G     | 603 | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 35  | c     | 515 | DGD  | C1D-O6D-C5D | -2.76 | 108.27      | 113.69   |
| 25  | N     | 614 | CLA  | C3D-C2D-C1D | 2.76  | 109.60      | 105.83   |
| 25  | n     | 614 | CLA  | C3D-C2D-C1D | 2.76  | 109.60      | 105.83   |
| 25  | b     | 611 | CLA  | CHD-C1D-C2D | 2.76  | 131.27      | 125.48   |
| 25  | 2     | 602 | CLA  | CHD-C4C-C3C | 2.76  | 128.90      | 124.84   |
| 25  | 6     | 602 | CLA  | CHD-C4C-C3C | 2.76  | 128.90      | 124.84   |
| 25  | N     | 610 | CLA  | C3D-C2D-C1D | 2.76  | 109.59      | 105.83   |
| 28  | T     | 101 | BCR  | C33-C5-C6   | -2.76 | 121.43      | 124.53   |
| 25  | y     | 313 | CLA  | C4-C3-C5    | 2.76  | 119.91      | 115.27   |
| 25  | y     | 303 | CLA  | C3D-C2D-C1D | 2.76  | 109.59      | 105.83   |
| 39  | s     | 315 | LUT  | C22-C23-C24 | 2.76  | 114.88      | 111.74   |
| 24  | 6     | 603 | CHL  | CHC-C1C-NC  | 2.75  | 128.38      | 124.20   |
| 25  | b     | 616 | CLA  | C3D-C2D-C1D | 2.75  | 109.59      | 105.83   |
| 25  | y     | 314 | CLA  | C1B-CHB-C4A | -2.75 | 124.67      | 130.12   |
| 24  | Y     | 302 | CHL  | CAA-C2A-C3A | -2.75 | 105.25      | 112.78   |
| 24  | y     | 302 | CHL  | CAA-C2A-C3A | -2.75 | 105.25      | 112.78   |
| 25  | y     | 312 | CLA  | C4-C3-C5    | 2.75  | 119.90      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | S     | 315 | LUT  | C22-C23-C24 | 2.75  | 114.87      | 111.74   |
| 28  | A     | 406 | BCR  | C33-C5-C6   | -2.75 | 121.44      | 124.53   |
| 28  | a     | 407 | BCR  | C33-C5-C6   | -2.75 | 121.44      | 124.53   |
| 32  | N     | 619 | AJP  | C01-C02-C03 | 2.75  | 118.07      | 112.09   |
| 24  | N     | 608 | CHL  | CHD-C1D-ND  | -2.75 | 121.93      | 124.45   |
| 25  | N     | 611 | CLA  | C4-C3-C5    | 2.75  | 119.89      | 115.27   |
| 25  | N     | 603 | CLA  | C4-C3-C5    | 2.75  | 119.89      | 115.27   |
| 25  | 6     | 604 | CLA  | C4-C3-C5    | 2.75  | 119.89      | 115.27   |
| 32  | S     | 319 | AJP  | O25-C26-O31 | 2.75  | 118.34      | 110.67   |
| 24  | G     | 605 | CHL  | CHD-C1D-ND  | -2.75 | 121.93      | 124.45   |
| 24  | g     | 605 | CHL  | CHD-C1D-ND  | -2.75 | 121.93      | 124.45   |
| 25  | Y     | 303 | CLA  | C3D-C2D-C1D | 2.74  | 109.58      | 105.83   |
| 25  | n     | 603 | CLA  | C4-C3-C5    | 2.74  | 119.89      | 115.27   |
| 25  | A     | 401 | CLA  | C4A-NA-C1A  | -2.74 | 105.47      | 106.71   |
| 35  | C     | 515 | DGD  | C1D-O6D-C5D | -2.74 | 108.31      | 113.69   |
| 24  | Y     | 302 | CHL  | C1-C2-C3    | 2.74  | 130.79      | 126.04   |
| 24  | y     | 302 | CHL  | C1-C2-C3    | 2.74  | 130.79      | 126.04   |
| 32  | n     | 619 | AJP  | C01-C02-C03 | 2.74  | 118.06      | 112.09   |
| 25  | c     | 509 | CLA  | C4-C3-C5    | 2.74  | 119.88      | 115.27   |
| 24  | G     | 601 | CHL  | O2A-CGA-CBA | 2.74  | 120.51      | 111.91   |
| 24  | g     | 601 | CHL  | O2A-CGA-CBA | 2.74  | 120.51      | 111.91   |
| 24  | G     | 609 | CHL  | C1-C2-C3    | 2.74  | 130.78      | 126.04   |
| 24  | Y     | 306 | CHL  | CHD-C1D-ND  | -2.74 | 121.94      | 124.45   |
| 28  | t     | 101 | BCR  | C33-C5-C6   | -2.74 | 121.45      | 124.53   |
| 25  | y     | 313 | CLA  | O1D-CGD-CBD | -2.74 | 118.88      | 124.48   |
| 25  | n     | 611 | CLA  | C4-C3-C5    | 2.74  | 119.88      | 115.27   |
| 25  | a     | 402 | CLA  | C4A-NA-C1A  | -2.74 | 105.47      | 106.71   |
| 25  | G     | 604 | CLA  | C2A-C1A-CHA | -2.74 | 119.07      | 123.86   |
| 32  | Y     | 324 | AJP  | C17-C16-C11 | -2.74 | 108.34      | 112.32   |
| 24  | S     | 307 | CHL  | CMB-C2B-C1B | -2.74 | 124.25      | 128.46   |
| 24  | s     | 307 | CHL  | CMB-C2B-C1B | -2.74 | 124.25      | 128.46   |
| 25  | C     | 505 | CLA  | C4-C3-C5    | 2.74  | 119.88      | 115.27   |
| 25  | R     | 608 | CLA  | O2A-CGA-CBA | 2.74  | 120.50      | 111.91   |
| 25  | B     | 605 | CLA  | C4-C3-C5    | 2.74  | 119.88      | 115.27   |
| 24  | 2     | 603 | CHL  | CHC-C1C-NC  | 2.74  | 128.36      | 124.20   |
| 25  | N     | 604 | CLA  | CHD-C1D-C2D | 2.74  | 131.22      | 125.48   |
| 25  | b     | 609 | CLA  | C2A-C1A-CHA | -2.74 | 119.08      | 123.86   |
| 25  | r     | 608 | CLA  | O2A-CGA-CBA | 2.73  | 120.49      | 111.91   |
| 25  | C     | 513 | CLA  | C4-C3-C5    | 2.73  | 119.87      | 115.27   |
| 24  | N     | 607 | CHL  | CMB-C2B-C1B | -2.73 | 124.27      | 128.46   |
| 25  | b     | 612 | CLA  | CHD-C1D-C2D | 2.73  | 131.21      | 125.48   |
| 25  | c     | 510 | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | Z     | 101 | BCR  | C24-C23-C22 | -2.73 | 122.11      | 126.23   |
| 28  | z     | 101 | BCR  | C24-C23-C22 | -2.73 | 122.11      | 126.23   |
| 32  | s     | 319 | AJP  | O25-C26-O31 | 2.73  | 118.30      | 110.67   |
| 28  | B     | 619 | BCR  | C33-C5-C6   | -2.73 | 121.46      | 124.53   |
| 28  | b     | 619 | BCR  | C33-C5-C6   | -2.73 | 121.46      | 124.53   |
| 25  | n     | 604 | CLA  | CHD-C1D-C2D | 2.73  | 131.20      | 125.48   |
| 25  | B     | 611 | CLA  | C4D-CHA-C1A | -2.73 | 117.93      | 121.25   |
| 28  | A     | 406 | BCR  | C27-C26-C25 | 2.73  | 126.69      | 122.73   |
| 28  | a     | 407 | BCR  | C27-C26-C25 | 2.73  | 126.69      | 122.73   |
| 25  | B     | 602 | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 25  | c     | 513 | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 25  | C     | 510 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.33   |
| 25  | c     | 510 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.33   |
| 25  | C     | 510 | CLA  | C1B-CHB-C4A | -2.72 | 124.72      | 130.12   |
| 25  | c     | 510 | CLA  | C1B-CHB-C4A | -2.72 | 124.72      | 130.12   |
| 25  | N     | 613 | CLA  | CHD-C1D-C2D | 2.72  | 131.19      | 125.48   |
| 28  | K     | 101 | BCR  | C33-C5-C6   | -2.72 | 121.47      | 124.53   |
| 28  | k     | 101 | BCR  | C33-C5-C6   | -2.72 | 121.47      | 124.53   |
| 25  | C     | 509 | CLA  | C4-C3-C5    | 2.72  | 119.85      | 115.27   |
| 25  | C     | 507 | CLA  | C3D-C2D-C1D | 2.72  | 109.55      | 105.83   |
| 25  | A     | 405 | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 25  | a     | 406 | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 24  | n     | 607 | CHL  | CMB-C2B-C1B | -2.72 | 124.28      | 128.46   |
| 24  | 6     | 601 | CHL  | C2A-C1A-CHA | 2.72  | 128.62      | 123.86   |
| 25  | B     | 609 | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 25  | R     | 614 | CLA  | O1D-CGD-CBD | -2.72 | 118.91      | 124.48   |
| 25  | b     | 611 | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 25  | C     | 511 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.33   |
| 25  | c     | 511 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.33   |
| 25  | C     | 507 | CLA  | C4D-CHA-C1A | -2.72 | 117.94      | 121.25   |
| 24  | y     | 309 | CHL  | CHD-C1D-ND  | -2.72 | 121.95      | 124.45   |
| 25  | r     | 614 | CLA  | O1D-CGD-CBD | -2.72 | 118.92      | 124.48   |
| 28  | A     | 406 | BCR  | C11-C10-C9  | -2.72 | 123.43      | 127.31   |
| 28  | a     | 407 | BCR  | C11-C10-C9  | -2.72 | 123.43      | 127.31   |
| 28  | B     | 619 | BCR  | C24-C23-C22 | -2.72 | 122.13      | 126.23   |
| 28  | b     | 619 | BCR  | C24-C23-C22 | -2.72 | 122.13      | 126.23   |
| 25  | N     | 614 | CLA  | CBA-CAA-C2A | -2.72 | 105.84      | 113.86   |
| 25  | B     | 611 | CLA  | C2A-C1A-CHA | -2.72 | 119.11      | 123.86   |
| 25  | g     | 613 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.33   |
| 24  | R     | 607 | CHL  | O2A-CGA-CBA | 2.72  | 120.43      | 111.91   |
| 25  | b     | 611 | CLA  | C4D-CHA-C1A | -2.72 | 117.94      | 121.25   |
| 25  | R     | 602 | CLA  | CHD-C1D-C2D | 2.72  | 131.18      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | s     | 311 | CLA  | C4-C3-C5    | 2.72  | 119.84      | 115.27   |
| 25  | A     | 401 | CLA  | C1B-CHB-C4A | -2.72 | 124.74      | 130.12   |
| 25  | a     | 402 | CLA  | C1B-CHB-C4A | -2.72 | 124.74      | 130.12   |
| 24  | n     | 607 | CHL  | O2A-CGA-O1A | -2.72 | 116.74      | 123.59   |
| 26  | s     | 318 | LHG  | O8-C23-C24  | 2.72  | 120.43      | 111.91   |
| 24  | N     | 607 | CHL  | O2A-CGA-O1A | -2.71 | 116.74      | 123.59   |
| 25  | B     | 613 | CLA  | O1D-CGD-CBD | -2.71 | 118.93      | 124.48   |
| 25  | b     | 613 | CLA  | O1D-CGD-CBD | -2.71 | 118.93      | 124.48   |
| 25  | 2     | 604 | CLA  | C4-C3-C5    | 2.71  | 119.84      | 115.27   |
| 25  | c     | 507 | CLA  | C3D-C2D-C1D | 2.71  | 109.53      | 105.83   |
| 25  | B     | 604 | CLA  | C4D-CHA-C1A | -2.71 | 117.95      | 121.25   |
| 25  | b     | 604 | CLA  | C4D-CHA-C1A | -2.71 | 117.95      | 121.25   |
| 24  | Y     | 310 | CHL  | CHD-C1D-ND  | -2.71 | 121.96      | 124.45   |
| 26  | S     | 318 | LHG  | O8-C23-C24  | 2.71  | 120.42      | 111.91   |
| 25  | C     | 504 | CLA  | C4D-C3D-CAD | -2.71 | 104.90      | 108.10   |
| 25  | c     | 504 | CLA  | C4D-C3D-CAD | -2.71 | 104.90      | 108.10   |
| 25  | S     | 313 | CLA  | C4-C3-C5    | 2.71  | 119.83      | 115.27   |
| 25  | s     | 313 | CLA  | C4-C3-C5    | 2.71  | 119.83      | 115.27   |
| 24  | y     | 307 | CHL  | OMC-CMC-C2C | -2.71 | 119.56      | 125.69   |
| 24  | Y     | 308 | CHL  | CMB-C2B-C1B | -2.71 | 124.30      | 128.46   |
| 25  | r     | 602 | CLA  | CHD-C1D-C2D | 2.71  | 131.16      | 125.48   |
| 40  | g     | 617 | NEX  | C5-C4-C3    | -2.71 | 108.54      | 111.75   |
| 25  | Y     | 313 | CLA  | O1D-CGD-CBD | -2.71 | 118.94      | 124.48   |
| 28  | I     | 101 | BCR  | C27-C26-C25 | 2.71  | 126.66      | 122.73   |
| 25  | B     | 612 | CLA  | CHD-C1D-C2D | 2.71  | 131.16      | 125.48   |
| 25  | n     | 612 | CLA  | C1D-CHD-C4C | -2.71 | 120.22      | 126.06   |
| 24  | Y     | 309 | CHL  | C2A-C1A-CHA | 2.71  | 128.59      | 123.86   |
| 32  | a     | 413 | AJP  | C61-C59-C58 | 2.71  | 119.34      | 113.00   |
| 30  | C     | 520 | LMG  | O8-C28-C29  | 2.71  | 120.40      | 111.91   |
| 25  | Y     | 315 | CLA  | O2D-CGD-O1D | -2.71 | 118.55      | 123.84   |
| 25  | b     | 602 | CLA  | C4-C3-C5    | 2.71  | 119.82      | 115.27   |
| 32  | y     | 324 | AJP  | C17-C16-C11 | -2.70 | 108.39      | 112.32   |
| 24  | Y     | 310 | CHL  | C1-C2-C3    | 2.70  | 130.72      | 126.04   |
| 24  | y     | 310 | CHL  | C1-C2-C3    | 2.70  | 130.72      | 126.04   |
| 25  | S     | 311 | CLA  | C4-C3-C5    | 2.70  | 119.82      | 115.27   |
| 24  | G     | 608 | CHL  | CHD-C1D-ND  | -2.70 | 121.97      | 124.45   |
| 24  | g     | 608 | CHL  | CHD-C1D-ND  | -2.70 | 121.97      | 124.45   |
| 25  | S     | 312 | CLA  | O2A-CGA-CBA | 2.70  | 120.39      | 111.91   |
| 25  | n     | 613 | CLA  | CHD-C1D-C2D | 2.70  | 131.15      | 125.48   |
| 28  | i     | 101 | BCR  | C27-C26-C25 | 2.70  | 126.66      | 122.73   |
| 25  | n     | 614 | CLA  | CBA-CAA-C2A | -2.70 | 105.89      | 113.86   |
| 24  | g     | 606 | CHL  | O2A-CGA-CBA | 2.70  | 120.39      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | y     | 309 | CHL  | C2A-C1A-CHA | 2.70  | 128.58      | 123.86   |
| 30  | c     | 520 | LMG  | O8-C28-C29  | 2.70  | 120.38      | 111.91   |
| 25  | g     | 604 | CLA  | C2A-C1A-CHA | -2.70 | 119.14      | 123.86   |
| 26  | 2     | 606 | LHG  | P-O6-C4     | -2.70 | 105.85      | 121.68   |
| 25  | G     | 613 | CLA  | C1D-ND-C4D  | -2.70 | 104.42      | 106.33   |
| 25  | R     | 601 | CLA  | C3D-C4D-CHA | 2.70  | 118.90      | 112.72   |
| 25  | r     | 601 | CLA  | C3D-C4D-CHA | 2.70  | 118.90      | 112.72   |
| 26  | Y     | 301 | LHG  | O8-C23-C24  | 2.70  | 120.38      | 111.91   |
| 26  | D     | 406 | LHG  | P-O6-C4     | -2.70 | 105.86      | 121.68   |
| 26  | d     | 406 | LHG  | P-O6-C4     | -2.70 | 105.86      | 121.68   |
| 26  | 6     | 606 | LHG  | P-O6-C4     | -2.70 | 105.86      | 121.68   |
| 24  | r     | 607 | CHL  | O2A-CGA-CBA | 2.70  | 120.38      | 111.91   |
| 25  | C     | 510 | CLA  | C4-C3-C5    | 2.70  | 119.81      | 115.27   |
| 25  | r     | 611 | CLA  | C3B-C4B-NB  | -2.70 | 105.72      | 109.21   |
| 24  | 2     | 601 | CHL  | C2A-C1A-CHA | 2.70  | 128.57      | 123.86   |
| 25  | N     | 602 | CLA  | C3D-C2D-C1D | 2.70  | 109.51      | 105.83   |
| 24  | G     | 606 | CHL  | O2A-CGA-CBA | 2.69  | 120.36      | 111.91   |
| 25  | R     | 611 | CLA  | C3B-C4B-NB  | -2.69 | 105.73      | 109.21   |
| 25  | y     | 315 | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 25  | y     | 305 | CLA  | O1D-CGD-CBD | -2.69 | 118.97      | 124.48   |
| 26  | y     | 301 | LHG  | O8-C23-C24  | 2.69  | 120.36      | 111.91   |
| 30  | a     | 409 | LMG  | C1-O6-C5    | -2.69 | 108.41      | 113.69   |
| 25  | Y     | 305 | CLA  | O1D-CGD-CBD | -2.69 | 118.98      | 124.48   |
| 25  | N     | 612 | CLA  | C1D-CHD-C4C | -2.69 | 120.25      | 126.06   |
| 28  | Z     | 101 | BCR  | C28-C27-C26 | -2.69 | 109.28      | 114.08   |
| 30  | A     | 408 | LMG  | C1-O6-C5    | -2.69 | 108.41      | 113.69   |
| 28  | I     | 101 | BCR  | C33-C5-C6   | -2.69 | 121.51      | 124.53   |
| 28  | K     | 101 | BCR  | C27-C26-C25 | 2.69  | 126.63      | 122.73   |
| 25  | C     | 512 | CLA  | O1D-CGD-CBD | -2.69 | 118.99      | 124.48   |
| 25  | c     | 512 | CLA  | O1D-CGD-CBD | -2.69 | 118.99      | 124.48   |
| 32  | A     | 412 | AJP  | C61-C59-C58 | 2.68  | 119.29      | 113.00   |
| 25  | S     | 303 | CLA  | CHD-C1D-C2D | 2.68  | 131.11      | 125.48   |
| 24  | y     | 310 | CHL  | CHD-C1D-ND  | -2.68 | 121.99      | 124.45   |
| 25  | s     | 312 | CLA  | O2A-CGA-CBA | 2.68  | 120.32      | 111.91   |
| 25  | C     | 504 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 40  | g     | 617 | NEX  | C39-C29-C30 | -2.68 | 119.17      | 122.92   |
| 25  | B     | 602 | CLA  | CHD-C1D-C2D | 2.68  | 131.10      | 125.48   |
| 25  | b     | 602 | CLA  | CHD-C1D-C2D | 2.68  | 131.10      | 125.48   |
| 25  | S     | 313 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 25  | s     | 313 | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 24  | y     | 308 | CHL  | CMB-C2B-C1B | -2.68 | 124.35      | 128.46   |
| 25  | G     | 602 | CLA  | C2A-C1A-CHA | -2.68 | 119.18      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 602 | CLA  | C2A-C1A-CHA | -2.68 | 119.18      | 123.86   |
| 25  | d     | 403 | CLA  | C4D-C3D-CAD | -2.68 | 104.94      | 108.10   |
| 28  | H     | 101 | BCR  | C2-C1-C6    | 2.68  | 114.60      | 110.48   |
| 25  | c     | 507 | CLA  | O2A-CGA-CBA | 2.68  | 120.31      | 111.91   |
| 25  | a     | 402 | CLA  | C4-C3-C5    | 2.68  | 119.77      | 115.27   |
| 32  | B     | 624 | AJP  | O84-C05-C06 | 2.68  | 116.77      | 107.38   |
| 32  | b     | 624 | AJP  | O84-C05-C06 | 2.68  | 116.77      | 107.38   |
| 25  | c     | 511 | CLA  | C4-C3-C5    | 2.68  | 119.77      | 115.27   |
| 24  | g     | 601 | CHL  | C1-C2-C3    | 2.67  | 130.67      | 126.04   |
| 28  | H     | 101 | BCR  | C24-C23-C22 | -2.67 | 122.20      | 126.23   |
| 25  | A     | 401 | CLA  | C4-C3-C5    | 2.67  | 119.77      | 115.27   |
| 25  | c     | 503 | CLA  | O1D-CGD-CBD | -2.67 | 119.02      | 124.48   |
| 24  | y     | 309 | CHL  | CMB-C2B-C1B | -2.67 | 124.36      | 128.46   |
| 28  | K     | 101 | BCR  | C2-C1-C6    | 2.67  | 114.59      | 110.48   |
| 28  | k     | 101 | BCR  | C2-C1-C6    | 2.67  | 114.59      | 110.48   |
| 40  | N     | 617 | NEX  | C28-C29-C30 | 2.67  | 123.04      | 118.94   |
| 25  | b     | 615 | CLA  | C4D-CHA-C1A | -2.67 | 118.00      | 121.25   |
| 25  | b     | 603 | CLA  | CHD-C1D-C2D | 2.67  | 131.08      | 125.48   |
| 25  | n     | 602 | CLA  | C3D-C2D-C1D | 2.67  | 109.47      | 105.83   |
| 40  | n     | 617 | NEX  | C28-C29-C30 | 2.67  | 123.03      | 118.94   |
| 32  | y     | 323 | AJP  | C06-C07-C08 | -2.67 | 99.49       | 104.34   |
| 41  | r     | 616 | XAT  | C20-C13-C14 | -2.66 | 119.19      | 122.92   |
| 28  | k     | 101 | BCR  | C27-C26-C25 | 2.66  | 126.60      | 122.73   |
| 25  | C     | 507 | CLA  | O2A-CGA-CBA | 2.66  | 120.27      | 111.91   |
| 32  | Y     | 323 | AJP  | C06-C07-C08 | -2.66 | 99.49       | 104.34   |
| 28  | z     | 101 | BCR  | C28-C27-C26 | -2.66 | 109.32      | 114.08   |
| 24  | Y     | 307 | CHL  | OMC-CMC-C2C | -2.66 | 119.67      | 125.69   |
| 25  | C     | 511 | CLA  | C4-C3-C5    | 2.66  | 119.75      | 115.27   |
| 28  | h     | 101 | BCR  | C24-C23-C22 | -2.66 | 122.22      | 126.23   |
| 25  | C     | 501 | CLA  | C4-C3-C5    | 2.66  | 119.75      | 115.27   |
| 28  | h     | 101 | BCR  | C2-C1-C6    | 2.66  | 114.58      | 110.48   |
| 25  | 6     | 602 | CLA  | C3D-C4D-CHA | 2.66  | 118.81      | 112.72   |
| 25  | Y     | 304 | CLA  | C4-C3-C5    | 2.66  | 119.74      | 115.27   |
| 27  | A     | 403 | PHO  | C4-C3-C5    | 2.66  | 119.74      | 115.27   |
| 27  | a     | 404 | PHO  | C4-C3-C5    | 2.66  | 119.74      | 115.27   |
| 24  | R     | 607 | CHL  | CMB-C2B-C1B | -2.66 | 124.38      | 128.46   |
| 24  | r     | 607 | CHL  | CMB-C2B-C1B | -2.66 | 124.38      | 128.46   |
| 25  | y     | 304 | CLA  | C4-C3-C5    | 2.66  | 119.74      | 115.27   |
| 25  | g     | 602 | CLA  | C1-C2-C3    | -2.66 | 121.45      | 126.04   |
| 25  | S     | 303 | CLA  | C4-C3-C5    | 2.66  | 119.74      | 115.27   |
| 28  | B     | 618 | BCR  | C33-C5-C6   | -2.66 | 121.55      | 124.53   |
| 28  | b     | 618 | BCR  | C33-C5-C6   | -2.66 | 121.55      | 124.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 6     | 602 | CLA  | O1D-CGD-CBD | -2.66 | 119.05      | 124.48   |
| 24  | 1     | 302 | CHL  | CMB-C2B-C1B | -2.66 | 124.38      | 128.46   |
| 25  | y     | 312 | CLA  | O2A-CGA-CBA | 2.66  | 120.24      | 111.91   |
| 25  | G     | 602 | CLA  | C3D-C2D-C1D | 2.65  | 109.45      | 105.83   |
| 25  | g     | 602 | CLA  | C3D-C2D-C1D | 2.65  | 109.45      | 105.83   |
| 25  | C     | 506 | CLA  | O2A-CGA-CBA | 2.65  | 120.23      | 111.91   |
| 25  | c     | 506 | CLA  | O2A-CGA-CBA | 2.65  | 120.23      | 111.91   |
| 25  | S     | 303 | CLA  | O1D-CGD-CBD | -2.65 | 119.06      | 124.48   |
| 25  | c     | 504 | CLA  | O2D-CGD-O1D | -2.65 | 118.65      | 123.84   |
| 25  | 2     | 604 | CLA  | C1B-CHB-C4A | -2.65 | 124.86      | 130.12   |
| 25  | 6     | 604 | CLA  | C1B-CHB-C4A | -2.65 | 124.86      | 130.12   |
| 25  | s     | 303 | CLA  | CHD-C1D-C2D | 2.65  | 131.04      | 125.48   |
| 28  | D     | 404 | BCR  | C28-C27-C26 | -2.65 | 109.34      | 114.08   |
| 25  | 2     | 602 | CLA  | C3D-C4D-CHA | 2.65  | 118.79      | 112.72   |
| 25  | s     | 303 | CLA  | O1D-CGD-CBD | -2.65 | 119.06      | 124.48   |
| 25  | n     | 603 | CLA  | CHD-C1D-C2D | 2.65  | 131.04      | 125.48   |
| 24  | G     | 601 | CHL  | C1-C2-C3    | 2.65  | 130.62      | 126.04   |
| 41  | R     | 616 | XAT  | C20-C13-C14 | -2.65 | 119.21      | 122.92   |
| 25  | S     | 311 | CLA  | C4D-CHA-C1A | -2.65 | 118.03      | 121.25   |
| 25  | s     | 311 | CLA  | C4D-CHA-C1A | -2.65 | 118.03      | 121.25   |
| 27  | A     | 403 | PHO  | O2A-CGA-CBA | 2.65  | 120.22      | 111.91   |
| 25  | Y     | 313 | CLA  | O2A-CGA-CBA | 2.65  | 120.21      | 111.91   |
| 25  | C     | 510 | CLA  | O2A-CGA-CBA | 2.65  | 120.21      | 111.91   |
| 24  | 5     | 302 | CHL  | CMB-C2B-C1B | -2.64 | 124.40      | 128.46   |
| 25  | c     | 510 | CLA  | O2A-CGA-CBA | 2.64  | 120.21      | 111.91   |
| 25  | 2     | 602 | CLA  | O1D-CGD-CBD | -2.64 | 119.07      | 124.48   |
| 24  | Y     | 309 | CHL  | CMB-C2B-C1B | -2.64 | 124.40      | 128.46   |
| 25  | B     | 615 | CLA  | C4D-CHA-C1A | -2.64 | 118.03      | 121.25   |
| 27  | a     | 404 | PHO  | O2A-CGA-CBA | 2.64  | 120.20      | 111.91   |
| 25  | N     | 603 | CLA  | CHD-C1D-C2D | 2.64  | 131.02      | 125.48   |
| 25  | D     | 403 | CLA  | C4D-C3D-CAD | -2.64 | 104.98      | 108.10   |
| 25  | B     | 606 | CLA  | C4-C3-C5    | 2.64  | 119.72      | 115.27   |
| 25  | b     | 606 | CLA  | C4-C3-C5    | 2.64  | 119.72      | 115.27   |
| 25  | c     | 501 | CLA  | C4-C3-C5    | 2.64  | 119.72      | 115.27   |
| 26  | S     | 318 | LHG  | P-O6-C4     | -2.64 | 106.19      | 121.68   |
| 32  | A     | 412 | AJP  | C58-C57-C56 | 2.64  | 114.66      | 110.85   |
| 32  | a     | 413 | AJP  | C58-C57-C56 | 2.64  | 114.66      | 110.85   |
| 25  | g     | 613 | CLA  | C4-C3-C5    | 2.64  | 119.71      | 115.27   |
| 26  | Y     | 301 | LHG  | P-O3-C3     | -2.64 | 106.20      | 121.68   |
| 26  | y     | 301 | LHG  | P-O3-C3     | -2.64 | 106.20      | 121.68   |
| 25  | B     | 603 | CLA  | CHD-C1D-C2D | 2.64  | 131.02      | 125.48   |
| 40  | N     | 617 | NEX  | C2-C1-C6    | 2.64  | 111.78      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | N     | 604 | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 32  | B     | 624 | AJP  | C06-C07-C08 | -2.64 | 99.54       | 104.34   |
| 32  | b     | 624 | AJP  | C06-C07-C08 | -2.64 | 99.54       | 104.34   |
| 25  | Y     | 312 | CLA  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 25  | s     | 303 | CLA  | C4-C3-C5    | 2.64  | 119.70      | 115.27   |
| 25  | n     | 613 | CLA  | C1B-CHB-C4A | -2.63 | 124.90      | 130.12   |
| 25  | c     | 508 | CLA  | C1D-ND-C4D  | -2.63 | 104.46      | 106.33   |
| 24  | n     | 607 | CHL  | CAA-C2A-C3A | -2.63 | 105.57      | 112.78   |
| 26  | s     | 318 | LHG  | P-O6-C4     | -2.63 | 106.24      | 121.68   |
| 26  | B     | 625 | LHG  | P-O6-C4     | -2.63 | 106.24      | 121.68   |
| 39  | G     | 615 | LUT  | C35-C15-C14 | -2.63 | 118.08      | 123.47   |
| 39  | g     | 615 | LUT  | C35-C15-C14 | -2.63 | 118.08      | 123.47   |
| 25  | b     | 606 | CLA  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 25  | B     | 613 | CLA  | O2D-CGD-O1D | -2.63 | 118.69      | 123.84   |
| 25  | b     | 613 | CLA  | O2D-CGD-O1D | -2.63 | 118.69      | 123.84   |
| 25  | G     | 602 | CLA  | C1-C2-C3    | -2.63 | 121.49      | 126.04   |
| 25  | n     | 604 | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 26  | C     | 518 | LHG  | O8-C23-C24  | 2.63  | 120.16      | 111.91   |
| 25  | G     | 613 | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 25  | N     | 613 | CLA  | C1B-CHB-C4A | -2.63 | 124.91      | 130.12   |
| 28  | B     | 618 | BCR  | C15-C16-C17 | -2.63 | 118.09      | 123.47   |
| 28  | b     | 618 | BCR  | C15-C16-C17 | -2.63 | 118.09      | 123.47   |
| 39  | r     | 615 | LUT  | C1-C2-C3    | 2.63  | 119.58      | 113.64   |
| 24  | N     | 607 | CHL  | CAA-C2A-C3A | -2.63 | 105.59      | 112.78   |
| 32  | g     | 618 | AJP  | C06-C07-C08 | -2.62 | 99.56       | 104.34   |
| 25  | c     | 512 | CLA  | C4-C3-C5    | 2.62  | 119.69      | 115.27   |
| 26  | b     | 625 | LHG  | P-O6-C4     | -2.62 | 106.30      | 121.68   |
| 28  | A     | 406 | BCR  | C24-C23-C22 | -2.62 | 122.27      | 126.23   |
| 28  | a     | 407 | BCR  | C24-C23-C22 | -2.62 | 122.27      | 126.23   |
| 28  | d     | 404 | BCR  | C28-C27-C26 | -2.62 | 109.39      | 114.08   |
| 25  | C     | 503 | CLA  | O1D-CGD-CBD | -2.62 | 119.12      | 124.48   |
| 24  | y     | 310 | CHL  | C2A-C1A-CHA | 2.62  | 128.44      | 123.86   |
| 29  | l     | 101 | SQD  | O7-S-C6     | 2.62  | 110.06      | 106.94   |
| 25  | R     | 610 | CLA  | C3D-C4D-CHA | 2.62  | 118.72      | 112.72   |
| 25  | C     | 501 | CLA  | O2A-CGA-CBA | 2.62  | 120.13      | 111.91   |
| 25  | b     | 611 | CLA  | C4-C3-C5    | 2.62  | 119.68      | 115.27   |
| 25  | C     | 509 | CLA  | CHD-C1D-C2D | 2.62  | 130.98      | 125.48   |
| 25  | A     | 405 | CLA  | C4D-CHA-C1A | -2.62 | 118.06      | 121.25   |
| 25  | a     | 406 | CLA  | C4D-CHA-C1A | -2.62 | 118.06      | 121.25   |
| 25  | B     | 606 | CLA  | O2A-CGA-CBA | 2.62  | 120.13      | 111.91   |
| 25  | g     | 612 | CLA  | O2A-CGA-CBA | 2.62  | 120.13      | 111.91   |
| 25  | r     | 609 | CLA  | O2A-CGA-CBA | 2.62  | 120.13      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | k     | 101 | BCR  | C24-C23-C22 | -2.62 | 122.28      | 126.23   |
| 32  | G     | 618 | AJP  | C06-C07-C08 | -2.62 | 99.58       | 104.34   |
| 39  | R     | 615 | LUT  | C1-C2-C3    | 2.62  | 119.55      | 113.64   |
| 25  | c     | 509 | CLA  | CHD-C1D-C2D | 2.62  | 130.97      | 125.48   |
| 32  | A     | 412 | AJP  | O40-C35-C36 | 2.62  | 114.70      | 109.51   |
| 25  | r     | 614 | CLA  | C4A-NA-C1A  | -2.62 | 105.53      | 106.71   |
| 32  | B     | 624 | AJP  | C24-C19-C18 | -2.62 | 106.94      | 111.74   |
| 32  | b     | 624 | AJP  | C24-C19-C18 | -2.62 | 106.94      | 111.74   |
| 25  | y     | 313 | CLA  | O2A-CGA-CBA | 2.62  | 120.12      | 111.91   |
| 25  | A     | 402 | CLA  | O2A-CGA-CBA | 2.62  | 120.11      | 111.91   |
| 24  | g     | 607 | CHL  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 32  | n     | 619 | AJP  | C04-C03-C02 | -2.62 | 106.29      | 111.81   |
| 25  | a     | 403 | CLA  | O2A-CGA-CBA | 2.61  | 120.11      | 111.91   |
| 26  | c     | 518 | LHG  | O8-C23-C24  | 2.61  | 120.11      | 111.91   |
| 25  | S     | 310 | CLA  | C1D-CHD-C4C | -2.61 | 120.42      | 126.06   |
| 25  | R     | 609 | CLA  | O2A-CGA-CBA | 2.61  | 120.11      | 111.91   |
| 28  | i     | 101 | BCR  | C33-C5-C6   | -2.61 | 121.59      | 124.53   |
| 40  | n     | 617 | NEX  | C2-C1-C6    | 2.61  | 111.75      | 109.21   |
| 24  | Y     | 310 | CHL  | CMB-C2B-C1B | -2.61 | 124.45      | 128.46   |
| 32  | B     | 624 | AJP  | C83-C06-C05 | -2.61 | 110.15      | 114.92   |
| 32  | b     | 624 | AJP  | C83-C06-C05 | -2.61 | 110.15      | 114.92   |
| 32  | A     | 412 | AJP  | C18-C17-C16 | -2.61 | 107.84      | 112.14   |
| 32  | S     | 319 | AJP  | C01-C02-C03 | 2.61  | 117.78      | 112.09   |
| 40  | G     | 617 | NEX  | C39-C29-C30 | -2.61 | 119.27      | 122.92   |
| 32  | a     | 413 | AJP  | O40-C35-C36 | 2.61  | 114.69      | 109.51   |
| 25  | g     | 613 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 25  | c     | 504 | CLA  | C2A-C3A-C4A | -2.61 | 97.65       | 101.87   |
| 25  | c     | 501 | CLA  | C4D-C3D-CAD | -2.61 | 105.02      | 108.10   |
| 25  | B     | 616 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 25  | b     | 616 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 25  | Y     | 314 | CLA  | CHD-C1D-C2D | 2.61  | 130.95      | 125.48   |
| 25  | y     | 314 | CLA  | CHD-C1D-C2D | 2.61  | 130.95      | 125.48   |
| 25  | G     | 613 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 29  | L     | 103 | SQD  | O7-S-C6     | 2.61  | 110.04      | 106.94   |
| 28  | k     | 101 | BCR  | C15-C14-C13 | -2.61 | 123.59      | 127.31   |
| 24  | n     | 609 | CHL  | C4D-CHA-C1A | 2.61  | 124.42      | 121.25   |
| 26  | L     | 102 | LHG  | O8-C23-C24  | 2.61  | 120.09      | 111.91   |
| 26  | l     | 103 | LHG  | O8-C23-C24  | 2.61  | 120.09      | 111.91   |
| 32  | a     | 413 | AJP  | C18-C17-C16 | -2.61 | 107.85      | 112.14   |
| 25  | G     | 612 | CLA  | O2A-CGA-CBA | 2.61  | 120.08      | 111.91   |
| 40  | g     | 617 | NEX  | C20-C13-C12 | 2.60  | 122.18      | 118.08   |
| 25  | r     | 608 | CLA  | C4-C3-C5    | 2.60  | 119.65      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | g     | 609 | CHL  | CHD-C1D-ND  | -2.60 | 122.06      | 124.45   |
| 25  | B     | 611 | CLA  | C4-C3-C5    | 2.60  | 119.65      | 115.27   |
| 25  | C     | 512 | CLA  | C4-C3-C5    | 2.60  | 119.65      | 115.27   |
| 40  | G     | 617 | NEX  | C10-C11-C12 | 2.60  | 131.34      | 123.22   |
| 25  | R     | 608 | CLA  | C4-C3-C5    | 2.60  | 119.65      | 115.27   |
| 25  | c     | 501 | CLA  | O2A-CGA-CBA | 2.60  | 120.07      | 111.91   |
| 28  | K     | 101 | BCR  | C24-C23-C22 | -2.60 | 122.31      | 126.23   |
| 24  | N     | 605 | CHL  | CMB-C2B-C1B | -2.60 | 124.47      | 128.46   |
| 24  | n     | 605 | CHL  | CMB-C2B-C1B | -2.60 | 124.47      | 128.46   |
| 24  | 2     | 603 | CHL  | CAA-C2A-C3A | -2.60 | 105.66      | 112.78   |
| 32  | A     | 412 | AJP  | C71-C69-C68 | 2.60  | 119.09      | 113.00   |
| 32  | a     | 413 | AJP  | C71-C69-C68 | 2.60  | 119.09      | 113.00   |
| 24  | 6     | 603 | CHL  | CAA-C2A-C3A | -2.60 | 105.66      | 112.78   |
| 28  | K     | 101 | BCR  | C15-C14-C13 | -2.60 | 123.60      | 127.31   |
| 25  | R     | 611 | CLA  | C2C-C1C-NC  | -2.60 | 107.54      | 109.97   |
| 26  | n     | 618 | LHG  | P-O6-C4     | -2.60 | 106.45      | 121.68   |
| 32  | B     | 624 | AJP  | C85-O84-C05 | 2.60  | 118.64      | 113.72   |
| 32  | b     | 624 | AJP  | C85-O84-C05 | 2.60  | 118.64      | 113.72   |
| 25  | r     | 611 | CLA  | CAD-C3D-C2D | 2.60  | 153.33      | 140.80   |
| 32  | s     | 319 | AJP  | C01-C02-C03 | 2.60  | 117.74      | 112.09   |
| 26  | Y     | 319 | LHG  | P-O3-C3     | -2.60 | 106.46      | 121.68   |
| 26  | y     | 319 | LHG  | P-O3-C3     | -2.60 | 106.46      | 121.68   |
| 25  | a     | 406 | CLA  | C1B-CHB-C4A | -2.60 | 124.97      | 130.12   |
| 32  | N     | 619 | AJP  | C18-C17-C16 | -2.60 | 107.86      | 112.14   |
| 24  | 2     | 603 | CHL  | CMB-C2B-C1B | -2.60 | 124.47      | 128.46   |
| 24  | 6     | 603 | CHL  | CMB-C2B-C1B | -2.60 | 124.47      | 128.46   |
| 25  | s     | 310 | CLA  | C3D-C2D-C1D | 2.59  | 109.37      | 105.83   |
| 25  | C     | 504 | CLA  | C2A-C3A-C4A | -2.59 | 97.68       | 101.87   |
| 25  | B     | 614 | CLA  | CHD-C1D-C2D | 2.59  | 130.92      | 125.48   |
| 25  | b     | 614 | CLA  | CHD-C1D-C2D | 2.59  | 130.92      | 125.48   |
| 32  | N     | 620 | AJP  | C19-C24-C23 | -2.59 | 106.47      | 112.92   |
| 32  | n     | 620 | AJP  | C19-C24-C23 | -2.59 | 106.47      | 112.92   |
| 24  | y     | 310 | CHL  | CMB-C2B-C1B | -2.59 | 124.48      | 128.46   |
| 24  | G     | 608 | CHL  | CMB-C2B-C1B | -2.59 | 124.48      | 128.46   |
| 25  | G     | 614 | CLA  | O2A-CGA-CBA | 2.59  | 120.04      | 111.91   |
| 25  | g     | 614 | CLA  | O2A-CGA-CBA | 2.59  | 120.04      | 111.91   |
| 24  | Y     | 310 | CHL  | C2A-C1A-CHA | 2.59  | 128.39      | 123.86   |
| 25  | r     | 610 | CLA  | C3D-C4D-CHA | 2.59  | 118.65      | 112.72   |
| 25  | B     | 612 | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 25  | b     | 612 | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 32  | y     | 321 | AJP  | C83-C06-C05 | -2.59 | 110.19      | 114.92   |
| 25  | s     | 310 | CLA  | C1D-CHD-C4C | -2.59 | 120.47      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | G     | 605 | CHL  | OMC-CMC-C2C | -2.59 | 119.83      | 125.69   |
| 25  | R     | 611 | CLA  | CAD-C3D-C2D | 2.59  | 153.30      | 140.80   |
| 24  | N     | 609 | CHL  | CMB-C2B-C1B | -2.59 | 124.48      | 128.46   |
| 26  | N     | 618 | LHG  | P-O6-C4     | -2.59 | 106.50      | 121.68   |
| 26  | b     | 621 | LHG  | P-O3-C3     | -2.59 | 106.50      | 121.68   |
| 26  | B     | 621 | LHG  | P-O3-C3     | -2.59 | 106.50      | 121.68   |
| 26  | n     | 618 | LHG  | O8-C23-C24  | 2.59  | 120.03      | 111.91   |
| 25  | C     | 512 | CLA  | O2D-CGD-O1D | -2.59 | 118.78      | 123.84   |
| 35  | B     | 626 | DGD  | O1G-C1A-C2A | 2.59  | 120.03      | 111.91   |
| 26  | C     | 518 | LHG  | P-O3-C3     | -2.59 | 106.51      | 121.68   |
| 24  | N     | 609 | CHL  | C4D-CHA-C1A | 2.59  | 124.40      | 121.25   |
| 26  | c     | 518 | LHG  | P-O3-C3     | -2.59 | 106.52      | 121.68   |
| 25  | c     | 512 | CLA  | O2D-CGD-O1D | -2.58 | 118.78      | 123.84   |
| 24  | l     | 301 | CHL  | CMB-C2B-C1B | -2.58 | 124.49      | 128.46   |
| 32  | N     | 619 | AJP  | C04-C03-C02 | -2.58 | 106.36      | 111.81   |
| 25  | R     | 602 | CLA  | C2A-C1A-CHA | -2.58 | 119.34      | 123.86   |
| 25  | r     | 602 | CLA  | C2A-C1A-CHA | -2.58 | 119.34      | 123.86   |
| 28  | I     | 101 | BCR  | C15-C14-C13 | -2.58 | 123.62      | 127.31   |
| 25  | C     | 511 | CLA  | C4D-CHA-C1A | -2.58 | 118.11      | 121.25   |
| 24  | g     | 605 | CHL  | C2A-C1A-CHA | 2.58  | 128.38      | 123.86   |
| 28  | B     | 618 | BCR  | C15-C14-C13 | -2.58 | 123.62      | 127.31   |
| 28  | b     | 618 | BCR  | C15-C14-C13 | -2.58 | 123.62      | 127.31   |
| 24  | g     | 608 | CHL  | CMB-C2B-C1B | -2.58 | 124.50      | 128.46   |
| 28  | Z     | 101 | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 40  | N     | 617 | NEX  | C40-C33-C34 | -2.58 | 119.31      | 122.92   |
| 32  | n     | 619 | AJP  | C18-C17-C16 | -2.58 | 107.89      | 112.14   |
| 25  | C     | 508 | CLA  | C1D-ND-C4D  | -2.58 | 104.50      | 106.33   |
| 24  | R     | 605 | CHL  | CMB-C2B-C1B | -2.58 | 124.50      | 128.46   |
| 25  | N     | 614 | CLA  | O1D-CGD-CBD | -2.58 | 119.21      | 124.48   |
| 35  | c     | 516 | DGD  | O1G-C1A-C2A | 2.58  | 120.00      | 111.91   |
| 35  | b     | 626 | DGD  | O1G-C1A-C2A | 2.58  | 120.00      | 111.91   |
| 24  | G     | 605 | CHL  | CMB-C2B-C1B | -2.58 | 124.50      | 128.46   |
| 25  | C     | 502 | CLA  | O1D-CGD-CBD | -2.58 | 119.21      | 124.48   |
| 25  | B     | 610 | CLA  | C4D-CHA-C1A | -2.58 | 118.11      | 121.25   |
| 25  | b     | 610 | CLA  | C4D-CHA-C1A | -2.58 | 118.11      | 121.25   |
| 24  | Y     | 310 | CHL  | O2A-CGA-CBA | 2.57  | 119.98      | 111.91   |
| 24  | y     | 310 | CHL  | O2A-CGA-CBA | 2.57  | 119.98      | 111.91   |
| 26  | s     | 301 | LHG  | P-O6-C4     | -2.57 | 106.59      | 121.68   |
| 24  | n     | 609 | CHL  | CMB-C2B-C1B | -2.57 | 124.51      | 128.46   |
| 32  | A     | 412 | AJP  | O25-C26-O31 | 2.57  | 117.86      | 110.67   |
| 32  | a     | 413 | AJP  | O25-C26-O31 | 2.57  | 117.86      | 110.67   |
| 25  | c     | 511 | CLA  | C4D-CHA-C1A | -2.57 | 118.12      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 321 | AJP  | C83-C06-C05 | -2.57 | 110.22      | 114.92   |
| 26  | 2     | 606 | LHG  | O8-C23-C24  | 2.57  | 119.98      | 111.91   |
| 25  | B     | 610 | CLA  | O1D-CGD-CBD | -2.57 | 119.22      | 124.48   |
| 25  | b     | 610 | CLA  | O1D-CGD-CBD | -2.57 | 119.22      | 124.48   |
| 24  | G     | 607 | CHL  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 28  | z     | 101 | BCR  | C33-C5-C6   | -2.57 | 121.64      | 124.53   |
| 25  | C     | 501 | CLA  | C4D-C3D-CAD | -2.57 | 105.07      | 108.10   |
| 24  | g     | 605 | CHL  | OMC-CMC-C2C | -2.57 | 119.88      | 125.69   |
| 25  | 2     | 605 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 25  | 6     | 605 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 25  | r     | 611 | CLA  | C2C-C1C-NC  | -2.57 | 107.56      | 109.97   |
| 24  | r     | 605 | CHL  | CMB-C2B-C1B | -2.57 | 124.52      | 128.46   |
| 25  | n     | 603 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 32  | y     | 321 | AJP  | C21-C20-C15 | -2.57 | 106.24      | 110.08   |
| 26  | N     | 618 | LHG  | O8-C23-C24  | 2.57  | 119.97      | 111.91   |
| 32  | Y     | 321 | AJP  | C21-C20-C15 | -2.57 | 106.24      | 110.08   |
| 35  | C     | 516 | DGD  | O1G-C1A-C2A | 2.57  | 119.96      | 111.91   |
| 26  | B     | 622 | LHG  | P-O6-C4     | -2.57 | 106.63      | 121.68   |
| 26  | b     | 622 | LHG  | P-O6-C4     | -2.57 | 106.63      | 121.68   |
| 28  | i     | 101 | BCR  | C15-C14-C13 | -2.57 | 123.65      | 127.31   |
| 26  | l     | 103 | LHG  | P-O6-C4     | -2.57 | 106.64      | 121.68   |
| 24  | 5     | 301 | CHL  | CMB-C2B-C1B | -2.57 | 124.52      | 128.46   |
| 25  | y     | 312 | CLA  | O1D-CGD-CBD | -2.57 | 119.23      | 124.48   |
| 24  | S     | 306 | CHL  | CMB-C2B-C1B | -2.56 | 124.52      | 128.46   |
| 24  | s     | 306 | CHL  | CMB-C2B-C1B | -2.56 | 124.52      | 128.46   |
| 26  | S     | 301 | LHG  | P-O3-C3     | -2.56 | 106.64      | 121.68   |
| 26  | s     | 301 | LHG  | P-O3-C3     | -2.56 | 106.64      | 121.68   |
| 39  | N     | 616 | LUT  | C2-C3-C4    | 2.56  | 113.81      | 110.30   |
| 24  | n     | 608 | CHL  | C2A-C1A-CHA | 2.56  | 128.34      | 123.86   |
| 26  | S     | 301 | LHG  | P-O6-C4     | -2.56 | 106.65      | 121.68   |
| 24  | 6     | 601 | CHL  | CMB-C2B-C1B | -2.56 | 124.52      | 128.46   |
| 24  | n     | 601 | CHL  | C4D-CHA-C1A | 2.56  | 124.37      | 121.25   |
| 26  | L     | 102 | LHG  | P-O6-C4     | -2.56 | 106.66      | 121.68   |
| 25  | b     | 609 | CLA  | O1D-CGD-CBD | -2.56 | 119.24      | 124.48   |
| 25  | n     | 614 | CLA  | O1D-CGD-CBD | -2.56 | 119.24      | 124.48   |
| 25  | A     | 405 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 24  | S     | 308 | CHL  | CMB-C2B-C1B | -2.56 | 124.53      | 128.46   |
| 24  | g     | 601 | CHL  | CMB-C2B-C1B | -2.56 | 124.53      | 128.46   |
| 24  | s     | 308 | CHL  | CMB-C2B-C1B | -2.56 | 124.53      | 128.46   |
| 25  | c     | 502 | CLA  | O1D-CGD-CBD | -2.56 | 119.25      | 124.48   |
| 25  | Y     | 304 | CLA  | CHD-C1D-C2D | 2.56  | 130.85      | 125.48   |
| 32  | Y     | 321 | AJP  | C85-O84-C05 | -2.56 | 108.87      | 113.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 321 | AJP  | C85-O84-C05 | -2.56 | 108.87      | 113.72   |
| 24  | 2     | 601 | CHL  | CMB-C2B-C1B | -2.56 | 124.53      | 128.46   |
| 24  | G     | 605 | CHL  | C2A-C1A-CHA | 2.56  | 128.33      | 123.86   |
| 25  | 6     | 602 | CLA  | C4-C3-C5    | 2.56  | 119.57      | 115.27   |
| 26  | d     | 406 | LHG  | O8-C23-C24  | 2.56  | 119.93      | 111.91   |
| 25  | b     | 612 | CLA  | O2A-CGA-CBA | 2.56  | 119.93      | 111.91   |
| 24  | G     | 608 | CHL  | C2A-C1A-CHA | 2.56  | 128.33      | 123.86   |
| 25  | N     | 603 | CLA  | O2A-CGA-CBA | 2.56  | 119.93      | 111.91   |
| 24  | g     | 608 | CHL  | C2A-C1A-CHA | 2.56  | 128.33      | 123.86   |
| 26  | D     | 406 | LHG  | O8-C23-C24  | 2.56  | 119.93      | 111.91   |
| 25  | 2     | 602 | CLA  | C4-C3-C5    | 2.55  | 119.57      | 115.27   |
| 24  | N     | 608 | CHL  | C2A-C1A-CHA | 2.55  | 128.32      | 123.86   |
| 25  | s     | 303 | CLA  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 26  | 6     | 606 | LHG  | O8-C23-C24  | 2.55  | 119.92      | 111.91   |
| 25  | S     | 310 | CLA  | C3D-C2D-C1D | 2.55  | 109.31      | 105.83   |
| 26  | b     | 621 | LHG  | P-O6-C4     | -2.55 | 106.71      | 121.68   |
| 24  | N     | 607 | CHL  | OMC-CMC-C2C | -2.55 | 119.92      | 125.69   |
| 25  | B     | 608 | CLA  | CHD-C1D-C2D | 2.55  | 130.83      | 125.48   |
| 39  | n     | 616 | LUT  | C2-C3-C4    | 2.55  | 113.80      | 110.30   |
| 25  | B     | 609 | CLA  | O1D-CGD-CBD | -2.55 | 119.26      | 124.48   |
| 25  | B     | 602 | CLA  | O2A-CGA-CBA | 2.55  | 119.92      | 111.91   |
| 24  | G     | 601 | CHL  | CMB-C2B-C1B | -2.55 | 124.54      | 128.46   |
| 24  | g     | 605 | CHL  | CMB-C2B-C1B | -2.55 | 124.54      | 128.46   |
| 32  | Y     | 324 | AJP  | C01-C02-C03 | 2.55  | 117.64      | 112.09   |
| 25  | B     | 612 | CLA  | O2A-CGA-CBA | 2.55  | 119.91      | 111.91   |
| 25  | c     | 512 | CLA  | C4A-NA-C1A  | -2.55 | 105.56      | 106.71   |
| 25  | b     | 608 | CLA  | CHD-C1D-C2D | 2.55  | 130.83      | 125.48   |
| 24  | n     | 607 | CHL  | OMC-CMC-C2C | -2.55 | 119.92      | 125.69   |
| 25  | b     | 602 | CLA  | O2A-CGA-CBA | 2.55  | 119.91      | 111.91   |
| 32  | n     | 619 | AJP  | C17-C16-C15 | -2.55 | 107.33      | 110.49   |
| 25  | y     | 304 | CLA  | CHD-C1D-C2D | 2.55  | 130.82      | 125.48   |
| 25  | C     | 503 | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 25  | c     | 503 | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 32  | n     | 620 | AJP  | C83-C06-C05 | -2.55 | 110.27      | 114.92   |
| 32  | y     | 324 | AJP  | C01-C02-C03 | 2.55  | 117.63      | 112.09   |
| 25  | r     | 601 | CLA  | O2A-CGA-CBA | 2.54  | 119.89      | 111.91   |
| 25  | Y     | 312 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 24  | S     | 302 | CHL  | CMB-C2B-C1B | -2.54 | 124.56      | 128.46   |
| 24  | R     | 613 | CHL  | CMB-C2B-C1B | -2.54 | 124.56      | 128.46   |
| 26  | B     | 621 | LHG  | P-O6-C4     | -2.54 | 106.77      | 121.68   |
| 25  | N     | 603 | CLA  | C4D-CHA-C1A | -2.54 | 118.15      | 121.25   |
| 25  | n     | 603 | CLA  | C4D-CHA-C1A | -2.54 | 118.15      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | N     | 601 | CHL  | C2C-C3C-C4C | 2.54  | 108.30      | 106.49   |
| 25  | C     | 502 | CLA  | C2A-C1A-CHA | -2.54 | 119.42      | 123.86   |
| 25  | g     | 604 | CLA  | O1D-CGD-CBD | -2.54 | 119.29      | 124.48   |
| 28  | I     | 101 | BCR  | C11-C10-C9  | -2.54 | 123.69      | 127.31   |
| 28  | i     | 101 | BCR  | C11-C10-C9  | -2.54 | 123.69      | 127.31   |
| 25  | R     | 612 | CLA  | C2D-C1D-ND  | -2.54 | 108.23      | 110.10   |
| 25  | r     | 612 | CLA  | C2D-C1D-ND  | -2.54 | 108.23      | 110.10   |
| 40  | N     | 617 | NEX  | C10-C11-C12 | 2.54  | 131.14      | 123.22   |
| 25  | a     | 402 | CLA  | C2A-C1A-CHA | -2.54 | 119.42      | 123.86   |
| 25  | s     | 310 | CLA  | C2A-C1A-CHA | -2.54 | 119.42      | 123.86   |
| 30  | A     | 408 | LMG  | O8-C28-C29  | 2.54  | 119.87      | 111.91   |
| 32  | y     | 322 | AJP  | C06-C07-C08 | -2.54 | 99.72       | 104.34   |
| 40  | n     | 617 | NEX  | C10-C11-C12 | 2.54  | 131.14      | 123.22   |
| 40  | n     | 617 | NEX  | C40-C33-C34 | -2.54 | 119.37      | 122.92   |
| 25  | S     | 303 | CLA  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 25  | Y     | 313 | CLA  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 24  | g     | 609 | CHL  | CMB-C2B-C1B | -2.54 | 124.57      | 128.46   |
| 25  | C     | 512 | CLA  | C4A-NA-C1A  | -2.54 | 105.57      | 106.71   |
| 32  | Y     | 322 | AJP  | C06-C07-C08 | -2.53 | 99.73       | 104.34   |
| 30  | A     | 410 | LMG  | O8-C28-C29  | 2.53  | 119.86      | 111.91   |
| 30  | a     | 411 | LMG  | O8-C28-C29  | 2.53  | 119.86      | 111.91   |
| 24  | n     | 601 | CHL  | C2C-C3C-C4C | 2.53  | 108.30      | 106.49   |
| 25  | G     | 613 | CLA  | O2A-CGA-CBA | 2.53  | 119.86      | 111.91   |
| 25  | R     | 601 | CLA  | O2A-CGA-CBA | 2.53  | 119.86      | 111.91   |
| 25  | c     | 505 | CLA  | CHD-C1D-C2D | 2.53  | 130.79      | 125.48   |
| 30  | a     | 409 | LMG  | O8-C28-C29  | 2.53  | 119.85      | 111.91   |
| 24  | G     | 609 | CHL  | CHD-C1D-ND  | -2.53 | 122.13      | 124.45   |
| 32  | N     | 619 | AJP  | C17-C16-C15 | -2.53 | 107.35      | 110.49   |
| 32  | N     | 620 | AJP  | C83-C06-C05 | -2.53 | 110.30      | 114.92   |
| 38  | f     | 101 | HEM  | CHA-C4D-ND  | 2.53  | 127.51      | 124.38   |
| 25  | S     | 305 | CLA  | C3D-C4D-CHA | 2.53  | 118.51      | 112.72   |
| 26  | B     | 625 | LHG  | O8-C23-C24  | 2.53  | 119.84      | 111.91   |
| 26  | b     | 625 | LHG  | O8-C23-C24  | 2.53  | 119.84      | 111.91   |
| 24  | R     | 607 | CHL  | C2A-C3A-C4A | 2.53  | 105.95      | 101.87   |
| 25  | y     | 313 | CLA  | O2D-CGD-O1D | -2.53 | 118.90      | 123.84   |
| 24  | r     | 613 | CHL  | CMB-C2B-C1B | -2.53 | 124.58      | 128.46   |
| 25  | n     | 602 | CLA  | C4-C3-C5    | 2.52  | 119.52      | 115.27   |
| 25  | R     | 614 | CLA  | C4A-NA-C1A  | -2.52 | 105.57      | 106.71   |
| 25  | G     | 604 | CLA  | O1D-CGD-CBD | -2.52 | 119.32      | 124.48   |
| 25  | D     | 402 | CLA  | C4-C3-C5    | 2.52  | 119.52      | 115.27   |
| 25  | S     | 310 | CLA  | C2A-C1A-CHA | -2.52 | 119.45      | 123.86   |
| 25  | G     | 603 | CLA  | O2D-CGD-O1D | -2.52 | 118.91      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | c     | 519 | LHG  | P-O3-C3     | -2.52 | 106.89      | 121.68   |
| 28  | H     | 101 | BCR  | C33-C5-C6   | -2.52 | 121.69      | 124.53   |
| 28  | h     | 101 | BCR  | C33-C5-C6   | -2.52 | 121.69      | 124.53   |
| 30  | d     | 407 | LMG  | O8-C28-C29  | 2.52  | 119.82      | 111.91   |
| 24  | Y     | 306 | CHL  | CMB-C2B-C1B | -2.52 | 124.59      | 128.46   |
| 26  | 2     | 606 | LHG  | P-O3-C3     | -2.52 | 106.89      | 121.68   |
| 26  | S     | 318 | LHG  | P-O3-C3     | -2.52 | 106.90      | 121.68   |
| 26  | s     | 318 | LHG  | P-O3-C3     | -2.52 | 106.90      | 121.68   |
| 25  | c     | 502 | CLA  | C2A-C1A-CHA | -2.52 | 119.45      | 123.86   |
| 26  | 6     | 606 | LHG  | P-O3-C3     | -2.52 | 106.90      | 121.68   |
| 26  | C     | 517 | LHG  | P-O6-C4     | -2.52 | 106.91      | 121.68   |
| 32  | y     | 323 | AJP  | C17-C16-C15 | -2.52 | 107.37      | 110.49   |
| 24  | G     | 609 | CHL  | CMB-C2B-C1B | -2.52 | 124.59      | 128.46   |
| 24  | N     | 601 | CHL  | C4D-CHA-C1A | 2.52  | 124.31      | 121.25   |
| 25  | R     | 609 | CLA  | O2D-CGD-O1D | -2.52 | 118.92      | 123.84   |
| 25  | r     | 609 | CLA  | O2D-CGD-O1D | -2.52 | 118.92      | 123.84   |
| 26  | C     | 519 | LHG  | P-O3-C3     | -2.52 | 106.92      | 121.68   |
| 26  | c     | 517 | LHG  | P-O6-C4     | -2.52 | 106.92      | 121.68   |
| 25  | d     | 402 | CLA  | C4-C3-C5    | 2.52  | 119.50      | 115.27   |
| 26  | c     | 517 | LHG  | P-O3-C3     | -2.52 | 106.93      | 121.68   |
| 24  | s     | 302 | CHL  | CMB-C2B-C1B | -2.52 | 124.60      | 128.46   |
| 25  | N     | 602 | CLA  | C4-C3-C5    | 2.52  | 119.50      | 115.27   |
| 25  | s     | 305 | CLA  | C3D-C4D-CHA | 2.52  | 118.48      | 112.72   |
| 30  | D     | 407 | LMG  | O8-C28-C29  | 2.51  | 119.80      | 111.91   |
| 25  | A     | 401 | CLA  | C2A-C1A-CHA | -2.51 | 119.46      | 123.86   |
| 40  | y     | 318 | NEX  | C30-C31-C32 | 2.51  | 131.06      | 123.22   |
| 24  | r     | 607 | CHL  | C2A-C3A-C4A | 2.51  | 105.93      | 101.87   |
| 26  | C     | 517 | LHG  | P-O3-C3     | -2.51 | 106.94      | 121.68   |
| 25  | B     | 606 | CLA  | C1D-ND-C4D  | -2.51 | 104.55      | 106.33   |
| 25  | b     | 606 | CLA  | C1D-ND-C4D  | -2.51 | 104.55      | 106.33   |
| 26  | B     | 625 | LHG  | P-O3-C3     | -2.51 | 106.95      | 121.68   |
| 26  | b     | 625 | LHG  | P-O3-C3     | -2.51 | 106.95      | 121.68   |
| 26  | d     | 406 | LHG  | P-O3-C3     | -2.51 | 106.95      | 121.68   |
| 40  | Y     | 318 | NEX  | C30-C31-C32 | 2.51  | 131.05      | 123.22   |
| 39  | g     | 616 | LUT  | C3-C4-C5    | 2.51  | 116.85      | 111.85   |
| 32  | Y     | 323 | AJP  | C17-C16-C15 | -2.51 | 107.38      | 110.49   |
| 25  | R     | 601 | CLA  | O2D-CGD-O1D | -2.51 | 118.93      | 123.84   |
| 26  | D     | 406 | LHG  | P-O3-C3     | -2.51 | 106.97      | 121.68   |
| 24  | n     | 606 | CHL  | CMB-C2B-C1B | -2.51 | 124.61      | 128.46   |
| 30  | B     | 620 | LMG  | O8-C28-C29  | 2.51  | 119.78      | 111.91   |
| 25  | R     | 609 | CLA  | O1D-CGD-CBD | -2.51 | 119.35      | 124.48   |
| 24  | N     | 606 | CHL  | CMB-C2B-C1B | -2.51 | 124.61      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | n     | 619 | AJP  | C06-C07-C08 | -2.51 | 99.78       | 104.34   |
| 25  | C     | 505 | CLA  | CHD-C1D-C2D | 2.51  | 130.74      | 125.48   |
| 25  | g     | 613 | CLA  | O2A-CGA-CBA | 2.51  | 119.77      | 111.91   |
| 25  | r     | 609 | CLA  | O1D-CGD-CBD | -2.50 | 119.36      | 124.48   |
| 25  | g     | 603 | CLA  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 26  | B     | 622 | LHG  | P-O3-C3     | -2.50 | 107.00      | 121.68   |
| 26  | b     | 622 | LHG  | P-O3-C3     | -2.50 | 107.00      | 121.68   |
| 30  | b     | 620 | LMG  | O8-C28-C29  | 2.50  | 119.76      | 111.91   |
| 25  | D     | 401 | CLA  | O2A-CGA-CBA | 2.50  | 119.76      | 111.91   |
| 25  | d     | 401 | CLA  | O2A-CGA-CBA | 2.50  | 119.76      | 111.91   |
| 25  | r     | 601 | CLA  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 24  | R     | 605 | CHL  | C2A-C3A-C4A | 2.50  | 105.91      | 101.87   |
| 26  | C     | 517 | LHG  | O8-C23-C24  | 2.50  | 119.75      | 111.91   |
| 26  | c     | 517 | LHG  | O8-C23-C24  | 2.50  | 119.75      | 111.91   |
| 24  | y     | 306 | CHL  | CMB-C2B-C1B | -2.50 | 124.62      | 128.46   |
| 25  | n     | 611 | CLA  | O2A-CGA-CBA | 2.50  | 119.75      | 111.91   |
| 40  | y     | 318 | NEX  | C24-C23-C22 | -2.50 | 105.94      | 110.77   |
| 26  | C     | 518 | LHG  | P-O6-C4     | -2.50 | 107.02      | 121.68   |
| 26  | c     | 518 | LHG  | P-O6-C4     | -2.50 | 107.02      | 121.68   |
| 28  | B     | 617 | BCR  | C28-C27-C26 | -2.50 | 109.61      | 114.08   |
| 28  | b     | 617 | BCR  | C28-C27-C26 | -2.50 | 109.61      | 114.08   |
| 25  | R     | 611 | CLA  | O1D-CGD-CBD | -2.50 | 119.37      | 124.48   |
| 32  | n     | 619 | AJP  | C17-C16-C11 | -2.50 | 108.69      | 112.32   |
| 32  | N     | 619 | AJP  | C06-C07-C08 | -2.50 | 99.80       | 104.34   |
| 25  | r     | 611 | CLA  | O1D-CGD-CBD | -2.50 | 119.38      | 124.48   |
| 26  | N     | 618 | LHG  | P-O3-C3     | -2.50 | 107.04      | 121.68   |
| 26  | b     | 621 | LHG  | O8-C23-C24  | 2.50  | 119.74      | 111.91   |
| 24  | r     | 605 | CHL  | C2A-C3A-C4A | 2.50  | 105.90      | 101.87   |
| 26  | n     | 618 | LHG  | P-O3-C3     | -2.50 | 107.05      | 121.68   |
| 24  | n     | 601 | CHL  | CMB-C2B-C1B | -2.50 | 124.63      | 128.46   |
| 39  | G     | 616 | LUT  | C3-C4-C5    | 2.49  | 116.82      | 111.85   |
| 25  | n     | 611 | CLA  | O2D-CGD-O1D | -2.49 | 118.96      | 123.84   |
| 40  | n     | 617 | NEX  | C26-C27-C28 | -2.49 | 120.72      | 125.99   |
| 26  | C     | 519 | LHG  | O8-C23-C24  | 2.49  | 119.73      | 111.91   |
| 26  | c     | 519 | LHG  | O8-C23-C24  | 2.49  | 119.73      | 111.91   |
| 25  | N     | 611 | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 25  | C     | 510 | CLA  | O1D-CGD-CBD | -2.49 | 119.38      | 124.48   |
| 25  | c     | 510 | CLA  | O1D-CGD-CBD | -2.49 | 119.38      | 124.48   |
| 25  | N     | 612 | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 25  | 2     | 602 | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 25  | 6     | 602 | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 25  | R     | 608 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | r     | 608 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |
| 28  | C     | 514 | BCR  | C15-C16-C17 | -2.49 | 118.37      | 123.47   |
| 28  | c     | 514 | BCR  | C15-C16-C17 | -2.49 | 118.37      | 123.47   |
| 39  | S     | 315 | LUT  | C1-C2-C3    | 2.49  | 119.27      | 113.64   |
| 25  | S     | 312 | CLA  | C4D-CHA-C1A | -2.49 | 118.22      | 121.25   |
| 25  | s     | 312 | CLA  | C4D-CHA-C1A | -2.49 | 118.22      | 121.25   |
| 28  | T     | 101 | BCR  | C27-C26-C25 | 2.49  | 126.35      | 122.73   |
| 28  | t     | 101 | BCR  | C27-C26-C25 | 2.49  | 126.35      | 122.73   |
| 40  | Y     | 318 | NEX  | C24-C23-C22 | -2.49 | 105.97      | 110.77   |
| 25  | s     | 314 | CLA  | O1D-CGD-CBD | -2.49 | 119.39      | 124.48   |
| 25  | R     | 611 | CLA  | O2A-CGA-CBA | 2.49  | 119.72      | 111.91   |
| 25  | B     | 609 | CLA  | CHD-C1D-C2D | 2.49  | 130.70      | 125.48   |
| 25  | S     | 311 | CLA  | O2A-CGA-CBA | 2.49  | 119.72      | 111.91   |
| 26  | B     | 621 | LHG  | O8-C23-C24  | 2.49  | 119.72      | 111.91   |
| 28  | B     | 619 | BCR  | C2-C1-C6    | 2.49  | 114.31      | 110.48   |
| 28  | b     | 619 | BCR  | C2-C1-C6    | 2.49  | 114.31      | 110.48   |
| 25  | N     | 611 | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 25  | r     | 611 | CLA  | O2A-CGA-CBA | 2.49  | 119.71      | 111.91   |
| 39  | s     | 315 | LUT  | C1-C2-C3    | 2.49  | 119.26      | 113.64   |
| 26  | L     | 102 | LHG  | P-O3-C3     | -2.49 | 107.10      | 121.68   |
| 39  | G     | 615 | LUT  | C1-C2-C3    | 2.49  | 119.26      | 113.64   |
| 26  | l     | 103 | LHG  | P-O3-C3     | -2.49 | 107.11      | 121.68   |
| 25  | r     | 604 | CLA  | O1D-CGD-CBD | -2.48 | 119.40      | 124.48   |
| 25  | S     | 312 | CLA  | CHB-C4A-NA  | -2.48 | 121.08      | 124.51   |
| 24  | 2     | 603 | CHL  | CHD-C1D-C2D | 2.48  | 130.69      | 125.48   |
| 24  | 6     | 603 | CHL  | CHD-C1D-C2D | 2.48  | 130.69      | 125.48   |
| 25  | C     | 509 | CLA  | O2A-CGA-CBA | 2.48  | 119.69      | 111.91   |
| 25  | s     | 311 | CLA  | O2A-CGA-CBA | 2.48  | 119.69      | 111.91   |
| 25  | C     | 512 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 25  | c     | 512 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 25  | N     | 603 | CLA  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 32  | N     | 619 | AJP  | C17-C16-C11 | -2.48 | 108.72      | 112.32   |
| 25  | C     | 503 | CLA  | O2D-CGD-O1D | -2.48 | 118.99      | 123.84   |
| 25  | g     | 604 | CLA  | C5-C3-C4    | 2.48  | 120.08      | 114.60   |
| 24  | N     | 601 | CHL  | CMB-C2B-C1B | -2.48 | 124.65      | 128.46   |
| 25  | R     | 604 | CLA  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 24  | S     | 308 | CHL  | C2A-C3A-C4A | 2.48  | 105.87      | 101.87   |
| 24  | s     | 308 | CHL  | C2A-C3A-C4A | 2.48  | 105.87      | 101.87   |
| 25  | r     | 614 | CLA  | C4D-CHA-C1A | -2.48 | 118.23      | 121.25   |
| 25  | C     | 510 | CLA  | O2D-CGD-O1D | -2.48 | 119.00      | 123.84   |
| 25  | c     | 510 | CLA  | O2D-CGD-O1D | -2.48 | 119.00      | 123.84   |
| 25  | n     | 614 | CLA  | O2D-CGD-O1D | -2.48 | 119.00      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | B     | 602 | CLA  | C1B-CHB-C4A | -2.48 | 125.21      | 130.12   |
| 25  | b     | 602 | CLA  | C1B-CHB-C4A | -2.48 | 125.21      | 130.12   |
| 25  | R     | 609 | CLA  | C2A-C1A-CHA | -2.48 | 119.53      | 123.86   |
| 25  | s     | 312 | CLA  | CHB-C4A-NA  | -2.48 | 121.09      | 124.51   |
| 39  | g     | 615 | LUT  | C1-C2-C3    | 2.48  | 119.23      | 113.64   |
| 25  | n     | 612 | CLA  | O2A-CGA-CBA | 2.47  | 119.67      | 111.91   |
| 25  | c     | 509 | CLA  | O2A-CGA-CBA | 2.47  | 119.67      | 111.91   |
| 40  | N     | 617 | NEX  | C26-C27-C28 | -2.47 | 120.76      | 125.99   |
| 38  | F     | 101 | HEM  | CHA-C4D-ND  | 2.47  | 127.44      | 124.38   |
| 25  | G     | 604 | CLA  | C5-C3-C4    | 2.47  | 120.07      | 114.60   |
| 25  | R     | 604 | CLA  | CAA-CBA-CGA | -2.47 | 106.03      | 113.25   |
| 25  | r     | 604 | CLA  | CAA-CBA-CGA | -2.47 | 106.03      | 113.25   |
| 24  | G     | 606 | CHL  | C2C-C3C-C4C | 2.47  | 108.25      | 106.49   |
| 25  | b     | 609 | CLA  | CHD-C1D-C2D | 2.47  | 130.66      | 125.48   |
| 30  | B     | 623 | LMG  | O8-C28-C29  | 2.47  | 119.66      | 111.91   |
| 30  | b     | 623 | LMG  | O8-C28-C29  | 2.47  | 119.66      | 111.91   |
| 32  | Y     | 324 | AJP  | C17-C16-C15 | -2.47 | 107.43      | 110.49   |
| 32  | y     | 324 | AJP  | C17-C16-C15 | -2.47 | 107.43      | 110.49   |
| 25  | G     | 612 | CLA  | C4D-CHA-C1A | -2.47 | 118.24      | 121.25   |
| 32  | Y     | 322 | AJP  | C20-C21-C22 | 2.47  | 118.14      | 114.09   |
| 39  | n     | 616 | LUT  | C11-C10-C9  | -2.47 | 123.79      | 127.31   |
| 32  | a     | 413 | AJP  | C57-C58-C59 | 2.47  | 114.91      | 109.66   |
| 26  | y     | 319 | LHG  | O8-C23-C24  | 2.46  | 119.64      | 111.91   |
| 32  | y     | 322 | AJP  | C20-C21-C22 | 2.46  | 118.13      | 114.09   |
| 25  | n     | 603 | CLA  | O1D-CGD-CBD | -2.46 | 119.44      | 124.48   |
| 25  | 2     | 605 | CLA  | CHD-C1D-C2D | 2.46  | 130.65      | 125.48   |
| 40  | Y     | 318 | NEX  | C19-C9-C10  | -2.46 | 119.47      | 122.92   |
| 26  | r     | 618 | LHG  | P-O3-C3     | -2.46 | 107.24      | 121.68   |
| 24  | G     | 609 | CHL  | OMC-CMC-C2C | -2.46 | 120.12      | 125.69   |
| 25  | B     | 615 | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 25  | b     | 615 | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 25  | r     | 608 | CLA  | C2A-C3A-C4A | -2.46 | 97.89       | 101.87   |
| 25  | y     | 304 | CLA  | O2A-CGA-CBA | 2.46  | 119.63      | 111.91   |
| 24  | y     | 302 | CHL  | CMB-C2B-C1B | -2.46 | 124.68      | 128.46   |
| 25  | g     | 611 | CLA  | CHD-C1D-C2D | 2.46  | 130.64      | 125.48   |
| 32  | A     | 412 | AJP  | C48-C47-C46 | -2.46 | 106.64      | 110.89   |
| 32  | a     | 413 | AJP  | C48-C47-C46 | -2.46 | 106.64      | 110.89   |
| 27  | A     | 404 | PHO  | O2A-CGA-CBA | 2.46  | 119.62      | 111.91   |
| 27  | a     | 405 | PHO  | O2A-CGA-CBA | 2.46  | 119.62      | 111.91   |
| 25  | r     | 601 | CLA  | CMB-C2B-C1B | -2.46 | 124.69      | 128.46   |
| 25  | r     | 609 | CLA  | C2A-C1A-CHA | -2.46 | 119.56      | 123.86   |
| 26  | R     | 618 | LHG  | O8-C23-C24  | 2.46  | 119.62      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | y     | 316 | LUT  | C1-C2-C3    | 2.46  | 119.19      | 113.64   |
| 26  | Y     | 319 | LHG  | O8-C23-C24  | 2.46  | 119.62      | 111.91   |
| 32  | Y     | 321 | AJP  | C21-C20-C19 | 2.46  | 109.91      | 107.14   |
| 32  | y     | 321 | AJP  | C21-C20-C19 | 2.46  | 109.91      | 107.14   |
| 25  | Y     | 304 | CLA  | O2A-CGA-CBA | 2.46  | 119.62      | 111.91   |
| 24  | y     | 306 | CHL  | OMC-CMC-C2C | -2.46 | 120.13      | 125.69   |
| 39  | Y     | 316 | LUT  | C1-C2-C3    | 2.46  | 119.19      | 113.64   |
| 25  | D     | 403 | CLA  | O1D-CGD-CBD | -2.45 | 119.46      | 124.48   |
| 40  | S     | 317 | NEX  | C1-C2-C3    | -2.45 | 108.10      | 113.64   |
| 25  | 6     | 605 | CLA  | CHD-C1D-C2D | 2.45  | 130.63      | 125.48   |
| 25  | S     | 314 | CLA  | O1D-CGD-CBD | -2.45 | 119.47      | 124.48   |
| 32  | B     | 624 | AJP  | O34-C29-C28 | -2.45 | 100.76      | 107.28   |
| 32  | b     | 624 | AJP  | O34-C29-C28 | -2.45 | 100.76      | 107.28   |
| 28  | A     | 406 | BCR  | C15-C16-C17 | -2.45 | 118.45      | 123.47   |
| 28  | a     | 407 | BCR  | C15-C16-C17 | -2.45 | 118.45      | 123.47   |
| 24  | N     | 606 | CHL  | OMC-CMC-C2C | -2.45 | 120.14      | 125.69   |
| 25  | c     | 503 | CLA  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 40  | y     | 318 | NEX  | C19-C9-C10  | -2.45 | 119.49      | 122.92   |
| 26  | R     | 618 | LHG  | P-O3-C3     | -2.45 | 107.31      | 121.68   |
| 25  | A     | 402 | CLA  | C2A-C1A-CHA | -2.45 | 119.57      | 123.86   |
| 25  | a     | 403 | CLA  | C2A-C1A-CHA | -2.45 | 119.57      | 123.86   |
| 32  | A     | 412 | AJP  | C57-C58-C59 | 2.45  | 114.88      | 109.66   |
| 25  | B     | 601 | CLA  | O2A-CGA-CBA | 2.45  | 119.60      | 111.91   |
| 25  | b     | 601 | CLA  | O2A-CGA-CBA | 2.45  | 119.60      | 111.91   |
| 28  | A     | 406 | BCR  | C2-C1-C6    | 2.45  | 114.25      | 110.48   |
| 28  | a     | 407 | BCR  | C2-C1-C6    | 2.45  | 114.25      | 110.48   |
| 25  | g     | 611 | CLA  | CMD-C2D-C1D | -2.45 | 120.40      | 124.71   |
| 40  | R     | 617 | NEX  | C1-C2-C3    | -2.45 | 108.11      | 113.64   |
| 24  | g     | 606 | CHL  | C2C-C3C-C4C | 2.45  | 108.23      | 106.49   |
| 24  | g     | 609 | CHL  | OMC-CMC-C2C | -2.45 | 120.15      | 125.69   |
| 25  | R     | 608 | CLA  | C2A-C3A-C4A | -2.45 | 97.92       | 101.87   |
| 24  | n     | 606 | CHL  | OMC-CMC-C2C | -2.45 | 120.15      | 125.69   |
| 24  | s     | 307 | CHL  | C2A-C3A-C4A | 2.45  | 105.82      | 101.87   |
| 25  | n     | 613 | CLA  | O1D-CGD-CBD | -2.45 | 119.48      | 124.48   |
| 40  | s     | 317 | NEX  | C1-C2-C3    | -2.45 | 108.12      | 113.64   |
| 25  | s     | 309 | CLA  | O1D-CGD-CBD | -2.45 | 119.48      | 124.48   |
| 24  | y     | 310 | CHL  | O2A-CGA-O1A | -2.45 | 117.42      | 123.59   |
| 26  | s     | 301 | LHG  | O8-C23-C24  | 2.45  | 119.58      | 111.91   |
| 25  | d     | 403 | CLA  | O1D-CGD-CBD | -2.44 | 119.48      | 124.48   |
| 25  | B     | 615 | CLA  | O2A-CGA-CBA | 2.44  | 119.58      | 111.91   |
| 25  | b     | 615 | CLA  | O2A-CGA-CBA | 2.44  | 119.58      | 111.91   |
| 24  | Y     | 310 | CHL  | O2A-CGA-O1A | -2.44 | 117.42      | 123.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | S     | 309 | CLA  | O1D-CGD-CBD | -2.44 | 119.48      | 124.48   |
| 25  | B     | 607 | CLA  | C4D-CHA-C1A | -2.44 | 118.28      | 121.25   |
| 25  | b     | 607 | CLA  | C4D-CHA-C1A | -2.44 | 118.28      | 121.25   |
| 39  | N     | 616 | LUT  | C11-C10-C9  | -2.44 | 123.83      | 127.31   |
| 25  | N     | 613 | CLA  | O1D-CGD-CBD | -2.44 | 119.49      | 124.48   |
| 24  | Y     | 306 | CHL  | OMC-CMC-C2C | -2.44 | 120.17      | 125.69   |
| 24  | y     | 302 | CHL  | C4D-CHA-C1A | 2.44  | 124.22      | 121.25   |
| 25  | S     | 305 | CLA  | C5-C3-C4    | 2.44  | 119.99      | 114.60   |
| 40  | R     | 617 | NEX  | C32-C33-C34 | 2.44  | 122.68      | 118.94   |
| 25  | Y     | 305 | CLA  | C5-C3-C4    | 2.44  | 119.99      | 114.60   |
| 41  | r     | 616 | XAT  | C31-C32-C33 | -2.44 | 119.57      | 126.42   |
| 25  | B     | 608 | CLA  | O2A-CGA-CBA | 2.44  | 119.55      | 111.91   |
| 32  | a     | 413 | AJP  | C24-C19-C18 | -2.44 | 107.28      | 111.74   |
| 25  | b     | 608 | CLA  | O2A-CGA-CBA | 2.43  | 119.55      | 111.91   |
| 25  | s     | 305 | CLA  | C5-C3-C4    | 2.43  | 119.98      | 114.60   |
| 25  | G     | 611 | CLA  | CMD-C2D-C1D | -2.43 | 120.42      | 124.71   |
| 25  | G     | 611 | CLA  | CHD-C1D-C2D | 2.43  | 130.59      | 125.48   |
| 25  | Y     | 311 | CLA  | O2A-CGA-CBA | 2.43  | 119.55      | 111.91   |
| 25  | y     | 311 | CLA  | O2A-CGA-CBA | 2.43  | 119.55      | 111.91   |
| 25  | S     | 313 | CLA  | O2A-CGA-CBA | 2.43  | 119.54      | 111.91   |
| 40  | r     | 617 | NEX  | C1-C2-C3    | -2.43 | 108.15      | 113.64   |
| 25  | C     | 506 | CLA  | O1D-CGD-CBD | -2.43 | 119.51      | 124.48   |
| 25  | c     | 506 | CLA  | O1D-CGD-CBD | -2.43 | 119.51      | 124.48   |
| 24  | S     | 307 | CHL  | C2A-C3A-C4A | 2.43  | 105.80      | 101.87   |
| 24  | g     | 609 | CHL  | C2A-C3A-C4A | 2.43  | 105.80      | 101.87   |
| 25  | C     | 512 | CLA  | C4D-CHA-C1A | -2.43 | 118.29      | 121.25   |
| 25  | R     | 602 | CLA  | O1D-CGD-CBD | -2.43 | 119.51      | 124.48   |
| 24  | Y     | 302 | CHL  | C4D-CHA-C1A | 2.43  | 124.20      | 121.25   |
| 25  | R     | 601 | CLA  | CMB-C2B-C1B | -2.43 | 124.73      | 128.46   |
| 41  | R     | 616 | XAT  | C31-C32-C33 | -2.43 | 119.59      | 126.42   |
| 25  | s     | 313 | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 26  | r     | 618 | LHG  | O8-C23-C24  | 2.43  | 119.53      | 111.91   |
| 25  | 2     | 604 | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 25  | 6     | 604 | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 25  | R     | 603 | CLA  | C3D-C4D-CHA | 2.43  | 118.28      | 112.72   |
| 25  | r     | 603 | CLA  | C3D-C4D-CHA | 2.43  | 118.28      | 112.72   |
| 32  | N     | 619 | AJP  | C29-C30-C32 | -2.43 | 108.34      | 112.60   |
| 40  | r     | 617 | NEX  | C32-C33-C34 | 2.43  | 122.67      | 118.94   |
| 25  | y     | 303 | CLA  | O2A-CGA-CBA | 2.43  | 119.52      | 111.91   |
| 25  | n     | 604 | CLA  | C5-C3-C4    | 2.43  | 119.96      | 114.60   |
| 25  | A     | 401 | CLA  | O2A-CGA-CBA | 2.43  | 119.52      | 111.91   |
| 25  | a     | 402 | CLA  | O2A-CGA-CBA | 2.43  | 119.52      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | N     | 604 | CLA  | C5-C3-C4    | 2.42  | 119.96      | 114.60   |
| 25  | Y     | 314 | CLA  | O1D-CGD-CBD | -2.42 | 119.52      | 124.48   |
| 25  | y     | 314 | CLA  | O1D-CGD-CBD | -2.42 | 119.52      | 124.48   |
| 25  | y     | 305 | CLA  | C5-C3-C4    | 2.42  | 119.96      | 114.60   |
| 25  | N     | 614 | CLA  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 24  | s     | 302 | CHL  | C2A-C3A-C4A | 2.42  | 105.78      | 101.87   |
| 26  | S     | 301 | LHG  | O8-C23-C24  | 2.42  | 119.51      | 111.91   |
| 25  | g     | 612 | CLA  | C4D-CHA-C1A | -2.42 | 118.30      | 121.25   |
| 25  | G     | 603 | CLA  | O2A-CGA-CBA | 2.42  | 119.50      | 111.91   |
| 32  | B     | 624 | AJP  | C26-O31-C30 | -2.42 | 108.94      | 113.69   |
| 32  | b     | 624 | AJP  | C26-O31-C30 | -2.42 | 108.94      | 113.69   |
| 25  | N     | 602 | CLA  | O2A-CGA-CBA | 2.42  | 119.50      | 111.91   |
| 24  | S     | 302 | CHL  | C2A-C3A-C4A | 2.42  | 105.78      | 101.87   |
| 38  | F     | 101 | HEM  | CHB-C1B-NB  | 2.42  | 127.37      | 124.38   |
| 32  | n     | 619 | AJP  | C29-C30-C32 | -2.42 | 108.36      | 112.60   |
| 28  | K     | 101 | BCR  | C38-C26-C25 | -2.42 | 121.81      | 124.53   |
| 24  | Y     | 302 | CHL  | CMB-C2B-C1B | -2.42 | 124.75      | 128.46   |
| 25  | b     | 610 | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 25  | Y     | 303 | CLA  | O2A-CGA-CBA | 2.42  | 119.49      | 111.91   |
| 25  | C     | 508 | CLA  | O2A-CGA-CBA | 2.42  | 119.49      | 111.91   |
| 25  | c     | 508 | CLA  | O2A-CGA-CBA | 2.42  | 119.49      | 111.91   |
| 39  | y     | 317 | LUT  | C2-C3-C4    | 2.42  | 113.61      | 110.30   |
| 25  | R     | 614 | CLA  | C4D-CHA-C1A | -2.41 | 118.31      | 121.25   |
| 25  | B     | 607 | CLA  | O1D-CGD-CBD | -2.41 | 119.54      | 124.48   |
| 25  | b     | 607 | CLA  | O1D-CGD-CBD | -2.41 | 119.54      | 124.48   |
| 24  | N     | 605 | CHL  | OMC-CMC-C2C | -2.41 | 120.23      | 125.69   |
| 24  | n     | 605 | CHL  | OMC-CMC-C2C | -2.41 | 120.23      | 125.69   |
| 25  | n     | 602 | CLA  | O2A-CGA-CBA | 2.41  | 119.48      | 111.91   |
| 39  | S     | 316 | LUT  | C2-C3-C4    | 2.41  | 113.61      | 110.30   |
| 39  | s     | 316 | LUT  | C2-C3-C4    | 2.41  | 113.61      | 110.30   |
| 28  | B     | 618 | BCR  | C24-C23-C22 | -2.41 | 122.59      | 126.23   |
| 28  | b     | 618 | BCR  | C24-C23-C22 | -2.41 | 122.59      | 126.23   |
| 35  | A     | 415 | DGD  | O1G-C1A-C2A | 2.41  | 119.48      | 111.91   |
| 35  | a     | 401 | DGD  | O1G-C1A-C2A | 2.41  | 119.48      | 111.91   |
| 25  | S     | 305 | CLA  | O2D-CGD-O1D | -2.41 | 119.12      | 123.84   |
| 24  | G     | 609 | CHL  | C2A-C3A-C4A | 2.41  | 105.77      | 101.87   |
| 24  | G     | 601 | CHL  | C4D-CHA-C1A | 2.41  | 124.18      | 121.25   |
| 24  | g     | 601 | CHL  | C4D-CHA-C1A | 2.41  | 124.18      | 121.25   |
| 25  | y     | 305 | CLA  | O2A-CGA-CBA | 2.41  | 119.47      | 111.91   |
| 24  | n     | 606 | CHL  | C2C-C3C-C4C | 2.41  | 108.21      | 106.49   |
| 25  | G     | 603 | CLA  | C2A-C1A-CHA | -2.41 | 119.64      | 123.86   |
| 25  | g     | 603 | CLA  | C2A-C1A-CHA | -2.41 | 119.64      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | Y     | 320 | AJP  | C83-C06-C05 | -2.41 | 110.52      | 114.92   |
| 24  | 2     | 601 | CHL  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 25  | y     | 313 | CLA  | C4A-NA-C1A  | -2.41 | 105.62      | 106.71   |
| 32  | y     | 322 | AJP  | C83-C06-C05 | -2.41 | 110.52      | 114.92   |
| 25  | g     | 603 | CLA  | O2A-CGA-CBA | 2.41  | 119.47      | 111.91   |
| 39  | S     | 316 | LUT  | C37-C21-C22 | -2.41 | 104.88      | 109.44   |
| 39  | s     | 316 | LUT  | C37-C21-C22 | -2.41 | 104.88      | 109.44   |
| 26  | r     | 618 | LHG  | P-O6-C4     | -2.41 | 107.56      | 121.68   |
| 32  | G     | 618 | AJP  | C03-C04-C05 | -2.41 | 107.77      | 111.93   |
| 26  | R     | 618 | LHG  | P-O6-C4     | -2.41 | 107.57      | 121.68   |
| 25  | Y     | 305 | CLA  | O2A-CGA-CBA | 2.41  | 119.46      | 111.91   |
| 25  | g     | 604 | CLA  | O2A-CGA-CBA | 2.41  | 119.46      | 111.91   |
| 24  | G     | 606 | CHL  | CMB-C2B-C1B | -2.40 | 124.77      | 128.46   |
| 28  | B     | 617 | BCR  | C7-C8-C9    | -2.40 | 122.60      | 126.23   |
| 28  | b     | 617 | BCR  | C7-C8-C9    | -2.40 | 122.60      | 126.23   |
| 25  | r     | 602 | CLA  | O1D-CGD-CBD | -2.40 | 119.56      | 124.48   |
| 25  | B     | 610 | CLA  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 25  | B     | 609 | CLA  | O2A-CGA-CBA | 2.40  | 119.44      | 111.91   |
| 25  | b     | 609 | CLA  | O2A-CGA-CBA | 2.40  | 119.44      | 111.91   |
| 32  | A     | 412 | AJP  | C24-C19-C18 | -2.40 | 107.34      | 111.74   |
| 25  | G     | 604 | CLA  | O2A-CGA-CBA | 2.40  | 119.44      | 111.91   |
| 32  | N     | 619 | AJP  | C83-C06-C05 | -2.40 | 110.53      | 114.92   |
| 25  | g     | 603 | CLA  | CHD-C1D-C2D | 2.40  | 130.52      | 125.48   |
| 32  | Y     | 322 | AJP  | C83-C06-C05 | -2.40 | 110.53      | 114.92   |
| 25  | n     | 612 | CLA  | CHB-C4A-NA  | -2.40 | 121.19      | 124.51   |
| 25  | s     | 305 | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 25  | G     | 604 | CLA  | CHD-C1D-C2D | 2.40  | 130.51      | 125.48   |
| 32  | y     | 320 | AJP  | C83-C06-C05 | -2.40 | 110.54      | 114.92   |
| 24  | 6     | 601 | CHL  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 24  | Y     | 308 | CHL  | O2A-CGA-CBA | 2.40  | 119.43      | 111.91   |
| 25  | B     | 611 | CLA  | O2A-CGA-CBA | 2.40  | 119.43      | 111.91   |
| 25  | b     | 611 | CLA  | O2A-CGA-CBA | 2.40  | 119.43      | 111.91   |
| 24  | S     | 302 | CHL  | C4D-CHA-C1A | 2.40  | 124.17      | 121.25   |
| 25  | 2     | 605 | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 25  | 6     | 605 | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 25  | G     | 614 | CLA  | O2D-CGD-O1D | -2.40 | 119.16      | 123.84   |
| 25  | S     | 312 | CLA  | O1D-CGD-CBD | -2.39 | 119.58      | 124.48   |
| 25  | b     | 605 | CLA  | O1D-CGD-CBD | -2.39 | 119.58      | 124.48   |
| 32  | g     | 618 | AJP  | C03-C04-C05 | -2.39 | 107.79      | 111.93   |
| 24  | r     | 605 | CHL  | OMC-CMC-C2C | -2.39 | 120.27      | 125.69   |
| 32  | n     | 619 | AJP  | C83-C06-C05 | -2.39 | 110.55      | 114.92   |
| 25  | y     | 311 | CLA  | CHD-C1D-C2D | 2.39  | 130.50      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | D     | 401 | CLA  | C5-C3-C4    | 2.39  | 119.89      | 114.60   |
| 25  | d     | 401 | CLA  | C5-C3-C4    | 2.39  | 119.89      | 114.60   |
| 25  | s     | 312 | CLA  | O1D-CGD-CBD | -2.39 | 119.59      | 124.48   |
| 24  | R     | 605 | CHL  | OMC-CMC-C2C | -2.39 | 120.28      | 125.69   |
| 25  | G     | 603 | CLA  | CHD-C1D-C2D | 2.39  | 130.50      | 125.48   |
| 24  | s     | 302 | CHL  | C4D-CHA-C1A | 2.39  | 124.16      | 121.25   |
| 28  | H     | 101 | BCR  | C29-C30-C25 | 2.39  | 114.16      | 110.48   |
| 28  | h     | 101 | BCR  | C29-C30-C25 | 2.39  | 114.16      | 110.48   |
| 32  | A     | 412 | AJP  | C27-C28-C29 | 2.39  | 115.14      | 109.68   |
| 32  | a     | 413 | AJP  | C27-C28-C29 | 2.39  | 115.14      | 109.68   |
| 25  | N     | 612 | CLA  | CHB-C4A-NA  | -2.39 | 121.20      | 124.51   |
| 25  | c     | 512 | CLA  | C4D-CHA-C1A | -2.39 | 118.34      | 121.25   |
| 39  | Y     | 317 | LUT  | C2-C3-C4    | 2.39  | 113.58      | 110.30   |
| 28  | B     | 618 | BCR  | C27-C26-C25 | 2.39  | 126.20      | 122.73   |
| 28  | b     | 618 | BCR  | C27-C26-C25 | 2.39  | 126.20      | 122.73   |
| 25  | s     | 313 | CLA  | C2D-C1D-ND  | -2.39 | 108.34      | 110.10   |
| 25  | Y     | 314 | CLA  | C2A-C1A-CHA | -2.39 | 119.68      | 123.86   |
| 28  | k     | 101 | BCR  | C38-C26-C25 | -2.39 | 121.85      | 124.53   |
| 32  | Y     | 321 | AJP  | C17-C16-C11 | -2.39 | 108.85      | 112.32   |
| 32  | y     | 321 | AJP  | C17-C16-C11 | -2.39 | 108.85      | 112.32   |
| 25  | 2     | 604 | CLA  | C3D-C4D-CHA | 2.39  | 118.18      | 112.72   |
| 25  | 6     | 604 | CLA  | C3D-C4D-CHA | 2.39  | 118.18      | 112.72   |
| 25  | r     | 604 | CLA  | C2D-C1D-ND  | -2.39 | 108.34      | 110.10   |
| 24  | y     | 308 | CHL  | O2A-CGA-CBA | 2.39  | 119.39      | 111.91   |
| 26  | B     | 622 | LHG  | O8-C23-C24  | 2.39  | 119.39      | 111.91   |
| 26  | b     | 622 | LHG  | O8-C23-C24  | 2.39  | 119.39      | 111.91   |
| 25  | Y     | 311 | CLA  | CHD-C1D-C2D | 2.39  | 130.48      | 125.48   |
| 25  | B     | 608 | CLA  | O1D-CGD-CBD | -2.38 | 119.60      | 124.48   |
| 25  | C     | 503 | CLA  | O2A-CGA-CBA | 2.38  | 119.39      | 111.91   |
| 25  | c     | 503 | CLA  | O2A-CGA-CBA | 2.38  | 119.39      | 111.91   |
| 25  | b     | 608 | CLA  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |
| 25  | R     | 610 | CLA  | O2A-CGA-CBA | 2.38  | 119.38      | 111.91   |
| 35  | c     | 515 | DGD  | O1G-C1A-C2A | 2.38  | 119.38      | 111.91   |
| 25  | D     | 402 | CLA  | C3A-C2A-C1A | -2.38 | 97.77       | 101.34   |
| 25  | d     | 402 | CLA  | C3A-C2A-C1A | -2.38 | 97.77       | 101.34   |
| 25  | B     | 605 | CLA  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |
| 26  | y     | 319 | LHG  | P-O6-C4     | -2.38 | 107.72      | 121.68   |
| 25  | A     | 401 | CLA  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 25  | a     | 402 | CLA  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 25  | r     | 610 | CLA  | O2A-CGA-CBA | 2.38  | 119.38      | 111.91   |
| 25  | y     | 314 | CLA  | C2A-C1A-CHA | -2.38 | 119.70      | 123.86   |
| 24  | y     | 307 | CHL  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | B     | 618 | BCR  | C11-C10-C9  | -2.38 | 123.91      | 127.31   |
| 28  | b     | 618 | BCR  | C11-C10-C9  | -2.38 | 123.91      | 127.31   |
| 24  | g     | 606 | CHL  | CMB-C2B-C1B | -2.38 | 124.81      | 128.46   |
| 25  | 6     | 602 | CLA  | C1D-ND-C4D  | 2.38  | 108.03      | 106.33   |
| 26  | y     | 301 | LHG  | P-O6-C4     | -2.38 | 107.73      | 121.68   |
| 24  | N     | 606 | CHL  | C2C-C3C-C4C | 2.38  | 108.18      | 106.49   |
| 25  | g     | 614 | CLA  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 24  | g     | 608 | CHL  | OMC-CMC-C2C | -2.38 | 120.31      | 125.69   |
| 32  | Y     | 324 | AJP  | C19-C24-C23 | -2.38 | 107.01      | 112.92   |
| 35  | C     | 515 | DGD  | O1G-C1A-C2A | 2.38  | 119.36      | 111.91   |
| 25  | S     | 311 | CLA  | O1D-CGD-CBD | -2.37 | 119.62      | 124.48   |
| 26  | Y     | 301 | LHG  | P-O6-C4     | -2.37 | 107.76      | 121.68   |
| 26  | Y     | 319 | LHG  | P-O6-C4     | -2.37 | 107.76      | 121.68   |
| 25  | 2     | 602 | CLA  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 40  | S     | 317 | NEX  | C5-C6-C1    | -2.37 | 117.34      | 119.70   |
| 32  | y     | 324 | AJP  | C21-C20-C19 | 2.37  | 109.81      | 107.14   |
| 24  | Y     | 307 | CHL  | O1D-CGD-CBD | -2.37 | 119.63      | 124.48   |
| 25  | b     | 609 | CLA  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 24  | 5     | 302 | CHL  | OMC-CMC-C2C | -2.37 | 120.33      | 125.69   |
| 24  | N     | 607 | CHL  | O2A-CGA-CBA | 2.37  | 119.34      | 111.91   |
| 32  | Y     | 324 | AJP  | C21-C20-C19 | 2.37  | 109.81      | 107.14   |
| 39  | R     | 615 | LUT  | C31-C30-C29 | -2.37 | 123.93      | 127.31   |
| 39  | r     | 615 | LUT  | C31-C30-C29 | -2.37 | 123.93      | 127.31   |
| 24  | G     | 608 | CHL  | OMC-CMC-C2C | -2.37 | 120.33      | 125.69   |
| 38  | f     | 101 | HEM  | CHB-C1B-NB  | 2.37  | 127.31      | 124.38   |
| 25  | C     | 504 | CLA  | C3D-C4D-CHA | 2.37  | 118.14      | 112.72   |
| 25  | c     | 504 | CLA  | C3D-C4D-CHA | 2.37  | 118.14      | 112.72   |
| 32  | y     | 324 | AJP  | C19-C24-C23 | -2.37 | 107.04      | 112.92   |
| 24  | g     | 609 | CHL  | C2A-C1A-CHA | 2.37  | 128.00      | 123.86   |
| 24  | 2     | 601 | CHL  | O1D-CGD-CBD | -2.37 | 119.64      | 124.48   |
| 24  | 6     | 601 | CHL  | O1D-CGD-CBD | -2.37 | 119.64      | 124.48   |
| 25  | c     | 507 | CLA  | O1D-CGD-CBD | -2.36 | 119.64      | 124.48   |
| 25  | s     | 311 | CLA  | O1D-CGD-CBD | -2.36 | 119.64      | 124.48   |
| 40  | n     | 617 | NEX  | C5-C6-C1    | -2.36 | 117.35      | 119.70   |
| 25  | B     | 609 | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 25  | R     | 604 | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 25  | B     | 611 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 25  | B     | 615 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 25  | b     | 611 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 25  | g     | 604 | CLA  | CHD-C1D-C2D | 2.36  | 130.44      | 125.48   |
| 24  | n     | 607 | CHL  | O2A-CGA-CBA | 2.36  | 119.33      | 111.91   |
| 25  | D     | 402 | CLA  | CHD-C1D-C2D | 2.36  | 130.44      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | d     | 402 | CLA  | CHD-C1D-C2D | 2.36  | 130.44      | 125.48   |
| 25  | g     | 614 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 25  | R     | 604 | CLA  | C2D-C1D-ND  | -2.36 | 108.36      | 110.10   |
| 25  | r     | 604 | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 25  | S     | 313 | CLA  | C2D-C1D-ND  | -2.36 | 108.36      | 110.10   |
| 32  | N     | 620 | AJP  | C21-C20-C19 | 2.36  | 109.80      | 107.14   |
| 40  | Y     | 318 | NEX  | O24-C25-C38 | 2.36  | 117.88      | 115.06   |
| 25  | R     | 609 | CLA  | C4D-CHA-C1A | -2.36 | 118.38      | 121.25   |
| 25  | R     | 612 | CLA  | O2A-CGA-CBA | 2.36  | 119.31      | 111.91   |
| 25  | C     | 507 | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 25  | r     | 612 | CLA  | O2A-CGA-CBA | 2.36  | 119.31      | 111.91   |
| 24  | l     | 302 | CHL  | OMC-CMC-C2C | -2.36 | 120.36      | 125.69   |
| 25  | r     | 614 | CLA  | O2D-CGD-O1D | -2.36 | 119.23      | 123.84   |
| 25  | N     | 604 | CLA  | O2A-CGA-CBA | 2.36  | 119.31      | 111.91   |
| 32  | n     | 620 | AJP  | C21-C20-C19 | 2.36  | 109.79      | 107.14   |
| 24  | n     | 607 | CHL  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 24  | N     | 607 | CHL  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 25  | R     | 614 | CLA  | O2D-CGD-O1D | -2.36 | 119.23      | 123.84   |
| 32  | Y     | 324 | AJP  | C18-C17-C16 | -2.36 | 108.26      | 112.14   |
| 32  | y     | 323 | AJP  | C21-C20-C19 | 2.36  | 109.79      | 107.14   |
| 25  | N     | 610 | CLA  | O1D-CGD-CBD | -2.36 | 119.67      | 124.48   |
| 25  | n     | 610 | CLA  | O1D-CGD-CBD | -2.36 | 119.67      | 124.48   |
| 25  | n     | 604 | CLA  | O2A-CGA-CBA | 2.35  | 119.30      | 111.91   |
| 25  | Y     | 305 | CLA  | O2D-CGD-O1D | -2.35 | 119.23      | 123.84   |
| 25  | b     | 606 | CLA  | O2D-CGD-O1D | -2.35 | 119.23      | 123.84   |
| 40  | N     | 617 | NEX  | C5-C6-C1    | -2.35 | 117.36      | 119.70   |
| 40  | s     | 317 | NEX  | C5-C6-C1    | -2.35 | 117.36      | 119.70   |
| 28  | H     | 101 | BCR  | C11-C10-C9  | -2.35 | 123.95      | 127.31   |
| 28  | h     | 101 | BCR  | C11-C10-C9  | -2.35 | 123.95      | 127.31   |
| 25  | R     | 614 | CLA  | C4D-C3D-CAD | -2.35 | 105.33      | 108.10   |
| 24  | Y     | 302 | CHL  | C2C-C3C-C4C | 2.35  | 108.16      | 106.49   |
| 24  | y     | 302 | CHL  | C2C-C3C-C4C | 2.35  | 108.16      | 106.49   |
| 25  | b     | 615 | CLA  | O1D-CGD-CBD | -2.35 | 119.68      | 124.48   |
| 25  | A     | 401 | CLA  | O1D-CGD-CBD | -2.35 | 119.68      | 124.48   |
| 25  | a     | 402 | CLA  | O1D-CGD-CBD | -2.35 | 119.68      | 124.48   |
| 32  | G     | 618 | AJP  | C18-C17-C16 | 2.35  | 116.00      | 112.14   |
| 25  | N     | 610 | CLA  | O2A-CGA-CBA | 2.35  | 119.28      | 111.91   |
| 25  | n     | 610 | CLA  | O2A-CGA-CBA | 2.35  | 119.28      | 111.91   |
| 25  | B     | 615 | CLA  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 25  | b     | 615 | CLA  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 33  | A     | 413 | BCT  | O3-C-O1     | -2.35 | 113.46      | 119.55   |
| 33  | a     | 414 | BCT  | O3-C-O1     | -2.35 | 113.46      | 119.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 324 | AJP  | C18-C17-C16 | -2.35 | 108.27      | 112.14   |
| 24  | G     | 607 | CHL  | OMC-CMC-C2C | -2.35 | 120.38      | 125.69   |
| 24  | g     | 607 | CHL  | OMC-CMC-C2C | -2.35 | 120.38      | 125.69   |
| 25  | N     | 613 | CLA  | CHD-C4C-C3C | -2.34 | 121.39      | 124.84   |
| 25  | 6     | 602 | CLA  | O2D-CGD-O1D | -2.34 | 119.26      | 123.84   |
| 25  | D     | 402 | CLA  | O2A-CGA-CBA | 2.34  | 119.26      | 111.91   |
| 25  | r     | 609 | CLA  | C4D-CHA-C1A | -2.34 | 118.40      | 121.25   |
| 25  | y     | 305 | CLA  | O2D-CGD-O1D | -2.34 | 119.26      | 123.84   |
| 32  | A     | 412 | AJP  | C85-O84-C05 | 2.34  | 118.15      | 113.72   |
| 32  | a     | 413 | AJP  | C85-O84-C05 | 2.34  | 118.15      | 113.72   |
| 24  | s     | 302 | CHL  | OMC-CMC-C2C | -2.34 | 120.40      | 125.69   |
| 32  | g     | 618 | AJP  | C18-C17-C16 | 2.34  | 115.99      | 112.14   |
| 25  | d     | 402 | CLA  | O2A-CGA-CBA | 2.34  | 119.24      | 111.91   |
| 25  | Y     | 313 | CLA  | C4A-NA-C1A  | -2.34 | 105.66      | 106.71   |
| 24  | Y     | 302 | CHL  | OMC-CMC-C2C | -2.34 | 120.40      | 125.69   |
| 24  | y     | 302 | CHL  | OMC-CMC-C2C | -2.34 | 120.40      | 125.69   |
| 25  | G     | 611 | CLA  | O1D-CGD-CBD | -2.34 | 119.70      | 124.48   |
| 28  | A     | 406 | BCR  | C38-C26-C25 | -2.34 | 121.91      | 124.53   |
| 28  | a     | 407 | BCR  | C38-C26-C25 | -2.34 | 121.91      | 124.53   |
| 25  | r     | 614 | CLA  | C4D-C3D-CAD | -2.34 | 105.34      | 108.10   |
| 24  | y     | 308 | CHL  | O1D-CGD-CBD | -2.34 | 119.70      | 124.48   |
| 25  | B     | 601 | CLA  | O1D-CGD-CBD | -2.34 | 119.70      | 124.48   |
| 25  | 2     | 602 | CLA  | C1D-ND-C4D  | 2.34  | 107.99      | 106.33   |
| 25  | b     | 601 | CLA  | O1D-CGD-CBD | -2.34 | 119.71      | 124.48   |
| 25  | c     | 501 | CLA  | C2A-C3A-C4A | -2.33 | 98.10       | 101.87   |
| 28  | I     | 101 | BCR  | C38-C26-C25 | -2.33 | 121.91      | 124.53   |
| 24  | l     | 302 | CHL  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 25  | B     | 611 | CLA  | O2D-CGD-O1D | -2.33 | 119.28      | 123.84   |
| 25  | b     | 611 | CLA  | O2D-CGD-O1D | -2.33 | 119.28      | 123.84   |
| 25  | g     | 611 | CLA  | O1D-CGD-CBD | -2.33 | 119.71      | 124.48   |
| 25  | c     | 507 | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 25  | B     | 606 | CLA  | O2D-CGD-O1D | -2.33 | 119.28      | 123.84   |
| 25  | R     | 603 | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 25  | r     | 603 | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 25  | C     | 513 | CLA  | C2A-C1A-CHA | -2.33 | 119.79      | 123.86   |
| 25  | c     | 513 | CLA  | C2A-C1A-CHA | -2.33 | 119.79      | 123.86   |
| 25  | G     | 614 | CLA  | O1D-CGD-CBD | -2.33 | 119.72      | 124.48   |
| 25  | S     | 305 | CLA  | O2A-CGA-CBA | 2.33  | 119.22      | 111.91   |
| 25  | s     | 305 | CLA  | O2A-CGA-CBA | 2.33  | 119.22      | 111.91   |
| 25  | Y     | 303 | CLA  | CMB-C2B-C1B | -2.33 | 124.89      | 128.46   |
| 24  | S     | 306 | CHL  | C2A-C3A-C4A | 2.33  | 105.63      | 101.87   |
| 24  | Y     | 308 | CHL  | O1D-CGD-CBD | -2.33 | 119.72      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 610 | CLA  | O2A-CGA-CBA | 2.33  | 119.21      | 111.91   |
| 28  | B     | 619 | BCR  | C27-C26-C25 | 2.33  | 126.11      | 122.73   |
| 28  | H     | 101 | BCR  | C27-C26-C25 | 2.33  | 126.11      | 122.73   |
| 28  | i     | 101 | BCR  | C38-C26-C25 | -2.33 | 121.92      | 124.53   |
| 25  | B     | 612 | CLA  | O1D-CGD-CBD | -2.32 | 119.73      | 124.48   |
| 25  | b     | 612 | CLA  | O1D-CGD-CBD | -2.32 | 119.73      | 124.48   |
| 25  | s     | 304 | CLA  | O1D-CGD-CBD | -2.32 | 119.73      | 124.48   |
| 24  | s     | 306 | CHL  | C2A-C3A-C4A | 2.32  | 105.62      | 101.87   |
| 25  | y     | 312 | CLA  | C4D-CHA-C1A | -2.32 | 118.43      | 121.25   |
| 24  | S     | 306 | CHL  | OMC-CMC-C2C | -2.32 | 120.44      | 125.69   |
| 32  | Y     | 323 | AJP  | C21-C20-C19 | 2.32  | 109.75      | 107.14   |
| 25  | n     | 613 | CLA  | CHD-C4C-C3C | -2.32 | 121.43      | 124.84   |
| 25  | S     | 304 | CLA  | O1D-CGD-CBD | -2.32 | 119.74      | 124.48   |
| 24  | s     | 308 | CHL  | OMC-CMC-C2C | -2.32 | 120.45      | 125.69   |
| 32  | N     | 620 | AJP  | O25-C26-O31 | 2.32  | 117.14      | 110.67   |
| 32  | n     | 620 | AJP  | O25-C26-O31 | 2.32  | 117.14      | 110.67   |
| 24  | g     | 601 | CHL  | OMC-CMC-C2C | -2.32 | 120.45      | 125.69   |
| 40  | y     | 318 | NEX  | O24-C25-C38 | 2.32  | 117.83      | 115.06   |
| 24  | G     | 609 | CHL  | C2A-C1A-CHA | 2.32  | 127.91      | 123.86   |
| 24  | G     | 601 | CHL  | OMC-CMC-C2C | -2.32 | 120.45      | 125.69   |
| 24  | R     | 613 | CHL  | OMC-CMC-C2C | -2.32 | 120.45      | 125.69   |
| 24  | s     | 306 | CHL  | OMC-CMC-C2C | -2.32 | 120.45      | 125.69   |
| 25  | B     | 607 | CLA  | O2D-CGD-O1D | -2.32 | 119.31      | 123.84   |
| 25  | b     | 607 | CLA  | O2D-CGD-O1D | -2.32 | 119.31      | 123.84   |
| 25  | b     | 613 | CLA  | O2A-CGA-CBA | 2.31  | 119.17      | 111.91   |
| 25  | C     | 507 | CLA  | C4-C3-C5    | 2.31  | 119.17      | 115.27   |
| 28  | b     | 619 | BCR  | C27-C26-C25 | 2.31  | 126.09      | 122.73   |
| 25  | d     | 403 | CLA  | C3D-C4D-CHA | 2.31  | 118.02      | 112.72   |
| 25  | s     | 305 | CLA  | C3C-C4C-NC  | -2.31 | 107.98      | 110.57   |
| 24  | S     | 302 | CHL  | OMC-CMC-C2C | -2.31 | 120.46      | 125.69   |
| 24  | N     | 605 | CHL  | C2A-C3A-C4A | 2.31  | 105.60      | 101.87   |
| 24  | s     | 307 | CHL  | OMC-CMC-C2C | -2.31 | 120.46      | 125.69   |
| 32  | S     | 319 | AJP  | C17-C16-C11 | -2.31 | 108.96      | 112.32   |
| 32  | s     | 319 | AJP  | C17-C16-C11 | -2.31 | 108.96      | 112.32   |
| 24  | n     | 607 | CHL  | C2C-C3C-C4C | 2.31  | 108.14      | 106.49   |
| 25  | n     | 610 | CLA  | CHD-C1D-C2D | 2.31  | 130.32      | 125.48   |
| 39  | R     | 615 | LUT  | C35-C34-C33 | -2.31 | 124.02      | 127.31   |
| 25  | B     | 616 | CLA  | O1D-CGD-CBD | -2.31 | 119.76      | 124.48   |
| 25  | b     | 616 | CLA  | O1D-CGD-CBD | -2.31 | 119.76      | 124.48   |
| 25  | d     | 401 | CLA  | O1D-CGD-CBD | -2.31 | 119.76      | 124.48   |
| 25  | C     | 507 | CLA  | C1D-CHD-C4C | -2.31 | 121.08      | 126.06   |
| 25  | c     | 507 | CLA  | C1D-CHD-C4C | -2.31 | 121.08      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | g     | 607 | CHL  | CAA-C2A-C3A | -2.31 | 106.46      | 112.78   |
| 25  | B     | 610 | CLA  | O2A-CGA-CBA | 2.31  | 119.15      | 111.91   |
| 25  | G     | 614 | CLA  | C2C-C1C-NC  | 2.31  | 112.13      | 109.97   |
| 40  | Y     | 318 | NEX  | C40-C33-C32 | 2.31  | 121.71      | 118.08   |
| 25  | n     | 604 | CLA  | C2A-C1A-CHA | -2.31 | 119.83      | 123.86   |
| 25  | S     | 305 | CLA  | C3C-C4C-NC  | -2.31 | 107.98      | 110.57   |
| 25  | B     | 608 | CLA  | O2D-CGD-O1D | -2.31 | 119.33      | 123.84   |
| 25  | c     | 505 | CLA  | O1D-CGD-CBD | -2.30 | 119.77      | 124.48   |
| 25  | C     | 513 | CLA  | O2A-CGA-CBA | 2.30  | 119.14      | 111.91   |
| 25  | c     | 513 | CLA  | O2A-CGA-CBA | 2.30  | 119.14      | 111.91   |
| 25  | y     | 315 | CLA  | C2C-C1C-NC  | 2.30  | 112.13      | 109.97   |
| 25  | D     | 403 | CLA  | C3D-C4D-CHA | 2.30  | 118.00      | 112.72   |
| 25  | B     | 613 | CLA  | O2A-CGA-CBA | 2.30  | 119.14      | 111.91   |
| 25  | C     | 501 | CLA  | C3D-C4D-CHA | 2.30  | 117.99      | 112.72   |
| 28  | h     | 101 | BCR  | C27-C26-C25 | 2.30  | 126.08      | 122.73   |
| 24  | r     | 613 | CHL  | OMC-CMC-C2C | -2.30 | 120.48      | 125.69   |
| 25  | C     | 501 | CLA  | C2A-C3A-C4A | -2.30 | 98.15       | 101.87   |
| 28  | B     | 618 | BCR  | C2-C1-C6    | 2.30  | 114.03      | 110.48   |
| 28  | b     | 618 | BCR  | C2-C1-C6    | 2.30  | 114.03      | 110.48   |
| 24  | y     | 309 | CHL  | OMC-CMC-C2C | -2.30 | 120.48      | 125.69   |
| 24  | S     | 308 | CHL  | OMC-CMC-C2C | -2.30 | 120.48      | 125.69   |
| 24  | S     | 307 | CHL  | OMC-CMC-C2C | -2.30 | 120.48      | 125.69   |
| 25  | y     | 303 | CLA  | CMB-C2B-C1B | -2.30 | 124.93      | 128.46   |
| 25  | c     | 501 | CLA  | C3D-C4D-CHA | 2.30  | 117.98      | 112.72   |
| 25  | B     | 603 | CLA  | O2A-CGA-CBA | 2.30  | 119.12      | 111.91   |
| 25  | b     | 603 | CLA  | O2A-CGA-CBA | 2.30  | 119.12      | 111.91   |
| 25  | G     | 604 | CLA  | O2D-CGD-O1D | -2.30 | 119.35      | 123.84   |
| 25  | b     | 608 | CLA  | O2D-CGD-O1D | -2.30 | 119.35      | 123.84   |
| 24  | l     | 302 | CHL  | O2A-CGA-CBA | 2.30  | 121.41      | 114.03   |
| 24  | N     | 609 | CHL  | C2A-C3A-C4A | 2.30  | 105.58      | 101.87   |
| 24  | n     | 609 | CHL  | C2A-C3A-C4A | 2.30  | 105.58      | 101.87   |
| 24  | G     | 607 | CHL  | CAA-C2A-C3A | -2.30 | 106.49      | 112.78   |
| 24  | N     | 607 | CHL  | C2C-C3C-C4C | 2.30  | 108.12      | 106.49   |
| 24  | n     | 605 | CHL  | C2A-C3A-C4A | 2.29  | 105.58      | 101.87   |
| 25  | b     | 604 | CLA  | O1D-CGD-CBD | -2.29 | 119.79      | 124.48   |
| 25  | C     | 505 | CLA  | O1D-CGD-CBD | -2.29 | 119.79      | 124.48   |
| 25  | r     | 608 | CLA  | O1D-CGD-CBD | -2.29 | 119.79      | 124.48   |
| 24  | Y     | 306 | CHL  | C2A-C3A-C4A | 2.29  | 105.57      | 101.87   |
| 25  | B     | 604 | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 24  | Y     | 309 | CHL  | OMC-CMC-C2C | -2.29 | 120.51      | 125.69   |
| 24  | N     | 601 | CHL  | C2A-C3A-C4A | 2.29  | 105.57      | 101.87   |
| 24  | G     | 606 | CHL  | OMC-CMC-C2C | -2.29 | 120.51      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | A     | 402 | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 25  | a     | 403 | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 24  | 5     | 302 | CHL  | O2A-CGA-CBA | 2.29  | 121.38      | 114.03   |
| 25  | c     | 502 | CLA  | O2D-CGD-O1D | -2.29 | 119.36      | 123.84   |
| 24  | 5     | 302 | CHL  | CHD-C1D-ND  | -2.29 | 122.35      | 124.45   |
| 25  | C     | 506 | CLA  | CHD-C1D-C2D | 2.29  | 130.28      | 125.48   |
| 25  | c     | 506 | CLA  | CHD-C1D-C2D | 2.29  | 130.28      | 125.48   |
| 25  | R     | 604 | CLA  | C4D-CHA-C1A | -2.29 | 118.47      | 121.25   |
| 25  | r     | 604 | CLA  | C4D-CHA-C1A | -2.29 | 118.47      | 121.25   |
| 39  | r     | 615 | LUT  | C35-C34-C33 | -2.29 | 124.05      | 127.31   |
| 24  | y     | 306 | CHL  | C2A-C3A-C4A | 2.29  | 105.56      | 101.87   |
| 32  | Y     | 320 | AJP  | O09-C08-C07 | 2.29  | 109.55      | 104.06   |
| 32  | y     | 320 | AJP  | O09-C08-C07 | 2.29  | 109.55      | 104.06   |
| 25  | n     | 602 | CLA  | C2A-C1A-CHA | -2.29 | 119.86      | 123.86   |
| 24  | g     | 606 | CHL  | OMC-CMC-C2C | -2.29 | 120.52      | 125.69   |
| 25  | Y     | 303 | CLA  | C2A-C1A-CHA | -2.28 | 119.86      | 123.86   |
| 25  | y     | 303 | CLA  | C2A-C1A-CHA | -2.28 | 119.86      | 123.86   |
| 25  | g     | 614 | CLA  | C2C-C1C-NC  | 2.28  | 112.11      | 109.97   |
| 25  | b     | 613 | CLA  | C2A-C1A-CHA | -2.28 | 119.87      | 123.86   |
| 24  | N     | 606 | CHL  | CBC-CAC-C3C | -2.28 | 106.14      | 112.43   |
| 24  | n     | 606 | CHL  | CBC-CAC-C3C | -2.28 | 106.14      | 112.43   |
| 25  | N     | 610 | CLA  | CHD-C1D-C2D | 2.28  | 130.26      | 125.48   |
| 25  | R     | 612 | CLA  | O1D-CGD-CBD | -2.28 | 119.82      | 124.48   |
| 25  | S     | 310 | CLA  | O2A-CGA-CBA | 2.28  | 119.06      | 111.91   |
| 24  | Y     | 302 | CHL  | C2A-C3A-C4A | 2.28  | 105.55      | 101.87   |
| 24  | y     | 302 | CHL  | C2A-C3A-C4A | 2.28  | 105.55      | 101.87   |
| 25  | B     | 606 | CLA  | O1D-CGD-CBD | -2.28 | 119.83      | 124.48   |
| 25  | g     | 614 | CLA  | CHD-C1D-C2D | 2.27  | 130.25      | 125.48   |
| 28  | T     | 101 | BCR  | C38-C26-C25 | -2.27 | 121.97      | 124.53   |
| 28  | t     | 101 | BCR  | C38-C26-C25 | -2.27 | 121.97      | 124.53   |
| 25  | N     | 604 | CLA  | C2A-C1A-CHA | -2.27 | 119.88      | 123.86   |
| 25  | D     | 401 | CLA  | O1D-CGD-CBD | -2.27 | 119.83      | 124.48   |
| 25  | Y     | 315 | CLA  | C2C-C1C-NC  | 2.27  | 112.10      | 109.97   |
| 25  | B     | 601 | CLA  | O2D-CGD-O1D | -2.27 | 119.39      | 123.84   |
| 25  | b     | 601 | CLA  | O2D-CGD-O1D | -2.27 | 119.39      | 123.84   |
| 25  | N     | 602 | CLA  | C2A-C1A-CHA | -2.27 | 119.89      | 123.86   |
| 25  | 2     | 602 | CLA  | CHC-C1C-C2C | 2.27  | 133.01      | 126.72   |
| 25  | 6     | 602 | CLA  | CHC-C1C-C2C | 2.27  | 133.01      | 126.72   |
| 25  | 2     | 604 | CLA  | C3C-C4C-NC  | -2.27 | 108.02      | 110.57   |
| 25  | 6     | 604 | CLA  | C3C-C4C-NC  | -2.27 | 108.02      | 110.57   |
| 25  | r     | 601 | CLA  | C3C-C4C-NC  | -2.27 | 108.02      | 110.57   |
| 24  | y     | 310 | CHL  | OMC-CMC-C2C | -2.27 | 120.55      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | Y     | 308 | CHL  | O2D-CGD-O1D | -2.27 | 119.40      | 123.84   |
| 25  | R     | 608 | CLA  | O1D-CGD-CBD | -2.27 | 119.84      | 124.48   |
| 24  | n     | 605 | CHL  | C2A-C1A-CHA | 2.27  | 127.83      | 123.86   |
| 25  | C     | 502 | CLA  | O2D-CGD-O1D | -2.27 | 119.40      | 123.84   |
| 25  | Y     | 313 | CLA  | C4D-CHA-C1A | -2.27 | 118.49      | 121.25   |
| 25  | r     | 612 | CLA  | O1D-CGD-CBD | -2.27 | 119.84      | 124.48   |
| 32  | Y     | 322 | AJP  | C19-C24-C23 | -2.27 | 107.28      | 112.92   |
| 32  | y     | 322 | AJP  | C19-C24-C23 | -2.27 | 107.28      | 112.92   |
| 40  | y     | 318 | NEX  | C40-C33-C32 | 2.27  | 121.65      | 118.08   |
| 25  | y     | 304 | CLA  | O1D-CGD-CBD | -2.27 | 119.84      | 124.48   |
| 25  | S     | 312 | CLA  | O2D-CGD-O1D | -2.27 | 119.41      | 123.84   |
| 24  | n     | 608 | CHL  | OMC-CMC-C2C | -2.27 | 120.56      | 125.69   |
| 25  | s     | 310 | CLA  | O2A-CGA-CBA | 2.27  | 119.02      | 111.91   |
| 28  | T     | 101 | BCR  | C15-C14-C13 | -2.27 | 124.08      | 127.31   |
| 25  | S     | 314 | CLA  | C3D-C4D-ND  | 2.27  | 113.90      | 110.24   |
| 25  | g     | 610 | CLA  | O1D-CGD-CBD | -2.27 | 119.85      | 124.48   |
| 25  | r     | 609 | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 25  | g     | 604 | CLA  | O2D-CGD-O1D | -2.27 | 119.41      | 123.84   |
| 25  | G     | 611 | CLA  | CAD-C3D-C2D | 2.27  | 151.73      | 140.80   |
| 25  | g     | 611 | CLA  | CAD-C3D-C2D | 2.27  | 151.73      | 140.80   |
| 25  | B     | 605 | CLA  | CBA-CAA-C2A | -2.26 | 107.18      | 113.86   |
| 25  | b     | 605 | CLA  | CBA-CAA-C2A | -2.26 | 107.18      | 113.86   |
| 25  | a     | 402 | CLA  | C4D-CHA-C1A | -2.26 | 118.49      | 121.25   |
| 24  | Y     | 310 | CHL  | OMC-CMC-C2C | -2.26 | 120.57      | 125.69   |
| 24  | n     | 601 | CHL  | C2A-C3A-C4A | 2.26  | 105.52      | 101.87   |
| 24  | r     | 607 | CHL  | OMC-CMC-C2C | -2.26 | 120.57      | 125.69   |
| 32  | S     | 319 | AJP  | C83-C06-C05 | -2.26 | 110.79      | 114.92   |
| 25  | R     | 609 | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 25  | c     | 505 | CLA  | C3D-C4D-ND  | 2.26  | 113.89      | 110.24   |
| 25  | c     | 503 | CLA  | C2A-C1A-CHA | -2.26 | 119.91      | 123.86   |
| 25  | c     | 513 | CLA  | O1D-CGD-CBD | -2.26 | 119.86      | 124.48   |
| 24  | y     | 308 | CHL  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 25  | B     | 613 | CLA  | C2A-C1A-CHA | -2.26 | 119.91      | 123.86   |
| 25  | Y     | 304 | CLA  | O1D-CGD-CBD | -2.26 | 119.86      | 124.48   |
| 24  | r     | 606 | CHL  | OMC-CMC-C2C | -2.26 | 120.58      | 125.69   |
| 24  | 5     | 301 | CHL  | OMC-CMC-C2C | -2.26 | 120.58      | 125.69   |
| 25  | C     | 503 | CLA  | C2A-C1A-CHA | -2.26 | 119.91      | 123.86   |
| 25  | B     | 614 | CLA  | O1D-CGD-CBD | -2.26 | 119.87      | 124.48   |
| 25  | b     | 614 | CLA  | O1D-CGD-CBD | -2.26 | 119.87      | 124.48   |
| 25  | G     | 614 | CLA  | CHD-C1D-C2D | 2.26  | 130.21      | 125.48   |
| 25  | R     | 601 | CLA  | C3C-C4C-NC  | -2.26 | 108.04      | 110.57   |
| 40  | G     | 617 | NEX  | C20-C13-C12 | 2.26  | 121.63      | 118.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | D     | 403 | CLA  | O2D-CGD-O1D | -2.26 | 119.43      | 123.84   |
| 25  | d     | 403 | CLA  | O2D-CGD-O1D | -2.26 | 119.43      | 123.84   |
| 25  | C     | 513 | CLA  | O1D-CGD-CBD | -2.25 | 119.87      | 124.48   |
| 24  | Y     | 308 | CHL  | OMC-CMC-C2C | -2.25 | 120.59      | 125.69   |
| 24  | N     | 609 | CHL  | OMC-CMC-C2C | -2.25 | 120.59      | 125.69   |
| 24  | n     | 609 | CHL  | OMC-CMC-C2C | -2.25 | 120.59      | 125.69   |
| 32  | G     | 618 | AJP  | C17-C18-C19 | 2.25  | 116.36      | 111.84   |
| 32  | g     | 618 | AJP  | C17-C18-C19 | 2.25  | 116.36      | 111.84   |
| 25  | 2     | 604 | CLA  | CAD-C3D-C2D | 2.25  | 151.67      | 140.80   |
| 25  | 6     | 604 | CLA  | CAD-C3D-C2D | 2.25  | 151.67      | 140.80   |
| 24  | N     | 608 | CHL  | OMC-CMC-C2C | -2.25 | 120.59      | 125.69   |
| 25  | B     | 605 | CLA  | O2D-CGD-O1D | -2.25 | 119.43      | 123.84   |
| 25  | b     | 605 | CLA  | O2D-CGD-O1D | -2.25 | 119.43      | 123.84   |
| 25  | A     | 405 | CLA  | O2A-CGA-CBA | 2.25  | 118.98      | 111.91   |
| 25  | a     | 406 | CLA  | O2A-CGA-CBA | 2.25  | 118.98      | 111.91   |
| 25  | b     | 606 | CLA  | O1D-CGD-CBD | -2.25 | 119.88      | 124.48   |
| 25  | n     | 614 | CLA  | CHD-C1D-C2D | 2.25  | 130.20      | 125.48   |
| 24  | N     | 606 | CHL  | C2A-C3A-C4A | 2.25  | 105.51      | 101.87   |
| 24  | n     | 606 | CHL  | C2A-C3A-C4A | 2.25  | 105.51      | 101.87   |
| 25  | s     | 312 | CLA  | O2D-CGD-O1D | -2.25 | 119.44      | 123.84   |
| 25  | A     | 401 | CLA  | C4D-CHA-C1A | -2.25 | 118.51      | 121.25   |
| 24  | y     | 308 | CHL  | OMC-CMC-C2C | -2.25 | 120.60      | 125.69   |
| 25  | D     | 403 | CLA  | C3B-C4B-NB  | -2.25 | 106.30      | 109.21   |
| 25  | S     | 311 | CLA  | O2D-CGD-O1D | -2.25 | 119.44      | 123.84   |
| 25  | s     | 311 | CLA  | O2D-CGD-O1D | -2.25 | 119.44      | 123.84   |
| 25  | C     | 505 | CLA  | C3D-C4D-ND  | 2.25  | 113.88      | 110.24   |
| 25  | B     | 606 | CLA  | C2A-C1A-CHA | -2.25 | 119.92      | 123.86   |
| 25  | b     | 606 | CLA  | C2A-C1A-CHA | -2.25 | 119.92      | 123.86   |
| 24  | g     | 601 | CHL  | O1D-CGD-CBD | -2.25 | 119.88      | 124.48   |
| 25  | c     | 513 | CLA  | CMB-C2B-C1B | -2.25 | 125.01      | 128.46   |
| 25  | Y     | 312 | CLA  | C4D-CHA-C1A | -2.25 | 118.51      | 121.25   |
| 24  | 2     | 601 | CHL  | C3C-C4C-NC  | -2.25 | 108.05      | 110.57   |
| 24  | 6     | 601 | CHL  | C3C-C4C-NC  | -2.25 | 108.05      | 110.57   |
| 25  | C     | 513 | CLA  | CMB-C2B-C1B | -2.25 | 125.01      | 128.46   |
| 25  | C     | 507 | CLA  | C4D-C3D-CAD | -2.25 | 105.45      | 108.10   |
| 25  | D     | 401 | CLA  | C2A-C1A-CHA | -2.25 | 119.93      | 123.86   |
| 25  | d     | 401 | CLA  | C2A-C1A-CHA | -2.25 | 119.93      | 123.86   |
| 25  | s     | 314 | CLA  | CHD-C1D-C2D | 2.25  | 130.19      | 125.48   |
| 24  | y     | 307 | CHL  | CMB-C2B-C1B | -2.25 | 125.01      | 128.46   |
| 24  | N     | 605 | CHL  | C2A-C1A-CHA | 2.25  | 127.78      | 123.86   |
| 40  | Y     | 318 | NEX  | C28-C29-C30 | 2.25  | 122.39      | 118.94   |
| 25  | S     | 305 | CLA  | C3B-C4B-NB  | -2.24 | 106.31      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | N     | 614 | CLA  | CHD-C1D-C2D | 2.24  | 130.19      | 125.48   |
| 32  | s     | 319 | AJP  | C83-C06-C05 | -2.24 | 110.82      | 114.92   |
| 25  | N     | 603 | CLA  | O2D-CGD-O1D | -2.24 | 119.45      | 123.84   |
| 24  | R     | 607 | CHL  | OMC-CMC-C2C | -2.24 | 120.61      | 125.69   |
| 25  | G     | 610 | CLA  | O1D-CGD-CBD | -2.24 | 119.89      | 124.48   |
| 25  | Y     | 311 | CLA  | O1D-CGD-CBD | -2.24 | 119.89      | 124.48   |
| 32  | a     | 413 | AJP  | O70-C65-C66 | 2.24  | 115.10      | 110.35   |
| 24  | G     | 601 | CHL  | C2C-C3C-C4C | 2.24  | 108.09      | 106.49   |
| 25  | D     | 402 | CLA  | O1D-CGD-CBD | -2.24 | 119.90      | 124.48   |
| 25  | d     | 402 | CLA  | O1D-CGD-CBD | -2.24 | 119.90      | 124.48   |
| 25  | 6     | 604 | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 28  | h     | 101 | BCR  | C38-C26-C25 | -2.24 | 122.01      | 124.53   |
| 25  | 2     | 604 | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 25  | C     | 506 | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 25  | c     | 506 | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 24  | R     | 606 | CHL  | OMC-CMC-C2C | -2.24 | 120.62      | 125.69   |
| 24  | G     | 601 | CHL  | O1D-CGD-CBD | -2.24 | 119.90      | 124.48   |
| 28  | H     | 101 | BCR  | C38-C26-C25 | -2.24 | 122.01      | 124.53   |
| 25  | y     | 311 | CLA  | O1D-CGD-CBD | -2.24 | 119.91      | 124.48   |
| 24  | G     | 606 | CHL  | O2A-CGA-O1A | -2.24 | 117.94      | 123.59   |
| 24  | Y     | 307 | CHL  | CMB-C2B-C1B | -2.24 | 125.03      | 128.46   |
| 25  | n     | 613 | CLA  | O2A-CGA-CBA | 2.24  | 118.93      | 111.91   |
| 25  | S     | 309 | CLA  | CHD-C1D-C2D | 2.24  | 130.17      | 125.48   |
| 25  | s     | 309 | CLA  | CHD-C1D-C2D | 2.24  | 130.17      | 125.48   |
| 25  | S     | 314 | CLA  | O2D-CGD-O1D | -2.24 | 119.47      | 123.84   |
| 25  | R     | 614 | CLA  | CHD-C1D-C2D | 2.24  | 130.17      | 125.48   |
| 25  | r     | 614 | CLA  | CHD-C1D-C2D | 2.24  | 130.17      | 125.48   |
| 24  | l     | 301 | CHL  | O2A-CGA-CBA | 2.24  | 121.21      | 114.03   |
| 24  | 5     | 301 | CHL  | O2A-CGA-CBA | 2.24  | 121.21      | 114.03   |
| 25  | r     | 603 | CLA  | O2A-CGA-CBA | 2.24  | 118.92      | 111.91   |
| 25  | r     | 603 | CLA  | C3B-C4B-NB  | -2.23 | 106.32      | 109.21   |
| 25  | C     | 502 | CLA  | O2A-CGA-CBA | 2.23  | 118.92      | 111.91   |
| 25  | c     | 502 | CLA  | O2A-CGA-CBA | 2.23  | 118.92      | 111.91   |
| 25  | s     | 314 | CLA  | C3D-C4D-ND  | 2.23  | 113.85      | 110.24   |
| 25  | N     | 614 | CLA  | O2A-CGA-CBA | 2.23  | 118.92      | 111.91   |
| 25  | c     | 507 | CLA  | C4D-C3D-CAD | -2.23 | 105.46      | 108.10   |
| 25  | s     | 305 | CLA  | C3B-C4B-NB  | -2.23 | 106.32      | 109.21   |
| 25  | C     | 501 | CLA  | C2A-C1A-CHA | -2.23 | 119.95      | 123.86   |
| 25  | c     | 501 | CLA  | C2A-C1A-CHA | -2.23 | 119.95      | 123.86   |
| 24  | Y     | 309 | CHL  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 32  | A     | 412 | AJP  | O70-C65-C66 | 2.23  | 115.07      | 110.35   |
| 25  | S     | 314 | CLA  | CHD-C1D-C2D | 2.23  | 130.16      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | n     | 614 | CLA  | O2A-CGA-CBA | 2.23  | 118.91      | 111.91   |
| 25  | B     | 612 | CLA  | C2A-C1A-CHA | -2.23 | 119.96      | 123.86   |
| 25  | y     | 313 | CLA  | C4D-CHA-C1A | -2.23 | 118.53      | 121.25   |
| 40  | y     | 318 | NEX  | C28-C29-C30 | 2.23  | 122.36      | 118.94   |
| 25  | A     | 401 | CLA  | C11-C12-C13 | -2.23 | 108.71      | 115.92   |
| 24  | Y     | 307 | CHL  | CBC-CAC-C3C | -2.23 | 106.28      | 112.43   |
| 25  | g     | 610 | CLA  | O2A-CGA-CBA | 2.23  | 118.91      | 111.91   |
| 25  | G     | 610 | CLA  | O2A-CGA-CBA | 2.23  | 118.91      | 111.91   |
| 28  | t     | 101 | BCR  | C15-C14-C13 | -2.23 | 124.13      | 127.31   |
| 25  | r     | 614 | CLA  | C3D-C4D-ND  | 2.23  | 113.84      | 110.24   |
| 24  | g     | 606 | CHL  | O2A-CGA-O1A | -2.23 | 117.97      | 123.59   |
| 32  | y     | 324 | AJP  | C83-C06-C05 | -2.23 | 110.85      | 114.92   |
| 32  | Y     | 320 | AJP  | O84-C85-C02 | 2.23  | 115.39      | 112.18   |
| 24  | R     | 607 | CHL  | O1D-CGD-CBD | -2.23 | 119.93      | 124.48   |
| 24  | r     | 607 | CHL  | O1D-CGD-CBD | -2.23 | 119.93      | 124.48   |
| 25  | r     | 608 | CLA  | O2D-CGD-O1D | -2.23 | 119.48      | 123.84   |
| 24  | S     | 306 | CHL  | O2D-CGD-O1D | -2.23 | 119.48      | 123.84   |
| 25  | N     | 613 | CLA  | O2A-CGA-CBA | 2.23  | 118.89      | 111.91   |
| 25  | n     | 603 | CLA  | O2D-CGD-O1D | -2.23 | 119.49      | 123.84   |
| 25  | r     | 602 | CLA  | O2D-CGD-O1D | -2.23 | 119.49      | 123.84   |
| 25  | R     | 614 | CLA  | CAD-C3D-C2D | 2.23  | 151.54      | 140.80   |
| 25  | r     | 614 | CLA  | CAD-C3D-C2D | 2.23  | 151.54      | 140.80   |
| 32  | Y     | 320 | AJP  | C11-C16-C15 | -2.22 | 105.35      | 109.23   |
| 32  | y     | 320 | AJP  | C11-C16-C15 | -2.22 | 105.35      | 109.23   |
| 25  | b     | 613 | CLA  | C4D-CHA-C1A | -2.22 | 118.54      | 121.25   |
| 25  | Y     | 312 | CLA  | O2D-CGD-O1D | -2.22 | 119.49      | 123.84   |
| 25  | B     | 602 | CLA  | O1D-CGD-CBD | -2.22 | 119.94      | 124.48   |
| 25  | b     | 602 | CLA  | O1D-CGD-CBD | -2.22 | 119.94      | 124.48   |
| 25  | a     | 402 | CLA  | C11-C12-C13 | -2.22 | 108.73      | 115.92   |
| 25  | d     | 403 | CLA  | C3B-C4B-NB  | -2.22 | 106.34      | 109.21   |
| 28  | D     | 404 | BCR  | C7-C8-C9    | -2.22 | 122.88      | 126.23   |
| 28  | d     | 404 | BCR  | C7-C8-C9    | -2.22 | 122.88      | 126.23   |
| 25  | R     | 614 | CLA  | C3D-C4D-ND  | 2.22  | 113.83      | 110.24   |
| 25  | C     | 509 | CLA  | C2A-C1A-CHA | -2.22 | 119.97      | 123.86   |
| 25  | c     | 509 | CLA  | C2A-C1A-CHA | -2.22 | 119.97      | 123.86   |
| 24  | s     | 306 | CHL  | O2D-CGD-O1D | -2.22 | 119.49      | 123.84   |
| 25  | Y     | 315 | CLA  | CMB-C2B-C1B | -2.22 | 125.05      | 128.46   |
| 25  | y     | 315 | CLA  | CMB-C2B-C1B | -2.22 | 125.05      | 128.46   |
| 24  | y     | 309 | CHL  | O2D-CGD-O1D | -2.22 | 119.49      | 123.84   |
| 25  | R     | 608 | CLA  | O2D-CGD-O1D | -2.22 | 119.49      | 123.84   |
| 24  | y     | 307 | CHL  | CBC-CAC-C3C | -2.22 | 106.31      | 112.43   |
| 24  | 1     | 301 | CHL  | OMC-CMC-C2C | -2.22 | 120.67      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | G     | 602 | CLA  | C6-C7-C8    | -2.22 | 108.75      | 115.92   |
| 25  | R     | 603 | CLA  | C3B-C4B-NB  | -2.22 | 106.34      | 109.21   |
| 25  | B     | 614 | CLA  | O2A-CGA-CBA | 2.22  | 118.87      | 111.91   |
| 25  | b     | 614 | CLA  | O2A-CGA-CBA | 2.22  | 118.87      | 111.91   |
| 24  | R     | 607 | CHL  | O2D-CGD-O1D | -2.22 | 119.50      | 123.84   |
| 25  | g     | 602 | CLA  | C6-C7-C8    | -2.22 | 108.75      | 115.92   |
| 25  | B     | 613 | CLA  | C4D-CHA-C1A | -2.22 | 118.55      | 121.25   |
| 25  | n     | 613 | CLA  | C6-C7-C8    | -2.22 | 108.75      | 115.92   |
| 24  | n     | 601 | CHL  | C2A-C1A-CHA | 2.22  | 127.73      | 123.86   |
| 25  | g     | 611 | CLA  | C11-C10-C8  | -2.22 | 108.76      | 115.92   |
| 24  | G     | 601 | CHL  | O2D-CGD-O1D | -2.22 | 119.51      | 123.84   |
| 29  | l     | 102 | SQD  | C1-C2-C3    | 2.22  | 114.61      | 110.00   |
| 25  | G     | 602 | CLA  | C3D-C4D-ND  | 2.22  | 113.82      | 110.24   |
| 25  | g     | 602 | CLA  | C3D-C4D-ND  | 2.22  | 113.82      | 110.24   |
| 40  | g     | 617 | NEX  | C32-C33-C34 | -2.22 | 115.54      | 118.94   |
| 25  | s     | 314 | CLA  | O2D-CGD-O1D | -2.21 | 119.51      | 123.84   |
| 28  | I     | 101 | BCR  | C7-C8-C9    | -2.21 | 122.89      | 126.23   |
| 24  | s     | 306 | CHL  | O1D-CGD-CBD | -2.21 | 119.95      | 124.48   |
| 28  | A     | 406 | BCR  | C7-C8-C9    | -2.21 | 122.89      | 126.23   |
| 28  | a     | 407 | BCR  | C7-C8-C9    | -2.21 | 122.89      | 126.23   |
| 24  | S     | 306 | CHL  | O1D-CGD-CBD | -2.21 | 119.96      | 124.48   |
| 28  | B     | 619 | BCR  | C15-C16-C17 | -2.21 | 118.94      | 123.47   |
| 28  | b     | 619 | BCR  | C15-C16-C17 | -2.21 | 118.94      | 123.47   |
| 24  | G     | 608 | CHL  | C2C-C3C-C4C | 2.21  | 108.07      | 106.49   |
| 40  | G     | 617 | NEX  | C32-C33-C34 | -2.21 | 115.55      | 118.94   |
| 25  | G     | 611 | CLA  | C11-C10-C8  | -2.21 | 108.77      | 115.92   |
| 25  | C     | 505 | CLA  | O2A-CGA-CBA | 2.21  | 118.85      | 111.91   |
| 28  | c     | 514 | BCR  | C15-C14-C13 | -2.21 | 124.15      | 127.31   |
| 29  | L     | 101 | SQD  | C1-C2-C3    | 2.21  | 114.60      | 110.00   |
| 32  | y     | 320 | AJP  | O84-C85-C02 | 2.21  | 115.37      | 112.18   |
| 40  | N     | 617 | NEX  | C5-C4-C3    | -2.21 | 109.13      | 111.75   |
| 39  | n     | 615 | LUT  | C1-C2-C3    | 2.21  | 118.63      | 113.64   |
| 25  | c     | 505 | CLA  | O2A-CGA-CBA | 2.21  | 118.84      | 111.91   |
| 40  | n     | 617 | NEX  | C17-C1-C6   | -2.21 | 108.50      | 110.47   |
| 25  | d     | 401 | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 25  | S     | 312 | CLA  | CHD-C1D-C2D | 2.21  | 130.11      | 125.48   |
| 25  | s     | 312 | CLA  | CHD-C1D-C2D | 2.21  | 130.11      | 125.48   |
| 25  | D     | 401 | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 25  | Y     | 312 | CLA  | C3D-C4D-ND  | 2.21  | 113.81      | 110.24   |
| 28  | D     | 404 | BCR  | C11-C10-C9  | -2.21 | 124.16      | 127.31   |
| 28  | d     | 404 | BCR  | C11-C10-C9  | -2.21 | 124.16      | 127.31   |
| 24  | g     | 607 | CHL  | C2A-C3A-C4A | 2.21  | 105.44      | 101.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | s     | 307 | CHL  | C4D-CHA-C1A | 2.21  | 123.94      | 121.25   |
| 24  | r     | 607 | CHL  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 24  | y     | 308 | CHL  | C2A-C3A-C4A | 2.21  | 105.43      | 101.87   |
| 28  | C     | 514 | BCR  | C8-C7-C6    | -2.21 | 121.01      | 127.20   |
| 32  | g     | 618 | AJP  | C83-C06-C05 | -2.21 | 110.89      | 114.92   |
| 25  | R     | 603 | CLA  | O2A-CGA-CBA | 2.21  | 118.83      | 111.91   |
| 32  | Y     | 324 | AJP  | C83-C06-C05 | -2.21 | 110.89      | 114.92   |
| 40  | n     | 617 | NEX  | C5-C4-C3    | -2.21 | 109.13      | 111.75   |
| 32  | Y     | 320 | AJP  | C24-C23-C22 | 2.20  | 113.34      | 111.00   |
| 32  | B     | 624 | AJP  | O60-C55-C56 | 2.20  | 115.02      | 110.35   |
| 32  | b     | 624 | AJP  | O60-C55-C56 | 2.20  | 115.02      | 110.35   |
| 24  | n     | 607 | CHL  | C2A-C1A-CHA | 2.20  | 127.71      | 123.86   |
| 25  | s     | 312 | CLA  | C3A-C2A-C1A | -2.20 | 98.04       | 101.34   |
| 32  | y     | 320 | AJP  | C24-C23-C22 | 2.20  | 113.34      | 111.00   |
| 25  | N     | 613 | CLA  | C6-C7-C8    | -2.20 | 108.80      | 115.92   |
| 24  | N     | 607 | CHL  | C2A-C1A-CHA | 2.20  | 127.71      | 123.86   |
| 24  | n     | 609 | CHL  | O1D-CGD-CBD | -2.20 | 119.98      | 124.48   |
| 24  | 6     | 601 | CHL  | OMC-CMC-C2C | -2.20 | 120.71      | 125.69   |
| 25  | 6     | 602 | CLA  | CAD-C3D-C2D | 2.20  | 151.42      | 140.80   |
| 25  | B     | 605 | CLA  | O2A-CGA-CBA | 2.20  | 118.81      | 111.91   |
| 25  | b     | 605 | CLA  | O2A-CGA-CBA | 2.20  | 118.81      | 111.91   |
| 25  | b     | 612 | CLA  | C2A-C1A-CHA | -2.20 | 120.01      | 123.86   |
| 28  | i     | 101 | BCR  | C7-C8-C9    | -2.20 | 122.91      | 126.23   |
| 39  | N     | 615 | LUT  | C1-C2-C3    | 2.20  | 118.61      | 113.64   |
| 25  | R     | 602 | CLA  | O2D-CGD-O1D | -2.20 | 119.54      | 123.84   |
| 24  | N     | 601 | CHL  | OMC-CMC-C2C | -2.20 | 120.72      | 125.69   |
| 25  | r     | 612 | CLA  | O2D-CGD-O1D | -2.20 | 119.54      | 123.84   |
| 24  | S     | 307 | CHL  | C4D-CHA-C1A | 2.20  | 123.92      | 121.25   |
| 24  | N     | 609 | CHL  | O1D-CGD-CBD | -2.20 | 119.99      | 124.48   |
| 25  | r     | 604 | CLA  | C4D-C3D-CAD | -2.19 | 105.51      | 108.10   |
| 25  | 2     | 602 | CLA  | CAD-C3D-C2D | 2.19  | 151.39      | 140.80   |
| 25  | S     | 312 | CLA  | C3A-C2A-C1A | -2.19 | 98.05       | 101.34   |
| 25  | r     | 610 | CLA  | CAD-C3D-C2D | 2.19  | 151.39      | 140.80   |
| 32  | Y     | 324 | AJP  | C04-C03-C02 | -2.19 | 107.18      | 111.81   |
| 24  | g     | 601 | CHL  | C2C-C3C-C4C | 2.19  | 108.05      | 106.49   |
| 28  | C     | 514 | BCR  | C2-C1-C6    | 2.19  | 113.86      | 110.48   |
| 24  | n     | 606 | CHL  | C4D-CHA-C1A | 2.19  | 123.92      | 121.25   |
| 25  | C     | 504 | CLA  | C6-C7-C8    | -2.19 | 108.83      | 115.92   |
| 24  | 2     | 601 | CHL  | C2C-C3C-C4C | 2.19  | 108.05      | 106.49   |
| 25  | G     | 602 | CLA  | C2C-C1C-NC  | 2.19  | 112.03      | 109.97   |
| 25  | g     | 602 | CLA  | C2C-C1C-NC  | 2.19  | 112.03      | 109.97   |
| 24  | 2     | 601 | CHL  | OMC-CMC-C2C | -2.19 | 120.73      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | y     | 324 | AJP  | C04-C03-C02 | -2.19 | 107.19      | 111.81   |
| 24  | R     | 607 | CHL  | C2C-C3C-C4C | 2.19  | 108.05      | 106.49   |
| 25  | R     | 610 | CLA  | CAD-C3D-C2D | 2.19  | 151.37      | 140.80   |
| 24  | n     | 606 | CHL  | C2A-C1A-CHA | 2.19  | 127.69      | 123.86   |
| 28  | c     | 514 | BCR  | C8-C7-C6    | -2.19 | 121.05      | 127.20   |
| 25  | r     | 612 | CLA  | C4D-CHA-C1A | -2.19 | 118.58      | 121.25   |
| 25  | Y     | 305 | CLA  | CHD-C1D-C2D | 2.19  | 130.07      | 125.48   |
| 25  | y     | 305 | CLA  | CHD-C1D-C2D | 2.19  | 130.07      | 125.48   |
| 28  | C     | 514 | BCR  | C15-C14-C13 | -2.19 | 124.19      | 127.31   |
| 24  | N     | 606 | CHL  | C2A-C1A-CHA | 2.19  | 127.69      | 123.86   |
| 25  | y     | 312 | CLA  | C3D-C4D-ND  | 2.19  | 113.78      | 110.24   |
| 28  | c     | 514 | BCR  | C2-C1-C6    | 2.19  | 113.85      | 110.48   |
| 28  | B     | 618 | BCR  | C38-C26-C25 | -2.19 | 122.07      | 124.53   |
| 28  | b     | 618 | BCR  | C38-C26-C25 | -2.19 | 122.07      | 124.53   |
| 25  | R     | 612 | CLA  | O2D-CGD-O1D | -2.19 | 119.56      | 123.84   |
| 25  | y     | 312 | CLA  | O2D-CGD-O1D | -2.19 | 119.56      | 123.84   |
| 25  | y     | 314 | CLA  | O2A-CGA-CBA | 2.19  | 118.77      | 111.91   |
| 25  | G     | 612 | CLA  | O1D-CGD-CBD | -2.18 | 120.01      | 124.48   |
| 25  | g     | 612 | CLA  | O1D-CGD-CBD | -2.18 | 120.01      | 124.48   |
| 25  | c     | 504 | CLA  | C6-C7-C8    | -2.18 | 108.86      | 115.92   |
| 24  | g     | 601 | CHL  | O2D-CGD-O1D | -2.18 | 119.57      | 123.84   |
| 25  | B     | 616 | CLA  | CHD-C1D-C2D | 2.18  | 130.06      | 125.48   |
| 25  | C     | 505 | CLA  | O2D-CGD-O1D | -2.18 | 119.57      | 123.84   |
| 25  | Y     | 305 | CLA  | C3D-C4D-ND  | 2.18  | 113.77      | 110.24   |
| 24  | n     | 601 | CHL  | OMC-CMC-C2C | -2.18 | 120.76      | 125.69   |
| 25  | S     | 303 | CLA  | C3D-C4D-ND  | 2.18  | 113.77      | 110.24   |
| 25  | g     | 612 | CLA  | C3D-C4D-ND  | 2.18  | 113.77      | 110.24   |
| 24  | Y     | 307 | CHL  | C1B-CHB-C4A | -2.18 | 125.80      | 130.12   |
| 25  | N     | 610 | CLA  | C1B-CHB-C4A | -2.18 | 125.80      | 130.12   |
| 25  | G     | 610 | CLA  | C1D-ND-C4D  | -2.18 | 104.79      | 106.33   |
| 25  | g     | 610 | CLA  | C1D-ND-C4D  | -2.18 | 104.79      | 106.33   |
| 24  | y     | 309 | CHL  | C2C-C3C-C4C | 2.18  | 108.04      | 106.49   |
| 25  | Y     | 314 | CLA  | O2A-CGA-CBA | 2.18  | 118.75      | 111.91   |
| 32  | G     | 618 | AJP  | C83-C06-C05 | -2.18 | 110.94      | 114.92   |
| 24  | N     | 606 | CHL  | O2D-CGD-O1D | -2.18 | 119.58      | 123.84   |
| 28  | K     | 101 | BCR  | C8-C7-C6    | -2.18 | 121.08      | 127.20   |
| 25  | G     | 603 | CLA  | C11-C10-C8  | -2.18 | 108.88      | 115.92   |
| 28  | B     | 619 | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |
| 28  | b     | 619 | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |
| 24  | Y     | 308 | CHL  | C2A-C3A-C4A | 2.18  | 105.39      | 101.87   |
| 28  | Z     | 101 | BCR  | C37-C22-C21 | -2.18 | 119.87      | 122.92   |
| 25  | C     | 511 | CLA  | O2A-CGA-CBA | 2.18  | 118.74      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | c     | 511 | CLA  | O2A-CGA-CBA | 2.18  | 118.74      | 111.91   |
| 25  | R     | 611 | CLA  | CHA-C4D-ND  | -2.18 | 127.94      | 132.50   |
| 25  | s     | 303 | CLA  | C3D-C4D-ND  | 2.18  | 113.76      | 110.24   |
| 28  | k     | 101 | BCR  | C8-C7-C6    | -2.18 | 121.09      | 127.20   |
| 25  | r     | 604 | CLA  | C2A-C1A-CHA | -2.18 | 120.06      | 123.86   |
| 24  | y     | 307 | CHL  | C1B-CHB-C4A | -2.17 | 125.81      | 130.12   |
| 24  | y     | 310 | CHL  | C2A-C3A-C4A | 2.17  | 105.38      | 101.87   |
| 24  | N     | 601 | CHL  | C2A-C1A-CHA | 2.17  | 127.66      | 123.86   |
| 25  | G     | 602 | CLA  | O2A-CGA-CBA | 2.17  | 118.73      | 111.91   |
| 25  | r     | 614 | CLA  | C2A-C1A-CHA | -2.17 | 120.06      | 123.86   |
| 24  | g     | 608 | CHL  | O1D-CGD-CBD | -2.17 | 120.04      | 124.48   |
| 39  | R     | 615 | LUT  | C22-C23-C24 | 2.17  | 114.21      | 111.74   |
| 39  | r     | 615 | LUT  | C22-C23-C24 | 2.17  | 114.21      | 111.74   |
| 25  | n     | 610 | CLA  | C1B-CHB-C4A | -2.17 | 125.81      | 130.12   |
| 25  | Y     | 312 | CLA  | C11-C10-C8  | -2.17 | 108.90      | 115.92   |
| 25  | y     | 312 | CLA  | C11-C10-C8  | -2.17 | 108.90      | 115.92   |
| 28  | z     | 101 | BCR  | C37-C22-C21 | -2.17 | 119.88      | 122.92   |
| 25  | G     | 612 | CLA  | C3D-C4D-ND  | 2.17  | 113.75      | 110.24   |
| 25  | c     | 505 | CLA  | O2D-CGD-O1D | -2.17 | 119.59      | 123.84   |
| 25  | R     | 604 | CLA  | C2A-C1A-CHA | -2.17 | 120.06      | 123.86   |
| 32  | N     | 619 | AJP  | C21-C20-C19 | 2.17  | 109.58      | 107.14   |
| 32  | n     | 619 | AJP  | C21-C20-C19 | 2.17  | 109.58      | 107.14   |
| 25  | B     | 604 | CLA  | O2A-CGA-CBA | 2.17  | 118.72      | 111.91   |
| 40  | s     | 317 | NEX  | C35-C15-C14 | -2.17 | 119.03      | 123.47   |
| 25  | g     | 602 | CLA  | O2A-CGA-CBA | 2.17  | 118.71      | 111.91   |
| 25  | A     | 401 | CLA  | C11-C10-C8  | -2.17 | 108.91      | 115.92   |
| 25  | a     | 402 | CLA  | C11-C10-C8  | -2.17 | 108.91      | 115.92   |
| 25  | b     | 616 | CLA  | CHD-C1D-C2D | 2.17  | 130.03      | 125.48   |
| 25  | 6     | 602 | CLA  | C6-C7-C8    | -2.17 | 108.91      | 115.92   |
| 25  | y     | 314 | CLA  | O2D-CGD-O1D | -2.17 | 119.60      | 123.84   |
| 25  | y     | 315 | CLA  | CHD-C1D-C2D | 2.17  | 130.02      | 125.48   |
| 25  | b     | 609 | CLA  | C3D-C4D-ND  | 2.17  | 113.74      | 110.24   |
| 24  | 6     | 601 | CHL  | C2C-C3C-C4C | 2.17  | 108.03      | 106.49   |
| 24  | G     | 608 | CHL  | O2D-CGD-O1D | -2.17 | 119.60      | 123.84   |
| 40  | N     | 617 | NEX  | C17-C1-C6   | -2.17 | 108.53      | 110.47   |
| 25  | b     | 604 | CLA  | O2A-CGA-CBA | 2.17  | 118.70      | 111.91   |
| 25  | s     | 305 | CLA  | CAD-C3D-C2D | 2.17  | 151.25      | 140.80   |
| 28  | Z     | 101 | BCR  | C8-C7-C6    | -2.17 | 121.12      | 127.20   |
| 24  | G     | 605 | CHL  | O2A-CGA-CBA | 2.16  | 120.98      | 114.03   |
| 24  | g     | 605 | CHL  | O2A-CGA-CBA | 2.16  | 120.98      | 114.03   |
| 25  | 2     | 604 | CLA  | CMB-C2B-C1B | -2.16 | 125.14      | 128.46   |
| 25  | 6     | 604 | CLA  | CMB-C2B-C1B | -2.16 | 125.14      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | N     | 606 | CHL  | C4D-CHA-C1A | 2.16  | 123.88      | 121.25   |
| 25  | 2     | 602 | CLA  | C6-C7-C8    | -2.16 | 108.93      | 115.92   |
| 25  | B     | 609 | CLA  | C3D-C4D-ND  | 2.16  | 113.74      | 110.24   |
| 25  | y     | 305 | CLA  | C3D-C4D-ND  | 2.16  | 113.74      | 110.24   |
| 24  | r     | 607 | CHL  | C2C-C3C-C4C | 2.16  | 108.03      | 106.49   |
| 25  | g     | 603 | CLA  | C11-C10-C8  | -2.16 | 108.93      | 115.92   |
| 24  | g     | 608 | CHL  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 25  | 2     | 602 | CLA  | C2C-C1C-NC  | -2.16 | 107.95      | 109.97   |
| 25  | 6     | 602 | CLA  | C2C-C1C-NC  | -2.16 | 107.95      | 109.97   |
| 25  | R     | 610 | CLA  | C3C-C4C-NC  | -2.16 | 108.15      | 110.57   |
| 25  | r     | 610 | CLA  | C3C-C4C-NC  | -2.16 | 108.15      | 110.57   |
| 25  | A     | 402 | CLA  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 25  | a     | 403 | CLA  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 24  | Y     | 308 | CHL  | O2A-CGA-O1A | -2.16 | 118.14      | 123.59   |
| 24  | y     | 308 | CHL  | O2A-CGA-O1A | -2.16 | 118.14      | 123.59   |
| 25  | r     | 611 | CLA  | CHA-C4D-ND  | -2.16 | 127.98      | 132.50   |
| 25  | S     | 305 | CLA  | CAD-C3D-C2D | 2.16  | 151.22      | 140.80   |
| 40  | S     | 317 | NEX  | C35-C15-C14 | -2.16 | 119.05      | 123.47   |
| 24  | N     | 609 | CHL  | C2C-C3C-C4C | 2.16  | 108.03      | 106.49   |
| 24  | n     | 609 | CHL  | C2C-C3C-C4C | 2.16  | 108.03      | 106.49   |
| 25  | c     | 506 | CLA  | C3D-C4D-ND  | 2.16  | 113.73      | 110.24   |
| 25  | N     | 613 | CLA  | O2D-CGD-O1D | -2.16 | 119.62      | 123.84   |
| 32  | y     | 320 | AJP  | C01-C02-C03 | 2.16  | 116.79      | 112.09   |
| 25  | r     | 601 | CLA  | CAD-C3D-C2D | 2.16  | 151.21      | 140.80   |
| 25  | Y     | 315 | CLA  | CHD-C1D-C2D | 2.16  | 130.01      | 125.48   |
| 24  | 6     | 603 | CHL  | C2C-C3C-C4C | 2.16  | 108.03      | 106.49   |
| 24  | G     | 607 | CHL  | C2A-C3A-C4A | 2.16  | 105.35      | 101.87   |
| 24  | Y     | 310 | CHL  | C2A-C3A-C4A | 2.16  | 105.35      | 101.87   |
| 25  | B     | 613 | CLA  | C6-C7-C8    | -2.16 | 108.95      | 115.92   |
| 25  | b     | 613 | CLA  | C6-C7-C8    | -2.16 | 108.95      | 115.92   |
| 32  | Y     | 320 | AJP  | C01-C02-C03 | 2.16  | 116.78      | 112.09   |
| 25  | Y     | 314 | CLA  | O2D-CGD-O1D | -2.16 | 119.62      | 123.84   |
| 25  | r     | 601 | CLA  | C3B-C4B-NB  | -2.16 | 106.42      | 109.21   |
| 25  | C     | 512 | CLA  | O2A-CGA-CBA | 2.16  | 118.67      | 111.91   |
| 25  | R     | 604 | CLA  | C4A-NA-C1A  | -2.16 | 105.74      | 106.71   |
| 25  | r     | 604 | CLA  | C4A-NA-C1A  | -2.16 | 105.74      | 106.71   |
| 25  | c     | 504 | CLA  | C3B-C4B-NB  | -2.15 | 106.42      | 109.21   |
| 25  | B     | 602 | CLA  | O2D-CGD-O1D | -2.15 | 119.63      | 123.84   |
| 25  | b     | 602 | CLA  | O2D-CGD-O1D | -2.15 | 119.63      | 123.84   |
| 25  | C     | 504 | CLA  | C3B-C4B-NB  | -2.15 | 106.42      | 109.21   |
| 25  | n     | 613 | CLA  | C2C-C1C-NC  | 2.15  | 111.99      | 109.97   |
| 25  | y     | 303 | CLA  | C1B-CHB-C4A | -2.15 | 125.85      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | Y     | 307 | CHL  | C2A-C3A-C4A | 2.15  | 105.35      | 101.87   |
| 24  | y     | 307 | CHL  | C2A-C3A-C4A | 2.15  | 105.35      | 101.87   |
| 24  | 2     | 603 | CHL  | C2C-C3C-C4C | 2.15  | 108.02      | 106.49   |
| 25  | c     | 512 | CLA  | O2A-CGA-CBA | 2.15  | 118.66      | 111.91   |
| 25  | R     | 601 | CLA  | CAD-C3D-C2D | 2.15  | 151.18      | 140.80   |
| 28  | z     | 101 | BCR  | C8-C7-C6    | -2.15 | 121.16      | 127.20   |
| 25  | b     | 602 | CLA  | C11-C10-C8  | -2.15 | 108.97      | 115.92   |
| 25  | R     | 608 | CLA  | CAA-CBA-CGA | -2.15 | 106.97      | 113.25   |
| 25  | C     | 502 | CLA  | CHD-C1D-C2D | 2.15  | 129.99      | 125.48   |
| 25  | c     | 502 | CLA  | CHD-C1D-C2D | 2.15  | 129.99      | 125.48   |
| 24  | s     | 308 | CHL  | C4D-CHA-C1A | 2.15  | 123.86      | 121.25   |
| 25  | C     | 509 | CLA  | O1D-CGD-CBD | -2.15 | 120.09      | 124.48   |
| 39  | n     | 615 | LUT  | C15-C35-C34 | -2.15 | 119.07      | 123.47   |
| 41  | r     | 616 | XAT  | C11-C12-C13 | -2.15 | 120.38      | 126.42   |
| 25  | B     | 612 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 25  | b     | 612 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 39  | N     | 615 | LUT  | C15-C35-C34 | -2.15 | 119.08      | 123.47   |
| 25  | G     | 611 | CLA  | C6-C7-C8    | -2.15 | 108.98      | 115.92   |
| 25  | R     | 604 | CLA  | C4D-C3D-CAD | -2.15 | 105.57      | 108.10   |
| 32  | A     | 412 | AJP  | C83-C06-C05 | -2.15 | 111.00      | 114.92   |
| 32  | a     | 413 | AJP  | C83-C06-C05 | -2.15 | 111.00      | 114.92   |
| 25  | N     | 602 | CLA  | C16-C15-C13 | -2.15 | 108.98      | 115.92   |
| 25  | R     | 614 | CLA  | C2A-C1A-CHA | -2.15 | 120.11      | 123.86   |
| 25  | c     | 513 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 25  | B     | 604 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 25  | b     | 604 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 25  | n     | 602 | CLA  | C16-C15-C13 | -2.14 | 108.99      | 115.92   |
| 24  | y     | 306 | CHL  | C4D-CHA-C1A | 2.14  | 123.86      | 121.25   |
| 24  | G     | 608 | CHL  | O1D-CGD-CBD | -2.14 | 120.10      | 124.48   |
| 24  | N     | 607 | CHL  | C1-C2-C3    | 2.14  | 129.75      | 126.04   |
| 24  | Y     | 308 | CHL  | C3C-C4C-NC  | -2.14 | 108.17      | 110.57   |
| 24  | S     | 306 | CHL  | C4D-CHA-C1A | 2.14  | 123.86      | 121.25   |
| 24  | s     | 306 | CHL  | C4D-CHA-C1A | 2.14  | 123.86      | 121.25   |
| 25  | Y     | 313 | CLA  | C2C-C1C-NC  | 2.14  | 111.98      | 109.97   |
| 25  | R     | 603 | CLA  | C3C-C4C-NC  | -2.14 | 108.17      | 110.57   |
| 24  | R     | 606 | CHL  | O2A-CGA-CBA | 2.14  | 120.91      | 114.03   |
| 25  | n     | 613 | CLA  | O2D-CGD-O1D | -2.14 | 119.65      | 123.84   |
| 25  | G     | 610 | CLA  | C2D-C1D-ND  | -2.14 | 108.53      | 110.10   |
| 25  | b     | 616 | CLA  | C3D-C4D-ND  | 2.14  | 113.70      | 110.24   |
| 25  | C     | 513 | CLA  | O2D-CGD-O1D | -2.14 | 119.66      | 123.84   |
| 41  | R     | 616 | XAT  | C11-C12-C13 | -2.14 | 120.41      | 126.42   |
| 32  | y     | 323 | AJP  | O84-C05-C06 | 2.14  | 114.88      | 107.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | g     | 611 | CLA  | C6-C7-C8    | -2.14 | 109.01      | 115.92   |
| 32  | a     | 413 | AJP  | C06-C07-C08 | -2.14 | 100.45      | 104.34   |
| 25  | Y     | 303 | CLA  | C1B-CHB-C4A | -2.14 | 125.88      | 130.12   |
| 24  | R     | 606 | CHL  | C2C-C3C-C4C | 2.14  | 108.01      | 106.49   |
| 24  | N     | 606 | CHL  | O2A-CGA-CBA | 2.14  | 120.89      | 114.03   |
| 25  | S     | 314 | CLA  | O2A-CGA-CBA | 2.14  | 118.61      | 111.91   |
| 25  | s     | 314 | CLA  | O2A-CGA-CBA | 2.14  | 118.61      | 111.91   |
| 40  | g     | 617 | NEX  | C10-C11-C12 | 2.14  | 129.88      | 123.22   |
| 25  | c     | 504 | CLA  | C3C-C4C-NC  | -2.13 | 108.18      | 110.57   |
| 25  | B     | 602 | CLA  | C11-C10-C8  | -2.13 | 109.02      | 115.92   |
| 25  | B     | 615 | CLA  | CHD-C1D-C2D | 2.13  | 129.96      | 125.48   |
| 25  | B     | 604 | CLA  | CBA-CAA-C2A | -2.13 | 107.57      | 113.86   |
| 25  | b     | 604 | CLA  | CBA-CAA-C2A | -2.13 | 107.57      | 113.86   |
| 24  | n     | 606 | CHL  | O2A-CGA-CBA | 2.13  | 120.88      | 114.03   |
| 25  | c     | 512 | CLA  | CBA-CAA-C2A | -2.13 | 107.57      | 113.86   |
| 24  | y     | 308 | CHL  | C3C-C4C-NC  | -2.13 | 108.18      | 110.57   |
| 25  | r     | 608 | CLA  | CAA-CBA-CGA | -2.13 | 107.02      | 113.25   |
| 24  | r     | 606 | CHL  | O2A-CGA-CBA | 2.13  | 120.88      | 114.03   |
| 25  | r     | 602 | CLA  | C3D-C4D-ND  | 2.13  | 113.69      | 110.24   |
| 25  | s     | 310 | CLA  | O1D-CGD-CBD | -2.13 | 120.12      | 124.48   |
| 25  | R     | 612 | CLA  | C4D-CHA-C1A | -2.13 | 118.65      | 121.25   |
| 25  | G     | 611 | CLA  | C2A-C1A-CHA | -2.13 | 120.13      | 123.86   |
| 25  | g     | 611 | CLA  | C2A-C1A-CHA | -2.13 | 120.13      | 123.86   |
| 25  | S     | 310 | CLA  | O1D-CGD-CBD | -2.13 | 120.12      | 124.48   |
| 25  | N     | 612 | CLA  | O1D-CGD-CBD | -2.13 | 120.12      | 124.48   |
| 32  | S     | 319 | AJP  | C06-C07-C08 | -2.13 | 100.47      | 104.34   |
| 32  | Y     | 323 | AJP  | O84-C05-C06 | 2.13  | 114.85      | 107.38   |
| 24  | g     | 601 | CHL  | O2A-CGA-O1A | -2.13 | 118.22      | 123.59   |
| 25  | R     | 603 | CLA  | CAD-C3D-C2D | 2.13  | 151.07      | 140.80   |
| 25  | r     | 603 | CLA  | CAD-C3D-C2D | 2.13  | 151.07      | 140.80   |
| 29  | l     | 101 | SQD  | O9-S-O7     | 2.13  | 121.32      | 113.95   |
| 24  | Y     | 302 | CHL  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 28  | B     | 619 | BCR  | C8-C7-C6    | -2.13 | 121.22      | 127.20   |
| 28  | b     | 619 | BCR  | C8-C7-C6    | -2.13 | 121.22      | 127.20   |
| 25  | B     | 603 | CLA  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 25  | b     | 603 | CLA  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 28  | z     | 101 | BCR  | C29-C30-C25 | 2.13  | 113.75      | 110.48   |
| 24  | S     | 302 | CHL  | C2C-C3C-C4C | 2.13  | 108.00      | 106.49   |
| 24  | s     | 302 | CHL  | C2C-C3C-C4C | 2.13  | 108.00      | 106.49   |
| 25  | B     | 614 | CLA  | O2D-CGD-O1D | -2.13 | 119.68      | 123.84   |
| 25  | b     | 614 | CLA  | O2D-CGD-O1D | -2.13 | 119.68      | 123.84   |
| 25  | C     | 511 | CLA  | C11-C12-C13 | -2.13 | 109.05      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | G     | 618 | AJP  | C85-O84-C05 | 2.13  | 117.75      | 113.72   |
| 25  | R     | 602 | CLA  | C3D-C4D-ND  | 2.13  | 113.68      | 110.24   |
| 24  | N     | 605 | CHL  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 25  | R     | 611 | CLA  | O2D-CGD-O1D | -2.13 | 119.68      | 123.84   |
| 25  | N     | 611 | CLA  | C3D-C4D-ND  | 2.12  | 113.67      | 110.24   |
| 25  | c     | 509 | CLA  | O1D-CGD-CBD | -2.12 | 120.14      | 124.48   |
| 25  | n     | 612 | CLA  | O1D-CGD-CBD | -2.12 | 120.14      | 124.48   |
| 25  | D     | 403 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 25  | d     | 403 | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 24  | g     | 607 | CHL  | O2A-CGA-O1A | -2.12 | 118.00      | 123.30   |
| 24  | G     | 601 | CHL  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 24  | y     | 302 | CHL  | O1D-CGD-CBD | -2.12 | 120.14      | 124.48   |
| 25  | C     | 508 | CLA  | C2A-C1A-CHA | -2.12 | 120.15      | 123.86   |
| 24  | s     | 307 | CHL  | O2A-CGA-CBA | 2.12  | 120.85      | 114.03   |
| 25  | G     | 602 | CLA  | C16-C15-C13 | -2.12 | 109.06      | 115.92   |
| 32  | A     | 412 | AJP  | C06-C07-C08 | -2.12 | 100.48      | 104.34   |
| 25  | y     | 311 | CLA  | C3D-C4D-ND  | 2.12  | 113.67      | 110.24   |
| 24  | n     | 606 | CHL  | O2D-CGD-O1D | -2.12 | 119.69      | 123.84   |
| 25  | c     | 511 | CLA  | C11-C12-C13 | -2.12 | 109.06      | 115.92   |
| 25  | n     | 613 | CLA  | C11-C10-C8  | -2.12 | 109.07      | 115.92   |
| 25  | c     | 508 | CLA  | C2A-C1A-CHA | -2.12 | 120.15      | 123.86   |
| 25  | r     | 602 | CLA  | O2A-CGA-CBA | 2.12  | 118.56      | 111.91   |
| 24  | 6     | 601 | CHL  | C2A-C3A-C4A | 2.12  | 105.29      | 101.87   |
| 24  | g     | 609 | CHL  | C2C-C3C-C4C | 2.12  | 108.00      | 106.49   |
| 25  | B     | 616 | CLA  | O2D-CGD-O1D | -2.12 | 119.69      | 123.84   |
| 25  | g     | 602 | CLA  | C16-C15-C13 | -2.12 | 109.07      | 115.92   |
| 25  | C     | 506 | CLA  | C3D-C4D-ND  | 2.12  | 113.67      | 110.24   |
| 25  | N     | 611 | CLA  | C6-C7-C8    | -2.12 | 109.07      | 115.92   |
| 25  | n     | 611 | CLA  | C6-C7-C8    | -2.12 | 109.07      | 115.92   |
| 24  | Y     | 306 | CHL  | C4D-CHA-C1A | 2.12  | 123.83      | 121.25   |
| 29  | L     | 103 | SQD  | O9-S-O7     | 2.12  | 121.28      | 113.95   |
| 28  | c     | 514 | BCR  | C24-C23-C22 | -2.12 | 123.03      | 126.23   |
| 24  | S     | 308 | CHL  | C4D-CHA-C1A | 2.12  | 123.83      | 121.25   |
| 25  | g     | 610 | CLA  | C2D-C1D-ND  | -2.12 | 108.54      | 110.10   |
| 25  | R     | 601 | CLA  | C3B-C4B-NB  | -2.12 | 106.47      | 109.21   |
| 24  | S     | 307 | CHL  | O2A-CGA-CBA | 2.12  | 120.83      | 114.03   |
| 40  | G     | 617 | NEX  | C15-C35-C34 | -2.12 | 119.14      | 123.47   |
| 29  | l     | 102 | SQD  | O9-S-O7     | 2.12  | 121.28      | 113.95   |
| 25  | C     | 512 | CLA  | CBA-CAA-C2A | -2.12 | 107.61      | 113.86   |
| 25  | G     | 611 | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.33   |
| 28  | D     | 404 | BCR  | C29-C30-C25 | 2.12  | 113.74      | 110.48   |
| 28  | d     | 404 | BCR  | C29-C30-C25 | 2.12  | 113.74      | 110.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 504 | CLA  | C3C-C4C-NC  | -2.12 | 108.20      | 110.57   |
| 29  | A     | 411 | SQD  | O9-S-O7     | 2.12  | 121.27      | 113.95   |
| 29  | a     | 412 | SQD  | O9-S-O7     | 2.12  | 121.27      | 113.95   |
| 24  | Y     | 306 | CHL  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 25  | r     | 602 | CLA  | CAA-CBA-CGA | -2.12 | 107.07      | 113.25   |
| 25  | G     | 602 | CLA  | CHD-C4C-C3C | -2.12 | 121.73      | 124.84   |
| 32  | g     | 618 | AJP  | C85-O84-C05 | 2.12  | 117.73      | 113.72   |
| 25  | R     | 609 | CLA  | CAA-CBA-CGA | -2.11 | 107.07      | 113.25   |
| 25  | b     | 616 | CLA  | O2D-CGD-O1D | -2.11 | 119.70      | 123.84   |
| 25  | r     | 611 | CLA  | O2D-CGD-O1D | -2.11 | 119.70      | 123.84   |
| 25  | Y     | 311 | CLA  | C1B-CHB-C4A | -2.11 | 125.93      | 130.12   |
| 40  | g     | 617 | NEX  | C15-C35-C34 | -2.11 | 119.14      | 123.47   |
| 40  | y     | 318 | NEX  | C11-C12-C13 | -2.11 | 120.48      | 126.42   |
| 32  | B     | 624 | AJP  | O09-C08-C07 | 2.11  | 109.13      | 104.06   |
| 32  | b     | 624 | AJP  | O09-C08-C07 | 2.11  | 109.13      | 104.06   |
| 25  | N     | 613 | CLA  | C2C-C1C-NC  | 2.11  | 111.95      | 109.97   |
| 25  | y     | 313 | CLA  | C2C-C1C-NC  | 2.11  | 111.95      | 109.97   |
| 25  | g     | 611 | CLA  | O2D-CGD-O1D | -2.11 | 119.71      | 123.84   |
| 25  | G     | 611 | CLA  | C4D-C3D-CAD | -2.11 | 105.61      | 108.10   |
| 25  | g     | 611 | CLA  | C4D-C3D-CAD | -2.11 | 105.61      | 108.10   |
| 25  | N     | 611 | CLA  | C4D-CHA-C1A | -2.11 | 118.68      | 121.25   |
| 25  | n     | 611 | CLA  | C4D-CHA-C1A | -2.11 | 118.68      | 121.25   |
| 25  | Y     | 312 | CLA  | C2C-C1C-NC  | 2.11  | 111.95      | 109.97   |
| 25  | y     | 312 | CLA  | C2C-C1C-NC  | 2.11  | 111.95      | 109.97   |
| 25  | C     | 506 | CLA  | C11-C12-C13 | -2.11 | 109.09      | 115.92   |
| 25  | c     | 506 | CLA  | C11-C12-C13 | -2.11 | 109.09      | 115.92   |
| 25  | r     | 612 | CLA  | C2A-C3A-C4A | -2.11 | 98.46       | 101.87   |
| 25  | R     | 612 | CLA  | C11-C10-C8  | -2.11 | 109.09      | 115.92   |
| 25  | b     | 615 | CLA  | CHD-C1D-C2D | 2.11  | 129.91      | 125.48   |
| 28  | h     | 101 | BCR  | C16-C15-C14 | -2.11 | 119.15      | 123.47   |
| 32  | s     | 319 | AJP  | C06-C07-C08 | -2.11 | 100.50      | 104.34   |
| 24  | 5     | 301 | CHL  | O2D-CGD-O1D | -2.11 | 119.71      | 123.84   |
| 25  | D     | 403 | CLA  | CAA-CBA-CGA | -2.11 | 107.09      | 113.25   |
| 25  | d     | 403 | CLA  | CAA-CBA-CGA | -2.11 | 107.09      | 113.25   |
| 28  | C     | 514 | BCR  | C24-C23-C22 | -2.11 | 123.05      | 126.23   |
| 29  | L     | 101 | SQD  | O9-S-O7     | 2.11  | 121.25      | 113.95   |
| 24  | 2     | 601 | CHL  | C2A-C3A-C4A | 2.11  | 105.28      | 101.87   |
| 25  | R     | 610 | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 25  | r     | 610 | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 25  | B     | 604 | CLA  | C16-C15-C13 | -2.11 | 109.11      | 115.92   |
| 25  | b     | 604 | CLA  | C16-C15-C13 | -2.11 | 109.11      | 115.92   |
| 40  | Y     | 318 | NEX  | C11-C12-C13 | -2.11 | 120.49      | 126.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | R     | 602 | CLA  | CAA-CBA-CGA | -2.11 | 107.09      | 113.25   |
| 25  | N     | 610 | CLA  | O2D-CGD-O1D | -2.11 | 119.72      | 123.84   |
| 25  | n     | 610 | CLA  | O2D-CGD-O1D | -2.11 | 119.72      | 123.84   |
| 25  | R     | 612 | CLA  | C2A-C3A-C4A | -2.11 | 98.47       | 101.87   |
| 24  | g     | 605 | CHL  | C2C-C3C-C4C | 2.11  | 107.99      | 106.49   |
| 25  | Y     | 303 | CLA  | C3D-C4D-ND  | 2.11  | 113.65      | 110.24   |
| 25  | d     | 403 | CLA  | CAD-C3D-C2D | 2.11  | 150.97      | 140.80   |
| 25  | N     | 613 | CLA  | CBA-CAA-C2A | -2.11 | 107.64      | 113.86   |
| 25  | c     | 507 | CLA  | O2D-CGD-O1D | -2.11 | 119.72      | 123.84   |
| 24  | l     | 301 | CHL  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 39  | s     | 316 | LUT  | C12-C13-C14 | -2.11 | 115.71      | 118.94   |
| 24  | G     | 607 | CHL  | O2A-CGA-O1A | -2.11 | 118.05      | 123.30   |
| 24  | g     | 608 | CHL  | C2C-C3C-C4C | 2.11  | 107.99      | 106.49   |
| 24  | n     | 605 | CHL  | O1D-CGD-CBD | -2.11 | 120.18      | 124.48   |
| 25  | c     | 504 | CLA  | O2A-CGA-CBA | 2.10  | 118.51      | 111.91   |
| 24  | n     | 607 | CHL  | C1-C2-C3    | 2.10  | 129.68      | 126.04   |
| 25  | R     | 602 | CLA  | O2A-CGA-CBA | 2.10  | 118.51      | 111.91   |
| 25  | a     | 406 | CLA  | O1D-CGD-CBD | -2.10 | 120.18      | 124.48   |
| 25  | c     | 510 | CLA  | C11-C10-C8  | -2.10 | 109.12      | 115.92   |
| 24  | S     | 308 | CHL  | O2A-CGA-CBA | 2.10  | 120.79      | 114.03   |
| 24  | Y     | 309 | CHL  | O1D-CGD-CBD | -2.10 | 120.18      | 124.48   |
| 28  | Z     | 101 | BCR  | C29-C30-C25 | 2.10  | 113.72      | 110.48   |
| 24  | s     | 308 | CHL  | O2A-CGA-CBA | 2.10  | 120.78      | 114.03   |
| 25  | C     | 510 | CLA  | C11-C10-C8  | -2.10 | 109.12      | 115.92   |
| 25  | N     | 602 | CLA  | C2C-C1C-NC  | 2.10  | 111.94      | 109.97   |
| 25  | n     | 602 | CLA  | C2C-C1C-NC  | 2.10  | 111.94      | 109.97   |
| 24  | N     | 605 | CHL  | C2C-C3C-C4C | 2.10  | 107.99      | 106.49   |
| 24  | n     | 605 | CHL  | C2C-C3C-C4C | 2.10  | 107.99      | 106.49   |
| 39  | N     | 615 | LUT  | C7-C8-C9    | 2.10  | 129.41      | 126.23   |
| 25  | G     | 614 | CLA  | C4D-CHA-C1A | -2.10 | 118.69      | 121.25   |
| 25  | g     | 614 | CLA  | C4D-CHA-C1A | -2.10 | 118.69      | 121.25   |
| 25  | N     | 613 | CLA  | C11-C10-C8  | -2.10 | 109.13      | 115.92   |
| 25  | n     | 602 | CLA  | C11-C12-C13 | -2.10 | 109.13      | 115.92   |
| 25  | y     | 303 | CLA  | C3D-C4D-ND  | 2.10  | 113.64      | 110.24   |
| 25  | G     | 614 | CLA  | C2A-C1A-CHA | -2.10 | 120.19      | 123.86   |
| 25  | G     | 611 | CLA  | O2A-CGA-CBA | 2.10  | 118.50      | 111.91   |
| 24  | 2     | 603 | CHL  | C3D-C4D-ND  | 2.10  | 113.64      | 110.24   |
| 25  | D     | 403 | CLA  | CAD-C3D-C2D | 2.10  | 150.93      | 140.80   |
| 25  | A     | 405 | CLA  | O1D-CGD-CBD | -2.10 | 120.19      | 124.48   |
| 25  | c     | 513 | CLA  | C6-C7-C8    | -2.10 | 109.13      | 115.92   |
| 25  | g     | 611 | CLA  | O2A-CGA-CBA | 2.10  | 118.50      | 111.91   |
| 25  | b     | 603 | CLA  | C3D-C4D-ND  | 2.10  | 113.63      | 110.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | y     | 309 | CHL  | O1D-CGD-CBD | -2.10 | 120.19      | 124.48   |
| 25  | Y     | 304 | CLA  | C16-C15-C13 | -2.10 | 109.13      | 115.92   |
| 24  | 2     | 603 | CHL  | O2A-CGA-CBA | 2.10  | 120.77      | 114.03   |
| 28  | H     | 101 | BCR  | C16-C15-C14 | -2.10 | 119.17      | 123.47   |
| 25  | C     | 504 | CLA  | O2A-CGA-CBA | 2.10  | 118.50      | 111.91   |
| 25  | c     | 511 | CLA  | C6-C7-C8    | -2.10 | 109.14      | 115.92   |
| 24  | Y     | 309 | CHL  | C2C-C3C-C4C | 2.10  | 107.98      | 106.49   |
| 25  | r     | 612 | CLA  | C11-C10-C8  | -2.10 | 109.14      | 115.92   |
| 25  | N     | 602 | CLA  | C11-C12-C13 | -2.10 | 109.14      | 115.92   |
| 25  | n     | 611 | CLA  | C3D-C4D-ND  | 2.10  | 113.63      | 110.24   |
| 28  | K     | 101 | BCR  | C11-C10-C9  | -2.10 | 124.32      | 127.31   |
| 24  | 6     | 603 | CHL  | O2A-CGA-CBA | 2.10  | 120.77      | 114.03   |
| 25  | r     | 609 | CLA  | CAA-CBA-CGA | -2.10 | 107.13      | 113.25   |
| 25  | C     | 511 | CLA  | C6-C7-C8    | -2.10 | 109.14      | 115.92   |
| 24  | G     | 607 | CHL  | C2C-C3C-C4C | 2.10  | 107.98      | 106.49   |
| 25  | C     | 513 | CLA  | C6-C7-C8    | -2.10 | 109.14      | 115.92   |
| 25  | g     | 614 | CLA  | C2A-C1A-CHA | -2.09 | 120.20      | 123.86   |
| 25  | y     | 311 | CLA  | C1B-CHB-C4A | -2.09 | 125.97      | 130.12   |
| 39  | S     | 316 | LUT  | C12-C13-C14 | -2.09 | 115.73      | 118.94   |
| 24  | y     | 306 | CHL  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 24  | 1     | 301 | CHL  | O2D-CGD-O1D | -2.09 | 119.74      | 123.84   |
| 24  | 5     | 301 | CHL  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 24  | 1     | 301 | CHL  | C2A-C1A-CHA | 2.09  | 127.52      | 123.86   |
| 39  | n     | 615 | LUT  | C7-C8-C9    | 2.09  | 129.40      | 126.23   |
| 25  | g     | 611 | CLA  | C1D-ND-C4D  | -2.09 | 104.85      | 106.33   |
| 25  | n     | 613 | CLA  | CBA-CAA-C2A | -2.09 | 107.69      | 113.86   |
| 25  | C     | 501 | CLA  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 25  | c     | 501 | CLA  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 39  | S     | 315 | LUT  | C37-C21-C22 | -2.09 | 105.47      | 109.44   |
| 39  | s     | 315 | LUT  | C37-C21-C22 | -2.09 | 105.47      | 109.44   |
| 24  | 6     | 603 | CHL  | C3D-C4D-ND  | 2.09  | 113.62      | 110.24   |
| 28  | B     | 619 | BCR  | C15-C14-C13 | -2.09 | 124.33      | 127.31   |
| 28  | b     | 619 | BCR  | C15-C14-C13 | -2.09 | 124.33      | 127.31   |
| 25  | c     | 512 | CLA  | C11-C12-C13 | -2.09 | 109.16      | 115.92   |
| 28  | H     | 101 | BCR  | C8-C7-C6    | -2.09 | 121.33      | 127.20   |
| 28  | h     | 101 | BCR  | C8-C7-C6    | -2.09 | 121.33      | 127.20   |
| 25  | C     | 507 | CLA  | O2D-CGD-O1D | -2.09 | 119.75      | 123.84   |
| 24  | R     | 613 | CHL  | C2C-C3C-C4C | 2.09  | 107.98      | 106.49   |
| 26  | c     | 519 | LHG  | P-O6-C4     | -2.09 | 109.42      | 121.68   |
| 25  | S     | 304 | CLA  | O2D-CGD-O1D | -2.09 | 119.75      | 123.84   |
| 25  | y     | 304 | CLA  | C16-C15-C13 | -2.09 | 109.17      | 115.92   |
| 26  | C     | 519 | LHG  | P-O6-C4     | -2.09 | 109.43      | 121.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | y     | 306 | CHL  | C2C-C3C-C4C | 2.09  | 107.98      | 106.49   |
| 25  | Y     | 304 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | y     | 304 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | r     | 603 | CLA  | C3C-C4C-NC  | -2.09 | 108.23      | 110.57   |
| 25  | B     | 607 | CLA  | O2A-CGA-CBA | 2.09  | 118.46      | 111.91   |
| 25  | b     | 607 | CLA  | O2A-CGA-CBA | 2.09  | 118.46      | 111.91   |
| 25  | C     | 504 | CLA  | CAD-C3D-C2D | 2.09  | 150.87      | 140.80   |
| 25  | B     | 616 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | N     | 603 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | n     | 603 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | D     | 402 | CLA  | C16-C15-C13 | -2.09 | 109.17      | 115.92   |
| 25  | d     | 402 | CLA  | C16-C15-C13 | -2.09 | 109.17      | 115.92   |
| 24  | S     | 306 | CHL  | O2A-CGA-O1A | -2.09 | 118.10      | 123.30   |
| 25  | Y     | 313 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 24  | G     | 609 | CHL  | C2C-C3C-C4C | 2.09  | 107.98      | 106.49   |
| 25  | C     | 512 | CLA  | C11-C12-C13 | -2.09 | 109.18      | 115.92   |
| 25  | G     | 611 | CLA  | O2D-CGD-O1D | -2.09 | 119.76      | 123.84   |
| 24  | R     | 607 | CHL  | O2A-CGA-O1A | -2.09 | 118.33      | 123.59   |
| 25  | Y     | 311 | CLA  | C3D-C4D-ND  | 2.09  | 113.61      | 110.24   |
| 25  | c     | 504 | CLA  | CAD-C3D-C2D | 2.09  | 150.86      | 140.80   |
| 25  | s     | 304 | CLA  | O2D-CGD-O1D | -2.08 | 119.76      | 123.84   |
| 24  | S     | 308 | CHL  | C2C-C3C-C4C | 2.08  | 107.97      | 106.49   |
| 25  | b     | 601 | CLA  | C1D-CHD-C4C | -2.08 | 121.56      | 126.06   |
| 25  | B     | 603 | CLA  | C3D-C4D-ND  | 2.08  | 113.61      | 110.24   |
| 25  | R     | 609 | CLA  | C11-C12-C13 | -2.08 | 109.19      | 115.92   |
| 25  | c     | 508 | CLA  | C16-C15-C13 | -2.08 | 109.19      | 115.92   |
| 32  | B     | 624 | AJP  | C24-C19-C20 | 2.08  | 114.87      | 112.66   |
| 32  | b     | 624 | AJP  | C24-C19-C20 | 2.08  | 114.87      | 112.66   |
| 25  | C     | 503 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 25  | c     | 503 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 25  | B     | 607 | CLA  | C1B-CHB-C4A | -2.08 | 125.99      | 130.12   |
| 25  | B     | 606 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 25  | b     | 606 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 25  | S     | 303 | CLA  | O2A-CGA-CBA | 2.08  | 118.44      | 111.91   |
| 25  | s     | 303 | CLA  | O2A-CGA-CBA | 2.08  | 118.44      | 111.91   |
| 25  | n     | 611 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 25  | d     | 403 | CLA  | C6-C7-C8    | -2.08 | 109.19      | 115.92   |
| 25  | y     | 313 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 24  | r     | 606 | CHL  | C2C-C3C-C4C | 2.08  | 107.97      | 106.49   |
| 25  | R     | 602 | CLA  | C11-C10-C8  | -2.08 | 109.19      | 115.92   |
| 24  | r     | 605 | CHL  | C4D-CHA-C1A | 2.08  | 123.78      | 121.25   |
| 24  | s     | 306 | CHL  | O2A-CGA-O1A | -2.08 | 118.12      | 123.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | r     | 609 | CLA  | C11-C12-C13 | -2.08 | 109.20      | 115.92   |
| 25  | Y     | 313 | CLA  | C1B-CHB-C4A | -2.08 | 126.00      | 130.12   |
| 25  | B     | 608 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 25  | b     | 608 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 25  | B     | 601 | CLA  | C1D-CHD-C4C | -2.08 | 121.57      | 126.06   |
| 25  | n     | 604 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 25  | A     | 405 | CLA  | C6-C7-C8    | -2.08 | 109.20      | 115.92   |
| 25  | g     | 602 | CLA  | CHD-C4C-C3C | -2.08 | 121.79      | 124.84   |
| 24  | r     | 607 | CHL  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 28  | B     | 618 | BCR  | C29-C30-C25 | 2.08  | 113.68      | 110.48   |
| 28  | b     | 618 | BCR  | C29-C30-C25 | 2.08  | 113.68      | 110.48   |
| 25  | D     | 403 | CLA  | C3C-C4C-NC  | -2.08 | 108.24      | 110.57   |
| 25  | d     | 403 | CLA  | C3C-C4C-NC  | -2.08 | 108.24      | 110.57   |
| 25  | C     | 508 | CLA  | C16-C15-C13 | -2.08 | 109.21      | 115.92   |
| 24  | r     | 613 | CHL  | C2C-C3C-C4C | 2.08  | 107.97      | 106.49   |
| 25  | N     | 611 | CLA  | C11-C10-C8  | -2.08 | 109.21      | 115.92   |
| 25  | N     | 610 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 25  | n     | 610 | CLA  | C3D-C4D-ND  | 2.08  | 113.60      | 110.24   |
| 25  | B     | 609 | CLA  | C11-C12-C13 | -2.08 | 109.21      | 115.92   |
| 25  | b     | 609 | CLA  | C11-C12-C13 | -2.08 | 109.21      | 115.92   |
| 24  | g     | 607 | CHL  | C2C-C3C-C4C | 2.07  | 107.97      | 106.49   |
| 24  | R     | 605 | CHL  | O1D-CGD-CBD | -2.07 | 120.24      | 124.48   |
| 24  | r     | 605 | CHL  | O1D-CGD-CBD | -2.07 | 120.24      | 124.48   |
| 28  | k     | 101 | BCR  | C11-C10-C9  | -2.07 | 124.35      | 127.31   |
| 25  | B     | 609 | CLA  | C16-C15-C13 | -2.07 | 109.22      | 115.92   |
| 25  | b     | 609 | CLA  | C16-C15-C13 | -2.07 | 109.22      | 115.92   |
| 28  | C     | 514 | BCR  | C27-C26-C25 | 2.07  | 125.74      | 122.73   |
| 28  | c     | 514 | BCR  | C27-C26-C25 | 2.07  | 125.74      | 122.73   |
| 25  | 6     | 602 | CLA  | CMB-C2B-C1B | -2.07 | 125.28      | 128.46   |
| 25  | a     | 406 | CLA  | C6-C7-C8    | -2.07 | 109.22      | 115.92   |
| 24  | S     | 302 | CHL  | O2A-CGA-CBA | 2.07  | 120.69      | 114.03   |
| 24  | s     | 302 | CHL  | O2A-CGA-CBA | 2.07  | 120.69      | 114.03   |
| 29  | A     | 407 | SQD  | O9-S-C6     | 2.07  | 109.40      | 106.94   |
| 29  | a     | 408 | SQD  | O9-S-C6     | 2.07  | 109.40      | 106.94   |
| 32  | Y     | 324 | AJP  | C85-O84-C05 | 2.07  | 117.64      | 113.72   |
| 32  | y     | 324 | AJP  | C85-O84-C05 | 2.07  | 117.64      | 113.72   |
| 25  | y     | 312 | CLA  | CAD-C3D-C2D | 2.07  | 150.79      | 140.80   |
| 25  | a     | 403 | CLA  | C6-C7-C8    | -2.07 | 109.23      | 115.92   |
| 25  | S     | 314 | CLA  | C1B-CHB-C4A | -2.07 | 126.02      | 130.12   |
| 25  | B     | 603 | CLA  | C6-C7-C8    | -2.07 | 109.23      | 115.92   |
| 25  | b     | 603 | CLA  | C6-C7-C8    | -2.07 | 109.23      | 115.92   |
| 25  | c     | 501 | CLA  | C6-C7-C8    | -2.07 | 109.23      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | D     | 403 | CLA  | C6-C7-C8    | -2.07 | 109.23      | 115.92   |
| 25  | 6     | 602 | CLA  | C3B-C4B-NB  | -2.07 | 106.54      | 109.21   |
| 28  | T     | 101 | BCR  | C24-C23-C22 | -2.07 | 123.11      | 126.23   |
| 28  | t     | 101 | BCR  | C24-C23-C22 | -2.07 | 123.11      | 126.23   |
| 25  | r     | 602 | CLA  | C11-C10-C8  | -2.07 | 109.24      | 115.92   |
| 24  | R     | 605 | CHL  | O2A-CGA-O1A | -2.07 | 118.15      | 123.30   |
| 24  | r     | 605 | CHL  | O2A-CGA-O1A | -2.07 | 118.15      | 123.30   |
| 25  | s     | 313 | CLA  | CAD-C3D-C2D | 2.07  | 150.77      | 140.80   |
| 40  | n     | 617 | NEX  | C11-C10-C9  | 2.07  | 130.26      | 127.31   |
| 25  | y     | 313 | CLA  | C1B-CHB-C4A | -2.07 | 126.03      | 130.12   |
| 24  | y     | 302 | CHL  | O2D-CGD-O1D | -2.07 | 119.80      | 123.84   |
| 24  | R     | 605 | CHL  | O2A-CGA-CBA | 2.06  | 120.66      | 114.03   |
| 24  | r     | 605 | CHL  | O2A-CGA-CBA | 2.06  | 120.66      | 114.03   |
| 25  | b     | 607 | CLA  | C1B-CHB-C4A | -2.06 | 126.03      | 130.12   |
| 24  | 1     | 301 | CHL  | C4D-CHA-C1A | 2.06  | 123.76      | 121.25   |
| 25  | A     | 402 | CLA  | C6-C7-C8    | -2.06 | 109.25      | 115.92   |
| 25  | Y     | 312 | CLA  | CAD-C3D-C2D | 2.06  | 150.75      | 140.80   |
| 25  | R     | 608 | CLA  | C2A-C1A-CHA | -2.06 | 120.25      | 123.86   |
| 25  | s     | 313 | CLA  | C4D-CHA-C1A | -2.06 | 118.74      | 121.25   |
| 25  | B     | 609 | CLA  | C11-C10-C8  | -2.06 | 109.25      | 115.92   |
| 25  | C     | 501 | CLA  | C6-C7-C8    | -2.06 | 109.25      | 115.92   |
| 25  | b     | 612 | CLA  | C11-C10-C8  | -2.06 | 109.25      | 115.92   |
| 24  | Y     | 302 | CHL  | O2D-CGD-O1D | -2.06 | 119.81      | 123.84   |
| 25  | 2     | 602 | CLA  | CMB-C2B-C1B | -2.06 | 125.30      | 128.46   |
| 25  | c     | 501 | CLA  | CAD-C3D-C2D | 2.06  | 150.74      | 140.80   |
| 25  | B     | 612 | CLA  | C11-C10-C8  | -2.06 | 109.26      | 115.92   |
| 25  | C     | 505 | CLA  | CMB-C2B-C1B | -2.06 | 125.30      | 128.46   |
| 25  | g     | 612 | CLA  | CHD-C1D-C2D | 2.06  | 129.80      | 125.48   |
| 24  | 5     | 301 | CHL  | C2A-C1A-CHA | 2.06  | 127.46      | 123.86   |
| 25  | G     | 612 | CLA  | CHD-C1D-C2D | 2.06  | 129.80      | 125.48   |
| 25  | c     | 513 | CLA  | CAA-CBA-CGA | -2.06 | 107.24      | 113.25   |
| 24  | R     | 605 | CHL  | C2C-C3C-C4C | 2.06  | 107.96      | 106.49   |
| 24  | s     | 308 | CHL  | C2C-C3C-C4C | 2.06  | 107.96      | 106.49   |
| 25  | B     | 615 | CLA  | C11-C12-C13 | -2.06 | 109.27      | 115.92   |
| 25  | b     | 615 | CLA  | C11-C12-C13 | -2.06 | 109.27      | 115.92   |
| 25  | B     | 614 | CLA  | C3D-C4D-ND  | 2.06  | 113.57      | 110.24   |
| 25  | b     | 614 | CLA  | C3D-C4D-ND  | 2.06  | 113.57      | 110.24   |
| 25  | y     | 315 | CLA  | C3D-C4D-ND  | 2.06  | 113.57      | 110.24   |
| 25  | C     | 511 | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 25  | c     | 511 | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 25  | B     | 603 | CLA  | C4D-CHA-C1A | -2.06 | 118.75      | 121.25   |
| 25  | b     | 603 | CLA  | C4D-CHA-C1A | -2.06 | 118.75      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 513 | CLA  | CAA-CBA-CGA | -2.06 | 107.24      | 113.25   |
| 25  | B     | 602 | CLA  | C11-C12-C13 | -2.06 | 109.27      | 115.92   |
| 25  | B     | 612 | CLA  | C16-C15-C13 | -2.06 | 109.27      | 115.92   |
| 25  | b     | 612 | CLA  | C16-C15-C13 | -2.06 | 109.27      | 115.92   |
| 25  | g     | 613 | CLA  | C11-C10-C8  | -2.06 | 109.27      | 115.92   |
| 25  | S     | 313 | CLA  | C4D-CHA-C1A | -2.06 | 118.75      | 121.25   |
| 25  | B     | 601 | CLA  | C1D-ND-C4D  | -2.06 | 104.87      | 106.33   |
| 25  | b     | 601 | CLA  | C1D-ND-C4D  | -2.06 | 104.87      | 106.33   |
| 25  | g     | 604 | CLA  | C3D-C4D-ND  | 2.06  | 113.56      | 110.24   |
| 40  | G     | 617 | NEX  | C35-C15-C14 | -2.06 | 119.26      | 123.47   |
| 25  | G     | 613 | CLA  | C11-C10-C8  | -2.06 | 109.28      | 115.92   |
| 25  | C     | 501 | CLA  | CAD-C3D-C2D | 2.05  | 150.71      | 140.80   |
| 40  | g     | 617 | NEX  | C12-C13-C14 | -2.05 | 115.79      | 118.94   |
| 25  | C     | 508 | CLA  | C6-C7-C8    | -2.05 | 109.28      | 115.92   |
| 25  | A     | 405 | CLA  | O2D-CGD-O1D | -2.05 | 119.82      | 123.84   |
| 25  | a     | 406 | CLA  | O2D-CGD-O1D | -2.05 | 119.82      | 123.84   |
| 24  | G     | 605 | CHL  | C2C-C3C-C4C | 2.05  | 107.95      | 106.49   |
| 25  | S     | 313 | CLA  | CAD-C3D-C2D | 2.05  | 150.70      | 140.80   |
| 24  | n     | 606 | CHL  | O1D-CGD-CBD | -2.05 | 120.29      | 124.48   |
| 24  | R     | 605 | CHL  | C4D-CHA-C1A | 2.05  | 123.75      | 121.25   |
| 24  | 5     | 301 | CHL  | C4D-CHA-C1A | 2.05  | 123.75      | 121.25   |
| 25  | c     | 502 | CLA  | C2C-C1C-NC  | 2.05  | 111.89      | 109.97   |
| 25  | 2     | 602 | CLA  | C3B-C4B-NB  | -2.05 | 106.56      | 109.21   |
| 32  | B     | 624 | AJP  | C15-C20-C19 | -2.05 | 105.70      | 108.58   |
| 32  | b     | 624 | AJP  | C15-C20-C19 | -2.05 | 105.70      | 108.58   |
| 25  | b     | 602 | CLA  | C11-C12-C13 | -2.05 | 109.30      | 115.92   |
| 25  | N     | 604 | CLA  | C3D-C4D-ND  | 2.05  | 113.55      | 110.24   |
| 24  | g     | 609 | CHL  | O1D-CGD-CBD | -2.05 | 120.29      | 124.48   |
| 25  | b     | 609 | CLA  | C11-C10-C8  | -2.05 | 109.30      | 115.92   |
| 40  | N     | 617 | NEX  | C11-C10-C9  | 2.05  | 130.23      | 127.31   |
| 40  | y     | 318 | NEX  | C31-C32-C33 | 2.05  | 132.17      | 126.42   |
| 25  | c     | 508 | CLA  | C6-C7-C8    | -2.05 | 109.30      | 115.92   |
| 25  | Y     | 311 | CLA  | C6-C7-C8    | -2.05 | 109.31      | 115.92   |
| 25  | y     | 311 | CLA  | C6-C7-C8    | -2.05 | 109.31      | 115.92   |
| 24  | G     | 606 | CHL  | CBC-CAC-C3C | -2.05 | 106.79      | 112.43   |
| 28  | I     | 101 | BCR  | C2-C1-C6    | 2.05  | 113.63      | 110.48   |
| 25  | g     | 614 | CLA  | C3D-C4D-ND  | 2.05  | 113.55      | 110.24   |
| 25  | G     | 610 | CLA  | C4D-C3D-CAD | -2.04 | 105.69      | 108.10   |
| 25  | g     | 610 | CLA  | C4D-C3D-CAD | -2.04 | 105.69      | 108.10   |
| 24  | s     | 308 | CHL  | O1D-CGD-CBD | -2.04 | 120.30      | 124.48   |
| 39  | Y     | 316 | LUT  | C22-C23-C24 | 2.04  | 114.07      | 111.74   |
| 25  | C     | 510 | CLA  | CAC-C3C-C4C | 2.04  | 127.46      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | G     | 611 | CLA  | CAA-CBA-CGA | -2.04 | 107.28      | 113.25   |
| 25  | c     | 505 | CLA  | CMB-C2B-C1B | -2.04 | 125.32      | 128.46   |
| 24  | g     | 606 | CHL  | CBC-CAC-C3C | -2.04 | 106.80      | 112.43   |
| 25  | n     | 611 | CLA  | CAD-C3D-C2D | 2.04  | 150.66      | 140.80   |
| 25  | C     | 502 | CLA  | C16-C15-C13 | -2.04 | 109.32      | 115.92   |
| 25  | Y     | 315 | CLA  | C3D-C4D-ND  | 2.04  | 113.54      | 110.24   |
| 24  | S     | 307 | CHL  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 24  | Y     | 307 | CHL  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 25  | r     | 608 | CLA  | C2A-C1A-CHA | -2.04 | 120.29      | 123.86   |
| 25  | c     | 502 | CLA  | C16-C15-C13 | -2.04 | 109.32      | 115.92   |
| 24  | G     | 609 | CHL  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 25  | Y     | 313 | CLA  | C11-C10-C8  | -2.04 | 109.33      | 115.92   |
| 24  | y     | 307 | CHL  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 24  | S     | 308 | CHL  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 25  | c     | 508 | CLA  | C4D-CHA-C1A | -2.04 | 118.77      | 121.25   |
| 40  | g     | 617 | NEX  | C35-C15-C14 | -2.04 | 119.30      | 123.47   |
| 25  | S     | 303 | CLA  | C6-C7-C8    | -2.04 | 109.33      | 115.92   |
| 25  | B     | 601 | CLA  | CAD-C3D-C2D | 2.04  | 150.64      | 140.80   |
| 25  | b     | 601 | CLA  | CAD-C3D-C2D | 2.04  | 150.64      | 140.80   |
| 24  | s     | 306 | CHL  | C2C-C3C-C4C | 2.04  | 107.94      | 106.49   |
| 25  | B     | 607 | CLA  | C6-C7-C8    | -2.04 | 109.33      | 115.92   |
| 25  | C     | 503 | CLA  | C11-C12-C13 | -2.04 | 109.33      | 115.92   |
| 25  | c     | 503 | CLA  | C11-C12-C13 | -2.04 | 109.33      | 115.92   |
| 25  | N     | 611 | CLA  | CAD-C3D-C2D | 2.04  | 150.63      | 140.80   |
| 24  | Y     | 306 | CHL  | C2C-C3C-C4C | 2.04  | 107.94      | 106.49   |
| 25  | g     | 611 | CLA  | CAA-CBA-CGA | -2.04 | 107.30      | 113.25   |
| 25  | b     | 608 | CLA  | C16-C15-C13 | -2.04 | 109.34      | 115.92   |
| 25  | R     | 609 | CLA  | C11-C10-C8  | -2.04 | 109.34      | 115.92   |
| 25  | b     | 607 | CLA  | C6-C7-C8    | -2.04 | 109.34      | 115.92   |
| 30  | a     | 409 | LMG  | C6-C5-C4    | -2.04 | 108.23      | 113.00   |
| 32  | A     | 412 | AJP  | C17-C16-C15 | -2.04 | 107.97      | 110.49   |
| 32  | a     | 413 | AJP  | C17-C16-C15 | -2.04 | 107.97      | 110.49   |
| 28  | b     | 618 | BCR  | C8-C7-C6    | -2.04 | 121.48      | 127.20   |
| 24  | r     | 605 | CHL  | C2C-C3C-C4C | 2.04  | 107.94      | 106.49   |
| 39  | N     | 615 | LUT  | C35-C34-C33 | 2.04  | 130.22      | 127.31   |
| 25  | N     | 603 | CLA  | C11-C12-C13 | -2.04 | 109.34      | 115.92   |
| 25  | n     | 603 | CLA  | C11-C12-C13 | -2.04 | 109.34      | 115.92   |
| 25  | y     | 313 | CLA  | C11-C10-C8  | -2.04 | 109.34      | 115.92   |
| 25  | B     | 608 | CLA  | C16-C15-C13 | -2.04 | 109.34      | 115.92   |
| 25  | C     | 505 | CLA  | C11-C10-C8  | -2.03 | 109.34      | 115.92   |
| 24  | n     | 605 | CHL  | C4D-CHA-C1A | 2.03  | 123.72      | 121.25   |
| 25  | s     | 314 | CLA  | C1B-CHB-C4A | -2.03 | 126.09      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | l     | 302 | CHL  | C2A-C1A-CHA | 2.03  | 127.41      | 123.86   |
| 25  | c     | 512 | CLA  | C11-C10-C8  | -2.03 | 109.35      | 115.92   |
| 25  | s     | 303 | CLA  | C6-C7-C8    | -2.03 | 109.35      | 115.92   |
| 25  | C     | 512 | CLA  | C11-C10-C8  | -2.03 | 109.35      | 115.92   |
| 25  | B     | 602 | CLA  | C2A-C1A-CHA | -2.03 | 120.31      | 123.86   |
| 25  | B     | 611 | CLA  | C11-C12-C13 | -2.03 | 109.36      | 115.92   |
| 25  | C     | 501 | CLA  | C16-C15-C13 | -2.03 | 109.36      | 115.92   |
| 25  | b     | 611 | CLA  | C11-C12-C13 | -2.03 | 109.36      | 115.92   |
| 25  | c     | 501 | CLA  | C16-C15-C13 | -2.03 | 109.36      | 115.92   |
| 24  | s     | 307 | CHL  | O1D-CGD-CBD | -2.03 | 120.33      | 124.48   |
| 24  | N     | 609 | CHL  | O2D-CGD-O1D | -2.03 | 119.87      | 123.84   |
| 24  | S     | 302 | CHL  | O2A-CGA-O1A | -2.03 | 118.24      | 123.30   |
| 24  | s     | 302 | CHL  | O2A-CGA-O1A | -2.03 | 118.24      | 123.30   |
| 25  | n     | 612 | CLA  | CAD-C3D-C2D | 2.03  | 150.59      | 140.80   |
| 28  | i     | 101 | BCR  | C2-C1-C6    | 2.03  | 113.61      | 110.48   |
| 25  | S     | 304 | CLA  | CAD-C3D-C2D | 2.03  | 150.59      | 140.80   |
| 25  | s     | 304 | CLA  | CAD-C3D-C2D | 2.03  | 150.59      | 140.80   |
| 27  | A     | 404 | PHO  | C16-C15-C13 | -2.03 | 109.36      | 115.92   |
| 27  | a     | 405 | PHO  | C16-C15-C13 | -2.03 | 109.36      | 115.92   |
| 28  | B     | 618 | BCR  | C8-C7-C6    | -2.03 | 121.50      | 127.20   |
| 25  | G     | 610 | CLA  | C11-C10-C8  | -2.03 | 109.36      | 115.92   |
| 28  | A     | 406 | BCR  | C20-C21-C22 | -2.03 | 124.42      | 127.31   |
| 28  | a     | 407 | BCR  | C20-C21-C22 | -2.03 | 124.42      | 127.31   |
| 40  | Y     | 318 | NEX  | C31-C32-C33 | 2.03  | 132.11      | 126.42   |
| 25  | G     | 614 | CLA  | C3D-C4D-ND  | 2.03  | 113.52      | 110.24   |
| 25  | r     | 604 | CLA  | CAD-C3D-C2D | 2.03  | 150.58      | 140.80   |
| 28  | T     | 101 | BCR  | C8-C7-C6    | -2.03 | 121.51      | 127.20   |
| 29  | A     | 407 | SQD  | O9-S-O7     | 2.03  | 120.96      | 113.95   |
| 29  | a     | 408 | SQD  | O9-S-O7     | 2.03  | 120.96      | 113.95   |
| 24  | Y     | 309 | CHL  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 24  | y     | 309 | CHL  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 25  | N     | 612 | CLA  | CAD-C3D-C2D | 2.03  | 150.57      | 140.80   |
| 32  | B     | 624 | AJP  | C04-C05-C06 | 2.03  | 119.86      | 115.69   |
| 32  | b     | 624 | AJP  | C04-C05-C06 | 2.03  | 119.86      | 115.69   |
| 24  | S     | 306 | CHL  | C2C-C3C-C4C | 2.03  | 107.93      | 106.49   |
| 25  | C     | 507 | CLA  | CAD-C3D-C2D | 2.03  | 150.57      | 140.80   |
| 25  | B     | 609 | CLA  | C6-C7-C8    | -2.02 | 109.37      | 115.92   |
| 25  | b     | 609 | CLA  | C6-C7-C8    | -2.02 | 109.37      | 115.92   |
| 24  | n     | 609 | CHL  | O2D-CGD-O1D | -2.02 | 119.88      | 123.84   |
| 25  | c     | 505 | CLA  | C11-C10-C8  | -2.02 | 109.38      | 115.92   |
| 25  | C     | 511 | CLA  | O2D-CGD-O1D | -2.02 | 119.88      | 123.84   |
| 25  | r     | 609 | CLA  | C11-C10-C8  | -2.02 | 109.38      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 503 | CLA  | C3D-C4D-ND  | 2.02  | 113.51      | 110.24   |
| 24  | S     | 308 | CHL  | C2A-C1A-CHA | 2.02  | 127.40      | 123.86   |
| 24  | s     | 308 | CHL  | C2A-C1A-CHA | 2.02  | 127.40      | 123.86   |
| 25  | B     | 615 | CLA  | C16-C15-C13 | -2.02 | 109.38      | 115.92   |
| 25  | b     | 615 | CLA  | C16-C15-C13 | -2.02 | 109.38      | 115.92   |
| 28  | t     | 101 | BCR  | C8-C7-C6    | -2.02 | 121.52      | 127.20   |
| 25  | S     | 309 | CLA  | O2D-CGD-O1D | -2.02 | 119.88      | 123.84   |
| 25  | R     | 604 | CLA  | CAD-C3D-C2D | 2.02  | 150.56      | 140.80   |
| 25  | c     | 507 | CLA  | CAD-C3D-C2D | 2.02  | 150.56      | 140.80   |
| 25  | C     | 513 | CLA  | C11-C12-C13 | -2.02 | 109.38      | 115.92   |
| 25  | c     | 513 | CLA  | C11-C12-C13 | -2.02 | 109.38      | 115.92   |
| 25  | n     | 603 | CLA  | C6-C7-C8    | -2.02 | 109.39      | 115.92   |
| 28  | I     | 101 | BCR  | C8-C7-C6    | -2.02 | 121.53      | 127.20   |
| 25  | G     | 604 | CLA  | C3D-C4D-ND  | 2.02  | 113.51      | 110.24   |
| 25  | R     | 602 | CLA  | C6-C7-C8    | -2.02 | 109.39      | 115.92   |
| 27  | a     | 405 | PHO  | C11-C12-C13 | -2.02 | 109.39      | 115.92   |
| 25  | C     | 501 | CLA  | O2D-CGD-O1D | -2.02 | 119.89      | 123.84   |
| 25  | c     | 501 | CLA  | O2D-CGD-O1D | -2.02 | 119.89      | 123.84   |
| 25  | B     | 603 | CLA  | O2D-CGD-O1D | -2.02 | 119.89      | 123.84   |
| 25  | b     | 603 | CLA  | O2D-CGD-O1D | -2.02 | 119.89      | 123.84   |
| 25  | C     | 508 | CLA  | C4D-CHA-C1A | -2.02 | 118.79      | 121.25   |
| 25  | c     | 511 | CLA  | O2D-CGD-O1D | -2.02 | 119.89      | 123.84   |
| 24  | r     | 606 | CHL  | C2A-C3A-C4A | 2.02  | 105.13      | 101.87   |
| 27  | A     | 404 | PHO  | C11-C12-C13 | -2.02 | 109.40      | 115.92   |
| 24  | S     | 306 | CHL  | O2A-CGA-CBA | 2.02  | 120.51      | 114.03   |
| 24  | s     | 306 | CHL  | O2A-CGA-CBA | 2.02  | 120.51      | 114.03   |
| 25  | R     | 604 | CLA  | C1D-CHD-C4C | -2.02 | 121.71      | 126.06   |
| 28  | z     | 101 | BCR  | C16-C15-C14 | -2.02 | 119.34      | 123.47   |
| 25  | N     | 602 | CLA  | C11-C10-C8  | -2.02 | 109.40      | 115.92   |
| 25  | n     | 602 | CLA  | C11-C10-C8  | -2.02 | 109.40      | 115.92   |
| 25  | r     | 602 | CLA  | C6-C7-C8    | -2.02 | 109.40      | 115.92   |
| 25  | G     | 613 | CLA  | CHD-C4C-C3C | -2.02 | 121.88      | 124.84   |
| 25  | C     | 510 | CLA  | CAD-C3D-C2D | 2.02  | 150.53      | 140.80   |
| 25  | c     | 510 | CLA  | CAD-C3D-C2D | 2.02  | 150.53      | 140.80   |
| 24  | G     | 609 | CHL  | O2D-CGD-O1D | -2.02 | 119.90      | 123.84   |
| 24  | r     | 613 | CHL  | C2A-C1A-CHA | 2.02  | 127.37      | 123.85   |
| 25  | n     | 610 | CLA  | C11-C10-C8  | -2.01 | 109.41      | 115.92   |
| 25  | s     | 309 | CLA  | O2D-CGD-O1D | -2.01 | 119.90      | 123.84   |
| 25  | c     | 504 | CLA  | C11-C10-C8  | -2.01 | 109.41      | 115.92   |
| 25  | C     | 504 | CLA  | C11-C10-C8  | -2.01 | 109.41      | 115.92   |
| 25  | R     | 609 | CLA  | C6-C7-C8    | -2.01 | 109.41      | 115.92   |
| 32  | N     | 620 | AJP  | C20-C21-C22 | 2.01  | 117.39      | 114.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | B     | 611 | CLA  | C16-C15-C13 | -2.01 | 109.41      | 115.92   |
| 25  | b     | 611 | CLA  | C16-C15-C13 | -2.01 | 109.41      | 115.92   |
| 25  | S     | 310 | CLA  | CHB-C4A-NA  | -2.01 | 121.73      | 124.51   |
| 25  | B     | 601 | CLA  | C4D-C3D-CAD | -2.01 | 105.72      | 108.10   |
| 25  | b     | 601 | CLA  | C4D-C3D-CAD | -2.01 | 105.72      | 108.10   |
| 24  | N     | 605 | CHL  | C4D-CHA-C1A | 2.01  | 123.70      | 121.25   |
| 25  | B     | 613 | CLA  | C3D-C4D-ND  | 2.01  | 113.49      | 110.24   |
| 25  | r     | 609 | CLA  | C6-C7-C8    | -2.01 | 109.41      | 115.92   |
| 25  | r     | 612 | CLA  | CAD-C3D-C2D | 2.01  | 150.51      | 140.80   |
| 25  | Y     | 311 | CLA  | C11-C10-C8  | -2.01 | 109.41      | 115.92   |
| 25  | c     | 510 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 25  | c     | 512 | CLA  | C16-C15-C13 | -2.01 | 109.42      | 115.92   |
| 25  | G     | 610 | CLA  | CAD-C3D-C2D | 2.01  | 150.50      | 140.80   |
| 25  | N     | 603 | CLA  | C6-C7-C8    | -2.01 | 109.42      | 115.92   |
| 25  | y     | 311 | CLA  | C11-C10-C8  | -2.01 | 109.42      | 115.92   |
| 25  | b     | 613 | CLA  | C3D-C4D-ND  | 2.01  | 113.49      | 110.24   |
| 28  | i     | 101 | BCR  | C8-C7-C6    | -2.01 | 121.56      | 127.20   |
| 25  | N     | 610 | CLA  | C11-C10-C8  | -2.01 | 109.42      | 115.92   |
| 39  | n     | 615 | LUT  | C35-C34-C33 | 2.01  | 130.18      | 127.31   |
| 25  | N     | 602 | CLA  | C3D-C4D-ND  | 2.01  | 113.49      | 110.24   |
| 24  | G     | 606 | CHL  | C2A-C1A-CHA | 2.01  | 127.37      | 123.86   |
| 39  | y     | 316 | LUT  | C22-C23-C24 | 2.01  | 114.03      | 111.74   |
| 25  | 2     | 605 | CLA  | C2A-C3A-C4A | -2.01 | 98.62       | 101.87   |
| 25  | B     | 610 | CLA  | C16-C15-C13 | -2.01 | 109.43      | 115.92   |
| 25  | b     | 605 | CLA  | C16-C15-C13 | -2.01 | 109.43      | 115.92   |
| 25  | b     | 610 | CLA  | C16-C15-C13 | -2.01 | 109.43      | 115.92   |
| 25  | s     | 303 | CLA  | C11-C10-C8  | -2.01 | 109.43      | 115.92   |
| 32  | G     | 618 | AJP  | C29-C30-C32 | -2.01 | 109.08      | 112.60   |
| 32  | g     | 618 | AJP  | C29-C30-C32 | -2.01 | 109.08      | 112.60   |
| 25  | g     | 610 | CLA  | CAD-C3D-C2D | 2.01  | 150.49      | 140.80   |
| 30  | A     | 408 | LMG  | C6-C5-C4    | -2.01 | 108.30      | 113.00   |
| 24  | Y     | 302 | CHL  | C3C-C4C-NC  | -2.01 | 108.32      | 110.57   |
| 24  | y     | 302 | CHL  | C3C-C4C-NC  | -2.01 | 108.32      | 110.57   |
| 24  | s     | 307 | CHL  | O2D-CGD-O1D | -2.01 | 119.91      | 123.84   |
| 25  | n     | 602 | CLA  | C3D-C4D-ND  | 2.01  | 113.48      | 110.24   |
| 25  | R     | 612 | CLA  | CAD-C3D-C2D | 2.01  | 150.48      | 140.80   |
| 25  | B     | 602 | CLA  | C4D-CHA-C1A | -2.01 | 118.81      | 121.25   |
| 24  | Y     | 302 | CHL  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 24  | y     | 302 | CHL  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 25  | Y     | 304 | CLA  | CAD-C3D-C2D | 2.01  | 150.48      | 140.80   |
| 25  | y     | 304 | CLA  | CAD-C3D-C2D | 2.01  | 150.48      | 140.80   |
| 25  | C     | 509 | CLA  | C11-C12-C13 | -2.01 | 109.44      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 604 | CLA  | C11-C10-C8  | -2.01 | 109.44      | 115.92   |
| 25  | C     | 512 | CLA  | C16-C15-C13 | -2.00 | 109.44      | 115.92   |
| 25  | C     | 502 | CLA  | C2C-C1C-NC  | 2.00  | 111.85      | 109.97   |
| 41  | R     | 616 | XAT  | C32-C33-C34 | 2.00  | 122.02      | 118.94   |
| 41  | r     | 616 | XAT  | C32-C33-C34 | 2.00  | 122.02      | 118.94   |
| 24  | G     | 601 | CHL  | C3C-C4C-NC  | -2.00 | 108.32      | 110.57   |
| 25  | r     | 602 | CLA  | CAD-C3D-C2D | 2.00  | 150.47      | 140.80   |
| 25  | C     | 511 | CLA  | C11-C10-C8  | -2.00 | 109.44      | 115.92   |
| 24  | R     | 605 | CHL  | O2D-CGD-O1D | -2.00 | 119.92      | 123.84   |
| 24  | r     | 605 | CHL  | O2D-CGD-O1D | -2.00 | 119.92      | 123.84   |
| 25  | D     | 402 | CLA  | C6-C7-C8    | -2.00 | 109.44      | 115.92   |
| 25  | d     | 402 | CLA  | C6-C7-C8    | -2.00 | 109.44      | 115.92   |
| 25  | B     | 605 | CLA  | C16-C15-C13 | -2.00 | 109.44      | 115.92   |
| 24  | R     | 613 | CHL  | C2A-C1A-CHA | 2.00  | 127.35      | 123.85   |
| 28  | Z     | 101 | BCR  | C16-C15-C14 | -2.00 | 119.37      | 123.47   |
| 25  | Y     | 303 | CLA  | CHD-C1D-C2D | 2.00  | 129.68      | 125.48   |
| 25  | y     | 303 | CLA  | CHD-C1D-C2D | 2.00  | 129.68      | 125.48   |
| 39  | G     | 615 | LUT  | C37-C21-C22 | -2.00 | 105.64      | 109.44   |
| 39  | g     | 615 | LUT  | C37-C21-C22 | -2.00 | 105.64      | 109.44   |
| 25  | b     | 602 | CLA  | C2A-C1A-CHA | -2.00 | 120.36      | 123.86   |
| 25  | R     | 602 | CLA  | CAD-C3D-C2D | 2.00  | 150.46      | 140.80   |
| 24  | R     | 606 | CHL  | C2A-C3A-C4A | 2.00  | 105.10      | 101.87   |
| 25  | r     | 604 | CLA  | C1D-CHD-C4C | -2.00 | 121.74      | 126.06   |
| 32  | n     | 620 | AJP  | C20-C21-C22 | 2.00  | 117.37      | 114.09   |
| 25  | C     | 506 | CLA  | C11-C10-C8  | -2.00 | 109.45      | 115.92   |
| 25  | C     | 508 | CLA  | C11-C10-C8  | -2.00 | 109.45      | 115.92   |
| 25  | c     | 506 | CLA  | C11-C10-C8  | -2.00 | 109.45      | 115.92   |
| 39  | Y     | 316 | LUT  | C37-C21-C22 | -2.00 | 105.65      | 109.44   |
| 25  | c     | 503 | CLA  | C3D-C4D-ND  | 2.00  | 113.47      | 110.24   |
| 25  | A     | 402 | CLA  | CAD-C3D-C2D | 2.00  | 150.45      | 140.80   |
| 25  | a     | 403 | CLA  | CAD-C3D-C2D | 2.00  | 150.45      | 140.80   |
| 25  | C     | 512 | CLA  | C6-C7-C8    | -2.00 | 109.45      | 115.92   |

All (734) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | 1     | 301 | CHL  | ND   |
| 24  | 1     | 301 | CHL  | NA   |
| 24  | 1     | 301 | CHL  | NC   |
| 24  | 1     | 302 | CHL  | ND   |
| 24  | 1     | 302 | CHL  | NA   |
| 24  | 1     | 302 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | 2     | 601 | CHL  | ND   |
| 24  | 2     | 601 | CHL  | NA   |
| 24  | 2     | 601 | CHL  | NC   |
| 24  | 2     | 603 | CHL  | ND   |
| 24  | 2     | 603 | CHL  | NA   |
| 24  | 2     | 603 | CHL  | NC   |
| 24  | S     | 302 | CHL  | ND   |
| 24  | S     | 302 | CHL  | NC   |
| 24  | S     | 306 | CHL  | ND   |
| 24  | S     | 306 | CHL  | NA   |
| 24  | S     | 306 | CHL  | NC   |
| 24  | S     | 307 | CHL  | ND   |
| 24  | S     | 307 | CHL  | NA   |
| 24  | S     | 307 | CHL  | NC   |
| 24  | S     | 308 | CHL  | ND   |
| 24  | S     | 308 | CHL  | NA   |
| 24  | S     | 308 | CHL  | NC   |
| 24  | G     | 601 | CHL  | ND   |
| 24  | G     | 601 | CHL  | NC   |
| 24  | G     | 605 | CHL  | ND   |
| 24  | G     | 605 | CHL  | NA   |
| 24  | G     | 605 | CHL  | NC   |
| 24  | G     | 606 | CHL  | ND   |
| 24  | G     | 606 | CHL  | NA   |
| 24  | G     | 606 | CHL  | NC   |
| 24  | G     | 607 | CHL  | ND   |
| 24  | G     | 607 | CHL  | NC   |
| 24  | G     | 608 | CHL  | ND   |
| 24  | G     | 608 | CHL  | NA   |
| 24  | G     | 608 | CHL  | NC   |
| 24  | G     | 609 | CHL  | ND   |
| 24  | G     | 609 | CHL  | NA   |
| 24  | G     | 609 | CHL  | NC   |
| 24  | N     | 601 | CHL  | ND   |
| 24  | N     | 601 | CHL  | NC   |
| 24  | N     | 605 | CHL  | ND   |
| 24  | N     | 605 | CHL  | NA   |
| 24  | N     | 605 | CHL  | NC   |
| 24  | N     | 606 | CHL  | ND   |
| 24  | N     | 606 | CHL  | NC   |
| 24  | N     | 607 | CHL  | ND   |
| 24  | N     | 607 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | N     | 608 | CHL  | ND   |
| 24  | N     | 608 | CHL  | NA   |
| 24  | N     | 608 | CHL  | NC   |
| 24  | N     | 609 | CHL  | ND   |
| 24  | N     | 609 | CHL  | NC   |
| 24  | Y     | 302 | CHL  | ND   |
| 24  | Y     | 302 | CHL  | NC   |
| 24  | Y     | 306 | CHL  | ND   |
| 24  | Y     | 306 | CHL  | NA   |
| 24  | Y     | 306 | CHL  | NC   |
| 24  | Y     | 307 | CHL  | ND   |
| 24  | Y     | 307 | CHL  | NA   |
| 24  | Y     | 307 | CHL  | NC   |
| 24  | Y     | 308 | CHL  | ND   |
| 24  | Y     | 308 | CHL  | NC   |
| 24  | Y     | 309 | CHL  | ND   |
| 24  | Y     | 309 | CHL  | NA   |
| 24  | Y     | 309 | CHL  | NC   |
| 24  | Y     | 310 | CHL  | ND   |
| 24  | Y     | 310 | CHL  | NA   |
| 24  | Y     | 310 | CHL  | NC   |
| 24  | R     | 605 | CHL  | ND   |
| 24  | R     | 605 | CHL  | NA   |
| 24  | R     | 605 | CHL  | NC   |
| 24  | R     | 606 | CHL  | ND   |
| 24  | R     | 606 | CHL  | NA   |
| 24  | R     | 606 | CHL  | NC   |
| 24  | R     | 607 | CHL  | ND   |
| 24  | R     | 607 | CHL  | NA   |
| 24  | R     | 607 | CHL  | NC   |
| 24  | R     | 613 | CHL  | ND   |
| 24  | R     | 613 | CHL  | NA   |
| 24  | R     | 613 | CHL  | NC   |
| 24  | 5     | 301 | CHL  | ND   |
| 24  | 5     | 301 | CHL  | NA   |
| 24  | 5     | 301 | CHL  | NC   |
| 24  | 5     | 302 | CHL  | ND   |
| 24  | 5     | 302 | CHL  | NA   |
| 24  | 5     | 302 | CHL  | NC   |
| 24  | 6     | 601 | CHL  | ND   |
| 24  | 6     | 601 | CHL  | NA   |
| 24  | 6     | 601 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | 6     | 603 | CHL  | ND   |
| 24  | 6     | 603 | CHL  | NA   |
| 24  | 6     | 603 | CHL  | NC   |
| 24  | s     | 302 | CHL  | ND   |
| 24  | s     | 302 | CHL  | NC   |
| 24  | s     | 306 | CHL  | ND   |
| 24  | s     | 306 | CHL  | NA   |
| 24  | s     | 306 | CHL  | NC   |
| 24  | s     | 307 | CHL  | ND   |
| 24  | s     | 307 | CHL  | NA   |
| 24  | s     | 307 | CHL  | NC   |
| 24  | s     | 308 | CHL  | ND   |
| 24  | s     | 308 | CHL  | NA   |
| 24  | s     | 308 | CHL  | NC   |
| 24  | g     | 601 | CHL  | ND   |
| 24  | g     | 601 | CHL  | NC   |
| 24  | g     | 605 | CHL  | ND   |
| 24  | g     | 605 | CHL  | NA   |
| 24  | g     | 605 | CHL  | NC   |
| 24  | g     | 606 | CHL  | ND   |
| 24  | g     | 606 | CHL  | NA   |
| 24  | g     | 606 | CHL  | NC   |
| 24  | g     | 607 | CHL  | ND   |
| 24  | g     | 607 | CHL  | NC   |
| 24  | g     | 608 | CHL  | ND   |
| 24  | g     | 608 | CHL  | NA   |
| 24  | g     | 608 | CHL  | NC   |
| 24  | g     | 609 | CHL  | ND   |
| 24  | g     | 609 | CHL  | NA   |
| 24  | g     | 609 | CHL  | NC   |
| 24  | n     | 601 | CHL  | ND   |
| 24  | n     | 601 | CHL  | NC   |
| 24  | n     | 605 | CHL  | ND   |
| 24  | n     | 605 | CHL  | NA   |
| 24  | n     | 605 | CHL  | NC   |
| 24  | n     | 606 | CHL  | ND   |
| 24  | n     | 606 | CHL  | NC   |
| 24  | n     | 607 | CHL  | ND   |
| 24  | n     | 607 | CHL  | NC   |
| 24  | n     | 608 | CHL  | ND   |
| 24  | n     | 608 | CHL  | NA   |
| 24  | n     | 608 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | n     | 609 | CHL  | ND   |
| 24  | n     | 609 | CHL  | NC   |
| 24  | y     | 302 | CHL  | ND   |
| 24  | y     | 302 | CHL  | NC   |
| 24  | y     | 306 | CHL  | ND   |
| 24  | y     | 306 | CHL  | NA   |
| 24  | y     | 306 | CHL  | NC   |
| 24  | y     | 307 | CHL  | ND   |
| 24  | y     | 307 | CHL  | NA   |
| 24  | y     | 307 | CHL  | NC   |
| 24  | y     | 308 | CHL  | ND   |
| 24  | y     | 308 | CHL  | NC   |
| 24  | y     | 309 | CHL  | ND   |
| 24  | y     | 309 | CHL  | NA   |
| 24  | y     | 309 | CHL  | NC   |
| 24  | y     | 310 | CHL  | ND   |
| 24  | y     | 310 | CHL  | NA   |
| 24  | y     | 310 | CHL  | NC   |
| 24  | r     | 605 | CHL  | ND   |
| 24  | r     | 605 | CHL  | NA   |
| 24  | r     | 605 | CHL  | NC   |
| 24  | r     | 606 | CHL  | ND   |
| 24  | r     | 606 | CHL  | NA   |
| 24  | r     | 606 | CHL  | NC   |
| 24  | r     | 607 | CHL  | ND   |
| 24  | r     | 607 | CHL  | NA   |
| 24  | r     | 607 | CHL  | NC   |
| 24  | r     | 613 | CHL  | ND   |
| 24  | r     | 613 | CHL  | NA   |
| 24  | r     | 613 | CHL  | NC   |
| 25  | 2     | 602 | CLA  | ND   |
| 25  | 2     | 604 | CLA  | ND   |
| 25  | 2     | 605 | CLA  | ND   |
| 25  | A     | 401 | CLA  | ND   |
| 25  | A     | 402 | CLA  | ND   |
| 25  | A     | 405 | CLA  | ND   |
| 25  | B     | 601 | CLA  | ND   |
| 25  | B     | 602 | CLA  | ND   |
| 25  | B     | 603 | CLA  | ND   |
| 25  | B     | 604 | CLA  | ND   |
| 25  | B     | 605 | CLA  | ND   |
| 25  | B     | 606 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | B     | 607 | CLA  | ND   |
| 25  | B     | 608 | CLA  | ND   |
| 25  | B     | 609 | CLA  | ND   |
| 25  | B     | 610 | CLA  | ND   |
| 25  | B     | 611 | CLA  | ND   |
| 25  | B     | 612 | CLA  | ND   |
| 25  | B     | 613 | CLA  | ND   |
| 25  | B     | 614 | CLA  | ND   |
| 25  | B     | 615 | CLA  | ND   |
| 25  | B     | 616 | CLA  | ND   |
| 25  | C     | 501 | CLA  | ND   |
| 25  | C     | 502 | CLA  | ND   |
| 25  | C     | 503 | CLA  | ND   |
| 25  | C     | 504 | CLA  | ND   |
| 25  | C     | 505 | CLA  | ND   |
| 25  | C     | 506 | CLA  | ND   |
| 25  | C     | 507 | CLA  | ND   |
| 25  | C     | 508 | CLA  | ND   |
| 25  | C     | 509 | CLA  | ND   |
| 25  | C     | 510 | CLA  | ND   |
| 25  | C     | 511 | CLA  | ND   |
| 25  | C     | 512 | CLA  | ND   |
| 25  | C     | 513 | CLA  | ND   |
| 25  | D     | 401 | CLA  | ND   |
| 25  | D     | 402 | CLA  | ND   |
| 25  | D     | 403 | CLA  | ND   |
| 25  | S     | 303 | CLA  | ND   |
| 25  | S     | 304 | CLA  | ND   |
| 25  | S     | 305 | CLA  | ND   |
| 25  | S     | 309 | CLA  | ND   |
| 25  | S     | 310 | CLA  | ND   |
| 25  | S     | 311 | CLA  | ND   |
| 25  | S     | 312 | CLA  | ND   |
| 25  | S     | 313 | CLA  | ND   |
| 25  | S     | 314 | CLA  | ND   |
| 25  | G     | 602 | CLA  | ND   |
| 25  | G     | 603 | CLA  | ND   |
| 25  | G     | 604 | CLA  | ND   |
| 25  | G     | 610 | CLA  | ND   |
| 25  | G     | 611 | CLA  | ND   |
| 25  | G     | 612 | CLA  | ND   |
| 25  | G     | 613 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | G     | 614 | CLA  | ND   |
| 25  | N     | 602 | CLA  | ND   |
| 25  | N     | 603 | CLA  | ND   |
| 25  | N     | 604 | CLA  | ND   |
| 25  | N     | 610 | CLA  | ND   |
| 25  | N     | 611 | CLA  | ND   |
| 25  | N     | 612 | CLA  | ND   |
| 25  | N     | 613 | CLA  | ND   |
| 25  | N     | 614 | CLA  | ND   |
| 25  | Y     | 303 | CLA  | ND   |
| 25  | Y     | 304 | CLA  | ND   |
| 25  | Y     | 305 | CLA  | ND   |
| 25  | Y     | 311 | CLA  | ND   |
| 25  | Y     | 312 | CLA  | ND   |
| 25  | Y     | 313 | CLA  | ND   |
| 25  | Y     | 314 | CLA  | ND   |
| 25  | Y     | 315 | CLA  | ND   |
| 25  | R     | 601 | CLA  | ND   |
| 25  | R     | 602 | CLA  | ND   |
| 25  | R     | 603 | CLA  | ND   |
| 25  | R     | 604 | CLA  | ND   |
| 25  | R     | 608 | CLA  | ND   |
| 25  | R     | 609 | CLA  | ND   |
| 25  | R     | 610 | CLA  | ND   |
| 25  | R     | 611 | CLA  | ND   |
| 25  | R     | 612 | CLA  | ND   |
| 25  | R     | 614 | CLA  | ND   |
| 25  | 6     | 602 | CLA  | ND   |
| 25  | 6     | 604 | CLA  | ND   |
| 25  | 6     | 605 | CLA  | ND   |
| 25  | a     | 402 | CLA  | ND   |
| 25  | a     | 403 | CLA  | ND   |
| 25  | a     | 406 | CLA  | ND   |
| 25  | b     | 601 | CLA  | ND   |
| 25  | b     | 602 | CLA  | ND   |
| 25  | b     | 603 | CLA  | ND   |
| 25  | b     | 604 | CLA  | ND   |
| 25  | b     | 605 | CLA  | ND   |
| 25  | b     | 606 | CLA  | ND   |
| 25  | b     | 607 | CLA  | ND   |
| 25  | b     | 608 | CLA  | ND   |
| 25  | b     | 609 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | b     | 610 | CLA  | ND   |
| 25  | b     | 611 | CLA  | ND   |
| 25  | b     | 612 | CLA  | ND   |
| 25  | b     | 613 | CLA  | ND   |
| 25  | b     | 614 | CLA  | ND   |
| 25  | b     | 615 | CLA  | ND   |
| 25  | b     | 616 | CLA  | ND   |
| 25  | c     | 501 | CLA  | ND   |
| 25  | c     | 502 | CLA  | ND   |
| 25  | c     | 503 | CLA  | ND   |
| 25  | c     | 504 | CLA  | ND   |
| 25  | c     | 505 | CLA  | ND   |
| 25  | c     | 506 | CLA  | ND   |
| 25  | c     | 507 | CLA  | ND   |
| 25  | c     | 508 | CLA  | ND   |
| 25  | c     | 509 | CLA  | ND   |
| 25  | c     | 510 | CLA  | ND   |
| 25  | c     | 511 | CLA  | ND   |
| 25  | c     | 512 | CLA  | ND   |
| 25  | c     | 513 | CLA  | ND   |
| 25  | d     | 401 | CLA  | ND   |
| 25  | d     | 402 | CLA  | ND   |
| 25  | d     | 403 | CLA  | ND   |
| 25  | s     | 303 | CLA  | ND   |
| 25  | s     | 304 | CLA  | ND   |
| 25  | s     | 305 | CLA  | ND   |
| 25  | s     | 309 | CLA  | ND   |
| 25  | s     | 310 | CLA  | ND   |
| 25  | s     | 311 | CLA  | ND   |
| 25  | s     | 312 | CLA  | ND   |
| 25  | s     | 313 | CLA  | ND   |
| 25  | s     | 314 | CLA  | ND   |
| 25  | g     | 602 | CLA  | ND   |
| 25  | g     | 603 | CLA  | ND   |
| 25  | g     | 604 | CLA  | ND   |
| 25  | g     | 610 | CLA  | ND   |
| 25  | g     | 611 | CLA  | ND   |
| 25  | g     | 612 | CLA  | ND   |
| 25  | g     | 613 | CLA  | ND   |
| 25  | g     | 614 | CLA  | ND   |
| 25  | n     | 602 | CLA  | ND   |
| 25  | n     | 603 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | n     | 604 | CLA  | ND   |
| 25  | n     | 610 | CLA  | ND   |
| 25  | n     | 611 | CLA  | ND   |
| 25  | n     | 612 | CLA  | ND   |
| 25  | n     | 613 | CLA  | ND   |
| 25  | n     | 614 | CLA  | ND   |
| 25  | y     | 303 | CLA  | ND   |
| 25  | y     | 304 | CLA  | ND   |
| 25  | y     | 305 | CLA  | ND   |
| 25  | y     | 311 | CLA  | ND   |
| 25  | y     | 312 | CLA  | ND   |
| 25  | y     | 313 | CLA  | ND   |
| 25  | y     | 314 | CLA  | ND   |
| 25  | y     | 315 | CLA  | ND   |
| 25  | r     | 601 | CLA  | ND   |
| 25  | r     | 602 | CLA  | ND   |
| 25  | r     | 603 | CLA  | ND   |
| 25  | r     | 604 | CLA  | ND   |
| 25  | r     | 608 | CLA  | ND   |
| 25  | r     | 609 | CLA  | ND   |
| 25  | r     | 610 | CLA  | ND   |
| 25  | r     | 611 | CLA  | ND   |
| 25  | r     | 612 | CLA  | ND   |
| 25  | r     | 614 | CLA  | ND   |
| 32  | A     | 412 | AJP  | C56  |
| 32  | A     | 412 | AJP  | C68  |
| 32  | A     | 412 | AJP  | C69  |
| 32  | A     | 412 | AJP  | C65  |
| 32  | A     | 412 | AJP  | C59  |
| 32  | A     | 412 | AJP  | C55  |
| 32  | A     | 412 | AJP  | C27  |
| 32  | A     | 412 | AJP  | C23  |
| 32  | A     | 412 | AJP  | C47  |
| 32  | A     | 412 | AJP  | C38  |
| 32  | A     | 412 | AJP  | C39  |
| 32  | A     | 412 | AJP  | C11  |
| 32  | A     | 412 | AJP  | C28  |
| 32  | A     | 412 | AJP  | C22  |
| 32  | A     | 412 | AJP  | C12  |
| 32  | A     | 412 | AJP  | C48  |
| 32  | A     | 412 | AJP  | C16  |
| 32  | A     | 412 | AJP  | C08  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | A     | 412 | AJP  | C36  |
| 32  | A     | 412 | AJP  | C26  |
| 32  | A     | 412 | AJP  | C37  |
| 32  | A     | 412 | AJP  | C02  |
| 32  | A     | 412 | AJP  | C57  |
| 32  | A     | 412 | AJP  | C10  |
| 32  | A     | 412 | AJP  | C15  |
| 32  | A     | 412 | AJP  | C20  |
| 32  | A     | 412 | AJP  | C07  |
| 32  | A     | 412 | AJP  | C19  |
| 32  | A     | 412 | AJP  | C67  |
| 32  | A     | 412 | AJP  | C66  |
| 32  | A     | 412 | AJP  | C35  |
| 32  | A     | 412 | AJP  | C45  |
| 32  | A     | 412 | AJP  | C46  |
| 32  | A     | 412 | AJP  | C30  |
| 32  | B     | 624 | AJP  | C68  |
| 32  | B     | 624 | AJP  | C56  |
| 32  | B     | 624 | AJP  | C65  |
| 32  | B     | 624 | AJP  | C59  |
| 32  | B     | 624 | AJP  | C69  |
| 32  | B     | 624 | AJP  | C55  |
| 32  | B     | 624 | AJP  | C27  |
| 32  | B     | 624 | AJP  | C23  |
| 32  | B     | 624 | AJP  | C47  |
| 32  | B     | 624 | AJP  | C38  |
| 32  | B     | 624 | AJP  | C39  |
| 32  | B     | 624 | AJP  | C11  |
| 32  | B     | 624 | AJP  | C28  |
| 32  | B     | 624 | AJP  | C22  |
| 32  | B     | 624 | AJP  | C12  |
| 32  | B     | 624 | AJP  | C48  |
| 32  | B     | 624 | AJP  | C16  |
| 32  | B     | 624 | AJP  | C08  |
| 32  | B     | 624 | AJP  | C37  |
| 32  | B     | 624 | AJP  | C26  |
| 32  | B     | 624 | AJP  | C36  |
| 32  | B     | 624 | AJP  | C02  |
| 32  | B     | 624 | AJP  | C57  |
| 32  | B     | 624 | AJP  | C10  |
| 32  | B     | 624 | AJP  | C15  |
| 32  | B     | 624 | AJP  | C20  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | B     | 624 | AJP  | C07  |
| 32  | B     | 624 | AJP  | C19  |
| 32  | B     | 624 | AJP  | C67  |
| 32  | B     | 624 | AJP  | C66  |
| 32  | B     | 624 | AJP  | C35  |
| 32  | B     | 624 | AJP  | C45  |
| 32  | B     | 624 | AJP  | C46  |
| 32  | B     | 624 | AJP  | C30  |
| 32  | S     | 319 | AJP  | C15  |
| 32  | S     | 319 | AJP  | C20  |
| 32  | S     | 319 | AJP  | C23  |
| 32  | S     | 319 | AJP  | C07  |
| 32  | S     | 319 | AJP  | C19  |
| 32  | S     | 319 | AJP  | C26  |
| 32  | S     | 319 | AJP  | C11  |
| 32  | S     | 319 | AJP  | C02  |
| 32  | S     | 319 | AJP  | C22  |
| 32  | S     | 319 | AJP  | C12  |
| 32  | S     | 319 | AJP  | C28  |
| 32  | S     | 319 | AJP  | C30  |
| 32  | S     | 319 | AJP  | C10  |
| 32  | S     | 319 | AJP  | C16  |
| 32  | S     | 319 | AJP  | C27  |
| 32  | G     | 618 | AJP  | C15  |
| 32  | G     | 618 | AJP  | C07  |
| 32  | G     | 618 | AJP  | C19  |
| 32  | G     | 618 | AJP  | C23  |
| 32  | G     | 618 | AJP  | C26  |
| 32  | G     | 618 | AJP  | C11  |
| 32  | G     | 618 | AJP  | C02  |
| 32  | G     | 618 | AJP  | C22  |
| 32  | G     | 618 | AJP  | C28  |
| 32  | G     | 618 | AJP  | C12  |
| 32  | G     | 618 | AJP  | C20  |
| 32  | G     | 618 | AJP  | C30  |
| 32  | G     | 618 | AJP  | C10  |
| 32  | G     | 618 | AJP  | C16  |
| 32  | G     | 618 | AJP  | C27  |
| 32  | N     | 619 | AJP  | C15  |
| 32  | N     | 619 | AJP  | C20  |
| 32  | N     | 619 | AJP  | C23  |
| 32  | N     | 619 | AJP  | C07  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | N     | 619 | AJP  | C19  |
| 32  | N     | 619 | AJP  | C26  |
| 32  | N     | 619 | AJP  | C11  |
| 32  | N     | 619 | AJP  | C02  |
| 32  | N     | 619 | AJP  | C22  |
| 32  | N     | 619 | AJP  | C28  |
| 32  | N     | 619 | AJP  | C12  |
| 32  | N     | 619 | AJP  | C30  |
| 32  | N     | 619 | AJP  | C10  |
| 32  | N     | 619 | AJP  | C16  |
| 32  | N     | 619 | AJP  | C27  |
| 32  | N     | 620 | AJP  | C08  |
| 32  | N     | 620 | AJP  | C15  |
| 32  | N     | 620 | AJP  | C20  |
| 32  | N     | 620 | AJP  | C23  |
| 32  | N     | 620 | AJP  | C07  |
| 32  | N     | 620 | AJP  | C19  |
| 32  | N     | 620 | AJP  | C26  |
| 32  | N     | 620 | AJP  | C02  |
| 32  | N     | 620 | AJP  | C11  |
| 32  | N     | 620 | AJP  | C22  |
| 32  | N     | 620 | AJP  | C28  |
| 32  | N     | 620 | AJP  | C12  |
| 32  | N     | 620 | AJP  | C30  |
| 32  | N     | 620 | AJP  | C10  |
| 32  | N     | 620 | AJP  | C16  |
| 32  | N     | 620 | AJP  | C27  |
| 32  | Y     | 320 | AJP  | C15  |
| 32  | Y     | 320 | AJP  | C20  |
| 32  | Y     | 320 | AJP  | C07  |
| 32  | Y     | 320 | AJP  | C19  |
| 32  | Y     | 320 | AJP  | C23  |
| 32  | Y     | 320 | AJP  | C10  |
| 32  | Y     | 320 | AJP  | C26  |
| 32  | Y     | 320 | AJP  | C11  |
| 32  | Y     | 320 | AJP  | C02  |
| 32  | Y     | 320 | AJP  | C22  |
| 32  | Y     | 320 | AJP  | C28  |
| 32  | Y     | 320 | AJP  | C12  |
| 32  | Y     | 320 | AJP  | C30  |
| 32  | Y     | 320 | AJP  | C16  |
| 32  | Y     | 320 | AJP  | C27  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | Y     | 321 | AJP  | C08  |
| 32  | Y     | 321 | AJP  | C15  |
| 32  | Y     | 321 | AJP  | C20  |
| 32  | Y     | 321 | AJP  | C23  |
| 32  | Y     | 321 | AJP  | C07  |
| 32  | Y     | 321 | AJP  | C19  |
| 32  | Y     | 321 | AJP  | C26  |
| 32  | Y     | 321 | AJP  | C02  |
| 32  | Y     | 321 | AJP  | C11  |
| 32  | Y     | 321 | AJP  | C22  |
| 32  | Y     | 321 | AJP  | C28  |
| 32  | Y     | 321 | AJP  | C12  |
| 32  | Y     | 321 | AJP  | C30  |
| 32  | Y     | 321 | AJP  | C10  |
| 32  | Y     | 321 | AJP  | C16  |
| 32  | Y     | 321 | AJP  | C27  |
| 32  | Y     | 322 | AJP  | C15  |
| 32  | Y     | 322 | AJP  | C20  |
| 32  | Y     | 322 | AJP  | C23  |
| 32  | Y     | 322 | AJP  | C07  |
| 32  | Y     | 322 | AJP  | C19  |
| 32  | Y     | 322 | AJP  | C26  |
| 32  | Y     | 322 | AJP  | C11  |
| 32  | Y     | 322 | AJP  | C02  |
| 32  | Y     | 322 | AJP  | C22  |
| 32  | Y     | 322 | AJP  | C28  |
| 32  | Y     | 322 | AJP  | C12  |
| 32  | Y     | 322 | AJP  | C30  |
| 32  | Y     | 322 | AJP  | C10  |
| 32  | Y     | 322 | AJP  | C16  |
| 32  | Y     | 322 | AJP  | C27  |
| 32  | Y     | 323 | AJP  | C15  |
| 32  | Y     | 323 | AJP  | C20  |
| 32  | Y     | 323 | AJP  | C23  |
| 32  | Y     | 323 | AJP  | C07  |
| 32  | Y     | 323 | AJP  | C19  |
| 32  | Y     | 323 | AJP  | C26  |
| 32  | Y     | 323 | AJP  | C11  |
| 32  | Y     | 323 | AJP  | C02  |
| 32  | Y     | 323 | AJP  | C22  |
| 32  | Y     | 323 | AJP  | C28  |
| 32  | Y     | 323 | AJP  | C12  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | Y     | 323 | AJP  | C30  |
| 32  | Y     | 323 | AJP  | C10  |
| 32  | Y     | 323 | AJP  | C16  |
| 32  | Y     | 323 | AJP  | C27  |
| 32  | Y     | 324 | AJP  | C15  |
| 32  | Y     | 324 | AJP  | C20  |
| 32  | Y     | 324 | AJP  | C23  |
| 32  | Y     | 324 | AJP  | C07  |
| 32  | Y     | 324 | AJP  | C19  |
| 32  | Y     | 324 | AJP  | C26  |
| 32  | Y     | 324 | AJP  | C11  |
| 32  | Y     | 324 | AJP  | C02  |
| 32  | Y     | 324 | AJP  | C22  |
| 32  | Y     | 324 | AJP  | C28  |
| 32  | Y     | 324 | AJP  | C12  |
| 32  | Y     | 324 | AJP  | C30  |
| 32  | Y     | 324 | AJP  | C10  |
| 32  | Y     | 324 | AJP  | C16  |
| 32  | Y     | 324 | AJP  | C27  |
| 32  | a     | 413 | AJP  | C56  |
| 32  | a     | 413 | AJP  | C68  |
| 32  | a     | 413 | AJP  | C69  |
| 32  | a     | 413 | AJP  | C65  |
| 32  | a     | 413 | AJP  | C59  |
| 32  | a     | 413 | AJP  | C55  |
| 32  | a     | 413 | AJP  | C27  |
| 32  | a     | 413 | AJP  | C23  |
| 32  | a     | 413 | AJP  | C47  |
| 32  | a     | 413 | AJP  | C38  |
| 32  | a     | 413 | AJP  | C39  |
| 32  | a     | 413 | AJP  | C11  |
| 32  | a     | 413 | AJP  | C28  |
| 32  | a     | 413 | AJP  | C22  |
| 32  | a     | 413 | AJP  | C12  |
| 32  | a     | 413 | AJP  | C48  |
| 32  | a     | 413 | AJP  | C16  |
| 32  | a     | 413 | AJP  | C08  |
| 32  | a     | 413 | AJP  | C36  |
| 32  | a     | 413 | AJP  | C26  |
| 32  | a     | 413 | AJP  | C37  |
| 32  | a     | 413 | AJP  | C02  |
| 32  | a     | 413 | AJP  | C57  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | a     | 413 | AJP  | C10  |
| 32  | a     | 413 | AJP  | C15  |
| 32  | a     | 413 | AJP  | C20  |
| 32  | a     | 413 | AJP  | C07  |
| 32  | a     | 413 | AJP  | C19  |
| 32  | a     | 413 | AJP  | C67  |
| 32  | a     | 413 | AJP  | C66  |
| 32  | a     | 413 | AJP  | C35  |
| 32  | a     | 413 | AJP  | C45  |
| 32  | a     | 413 | AJP  | C46  |
| 32  | a     | 413 | AJP  | C30  |
| 32  | b     | 624 | AJP  | C68  |
| 32  | b     | 624 | AJP  | C56  |
| 32  | b     | 624 | AJP  | C65  |
| 32  | b     | 624 | AJP  | C59  |
| 32  | b     | 624 | AJP  | C69  |
| 32  | b     | 624 | AJP  | C55  |
| 32  | b     | 624 | AJP  | C27  |
| 32  | b     | 624 | AJP  | C23  |
| 32  | b     | 624 | AJP  | C47  |
| 32  | b     | 624 | AJP  | C38  |
| 32  | b     | 624 | AJP  | C39  |
| 32  | b     | 624 | AJP  | C11  |
| 32  | b     | 624 | AJP  | C28  |
| 32  | b     | 624 | AJP  | C22  |
| 32  | b     | 624 | AJP  | C12  |
| 32  | b     | 624 | AJP  | C48  |
| 32  | b     | 624 | AJP  | C16  |
| 32  | b     | 624 | AJP  | C08  |
| 32  | b     | 624 | AJP  | C37  |
| 32  | b     | 624 | AJP  | C26  |
| 32  | b     | 624 | AJP  | C36  |
| 32  | b     | 624 | AJP  | C02  |
| 32  | b     | 624 | AJP  | C57  |
| 32  | b     | 624 | AJP  | C10  |
| 32  | b     | 624 | AJP  | C15  |
| 32  | b     | 624 | AJP  | C20  |
| 32  | b     | 624 | AJP  | C07  |
| 32  | b     | 624 | AJP  | C19  |
| 32  | b     | 624 | AJP  | C67  |
| 32  | b     | 624 | AJP  | C66  |
| 32  | b     | 624 | AJP  | C35  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | b     | 624 | AJP  | C45  |
| 32  | b     | 624 | AJP  | C46  |
| 32  | b     | 624 | AJP  | C30  |
| 32  | s     | 319 | AJP  | C15  |
| 32  | s     | 319 | AJP  | C20  |
| 32  | s     | 319 | AJP  | C23  |
| 32  | s     | 319 | AJP  | C07  |
| 32  | s     | 319 | AJP  | C19  |
| 32  | s     | 319 | AJP  | C26  |
| 32  | s     | 319 | AJP  | C11  |
| 32  | s     | 319 | AJP  | C02  |
| 32  | s     | 319 | AJP  | C22  |
| 32  | s     | 319 | AJP  | C28  |
| 32  | s     | 319 | AJP  | C12  |
| 32  | s     | 319 | AJP  | C30  |
| 32  | s     | 319 | AJP  | C10  |
| 32  | s     | 319 | AJP  | C16  |
| 32  | s     | 319 | AJP  | C27  |
| 32  | g     | 618 | AJP  | C15  |
| 32  | g     | 618 | AJP  | C07  |
| 32  | g     | 618 | AJP  | C19  |
| 32  | g     | 618 | AJP  | C23  |
| 32  | g     | 618 | AJP  | C26  |
| 32  | g     | 618 | AJP  | C11  |
| 32  | g     | 618 | AJP  | C02  |
| 32  | g     | 618 | AJP  | C22  |
| 32  | g     | 618 | AJP  | C28  |
| 32  | g     | 618 | AJP  | C12  |
| 32  | g     | 618 | AJP  | C20  |
| 32  | g     | 618 | AJP  | C30  |
| 32  | g     | 618 | AJP  | C10  |
| 32  | g     | 618 | AJP  | C16  |
| 32  | g     | 618 | AJP  | C27  |
| 32  | n     | 619 | AJP  | C15  |
| 32  | n     | 619 | AJP  | C20  |
| 32  | n     | 619 | AJP  | C23  |
| 32  | n     | 619 | AJP  | C07  |
| 32  | n     | 619 | AJP  | C19  |
| 32  | n     | 619 | AJP  | C26  |
| 32  | n     | 619 | AJP  | C11  |
| 32  | n     | 619 | AJP  | C02  |
| 32  | n     | 619 | AJP  | C22  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | n     | 619 | AJP  | C28  |
| 32  | n     | 619 | AJP  | C12  |
| 32  | n     | 619 | AJP  | C30  |
| 32  | n     | 619 | AJP  | C10  |
| 32  | n     | 619 | AJP  | C16  |
| 32  | n     | 619 | AJP  | C27  |
| 32  | n     | 620 | AJP  | C08  |
| 32  | n     | 620 | AJP  | C15  |
| 32  | n     | 620 | AJP  | C20  |
| 32  | n     | 620 | AJP  | C23  |
| 32  | n     | 620 | AJP  | C07  |
| 32  | n     | 620 | AJP  | C19  |
| 32  | n     | 620 | AJP  | C26  |
| 32  | n     | 620 | AJP  | C02  |
| 32  | n     | 620 | AJP  | C11  |
| 32  | n     | 620 | AJP  | C22  |
| 32  | n     | 620 | AJP  | C28  |
| 32  | n     | 620 | AJP  | C12  |
| 32  | n     | 620 | AJP  | C30  |
| 32  | n     | 620 | AJP  | C10  |
| 32  | n     | 620 | AJP  | C16  |
| 32  | n     | 620 | AJP  | C27  |
| 32  | y     | 320 | AJP  | C15  |
| 32  | y     | 320 | AJP  | C20  |
| 32  | y     | 320 | AJP  | C07  |
| 32  | y     | 320 | AJP  | C19  |
| 32  | y     | 320 | AJP  | C23  |
| 32  | y     | 320 | AJP  | C10  |
| 32  | y     | 320 | AJP  | C26  |
| 32  | y     | 320 | AJP  | C11  |
| 32  | y     | 320 | AJP  | C02  |
| 32  | y     | 320 | AJP  | C22  |
| 32  | y     | 320 | AJP  | C28  |
| 32  | y     | 320 | AJP  | C12  |
| 32  | y     | 320 | AJP  | C30  |
| 32  | y     | 320 | AJP  | C16  |
| 32  | y     | 320 | AJP  | C27  |
| 32  | y     | 321 | AJP  | C08  |
| 32  | y     | 321 | AJP  | C15  |
| 32  | y     | 321 | AJP  | C20  |
| 32  | y     | 321 | AJP  | C23  |
| 32  | y     | 321 | AJP  | C07  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | y     | 321 | AJP  | C19  |
| 32  | y     | 321 | AJP  | C26  |
| 32  | y     | 321 | AJP  | C02  |
| 32  | y     | 321 | AJP  | C11  |
| 32  | y     | 321 | AJP  | C22  |
| 32  | y     | 321 | AJP  | C28  |
| 32  | y     | 321 | AJP  | C12  |
| 32  | y     | 321 | AJP  | C30  |
| 32  | y     | 321 | AJP  | C10  |
| 32  | y     | 321 | AJP  | C16  |
| 32  | y     | 321 | AJP  | C27  |
| 32  | y     | 322 | AJP  | C15  |
| 32  | y     | 322 | AJP  | C20  |
| 32  | y     | 322 | AJP  | C23  |
| 32  | y     | 322 | AJP  | C07  |
| 32  | y     | 322 | AJP  | C19  |
| 32  | y     | 322 | AJP  | C26  |
| 32  | y     | 322 | AJP  | C11  |
| 32  | y     | 322 | AJP  | C02  |
| 32  | y     | 322 | AJP  | C22  |
| 32  | y     | 322 | AJP  | C28  |
| 32  | y     | 322 | AJP  | C12  |
| 32  | y     | 322 | AJP  | C30  |
| 32  | y     | 322 | AJP  | C10  |
| 32  | y     | 322 | AJP  | C16  |
| 32  | y     | 322 | AJP  | C27  |
| 32  | y     | 323 | AJP  | C15  |
| 32  | y     | 323 | AJP  | C20  |
| 32  | y     | 323 | AJP  | C23  |
| 32  | y     | 323 | AJP  | C07  |
| 32  | y     | 323 | AJP  | C19  |
| 32  | y     | 323 | AJP  | C26  |
| 32  | y     | 323 | AJP  | C11  |
| 32  | y     | 323 | AJP  | C02  |
| 32  | y     | 323 | AJP  | C22  |
| 32  | y     | 323 | AJP  | C28  |
| 32  | y     | 323 | AJP  | C12  |
| 32  | y     | 323 | AJP  | C30  |
| 32  | y     | 323 | AJP  | C10  |
| 32  | y     | 323 | AJP  | C16  |
| 32  | y     | 323 | AJP  | C27  |
| 32  | y     | 324 | AJP  | C15  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | y     | 324 | AJP  | C20  |
| 32  | y     | 324 | AJP  | C23  |
| 32  | y     | 324 | AJP  | C07  |
| 32  | y     | 324 | AJP  | C19  |
| 32  | y     | 324 | AJP  | C26  |
| 32  | y     | 324 | AJP  | C11  |
| 32  | y     | 324 | AJP  | C02  |
| 32  | y     | 324 | AJP  | C22  |
| 32  | y     | 324 | AJP  | C28  |
| 32  | y     | 324 | AJP  | C12  |
| 32  | y     | 324 | AJP  | C30  |
| 32  | y     | 324 | AJP  | C10  |
| 32  | y     | 324 | AJP  | C16  |
| 32  | y     | 324 | AJP  | C27  |

All (3987) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 1     | 302 | CHL  | C1A-C2A-CAA-CBA |
| 24  | 1     | 302 | CHL  | C3A-C2A-CAA-CBA |
| 24  | 2     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | 2     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | 2     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | 2     | 601 | CHL  | CBD-CGD-O2D-CED |
| 24  | 2     | 601 | CHL  | C6-C7-C8-C10    |
| 24  | 2     | 603 | CHL  | C1C-C2C-CMC-OMC |
| 24  | 2     | 603 | CHL  | C3C-C2C-CMC-OMC |
| 24  | 2     | 603 | CHL  | CAD-CBD-CGD-O1D |
| 24  | 2     | 603 | CHL  | CBD-CGD-O2D-CED |
| 24  | S     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 24  | S     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 24  | S     | 306 | CHL  | CAD-CBD-CGD-O1D |
| 24  | S     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 24  | S     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 24  | G     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | G     | 601 | CHL  | C2-C3-C5-C6     |
| 24  | G     | 601 | CHL  | C11-C10-C8-C7   |
| 24  | G     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 24  | G     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 24  | G     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 24  | G     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 24  | G     | 607 | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | G     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 24  | G     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 24  | G     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 24  | G     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 24  | G     | 608 | CHL  | CBD-CGD-O2D-CED |
| 24  | G     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 24  | G     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 24  | N     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 24  | N     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | N     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | N     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 24  | N     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | N     | 601 | CHL  | C2-C3-C5-C6     |
| 24  | N     | 601 | CHL  | C4-C3-C5-C6     |
| 24  | N     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 24  | N     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 24  | N     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 24  | N     | 607 | CHL  | CAD-CBD-CGD-O2D |
| 24  | N     | 607 | CHL  | C4-C3-C5-C6     |
| 24  | N     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 24  | N     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 24  | N     | 608 | CHL  | CHA-CBD-CGD-O2D |
| 24  | N     | 609 | CHL  | C1A-C2A-CAA-CBA |
| 24  | N     | 609 | CHL  | C3A-C2A-CAA-CBA |
| 24  | N     | 609 | CHL  | C11-C10-C8-C9   |
| 24  | Y     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 24  | Y     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 24  | Y     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 24  | Y     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 24  | Y     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 24  | Y     | 309 | CHL  | CHA-CBD-CGD-O2D |
| 24  | Y     | 309 | CHL  | C14-C13-C15-C16 |
| 24  | Y     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 24  | R     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 24  | R     | 606 | CHL  | CHA-CBD-CGD-O1D |
| 24  | R     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 24  | R     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 24  | R     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 24  | R     | 613 | CHL  | CHA-CBD-CGD-O1D |
| 24  | R     | 613 | CHL  | CHA-CBD-CGD-O2D |
| 24  | R     | 613 | CHL  | CAD-CBD-CGD-O1D |
| 24  | 5     | 302 | CHL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 5     | 302 | CHL  | C3A-C2A-CAA-CBA |
| 24  | 6     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | 6     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | 6     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | 6     | 601 | CHL  | CBD-CGD-O2D-CED |
| 24  | 6     | 601 | CHL  | C6-C7-C8-C10    |
| 24  | 6     | 603 | CHL  | C1C-C2C-CMC-OMC |
| 24  | 6     | 603 | CHL  | C3C-C2C-CMC-OMC |
| 24  | 6     | 603 | CHL  | CAD-CBD-CGD-O1D |
| 24  | 6     | 603 | CHL  | CBD-CGD-O2D-CED |
| 24  | s     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 24  | s     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 24  | s     | 306 | CHL  | CAD-CBD-CGD-O1D |
| 24  | s     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 24  | s     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 24  | g     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | g     | 601 | CHL  | C2-C3-C5-C6     |
| 24  | g     | 601 | CHL  | C11-C10-C8-C7   |
| 24  | g     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 24  | g     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 24  | g     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 24  | g     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 24  | g     | 607 | CHL  | CHA-CBD-CGD-O1D |
| 24  | g     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 24  | g     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 24  | g     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 24  | g     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 24  | g     | 608 | CHL  | CBD-CGD-O2D-CED |
| 24  | g     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 24  | g     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 24  | n     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | n     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 24  | n     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 24  | n     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | n     | 601 | CHL  | C2-C3-C5-C6     |
| 24  | n     | 601 | CHL  | C4-C3-C5-C6     |
| 24  | n     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 24  | n     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 24  | n     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 24  | n     | 607 | CHL  | CAD-CBD-CGD-O2D |
| 24  | n     | 607 | CHL  | C4-C3-C5-C6     |
| 24  | n     | 608 | CHL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | n     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 24  | n     | 608 | CHL  | CHA-CBD-CGD-O2D |
| 24  | n     | 609 | CHL  | C1A-C2A-CAA-CBA |
| 24  | n     | 609 | CHL  | C3A-C2A-CAA-CBA |
| 24  | n     | 609 | CHL  | C11-C10-C8-C9   |
| 24  | y     | 302 | CHL  | C1C-C2C-CMC-OMC |
| 24  | y     | 302 | CHL  | C3C-C2C-CMC-OMC |
| 24  | y     | 302 | CHL  | CHA-CBD-CGD-O2D |
| 24  | y     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 24  | y     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 24  | y     | 309 | CHL  | CHA-CBD-CGD-O2D |
| 24  | y     | 309 | CHL  | C14-C13-C15-C16 |
| 24  | y     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 24  | r     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 24  | r     | 606 | CHL  | CHA-CBD-CGD-O1D |
| 24  | r     | 606 | CHL  | CHA-CBD-CGD-O2D |
| 24  | r     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 24  | r     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 24  | r     | 613 | CHL  | CHA-CBD-CGD-O1D |
| 24  | r     | 613 | CHL  | CHA-CBD-CGD-O2D |
| 24  | r     | 613 | CHL  | CAD-CBD-CGD-O1D |
| 25  | 2     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 2     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 25  | 2     | 602 | CLA  | CAD-CBD-CGD-O1D |
| 25  | 2     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 25  | 2     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 604 | CLA  | C2-C3-C5-C6     |
| 25  | 2     | 605 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 2     | 605 | CLA  | C3A-C2A-CAA-CBA |
| 25  | A     | 402 | CLA  | CHA-CBD-CGD-O2D |
| 25  | B     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 25  | B     | 601 | CLA  | CAD-CBD-CGD-O1D |
| 25  | B     | 601 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 602 | CLA  | C2-C3-C5-C6     |
| 25  | B     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 604 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 604 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 25  | B     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 612 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 25  | B     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 25  | B     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 25  | C     | 504 | CLA  | C4-C3-C5-C6     |
| 25  | C     | 506 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C2-C3-C5-C6     |
| 25  | C     | 507 | CLA  | C11-C10-C8-C9   |
| 25  | D     | 401 | CLA  | CHA-CBD-CGD-O2D |
| 25  | D     | 402 | CLA  | C1A-C2A-CAA-CBA |
| 25  | D     | 402 | CLA  | C3A-C2A-CAA-CBA |
| 25  | D     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 25  | D     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 25  | S     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 25  | S     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 25  | S     | 305 | CLA  | CHA-CBD-CGD-O2D |
| 25  | S     | 305 | CLA  | CBD-CGD-O2D-CED |
| 25  | S     | 310 | CLA  | C1-C2-C3-C4     |
| 25  | S     | 310 | CLA  | C2-C3-C5-C6     |
| 25  | S     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 25  | S     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 25  | S     | 311 | CLA  | CAD-CBD-CGD-O1D |
| 25  | S     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 25  | S     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 25  | S     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | G     | 610 | CLA  | CBD-CGD-O2D-CED |
| 25  | G     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 611 | CLA  | CAD-CBD-CGD-O1D |
| 25  | G     | 611 | CLA  | CAD-CBD-CGD-O2D |
| 25  | G     | 611 | CLA  | C2-C3-C5-C6     |
| 25  | G     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 25  | N     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | N     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | N     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | N     | 610 | CLA  | C1-C2-C3-C4     |
| 25  | N     | 610 | CLA  | C4-C3-C5-C6     |
| 25  | N     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | N     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | N     | 613 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | N     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | N     | 614 | CLA  | CBD-CGD-O2D-CED |
| 25  | Y     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 25  | Y     | 305 | CLA  | CBD-CGD-O2D-CED |
| 25  | Y     | 311 | CLA  | CBD-CGD-O2D-CED |
| 25  | Y     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 25  | Y     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 25  | Y     | 314 | CLA  | CHA-CBD-CGD-O1D |
| 25  | Y     | 314 | CLA  | C14-C13-C15-C16 |
| 25  | Y     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 25  | Y     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 25  | Y     | 315 | CLA  | CBD-CGD-O2D-CED |
| 25  | Y     | 315 | CLA  | O1D-CGD-O2D-CED |
| 25  | R     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 25  | R     | 603 | CLA  | CBD-CGD-O2D-CED |
| 25  | R     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | R     | 608 | CLA  | CHA-CBD-CGD-O2D |
| 25  | R     | 608 | CLA  | CBD-CGD-O2D-CED |
| 25  | R     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 25  | R     | 611 | CLA  | CBD-CGD-O2D-CED |
| 25  | R     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 25  | R     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 6     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 6     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 25  | 6     | 602 | CLA  | CAD-CBD-CGD-O1D |
| 25  | 6     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 25  | 6     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | 6     | 604 | CLA  | C2-C3-C5-C6     |
| 25  | 6     | 605 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 6     | 605 | CLA  | C3A-C2A-CAA-CBA |
| 25  | a     | 403 | CLA  | CHA-CBD-CGD-O2D |
| 25  | b     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 25  | b     | 601 | CLA  | CAD-CBD-CGD-O1D |
| 25  | b     | 601 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 602 | CLA  | C2-C3-C5-C6     |
| 25  | b     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 604 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | b     | 604 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 604 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 25  | b     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 25  | b     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 25  | b     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 25  | b     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 25  | c     | 504 | CLA  | C4-C3-C5-C6     |
| 25  | c     | 506 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 507 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 507 | CLA  | C11-C10-C8-C9   |
| 25  | d     | 401 | CLA  | CHA-CBD-CGD-O2D |
| 25  | d     | 402 | CLA  | C1A-C2A-CAA-CBA |
| 25  | d     | 402 | CLA  | C3A-C2A-CAA-CBA |
| 25  | d     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 25  | d     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 25  | s     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 25  | s     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 25  | s     | 305 | CLA  | CHA-CBD-CGD-O2D |
| 25  | s     | 305 | CLA  | CBD-CGD-O2D-CED |
| 25  | s     | 310 | CLA  | C1-C2-C3-C4     |
| 25  | s     | 310 | CLA  | C2-C3-C5-C6     |
| 25  | s     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 25  | s     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 25  | s     | 311 | CLA  | CAD-CBD-CGD-O1D |
| 25  | s     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 25  | s     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 25  | s     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 610 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 611 | CLA  | CAD-CBD-CGD-O1D |
| 25  | g     | 611 | CLA  | CAD-CBD-CGD-O2D |
| 25  | g     | 611 | CLA  | C2-C3-C5-C6     |
| 25  | g     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 25  | n     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | n     | 604 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | n     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | n     | 610 | CLA  | C1-C2-C3-C4     |
| 25  | n     | 610 | CLA  | C4-C3-C5-C6     |
| 25  | n     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | n     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | n     | 613 | CLA  | CHA-CBD-CGD-O1D |
| 25  | n     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 614 | CLA  | CBD-CGD-O2D-CED |
| 25  | y     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 25  | y     | 305 | CLA  | CBD-CGD-O2D-CED |
| 25  | y     | 311 | CLA  | CBD-CGD-O2D-CED |
| 25  | y     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 25  | y     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 25  | y     | 314 | CLA  | CHA-CBD-CGD-O1D |
| 25  | y     | 314 | CLA  | C14-C13-C15-C16 |
| 25  | y     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 25  | y     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 25  | y     | 315 | CLA  | CBD-CGD-O2D-CED |
| 25  | y     | 315 | CLA  | O1D-CGD-O2D-CED |
| 25  | r     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 25  | r     | 603 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | r     | 608 | CLA  | CHA-CBD-CGD-O2D |
| 25  | r     | 608 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 25  | r     | 611 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 25  | r     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 26  | 2     | 606 | LHG  | C3-O3-P-O4      |
| 26  | 2     | 606 | LHG  | C3-O3-P-O6      |
| 26  | 2     | 606 | LHG  | O7-C5-C6-O8     |
| 26  | C     | 517 | LHG  | C1-C2-C3-O3     |
| 26  | C     | 518 | LHG  | C3-O3-P-O6      |
| 26  | C     | 518 | LHG  | C8-C7-O7-C5     |
| 26  | C     | 519 | LHG  | C4-O6-P-O4      |
| 26  | C     | 519 | LHG  | C4-O6-P-O5      |
| 26  | C     | 519 | LHG  | C8-C7-O7-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | D     | 406 | LHG  | O1-C1-C2-O2     |
| 26  | D     | 406 | LHG  | O1-C1-C2-C3     |
| 26  | D     | 406 | LHG  | C1-C2-C3-O3     |
| 26  | L     | 102 | LHG  | C4-O6-P-O4      |
| 26  | L     | 102 | LHG  | C4-O6-P-O5      |
| 26  | S     | 301 | LHG  | O1-C1-C2-C3     |
| 26  | S     | 318 | LHG  | O1-C1-C2-C3     |
| 26  | N     | 618 | LHG  | O1-C1-C2-C3     |
| 26  | Y     | 301 | LHG  | C1-C2-C3-O3     |
| 26  | Y     | 319 | LHG  | O1-C1-C2-C3     |
| 26  | Y     | 319 | LHG  | C3-O3-P-O4      |
| 26  | Y     | 319 | LHG  | C3-O3-P-O5      |
| 26  | Y     | 319 | LHG  | C3-O3-P-O6      |
| 26  | 6     | 606 | LHG  | C3-O3-P-O4      |
| 26  | 6     | 606 | LHG  | C3-O3-P-O6      |
| 26  | 6     | 606 | LHG  | O7-C5-C6-O8     |
| 26  | c     | 517 | LHG  | C1-C2-C3-O3     |
| 26  | c     | 518 | LHG  | C3-O3-P-O6      |
| 26  | c     | 518 | LHG  | C8-C7-O7-C5     |
| 26  | c     | 519 | LHG  | C4-O6-P-O5      |
| 26  | c     | 519 | LHG  | C8-C7-O7-C5     |
| 26  | d     | 406 | LHG  | O1-C1-C2-O2     |
| 26  | d     | 406 | LHG  | O1-C1-C2-C3     |
| 26  | d     | 406 | LHG  | C1-C2-C3-O3     |
| 26  | l     | 103 | LHG  | C4-O6-P-O4      |
| 26  | l     | 103 | LHG  | C4-O6-P-O5      |
| 26  | s     | 301 | LHG  | O1-C1-C2-C3     |
| 26  | s     | 318 | LHG  | O1-C1-C2-C3     |
| 26  | n     | 618 | LHG  | O1-C1-C2-C3     |
| 26  | y     | 301 | LHG  | C1-C2-C3-O3     |
| 26  | y     | 319 | LHG  | O1-C1-C2-C3     |
| 26  | y     | 319 | LHG  | C3-O3-P-O4      |
| 26  | y     | 319 | LHG  | C3-O3-P-O5      |
| 26  | y     | 319 | LHG  | C3-O3-P-O6      |
| 27  | A     | 403 | PHO  | O1A-CGA-O2A-C1  |
| 27  | a     | 404 | PHO  | O1A-CGA-O2A-C1  |
| 28  | A     | 406 | BCR  | C14-C15-C16-C17 |
| 28  | A     | 406 | BCR  | C16-C17-C18-C19 |
| 28  | A     | 406 | BCR  | C16-C17-C18-C36 |
| 28  | B     | 618 | BCR  | C23-C24-C25-C30 |
| 28  | D     | 404 | BCR  | C1-C6-C7-C8     |
| 28  | D     | 404 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | H     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | H     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | H     | 101 | BCR  | C22-C23-C24-C25 |
| 28  | I     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | K     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | T     | 101 | BCR  | C11-C10-C9-C8   |
| 28  | T     | 101 | BCR  | C11-C10-C9-C34  |
| 28  | T     | 101 | BCR  | C11-C12-C13-C35 |
| 28  | T     | 101 | BCR  | C13-C14-C15-C16 |
| 28  | T     | 101 | BCR  | C21-C22-C23-C24 |
| 28  | T     | 101 | BCR  | C37-C22-C23-C24 |
| 28  | T     | 101 | BCR  | C22-C23-C24-C25 |
| 28  | Z     | 101 | BCR  | C1-C6-C7-C8     |
| 28  | Z     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | Z     | 101 | BCR  | C11-C12-C13-C35 |
| 28  | Z     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | Z     | 101 | BCR  | C21-C22-C23-C24 |
| 28  | Z     | 101 | BCR  | C37-C22-C23-C24 |
| 28  | a     | 407 | BCR  | C14-C15-C16-C17 |
| 28  | a     | 407 | BCR  | C16-C17-C18-C19 |
| 28  | a     | 407 | BCR  | C16-C17-C18-C36 |
| 28  | b     | 618 | BCR  | C23-C24-C25-C30 |
| 28  | d     | 404 | BCR  | C1-C6-C7-C8     |
| 28  | d     | 404 | BCR  | C7-C8-C9-C10    |
| 28  | h     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | h     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | h     | 101 | BCR  | C22-C23-C24-C25 |
| 28  | i     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | k     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | t     | 101 | BCR  | C11-C10-C9-C8   |
| 28  | t     | 101 | BCR  | C11-C10-C9-C34  |
| 28  | t     | 101 | BCR  | C11-C12-C13-C35 |
| 28  | t     | 101 | BCR  | C13-C14-C15-C16 |
| 28  | t     | 101 | BCR  | C21-C22-C23-C24 |
| 28  | t     | 101 | BCR  | C37-C22-C23-C24 |
| 28  | t     | 101 | BCR  | C22-C23-C24-C25 |
| 28  | z     | 101 | BCR  | C1-C6-C7-C8     |
| 28  | z     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | z     | 101 | BCR  | C11-C12-C13-C35 |
| 28  | z     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | z     | 101 | BCR  | C21-C22-C23-C24 |
| 28  | z     | 101 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | A     | 407 | SQD  | C2-C1-O6-C44    |
| 29  | A     | 407 | SQD  | O5-C1-O6-C44    |
| 29  | A     | 407 | SQD  | O49-C7-O47-C45  |
| 29  | A     | 407 | SQD  | O5-C5-C6-S      |
| 29  | A     | 411 | SQD  | O5-C1-O6-C44    |
| 29  | A     | 411 | SQD  | O5-C5-C6-S      |
| 29  | L     | 101 | SQD  | O47-C45-C46-O48 |
| 29  | L     | 103 | SQD  | C2-C1-O6-C44    |
| 29  | L     | 103 | SQD  | O5-C1-O6-C44    |
| 29  | L     | 103 | SQD  | O49-C7-O47-C45  |
| 29  | L     | 103 | SQD  | C8-C7-O47-C45   |
| 29  | L     | 103 | SQD  | O5-C5-C6-S      |
| 29  | a     | 408 | SQD  | C2-C1-O6-C44    |
| 29  | a     | 408 | SQD  | O5-C1-O6-C44    |
| 29  | a     | 408 | SQD  | O49-C7-O47-C45  |
| 29  | a     | 408 | SQD  | O5-C5-C6-S      |
| 29  | a     | 412 | SQD  | O5-C1-O6-C44    |
| 29  | a     | 412 | SQD  | O5-C5-C6-S      |
| 29  | l     | 101 | SQD  | C2-C1-O6-C44    |
| 29  | l     | 101 | SQD  | O5-C1-O6-C44    |
| 29  | l     | 101 | SQD  | O49-C7-O47-C45  |
| 29  | l     | 101 | SQD  | C8-C7-O47-C45   |
| 29  | l     | 101 | SQD  | O5-C5-C6-S      |
| 29  | l     | 102 | SQD  | O47-C45-C46-O48 |
| 30  | A     | 410 | LMG  | O7-C8-C9-O8     |
| 30  | B     | 623 | LMG  | C2-C1-O1-C7     |
| 30  | B     | 623 | LMG  | O6-C1-O1-C7     |
| 30  | B     | 623 | LMG  | O9-C10-O7-C8    |
| 30  | C     | 520 | LMG  | C2-C1-O1-C7     |
| 30  | C     | 520 | LMG  | O9-C10-O7-C8    |
| 30  | a     | 411 | LMG  | O7-C8-C9-O8     |
| 30  | b     | 623 | LMG  | C2-C1-O1-C7     |
| 30  | b     | 623 | LMG  | O6-C1-O1-C7     |
| 30  | b     | 623 | LMG  | O9-C10-O7-C8    |
| 30  | c     | 520 | LMG  | C2-C1-O1-C7     |
| 30  | c     | 520 | LMG  | O9-C10-O7-C8    |
| 32  | A     | 412 | AJP  | C22-C23-O25-C26 |
| 32  | S     | 319 | AJP  | C29-C30-C32-O33 |
| 32  | S     | 319 | AJP  | O31-C30-C32-O33 |
| 32  | N     | 620 | AJP  | C22-C23-O25-C26 |
| 32  | N     | 620 | AJP  | C27-C26-O25-C23 |
| 32  | N     | 620 | AJP  | C29-C30-C32-O33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | N     | 620 | AJP  | O31-C30-C32-O33 |
| 32  | Y     | 320 | AJP  | O31-C30-C32-O33 |
| 32  | Y     | 321 | AJP  | C24-C23-O25-C26 |
| 32  | Y     | 321 | AJP  | C29-C30-C32-O33 |
| 32  | Y     | 321 | AJP  | O31-C30-C32-O33 |
| 32  | Y     | 324 | AJP  | C29-C30-C32-O33 |
| 32  | Y     | 324 | AJP  | O31-C30-C32-O33 |
| 32  | a     | 413 | AJP  | C22-C23-O25-C26 |
| 32  | s     | 319 | AJP  | C29-C30-C32-O33 |
| 32  | s     | 319 | AJP  | O31-C30-C32-O33 |
| 32  | n     | 620 | AJP  | C22-C23-O25-C26 |
| 32  | n     | 620 | AJP  | C27-C26-O25-C23 |
| 32  | n     | 620 | AJP  | C29-C30-C32-O33 |
| 32  | n     | 620 | AJP  | O31-C30-C32-O33 |
| 32  | y     | 320 | AJP  | O31-C30-C32-O33 |
| 32  | y     | 321 | AJP  | C24-C23-O25-C26 |
| 32  | y     | 321 | AJP  | C29-C30-C32-O33 |
| 32  | y     | 321 | AJP  | O31-C30-C32-O33 |
| 32  | y     | 324 | AJP  | C29-C30-C32-O33 |
| 32  | y     | 324 | AJP  | O31-C30-C32-O33 |
| 35  | A     | 415 | DGD  | C2A-C1A-O1G-C1G |
| 35  | A     | 415 | DGD  | O1A-C1A-O1G-C1G |
| 35  | A     | 415 | DGD  | C2B-C1B-O2G-C2G |
| 35  | A     | 415 | DGD  | C2D-C1D-O3G-C3G |
| 35  | A     | 415 | DGD  | O6D-C1D-O3G-C3G |
| 35  | C     | 516 | DGD  | C2D-C1D-O3G-C3G |
| 35  | C     | 516 | DGD  | C2E-C1E-O5D-C6D |
| 35  | C     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 35  | a     | 401 | DGD  | C2A-C1A-O1G-C1G |
| 35  | a     | 401 | DGD  | O1A-C1A-O1G-C1G |
| 35  | a     | 401 | DGD  | C2B-C1B-O2G-C2G |
| 35  | a     | 401 | DGD  | C2D-C1D-O3G-C3G |
| 35  | a     | 401 | DGD  | O6D-C1D-O3G-C3G |
| 35  | c     | 516 | DGD  | C2D-C1D-O3G-C3G |
| 35  | c     | 516 | DGD  | C2E-C1E-O5D-C6D |
| 35  | c     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 39  | N     | 616 | LUT  | C7-C8-C9-C10    |
| 39  | N     | 616 | LUT  | C7-C8-C9-C19    |
| 39  | n     | 616 | LUT  | C7-C8-C9-C10    |
| 39  | n     | 616 | LUT  | C7-C8-C9-C19    |
| 40  | S     | 317 | NEX  | C11-C12-C13-C14 |
| 40  | S     | 317 | NEX  | C11-C12-C13-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 40  | G     | 617 | NEX  | C9-C10-C11-C12  |
| 40  | G     | 617 | NEX  | C11-C12-C13-C20 |
| 40  | G     | 617 | NEX  | C21-C26-C27-C28 |
| 40  | G     | 617 | NEX  | C25-C26-C27-C28 |
| 40  | G     | 617 | NEX  | C27-C28-C29-C30 |
| 40  | G     | 617 | NEX  | C27-C28-C29-C39 |
| 40  | N     | 617 | NEX  | C7-C8-C9-C10    |
| 40  | N     | 617 | NEX  | C27-C28-C29-C30 |
| 40  | N     | 617 | NEX  | C27-C28-C29-C39 |
| 40  | N     | 617 | NEX  | C31-C32-C33-C34 |
| 40  | N     | 617 | NEX  | C31-C32-C33-C40 |
| 40  | Y     | 318 | NEX  | C9-C10-C11-C12  |
| 40  | Y     | 318 | NEX  | C21-C26-C27-C28 |
| 40  | Y     | 318 | NEX  | C27-C28-C29-C30 |
| 40  | Y     | 318 | NEX  | C27-C28-C29-C39 |
| 40  | R     | 617 | NEX  | C9-C10-C11-C12  |
| 40  | R     | 617 | NEX  | C11-C12-C13-C14 |
| 40  | R     | 617 | NEX  | C11-C12-C13-C20 |
| 40  | s     | 317 | NEX  | C11-C12-C13-C14 |
| 40  | s     | 317 | NEX  | C11-C12-C13-C20 |
| 40  | g     | 617 | NEX  | C9-C10-C11-C12  |
| 40  | g     | 617 | NEX  | C11-C12-C13-C20 |
| 40  | g     | 617 | NEX  | C21-C26-C27-C28 |
| 40  | g     | 617 | NEX  | C25-C26-C27-C28 |
| 40  | g     | 617 | NEX  | C27-C28-C29-C30 |
| 40  | g     | 617 | NEX  | C27-C28-C29-C39 |
| 40  | n     | 617 | NEX  | C7-C8-C9-C10    |
| 40  | n     | 617 | NEX  | C27-C28-C29-C30 |
| 40  | n     | 617 | NEX  | C27-C28-C29-C39 |
| 40  | n     | 617 | NEX  | C31-C32-C33-C34 |
| 40  | n     | 617 | NEX  | C31-C32-C33-C40 |
| 40  | y     | 318 | NEX  | C9-C10-C11-C12  |
| 40  | y     | 318 | NEX  | C21-C26-C27-C28 |
| 40  | y     | 318 | NEX  | C27-C28-C29-C30 |
| 40  | y     | 318 | NEX  | C27-C28-C29-C39 |
| 40  | r     | 617 | NEX  | C9-C10-C11-C12  |
| 40  | r     | 617 | NEX  | C11-C12-C13-C14 |
| 40  | r     | 617 | NEX  | C11-C12-C13-C20 |
| 24  | Y     | 308 | CHL  | C2C-C3C-CAC-CBC |
| 24  | Y     | 308 | CHL  | C4C-C3C-CAC-CBC |
| 24  | y     | 308 | CHL  | C2C-C3C-CAC-CBC |
| 24  | y     | 308 | CHL  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | N     | 602 | CLA  | C4C-C3C-CAC-CBC |
| 25  | n     | 602 | CLA  | C4C-C3C-CAC-CBC |
| 32  | B     | 624 | AJP  | C30-C29-O34-C35 |
| 32  | b     | 624 | AJP  | C30-C29-O34-C35 |
| 25  | 2     | 604 | CLA  | O1D-CGD-O2D-CED |
| 25  | 2     | 605 | CLA  | O1D-CGD-O2D-CED |
| 25  | B     | 605 | CLA  | O1D-CGD-O2D-CED |
| 25  | S     | 305 | CLA  | O1D-CGD-O2D-CED |
| 25  | G     | 604 | CLA  | O1D-CGD-O2D-CED |
| 25  | G     | 610 | CLA  | O1D-CGD-O2D-CED |
| 25  | Y     | 311 | CLA  | O1D-CGD-O2D-CED |
| 25  | 6     | 604 | CLA  | O1D-CGD-O2D-CED |
| 25  | 6     | 605 | CLA  | O1D-CGD-O2D-CED |
| 25  | b     | 605 | CLA  | O1D-CGD-O2D-CED |
| 25  | s     | 305 | CLA  | O1D-CGD-O2D-CED |
| 25  | g     | 604 | CLA  | O1D-CGD-O2D-CED |
| 25  | g     | 610 | CLA  | O1D-CGD-O2D-CED |
| 25  | y     | 311 | CLA  | O1D-CGD-O2D-CED |
| 32  | B     | 624 | AJP  | O70-C65-O64-C57 |
| 32  | b     | 624 | AJP  | O70-C65-O64-C57 |
| 25  | G     | 614 | CLA  | C2C-C3C-CAC-CBC |
| 25  | G     | 614 | CLA  | C4C-C3C-CAC-CBC |
| 25  | N     | 602 | CLA  | C2C-C3C-CAC-CBC |
| 25  | g     | 614 | CLA  | C2C-C3C-CAC-CBC |
| 25  | g     | 614 | CLA  | C4C-C3C-CAC-CBC |
| 25  | n     | 602 | CLA  | C2C-C3C-CAC-CBC |
| 24  | 2     | 601 | CHL  | O1D-CGD-O2D-CED |
| 24  | N     | 608 | CHL  | O1D-CGD-O2D-CED |
| 24  | 6     | 601 | CHL  | O1D-CGD-O2D-CED |
| 24  | n     | 608 | CHL  | O1D-CGD-O2D-CED |
| 25  | A     | 401 | CLA  | O1D-CGD-O2D-CED |
| 25  | S     | 313 | CLA  | O1D-CGD-O2D-CED |
| 25  | N     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | R     | 603 | CLA  | O1D-CGD-O2D-CED |
| 25  | R     | 611 | CLA  | O1D-CGD-O2D-CED |
| 25  | a     | 402 | CLA  | O1D-CGD-O2D-CED |
| 25  | s     | 313 | CLA  | O1D-CGD-O2D-CED |
| 25  | n     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | r     | 603 | CLA  | O1D-CGD-O2D-CED |
| 25  | r     | 611 | CLA  | O1D-CGD-O2D-CED |
| 24  | N     | 607 | CHL  | CBD-CGD-O2D-CED |
| 24  | N     | 608 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | Y     | 309 | CHL  | CBD-CGD-O2D-CED |
| 24  | Y     | 310 | CHL  | CBD-CGD-O2D-CED |
| 24  | R     | 606 | CHL  | CBD-CGD-O2D-CED |
| 24  | n     | 607 | CHL  | CBD-CGD-O2D-CED |
| 24  | n     | 608 | CHL  | CBD-CGD-O2D-CED |
| 24  | y     | 309 | CHL  | CBD-CGD-O2D-CED |
| 24  | y     | 310 | CHL  | CBD-CGD-O2D-CED |
| 24  | r     | 606 | CHL  | CBD-CGD-O2D-CED |
| 25  | 2     | 605 | CLA  | CBD-CGD-O2D-CED |
| 25  | A     | 401 | CLA  | CBD-CGD-O2D-CED |
| 25  | B     | 605 | CLA  | CBD-CGD-O2D-CED |
| 25  | C     | 502 | CLA  | CBD-CGD-O2D-CED |
| 25  | C     | 503 | CLA  | CBD-CGD-O2D-CED |
| 25  | S     | 304 | CLA  | CBD-CGD-O2D-CED |
| 25  | S     | 309 | CLA  | CBD-CGD-O2D-CED |
| 25  | S     | 313 | CLA  | CBD-CGD-O2D-CED |
| 25  | G     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | N     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | N     | 610 | CLA  | CBD-CGD-O2D-CED |
| 25  | N     | 611 | CLA  | CBD-CGD-O2D-CED |
| 25  | R     | 609 | CLA  | CBD-CGD-O2D-CED |
| 25  | 6     | 605 | CLA  | CBD-CGD-O2D-CED |
| 25  | a     | 402 | CLA  | CBD-CGD-O2D-CED |
| 25  | b     | 605 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 502 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 503 | CLA  | CBD-CGD-O2D-CED |
| 25  | s     | 304 | CLA  | CBD-CGD-O2D-CED |
| 25  | s     | 309 | CLA  | CBD-CGD-O2D-CED |
| 25  | s     | 313 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 604 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 610 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 611 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 609 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 2     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 2     | 605 | CLA  | O1A-CGA-O2A-C1  |
| 25  | G     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 6     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 6     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 6     | 605 | CLA  | O1A-CGA-O2A-C1  |
| 25  | g     | 614 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | Y     | 322 | AJP  | O31-C26-O25-C23 |
| 32  | y     | 322 | AJP  | O31-C26-O25-C23 |
| 32  | Y     | 324 | AJP  | C27-C26-O25-C23 |
| 32  | y     | 324 | AJP  | C27-C26-O25-C23 |
| 24  | G     | 608 | CHL  | O1D-CGD-O2D-CED |
| 24  | Y     | 309 | CHL  | O1D-CGD-O2D-CED |
| 24  | g     | 608 | CHL  | O1D-CGD-O2D-CED |
| 24  | y     | 309 | CHL  | O1D-CGD-O2D-CED |
| 25  | S     | 304 | CLA  | O1D-CGD-O2D-CED |
| 25  | G     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | N     | 614 | CLA  | O1D-CGD-O2D-CED |
| 25  | R     | 608 | CLA  | O1D-CGD-O2D-CED |
| 25  | s     | 304 | CLA  | O1D-CGD-O2D-CED |
| 25  | g     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | n     | 614 | CLA  | O1D-CGD-O2D-CED |
| 25  | r     | 608 | CLA  | O1D-CGD-O2D-CED |
| 24  | S     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 24  | s     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 25  | R     | 608 | CLA  | C4C-C3C-CAC-CBC |
| 25  | r     | 608 | CLA  | C4C-C3C-CAC-CBC |
| 32  | A     | 412 | AJP  | O60-C55-O54-C36 |
| 32  | Y     | 323 | AJP  | O31-C26-O25-C23 |
| 32  | a     | 413 | AJP  | O60-C55-O54-C36 |
| 32  | y     | 323 | AJP  | O31-C26-O25-C23 |
| 32  | B     | 624 | AJP  | C66-C65-O64-C57 |
| 32  | N     | 619 | AJP  | C27-C26-O25-C23 |
| 32  | b     | 624 | AJP  | C66-C65-O64-C57 |
| 32  | n     | 619 | AJP  | C27-C26-O25-C23 |
| 25  | C     | 502 | CLA  | O1D-CGD-O2D-CED |
| 25  | N     | 610 | CLA  | O1D-CGD-O2D-CED |
| 25  | N     | 611 | CLA  | O1D-CGD-O2D-CED |
| 25  | Y     | 314 | CLA  | O1D-CGD-O2D-CED |
| 25  | c     | 502 | CLA  | O1D-CGD-O2D-CED |
| 25  | n     | 610 | CLA  | O1D-CGD-O2D-CED |
| 25  | n     | 611 | CLA  | O1D-CGD-O2D-CED |
| 25  | y     | 314 | CLA  | O1D-CGD-O2D-CED |
| 25  | 2     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 2     | 605 | CLA  | CBA-CGA-O2A-C1  |
| 25  | G     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 6     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 6     | 605 | CLA  | CBA-CGA-O2A-C1  |
| 25  | g     | 614 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | R     | 607 | CHL  | CBD-CGD-O2D-CED |
| 24  | r     | 607 | CHL  | CBD-CGD-O2D-CED |
| 25  | B     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | N     | 602 | CLA  | CBD-CGD-O2D-CED |
| 25  | Y     | 314 | CLA  | CBD-CGD-O2D-CED |
| 25  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 602 | CLA  | CBD-CGD-O2D-CED |
| 25  | y     | 314 | CLA  | CBD-CGD-O2D-CED |
| 24  | S     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 24  | s     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 25  | N     | 613 | CLA  | C2C-C3C-CAC-CBC |
| 25  | N     | 613 | CLA  | C4C-C3C-CAC-CBC |
| 25  | n     | 613 | CLA  | C2C-C3C-CAC-CBC |
| 25  | n     | 613 | CLA  | C4C-C3C-CAC-CBC |
| 25  | B     | 616 | CLA  | O1A-CGA-O2A-C1  |
| 25  | R     | 608 | CLA  | O1A-CGA-O2A-C1  |
| 25  | R     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 25  | R     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 616 | CLA  | O1A-CGA-O2A-C1  |
| 25  | r     | 608 | CLA  | O1A-CGA-O2A-C1  |
| 25  | r     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 25  | r     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 26  | L     | 102 | LHG  | O10-C23-O8-C6   |
| 26  | l     | 103 | LHG  | O10-C23-O8-C6   |
| 24  | 2     | 603 | CHL  | O1D-CGD-O2D-CED |
| 24  | R     | 606 | CHL  | O1D-CGD-O2D-CED |
| 24  | 6     | 603 | CHL  | O1D-CGD-O2D-CED |
| 24  | r     | 606 | CHL  | O1D-CGD-O2D-CED |
| 25  | B     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | S     | 309 | CLA  | O1D-CGD-O2D-CED |
| 25  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 25  | s     | 309 | CLA  | O1D-CGD-O2D-CED |
| 25  | R     | 608 | CLA  | C2C-C3C-CAC-CBC |
| 25  | r     | 608 | CLA  | C2C-C3C-CAC-CBC |
| 32  | S     | 319 | AJP  | C27-C26-O25-C23 |
| 32  | s     | 319 | AJP  | C27-C26-O25-C23 |
| 26  | C     | 518 | LHG  | O9-C7-O7-C5     |
| 26  | C     | 519 | LHG  | O9-C7-O7-C5     |
| 26  | c     | 518 | LHG  | O9-C7-O7-C5     |
| 26  | c     | 519 | LHG  | O9-C7-O7-C5     |
| 35  | A     | 415 | DGD  | O1B-C1B-O2G-C2G |
| 35  | a     | 401 | DGD  | O1B-C1B-O2G-C2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | G     | 609 | CHL  | C3-C5-C6-C7     |
| 24  | N     | 608 | CHL  | C3-C5-C6-C7     |
| 24  | Y     | 308 | CHL  | C3-C5-C6-C7     |
| 24  | g     | 609 | CHL  | C3-C5-C6-C7     |
| 24  | n     | 608 | CHL  | C3-C5-C6-C7     |
| 24  | y     | 308 | CHL  | C3-C5-C6-C7     |
| 25  | B     | 614 | CLA  | C3-C5-C6-C7     |
| 25  | B     | 616 | CLA  | C3-C5-C6-C7     |
| 25  | C     | 512 | CLA  | C3-C5-C6-C7     |
| 25  | b     | 614 | CLA  | C3-C5-C6-C7     |
| 25  | b     | 616 | CLA  | C3-C5-C6-C7     |
| 25  | c     | 512 | CLA  | C3-C5-C6-C7     |
| 25  | B     | 616 | CLA  | CBA-CGA-O2A-C1  |
| 25  | G     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 25  | b     | 616 | CLA  | CBA-CGA-O2A-C1  |
| 25  | g     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 25  | r     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 25  | r     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 26  | L     | 102 | LHG  | C24-C23-O8-C6   |
| 26  | l     | 103 | LHG  | C24-C23-O8-C6   |
| 27  | A     | 403 | PHO  | CBA-CGA-O2A-C1  |
| 27  | a     | 404 | PHO  | CBA-CGA-O2A-C1  |
| 29  | L     | 103 | SQD  | C24-C23-O48-C46 |
| 29  | l     | 101 | SQD  | C24-C23-O48-C46 |
| 24  | N     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 24  | n     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 29  | A     | 407 | SQD  | C8-C7-O47-C45   |
| 29  | a     | 408 | SQD  | C8-C7-O47-C45   |
| 30  | B     | 623 | LMG  | C11-C10-O7-C8   |
| 30  | C     | 520 | LMG  | C11-C10-O7-C8   |
| 30  | b     | 623 | LMG  | C11-C10-O7-C8   |
| 30  | c     | 520 | LMG  | C11-C10-O7-C8   |
| 25  | G     | 603 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 603 | CLA  | CBD-CGD-O2D-CED |
| 25  | B     | 616 | CLA  | C2C-C3C-CAC-CBC |
| 25  | b     | 616 | CLA  | C2C-C3C-CAC-CBC |
| 25  | D     | 403 | CLA  | O1A-CGA-O2A-C1  |
| 25  | d     | 403 | CLA  | O1A-CGA-O2A-C1  |
| 26  | C     | 519 | LHG  | O10-C23-O8-C6   |
| 26  | c     | 519 | LHG  | O10-C23-O8-C6   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | y     | 304 | CLA  | C2C-C3C-CAC-CBC |
| 25  | Y     | 304 | CLA  | C2C-C3C-CAC-CBC |
| 25  | 2     | 604 | CLA  | C4-C3-C5-C6     |
| 25  | B     | 602 | CLA  | C4-C3-C5-C6     |
| 25  | S     | 303 | CLA  | C4-C3-C5-C6     |
| 25  | G     | 611 | CLA  | C4-C3-C5-C6     |
| 25  | R     | 609 | CLA  | C4-C3-C5-C6     |
| 25  | 6     | 604 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 602 | CLA  | C4-C3-C5-C6     |
| 25  | s     | 303 | CLA  | C4-C3-C5-C6     |
| 25  | g     | 611 | CLA  | C4-C3-C5-C6     |
| 25  | r     | 609 | CLA  | C4-C3-C5-C6     |
| 30  | A     | 408 | LMG  | C4-C5-C6-O5     |
| 30  | a     | 409 | LMG  | C4-C5-C6-O5     |
| 24  | N     | 607 | CHL  | C2-C3-C5-C6     |
| 24  | n     | 607 | CHL  | C2-C3-C5-C6     |
| 25  | C     | 504 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 504 | CLA  | C2-C3-C5-C6     |
| 24  | G     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 24  | Y     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 24  | R     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 24  | g     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 24  | y     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 24  | r     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 25  | 2     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | B     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 25  | G     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 25  | 6     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 25  | c     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 25  | g     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 24  | G     | 608 | CHL  | C3-C5-C6-C7     |
| 24  | N     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | R     | 607 | CHL  | C3-C5-C6-C7     |
| 24  | g     | 608 | CHL  | C3-C5-C6-C7     |
| 24  | n     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | r     | 607 | CHL  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | C     | 504 | CLA  | C3-C5-C6-C7     |
| 25  | c     | 504 | CLA  | C3-C5-C6-C7     |
| 25  | S     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 25  | s     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 35  | C     | 515 | DGD  | C4E-C5E-C6E-O5E |
| 35  | c     | 515 | DGD  | C4E-C5E-C6E-O5E |
| 24  | N     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 24  | n     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 24  | Y     | 310 | CHL  | O1D-CGD-O2D-CED |
| 24  | y     | 310 | CHL  | O1D-CGD-O2D-CED |
| 25  | B     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 25  | C     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 25  | S     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 25  | c     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 25  | s     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 29  | L     | 103 | SQD  | O10-C23-O48-C46 |
| 29  | l     | 101 | SQD  | O10-C23-O48-C46 |
| 25  | Y     | 305 | CLA  | C2C-C3C-CAC-CBC |
| 25  | y     | 305 | CLA  | C2C-C3C-CAC-CBC |
| 39  | S     | 316 | LUT  | C33-C34-C35-C15 |
| 39  | s     | 316 | LUT  | C33-C34-C35-C15 |
| 40  | N     | 617 | NEX  | C9-C10-C11-C12  |
| 40  | n     | 617 | NEX  | C9-C10-C11-C12  |
| 32  | A     | 412 | AJP  | O70-C69-C71-O72 |
| 32  | a     | 413 | AJP  | O70-C69-C71-O72 |
| 29  | L     | 101 | SQD  | C10-C11-C12-C13 |
| 29  | l     | 102 | SQD  | C10-C11-C12-C13 |
| 35  | C     | 516 | DGD  | CCA-CDA-CEA-CFA |
| 35  | c     | 516 | DGD  | CCA-CDA-CEA-CFA |
| 25  | C     | 504 | CLA  | CBD-CGD-O2D-CED |
| 25  | C     | 508 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 504 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 508 | CLA  | CBD-CGD-O2D-CED |
| 26  | B     | 622 | LHG  | O2-C2-C3-O3     |
| 26  | C     | 517 | LHG  | O2-C2-C3-O3     |
| 26  | D     | 406 | LHG  | O2-C2-C3-O3     |
| 26  | S     | 301 | LHG  | O2-C2-C3-O3     |
| 26  | b     | 622 | LHG  | O2-C2-C3-O3     |
| 26  | c     | 517 | LHG  | O2-C2-C3-O3     |
| 26  | d     | 406 | LHG  | O2-C2-C3-O3     |
| 26  | s     | 301 | LHG  | O2-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | N     | 613 | CLA  | C3-C5-C6-C7     |
| 25  | R     | 603 | CLA  | C3-C5-C6-C7     |
| 25  | R     | 608 | CLA  | C3-C5-C6-C7     |
| 25  | n     | 613 | CLA  | C3-C5-C6-C7     |
| 25  | r     | 603 | CLA  | C3-C5-C6-C7     |
| 25  | r     | 608 | CLA  | C3-C5-C6-C7     |
| 24  | Y     | 310 | CHL  | CBA-CGA-O2A-C1  |
| 24  | y     | 310 | CHL  | CBA-CGA-O2A-C1  |
| 25  | 2     | 602 | CLA  | CBA-CGA-O2A-C1  |
| 25  | B     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 6     | 602 | CLA  | CBA-CGA-O2A-C1  |
| 25  | b     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 26  | C     | 519 | LHG  | C24-C23-O8-C6   |
| 26  | c     | 519 | LHG  | C24-C23-O8-C6   |
| 25  | C     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 25  | C     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 25  | c     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 25  | c     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 2     | 606 | LHG  | C8-C7-O7-C5     |
| 26  | C     | 517 | LHG  | C8-C7-O7-C5     |
| 26  | 6     | 606 | LHG  | C8-C7-O7-C5     |
| 26  | c     | 517 | LHG  | C8-C7-O7-C5     |
| 29  | L     | 101 | SQD  | C8-C7-O47-C45   |
| 29  | l     | 102 | SQD  | C8-C7-O47-C45   |
| 32  | B     | 624 | AJP  | O31-C26-O25-C23 |
| 32  | b     | 624 | AJP  | O31-C26-O25-C23 |
| 32  | A     | 412 | AJP  | C27-C26-O25-C23 |
| 32  | a     | 413 | AJP  | C27-C26-O25-C23 |
| 32  | B     | 624 | AJP  | C38-C39-C41-O42 |
| 32  | b     | 624 | AJP  | C38-C39-C41-O42 |
| 29  | L     | 103 | SQD  | C10-C11-C12-C13 |
| 29  | l     | 101 | SQD  | C10-C11-C12-C13 |
| 30  | B     | 620 | LMG  | C39-C40-C41-C42 |
| 35  | B     | 626 | DGD  | O6E-C5E-C6E-O5E |
| 35  | b     | 626 | DGD  | O6E-C5E-C6E-O5E |
| 30  | b     | 620 | LMG  | C39-C40-C41-C42 |
| 25  | B     | 601 | CLA  | C3-C5-C6-C7     |
| 25  | b     | 601 | CLA  | C3-C5-C6-C7     |
| 24  | N     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 24  | n     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 25  | C     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 608 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 25  | r     | 608 | CLA  | CBA-CGA-O2A-C1  |
| 30  | A     | 408 | LMG  | O6-C5-C6-O5     |
| 30  | a     | 409 | LMG  | O6-C5-C6-O5     |
| 35  | C     | 515 | DGD  | O6E-C5E-C6E-O5E |
| 35  | c     | 515 | DGD  | O6E-C5E-C6E-O5E |
| 24  | G     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 24  | g     | 608 | CHL  | C2C-C3C-CAC-CBC |
| 25  | G     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 25  | g     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 24  | 2     | 601 | CHL  | C4-C3-C5-C6     |
| 24  | G     | 601 | CHL  | C4-C3-C5-C6     |
| 24  | 6     | 601 | CHL  | C4-C3-C5-C6     |
| 24  | g     | 601 | CHL  | C4-C3-C5-C6     |
| 25  | C     | 507 | CLA  | C4-C3-C5-C6     |
| 25  | c     | 507 | CLA  | C4-C3-C5-C6     |
| 24  | 2     | 601 | CHL  | C2-C3-C5-C6     |
| 24  | 6     | 601 | CHL  | C2-C3-C5-C6     |
| 25  | N     | 610 | CLA  | C2-C3-C5-C6     |
| 25  | n     | 610 | CLA  | C2-C3-C5-C6     |
| 24  | 1     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 24  | 5     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 25  | S     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 25  | N     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 25  | Y     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | s     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 25  | n     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 25  | y     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 32  | A     | 412 | AJP  | C38-C39-C41-O42 |
| 32  | a     | 413 | AJP  | C38-C39-C41-O42 |
| 30  | A     | 408 | LMG  | O6-C1-O1-C7     |
| 30  | a     | 409 | LMG  | O6-C1-O1-C7     |
| 27  | A     | 403 | PHO  | C3-C5-C6-C7     |
| 27  | a     | 404 | PHO  | C3-C5-C6-C7     |
| 26  | Y     | 319 | LHG  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | y     | 319 | LHG  | C29-C30-C31-C32 |
| 25  | B     | 616 | CLA  | C4C-C3C-CAC-CBC |
| 25  | Y     | 304 | CLA  | C4C-C3C-CAC-CBC |
| 25  | b     | 616 | CLA  | C4C-C3C-CAC-CBC |
| 25  | y     | 304 | CLA  | C4C-C3C-CAC-CBC |
| 24  | Y     | 302 | CHL  | C2C-C3C-CAC-CBC |
| 24  | y     | 302 | CHL  | C2C-C3C-CAC-CBC |
| 25  | G     | 611 | CLA  | C2C-C3C-CAC-CBC |
| 25  | g     | 611 | CLA  | C2C-C3C-CAC-CBC |
| 26  | B     | 622 | LHG  | C1-C2-C3-O3     |
| 26  | L     | 102 | LHG  | C1-C2-C3-O3     |
| 26  | S     | 301 | LHG  | C1-C2-C3-O3     |
| 26  | b     | 622 | LHG  | C1-C2-C3-O3     |
| 26  | l     | 103 | LHG  | C1-C2-C3-O3     |
| 26  | s     | 301 | LHG  | C1-C2-C3-O3     |
| 26  | C     | 517 | LHG  | O9-C7-O7-C5     |
| 26  | c     | 517 | LHG  | O9-C7-O7-C5     |
| 29  | L     | 101 | SQD  | O49-C7-O47-C45  |
| 29  | l     | 102 | SQD  | O49-C7-O47-C45  |
| 25  | N     | 603 | CLA  | C3-C5-C6-C7     |
| 25  | n     | 603 | CLA  | C3-C5-C6-C7     |
| 24  | N     | 607 | CHL  | O1D-CGD-O2D-CED |
| 24  | n     | 607 | CHL  | O1D-CGD-O2D-CED |
| 25  | C     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 25  | C     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 25  | C     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 25  | D     | 403 | CLA  | CBA-CGA-O2A-C1  |
| 25  | N     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 25  | d     | 403 | CLA  | CBA-CGA-O2A-C1  |
| 25  | n     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 26  | B     | 622 | LHG  | C24-C23-O8-C6   |
| 26  | Y     | 319 | LHG  | C24-C23-O8-C6   |
| 26  | b     | 622 | LHG  | C24-C23-O8-C6   |
| 26  | y     | 319 | LHG  | C24-C23-O8-C6   |
| 25  | R     | 602 | CLA  | CBD-CGD-O2D-CED |
| 25  | R     | 614 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 602 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 614 | CLA  | CBD-CGD-O2D-CED |
| 39  | N     | 615 | LUT  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | N     | 604 | CLA  | C2C-C3C-CAC-CBC |
| 25  | n     | 604 | CLA  | C2C-C3C-CAC-CBC |
| 24  | G     | 609 | CHL  | C10-C11-C12-C13 |
| 24  | g     | 609 | CHL  | C10-C11-C12-C13 |
| 35  | C     | 515 | DGD  | C2A-C3A-C4A-C5A |
| 35  | c     | 515 | DGD  | C2A-C3A-C4A-C5A |
| 24  | R     | 607 | CHL  | C5-C6-C7-C8     |
| 24  | r     | 607 | CHL  | C5-C6-C7-C8     |
| 25  | S     | 303 | CLA  | C10-C11-C12-C13 |
| 25  | Y     | 304 | CLA  | C13-C15-C16-C17 |
| 25  | s     | 303 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 304 | CLA  | C13-C15-C16-C17 |
| 26  | L     | 102 | LHG  | O2-C2-C3-O3     |
| 26  | l     | 103 | LHG  | O2-C2-C3-O3     |
| 25  | G     | 612 | CLA  | C3-C5-C6-C7     |
| 26  | Y     | 301 | LHG  | C23-C24-C25-C26 |
| 26  | R     | 618 | LHG  | C23-C24-C25-C26 |
| 26  | y     | 301 | LHG  | C23-C24-C25-C26 |
| 26  | r     | 618 | LHG  | C23-C24-C25-C26 |
| 30  | A     | 408 | LMG  | C2-C1-O1-C7     |
| 30  | a     | 409 | LMG  | C2-C1-O1-C7     |
| 26  | S     | 301 | LHG  | C14-C15-C16-C17 |
| 26  | s     | 301 | LHG  | C14-C15-C16-C17 |
| 24  | n     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 25  | N     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 25  | n     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 25  | R     | 609 | CLA  | C2-C3-C5-C6     |
| 25  | r     | 609 | CLA  | C2-C3-C5-C6     |
| 24  | G     | 601 | CHL  | C11-C12-C13-C14 |
| 24  | G     | 608 | CHL  | C11-C10-C8-C9   |
| 24  | G     | 608 | CHL  | C14-C13-C15-C16 |
| 24  | G     | 609 | CHL  | C6-C7-C8-C9     |
| 24  | N     | 608 | CHL  | C11-C10-C8-C9   |
| 24  | N     | 609 | CHL  | C11-C12-C13-C14 |
| 24  | Y     | 302 | CHL  | C11-C12-C13-C14 |
| 24  | Y     | 309 | CHL  | C11-C10-C8-C9   |
| 24  | g     | 601 | CHL  | C11-C12-C13-C14 |
| 24  | g     | 608 | CHL  | C11-C10-C8-C9   |
| 24  | g     | 608 | CHL  | C14-C13-C15-C16 |
| 24  | g     | 609 | CHL  | C6-C7-C8-C9     |
| 24  | n     | 608 | CHL  | C11-C10-C8-C9   |
| 24  | n     | 609 | CHL  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | y     | 302 | CHL  | C11-C12-C13-C14 |
| 24  | y     | 309 | CHL  | C11-C10-C8-C9   |
| 25  | A     | 402 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 602 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 607 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 608 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 609 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 613 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 613 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 614 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 614 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 615 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 501 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 503 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 506 | CLA  | C6-C7-C8-C9     |
| 25  | C     | 507 | CLA  | C11-C12-C13-C14 |
| 25  | C     | 509 | CLA  | C6-C7-C8-C9     |
| 25  | C     | 511 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 513 | CLA  | C14-C13-C15-C16 |
| 25  | S     | 303 | CLA  | C11-C10-C8-C9   |
| 25  | N     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | N     | 612 | CLA  | C6-C7-C8-C9     |
| 25  | N     | 612 | CLA  | C11-C10-C8-C9   |
| 25  | Y     | 303 | CLA  | C11-C10-C8-C9   |
| 25  | Y     | 304 | CLA  | C11-C10-C8-C9   |
| 25  | Y     | 312 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 314 | CLA  | C6-C7-C8-C9     |
| 25  | R     | 603 | CLA  | C11-C10-C8-C9   |
| 25  | R     | 608 | CLA  | C6-C7-C8-C9     |
| 25  | R     | 612 | CLA  | C6-C7-C8-C9     |
| 25  | a     | 403 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 602 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 607 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 608 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 609 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 613 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 613 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 614 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 614 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 615 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 501 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 503 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 506 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 507 | CLA  | C11-C12-C13-C14 |
| 25  | c     | 509 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 511 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 513 | CLA  | C14-C13-C15-C16 |
| 25  | s     | 303 | CLA  | C11-C10-C8-C9   |
| 25  | n     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | n     | 612 | CLA  | C6-C7-C8-C9     |
| 25  | n     | 612 | CLA  | C11-C10-C8-C9   |
| 25  | y     | 303 | CLA  | C11-C10-C8-C9   |
| 25  | y     | 304 | CLA  | C11-C10-C8-C9   |
| 25  | y     | 312 | CLA  | C6-C7-C8-C9     |
| 25  | y     | 314 | CLA  | C6-C7-C8-C9     |
| 25  | r     | 603 | CLA  | C11-C10-C8-C9   |
| 25  | r     | 608 | CLA  | C6-C7-C8-C9     |
| 25  | r     | 612 | CLA  | C6-C7-C8-C9     |
| 27  | A     | 403 | PHO  | C14-C13-C15-C16 |
| 27  | a     | 404 | PHO  | C14-C13-C15-C16 |
| 25  | C     | 505 | CLA  | C15-C16-C17-C18 |
| 25  | c     | 505 | CLA  | C15-C16-C17-C18 |
| 25  | r     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 28  | H     | 101 | BCR  | C37-C22-C23-C24 |
| 28  | K     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | h     | 101 | BCR  | C37-C22-C23-C24 |
| 28  | k     | 101 | BCR  | C7-C8-C9-C34    |
| 39  | N     | 615 | LUT  | C11-C12-C13-C20 |
| 39  | Y     | 317 | LUT  | C7-C8-C9-C19    |
| 39  | n     | 615 | LUT  | C11-C12-C13-C20 |
| 39  | y     | 317 | LUT  | C7-C8-C9-C19    |
| 28  | H     | 101 | BCR  | C21-C22-C23-C24 |
| 28  | h     | 101 | BCR  | C21-C22-C23-C24 |
| 39  | N     | 615 | LUT  | C11-C12-C13-C14 |
| 39  | Y     | 317 | LUT  | C7-C8-C9-C10    |
| 39  | n     | 615 | LUT  | C11-C12-C13-C14 |
| 39  | y     | 317 | LUT  | C7-C8-C9-C10    |
| 26  | 2     | 606 | LHG  | O9-C7-O7-C5     |
| 26  | 6     | 606 | LHG  | O9-C7-O7-C5     |
| 25  | R     | 614 | CLA  | C2C-C3C-CAC-CBC |
| 25  | r     | 614 | CLA  | C2C-C3C-CAC-CBC |
| 29  | L     | 103 | SQD  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | l     | 101 | SQD  | C23-C24-C25-C26 |
| 24  | N     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 24  | N     | 607 | CHL  | C8-C10-C11-C12  |
| 24  | Y     | 302 | CHL  | C8-C10-C11-C12  |
| 24  | n     | 607 | CHL  | C8-C10-C11-C12  |
| 24  | y     | 302 | CHL  | C8-C10-C11-C12  |
| 25  | B     | 616 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 616 | CLA  | C5-C6-C7-C8     |
| 24  | G     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 24  | g     | 601 | CHL  | C2C-C3C-CAC-CBC |
| 25  | g     | 612 | CLA  | C3-C5-C6-C7     |
| 24  | Y     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 24  | y     | 302 | CHL  | CBA-CGA-O2A-C1  |
| 24  | 2     | 601 | CHL  | C10-C11-C12-C13 |
| 24  | G     | 601 | CHL  | C8-C10-C11-C12  |
| 24  | G     | 608 | CHL  | C10-C11-C12-C13 |
| 24  | G     | 608 | CHL  | C13-C15-C16-C17 |
| 24  | 6     | 601 | CHL  | C10-C11-C12-C13 |
| 24  | g     | 601 | CHL  | C8-C10-C11-C12  |
| 24  | g     | 608 | CHL  | C10-C11-C12-C13 |
| 24  | g     | 608 | CHL  | C13-C15-C16-C17 |
| 25  | B     | 611 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 611 | CLA  | C15-C16-C17-C18 |
| 25  | B     | 613 | CLA  | C13-C15-C16-C17 |
| 25  | N     | 603 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 613 | CLA  | C5-C6-C7-C8     |
| 25  | Y     | 314 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 611 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 611 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 613 | CLA  | C13-C15-C16-C17 |
| 25  | n     | 603 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 613 | CLA  | C5-C6-C7-C8     |
| 25  | y     | 314 | CLA  | C13-C15-C16-C17 |
| 26  | B     | 625 | LHG  | C7-C8-C9-C10    |
| 26  | b     | 625 | LHG  | C7-C8-C9-C10    |
| 30  | B     | 620 | LMG  | C28-C29-C30-C31 |
| 30  | b     | 620 | LMG  | C28-C29-C30-C31 |
| 32  | A     | 412 | AJP  | O40-C35-O34-C29 |
| 32  | a     | 413 | AJP  | O40-C35-O34-C29 |
| 24  | R     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 24  | r     | 606 | CHL  | C2C-C3C-CAC-CBC |
| 26  | Y     | 319 | LHG  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | y     | 319 | LHG  | C33-C34-C35-C36 |
| 30  | D     | 407 | LMG  | O6-C5-C6-O5     |
| 30  | d     | 407 | LMG  | O6-C5-C6-O5     |
| 24  | N     | 601 | CHL  | C5-C6-C7-C8     |
| 24  | N     | 607 | CHL  | C10-C11-C12-C13 |
| 24  | N     | 609 | CHL  | C13-C15-C16-C17 |
| 24  | n     | 601 | CHL  | C5-C6-C7-C8     |
| 24  | n     | 607 | CHL  | C10-C11-C12-C13 |
| 24  | n     | 609 | CHL  | C13-C15-C16-C17 |
| 25  | B     | 601 | CLA  | C10-C11-C12-C13 |
| 25  | B     | 607 | CLA  | C8-C10-C11-C12  |
| 25  | B     | 614 | CLA  | C5-C6-C7-C8     |
| 25  | C     | 503 | CLA  | C5-C6-C7-C8     |
| 25  | D     | 403 | CLA  | C10-C11-C12-C13 |
| 25  | S     | 310 | CLA  | C5-C6-C7-C8     |
| 25  | G     | 612 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 602 | CLA  | C5-C6-C7-C8     |
| 25  | N     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | N     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | Y     | 311 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 601 | CLA  | C10-C11-C12-C13 |
| 25  | b     | 607 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 614 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 503 | CLA  | C5-C6-C7-C8     |
| 25  | d     | 403 | CLA  | C10-C11-C12-C13 |
| 25  | s     | 310 | CLA  | C5-C6-C7-C8     |
| 25  | g     | 612 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 602 | CLA  | C5-C6-C7-C8     |
| 25  | n     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | n     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | y     | 311 | CLA  | C8-C10-C11-C12  |
| 26  | N     | 618 | LHG  | O1-C1-C2-O2     |
| 26  | n     | 618 | LHG  | O1-C1-C2-O2     |
| 26  | B     | 621 | LHG  | C7-C8-C9-C10    |
| 26  | C     | 518 | LHG  | C7-C8-C9-C10    |
| 26  | C     | 519 | LHG  | C23-C24-C25-C26 |
| 26  | b     | 621 | LHG  | C7-C8-C9-C10    |
| 26  | c     | 518 | LHG  | C7-C8-C9-C10    |
| 26  | c     | 519 | LHG  | C23-C24-C25-C26 |
| 30  | B     | 623 | LMG  | C28-C29-C30-C31 |
| 30  | b     | 623 | LMG  | C28-C29-C30-C31 |
| 24  | G     | 608 | CHL  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | g     | 608 | CHL  | C5-C6-C7-C8     |
| 25  | A     | 405 | CLA  | C10-C11-C12-C13 |
| 25  | a     | 406 | CLA  | C10-C11-C12-C13 |
| 25  | B     | 604 | CLA  | C3-C5-C6-C7     |
| 25  | b     | 604 | CLA  | C3-C5-C6-C7     |
| 25  | y     | 305 | CLA  | C4C-C3C-CAC-CBC |
| 25  | Y     | 305 | CLA  | C4C-C3C-CAC-CBC |
| 25  | Y     | 313 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 313 | CLA  | C10-C11-C12-C13 |
| 26  | 2     | 606 | LHG  | C23-C24-C25-C26 |
| 26  | B     | 622 | LHG  | C7-C8-C9-C10    |
| 26  | 6     | 606 | LHG  | C23-C24-C25-C26 |
| 26  | b     | 622 | LHG  | C7-C8-C9-C10    |
| 29  | L     | 101 | SQD  | C23-C24-C25-C26 |
| 29  | l     | 102 | SQD  | C23-C24-C25-C26 |
| 25  | N     | 612 | CLA  | CBD-CGD-O2D-CED |
| 25  | n     | 612 | CLA  | CBD-CGD-O2D-CED |
| 26  | S     | 301 | LHG  | C31-C32-C33-C34 |
| 26  | s     | 301 | LHG  | C31-C32-C33-C34 |
| 25  | B     | 607 | CLA  | C5-C6-C7-C8     |
| 25  | S     | 303 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 607 | CLA  | C5-C6-C7-C8     |
| 25  | s     | 303 | CLA  | C8-C10-C11-C12  |
| 24  | G     | 601 | CHL  | C12-C13-C15-C16 |
| 24  | N     | 607 | CHL  | C6-C7-C8-C10    |
| 24  | N     | 609 | CHL  | C11-C12-C13-C15 |
| 24  | g     | 601 | CHL  | C12-C13-C15-C16 |
| 24  | n     | 607 | CHL  | C6-C7-C8-C10    |
| 24  | n     | 609 | CHL  | C11-C12-C13-C15 |
| 25  | B     | 607 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 611 | CLA  | C12-C13-C15-C16 |
| 25  | B     | 613 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 503 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 510 | CLA  | C11-C12-C13-C15 |
| 25  | D     | 403 | CLA  | C12-C13-C15-C16 |
| 25  | S     | 303 | CLA  | C11-C12-C13-C15 |
| 25  | G     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | N     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | Y     | 313 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 607 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 611 | CLA  | C12-C13-C15-C16 |
| 25  | b     | 613 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 503 | CLA  | C11-C10-C8-C7   |
| 25  | c     | 510 | CLA  | C11-C12-C13-C15 |
| 25  | d     | 403 | CLA  | C12-C13-C15-C16 |
| 25  | s     | 303 | CLA  | C11-C12-C13-C15 |
| 25  | g     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | n     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | y     | 313 | CLA  | C6-C7-C8-C10    |
| 26  | Y     | 319 | LHG  | O10-C23-O8-C6   |
| 26  | y     | 319 | LHG  | O10-C23-O8-C6   |
| 39  | S     | 316 | LUT  | C13-C14-C15-C35 |
| 39  | s     | 316 | LUT  | C13-C14-C15-C35 |
| 39  | n     | 615 | LUT  | C9-C10-C11-C12  |
| 40  | N     | 617 | NEX  | C33-C34-C35-C15 |
| 40  | n     | 617 | NEX  | C33-C34-C35-C15 |
| 25  | S     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 25  | Y     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 25  | Y     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 25  | s     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 25  | y     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 25  | y     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 25  | Y     | 305 | CLA  | O1D-CGD-O2D-CED |
| 25  | y     | 305 | CLA  | O1D-CGD-O2D-CED |
| 25  | B     | 610 | CLA  | C15-C16-C17-C18 |
| 25  | C     | 507 | CLA  | C13-C15-C16-C17 |
| 25  | C     | 510 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 610 | CLA  | C15-C16-C17-C18 |
| 25  | c     | 507 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 510 | CLA  | C13-C15-C16-C17 |
| 35  | C     | 516 | DGD  | C8B-C9B-CAB-CBB |
| 35  | c     | 516 | DGD  | C8B-C9B-CAB-CBB |
| 26  | B     | 622 | LHG  | O10-C23-O8-C6   |
| 26  | b     | 622 | LHG  | O10-C23-O8-C6   |
| 25  | R     | 601 | CLA  | CBD-CGD-O2D-CED |
| 25  | r     | 601 | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 412 | AJP  | C58-C59-C61-O62 |
| 32  | a     | 413 | AJP  | C58-C59-C61-O62 |
| 25  | G     | 602 | CLA  | C10-C11-C12-C13 |
| 25  | g     | 602 | CLA  | C10-C11-C12-C13 |
| 30  | D     | 407 | LMG  | C31-C32-C33-C34 |
| 30  | d     | 407 | LMG  | C31-C32-C33-C34 |
| 26  | N     | 618 | LHG  | O2-C2-C3-O3     |
| 26  | n     | 618 | LHG  | O2-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 2     | 604 | CLA  | C3-C5-C6-C7     |
| 25  | B     | 607 | CLA  | C3-C5-C6-C7     |
| 25  | 6     | 604 | CLA  | C3-C5-C6-C7     |
| 25  | b     | 607 | CLA  | C3-C5-C6-C7     |
| 24  | Y     | 310 | CHL  | C5-C6-C7-C8     |
| 24  | y     | 310 | CHL  | C5-C6-C7-C8     |
| 25  | B     | 607 | CLA  | C10-C11-C12-C13 |
| 25  | D     | 402 | CLA  | C15-C16-C17-C18 |
| 25  | Y     | 303 | CLA  | C10-C11-C12-C13 |
| 25  | Y     | 304 | CLA  | C10-C11-C12-C13 |
| 25  | Y     | 311 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 607 | CLA  | C10-C11-C12-C13 |
| 25  | d     | 402 | CLA  | C15-C16-C17-C18 |
| 25  | y     | 303 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 304 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 311 | CLA  | C5-C6-C7-C8     |
| 30  | B     | 623 | LMG  | C29-C28-O8-C9   |
| 30  | b     | 623 | LMG  | C29-C28-O8-C9   |
| 32  | B     | 624 | AJP  | C38-C37-O44-C45 |
| 32  | b     | 624 | AJP  | C38-C37-O44-C45 |
| 24  | G     | 601 | CHL  | C10-C11-C12-C13 |
| 24  | N     | 609 | CHL  | C8-C10-C11-C12  |
| 24  | Y     | 309 | CHL  | C8-C10-C11-C12  |
| 24  | g     | 601 | CHL  | C10-C11-C12-C13 |
| 24  | n     | 609 | CHL  | C8-C10-C11-C12  |
| 24  | y     | 309 | CHL  | C8-C10-C11-C12  |
| 25  | B     | 607 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 611 | CLA  | C8-C10-C11-C12  |
| 25  | C     | 503 | CLA  | C15-C16-C17-C18 |
| 25  | N     | 613 | CLA  | C10-C11-C12-C13 |
| 25  | Y     | 313 | CLA  | C8-C10-C11-C12  |
| 25  | R     | 603 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 607 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 611 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 503 | CLA  | C15-C16-C17-C18 |
| 25  | n     | 613 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 313 | CLA  | C8-C10-C11-C12  |
| 25  | r     | 603 | CLA  | C8-C10-C11-C12  |
| 26  | C     | 517 | LHG  | C10-C11-C12-C13 |
| 26  | c     | 517 | LHG  | C10-C11-C12-C13 |
| 35  | C     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 35  | c     | 516 | DGD  | O6D-C5D-C6D-O5D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | Y     | 320 | AJP  | C27-C26-O25-C23 |
| 32  | y     | 320 | AJP  | C27-C26-O25-C23 |
| 29  | A     | 411 | SQD  | C8-C7-O47-C45   |
| 29  | a     | 412 | SQD  | C8-C7-O47-C45   |
| 24  | Y     | 309 | CHL  | C13-C15-C16-C17 |
| 24  | y     | 309 | CHL  | C13-C15-C16-C17 |
| 25  | B     | 604 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 609 | CLA  | C15-C16-C17-C18 |
| 25  | B     | 616 | CLA  | C13-C15-C16-C17 |
| 25  | C     | 513 | CLA  | C8-C10-C11-C12  |
| 25  | G     | 610 | CLA  | C8-C10-C11-C12  |
| 25  | N     | 612 | CLA  | C5-C6-C7-C8     |
| 25  | R     | 608 | CLA  | C8-C10-C11-C12  |
| 25  | R     | 612 | CLA  | C10-C11-C12-C13 |
| 25  | b     | 604 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 609 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 616 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 513 | CLA  | C8-C10-C11-C12  |
| 25  | g     | 610 | CLA  | C8-C10-C11-C12  |
| 25  | n     | 612 | CLA  | C5-C6-C7-C8     |
| 25  | r     | 608 | CLA  | C8-C10-C11-C12  |
| 25  | r     | 612 | CLA  | C10-C11-C12-C13 |
| 24  | N     | 607 | CHL  | C1-C2-C3-C5     |
| 24  | n     | 607 | CHL  | C1-C2-C3-C5     |
| 26  | C     | 519 | LHG  | C4-O6-P-O3      |
| 26  | L     | 102 | LHG  | C4-O6-P-O3      |
| 26  | N     | 618 | LHG  | C3-O3-P-O6      |
| 26  | c     | 519 | LHG  | C4-O6-P-O3      |
| 26  | l     | 103 | LHG  | C4-O6-P-O3      |
| 26  | n     | 618 | LHG  | C3-O3-P-O6      |
| 26  | Y     | 319 | LHG  | C23-C24-C25-C26 |
| 26  | y     | 319 | LHG  | C23-C24-C25-C26 |
| 32  | B     | 624 | AJP  | O60-C59-C61-O62 |
| 32  | b     | 624 | AJP  | O60-C59-C61-O62 |
| 25  | C     | 510 | CLA  | C15-C16-C17-C18 |
| 25  | G     | 613 | CLA  | C15-C16-C17-C18 |
| 25  | c     | 510 | CLA  | C15-C16-C17-C18 |
| 26  | N     | 618 | LHG  | C1-C2-C3-O3     |
| 26  | n     | 618 | LHG  | C1-C2-C3-O3     |
| 29  | A     | 411 | SQD  | O49-C7-O47-C45  |
| 29  | a     | 412 | SQD  | O49-C7-O47-C45  |
| 25  | S     | 310 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | s     | 310 | CLA  | C4-C3-C5-C6     |
| 25  | C     | 504 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 504 | CLA  | C5-C6-C7-C8     |
| 25  | g     | 613 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 409 | PL9  | C2-C3-C7-C8     |
| 31  | a     | 410 | PL9  | C2-C3-C7-C8     |
| 25  | A     | 401 | CLA  | C2C-C3C-CAC-CBC |
| 25  | N     | 603 | CLA  | C2C-C3C-CAC-CBC |
| 25  | a     | 402 | CLA  | C2C-C3C-CAC-CBC |
| 25  | n     | 603 | CLA  | C2C-C3C-CAC-CBC |
| 30  | A     | 410 | LMG  | C35-C36-C37-C38 |
| 30  | a     | 411 | LMG  | C35-C36-C37-C38 |
| 25  | C     | 513 | CLA  | C2A-CAA-CBA-CGA |
| 25  | S     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 25  | N     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | c     | 513 | CLA  | C2A-CAA-CBA-CGA |
| 25  | s     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 25  | n     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 504 | CLA  | C11-C12-C13-C14 |
| 25  | G     | 613 | CLA  | C16-C17-C18-C19 |
| 25  | R     | 609 | CLA  | C16-C17-C18-C20 |
| 25  | c     | 504 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 613 | CLA  | C16-C17-C18-C19 |
| 25  | r     | 609 | CLA  | C16-C17-C18-C20 |
| 30  | A     | 410 | LMG  | O6-C5-C6-O5     |
| 30  | a     | 411 | LMG  | O6-C5-C6-O5     |
| 24  | G     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 24  | g     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 35  | C     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 35  | c     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 26  | Y     | 319 | LHG  | C11-C12-C13-C14 |
| 26  | y     | 319 | LHG  | C11-C12-C13-C14 |
| 29  | A     | 407 | SQD  | C11-C12-C13-C14 |
| 29  | a     | 408 | SQD  | C11-C12-C13-C14 |
| 24  | G     | 608 | CHL  | C8-C10-C11-C12  |
| 28  | H     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | T     | 101 | BCR  | C35-C13-C14-C15 |
| 28  | h     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | t     | 101 | BCR  | C35-C13-C14-C15 |
| 26  | 2     | 606 | LHG  | C15-C16-C17-C18 |
| 26  | B     | 625 | LHG  | C25-C26-C27-C28 |
| 26  | C     | 517 | LHG  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | L     | 102 | LHG  | C27-C28-C29-C30 |
| 26  | 6     | 606 | LHG  | C15-C16-C17-C18 |
| 26  | b     | 625 | LHG  | C25-C26-C27-C28 |
| 26  | c     | 517 | LHG  | C34-C35-C36-C37 |
| 26  | l     | 103 | LHG  | C27-C28-C29-C30 |
| 29  | L     | 103 | SQD  | C11-C10-C9-C8   |
| 29  | L     | 103 | SQD  | C9-C10-C11-C12  |
| 29  | l     | 101 | SQD  | C11-C10-C9-C8   |
| 29  | l     | 101 | SQD  | C9-C10-C11-C12  |
| 30  | A     | 410 | LMG  | C37-C38-C39-C40 |
| 30  | D     | 407 | LMG  | C13-C14-C15-C16 |
| 30  | a     | 411 | LMG  | C37-C38-C39-C40 |
| 30  | d     | 407 | LMG  | C13-C14-C15-C16 |
| 24  | n     | 609 | CHL  | O1D-CGD-O2D-CED |
| 24  | Y     | 302 | CHL  | C16-C17-C18-C19 |
| 24  | y     | 302 | CHL  | C16-C17-C18-C19 |
| 25  | B     | 608 | CLA  | C16-C17-C18-C19 |
| 25  | N     | 612 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 608 | CLA  | C16-C17-C18-C19 |
| 25  | n     | 612 | CLA  | C11-C12-C13-C14 |
| 25  | y     | 313 | CLA  | C11-C12-C13-C15 |
| 26  | S     | 301 | LHG  | C26-C27-C28-C29 |
| 26  | s     | 301 | LHG  | C26-C27-C28-C29 |
| 26  | y     | 301 | LHG  | C26-C27-C28-C29 |
| 30  | A     | 408 | LMG  | C30-C31-C32-C33 |
| 30  | D     | 407 | LMG  | C12-C13-C14-C15 |
| 30  | a     | 409 | LMG  | C30-C31-C32-C33 |
| 35  | C     | 515 | DGD  | C5A-C6A-C7A-C8A |
| 35  | C     | 515 | DGD  | C7B-C8B-C9B-CAB |
| 35  | c     | 515 | DGD  | C5A-C6A-C7A-C8A |
| 35  | c     | 515 | DGD  | C7B-C8B-C9B-CAB |
| 26  | C     | 519 | LHG  | C4-C5-O7-C7     |
| 26  | c     | 519 | LHG  | C4-C5-O7-C7     |
| 24  | N     | 609 | CHL  | O1D-CGD-O2D-CED |
| 24  | g     | 608 | CHL  | C8-C10-C11-C12  |
| 25  | G     | 614 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 614 | CLA  | CBD-CGD-O2D-CED |
| 26  | Y     | 301 | LHG  | C26-C27-C28-C29 |
| 30  | B     | 623 | LMG  | C31-C32-C33-C34 |
| 30  | b     | 623 | LMG  | C31-C32-C33-C34 |
| 30  | d     | 407 | LMG  | C12-C13-C14-C15 |
| 35  | C     | 515 | DGD  | C4A-C5A-C6A-C7A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | c     | 515 | DGD  | C4A-C5A-C6A-C7A |
| 24  | G     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 24  | g     | 608 | CHL  | C4C-C3C-CAC-CBC |
| 26  | 2     | 606 | LHG  | C14-C15-C16-C17 |
| 26  | B     | 621 | LHG  | C26-C27-C28-C29 |
| 26  | D     | 406 | LHG  | C33-C34-C35-C36 |
| 26  | N     | 618 | LHG  | C26-C27-C28-C29 |
| 26  | N     | 618 | LHG  | C27-C28-C29-C30 |
| 26  | Y     | 319 | LHG  | C13-C14-C15-C16 |
| 26  | 6     | 606 | LHG  | C14-C15-C16-C17 |
| 26  | b     | 621 | LHG  | C26-C27-C28-C29 |
| 26  | d     | 406 | LHG  | C33-C34-C35-C36 |
| 26  | n     | 618 | LHG  | C26-C27-C28-C29 |
| 26  | n     | 618 | LHG  | C27-C28-C29-C30 |
| 26  | y     | 319 | LHG  | C13-C14-C15-C16 |
| 25  | C     | 503 | CLA  | O1D-CGD-O2D-CED |
| 26  | Y     | 301 | LHG  | O2-C2-C3-O3     |
| 26  | Y     | 319 | LHG  | O2-C2-C3-O3     |
| 26  | y     | 301 | LHG  | O2-C2-C3-O3     |
| 26  | y     | 319 | LHG  | O2-C2-C3-O3     |
| 26  | R     | 618 | LHG  | C9-C10-C11-C12  |
| 26  | r     | 618 | LHG  | C9-C10-C11-C12  |
| 35  | C     | 516 | DGD  | CBB-CCB-CDB-CEB |
| 35  | c     | 516 | DGD  | CBB-CCB-CDB-CEB |
| 35  | C     | 516 | DGD  | C1A-C2A-C3A-C4A |
| 35  | c     | 516 | DGD  | C1A-C2A-C3A-C4A |
| 25  | c     | 503 | CLA  | O1D-CGD-O2D-CED |
| 28  | T     | 101 | BCR  | C20-C21-C22-C23 |
| 28  | t     | 101 | BCR  | C20-C21-C22-C23 |
| 26  | B     | 622 | LHG  | C13-C14-C15-C16 |
| 26  | B     | 622 | LHG  | C18-C19-C20-C21 |
| 26  | C     | 519 | LHG  | C28-C29-C30-C31 |
| 26  | b     | 622 | LHG  | C13-C14-C15-C16 |
| 26  | b     | 622 | LHG  | C18-C19-C20-C21 |
| 26  | c     | 519 | LHG  | C28-C29-C30-C31 |
| 29  | L     | 101 | SQD  | C27-C28-C29-C30 |
| 35  | B     | 626 | DGD  | CBB-CCB-CDB-CEB |
| 35  | b     | 626 | DGD  | CBB-CCB-CDB-CEB |
| 24  | Y     | 310 | CHL  | O1A-CGA-O2A-C1  |
| 24  | y     | 310 | CHL  | O1A-CGA-O2A-C1  |
| 25  | A     | 405 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 612 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | Y     | 313 | CLA  | C11-C12-C13-C15 |
| 25  | a     | 406 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 612 | CLA  | C16-C17-C18-C20 |
| 25  | Y     | 304 | CLA  | C4-C3-C5-C6     |
| 25  | Y     | 312 | CLA  | C4-C3-C5-C6     |
| 25  | y     | 304 | CLA  | C4-C3-C5-C6     |
| 25  | y     | 312 | CLA  | C4-C3-C5-C6     |
| 26  | B     | 621 | LHG  | C27-C28-C29-C30 |
| 26  | B     | 622 | LHG  | C12-C13-C14-C15 |
| 26  | S     | 318 | LHG  | C33-C34-C35-C36 |
| 26  | b     | 621 | LHG  | C27-C28-C29-C30 |
| 26  | b     | 622 | LHG  | C12-C13-C14-C15 |
| 26  | s     | 318 | LHG  | C33-C34-C35-C36 |
| 26  | n     | 618 | LHG  | C32-C33-C34-C35 |
| 29  | A     | 411 | SQD  | C11-C12-C13-C14 |
| 29  | A     | 411 | SQD  | C12-C13-C14-C15 |
| 29  | a     | 412 | SQD  | C11-C12-C13-C14 |
| 29  | a     | 412 | SQD  | C12-C13-C14-C15 |
| 29  | l     | 102 | SQD  | C27-C28-C29-C30 |
| 30  | B     | 623 | LMG  | C32-C33-C34-C35 |
| 30  | b     | 623 | LMG  | C32-C33-C34-C35 |
| 24  | G     | 601 | CHL  | C11-C10-C8-C9   |
| 24  | g     | 601 | CHL  | C11-C10-C8-C9   |
| 25  | B     | 604 | CLA  | C11-C10-C8-C9   |
| 25  | S     | 303 | CLA  | C11-C12-C13-C14 |
| 25  | G     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | N     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 604 | CLA  | C11-C10-C8-C9   |
| 25  | s     | 303 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | n     | 603 | CLA  | C6-C7-C8-C9     |
| 24  | S     | 307 | CHL  | O1D-CGD-O2D-CED |
| 24  | s     | 307 | CHL  | O1D-CGD-O2D-CED |
| 26  | D     | 406 | LHG  | C7-C8-C9-C10    |
| 26  | d     | 406 | LHG  | C7-C8-C9-C10    |
| 26  | 2     | 606 | LHG  | C30-C31-C32-C33 |
| 26  | B     | 625 | LHG  | C10-C11-C12-C13 |
| 26  | S     | 318 | LHG  | C10-C11-C12-C13 |
| 26  | N     | 618 | LHG  | C32-C33-C34-C35 |
| 26  | 6     | 606 | LHG  | C30-C31-C32-C33 |
| 26  | b     | 625 | LHG  | C10-C11-C12-C13 |
| 26  | s     | 318 | LHG  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | L     | 103 | SQD  | C13-C14-C15-C16 |
| 29  | l     | 101 | SQD  | C13-C14-C15-C16 |
| 30  | B     | 620 | LMG  | C18-C19-C20-C21 |
| 30  | b     | 620 | LMG  | C18-C19-C20-C21 |
| 35  | B     | 626 | DGD  | C7B-C8B-C9B-CAB |
| 35  | C     | 516 | DGD  | CAB-CBB-CCB-CDB |
| 35  | b     | 626 | DGD  | C7B-C8B-C9B-CAB |
| 35  | c     | 516 | DGD  | CAB-CBB-CCB-CDB |
| 25  | 2     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | 6     | 602 | CLA  | C8-C10-C11-C12  |
| 30  | C     | 520 | LMG  | O6-C5-C6-O5     |
| 25  | B     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 25  | G     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 25  | g     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 25  | B     | 607 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 607 | CLA  | O1A-CGA-O2A-C1  |
| 32  | G     | 618 | AJP  | C27-C26-O25-C23 |
| 32  | g     | 618 | AJP  | C27-C26-O25-C23 |
| 26  | L     | 102 | LHG  | C30-C31-C32-C33 |
| 26  | l     | 103 | LHG  | C30-C31-C32-C33 |
| 26  | B     | 621 | LHG  | O1-C1-C2-C3     |
| 26  | B     | 625 | LHG  | O1-C1-C2-C3     |
| 26  | C     | 519 | LHG  | O1-C1-C2-C3     |
| 26  | b     | 621 | LHG  | O1-C1-C2-C3     |
| 26  | b     | 625 | LHG  | O1-C1-C2-C3     |
| 26  | c     | 519 | LHG  | O1-C1-C2-C3     |
| 28  | T     | 101 | BCR  | C11-C12-C13-C14 |
| 28  | t     | 101 | BCR  | C11-C12-C13-C14 |
| 40  | G     | 617 | NEX  | C11-C12-C13-C14 |
| 40  | g     | 617 | NEX  | C11-C12-C13-C14 |
| 30  | B     | 623 | LMG  | C33-C34-C35-C36 |
| 30  | C     | 520 | LMG  | C16-C17-C18-C19 |
| 30  | b     | 623 | LMG  | C33-C34-C35-C36 |
| 30  | c     | 520 | LMG  | C16-C17-C18-C19 |
| 35  | c     | 516 | DGD  | C8A-C9A-CAA-CBA |
| 26  | S     | 301 | LHG  | C7-C8-C9-C10    |
| 26  | s     | 301 | LHG  | C7-C8-C9-C10    |
| 26  | S     | 318 | LHG  | C12-C13-C14-C15 |
| 26  | s     | 318 | LHG  | C12-C13-C14-C15 |
| 26  | n     | 618 | LHG  | C15-C16-C17-C18 |
| 30  | A     | 408 | LMG  | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | a     | 409 | LMG  | C36-C37-C38-C39 |
| 35  | C     | 516 | DGD  | C8A-C9A-CAA-CBA |
| 30  | c     | 520 | LMG  | O6-C5-C6-O5     |
| 25  | C     | 504 | CLA  | C11-C12-C13-C15 |
| 25  | G     | 613 | CLA  | C16-C17-C18-C20 |
| 25  | c     | 504 | CLA  | C11-C12-C13-C15 |
| 25  | g     | 613 | CLA  | C16-C17-C18-C20 |
| 30  | B     | 623 | LMG  | C8-C9-O8-C28    |
| 30  | b     | 623 | LMG  | C8-C9-O8-C28    |
| 25  | D     | 402 | CLA  | C13-C15-C16-C17 |
| 25  | d     | 402 | CLA  | C13-C15-C16-C17 |
| 26  | 2     | 606 | LHG  | C12-C13-C14-C15 |
| 26  | B     | 621 | LHG  | C25-C26-C27-C28 |
| 26  | B     | 621 | LHG  | C32-C33-C34-C35 |
| 26  | C     | 518 | LHG  | C32-C33-C34-C35 |
| 26  | D     | 406 | LHG  | C32-C33-C34-C35 |
| 26  | N     | 618 | LHG  | C15-C16-C17-C18 |
| 26  | 6     | 606 | LHG  | C12-C13-C14-C15 |
| 26  | b     | 621 | LHG  | C25-C26-C27-C28 |
| 26  | b     | 621 | LHG  | C32-C33-C34-C35 |
| 26  | c     | 518 | LHG  | C32-C33-C34-C35 |
| 26  | d     | 406 | LHG  | C32-C33-C34-C35 |
| 29  | L     | 103 | SQD  | C32-C33-C34-C35 |
| 29  | l     | 101 | SQD  | C32-C33-C34-C35 |
| 35  | A     | 415 | DGD  | C8B-C9B-CAB-CBB |
| 35  | a     | 401 | DGD  | C8B-C9B-CAB-CBB |
| 24  | R     | 605 | CHL  | CBD-CGD-O2D-CED |
| 24  | r     | 605 | CHL  | CBD-CGD-O2D-CED |
| 29  | A     | 411 | SQD  | C23-C24-C25-C26 |
| 29  | a     | 412 | SQD  | C23-C24-C25-C26 |
| 25  | C     | 506 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 506 | CLA  | C13-C15-C16-C17 |
| 26  | S     | 318 | LHG  | C11-C12-C13-C14 |
| 26  | s     | 318 | LHG  | C11-C12-C13-C14 |
| 26  | n     | 618 | LHG  | C34-C35-C36-C37 |
| 26  | y     | 319 | LHG  | C24-C25-C26-C27 |
| 29  | A     | 411 | SQD  | C16-C17-C18-C19 |
| 29  | a     | 412 | SQD  | C16-C17-C18-C19 |
| 25  | g     | 611 | CLA  | C3-C5-C6-C7     |
| 26  | C     | 517 | LHG  | C24-C23-O8-C6   |
| 26  | c     | 517 | LHG  | C24-C23-O8-C6   |
| 26  | N     | 618 | LHG  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | Y     | 319 | LHG  | C24-C25-C26-C27 |
| 35  | A     | 415 | DGD  | C8A-C9A-CAA-CBA |
| 35  | a     | 401 | DGD  | C8A-C9A-CAA-CBA |
| 24  | 2     | 603 | CHL  | C3A-C2A-CAA-CBA |
| 24  | G     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 24  | N     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 24  | Y     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 24  | R     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 24  | R     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 24  | 6     | 603 | CHL  | C3A-C2A-CAA-CBA |
| 24  | g     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 24  | n     | 608 | CHL  | C3A-C2A-CAA-CBA |
| 24  | y     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 24  | r     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 24  | r     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 25  | S     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 25  | Y     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 25  | Y     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 25  | s     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 25  | y     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 25  | y     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 25  | C     | 508 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 508 | CLA  | C13-C15-C16-C17 |
| 26  | B     | 621 | LHG  | C24-C25-C26-C27 |
| 26  | C     | 519 | LHG  | C25-C26-C27-C28 |
| 26  | b     | 621 | LHG  | C24-C25-C26-C27 |
| 26  | c     | 519 | LHG  | C25-C26-C27-C28 |
| 30  | B     | 623 | LMG  | C11-C12-C13-C14 |
| 30  | b     | 623 | LMG  | C11-C12-C13-C14 |
| 30  | B     | 623 | LMG  | O10-C28-O8-C9   |
| 30  | b     | 623 | LMG  | O10-C28-O8-C9   |
| 25  | B     | 608 | CLA  | C16-C17-C18-C20 |
| 25  | N     | 613 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 608 | CLA  | C16-C17-C18-C20 |
| 25  | n     | 613 | CLA  | C11-C12-C13-C14 |
| 24  | 2     | 603 | CHL  | C2C-C3C-CAC-CBC |
| 24  | R     | 613 | CHL  | C2C-C3C-CAC-CBC |
| 24  | 6     | 603 | CHL  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | A     | 408 | LMG  | C16-C17-C18-C19 |
| 30  | A     | 408 | LMG  | C34-C35-C36-C37 |
| 30  | a     | 409 | LMG  | C16-C17-C18-C19 |
| 30  | a     | 409 | LMG  | C34-C35-C36-C37 |
| 35  | B     | 626 | DGD  | CBA-CCA-CDA-CEA |
| 35  | b     | 626 | DGD  | CBA-CCA-CDA-CEA |
| 26  | S     | 301 | LHG  | C4-C5-C6-O8     |
| 26  | s     | 301 | LHG  | C4-C5-C6-O8     |
| 26  | C     | 517 | LHG  | C27-C28-C29-C30 |
| 26  | C     | 519 | LHG  | C9-C10-C11-C12  |
| 26  | S     | 318 | LHG  | C17-C18-C19-C20 |
| 26  | c     | 517 | LHG  | C27-C28-C29-C30 |
| 26  | c     | 519 | LHG  | C9-C10-C11-C12  |
| 26  | s     | 318 | LHG  | C17-C18-C19-C20 |
| 30  | B     | 623 | LMG  | C30-C31-C32-C33 |
| 25  | A     | 405 | CLA  | C3-C5-C6-C7     |
| 25  | G     | 611 | CLA  | C3-C5-C6-C7     |
| 25  | a     | 406 | CLA  | C3-C5-C6-C7     |
| 30  | D     | 407 | LMG  | C28-C29-C30-C31 |
| 30  | d     | 407 | LMG  | C28-C29-C30-C31 |
| 24  | r     | 613 | CHL  | C2C-C3C-CAC-CBC |
| 30  | b     | 623 | LMG  | C30-C31-C32-C33 |
| 25  | B     | 606 | CLA  | C2-C3-C5-C6     |
| 25  | B     | 609 | CLA  | C2-C3-C5-C6     |
| 25  | C     | 510 | CLA  | C2-C3-C5-C6     |
| 25  | S     | 311 | CLA  | C2-C3-C5-C6     |
| 25  | N     | 612 | CLA  | C2-C3-C5-C6     |
| 25  | b     | 606 | CLA  | C2-C3-C5-C6     |
| 25  | b     | 609 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 510 | CLA  | C2-C3-C5-C6     |
| 25  | s     | 311 | CLA  | C2-C3-C5-C6     |
| 25  | n     | 612 | CLA  | C2-C3-C5-C6     |
| 26  | Y     | 301 | LHG  | C8-C7-O7-C5     |
| 26  | y     | 301 | LHG  | C8-C7-O7-C5     |
| 24  | Y     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 24  | y     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 26  | S     | 301 | LHG  | O1-C1-C2-O2     |
| 26  | S     | 318 | LHG  | O1-C1-C2-O2     |
| 26  | Y     | 319 | LHG  | O1-C1-C2-O2     |
| 26  | s     | 301 | LHG  | O1-C1-C2-O2     |
| 26  | s     | 318 | LHG  | O1-C1-C2-O2     |
| 26  | y     | 319 | LHG  | O1-C1-C2-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | L     | 102 | LHG  | C29-C30-C31-C32 |
| 26  | l     | 103 | LHG  | C29-C30-C31-C32 |
| 29  | L     | 103 | SQD  | C26-C27-C28-C29 |
| 29  | l     | 101 | SQD  | C26-C27-C28-C29 |
| 35  | C     | 515 | DGD  | C6B-C7B-C8B-C9B |
| 35  | c     | 515 | DGD  | C6B-C7B-C8B-C9B |
| 25  | B     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 35  | C     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 35  | c     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 26  | S     | 318 | LHG  | O2-C2-C3-O3     |
| 26  | s     | 318 | LHG  | O2-C2-C3-O3     |
| 24  | Y     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 24  | y     | 302 | CHL  | C4C-C3C-CAC-CBC |
| 26  | S     | 301 | LHG  | C24-C25-C26-C27 |
| 26  | s     | 301 | LHG  | C24-C25-C26-C27 |
| 26  | L     | 102 | LHG  | C31-C32-C33-C34 |
| 26  | c     | 518 | LHG  | C31-C32-C33-C34 |
| 26  | l     | 103 | LHG  | C31-C32-C33-C34 |
| 30  | a     | 409 | LMG  | C13-C14-C15-C16 |
| 25  | B     | 610 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 610 | CLA  | C13-C15-C16-C17 |
| 26  | C     | 518 | LHG  | C31-C32-C33-C34 |
| 30  | A     | 408 | LMG  | C13-C14-C15-C16 |
| 30  | B     | 623 | LMG  | C16-C17-C18-C19 |
| 30  | b     | 623 | LMG  | C16-C17-C18-C19 |
| 24  | N     | 608 | CHL  | C2-C1-O2A-CGA   |
| 24  | n     | 608 | CHL  | C2-C1-O2A-CGA   |
| 35  | B     | 626 | DGD  | C4E-C5E-C6E-O5E |
| 35  | b     | 626 | DGD  | C4E-C5E-C6E-O5E |
| 25  | G     | 611 | CLA  | C4C-C3C-CAC-CBC |
| 25  | g     | 611 | CLA  | C4C-C3C-CAC-CBC |
| 25  | r     | 614 | CLA  | C4C-C3C-CAC-CBC |
| 26  | L     | 102 | LHG  | C28-C29-C30-C31 |
| 26  | L     | 102 | LHG  | C34-C35-C36-C37 |
| 26  | l     | 103 | LHG  | C28-C29-C30-C31 |
| 26  | l     | 103 | LHG  | C34-C35-C36-C37 |
| 35  | B     | 626 | DGD  | CCB-CDB-CEB-CFB |
| 35  | C     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 35  | b     | 626 | DGD  | CCB-CDB-CEB-CFB |
| 25  | B     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | C     | 505 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | b     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 505 | CLA  | C5-C6-C7-C8     |
| 25  | R     | 614 | CLA  | C4C-C3C-CAC-CBC |
| 35  | c     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 28  | B     | 617 | BCR  | C1-C6-C7-C8     |
| 28  | B     | 617 | BCR  | C5-C6-C7-C8     |
| 28  | B     | 618 | BCR  | C23-C24-C25-C26 |
| 28  | B     | 619 | BCR  | C23-C24-C25-C30 |
| 28  | D     | 404 | BCR  | C5-C6-C7-C8     |
| 28  | T     | 101 | BCR  | C23-C24-C25-C26 |
| 28  | T     | 101 | BCR  | C23-C24-C25-C30 |
| 28  | Z     | 101 | BCR  | C5-C6-C7-C8     |
| 28  | b     | 617 | BCR  | C1-C6-C7-C8     |
| 28  | b     | 617 | BCR  | C5-C6-C7-C8     |
| 28  | b     | 618 | BCR  | C23-C24-C25-C26 |
| 28  | b     | 619 | BCR  | C23-C24-C25-C30 |
| 28  | d     | 404 | BCR  | C5-C6-C7-C8     |
| 28  | t     | 101 | BCR  | C23-C24-C25-C26 |
| 28  | t     | 101 | BCR  | C23-C24-C25-C30 |
| 28  | z     | 101 | BCR  | C5-C6-C7-C8     |
| 39  | G     | 615 | LUT  | C5-C6-C7-C8     |
| 39  | N     | 615 | LUT  | C1-C6-C7-C8     |
| 39  | N     | 615 | LUT  | C5-C6-C7-C8     |
| 39  | N     | 616 | LUT  | C1-C6-C7-C8     |
| 39  | N     | 616 | LUT  | C5-C6-C7-C8     |
| 39  | Y     | 316 | LUT  | C1-C6-C7-C8     |
| 39  | Y     | 316 | LUT  | C5-C6-C7-C8     |
| 39  | R     | 615 | LUT  | C5-C6-C7-C8     |
| 39  | g     | 615 | LUT  | C5-C6-C7-C8     |
| 39  | n     | 615 | LUT  | C1-C6-C7-C8     |
| 39  | n     | 615 | LUT  | C5-C6-C7-C8     |
| 39  | n     | 616 | LUT  | C1-C6-C7-C8     |
| 39  | n     | 616 | LUT  | C5-C6-C7-C8     |
| 39  | y     | 316 | LUT  | C1-C6-C7-C8     |
| 39  | y     | 316 | LUT  | C5-C6-C7-C8     |
| 39  | r     | 615 | LUT  | C5-C6-C7-C8     |
| 25  | N     | 604 | CLA  | C4C-C3C-CAC-CBC |
| 25  | G     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | G     | 603 | CLA  | C10-C11-C12-C13 |
| 25  | g     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | g     | 603 | CLA  | C10-C11-C12-C13 |
| 30  | D     | 407 | LMG  | C11-C10-O7-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | d     | 407 | LMG  | C11-C10-O7-C8   |
| 29  | A     | 411 | SQD  | C29-C30-C31-C32 |
| 29  | L     | 103 | SQD  | C27-C28-C29-C30 |
| 29  | a     | 412 | SQD  | C29-C30-C31-C32 |
| 29  | l     | 101 | SQD  | C27-C28-C29-C30 |
| 26  | s     | 318 | LHG  | C23-C24-C25-C26 |
| 35  | A     | 415 | DGD  | C1B-C2B-C3B-C4B |
| 35  | a     | 401 | DGD  | C1B-C2B-C3B-C4B |
| 25  | n     | 604 | CLA  | C4C-C3C-CAC-CBC |
| 26  | D     | 406 | LHG  | C26-C27-C28-C29 |
| 26  | d     | 406 | LHG  | C26-C27-C28-C29 |
| 24  | Y     | 309 | CHL  | C10-C11-C12-C13 |
| 24  | y     | 309 | CHL  | C10-C11-C12-C13 |
| 25  | A     | 401 | CLA  | C15-C16-C17-C18 |
| 25  | B     | 605 | CLA  | C5-C6-C7-C8     |
| 25  | C     | 511 | CLA  | C10-C11-C12-C13 |
| 25  | a     | 402 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 605 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 511 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 612 | CLA  | C4-C3-C5-C6     |
| 25  | R     | 608 | CLA  | C4-C3-C5-C6     |
| 25  | n     | 612 | CLA  | C4-C3-C5-C6     |
| 25  | r     | 608 | CLA  | C4-C3-C5-C6     |
| 24  | N     | 609 | CHL  | C2-C3-C5-C6     |
| 24  | n     | 609 | CHL  | C2-C3-C5-C6     |
| 25  | A     | 405 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 602 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 602 | CLA  | C12-C13-C15-C16 |
| 25  | B     | 604 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 610 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 611 | CLA  | C2-C3-C5-C6     |
| 25  | B     | 615 | CLA  | C2-C3-C5-C6     |
| 25  | C     | 501 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C12-C13-C15-C16 |
| 25  | S     | 303 | CLA  | C11-C10-C8-C7   |
| 25  | S     | 313 | CLA  | C2-C3-C5-C6     |
| 25  | G     | 602 | CLA  | C11-C10-C8-C7   |
| 25  | G     | 602 | CLA  | C12-C13-C15-C16 |
| 25  | Y     | 303 | CLA  | C11-C10-C8-C7   |
| 25  | Y     | 304 | CLA  | C6-C7-C8-C10    |
| 25  | Y     | 312 | CLA  | C2-C3-C5-C6     |
| 25  | R     | 608 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | a     | 406 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 602 | CLA  | C12-C13-C15-C16 |
| 25  | b     | 604 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 610 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 611 | CLA  | C2-C3-C5-C6     |
| 25  | b     | 615 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 501 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 507 | CLA  | C12-C13-C15-C16 |
| 25  | s     | 303 | CLA  | C11-C10-C8-C7   |
| 25  | s     | 313 | CLA  | C2-C3-C5-C6     |
| 25  | g     | 602 | CLA  | C11-C10-C8-C7   |
| 25  | g     | 602 | CLA  | C12-C13-C15-C16 |
| 25  | y     | 303 | CLA  | C11-C10-C8-C7   |
| 25  | y     | 304 | CLA  | C6-C7-C8-C10    |
| 25  | y     | 312 | CLA  | C2-C3-C5-C6     |
| 25  | r     | 608 | CLA  | C6-C7-C8-C10    |
| 26  | C     | 517 | LHG  | O10-C23-O8-C6   |
| 26  | c     | 517 | LHG  | O10-C23-O8-C6   |
| 30  | B     | 623 | LMG  | C17-C18-C19-C20 |
| 30  | b     | 623 | LMG  | C17-C18-C19-C20 |
| 24  | N     | 608 | CHL  | C15-C16-C17-C18 |
| 24  | n     | 608 | CHL  | C15-C16-C17-C18 |
| 25  | G     | 611 | CLA  | C8-C10-C11-C12  |
| 25  | R     | 609 | CLA  | C13-C15-C16-C17 |
| 25  | g     | 611 | CLA  | C8-C10-C11-C12  |
| 25  | r     | 609 | CLA  | C13-C15-C16-C17 |
| 24  | R     | 607 | CHL  | C11-C12-C13-C14 |
| 24  | r     | 607 | CHL  | C11-C12-C13-C14 |
| 25  | R     | 602 | CLA  | C11-C12-C13-C15 |
| 25  | R     | 609 | CLA  | C16-C17-C18-C19 |
| 25  | r     | 602 | CLA  | C11-C12-C13-C15 |
| 25  | r     | 609 | CLA  | C16-C17-C18-C19 |
| 26  | S     | 318 | LHG  | C23-C24-C25-C26 |
| 30  | D     | 407 | LMG  | C20-C21-C22-C23 |
| 30  | d     | 407 | LMG  | C20-C21-C22-C23 |
| 25  | 2     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 25  | 6     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 513 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 513 | CLA  | C5-C6-C7-C8     |
| 27  | A     | 403 | PHO  | C13-C15-C16-C17 |
| 27  | a     | 404 | PHO  | C13-C15-C16-C17 |
| 26  | D     | 406 | LHG  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | d     | 406 | LHG  | C25-C26-C27-C28 |
| 30  | A     | 408 | LMG  | C35-C36-C37-C38 |
| 30  | a     | 409 | LMG  | C35-C36-C37-C38 |
| 24  | y     | 309 | CHL  | O1A-CGA-O2A-C1  |
| 30  | D     | 407 | LMG  | C29-C30-C31-C32 |
| 30  | d     | 407 | LMG  | C29-C30-C31-C32 |
| 25  | S     | 311 | CLA  | C11-C10-C8-C7   |
| 25  | s     | 311 | CLA  | C11-C10-C8-C7   |
| 29  | L     | 103 | SQD  | C12-C13-C14-C15 |
| 29  | l     | 101 | SQD  | C12-C13-C14-C15 |
| 30  | C     | 520 | LMG  | C11-C12-C13-C14 |
| 30  | c     | 520 | LMG  | C11-C12-C13-C14 |
| 24  | Y     | 309 | CHL  | O1A-CGA-O2A-C1  |
| 26  | B     | 625 | LHG  | C32-C33-C34-C35 |
| 26  | b     | 625 | LHG  | C32-C33-C34-C35 |
| 30  | A     | 408 | LMG  | C29-C30-C31-C32 |
| 30  | a     | 409 | LMG  | C29-C30-C31-C32 |
| 26  | L     | 102 | LHG  | O6-C4-C5-O7     |
| 26  | l     | 103 | LHG  | O6-C4-C5-O7     |
| 26  | S     | 318 | LHG  | C31-C32-C33-C34 |
| 26  | s     | 318 | LHG  | C31-C32-C33-C34 |
| 29  | A     | 407 | SQD  | C17-C18-C19-C20 |
| 29  | a     | 408 | SQD  | C17-C18-C19-C20 |
| 35  | C     | 516 | DGD  | CCB-CDB-CEB-CFB |
| 35  | c     | 516 | DGD  | CCB-CDB-CEB-CFB |
| 32  | A     | 412 | AJP  | C68-C69-C71-O72 |
| 32  | a     | 413 | AJP  | C68-C69-C71-O72 |
| 25  | C     | 508 | CLA  | C15-C16-C17-C18 |
| 25  | N     | 602 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 602 | CLA  | C10-C11-C12-C13 |
| 25  | C     | 512 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 512 | CLA  | CBD-CGD-O2D-CED |
| 26  | B     | 625 | LHG  | C15-C16-C17-C18 |
| 26  | C     | 519 | LHG  | C12-C13-C14-C15 |
| 26  | c     | 519 | LHG  | C12-C13-C14-C15 |
| 25  | G     | 613 | CLA  | C3-C5-C6-C7     |
| 25  | g     | 613 | CLA  | C3-C5-C6-C7     |
| 26  | b     | 625 | LHG  | C15-C16-C17-C18 |
| 29  | L     | 103 | SQD  | C15-C16-C17-C18 |
| 29  | l     | 101 | SQD  | C15-C16-C17-C18 |
| 25  | c     | 508 | CLA  | C15-C16-C17-C18 |
| 26  | S     | 301 | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | s     | 301 | LHG  | O7-C5-C6-O8     |
| 29  | A     | 411 | SQD  | O6-C44-C45-O47  |
| 29  | a     | 412 | SQD  | O6-C44-C45-O47  |
| 30  | B     | 623 | LMG  | C19-C20-C21-C22 |
| 30  | b     | 623 | LMG  | C19-C20-C21-C22 |
| 35  | A     | 415 | DGD  | CBB-CCB-CDB-CEB |
| 35  | B     | 626 | DGD  | C3B-C4B-C5B-C6B |
| 35  | a     | 401 | DGD  | CBB-CCB-CDB-CEB |
| 35  | b     | 626 | DGD  | C3B-C4B-C5B-C6B |
| 25  | G     | 610 | CLA  | C2-C3-C5-C6     |
| 25  | Y     | 311 | CLA  | C2-C3-C5-C6     |
| 25  | g     | 610 | CLA  | C2-C3-C5-C6     |
| 25  | y     | 311 | CLA  | C2-C3-C5-C6     |
| 31  | D     | 405 | PL9  | C4-C3-C7-C8     |
| 31  | d     | 405 | PL9  | C4-C3-C7-C8     |
| 24  | N     | 607 | CHL  | C6-C7-C8-C9     |
| 24  | n     | 607 | CHL  | C6-C7-C8-C9     |
| 25  | A     | 405 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 604 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 607 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 611 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 615 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 510 | CLA  | C11-C12-C13-C14 |
| 25  | G     | 602 | CLA  | C14-C13-C15-C16 |
| 25  | G     | 603 | CLA  | C11-C10-C8-C9   |
| 25  | G     | 610 | CLA  | C14-C13-C15-C16 |
| 25  | N     | 603 | CLA  | C14-C13-C15-C16 |
| 25  | N     | 610 | CLA  | C11-C12-C13-C14 |
| 25  | a     | 406 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 603 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 604 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 607 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 611 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 615 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 507 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 510 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 602 | CLA  | C14-C13-C15-C16 |
| 25  | g     | 603 | CLA  | C11-C10-C8-C9   |
| 25  | g     | 610 | CLA  | C14-C13-C15-C16 |
| 25  | n     | 603 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | n     | 610 | CLA  | C11-C12-C13-C14 |
| 27  | A     | 403 | PHO  | C11-C10-C8-C9   |
| 27  | a     | 404 | PHO  | C11-C10-C8-C9   |
| 24  | G     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 26  | S     | 318 | LHG  | C29-C30-C31-C32 |
| 26  | s     | 318 | LHG  | C29-C30-C31-C32 |
| 24  | N     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 24  | n     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 25  | B     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 25  | B     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | S     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 25  | S     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | s     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 25  | s     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 24  | S     | 306 | CHL  | O1D-CGD-O2D-CED |
| 24  | s     | 306 | CHL  | O1D-CGD-O2D-CED |
| 24  | G     | 601 | CHL  | C13-C15-C16-C17 |
| 24  | g     | 601 | CHL  | C13-C15-C16-C17 |
| 25  | C     | 506 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 613 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 506 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 613 | CLA  | C8-C10-C11-C12  |
| 24  | g     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 26  | C     | 519 | LHG  | C30-C31-C32-C33 |
| 26  | c     | 519 | LHG  | C30-C31-C32-C33 |
| 35  | A     | 415 | DGD  | C7A-C8A-C9A-CAA |
| 35  | a     | 401 | DGD  | C7A-C8A-C9A-CAA |
| 24  | 2     | 603 | CHL  | C1A-C2A-CAA-CBA |
| 24  | R     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 24  | 6     | 603 | CHL  | C1A-C2A-CAA-CBA |
| 24  | n     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 24  | r     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 25  | A     | 402 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | C     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 25  | S     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 25  | S     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 611 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | Y     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 25  | Y     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 25  | Y     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | a     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 25  | b     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | c     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 25  | s     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 25  | s     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | y     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 25  | y     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 25  | y     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 25  | N     | 613 | CLA  | C11-C12-C13-C15 |
| 25  | R     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | R     | 603 | CLA  | C11-C12-C13-C14 |
| 25  | n     | 613 | CLA  | C11-C12-C13-C15 |
| 25  | r     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | r     | 603 | CLA  | C11-C12-C13-C14 |
| 26  | Y     | 301 | LHG  | O9-C7-O7-C5     |
| 26  | y     | 301 | LHG  | O9-C7-O7-C5     |
| 30  | D     | 407 | LMG  | O9-C10-O7-C8    |
| 30  | d     | 407 | LMG  | O9-C10-O7-C8    |
| 26  | L     | 102 | LHG  | C8-C7-O7-C5     |
| 26  | l     | 103 | LHG  | C8-C7-O7-C5     |
| 24  | N     | 607 | CHL  | C13-C15-C16-C17 |
| 24  | n     | 607 | CHL  | C13-C15-C16-C17 |
| 24  | 2     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | G     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | 6     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | g     | 601 | CHL  | C3-C5-C6-C7     |
| 24  | r     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 25  | C     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 602 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 602 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | d     | 403 | CLA  | C8-C10-C11-C12  |
| 26  | S     | 301 | LHG  | O6-C4-C5-C6     |
| 26  | N     | 618 | LHG  | O6-C4-C5-C6     |
| 26  | s     | 301 | LHG  | O6-C4-C5-C6     |
| 26  | n     | 618 | LHG  | O6-C4-C5-C6     |
| 24  | R     | 606 | CHL  | C4C-C3C-CAC-CBC |
| 30  | B     | 620 | LMG  | C17-C18-C19-C20 |
| 30  | b     | 620 | LMG  | C17-C18-C19-C20 |
| 25  | D     | 403 | CLA  | C8-C10-C11-C12  |
| 26  | C     | 517 | LHG  | C14-C15-C16-C17 |
| 26  | c     | 517 | LHG  | C14-C15-C16-C17 |
| 29  | L     | 103 | SQD  | C31-C32-C33-C34 |
| 29  | l     | 101 | SQD  | C31-C32-C33-C34 |
| 35  | A     | 415 | DGD  | C9B-CAB-CBB-CCB |
| 35  | a     | 401 | DGD  | C9B-CAB-CBB-CCB |
| 24  | G     | 609 | CHL  | O1D-CGD-O2D-CED |
| 32  | B     | 624 | AJP  | C56-C57-O64-C65 |
| 32  | b     | 624 | AJP  | C56-C57-O64-C65 |
| 25  | Y     | 312 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 312 | CLA  | C10-C11-C12-C13 |
| 26  | Y     | 319 | LHG  | C25-C26-C27-C28 |
| 35  | A     | 415 | DGD  | C6B-C7B-C8B-C9B |
| 35  | a     | 401 | DGD  | C6B-C7B-C8B-C9B |
| 26  | S     | 318 | LHG  | C1-C2-C3-O3     |
| 26  | Y     | 319 | LHG  | C1-C2-C3-O3     |
| 26  | s     | 318 | LHG  | C1-C2-C3-O3     |
| 26  | y     | 319 | LHG  | C1-C2-C3-O3     |
| 24  | N     | 609 | CHL  | C4-C3-C5-C6     |
| 24  | n     | 609 | CHL  | C4-C3-C5-C6     |
| 26  | c     | 518 | LHG  | C24-C25-C26-C27 |
| 26  | y     | 319 | LHG  | C25-C26-C27-C28 |
| 30  | B     | 620 | LMG  | C37-C38-C39-C40 |
| 25  | c     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 26  | C     | 518 | LHG  | C24-C25-C26-C27 |
| 30  | b     | 620 | LMG  | C37-C38-C39-C40 |
| 24  | l     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 24  | R     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 24  | r     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 25  | B     | 608 | CLA  | C2A-CAA-CBA-CGA |
| 25  | N     | 611 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 608 | CLA  | C2A-CAA-CBA-CGA |
| 25  | n     | 611 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 603 | CLA  | C16-C17-C18-C20 |
| 25  | C     | 513 | CLA  | C16-C17-C18-C19 |
| 25  | b     | 603 | CLA  | C16-C17-C18-C20 |
| 25  | c     | 513 | CLA  | C16-C17-C18-C19 |
| 24  | g     | 609 | CHL  | O1D-CGD-O2D-CED |
| 26  | B     | 621 | LHG  | C4-C5-C6-O8     |
| 26  | b     | 621 | LHG  | C4-C5-C6-O8     |
| 30  | A     | 408 | LMG  | C7-C8-C9-O8     |
| 30  | a     | 409 | LMG  | C7-C8-C9-O8     |
| 35  | B     | 626 | DGD  | C1G-C2G-C3G-O3G |
| 35  | b     | 626 | DGD  | C1G-C2G-C3G-O3G |
| 26  | 2     | 606 | LHG  | C29-C30-C31-C32 |
| 26  | 6     | 606 | LHG  | C29-C30-C31-C32 |
| 24  | g     | 601 | CHL  | C5-C6-C7-C8     |
| 25  | B     | 603 | CLA  | C15-C16-C17-C18 |
| 25  | B     | 606 | CLA  | C13-C15-C16-C17 |
| 25  | C     | 504 | CLA  | C10-C11-C12-C13 |
| 25  | R     | 609 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 603 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 606 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 504 | CLA  | C10-C11-C12-C13 |
| 25  | r     | 609 | CLA  | C5-C6-C7-C8     |
| 25  | S     | 303 | CLA  | C14-C13-C15-C16 |
| 25  | s     | 303 | CLA  | C14-C13-C15-C16 |
| 26  | Y     | 319 | LHG  | C34-C35-C36-C37 |
| 26  | y     | 319 | LHG  | C34-C35-C36-C37 |
| 35  | B     | 626 | DGD  | C1A-C2A-C3A-C4A |
| 35  | b     | 626 | DGD  | C1A-C2A-C3A-C4A |
| 24  | G     | 601 | CHL  | C5-C6-C7-C8     |
| 26  | S     | 318 | LHG  | C25-C26-C27-C28 |
| 26  | s     | 318 | LHG  | C25-C26-C27-C28 |
| 25  | C     | 504 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 504 | CLA  | C8-C10-C11-C12  |
| 30  | B     | 623 | LMG  | O6-C5-C6-O5     |
| 30  | b     | 623 | LMG  | O6-C5-C6-O5     |
| 25  | G     | 613 | CLA  | C4-C3-C5-C6     |
| 25  | g     | 613 | CLA  | C4-C3-C5-C6     |
| 25  | n     | 602 | CLA  | C4-C3-C5-C6     |
| 32  | B     | 624 | AJP  | C58-C57-O64-C65 |
| 32  | b     | 624 | AJP  | C58-C57-O64-C65 |
| 35  | A     | 415 | DGD  | C3B-C4B-C5B-C6B |
| 35  | a     | 401 | DGD  | C3B-C4B-C5B-C6B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | N     | 612 | CLA  | C11-C12-C13-C15 |
| 25  | n     | 612 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 25  | r     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 29  | A     | 407 | SQD  | C10-C11-C12-C13 |
| 29  | a     | 408 | SQD  | C10-C11-C12-C13 |
| 24  | G     | 609 | CHL  | CBD-CGD-O2D-CED |
| 24  | g     | 609 | CHL  | CBD-CGD-O2D-CED |
| 25  | B     | 616 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 616 | CLA  | C8-C10-C11-C12  |
| 26  | R     | 618 | LHG  | C28-C29-C30-C31 |
| 26  | r     | 618 | LHG  | C28-C29-C30-C31 |
| 24  | 5     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 25  | N     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 25  | n     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 24  | G     | 601 | CHL  | C2-C1-O2A-CGA   |
| 24  | g     | 601 | CHL  | C2-C1-O2A-CGA   |
| 29  | A     | 411 | SQD  | C30-C31-C32-C33 |
| 35  | C     | 516 | DGD  | C2A-C1A-O1G-C1G |
| 35  | c     | 516 | DGD  | C2A-C1A-O1G-C1G |
| 26  | C     | 517 | LHG  | O6-C4-C5-O7     |
| 26  | c     | 517 | LHG  | O6-C4-C5-O7     |
| 25  | 2     | 602 | CLA  | C11-C12-C13-C15 |
| 25  | 6     | 602 | CLA  | C11-C12-C13-C15 |
| 29  | a     | 412 | SQD  | C30-C31-C32-C33 |
| 24  | Y     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 24  | y     | 302 | CHL  | O1A-CGA-O2A-C1  |
| 26  | b     | 622 | LHG  | C26-C27-C28-C29 |
| 30  | A     | 410 | LMG  | C36-C37-C38-C39 |
| 30  | a     | 411 | LMG  | C36-C37-C38-C39 |
| 35  | A     | 415 | DGD  | C1A-C2A-C3A-C4A |
| 35  | a     | 401 | DGD  | C1A-C2A-C3A-C4A |
| 28  | I     | 101 | BCR  | C20-C21-C22-C23 |
| 28  | i     | 101 | BCR  | C20-C21-C22-C23 |
| 25  | A     | 401 | CLA  | C4C-C3C-CAC-CBC |
| 25  | a     | 402 | CLA  | C4C-C3C-CAC-CBC |
| 26  | B     | 622 | LHG  | C26-C27-C28-C29 |
| 26  | B     | 621 | LHG  | O7-C5-C6-O8     |
| 26  | N     | 618 | LHG  | O7-C5-C6-O8     |
| 26  | b     | 621 | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | n     | 618 | LHG  | O7-C5-C6-O8     |
| 29  | A     | 407 | SQD  | O6-C44-C45-O47  |
| 29  | a     | 408 | SQD  | O6-C44-C45-O47  |
| 30  | C     | 520 | LMG  | O7-C8-C9-O8     |
| 30  | c     | 520 | LMG  | O7-C8-C9-O8     |
| 26  | L     | 102 | LHG  | C10-C11-C12-C13 |
| 26  | l     | 103 | LHG  | C10-C11-C12-C13 |
| 30  | A     | 410 | LMG  | C40-C41-C42-C43 |
| 30  | a     | 411 | LMG  | C40-C41-C42-C43 |
| 35  | C     | 516 | DGD  | C2B-C3B-C4B-C5B |
| 25  | B     | 606 | CLA  | C4-C3-C5-C6     |
| 25  | N     | 602 | CLA  | C4-C3-C5-C6     |
| 25  | Y     | 313 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 606 | CLA  | C4-C3-C5-C6     |
| 25  | y     | 313 | CLA  | C4-C3-C5-C6     |
| 25  | n     | 603 | CLA  | C4C-C3C-CAC-CBC |
| 26  | N     | 618 | LHG  | C31-C32-C33-C34 |
| 35  | c     | 516 | DGD  | C2B-C3B-C4B-C5B |
| 24  | G     | 608 | CHL  | C11-C10-C8-C7   |
| 24  | Y     | 302 | CHL  | C12-C13-C15-C16 |
| 24  | Y     | 309 | CHL  | C12-C13-C15-C16 |
| 24  | g     | 608 | CHL  | C11-C10-C8-C7   |
| 24  | y     | 302 | CHL  | C12-C13-C15-C16 |
| 24  | y     | 309 | CHL  | C12-C13-C15-C16 |
| 25  | B     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 604 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 613 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 613 | CLA  | C12-C13-C15-C16 |
| 25  | B     | 614 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 615 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C6-C7-C8-C10    |
| 25  | C     | 509 | CLA  | C6-C7-C8-C10    |
| 25  | C     | 509 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 511 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 511 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 512 | CLA  | C12-C13-C15-C16 |
| 25  | D     | 403 | CLA  | C2-C3-C5-C6     |
| 25  | S     | 303 | CLA  | C6-C7-C8-C10    |
| 25  | G     | 610 | CLA  | C12-C13-C15-C16 |
| 25  | N     | 603 | CLA  | C11-C10-C8-C7   |
| 25  | N     | 603 | CLA  | C11-C12-C13-C15 |
| 25  | Y     | 304 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | Y     | 304 | CLA  | C11-C10-C8-C7   |
| 25  | R     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 602 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 604 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 613 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 613 | CLA  | C12-C13-C15-C16 |
| 25  | b     | 614 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 615 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 507 | CLA  | C6-C7-C8-C10    |
| 25  | c     | 509 | CLA  | C6-C7-C8-C10    |
| 25  | c     | 509 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 511 | CLA  | C11-C10-C8-C7   |
| 25  | c     | 511 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 512 | CLA  | C12-C13-C15-C16 |
| 25  | d     | 403 | CLA  | C2-C3-C5-C6     |
| 25  | s     | 303 | CLA  | C6-C7-C8-C10    |
| 25  | g     | 610 | CLA  | C12-C13-C15-C16 |
| 25  | n     | 603 | CLA  | C11-C10-C8-C7   |
| 25  | n     | 603 | CLA  | C11-C12-C13-C15 |
| 25  | y     | 304 | CLA  | C2-C3-C5-C6     |
| 25  | y     | 304 | CLA  | C11-C10-C8-C7   |
| 25  | r     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | r     | 612 | CLA  | C6-C7-C8-C10    |
| 24  | Y     | 310 | CHL  | C3-C5-C6-C7     |
| 24  | y     | 310 | CHL  | C3-C5-C6-C7     |
| 25  | N     | 603 | CLA  | C4C-C3C-CAC-CBC |
| 26  | b     | 625 | LHG  | C12-C13-C14-C15 |
| 26  | n     | 618 | LHG  | C31-C32-C33-C34 |
| 25  | B     | 601 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 601 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 605 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 504 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 508 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 510 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 511 | CLA  | C11-C12-C13-C14 |
| 25  | C     | 512 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 513 | CLA  | C11-C10-C8-C9   |
| 25  | D     | 403 | CLA  | C14-C13-C15-C16 |
| 25  | Y     | 313 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 313 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 601 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | b     | 601 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 605 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 504 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 508 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 510 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 511 | CLA  | C11-C12-C13-C14 |
| 25  | c     | 512 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 513 | CLA  | C11-C10-C8-C9   |
| 25  | d     | 403 | CLA  | C14-C13-C15-C16 |
| 25  | y     | 313 | CLA  | C6-C7-C8-C9     |
| 25  | y     | 313 | CLA  | C11-C10-C8-C9   |
| 26  | B     | 625 | LHG  | C12-C13-C14-C15 |
| 26  | y     | 301 | LHG  | C13-C14-C15-C16 |
| 25  | B     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 25  | N     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 25  | b     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 25  | n     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 603 | CLA  | C10-C11-C12-C13 |
| 25  | R     | 612 | CLA  | C5-C6-C7-C8     |
| 25  | r     | 603 | CLA  | C10-C11-C12-C13 |
| 25  | r     | 612 | CLA  | C5-C6-C7-C8     |
| 26  | Y     | 301 | LHG  | C13-C14-C15-C16 |
| 25  | R     | 610 | CLA  | C2C-C3C-CAC-CBC |
| 25  | r     | 610 | CLA  | C2C-C3C-CAC-CBC |
| 26  | 2     | 606 | LHG  | C17-C18-C19-C20 |
| 26  | 6     | 606 | LHG  | C17-C18-C19-C20 |
| 30  | B     | 620 | LMG  | C22-C23-C24-C25 |
| 30  | b     | 620 | LMG  | C22-C23-C24-C25 |
| 26  | B     | 622 | LHG  | C14-C15-C16-C17 |
| 26  | b     | 622 | LHG  | C14-C15-C16-C17 |
| 25  | C     | 513 | CLA  | C3-C5-C6-C7     |
| 25  | c     | 513 | CLA  | C3-C5-C6-C7     |
| 25  | R     | 609 | CLA  | O1D-CGD-O2D-CED |
| 25  | r     | 609 | CLA  | O1D-CGD-O2D-CED |
| 25  | B     | 611 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 610 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 611 | CLA  | C10-C11-C12-C13 |
| 26  | B     | 621 | LHG  | C11-C10-C9-C8   |
| 26  | N     | 618 | LHG  | C35-C36-C37-C38 |
| 26  | b     | 621 | LHG  | C11-C10-C9-C8   |
| 26  | n     | 618 | LHG  | C35-C36-C37-C38 |
| 26  | C     | 519 | LHG  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | c     | 519 | LHG  | C34-C35-C36-C37 |
| 35  | C     | 515 | DGD  | C4B-C5B-C6B-C7B |
| 25  | C     | 506 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 506 | CLA  | C5-C6-C7-C8     |
| 25  | n     | 610 | CLA  | C13-C15-C16-C17 |
| 32  | G     | 618 | AJP  | O31-C30-C32-O33 |
| 32  | g     | 618 | AJP  | O31-C30-C32-O33 |
| 35  | c     | 515 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 516 | DGD  | O6D-C1D-O3G-C3G |
| 35  | c     | 516 | DGD  | O6D-C1D-O3G-C3G |
| 26  | L     | 102 | LHG  | O6-C4-C5-C6     |
| 26  | l     | 103 | LHG  | O6-C4-C5-C6     |
| 29  | L     | 103 | SQD  | C11-C12-C13-C14 |
| 29  | l     | 101 | SQD  | C11-C12-C13-C14 |
| 28  | T     | 101 | BCR  | C10-C11-C12-C13 |
| 28  | t     | 101 | BCR  | C10-C11-C12-C13 |
| 24  | 6     | 601 | CHL  | C15-C16-C17-C18 |
| 26  | N     | 618 | LHG  | C16-C17-C18-C19 |
| 26  | n     | 618 | LHG  | C16-C17-C18-C19 |
| 35  | A     | 415 | DGD  | CCB-CDB-CEB-CFB |
| 35  | a     | 401 | DGD  | CCB-CDB-CEB-CFB |
| 24  | R     | 607 | CHL  | C4-C3-C5-C6     |
| 24  | r     | 607 | CHL  | C4-C3-C5-C6     |
| 25  | N     | 613 | CLA  | C4-C3-C5-C6     |
| 25  | Y     | 311 | CLA  | C4-C3-C5-C6     |
| 25  | n     | 613 | CLA  | C4-C3-C5-C6     |
| 25  | y     | 311 | CLA  | C4-C3-C5-C6     |
| 24  | 2     | 601 | CHL  | C15-C16-C17-C18 |
| 26  | Y     | 301 | LHG  | C32-C33-C34-C35 |
| 26  | y     | 301 | LHG  | C32-C33-C34-C35 |
| 25  | S     | 311 | CLA  | C11-C10-C8-C9   |
| 25  | s     | 311 | CLA  | C11-C10-C8-C9   |
| 25  | Y     | 312 | CLA  | C11-C12-C13-C15 |
| 25  | y     | 312 | CLA  | C11-C12-C13-C15 |
| 25  | R     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 510 | CLA  | C2C-C3C-CAC-CBC |
| 25  | c     | 510 | CLA  | C2C-C3C-CAC-CBC |
| 35  | A     | 415 | DGD  | C2A-C3A-C4A-C5A |
| 35  | a     | 401 | DGD  | C2A-C3A-C4A-C5A |
| 24  | N     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 24  | Y     | 306 | CHL  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | R     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 24  | n     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 24  | y     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 24  | r     | 607 | CHL  | C3A-C2A-CAA-CBA |
| 25  | S     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 25  | Y     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 25  | s     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 25  | y     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 24  | 5     | 301 | CHL  | C2C-C3C-CAC-CBC |
| 26  | B     | 625 | LHG  | C14-C15-C16-C17 |
| 26  | b     | 625 | LHG  | C14-C15-C16-C17 |
| 25  | 2     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 603 | CLA  | C16-C17-C18-C19 |
| 25  | R     | 603 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 603 | CLA  | C16-C17-C18-C19 |
| 25  | r     | 603 | CLA  | C11-C12-C13-C15 |
| 24  | 1     | 301 | CHL  | C2C-C3C-CAC-CBC |
| 25  | c     | 512 | CLA  | C2C-C3C-CAC-CBC |
| 25  | 2     | 605 | CLA  | O2A-C1-C2-C3    |
| 25  | 6     | 605 | CLA  | O2A-C1-C2-C3    |
| 25  | C     | 510 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 510 | CLA  | C8-C10-C11-C12  |
| 24  | n     | 606 | CHL  | O1D-CGD-O2D-CED |
| 29  | A     | 411 | SQD  | O6-C44-C45-C46  |
| 29  | a     | 412 | SQD  | O6-C44-C45-C46  |
| 30  | B     | 623 | LMG  | C7-C8-C9-O8     |
| 30  | b     | 623 | LMG  | C7-C8-C9-O8     |
| 26  | L     | 102 | LHG  | O9-C7-O7-C5     |
| 26  | l     | 103 | LHG  | O9-C7-O7-C5     |
| 25  | C     | 512 | CLA  | C2C-C3C-CAC-CBC |
| 29  | A     | 411 | SQD  | C25-C26-C27-C28 |
| 29  | a     | 412 | SQD  | C25-C26-C27-C28 |
| 26  | D     | 406 | LHG  | C34-C35-C36-C37 |
| 29  | L     | 103 | SQD  | C30-C31-C32-C33 |
| 29  | l     | 101 | SQD  | C30-C31-C32-C33 |
| 26  | d     | 406 | LHG  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | C     | 516 | DGD  | CAA-CBA-CCA-CDA |
| 35  | c     | 516 | DGD  | CAA-CBA-CCA-CDA |
| 24  | N     | 606 | CHL  | O1D-CGD-O2D-CED |
| 26  | 2     | 606 | LHG  | C27-C28-C29-C30 |
| 26  | 6     | 606 | LHG  | C27-C28-C29-C30 |
| 29  | L     | 101 | SQD  | C29-C30-C31-C32 |
| 29  | l     | 102 | SQD  | C29-C30-C31-C32 |
| 25  | B     | 615 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 615 | CLA  | C8-C10-C11-C12  |
| 25  | C     | 513 | CLA  | C16-C17-C18-C20 |
| 25  | 6     | 602 | CLA  | C11-C12-C13-C14 |
| 25  | c     | 513 | CLA  | C16-C17-C18-C20 |
| 25  | R     | 608 | CLA  | C2-C3-C5-C6     |
| 25  | r     | 608 | CLA  | C2-C3-C5-C6     |
| 26  | 2     | 606 | LHG  | C35-C36-C37-C38 |
| 30  | b     | 623 | LMG  | C15-C16-C17-C18 |
| 26  | N     | 618 | LHG  | C19-C20-C21-C22 |
| 26  | 6     | 606 | LHG  | C35-C36-C37-C38 |
| 30  | B     | 623 | LMG  | C15-C16-C17-C18 |
| 24  | G     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 24  | N     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 24  | Y     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 24  | Y     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 24  | g     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 24  | n     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 24  | y     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 24  | y     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 26  | n     | 618 | LHG  | C19-C20-C21-C22 |
| 25  | Y     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 25  | y     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 26  | C     | 519 | LHG  | O1-C1-C2-O2     |
| 26  | c     | 519 | LHG  | O1-C1-C2-O2     |
| 25  | B     | 612 | CLA  | C10-C11-C12-C13 |
| 25  | G     | 610 | CLA  | C10-C11-C12-C13 |
| 25  | N     | 603 | CLA  | C8-C10-C11-C12  |
| 25  | b     | 612 | CLA  | C10-C11-C12-C13 |
| 25  | g     | 610 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 603 | CLA  | C8-C10-C11-C12  |
| 26  | B     | 621 | LHG  | O6-C4-C5-O7     |
| 26  | S     | 301 | LHG  | O6-C4-C5-O7     |
| 26  | N     | 618 | LHG  | O6-C4-C5-O7     |
| 26  | b     | 621 | LHG  | O6-C4-C5-O7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | s     | 301 | LHG  | O6-C4-C5-O7     |
| 26  | n     | 618 | LHG  | O6-C4-C5-O7     |
| 24  | r     | 613 | CHL  | C4C-C3C-CAC-CBC |
| 25  | 2     | 605 | CLA  | C2C-C3C-CAC-CBC |
| 35  | C     | 516 | DGD  | O1A-C1A-O1G-C1G |
| 35  | c     | 516 | DGD  | O1A-C1A-O1G-C1G |
| 25  | C     | 503 | CLA  | C16-C17-C18-C19 |
| 25  | Y     | 312 | CLA  | C11-C12-C13-C14 |
| 25  | c     | 503 | CLA  | C16-C17-C18-C19 |
| 25  | y     | 312 | CLA  | C11-C12-C13-C14 |
| 24  | R     | 613 | CHL  | C4C-C3C-CAC-CBC |
| 25  | 6     | 605 | CLA  | C2C-C3C-CAC-CBC |
| 24  | Y     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 24  | y     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 25  | R     | 612 | CLA  | C3-C5-C6-C7     |
| 26  | L     | 102 | LHG  | O7-C5-C6-O8     |
| 26  | l     | 103 | LHG  | O7-C5-C6-O8     |
| 29  | A     | 407 | SQD  | O47-C45-C46-O48 |
| 29  | a     | 408 | SQD  | O47-C45-C46-O48 |
| 30  | B     | 623 | LMG  | O7-C8-C9-O8     |
| 30  | b     | 623 | LMG  | O7-C8-C9-O8     |
| 24  | Y     | 309 | CHL  | CBA-CGA-O2A-C1  |
| 24  | y     | 309 | CHL  | CBA-CGA-O2A-C1  |
| 25  | B     | 608 | CLA  | CBA-CGA-O2A-C1  |
| 24  | Y     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 24  | y     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 35  | B     | 626 | DGD  | CDB-CEB-CFB-CGB |
| 25  | G     | 602 | CLA  | C16-C17-C18-C20 |
| 25  | g     | 602 | CLA  | C16-C17-C18-C20 |
| 24  | Y     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 24  | y     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 26  | y     | 301 | LHG  | C27-C28-C29-C30 |
| 35  | b     | 626 | DGD  | CDB-CEB-CFB-CGB |
| 35  | B     | 626 | DGD  | O6D-C1D-O3G-C3G |
| 35  | b     | 626 | DGD  | O6D-C1D-O3G-C3G |
| 25  | B     | 601 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 601 | CLA  | C5-C6-C7-C8     |
| 26  | B     | 625 | LHG  | C1-C2-C3-O3     |
| 26  | b     | 625 | LHG  | C1-C2-C3-O3     |
| 29  | L     | 101 | SQD  | C28-C29-C30-C31 |
| 29  | l     | 102 | SQD  | C28-C29-C30-C31 |
| 25  | r     | 612 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | G     | 608 | CHL  | C2-C1-O2A-CGA   |
| 24  | g     | 608 | CHL  | C2-C1-O2A-CGA   |
| 25  | G     | 611 | CLA  | C2-C1-O2A-CGA   |
| 25  | g     | 611 | CLA  | C2-C1-O2A-CGA   |
| 25  | N     | 613 | CLA  | C2-C3-C5-C6     |
| 25  | n     | 613 | CLA  | C2-C3-C5-C6     |
| 26  | Y     | 301 | LHG  | C27-C28-C29-C30 |
| 25  | B     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 607 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 603 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 607 | CLA  | C15-C16-C17-C18 |
| 32  | Y     | 321 | AJP  | C27-C26-O25-C23 |
| 32  | y     | 321 | AJP  | C27-C26-O25-C23 |
| 26  | Y     | 301 | LHG  | O8-C23-C24-C25  |
| 26  | y     | 301 | LHG  | O8-C23-C24-C25  |
| 24  | 2     | 601 | CHL  | C6-C7-C8-C9     |
| 24  | G     | 608 | CHL  | C6-C7-C8-C9     |
| 24  | 6     | 601 | CHL  | C6-C7-C8-C9     |
| 24  | g     | 608 | CHL  | C6-C7-C8-C9     |
| 25  | B     | 607 | CLA  | C6-C7-C8-C9     |
| 25  | B     | 613 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 502 | CLA  | C11-C10-C8-C9   |
| 25  | S     | 303 | CLA  | C6-C7-C8-C9     |
| 25  | G     | 610 | CLA  | C11-C12-C13-C14 |
| 25  | N     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | Y     | 303 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 607 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 613 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 502 | CLA  | C11-C10-C8-C9   |
| 25  | s     | 303 | CLA  | C6-C7-C8-C9     |
| 25  | g     | 610 | CLA  | C11-C12-C13-C14 |
| 25  | n     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | y     | 303 | CLA  | C11-C12-C13-C14 |
| 27  | A     | 404 | PHO  | C6-C7-C8-C9     |
| 27  | a     | 405 | PHO  | C6-C7-C8-C9     |
| 25  | b     | 608 | CLA  | CBA-CGA-O2A-C1  |
| 26  | N     | 618 | LHG  | C10-C11-C12-C13 |
| 26  | R     | 618 | LHG  | C16-C17-C18-C19 |
| 26  | n     | 618 | LHG  | C10-C11-C12-C13 |
| 26  | Y     | 319 | LHG  | C17-C18-C19-C20 |
| 26  | y     | 319 | LHG  | C17-C18-C19-C20 |
| 26  | r     | 618 | LHG  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | y     | 312 | CLA  | C8-C10-C11-C12  |
| 26  | N     | 618 | LHG  | C2-C3-O3-P      |
| 26  | n     | 618 | LHG  | C2-C3-O3-P      |
| 26  | 2     | 606 | LHG  | C11-C10-C9-C8   |
| 26  | S     | 301 | LHG  | C17-C18-C19-C20 |
| 26  | 6     | 606 | LHG  | C11-C10-C9-C8   |
| 26  | s     | 301 | LHG  | C17-C18-C19-C20 |
| 25  | S     | 313 | CLA  | C6-C7-C8-C10    |
| 25  | s     | 313 | CLA  | C6-C7-C8-C10    |
| 28  | B     | 619 | BCR  | C23-C24-C25-C26 |
| 28  | K     | 101 | BCR  | C1-C6-C7-C8     |
| 28  | K     | 101 | BCR  | C5-C6-C7-C8     |
| 28  | b     | 619 | BCR  | C23-C24-C25-C26 |
| 28  | k     | 101 | BCR  | C1-C6-C7-C8     |
| 28  | k     | 101 | BCR  | C5-C6-C7-C8     |
| 39  | S     | 315 | LUT  | C1-C6-C7-C8     |
| 39  | R     | 615 | LUT  | C1-C6-C7-C8     |
| 39  | s     | 315 | LUT  | C1-C6-C7-C8     |
| 39  | r     | 615 | LUT  | C1-C6-C7-C8     |
| 25  | Y     | 312 | CLA  | C8-C10-C11-C12  |
| 28  | B     | 619 | BCR  | C7-C8-C9-C34    |
| 28  | b     | 619 | BCR  | C7-C8-C9-C34    |
| 35  | A     | 415 | DGD  | O6E-C5E-C6E-O5E |
| 35  | a     | 401 | DGD  | O6E-C5E-C6E-O5E |
| 26  | L     | 102 | LHG  | C16-C17-C18-C19 |
| 26  | S     | 301 | LHG  | C30-C31-C32-C33 |
| 26  | l     | 103 | LHG  | C16-C17-C18-C19 |
| 26  | s     | 301 | LHG  | C30-C31-C32-C33 |
| 28  | A     | 406 | BCR  | C17-C18-C19-C20 |
| 28  | a     | 407 | BCR  | C17-C18-C19-C20 |
| 24  | G     | 608 | CHL  | C15-C16-C17-C18 |
| 24  | g     | 608 | CHL  | C15-C16-C17-C18 |
| 38  | F     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 38  | f     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 26  | N     | 618 | LHG  | C8-C7-O7-C5     |
| 26  | n     | 618 | LHG  | C8-C7-O7-C5     |
| 26  | s     | 301 | LHG  | C33-C34-C35-C36 |
| 25  | R     | 611 | CLA  | C2C-C3C-CAC-CBC |
| 26  | S     | 301 | LHG  | C33-C34-C35-C36 |
| 24  | Y     | 302 | CHL  | C16-C17-C18-C20 |
| 24  | y     | 302 | CHL  | C16-C17-C18-C20 |
| 25  | A     | 405 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 612 | CLA  | C16-C17-C18-C19 |
| 25  | N     | 610 | CLA  | C16-C17-C18-C19 |
| 25  | Y     | 313 | CLA  | C11-C12-C13-C14 |
| 25  | a     | 406 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 612 | CLA  | C16-C17-C18-C19 |
| 25  | n     | 610 | CLA  | C16-C17-C18-C19 |
| 25  | y     | 313 | CLA  | C11-C12-C13-C14 |
| 26  | C     | 517 | LHG  | C33-C34-C35-C36 |
| 26  | c     | 517 | LHG  | C33-C34-C35-C36 |
| 29  | A     | 407 | SQD  | C13-C14-C15-C16 |
| 29  | a     | 408 | SQD  | C13-C14-C15-C16 |
| 25  | Y     | 314 | CLA  | C8-C10-C11-C12  |
| 25  | y     | 314 | CLA  | C8-C10-C11-C12  |
| 26  | C     | 517 | LHG  | O6-C4-C5-C6     |
| 26  | c     | 517 | LHG  | O6-C4-C5-C6     |
| 29  | A     | 407 | SQD  | C7-C8-C9-C10    |
| 29  | a     | 408 | SQD  | C7-C8-C9-C10    |
| 25  | r     | 611 | CLA  | C2C-C3C-CAC-CBC |
| 24  | G     | 601 | CHL  | C11-C12-C13-C15 |
| 24  | G     | 608 | CHL  | C12-C13-C15-C16 |
| 24  | G     | 609 | CHL  | C6-C7-C8-C10    |
| 24  | N     | 609 | CHL  | C11-C10-C8-C7   |
| 24  | Y     | 302 | CHL  | C11-C12-C13-C15 |
| 24  | Y     | 308 | CHL  | C6-C7-C8-C10    |
| 24  | Y     | 310 | CHL  | C2-C3-C5-C6     |
| 24  | g     | 601 | CHL  | C11-C12-C13-C15 |
| 24  | g     | 608 | CHL  | C12-C13-C15-C16 |
| 24  | g     | 609 | CHL  | C6-C7-C8-C10    |
| 24  | n     | 609 | CHL  | C11-C10-C8-C7   |
| 24  | y     | 302 | CHL  | C11-C12-C13-C15 |
| 24  | y     | 308 | CHL  | C6-C7-C8-C10    |
| 24  | y     | 310 | CHL  | C2-C3-C5-C6     |
| 25  | A     | 402 | CLA  | C12-C13-C15-C16 |
| 25  | B     | 601 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 606 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 614 | CLA  | C12-C13-C15-C16 |
| 25  | B     | 615 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 616 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 505 | CLA  | C2-C3-C5-C6     |
| 25  | C     | 506 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | C     | 507 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 508 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 509 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 513 | CLA  | C12-C13-C15-C16 |
| 25  | N     | 612 | CLA  | C6-C7-C8-C10    |
| 25  | N     | 612 | CLA  | C11-C10-C8-C7   |
| 25  | Y     | 313 | CLA  | C11-C10-C8-C7   |
| 25  | Y     | 314 | CLA  | C6-C7-C8-C10    |
| 25  | R     | 603 | CLA  | C11-C10-C8-C7   |
| 25  | R     | 612 | CLA  | C6-C7-C8-C10    |
| 25  | a     | 403 | CLA  | C12-C13-C15-C16 |
| 25  | b     | 601 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 606 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 614 | CLA  | C12-C13-C15-C16 |
| 25  | b     | 615 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 616 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 505 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 506 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 507 | CLA  | C11-C10-C8-C7   |
| 25  | c     | 507 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 508 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 509 | CLA  | C11-C10-C8-C7   |
| 25  | c     | 513 | CLA  | C12-C13-C15-C16 |
| 25  | n     | 612 | CLA  | C6-C7-C8-C10    |
| 25  | n     | 612 | CLA  | C11-C10-C8-C7   |
| 25  | y     | 313 | CLA  | C11-C10-C8-C7   |
| 25  | y     | 314 | CLA  | C6-C7-C8-C10    |
| 25  | r     | 603 | CLA  | C11-C10-C8-C7   |
| 27  | A     | 403 | PHO  | C12-C13-C15-C16 |
| 27  | a     | 404 | PHO  | C12-C13-C15-C16 |
| 28  | T     | 101 | BCR  | C19-C20-C21-C22 |
| 28  | t     | 101 | BCR  | C19-C20-C21-C22 |
| 24  | r     | 607 | CHL  | C11-C12-C13-C15 |
| 25  | N     | 603 | CLA  | C16-C17-C18-C20 |
| 25  | n     | 603 | CLA  | C16-C17-C18-C20 |
| 35  | B     | 626 | DGD  | C8A-C9A-CAA-CBA |
| 35  | b     | 626 | DGD  | C8A-C9A-CAA-CBA |
| 35  | b     | 626 | DGD  | CAB-CBB-CCB-CDB |
| 25  | A     | 405 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 613 | CLA  | C15-C16-C17-C18 |
| 25  | Y     | 314 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | a     | 406 | CLA  | C5-C6-C7-C8     |
| 25  | b     | 613 | CLA  | C15-C16-C17-C18 |
| 25  | y     | 314 | CLA  | C5-C6-C7-C8     |
| 35  | B     | 626 | DGD  | CAB-CBB-CCB-CDB |
| 24  | 6     | 603 | CHL  | C4C-C3C-CAC-CBC |
| 32  | G     | 618 | AJP  | C22-C23-O25-C26 |
| 32  | g     | 618 | AJP  | C22-C23-O25-C26 |
| 26  | y     | 301 | LHG  | C7-C8-C9-C10    |
| 24  | 2     | 603 | CHL  | C4C-C3C-CAC-CBC |
| 26  | L     | 102 | LHG  | C35-C36-C37-C38 |
| 26  | l     | 103 | LHG  | C35-C36-C37-C38 |
| 30  | c     | 520 | LMG  | C35-C36-C37-C38 |
| 24  | R     | 607 | CHL  | C11-C12-C13-C15 |
| 25  | B     | 607 | CLA  | CBA-CGA-O2A-C1  |
| 25  | R     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 25  | b     | 607 | CLA  | CBA-CGA-O2A-C1  |
| 25  | r     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 30  | C     | 520 | LMG  | C35-C36-C37-C38 |
| 25  | S     | 303 | CLA  | C12-C13-C15-C16 |
| 25  | s     | 303 | CLA  | C12-C13-C15-C16 |
| 26  | n     | 618 | LHG  | C33-C34-C35-C36 |
| 25  | S     | 303 | CLA  | CBD-CGD-O2D-CED |
| 25  | s     | 303 | CLA  | CBD-CGD-O2D-CED |
| 24  | Y     | 308 | CHL  | CAD-CBD-CGD-O2D |
| 24  | R     | 613 | CHL  | CAD-CBD-CGD-O2D |
| 24  | y     | 308 | CHL  | CAD-CBD-CGD-O2D |
| 24  | r     | 613 | CHL  | CAD-CBD-CGD-O2D |
| 25  | B     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 606 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 25  | S     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 25  | S     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 25  | G     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 25  | G     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 25  | N     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 25  | N     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 606 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 25  | s     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 25  | g     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 25  | g     | 610 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | n     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 25  | n     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | n     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 27  | A     | 403 | PHO  | CAD-CBD-CGD-O2D |
| 27  | a     | 404 | PHO  | CAD-CBD-CGD-O2D |
| 40  | N     | 617 | NEX  | C7-C8-C9-C19    |
| 40  | Y     | 318 | NEX  | C7-C8-C9-C19    |
| 40  | n     | 617 | NEX  | C7-C8-C9-C19    |
| 40  | y     | 318 | NEX  | C7-C8-C9-C19    |
| 26  | Y     | 301 | LHG  | C7-C8-C9-C10    |
| 29  | A     | 411 | SQD  | C13-C14-C15-C16 |
| 29  | a     | 412 | SQD  | C13-C14-C15-C16 |
| 28  | D     | 404 | BCR  | C22-C23-C24-C25 |
| 28  | d     | 404 | BCR  | C22-C23-C24-C25 |
| 26  | D     | 406 | LHG  | C24-C23-O8-C6   |
| 26  | d     | 406 | LHG  | C24-C23-O8-C6   |
| 25  | g     | 604 | CLA  | C2C-C3C-CAC-CBC |
| 26  | N     | 618 | LHG  | C33-C34-C35-C36 |
| 29  | A     | 407 | SQD  | C30-C31-C32-C33 |
| 29  | a     | 408 | SQD  | C30-C31-C32-C33 |
| 30  | C     | 520 | LMG  | C32-C33-C34-C35 |
| 30  | c     | 520 | LMG  | C32-C33-C34-C35 |
| 25  | B     | 605 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 605 | CLA  | C15-C16-C17-C18 |
| 26  | y     | 319 | LHG  | C35-C36-C37-C38 |
| 30  | B     | 623 | LMG  | C29-C30-C31-C32 |
| 30  | b     | 623 | LMG  | C29-C30-C31-C32 |
| 26  | 2     | 606 | LHG  | C2-C3-O3-P      |
| 26  | 2     | 606 | LHG  | C4-C5-C6-O8     |
| 26  | L     | 102 | LHG  | C4-C5-C6-O8     |
| 26  | S     | 318 | LHG  | C2-C3-O3-P      |
| 26  | 6     | 606 | LHG  | C2-C3-O3-P      |
| 26  | 6     | 606 | LHG  | C4-C5-C6-O8     |
| 26  | l     | 103 | LHG  | C4-C5-C6-O8     |
| 26  | s     | 318 | LHG  | C2-C3-O3-P      |
| 29  | L     | 101 | SQD  | C44-C45-C46-O48 |
| 29  | L     | 103 | SQD  | O6-C44-C45-C46  |
| 29  | l     | 101 | SQD  | O6-C44-C45-C46  |
| 29  | l     | 102 | SQD  | C44-C45-C46-O48 |
| 30  | A     | 410 | LMG  | C7-C8-C9-O8     |
| 30  | C     | 520 | LMG  | O1-C7-C8-C9     |
| 30  | a     | 411 | LMG  | C7-C8-C9-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | c     | 520 | LMG  | O1-C7-C8-C9     |
| 24  | n     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 26  | D     | 406 | LHG  | C30-C31-C32-C33 |
| 26  | Y     | 319 | LHG  | C35-C36-C37-C38 |
| 26  | d     | 406 | LHG  | C30-C31-C32-C33 |
| 24  | Y     | 302 | CHL  | C10-C11-C12-C13 |
| 24  | y     | 302 | CHL  | C10-C11-C12-C13 |
| 25  | A     | 405 | CLA  | C8-C10-C11-C12  |
| 25  | a     | 406 | CLA  | C8-C10-C11-C12  |
| 25  | c     | 512 | CLA  | C13-C15-C16-C17 |
| 25  | S     | 312 | CLA  | O2A-C1-C2-C3    |
| 25  | s     | 312 | CLA  | O2A-C1-C2-C3    |
| 25  | G     | 604 | CLA  | C2C-C3C-CAC-CBC |
| 25  | C     | 512 | CLA  | C13-C15-C16-C17 |
| 26  | C     | 518 | LHG  | C18-C19-C20-C21 |
| 26  | c     | 518 | LHG  | C18-C19-C20-C21 |
| 35  | C     | 516 | DGD  | C7A-C8A-C9A-CAA |
| 35  | c     | 516 | DGD  | C7A-C8A-C9A-CAA |
| 25  | A     | 402 | CLA  | C16-C17-C18-C20 |
| 25  | a     | 403 | CLA  | C16-C17-C18-C20 |
| 26  | C     | 519 | LHG  | C33-C34-C35-C36 |
| 26  | c     | 519 | LHG  | C33-C34-C35-C36 |
| 26  | B     | 625 | LHG  | O2-C2-C3-O3     |
| 26  | b     | 625 | LHG  | O2-C2-C3-O3     |
| 26  | n     | 618 | LHG  | O9-C7-O7-C5     |
| 24  | 2     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 24  | S     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 24  | G     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 24  | G     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 24  | N     | 608 | CHL  | CHA-CBD-CGD-O1D |
| 24  | 6     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 24  | s     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 24  | g     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 24  | g     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 24  | n     | 608 | CHL  | CHA-CBD-CGD-O1D |
| 25  | B     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | B     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 25  | C     | 502 | CLA  | CHA-CBD-CGD-O1D |
| 25  | C     | 505 | CLA  | CHA-CBD-CGD-O1D |
| 25  | C     | 505 | CLA  | CHA-CBD-CGD-O2D |
| 25  | C     | 507 | CLA  | CHA-CBD-CGD-O1D |
| 25  | S     | 305 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | N     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 25  | N     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | N     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 25  | Y     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 25  | Y     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 25  | Y     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 25  | Y     | 314 | CLA  | CHA-CBD-CGD-O2D |
| 25  | R     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 25  | R     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 25  | R     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | R     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 25  | R     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | b     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | b     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 25  | c     | 502 | CLA  | CHA-CBD-CGD-O1D |
| 25  | c     | 505 | CLA  | CHA-CBD-CGD-O1D |
| 25  | c     | 505 | CLA  | CHA-CBD-CGD-O2D |
| 25  | c     | 507 | CLA  | CHA-CBD-CGD-O1D |
| 25  | s     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 25  | g     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | n     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 25  | n     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | n     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 25  | y     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 25  | y     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 25  | y     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 25  | y     | 314 | CLA  | CHA-CBD-CGD-O2D |
| 25  | r     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 25  | r     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 25  | r     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 25  | r     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 25  | r     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | y     | 314 | CLA  | C3-C5-C6-C7     |
| 24  | G     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 24  | N     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 30  | B     | 620 | LMG  | C30-C31-C32-C33 |
| 30  | b     | 620 | LMG  | C30-C31-C32-C33 |
| 35  | B     | 626 | DGD  | C2D-C1D-O3G-C3G |
| 35  | b     | 626 | DGD  | C2D-C1D-O3G-C3G |
| 35  | A     | 415 | DGD  | O1G-C1G-C2G-O2G |
| 35  | B     | 626 | DGD  | O2G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | a     | 401 | DGD  | O1G-C1G-C2G-O2G |
| 35  | b     | 626 | DGD  | O2G-C2G-C3G-O3G |
| 26  | R     | 618 | LHG  | C11-C10-C9-C8   |
| 26  | r     | 618 | LHG  | C11-C10-C9-C8   |
| 24  | g     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 29  | A     | 407 | SQD  | C12-C13-C14-C15 |
| 29  | a     | 408 | SQD  | C12-C13-C14-C15 |
| 25  | G     | 612 | CLA  | C11-C12-C13-C14 |
| 25  | N     | 610 | CLA  | C16-C17-C18-C20 |
| 25  | g     | 612 | CLA  | C11-C12-C13-C14 |
| 25  | n     | 610 | CLA  | C16-C17-C18-C20 |
| 30  | D     | 407 | LMG  | C33-C34-C35-C36 |
| 30  | d     | 407 | LMG  | C33-C34-C35-C36 |
| 25  | Y     | 314 | CLA  | C3-C5-C6-C7     |
| 24  | Y     | 302 | CHL  | C4-C3-C5-C6     |
| 24  | y     | 302 | CHL  | C4-C3-C5-C6     |
| 25  | B     | 609 | CLA  | C4-C3-C5-C6     |
| 25  | S     | 313 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 609 | CLA  | C4-C3-C5-C6     |
| 25  | s     | 313 | CLA  | C4-C3-C5-C6     |
| 27  | A     | 403 | PHO  | C4-C3-C5-C6     |
| 27  | a     | 404 | PHO  | C4-C3-C5-C6     |
| 30  | B     | 620 | LMG  | C4-C5-C6-O5     |
| 30  | b     | 620 | LMG  | C4-C5-C6-O5     |
| 25  | Y     | 303 | CLA  | C2-C3-C5-C6     |
| 25  | y     | 303 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 409 | PL9  | C4-C3-C7-C8     |
| 31  | a     | 410 | PL9  | C4-C3-C7-C8     |
| 26  | N     | 618 | LHG  | O9-C7-O7-C5     |
| 25  | B     | 606 | CLA  | C11-C10-C8-C9   |
| 25  | B     | 616 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 509 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 606 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 616 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 509 | CLA  | C11-C10-C8-C9   |
| 26  | C     | 519 | LHG  | C18-C19-C20-C21 |
| 26  | c     | 519 | LHG  | C18-C19-C20-C21 |
| 25  | G     | 612 | CLA  | C2C-C3C-CAC-CBC |
| 25  | g     | 612 | CLA  | C2C-C3C-CAC-CBC |
| 26  | B     | 621 | LHG  | C13-C14-C15-C16 |
| 26  | b     | 621 | LHG  | C13-C14-C15-C16 |
| 25  | B     | 606 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | b     | 606 | CLA  | C10-C11-C12-C13 |
| 29  | A     | 411 | SQD  | C4-C5-C6-S      |
| 29  | L     | 103 | SQD  | C4-C5-C6-S      |
| 29  | a     | 412 | SQD  | C4-C5-C6-S      |
| 29  | l     | 101 | SQD  | C4-C5-C6-S      |
| 28  | Z     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | z     | 101 | BCR  | C7-C8-C9-C10    |
| 26  | S     | 301 | LHG  | C32-C33-C34-C35 |
| 25  | R     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 32  | Y     | 322 | AJP  | C29-C30-C32-O33 |
| 32  | y     | 322 | AJP  | C29-C30-C32-O33 |
| 25  | B     | 616 | CLA  | C16-C17-C18-C20 |
| 25  | S     | 310 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 304 | CLA  | C16-C17-C18-C19 |
| 25  | b     | 616 | CLA  | C16-C17-C18-C20 |
| 25  | s     | 310 | CLA  | C6-C7-C8-C9     |
| 25  | y     | 304 | CLA  | C16-C17-C18-C19 |
| 25  | C     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 26  | s     | 301 | LHG  | C32-C33-C34-C35 |
| 26  | L     | 102 | LHG  | C3-O3-P-O6      |
| 26  | l     | 103 | LHG  | C3-O3-P-O6      |
| 27  | A     | 403 | PHO  | C10-C11-C12-C13 |
| 27  | a     | 404 | PHO  | C10-C11-C12-C13 |
| 30  | B     | 620 | LMG  | C29-C30-C31-C32 |
| 30  | b     | 620 | LMG  | C29-C30-C31-C32 |
| 26  | 2     | 606 | LHG  | C3-O3-P-O5      |
| 26  | N     | 618 | LHG  | C3-O3-P-O4      |
| 26  | 6     | 606 | LHG  | C3-O3-P-O5      |
| 26  | c     | 519 | LHG  | C4-O6-P-O4      |
| 26  | n     | 618 | LHG  | C3-O3-P-O4      |
| 25  | C     | 503 | CLA  | C16-C17-C18-C20 |
| 25  | S     | 313 | CLA  | C6-C7-C8-C9     |
| 25  | G     | 602 | CLA  | C16-C17-C18-C19 |
| 25  | c     | 503 | CLA  | C16-C17-C18-C20 |
| 25  | s     | 313 | CLA  | C6-C7-C8-C9     |
| 25  | g     | 602 | CLA  | C16-C17-C18-C19 |
| 26  | B     | 622 | LHG  | C23-C24-C25-C26 |
| 29  | a     | 412 | SQD  | C31-C32-C33-C34 |
| 30  | A     | 410 | LMG  | O6-C1-O1-C7     |
| 30  | a     | 411 | LMG  | O6-C1-O1-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 25  | b     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 26  | 2     | 606 | LHG  | C13-C14-C15-C16 |
| 29  | A     | 411 | SQD  | C31-C32-C33-C34 |
| 30  | B     | 623 | LMG  | C21-C22-C23-C24 |
| 30  | b     | 623 | LMG  | C21-C22-C23-C24 |
| 25  | D     | 402 | CLA  | C10-C11-C12-C13 |
| 25  | d     | 402 | CLA  | C10-C11-C12-C13 |
| 26  | b     | 622 | LHG  | C23-C24-C25-C26 |
| 25  | 2     | 602 | CLA  | C3-C5-C6-C7     |
| 25  | Y     | 304 | CLA  | C3-C5-C6-C7     |
| 25  | 6     | 602 | CLA  | C3-C5-C6-C7     |
| 25  | y     | 304 | CLA  | C3-C5-C6-C7     |
| 26  | 6     | 606 | LHG  | C13-C14-C15-C16 |
| 25  | B     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 25  | C     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 25  | C     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 25  | S     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 25  | G     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 25  | Y     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 25  | R     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 25  | b     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 25  | c     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 25  | c     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 25  | s     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 25  | g     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 25  | y     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 25  | r     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 40  | G     | 617 | NEX  | C7-C8-C9-C10    |
| 40  | Y     | 318 | NEX  | C7-C8-C9-C10    |
| 40  | g     | 617 | NEX  | C7-C8-C9-C10    |
| 40  | y     | 318 | NEX  | C7-C8-C9-C10    |
| 26  | C     | 518 | LHG  | C11-C12-C13-C14 |
| 26  | c     | 518 | LHG  | C11-C12-C13-C14 |
| 30  | B     | 623 | LMG  | C35-C36-C37-C38 |
| 30  | b     | 623 | LMG  | C35-C36-C37-C38 |
| 25  | B     | 608 | CLA  | C5-C6-C7-C8     |
| 26  | c     | 518 | LHG  | C27-C28-C29-C30 |
| 26  | C     | 518 | LHG  | C27-C28-C29-C30 |
| 35  | C     | 515 | DGD  | C4D-C5D-C6D-O5D |
| 35  | c     | 515 | DGD  | C4D-C5D-C6D-O5D |
| 26  | C     | 517 | LHG  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | S     | 301 | LHG  | C11-C12-C13-C14 |
| 26  | s     | 301 | LHG  | C11-C12-C13-C14 |
| 30  | D     | 407 | LMG  | C17-C18-C19-C20 |
| 30  | d     | 407 | LMG  | C17-C18-C19-C20 |
| 24  | Y     | 309 | CHL  | C11-C10-C8-C7   |
| 24  | y     | 309 | CHL  | C11-C10-C8-C7   |
| 25  | B     | 609 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 614 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 615 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 508 | CLA  | C11-C12-C13-C15 |
| 25  | D     | 402 | CLA  | C11-C12-C13-C15 |
| 25  | N     | 613 | CLA  | C6-C7-C8-C10    |
| 25  | N     | 613 | CLA  | C11-C10-C8-C7   |
| 25  | Y     | 312 | CLA  | C6-C7-C8-C10    |
| 25  | R     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 609 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 614 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 615 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 508 | CLA  | C11-C12-C13-C15 |
| 25  | d     | 402 | CLA  | C11-C12-C13-C15 |
| 25  | n     | 613 | CLA  | C6-C7-C8-C10    |
| 25  | n     | 613 | CLA  | C11-C10-C8-C7   |
| 25  | y     | 312 | CLA  | C6-C7-C8-C10    |
| 25  | r     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 26  | c     | 517 | LHG  | C30-C31-C32-C33 |
| 25  | b     | 608 | CLA  | C5-C6-C7-C8     |
| 28  | T     | 101 | BCR  | C9-C10-C11-C12  |
| 28  | t     | 101 | BCR  | C9-C10-C11-C12  |
| 39  | N     | 615 | LUT  | C13-C14-C15-C35 |
| 39  | n     | 615 | LUT  | C13-C14-C15-C35 |
| 35  | C     | 515 | DGD  | O6D-C5D-C6D-O5D |
| 35  | c     | 515 | DGD  | O6D-C5D-C6D-O5D |
| 26  | N     | 618 | LHG  | C24-C25-C26-C27 |
| 26  | s     | 318 | LHG  | C9-C10-C11-C12  |
| 26  | n     | 618 | LHG  | C24-C25-C26-C27 |
| 26  | D     | 406 | LHG  | O10-C23-O8-C6   |
| 26  | d     | 406 | LHG  | O10-C23-O8-C6   |
| 26  | S     | 318 | LHG  | C9-C10-C11-C12  |
| 24  | R     | 607 | CHL  | C10-C11-C12-C13 |
| 24  | r     | 607 | CHL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | y     | 315 | CLA  | C2A-CAA-CBA-CGA |
| 29  | L     | 103 | SQD  | C29-C30-C31-C32 |
| 29  | l     | 101 | SQD  | C29-C30-C31-C32 |
| 24  | G     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | Y     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 24  | g     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 24  | y     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 29  | A     | 411 | SQD  | C44-C45-C46-O48 |
| 29  | a     | 412 | SQD  | C44-C45-C46-O48 |
| 30  | A     | 408 | LMG  | O1-C7-C8-C9     |
| 30  | a     | 409 | LMG  | O1-C7-C8-C9     |
| 29  | A     | 411 | SQD  | O47-C45-C46-O48 |
| 29  | L     | 103 | SQD  | O6-C44-C45-O47  |
| 29  | a     | 412 | SQD  | O47-C45-C46-O48 |
| 29  | l     | 101 | SQD  | O6-C44-C45-O47  |
| 30  | A     | 408 | LMG  | O1-C7-C8-O7     |
| 30  | A     | 408 | LMG  | O7-C8-C9-O8     |
| 30  | C     | 520 | LMG  | O1-C7-C8-O7     |
| 30  | D     | 407 | LMG  | O1-C7-C8-O7     |
| 30  | a     | 409 | LMG  | O1-C7-C8-O7     |
| 30  | a     | 409 | LMG  | O7-C8-C9-O8     |
| 30  | c     | 520 | LMG  | O1-C7-C8-O7     |
| 30  | d     | 407 | LMG  | O1-C7-C8-O7     |
| 26  | S     | 318 | LHG  | C11-C10-C9-C8   |
| 26  | s     | 318 | LHG  | C11-C10-C9-C8   |
| 25  | R     | 610 | CLA  | C4C-C3C-CAC-CBC |
| 25  | B     | 608 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 608 | CLA  | C4-C3-C5-C6     |
| 25  | r     | 610 | CLA  | C4C-C3C-CAC-CBC |
| 25  | Y     | 313 | CLA  | C2-C3-C5-C6     |
| 25  | y     | 313 | CLA  | C2-C3-C5-C6     |
| 24  | G     | 601 | CHL  | C14-C13-C15-C16 |
| 24  | g     | 601 | CHL  | C14-C13-C15-C16 |
| 25  | C     | 507 | CLA  | C6-C7-C8-C9     |
| 25  | C     | 509 | CLA  | C11-C12-C13-C14 |
| 25  | D     | 402 | CLA  | C11-C10-C8-C9   |
| 25  | D     | 402 | CLA  | C11-C12-C13-C14 |
| 25  | S     | 311 | CLA  | C6-C7-C8-C9     |
| 25  | N     | 603 | CLA  | C11-C12-C13-C14 |
| 25  | c     | 507 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 509 | CLA  | C11-C12-C13-C14 |
| 25  | d     | 402 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | d     | 402 | CLA  | C11-C12-C13-C14 |
| 25  | s     | 311 | CLA  | C6-C7-C8-C9     |
| 25  | n     | 603 | CLA  | C11-C12-C13-C14 |
| 25  | s     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 26  | N     | 618 | LHG  | C18-C19-C20-C21 |
| 24  | Y     | 302 | CHL  | C3-C5-C6-C7     |
| 24  | y     | 302 | CHL  | C3-C5-C6-C7     |
| 26  | n     | 618 | LHG  | C18-C19-C20-C21 |
| 29  | a     | 412 | SQD  | C17-C18-C19-C20 |
| 25  | S     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 24  | S     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 24  | s     | 307 | CHL  | C2A-CAA-CBA-CGA |
| 25  | Y     | 315 | CLA  | C2A-CAA-CBA-CGA |
| 26  | B     | 625 | LHG  | O1-C1-C2-O2     |
| 26  | b     | 625 | LHG  | O1-C1-C2-O2     |
| 26  | R     | 618 | LHG  | C12-C13-C14-C15 |
| 26  | r     | 618 | LHG  | C12-C13-C14-C15 |
| 29  | A     | 411 | SQD  | C17-C18-C19-C20 |
| 35  | B     | 626 | DGD  | C5A-C6A-C7A-C8A |
| 35  | b     | 626 | DGD  | C5A-C6A-C7A-C8A |
| 40  | G     | 617 | NEX  | C10-C11-C12-C13 |
| 40  | G     | 617 | NEX  | C30-C31-C32-C33 |
| 40  | Y     | 318 | NEX  | C30-C31-C32-C33 |
| 40  | g     | 617 | NEX  | C10-C11-C12-C13 |
| 40  | g     | 617 | NEX  | C30-C31-C32-C33 |
| 40  | y     | 318 | NEX  | C30-C31-C32-C33 |
| 26  | s     | 318 | LHG  | C15-C16-C17-C18 |
| 26  | S     | 318 | LHG  | C15-C16-C17-C18 |
| 26  | 2     | 606 | LHG  | C9-C10-C11-C12  |
| 26  | 6     | 606 | LHG  | C9-C10-C11-C12  |
| 26  | L     | 102 | LHG  | C26-C27-C28-C29 |
| 26  | l     | 103 | LHG  | C26-C27-C28-C29 |
| 27  | A     | 403 | PHO  | C2-C3-C5-C6     |
| 27  | a     | 404 | PHO  | C2-C3-C5-C6     |
| 25  | N     | 611 | CLA  | C10-C11-C12-C13 |
| 25  | n     | 611 | CLA  | C10-C11-C12-C13 |
| 26  | B     | 621 | LHG  | C30-C31-C32-C33 |
| 26  | b     | 621 | LHG  | C30-C31-C32-C33 |
| 30  | A     | 408 | LMG  | C32-C33-C34-C35 |
| 30  | a     | 409 | LMG  | C32-C33-C34-C35 |
| 24  | G     | 606 | CHL  | C1-C2-C3-C4     |
| 24  | Y     | 307 | CHL  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | g     | 606 | CHL  | C1-C2-C3-C4     |
| 24  | y     | 307 | CHL  | C1-C2-C3-C4     |
| 25  | S     | 312 | CLA  | C1-C2-C3-C4     |
| 25  | R     | 610 | CLA  | C1-C2-C3-C4     |
| 25  | R     | 611 | CLA  | C1-C2-C3-C4     |
| 25  | s     | 312 | CLA  | C1-C2-C3-C4     |
| 25  | r     | 610 | CLA  | C1-C2-C3-C4     |
| 25  | r     | 611 | CLA  | C1-C2-C3-C4     |
| 29  | L     | 101 | SQD  | C25-C26-C27-C28 |
| 29  | l     | 102 | SQD  | C25-C26-C27-C28 |
| 30  | C     | 520 | LMG  | C37-C38-C39-C40 |
| 30  | c     | 520 | LMG  | C37-C38-C39-C40 |
| 24  | y     | 302 | CHL  | C15-C16-C17-C18 |
| 26  | L     | 102 | LHG  | C6-C5-O7-C7     |
| 26  | l     | 103 | LHG  | C6-C5-O7-C7     |
| 29  | L     | 103 | SQD  | C44-C45-O47-C7  |
| 29  | l     | 101 | SQD  | C44-C45-O47-C7  |
| 25  | C     | 505 | CLA  | C2A-CAA-CBA-CGA |
| 25  | G     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | c     | 505 | CLA  | C2A-CAA-CBA-CGA |
| 25  | g     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 601 | CLA  | C2C-C3C-CAC-CBC |
| 29  | A     | 411 | SQD  | C32-C33-C34-C35 |
| 25  | y     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 24  | Y     | 308 | CHL  | C2-C1-O2A-CGA   |
| 24  | y     | 308 | CHL  | C2-C1-O2A-CGA   |
| 25  | A     | 401 | CLA  | C2-C1-O2A-CGA   |
| 25  | B     | 613 | CLA  | C2-C1-O2A-CGA   |
| 25  | a     | 402 | CLA  | C2-C1-O2A-CGA   |
| 25  | b     | 613 | CLA  | C2-C1-O2A-CGA   |
| 29  | a     | 412 | SQD  | C32-C33-C34-C35 |
| 35  | B     | 626 | DGD  | C7A-C8A-C9A-CAA |
| 25  | r     | 601 | CLA  | C2C-C3C-CAC-CBC |
| 26  | B     | 621 | LHG  | C31-C32-C33-C34 |
| 26  | b     | 621 | LHG  | C31-C32-C33-C34 |
| 35  | b     | 626 | DGD  | C7A-C8A-C9A-CAA |
| 29  | l     | 102 | SQD  | C11-C12-C13-C14 |
| 29  | L     | 101 | SQD  | C11-C12-C13-C14 |
| 24  | Y     | 302 | CHL  | C15-C16-C17-C18 |
| 25  | B     | 604 | CLA  | C10-C11-C12-C13 |
| 25  | b     | 604 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 304 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | r     | 612 | CLA  | C8-C10-C11-C12  |
| 25  | Y     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 35  | B     | 626 | DGD  | C6B-C7B-C8B-C9B |
| 25  | G     | 613 | CLA  | C10-C11-C12-C13 |
| 25  | Y     | 304 | CLA  | C15-C16-C17-C18 |
| 25  | R     | 612 | CLA  | C8-C10-C11-C12  |
| 25  | g     | 613 | CLA  | C10-C11-C12-C13 |
| 31  | D     | 405 | PL9  | C20-C19-C21-C22 |
| 31  | d     | 405 | PL9  | C20-C19-C21-C22 |
| 26  | B     | 622 | LHG  | C9-C10-C11-C12  |
| 26  | b     | 622 | LHG  | C9-C10-C11-C12  |
| 24  | N     | 605 | CHL  | O1D-CGD-O2D-CED |
| 39  | G     | 615 | LUT  | C1-C6-C7-C8     |
| 39  | g     | 615 | LUT  | C1-C6-C7-C8     |
| 25  | G     | 613 | CLA  | C2-C3-C5-C6     |
| 25  | g     | 613 | CLA  | C2-C3-C5-C6     |
| 25  | R     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 24  | n     | 605 | CHL  | O1D-CGD-O2D-CED |
| 25  | 2     | 605 | CLA  | C4C-C3C-CAC-CBC |
| 25  | 6     | 605 | CLA  | C4C-C3C-CAC-CBC |
| 35  | b     | 626 | DGD  | C6B-C7B-C8B-C9B |
| 30  | B     | 620 | LMG  | C36-C37-C38-C39 |
| 30  | b     | 620 | LMG  | C36-C37-C38-C39 |
| 25  | N     | 603 | CLA  | C16-C17-C18-C19 |
| 25  | n     | 603 | CLA  | C16-C17-C18-C19 |
| 29  | L     | 101 | SQD  | O5-C1-O6-C44    |
| 29  | l     | 102 | SQD  | O5-C1-O6-C44    |
| 29  | L     | 101 | SQD  | C2-C1-O6-C44    |
| 29  | l     | 102 | SQD  | C2-C1-O6-C44    |
| 30  | A     | 410 | LMG  | C2-C1-O1-C7     |
| 30  | a     | 411 | LMG  | C2-C1-O1-C7     |
| 24  | N     | 607 | CHL  | C5-C6-C7-C8     |
| 24  | n     | 607 | CHL  | C5-C6-C7-C8     |
| 26  | 2     | 606 | LHG  | C31-C32-C33-C34 |
| 26  | S     | 301 | LHG  | C25-C26-C27-C28 |
| 26  | B     | 621 | LHG  | C4-O6-P-O3      |
| 26  | B     | 622 | LHG  | C3-O3-P-O6      |
| 26  | C     | 517 | LHG  | C3-O3-P-O6      |
| 26  | D     | 406 | LHG  | C3-O3-P-O6      |
| 26  | S     | 318 | LHG  | C3-O3-P-O6      |
| 26  | N     | 618 | LHG  | C4-O6-P-O3      |
| 26  | Y     | 301 | LHG  | C3-O3-P-O6      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | R     | 618 | LHG  | C3-O3-P-O6      |
| 26  | b     | 621 | LHG  | C4-O6-P-O3      |
| 26  | b     | 622 | LHG  | C3-O3-P-O6      |
| 26  | c     | 517 | LHG  | C3-O3-P-O6      |
| 26  | d     | 406 | LHG  | C3-O3-P-O6      |
| 26  | s     | 318 | LHG  | C3-O3-P-O6      |
| 26  | n     | 618 | LHG  | C4-O6-P-O3      |
| 26  | y     | 301 | LHG  | C3-O3-P-O6      |
| 26  | r     | 618 | LHG  | C3-O3-P-O6      |
| 26  | 6     | 606 | LHG  | C31-C32-C33-C34 |
| 26  | s     | 301 | LHG  | C25-C26-C27-C28 |
| 30  | D     | 407 | LMG  | C21-C22-C23-C24 |
| 25  | r     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 26  | C     | 518 | LHG  | C11-C10-C9-C8   |
| 26  | c     | 518 | LHG  | C11-C10-C9-C8   |
| 30  | d     | 407 | LMG  | C21-C22-C23-C24 |
| 25  | g     | 602 | CLA  | CBD-CGD-O2D-CED |
| 26  | L     | 102 | LHG  | C17-C18-C19-C20 |
| 26  | l     | 103 | LHG  | C17-C18-C19-C20 |
| 30  | C     | 520 | LMG  | C7-C8-C9-O8     |
| 30  | c     | 520 | LMG  | C7-C8-C9-O8     |
| 35  | A     | 415 | DGD  | O1G-C1G-C2G-C3G |
| 35  | a     | 401 | DGD  | O1G-C1G-C2G-C3G |
| 25  | G     | 603 | CLA  | C4-C3-C5-C6     |
| 25  | g     | 603 | CLA  | C4-C3-C5-C6     |
| 35  | A     | 415 | DGD  | C5B-C6B-C7B-C8B |
| 35  | a     | 401 | DGD  | C5B-C6B-C7B-C8B |
| 24  | 2     | 601 | CHL  | C11-C10-C8-C7   |
| 24  | G     | 608 | CHL  | C6-C7-C8-C10    |
| 24  | 6     | 601 | CHL  | C11-C10-C8-C7   |
| 24  | g     | 608 | CHL  | C6-C7-C8-C10    |
| 25  | 2     | 602 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 608 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 505 | CLA  | C12-C13-C15-C16 |
| 25  | 6     | 602 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 608 | CLA  | C12-C13-C15-C16 |
| 25  | c     | 505 | CLA  | C12-C13-C15-C16 |
| 24  | G     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 24  | g     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 24  | Y     | 302 | CHL  | C14-C13-C15-C16 |
| 24  | Y     | 308 | CHL  | C6-C7-C8-C9     |
| 24  | y     | 302 | CHL  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | y     | 308 | CHL  | C6-C7-C8-C9     |
| 25  | B     | 614 | CLA  | C11-C12-C13-C14 |
| 25  | B     | 615 | CLA  | C11-C12-C13-C14 |
| 25  | N     | 613 | CLA  | C6-C7-C8-C9     |
| 25  | N     | 613 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 614 | CLA  | C11-C12-C13-C14 |
| 25  | b     | 615 | CLA  | C11-C12-C13-C14 |
| 25  | n     | 613 | CLA  | C6-C7-C8-C9     |
| 25  | n     | 613 | CLA  | C11-C10-C8-C9   |
| 24  | G     | 601 | CHL  | C15-C16-C17-C18 |
| 24  | g     | 601 | CHL  | C15-C16-C17-C18 |
| 26  | c     | 519 | LHG  | C14-C15-C16-C17 |
| 30  | B     | 620 | LMG  | C13-C14-C15-C16 |
| 30  | b     | 620 | LMG  | C13-C14-C15-C16 |
| 25  | G     | 602 | CLA  | CBD-CGD-O2D-CED |
| 25  | a     | 403 | CLA  | C16-C17-C18-C19 |
| 26  | C     | 519 | LHG  | C14-C15-C16-C17 |
| 30  | C     | 520 | LMG  | C31-C32-C33-C34 |
| 30  | c     | 520 | LMG  | C31-C32-C33-C34 |
| 26  | S     | 301 | LHG  | C16-C17-C18-C19 |
| 25  | G     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 25  | g     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 25  | Y     | 303 | CLA  | C5-C6-C7-C8     |
| 25  | y     | 303 | CLA  | C5-C6-C7-C8     |
| 26  | s     | 301 | LHG  | C16-C17-C18-C19 |
| 24  | Y     | 310 | CHL  | C4-C3-C5-C6     |
| 24  | y     | 310 | CHL  | C4-C3-C5-C6     |
| 25  | B     | 608 | CLA  | C2-C3-C5-C6     |
| 25  | b     | 608 | CLA  | C2-C3-C5-C6     |
| 25  | A     | 402 | CLA  | C16-C17-C18-C19 |
| 25  | N     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 25  | n     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 32  | Y     | 323 | AJP  | O31-C30-C32-O33 |
| 32  | y     | 323 | AJP  | O31-C30-C32-O33 |
| 28  | T     | 101 | BCR  | C6-C7-C8-C9     |
| 28  | t     | 101 | BCR  | C6-C7-C8-C9     |
| 25  | R     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 25  | r     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 25  | G     | 612 | CLA  | CBD-CGD-O2D-CED |
| 28  | A     | 406 | BCR  | C13-C14-C15-C16 |
| 28  | I     | 101 | BCR  | C9-C10-C11-C12  |
| 28  | a     | 407 | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | i     | 101 | BCR  | C9-C10-C11-C12  |
| 39  | Y     | 316 | LUT  | C33-C34-C35-C15 |
| 39  | y     | 316 | LUT  | C33-C34-C35-C15 |
| 26  | B     | 625 | LHG  | C28-C29-C30-C31 |
| 26  | b     | 625 | LHG  | C28-C29-C30-C31 |
| 30  | B     | 623 | LMG  | C18-C19-C20-C21 |
| 30  | b     | 623 | LMG  | C18-C19-C20-C21 |
| 26  | L     | 102 | LHG  | C32-C33-C34-C35 |
| 26  | l     | 103 | LHG  | C32-C33-C34-C35 |
| 25  | b     | 609 | CLA  | CBD-CGD-O2D-CED |
| 25  | g     | 612 | CLA  | CBD-CGD-O2D-CED |
| 29  | A     | 407 | SQD  | C29-C30-C31-C32 |
| 29  | a     | 408 | SQD  | C29-C30-C31-C32 |
| 25  | R     | 602 | CLA  | C4-C3-C5-C6     |
| 25  | r     | 602 | CLA  | C4-C3-C5-C6     |
| 25  | B     | 609 | CLA  | C5-C6-C7-C8     |
| 25  | G     | 610 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 609 | CLA  | C5-C6-C7-C8     |
| 25  | g     | 610 | CLA  | C13-C15-C16-C17 |
| 30  | B     | 620 | LMG  | O9-C10-O7-C8    |
| 30  | b     | 620 | LMG  | O9-C10-O7-C8    |
| 24  | N     | 609 | CHL  | C2-C1-O2A-CGA   |
| 24  | n     | 609 | CHL  | C2-C1-O2A-CGA   |
| 25  | C     | 506 | CLA  | C2-C1-O2A-CGA   |
| 25  | G     | 604 | CLA  | C2-C1-O2A-CGA   |
| 25  | c     | 506 | CLA  | C2-C1-O2A-CGA   |
| 25  | g     | 604 | CLA  | C2-C1-O2A-CGA   |
| 24  | N     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 24  | n     | 605 | CHL  | C2C-C3C-CAC-CBC |
| 26  | C     | 517 | LHG  | C35-C36-C37-C38 |
| 26  | c     | 517 | LHG  | C35-C36-C37-C38 |
| 24  | 1     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 24  | 5     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 25  | B     | 616 | CLA  | C2A-CAA-CBA-CGA |
| 25  | G     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 616 | CLA  | C2A-CAA-CBA-CGA |
| 25  | g     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 25  | B     | 609 | CLA  | CBD-CGD-O2D-CED |
| 25  | B     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 24  | R     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 24  | r     | 606 | CHL  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 303 | CLA  | C5-C6-C7-C8     |
| 25  | s     | 303 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 615 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 615 | CLA  | C4-C3-C5-C6     |
| 35  | B     | 626 | DGD  | CCA-CDA-CEA-CFA |
| 35  | b     | 626 | DGD  | CCA-CDA-CEA-CFA |
| 26  | B     | 622 | LHG  | C29-C30-C31-C32 |
| 26  | b     | 622 | LHG  | C29-C30-C31-C32 |
| 24  | Y     | 302 | CHL  | C6-C7-C8-C9     |
| 24  | y     | 302 | CHL  | C6-C7-C8-C9     |
| 25  | A     | 405 | CLA  | C11-C10-C8-C9   |
| 25  | C     | 504 | CLA  | C6-C7-C8-C9     |
| 25  | C     | 505 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 508 | CLA  | C11-C12-C13-C14 |
| 25  | G     | 610 | CLA  | C6-C7-C8-C9     |
| 25  | a     | 406 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 504 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 505 | CLA  | C14-C13-C15-C16 |
| 25  | c     | 508 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 610 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 311 | CLA  | C11-C12-C13-C14 |
| 25  | y     | 311 | CLA  | C11-C12-C13-C14 |
| 24  | Y     | 309 | CHL  | C2C-C3C-CAC-CBC |
| 24  | y     | 309 | CHL  | C2C-C3C-CAC-CBC |
| 35  | A     | 415 | DGD  | C3A-C4A-C5A-C6A |
| 35  | a     | 401 | DGD  | C3A-C4A-C5A-C6A |
| 30  | D     | 407 | LMG  | O1-C7-C8-C9     |
| 30  | d     | 407 | LMG  | O1-C7-C8-C9     |
| 35  | B     | 626 | DGD  | O1G-C1G-C2G-C3G |
| 35  | b     | 626 | DGD  | O1G-C1G-C2G-C3G |
| 39  | S     | 315 | LUT  | C40-C33-C34-C35 |
| 39  | G     | 615 | LUT  | C21-C26-C27-C28 |
| 39  | N     | 615 | LUT  | C21-C26-C27-C28 |
| 39  | R     | 615 | LUT  | C20-C13-C14-C15 |
| 39  | s     | 315 | LUT  | C40-C33-C34-C35 |
| 39  | g     | 615 | LUT  | C21-C26-C27-C28 |
| 39  | n     | 615 | LUT  | C21-C26-C27-C28 |
| 39  | r     | 615 | LUT  | C20-C13-C14-C15 |
| 40  | S     | 317 | NEX  | C11-C10-C9-C19  |
| 40  | S     | 317 | NEX  | C39-C29-C30-C31 |
| 40  | N     | 617 | NEX  | C39-C29-C30-C31 |
| 40  | R     | 617 | NEX  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 40  | s     | 317 | NEX  | C11-C10-C9-C19  |
| 40  | s     | 317 | NEX  | C39-C29-C30-C31 |
| 40  | n     | 617 | NEX  | C39-C29-C30-C31 |
| 40  | r     | 617 | NEX  | C39-C29-C30-C31 |
| 41  | R     | 616 | XAT  | C20-C13-C14-C15 |
| 41  | r     | 616 | XAT  | C20-C13-C14-C15 |
| 24  | r     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 26  | S     | 301 | LHG  | C19-C20-C21-C22 |
| 26  | s     | 301 | LHG  | C19-C20-C21-C22 |
| 24  | R     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 25  | Y     | 315 | CLA  | C2C-C3C-CAC-CBC |
| 32  | B     | 624 | AJP  | C36-C35-O34-C29 |
| 32  | b     | 624 | AJP  | C36-C35-O34-C29 |
| 35  | A     | 415 | DGD  | CAB-CBB-CCB-CDB |
| 35  | a     | 401 | DGD  | CAB-CBB-CCB-CDB |
| 24  | S     | 308 | CHL  | CAA-CBA-CGA-O1A |
| 24  | s     | 308 | CHL  | CAA-CBA-CGA-O1A |
| 29  | L     | 103 | SQD  | C46-C45-O47-C7  |
| 29  | l     | 101 | SQD  | C46-C45-O47-C7  |
| 25  | S     | 311 | CLA  | C4-C3-C5-C6     |
| 25  | s     | 311 | CLA  | C4-C3-C5-C6     |
| 24  | G     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 24  | Y     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 24  | R     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 24  | g     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 24  | y     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 24  | r     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 25  | G     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | G     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 25  | Y     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | g     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 25  | y     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 24  | 2     | 601 | CHL  | C12-C13-C15-C16 |
| 24  | 6     | 601 | CHL  | C12-C13-C15-C16 |
| 25  | A     | 402 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 607 | CLA  | C12-C13-C15-C16 |
| 25  | C     | 506 | CLA  | C6-C7-C8-C10    |
| 25  | D     | 402 | CLA  | C12-C13-C15-C16 |
| 25  | Y     | 314 | CLA  | C12-C13-C15-C16 |
| 25  | a     | 403 | CLA  | C11-C12-C13-C15 |
| 25  | b     | 607 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 506 | CLA  | C6-C7-C8-C10    |
| 25  | d     | 402 | CLA  | C12-C13-C15-C16 |
| 25  | y     | 314 | CLA  | C12-C13-C15-C16 |
| 35  | A     | 415 | DGD  | C7B-C8B-C9B-CAB |
| 35  | a     | 401 | DGD  | C7B-C8B-C9B-CAB |
| 32  | B     | 624 | AJP  | O40-C39-C41-O42 |
| 32  | b     | 624 | AJP  | O40-C39-C41-O42 |
| 24  | S     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 24  | s     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 25  | g     | 604 | CLA  | C4C-C3C-CAC-CBC |
| 25  | y     | 315 | CLA  | C2C-C3C-CAC-CBC |
| 25  | G     | 604 | CLA  | C4C-C3C-CAC-CBC |
| 26  | y     | 319 | LHG  | C9-C10-C11-C12  |
| 24  | Y     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 24  | y     | 302 | CHL  | C2A-CAA-CBA-CGA |
| 25  | B     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | N     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | R     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 25  | b     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 25  | n     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 25  | r     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 510 | CLA  | C10-C11-C12-C13 |
| 25  | c     | 510 | CLA  | C10-C11-C12-C13 |
| 25  | y     | 303 | CLA  | C2C-C3C-CAC-CBC |
| 25  | b     | 602 | CLA  | C10-C11-C12-C13 |
| 26  | Y     | 319 | LHG  | C9-C10-C11-C12  |
| 30  | B     | 620 | LMG  | C11-C10-O7-C8   |
| 30  | b     | 620 | LMG  | C11-C10-O7-C8   |
| 24  | G     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 24  | g     | 607 | CHL  | CAA-CBA-CGA-O2A |
| 25  | Y     | 303 | CLA  | C2C-C3C-CAC-CBC |
| 31  | D     | 405 | PL9  | C45-C44-C46-C47 |
| 31  | d     | 405 | PL9  | C45-C44-C46-C47 |
| 25  | B     | 602 | CLA  | C10-C11-C12-C13 |
| 24  | 1     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 24  | 5     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 24  | Y     | 302 | CHL  | C5-C6-C7-C8     |
| 39  | S     | 315 | LUT  | C32-C33-C34-C35 |
| 39  | R     | 615 | LUT  | C12-C13-C14-C15 |
| 39  | s     | 315 | LUT  | C32-C33-C34-C35 |
| 39  | r     | 615 | LUT  | C12-C13-C14-C15 |
| 40  | S     | 317 | NEX  | C11-C10-C9-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 40  | S     | 317 | NEX  | C28-C29-C30-C31 |
| 40  | N     | 617 | NEX  | C28-C29-C30-C31 |
| 40  | R     | 617 | NEX  | C28-C29-C30-C31 |
| 40  | s     | 317 | NEX  | C11-C10-C9-C8   |
| 40  | s     | 317 | NEX  | C28-C29-C30-C31 |
| 40  | n     | 617 | NEX  | C28-C29-C30-C31 |
| 40  | r     | 617 | NEX  | C28-C29-C30-C31 |
| 41  | R     | 616 | XAT  | C12-C13-C14-C15 |
| 41  | r     | 616 | XAT  | C12-C13-C14-C15 |
| 25  | S     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 25  | s     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 35  | C     | 515 | DGD  | O2G-C2G-C3G-O3G |
| 35  | c     | 515 | DGD  | O2G-C2G-C3G-O3G |
| 24  | y     | 302 | CHL  | C5-C6-C7-C8     |
| 39  | S     | 316 | LUT  | C9-C10-C11-C12  |
| 39  | s     | 316 | LUT  | C9-C10-C11-C12  |
| 25  | C     | 505 | CLA  | C10-C11-C12-C13 |
| 25  | c     | 505 | CLA  | C10-C11-C12-C13 |
| 29  | a     | 412 | SQD  | C14-C15-C16-C17 |
| 29  | A     | 411 | SQD  | C14-C15-C16-C17 |
| 24  | g     | 607 | CHL  | O1D-CGD-O2D-CED |
| 26  | b     | 622 | LHG  | C25-C26-C27-C28 |
| 25  | Y     | 312 | CLA  | C2-C1-O2A-CGA   |
| 25  | y     | 312 | CLA  | C2-C1-O2A-CGA   |
| 24  | Y     | 302 | CHL  | C2-C3-C5-C6     |
| 24  | y     | 302 | CHL  | C2-C3-C5-C6     |
| 25  | G     | 610 | CLA  | C15-C16-C17-C18 |
| 26  | B     | 622 | LHG  | C25-C26-C27-C28 |
| 24  | S     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 24  | s     | 302 | CHL  | CAA-CBA-CGA-O1A |
| 24  | G     | 607 | CHL  | O1D-CGD-O2D-CED |
| 35  | B     | 626 | DGD  | O2G-C1B-C2B-C3B |
| 25  | B     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | B     | 610 | CLA  | C11-C10-C8-C9   |
| 25  | B     | 613 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 610 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 613 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 510 | CLA  | C14-C13-C15-C16 |
| 25  | g     | 610 | CLA  | C15-C16-C17-C18 |
| 25  | N     | 612 | CLA  | C3-C5-C6-C7     |
| 25  | n     | 612 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | B     | 621 | LHG  | O8-C23-C24-C25  |
| 35  | b     | 626 | DGD  | O2G-C1B-C2B-C3B |
| 26  | B     | 622 | LHG  | C32-C33-C34-C35 |
| 26  | b     | 622 | LHG  | C32-C33-C34-C35 |
| 30  | A     | 410 | LMG  | C29-C30-C31-C32 |
| 25  | S     | 310 | CLA  | C6-C7-C8-C10    |
| 25  | G     | 612 | CLA  | C11-C12-C13-C15 |
| 25  | s     | 310 | CLA  | C6-C7-C8-C10    |
| 25  | g     | 612 | CLA  | C11-C12-C13-C15 |
| 28  | C     | 514 | BCR  | C1-C6-C7-C8     |
| 28  | c     | 514 | BCR  | C1-C6-C7-C8     |
| 39  | S     | 315 | LUT  | C5-C6-C7-C8     |
| 39  | s     | 315 | LUT  | C5-C6-C7-C8     |
| 25  | R     | 601 | CLA  | C4C-C3C-CAC-CBC |
| 30  | a     | 411 | LMG  | C29-C30-C31-C32 |
| 26  | b     | 621 | LHG  | O8-C23-C24-C25  |
| 32  | A     | 412 | AJP  | O31-C30-C32-O33 |
| 32  | a     | 413 | AJP  | O31-C30-C32-O33 |
| 26  | C     | 519 | LHG  | C31-C32-C33-C34 |
| 26  | c     | 519 | LHG  | C31-C32-C33-C34 |
| 39  | Y     | 317 | LUT  | C29-C30-C31-C32 |
| 39  | y     | 317 | LUT  | C29-C30-C31-C32 |
| 26  | R     | 618 | LHG  | C27-C28-C29-C30 |
| 25  | B     | 613 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 613 | CLA  | C4-C3-C5-C6     |
| 24  | R     | 607 | CHL  | C2-C3-C5-C6     |
| 24  | r     | 607 | CHL  | C2-C3-C5-C6     |
| 25  | N     | 602 | CLA  | C2-C3-C5-C6     |
| 25  | n     | 602 | CLA  | C2-C3-C5-C6     |
| 24  | Y     | 309 | CHL  | C3-C5-C6-C7     |
| 24  | y     | 309 | CHL  | C3-C5-C6-C7     |
| 26  | r     | 618 | LHG  | C27-C28-C29-C30 |
| 30  | B     | 620 | LMG  | C8-C7-O1-C1     |
| 30  | b     | 620 | LMG  | C8-C7-O1-C1     |
| 25  | r     | 601 | CLA  | C4C-C3C-CAC-CBC |
| 24  | S     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 24  | s     | 302 | CHL  | CAA-CBA-CGA-O2A |
| 25  | g     | 610 | CLA  | C5-C6-C7-C8     |
| 30  | C     | 520 | LMG  | C18-C19-C20-C21 |
| 30  | c     | 520 | LMG  | C18-C19-C20-C21 |
| 35  | C     | 515 | DGD  | C8B-C9B-CAB-CBB |
| 35  | c     | 515 | DGD  | C8B-C9B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | B     | 624 | AJP  | O40-C35-O34-C29 |
| 32  | b     | 624 | AJP  | O40-C35-O34-C29 |
| 25  | G     | 610 | CLA  | C5-C6-C7-C8     |
| 26  | B     | 621 | LHG  | O6-C4-C5-C6     |
| 26  | b     | 621 | LHG  | O6-C4-C5-C6     |
| 24  | N     | 608 | CHL  | C12-C13-C15-C16 |
| 24  | n     | 608 | CHL  | C12-C13-C15-C16 |
| 25  | G     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | G     | 603 | CLA  | C2-C3-C5-C6     |
| 25  | R     | 609 | CLA  | C11-C12-C13-C15 |
| 25  | g     | 602 | CLA  | C6-C7-C8-C10    |
| 25  | g     | 603 | CLA  | C2-C3-C5-C6     |
| 25  | r     | 609 | CLA  | C11-C12-C13-C15 |
| 26  | B     | 621 | LHG  | O1-C1-C2-O2     |
| 26  | b     | 621 | LHG  | O1-C1-C2-O2     |
| 25  | B     | 603 | CLA  | C1-C2-C3-C4     |
| 25  | B     | 607 | CLA  | C1-C2-C3-C4     |
| 25  | G     | 612 | CLA  | C1-C2-C3-C4     |
| 25  | b     | 603 | CLA  | C1-C2-C3-C4     |
| 25  | b     | 607 | CLA  | C1-C2-C3-C4     |
| 25  | g     | 612 | CLA  | C1-C2-C3-C4     |
| 24  | N     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 24  | n     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 24  | n     | 605 | CHL  | C2-C1-O2A-CGA   |
| 30  | B     | 623 | LMG  | C41-C42-C43-C44 |
| 30  | b     | 623 | LMG  | C41-C42-C43-C44 |
| 30  | B     | 623 | LMG  | O1-C7-C8-O7     |
| 30  | b     | 623 | LMG  | O1-C7-C8-O7     |
| 24  | N     | 605 | CHL  | C2-C1-O2A-CGA   |
| 24  | G     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 24  | S     | 308 | CHL  | CAA-CBA-CGA-O2A |
| 24  | s     | 308 | CHL  | CAA-CBA-CGA-O2A |
| 25  | Y     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 25  | R     | 601 | CLA  | O2A-C1-C2-C3    |
| 25  | r     | 601 | CLA  | O2A-C1-C2-C3    |
| 25  | R     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 25  | r     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 35  | C     | 515 | DGD  | O2G-C1B-C2B-C3B |
| 24  | g     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 30  | C     | 520 | LMG  | C39-C40-C41-C42 |
| 30  | c     | 520 | LMG  | C39-C40-C41-C42 |
| 35  | C     | 516 | DGD  | C5A-C6A-C7A-C8A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | c     | 516 | DGD  | C5A-C6A-C7A-C8A |
| 25  | B     | 606 | CLA  | C16-C17-C18-C19 |
| 25  | b     | 606 | CLA  | C16-C17-C18-C19 |
| 24  | G     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 24  | g     | 605 | CHL  | CAA-CBA-CGA-O2A |
| 25  | B     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 25  | s     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 28  | T     | 101 | BCR  | C20-C21-C22-C37 |
| 28  | t     | 101 | BCR  | C20-C21-C22-C37 |
| 29  | L     | 103 | SQD  | C16-C17-C18-C19 |
| 29  | l     | 101 | SQD  | C16-C17-C18-C19 |
| 25  | B     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 25  | b     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 35  | c     | 515 | DGD  | O2G-C1B-C2B-C3B |
| 25  | Y     | 303 | CLA  | C4C-C3C-CAC-CBC |
| 25  | b     | 607 | CLA  | C4-C3-C5-C6     |
| 24  | n     | 609 | CHL  | C10-C11-C12-C13 |
| 25  | N     | 610 | CLA  | C8-C10-C11-C12  |
| 25  | n     | 610 | CLA  | C8-C10-C11-C12  |
| 25  | y     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 31  | D     | 405 | PL9  | C43-C44-C46-C47 |
| 31  | d     | 405 | PL9  | C43-C44-C46-C47 |
| 24  | Y     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 24  | y     | 307 | CHL  | CAA-CBA-CGA-O2A |
| 25  | B     | 616 | CLA  | CAA-CBA-CGA-O2A |
| 25  | b     | 616 | CLA  | CAA-CBA-CGA-O2A |
| 25  | y     | 303 | CLA  | C4C-C3C-CAC-CBC |
| 24  | N     | 607 | CHL  | C11-C10-C8-C9   |
| 24  | n     | 607 | CHL  | C11-C10-C8-C9   |
| 25  | B     | 603 | CLA  | C14-C13-C15-C16 |
| 25  | B     | 611 | CLA  | C11-C12-C13-C14 |
| 25  | C     | 510 | CLA  | C14-C13-C15-C16 |
| 25  | G     | 613 | CLA  | C14-C13-C15-C16 |
| 25  | N     | 611 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 304 | CLA  | C6-C7-C8-C9     |
| 25  | b     | 603 | CLA  | C14-C13-C15-C16 |
| 25  | b     | 611 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 613 | CLA  | C14-C13-C15-C16 |
| 25  | n     | 611 | CLA  | C6-C7-C8-C9     |
| 25  | y     | 304 | CLA  | C6-C7-C8-C9     |
| 25  | S     | 305 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 25  | s     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 29  | A     | 407 | SQD  | C18-C19-C20-C21 |
| 29  | a     | 408 | SQD  | C18-C19-C20-C21 |
| 24  | N     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 24  | n     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 25  | B     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 25  | B     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 25  | C     | 505 | CLA  | C3A-C2A-CAA-CBA |
| 25  | G     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 25  | N     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 25  | b     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 25  | c     | 505 | CLA  | C3A-C2A-CAA-CBA |
| 25  | g     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 25  | n     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 26  | b     | 625 | LHG  | C11-C12-C13-C14 |
| 25  | B     | 604 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 604 | CLA  | C13-C15-C16-C17 |
| 25  | D     | 402 | CLA  | CAA-CBA-CGA-O2A |
| 25  | D     | 403 | CLA  | CAA-CBA-CGA-O2A |
| 25  | d     | 402 | CLA  | CAA-CBA-CGA-O2A |
| 25  | d     | 403 | CLA  | CAA-CBA-CGA-O2A |
| 26  | D     | 406 | LHG  | C29-C30-C31-C32 |
| 26  | d     | 406 | LHG  | C29-C30-C31-C32 |
| 24  | 2     | 603 | CHL  | CAD-CBD-CGD-O2D |
| 24  | Y     | 310 | CHL  | CAD-CBD-CGD-O2D |
| 24  | 6     | 603 | CHL  | CAD-CBD-CGD-O2D |
| 24  | y     | 310 | CHL  | CAD-CBD-CGD-O2D |
| 25  | 2     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 25  | B     | 616 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 501 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 508 | CLA  | CAD-CBD-CGD-O2D |
| 25  | C     | 513 | CLA  | CAD-CBD-CGD-O2D |
| 25  | D     | 403 | CLA  | CAD-CBD-CGD-O2D |
| 25  | S     | 314 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | N     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 25  | R     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 25  | R     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 25  | 6     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 25  | b     | 616 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 501 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 508 | CLA  | CAD-CBD-CGD-O2D |
| 25  | c     | 513 | CLA  | CAD-CBD-CGD-O2D |
| 25  | d     | 403 | CLA  | CAD-CBD-CGD-O2D |
| 25  | s     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 25  | s     | 314 | CLA  | CAD-CBD-CGD-O2D |
| 25  | g     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 25  | r     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 25  | r     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 40  | R     | 617 | NEX  | C7-C8-C9-C19    |
| 40  | r     | 617 | NEX  | C7-C8-C9-C19    |
| 25  | Y     | 304 | CLA  | C16-C17-C18-C20 |
| 25  | y     | 304 | CLA  | C16-C17-C18-C20 |
| 26  | B     | 625 | LHG  | C11-C12-C13-C14 |
| 24  | N     | 609 | CHL  | C10-C11-C12-C13 |
| 30  | A     | 408 | LMG  | O9-C10-O7-C8    |
| 30  | a     | 409 | LMG  | O9-C10-O7-C8    |
| 35  | C     | 516 | DGD  | O1B-C1B-O2G-C2G |
| 35  | c     | 516 | DGD  | O1B-C1B-O2G-C2G |
| 24  | Y     | 310 | CHL  | C2-C1-O2A-CGA   |
| 24  | y     | 310 | CHL  | C2-C1-O2A-CGA   |
| 25  | C     | 501 | CLA  | CAA-CBA-CGA-O2A |
| 25  | C     | 512 | CLA  | CAA-CBA-CGA-O2A |
| 25  | Y     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 25  | c     | 501 | CLA  | CAA-CBA-CGA-O2A |
| 25  | c     | 512 | CLA  | CAA-CBA-CGA-O2A |
| 25  | y     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 35  | A     | 415 | DGD  | O2G-C1B-C2B-C3B |
| 35  | a     | 401 | DGD  | O2G-C1B-C2B-C3B |
| 28  | B     | 617 | BCR  | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | b     | 617 | BCR  | C22-C23-C24-C25 |
| 26  | n     | 618 | LHG  | C29-C30-C31-C32 |
| 25  | B     | 607 | CLA  | C4-C3-C5-C6     |
| 25  | B     | 611 | CLA  | C4-C3-C5-C6     |
| 25  | b     | 611 | CLA  | C4-C3-C5-C6     |
| 30  | B     | 620 | LMG  | O6-C5-C6-O5     |
| 30  | b     | 620 | LMG  | O6-C5-C6-O5     |
| 24  | y     | 308 | CHL  | C5-C6-C7-C8     |
| 25  | B     | 608 | CLA  | C10-C11-C12-C13 |
| 25  | b     | 608 | CLA  | C10-C11-C12-C13 |
| 25  | S     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 25  | s     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 26  | N     | 618 | LHG  | C4-C5-C6-O8     |
| 26  | n     | 618 | LHG  | C4-C5-C6-O8     |
| 29  | A     | 407 | SQD  | O6-C44-C45-C46  |
| 29  | a     | 408 | SQD  | O6-C44-C45-C46  |
| 35  | C     | 515 | DGD  | C1G-C2G-C3G-O3G |
| 35  | c     | 515 | DGD  | C1G-C2G-C3G-O3G |
| 40  | G     | 617 | NEX  | O24-C26-C27-C28 |
| 40  | g     | 617 | NEX  | O24-C26-C27-C28 |
| 24  | y     | 309 | CHL  | C4C-C3C-CAC-CBC |
| 26  | N     | 618 | LHG  | C29-C30-C31-C32 |
| 24  | N     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 24  | Y     | 309 | CHL  | C4C-C3C-CAC-CBC |
| 24  | n     | 605 | CHL  | C4C-C3C-CAC-CBC |
| 26  | 2     | 606 | LHG  | O6-C4-C5-O7     |
| 26  | 6     | 606 | LHG  | O6-C4-C5-O7     |
| 24  | Y     | 308 | CHL  | C5-C6-C7-C8     |
| 26  | R     | 618 | LHG  | O7-C7-C8-C9     |
| 26  | r     | 618 | LHG  | O7-C7-C8-C9     |
| 29  | A     | 407 | SQD  | O47-C7-C8-C9    |
| 29  | a     | 408 | SQD  | O47-C7-C8-C9    |
| 35  | C     | 516 | DGD  | C6A-C7A-C8A-C9A |
| 25  | S     | 314 | CLA  | O2A-C1-C2-C3    |
| 25  | s     | 314 | CLA  | O2A-C1-C2-C3    |
| 35  | c     | 516 | DGD  | C6A-C7A-C8A-C9A |
| 24  | N     | 609 | CHL  | O2A-C1-C2-C3    |
| 24  | n     | 609 | CHL  | O2A-C1-C2-C3    |
| 29  | A     | 407 | SQD  | C14-C15-C16-C17 |
| 29  | a     | 408 | SQD  | C14-C15-C16-C17 |
| 24  | S     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 24  | s     | 306 | CHL  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | 6     | 606 | LHG  | C24-C25-C26-C27 |
| 24  | 1     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 24  | G     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | G     | 605 | CHL  | CHA-CBD-CGD-O1D |
| 24  | Y     | 309 | CHL  | CHA-CBD-CGD-O1D |
| 24  | 5     | 301 | CHL  | CHA-CBD-CGD-O2D |
| 24  | g     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 24  | g     | 605 | CHL  | CHA-CBD-CGD-O1D |
| 24  | y     | 309 | CHL  | CHA-CBD-CGD-O1D |
| 25  | 2     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 25  | B     | 601 | CLA  | CHA-CBD-CGD-O2D |
| 25  | B     | 607 | CLA  | CHA-CBD-CGD-O2D |
| 25  | B     | 610 | CLA  | CHA-CBD-CGD-O1D |
| 25  | B     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 25  | C     | 506 | CLA  | CHA-CBD-CGD-O2D |
| 25  | C     | 507 | CLA  | CHA-CBD-CGD-O2D |
| 25  | D     | 401 | CLA  | CHA-CBD-CGD-O1D |
| 25  | S     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 25  | S     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 25  | S     | 313 | CLA  | CHA-CBD-CGD-O2D |
| 25  | G     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 25  | G     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 25  | G     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 25  | G     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | G     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 25  | N     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 25  | Y     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 25  | R     | 601 | CLA  | CHA-CBD-CGD-O2D |
| 25  | 6     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 25  | b     | 601 | CLA  | CHA-CBD-CGD-O2D |
| 25  | b     | 607 | CLA  | CHA-CBD-CGD-O2D |
| 25  | b     | 610 | CLA  | CHA-CBD-CGD-O1D |
| 25  | b     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 25  | c     | 506 | CLA  | CHA-CBD-CGD-O2D |
| 25  | c     | 507 | CLA  | CHA-CBD-CGD-O2D |
| 25  | d     | 401 | CLA  | CHA-CBD-CGD-O1D |
| 25  | s     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 25  | s     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 25  | s     | 313 | CLA  | CHA-CBD-CGD-O2D |
| 25  | g     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 25  | g     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 25  | g     | 611 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | g     | 612 | CLA  | CHA-CBD-CGD-O2D |
| 25  | g     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 25  | n     | 612 | CLA  | CHA-CBD-CGD-O1D |
| 25  | y     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 25  | r     | 601 | CLA  | CHA-CBD-CGD-O2D |
| 26  | 2     | 606 | LHG  | C24-C25-C26-C27 |
| 26  | N     | 618 | LHG  | C9-C10-C11-C12  |
| 26  | n     | 618 | LHG  | C9-C10-C11-C12  |
| 26  | y     | 319 | LHG  | C15-C16-C17-C18 |
| 35  | C     | 516 | DGD  | CBA-CCA-CDA-CEA |
| 25  | N     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 25  | n     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 26  | D     | 406 | LHG  | O8-C23-C24-C25  |
| 26  | d     | 406 | LHG  | O8-C23-C24-C25  |
| 30  | A     | 410 | LMG  | C4-C5-C6-O5     |
| 30  | a     | 411 | LMG  | C4-C5-C6-O5     |
| 26  | D     | 406 | LHG  | C13-C14-C15-C16 |
| 35  | c     | 516 | DGD  | CBA-CCA-CDA-CEA |
| 26  | B     | 622 | LHG  | O7-C5-C6-O8     |
| 26  | b     | 622 | LHG  | O7-C5-C6-O8     |
| 26  | L     | 102 | LHG  | C23-C24-C25-C26 |
| 26  | l     | 103 | LHG  | C23-C24-C25-C26 |
| 24  | 6     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 25  | N     | 610 | CLA  | C5-C6-C7-C8     |
| 25  | n     | 610 | CLA  | C5-C6-C7-C8     |
| 24  | S     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 24  | s     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 26  | Y     | 319 | LHG  | C15-C16-C17-C18 |
| 26  | d     | 406 | LHG  | C13-C14-C15-C16 |
| 26  | 2     | 606 | LHG  | O10-C23-O8-C6   |
| 25  | B     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 25  | G     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 25  | g     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 25  | n     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 30  | C     | 520 | LMG  | O8-C28-C29-C30  |
| 24  | g     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 25  | D     | 403 | CLA  | C2A-CAA-CBA-CGA |
| 25  | d     | 403 | CLA  | C2A-CAA-CBA-CGA |
| 27  | A     | 403 | PHO  | CHA-CBD-CGD-O1D |
| 27  | a     | 404 | PHO  | CHA-CBD-CGD-O1D |
| 30  | D     | 407 | LMG  | C14-C15-C16-C17 |
| 30  | d     | 407 | LMG  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 2     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 25  | b     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | c     | 520 | LMG  | O8-C28-C29-C30  |
| 30  | a     | 411 | LMG  | C30-C31-C32-C33 |
| 24  | G     | 607 | CHL  | CAA-CBA-CGA-O1A |
| 24  | g     | 607 | CHL  | CAA-CBA-CGA-O1A |
| 25  | r     | 614 | CLA  | CAA-CBA-CGA-O1A |
| 26  | 6     | 606 | LHG  | O10-C23-O8-C6   |
| 24  | N     | 608 | CHL  | C11-C10-C8-C7   |
| 24  | n     | 608 | CHL  | C11-C10-C8-C7   |
| 25  | C     | 513 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 513 | CLA  | C11-C12-C13-C15 |
| 31  | D     | 405 | PL9  | C18-C19-C21-C22 |
| 31  | d     | 405 | PL9  | C18-C19-C21-C22 |
| 25  | B     | 616 | CLA  | C16-C17-C18-C19 |
| 25  | b     | 616 | CLA  | C16-C17-C18-C19 |
| 25  | C     | 508 | CLA  | C2C-C3C-CAC-CBC |
| 30  | A     | 410 | LMG  | C30-C31-C32-C33 |
| 24  | G     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 25  | N     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 25  | R     | 614 | CLA  | CAA-CBA-CGA-O1A |
| 25  | c     | 508 | CLA  | C2C-C3C-CAC-CBC |
| 25  | G     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | g     | 602 | CLA  | C6-C7-C8-C9     |
| 25  | Y     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 25  | y     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 26  | 2     | 606 | LHG  | C24-C23-O8-C6   |
| 26  | 6     | 606 | LHG  | C24-C23-O8-C6   |
| 24  | g     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 25  | N     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 25  | n     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 26  | y     | 301 | LHG  | O10-C23-C24-C25 |
| 25  | B     | 606 | CLA  | C16-C17-C18-C20 |
| 25  | b     | 606 | CLA  | C16-C17-C18-C20 |
| 24  | N     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 35  | C     | 516 | DGD  | C2B-C1B-O2G-C2G |
| 35  | c     | 516 | DGD  | C2B-C1B-O2G-C2G |
| 24  | G     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 26  | C     | 518 | LHG  | C23-C24-C25-C26 |
| 26  | Y     | 301 | LHG  | O10-C23-C24-C25 |
| 25  | C     | 510 | CLA  | C4C-C3C-CAC-CBC |
| 28  | D     | 404 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | I     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | d     | 404 | BCR  | C7-C8-C9-C34    |
| 25  | C     | 507 | CLA  | C5-C6-C7-C8     |
| 25  | g     | 611 | CLA  | C11-C12-C13-C14 |
| 32  | B     | 624 | AJP  | C56-C55-O54-C36 |
| 32  | b     | 624 | AJP  | C56-C55-O54-C36 |
| 25  | c     | 510 | CLA  | C4C-C3C-CAC-CBC |
| 26  | c     | 517 | LHG  | O1-C1-C2-C3     |
| 35  | C     | 515 | DGD  | CDB-CEB-CFB-CGB |
| 35  | C     | 515 | DGD  | O1B-C1B-C2B-C3B |
| 35  | c     | 515 | DGD  | O1B-C1B-C2B-C3B |
| 25  | C     | 507 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 507 | CLA  | CBA-CGA-O2A-C1  |
| 26  | Y     | 319 | LHG  | C28-C29-C30-C31 |
| 35  | c     | 515 | DGD  | CDB-CEB-CFB-CGB |
| 24  | G     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 24  | g     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 25  | 2     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | B     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 25  | N     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 25  | R     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 6     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 25  | b     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 25  | b     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 25  | n     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 25  | r     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 32  | Y     | 323 | AJP  | C29-C30-C32-O33 |
| 32  | y     | 323 | AJP  | C29-C30-C32-O33 |
| 26  | y     | 319 | LHG  | C28-C29-C30-C31 |
| 24  | N     | 607 | CHL  | C16-C17-C18-C20 |
| 24  | n     | 607 | CHL  | C16-C17-C18-C20 |
| 25  | G     | 611 | CLA  | C11-C12-C13-C14 |
| 35  | A     | 415 | DGD  | O1B-C1B-C2B-C3B |
| 35  | a     | 401 | DGD  | O1B-C1B-C2B-C3B |
| 25  | c     | 507 | CLA  | C5-C6-C7-C8     |
| 24  | n     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 25  | g     | 602 | CLA  | C13-C15-C16-C17 |
| 24  | y     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 25  | R     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 25  | r     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 26  | Y     | 319 | LHG  | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | y     | 319 | LHG  | C27-C28-C29-C30 |
| 29  | A     | 407 | SQD  | C44-C45-C46-O48 |
| 29  | a     | 408 | SQD  | C44-C45-C46-O48 |
| 30  | B     | 623 | LMG  | O1-C7-C8-C9     |
| 30  | b     | 623 | LMG  | O1-C7-C8-C9     |
| 25  | G     | 602 | CLA  | C13-C15-C16-C17 |
| 25  | C     | 512 | CLA  | C4C-C3C-CAC-CBC |
| 25  | c     | 512 | CLA  | C4C-C3C-CAC-CBC |
| 35  | C     | 515 | DGD  | C5B-C6B-C7B-C8B |
| 24  | Y     | 307 | CHL  | CAA-CBA-CGA-O1A |
| 25  | N     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 25  | n     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 35  | c     | 515 | DGD  | C5B-C6B-C7B-C8B |
| 25  | R     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 32  | Y     | 322 | AJP  | O31-C30-C32-O33 |
| 32  | y     | 322 | AJP  | O31-C30-C32-O33 |
| 25  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 25  | c     | 509 | CLA  | C13-C15-C16-C17 |
| 26  | c     | 518 | LHG  | C23-C24-C25-C26 |
| 30  | A     | 410 | LMG  | C34-C35-C36-C37 |
| 30  | a     | 411 | LMG  | C34-C35-C36-C37 |
| 25  | r     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 26  | B     | 625 | LHG  | C31-C32-C33-C34 |
| 26  | R     | 618 | LHG  | C14-C15-C16-C17 |
| 26  | r     | 618 | LHG  | C14-C15-C16-C17 |
| 26  | B     | 621 | LHG  | C3-O3-P-O5      |
| 26  | S     | 318 | LHG  | C3-O3-P-O5      |
| 26  | Y     | 301 | LHG  | C3-O3-P-O5      |
| 26  | b     | 621 | LHG  | C3-O3-P-O5      |
| 26  | s     | 318 | LHG  | C3-O3-P-O5      |
| 26  | y     | 301 | LHG  | C3-O3-P-O5      |
| 30  | A     | 408 | LMG  | C11-C10-O7-C8   |
| 26  | b     | 622 | LHG  | C16-C17-C18-C19 |
| 25  | G     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 25  | N     | 611 | CLA  | CAA-CBA-CGA-O1A |
| 25  | g     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 25  | n     | 611 | CLA  | CAA-CBA-CGA-O1A |
| 24  | n     | 609 | CHL  | CAA-CBA-CGA-O2A |
| 25  | N     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 26  | B     | 622 | LHG  | C16-C17-C18-C19 |
| 26  | b     | 625 | LHG  | C31-C32-C33-C34 |
| 28  | C     | 514 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | c     | 514 | BCR  | C5-C6-C7-C8     |
| 30  | B     | 623 | LMG  | C20-C21-C22-C23 |
| 30  | b     | 623 | LMG  | C20-C21-C22-C23 |
| 24  | G     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 24  | g     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 25  | B     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 25  | b     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 29  | A     | 407 | SQD  | O49-C7-C8-C9    |
| 29  | a     | 408 | SQD  | O49-C7-C8-C9    |
| 25  | C     | 501 | CLA  | O1A-CGA-O2A-C1  |
| 26  | S     | 318 | LHG  | C32-C33-C34-C35 |
| 30  | c     | 520 | LMG  | O10-C28-C29-C30 |
| 25  | c     | 501 | CLA  | O1A-CGA-O2A-C1  |
| 25  | C     | 508 | CLA  | C4C-C3C-CAC-CBC |
| 26  | s     | 318 | LHG  | C32-C33-C34-C35 |
| 30  | a     | 409 | LMG  | C11-C10-O7-C8   |
| 35  | C     | 516 | DGD  | C4E-C5E-C6E-O5E |
| 35  | c     | 516 | DGD  | C4E-C5E-C6E-O5E |
| 25  | n     | 611 | CLA  | C11-C12-C13-C15 |
| 25  | c     | 508 | CLA  | C4C-C3C-CAC-CBC |
| 24  | S     | 302 | CHL  | CAD-CBD-CGD-O1D |
| 24  | s     | 302 | CHL  | CAD-CBD-CGD-O1D |
| 25  | B     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 25  | C     | 506 | CLA  | CAD-CBD-CGD-O1D |
| 25  | C     | 508 | CLA  | CAD-CBD-CGD-O1D |
| 25  | N     | 610 | CLA  | CAD-CBD-CGD-O1D |
| 25  | b     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 25  | c     | 506 | CLA  | CAD-CBD-CGD-O1D |
| 25  | c     | 508 | CLA  | CAD-CBD-CGD-O1D |
| 25  | n     | 610 | CLA  | CAD-CBD-CGD-O1D |
| 26  | L     | 102 | LHG  | C4-C5-O7-C7     |
| 26  | l     | 103 | LHG  | C4-C5-O7-C7     |
| 25  | n     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 616 | CLA  | CAA-CBA-CGA-O1A |
| 25  | b     | 616 | CLA  | CAA-CBA-CGA-O1A |
| 26  | R     | 618 | LHG  | O9-C7-C8-C9     |
| 26  | r     | 618 | LHG  | O9-C7-C8-C9     |
| 30  | C     | 520 | LMG  | O10-C28-C29-C30 |
| 24  | N     | 609 | CHL  | CAA-CBA-CGA-O2A |
| 25  | g     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 25  | B     | 601 | CLA  | C6-C7-C8-C9     |
| 25  | C     | 512 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | C     | 513 | CLA  | C11-C12-C13-C14 |
| 25  | G     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | b     | 601 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 512 | CLA  | C6-C7-C8-C9     |
| 25  | c     | 513 | CLA  | C11-C12-C13-C14 |
| 25  | g     | 602 | CLA  | C11-C10-C8-C9   |
| 25  | y     | 311 | CLA  | C11-C10-C8-C9   |
| 25  | c     | 508 | CLA  | C5-C6-C7-C8     |
| 25  | N     | 611 | CLA  | C11-C12-C13-C15 |
| 25  | G     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 26  | Y     | 301 | LHG  | O7-C7-C8-C9     |
| 26  | y     | 301 | LHG  | O7-C7-C8-C9     |
| 35  | B     | 626 | DGD  | C9A-CAA-CBA-CCA |
| 25  | C     | 508 | CLA  | C5-C6-C7-C8     |
| 25  | y     | 303 | CLA  | C8-C10-C11-C12  |
| 35  | b     | 626 | DGD  | C9A-CAA-CBA-CCA |
| 25  | C     | 501 | CLA  | CAA-CBA-CGA-O1A |
| 25  | c     | 501 | CLA  | CAA-CBA-CGA-O1A |
| 24  | l     | 301 | CHL  | C4C-C3C-CAC-CBC |
| 24  | n     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 25  | S     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 25  | Y     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 25  | s     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 25  | B     | 605 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 605 | CLA  | C13-C15-C16-C17 |
| 26  | d     | 406 | LHG  | O10-C23-C24-C25 |
| 25  | C     | 510 | CLA  | C4-C3-C5-C6     |
| 25  | c     | 510 | CLA  | C4-C3-C5-C6     |
| 35  | C     | 516 | DGD  | C7B-C8B-C9B-CAB |
| 35  | c     | 516 | DGD  | C7B-C8B-C9B-CAB |
| 24  | Y     | 302 | CHL  | C6-C7-C8-C10    |
| 24  | y     | 302 | CHL  | C6-C7-C8-C10    |
| 25  | A     | 401 | CLA  | C11-C10-C8-C7   |
| 25  | B     | 601 | CLA  | C6-C7-C8-C10    |
| 25  | B     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 25  | B     | 605 | CLA  | C11-C12-C13-C15 |
| 25  | N     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | N     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 25  | R     | 602 | CLA  | C11-C10-C8-C7   |
| 25  | a     | 402 | CLA  | C11-C10-C8-C7   |
| 25  | b     | 601 | CLA  | C6-C7-C8-C10    |
| 25  | b     | 602 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | b     | 605 | CLA  | C11-C12-C13-C15 |
| 25  | n     | 603 | CLA  | C6-C7-C8-C10    |
| 25  | n     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 25  | r     | 602 | CLA  | C11-C10-C8-C7   |
| 39  | G     | 615 | LUT  | C25-C26-C27-C28 |
| 39  | N     | 615 | LUT  | C25-C26-C27-C28 |
| 39  | g     | 615 | LUT  | C25-C26-C27-C28 |
| 39  | n     | 615 | LUT  | C25-C26-C27-C28 |
| 25  | n     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 26  | D     | 406 | LHG  | O10-C23-C24-C25 |
| 24  | 5     | 301 | CHL  | C4C-C3C-CAC-CBC |
| 24  | N     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 25  | y     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 35  | c     | 516 | DGD  | O2G-C1B-C2B-C3B |
| 25  | Y     | 303 | CLA  | C8-C10-C11-C12  |
| 25  | Y     | 304 | CLA  | C8-C10-C11-C12  |
| 25  | y     | 304 | CLA  | C8-C10-C11-C12  |
| 28  | B     | 618 | BCR  | C21-C22-C23-C24 |
| 28  | I     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | b     | 618 | BCR  | C21-C22-C23-C24 |
| 28  | i     | 101 | BCR  | C7-C8-C9-C10    |
| 25  | N     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 39  | S     | 316 | LUT  | C29-C30-C31-C32 |
| 39  | G     | 615 | LUT  | C33-C34-C35-C15 |
| 39  | s     | 316 | LUT  | C29-C30-C31-C32 |
| 39  | g     | 615 | LUT  | C33-C34-C35-C15 |
| 29  | A     | 411 | SQD  | C28-C29-C30-C31 |
| 29  | a     | 412 | SQD  | C28-C29-C30-C31 |
| 26  | R     | 618 | LHG  | O8-C23-C24-C25  |
| 35  | C     | 516 | DGD  | O2G-C1B-C2B-C3B |
| 30  | d     | 407 | LMG  | C22-C23-C24-C25 |
| 35  | A     | 415 | DGD  | O6E-C1E-O5D-C6D |
| 35  | B     | 626 | DGD  | O6E-C1E-O5D-C6D |
| 35  | a     | 401 | DGD  | O6E-C1E-O5D-C6D |
| 35  | b     | 626 | DGD  | O6E-C1E-O5D-C6D |
| 25  | C     | 501 | CLA  | C15-C16-C17-C18 |
| 25  | c     | 501 | CLA  | C15-C16-C17-C18 |
| 30  | D     | 407 | LMG  | C22-C23-C24-C25 |
| 26  | Y     | 301 | LHG  | O9-C7-C8-C9     |
| 26  | y     | 301 | LHG  | O9-C7-C8-C9     |
| 24  | N     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 24  | n     | 606 | CHL  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 602 | CLA  | C8-C10-C11-C12  |
| 25  | g     | 602 | CLA  | C8-C10-C11-C12  |
| 32  | B     | 624 | AJP  | C28-C29-O34-C35 |
| 32  | b     | 624 | AJP  | C28-C29-O34-C35 |
| 25  | G     | 604 | CLA  | CAA-CBA-CGA-O2A |
| 25  | B     | 606 | CLA  | C15-C16-C17-C18 |
| 25  | b     | 606 | CLA  | C15-C16-C17-C18 |
| 24  | S     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 24  | s     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 25  | B     | 615 | CLA  | C13-C15-C16-C17 |
| 25  | b     | 615 | CLA  | C13-C15-C16-C17 |
| 26  | s     | 318 | LHG  | C34-C35-C36-C37 |
| 25  | G     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 25  | g     | 604 | CLA  | CAA-CBA-CGA-O2A |
| 26  | r     | 618 | LHG  | O8-C23-C24-C25  |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 40  | Y     | 318 | NEX  | C1-C2-C3-C4-C5-C6 |
| 40  | y     | 318 | NEX  | C1-C2-C3-C4-C5-C6 |

356 monomers are involved in 3261 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | a     | 403 | CLA  | 13      | 0            |
| 39  | r     | 615 | LUT  | 8       | 0            |
| 25  | R     | 602 | CLA  | 15      | 0            |
| 25  | C     | 510 | CLA  | 23      | 0            |
| 32  | y     | 322 | AJP  | 2       | 0            |
| 25  | S     | 303 | CLA  | 14      | 0            |
| 25  | G     | 603 | CLA  | 12      | 0            |
| 25  | B     | 612 | CLA  | 6       | 0            |
| 32  | n     | 619 | AJP  | 2       | 0            |
| 26  | b     | 622 | LHG  | 8       | 0            |
| 39  | N     | 616 | LUT  | 15      | 0            |
| 25  | R     | 604 | CLA  | 8       | 0            |
| 40  | g     | 617 | NEX  | 15      | 0            |
| 25  | c     | 511 | CLA  | 21      | 0            |
| 25  | s     | 303 | CLA  | 15      | 0            |
| 35  | B     | 626 | DGD  | 5       | 0            |
| 32  | Y     | 320 | AJP  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | n     | 614 | CLA  | 6       | 0            |
| 30  | A     | 410 | LMG  | 3       | 0            |
| 25  | Y     | 313 | CLA  | 9       | 0            |
| 26  | B     | 622 | LHG  | 8       | 0            |
| 40  | S     | 317 | NEX  | 6       | 0            |
| 25  | B     | 610 | CLA  | 14      | 0            |
| 25  | n     | 612 | CLA  | 10      | 0            |
| 26  | S     | 318 | LHG  | 5       | 0            |
| 25  | C     | 507 | CLA  | 6       | 0            |
| 25  | N     | 604 | CLA  | 9       | 0            |
| 27  | A     | 404 | PHO  | 14      | 0            |
| 25  | B     | 611 | CLA  | 7       | 0            |
| 25  | g     | 612 | CLA  | 9       | 0            |
| 25  | R     | 612 | CLA  | 19      | 0            |
| 25  | r     | 608 | CLA  | 17      | 0            |
| 25  | 2     | 602 | CLA  | 8       | 0            |
| 25  | S     | 313 | CLA  | 12      | 0            |
| 25  | n     | 602 | CLA  | 23      | 0            |
| 25  | 2     | 604 | CLA  | 19      | 0            |
| 30  | a     | 411 | LMG  | 3       | 0            |
| 30  | d     | 407 | LMG  | 3       | 0            |
| 24  | n     | 608 | CHL  | 9       | 0            |
| 32  | N     | 619 | AJP  | 2       | 0            |
| 24  | R     | 605 | CHL  | 8       | 0            |
| 24  | 2     | 601 | CHL  | 8       | 0            |
| 24  | n     | 606 | CHL  | 17      | 0            |
| 35  | A     | 415 | DGD  | 3       | 0            |
| 39  | g     | 615 | LUT  | 15      | 0            |
| 24  | N     | 609 | CHL  | 26      | 0            |
| 40  | R     | 617 | NEX  | 8       | 0            |
| 25  | s     | 314 | CLA  | 10      | 0            |
| 24  | N     | 608 | CHL  | 11      | 0            |
| 26  | s     | 301 | LHG  | 9       | 0            |
| 25  | n     | 604 | CLA  | 8       | 0            |
| 30  | A     | 408 | LMG  | 3       | 0            |
| 39  | S     | 316 | LUT  | 20      | 0            |
| 25  | g     | 610 | CLA  | 40      | 0            |
| 31  | a     | 410 | PL9  | 2       | 0            |
| 24  | N     | 605 | CHL  | 5       | 0            |
| 28  | B     | 617 | BCR  | 7       | 0            |
| 29  | L     | 101 | SQD  | 19      | 0            |
| 40  | y     | 318 | NEX  | 10      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | Y     | 315 | CLA  | 17      | 0            |
| 26  | d     | 406 | LHG  | 10      | 0            |
| 24  | s     | 308 | CHL  | 9       | 0            |
| 26  | l     | 103 | LHG  | 5       | 0            |
| 24  | Y     | 307 | CHL  | 14      | 0            |
| 24  | n     | 609 | CHL  | 29      | 0            |
| 26  | c     | 519 | LHG  | 4       | 0            |
| 25  | R     | 614 | CLA  | 11      | 0            |
| 24  | n     | 605 | CHL  | 5       | 0            |
| 25  | G     | 602 | CLA  | 12      | 0            |
| 24  | Y     | 302 | CHL  | 30      | 0            |
| 30  | C     | 520 | LMG  | 4       | 0            |
| 30  | b     | 623 | LMG  | 5       | 0            |
| 25  | C     | 508 | CLA  | 10      | 0            |
| 26  | 6     | 606 | LHG  | 14      | 0            |
| 28  | b     | 618 | BCR  | 8       | 0            |
| 25  | b     | 611 | CLA  | 7       | 0            |
| 25  | c     | 505 | CLA  | 10      | 0            |
| 25  | C     | 511 | CLA  | 20      | 0            |
| 25  | B     | 609 | CLA  | 11      | 0            |
| 25  | n     | 603 | CLA  | 33      | 0            |
| 24  | S     | 307 | CHL  | 6       | 0            |
| 25  | y     | 313 | CLA  | 9       | 0            |
| 35  | a     | 401 | DGD  | 3       | 0            |
| 24  | l     | 302 | CHL  | 9       | 0            |
| 25  | B     | 608 | CLA  | 8       | 0            |
| 25  | D     | 402 | CLA  | 19      | 0            |
| 26  | L     | 102 | LHG  | 5       | 0            |
| 28  | Z     | 101 | BCR  | 5       | 0            |
| 28  | b     | 619 | BCR  | 4       | 0            |
| 25  | 2     | 605 | CLA  | 6       | 0            |
| 25  | b     | 616 | CLA  | 15      | 0            |
| 28  | a     | 407 | BCR  | 5       | 0            |
| 29  | A     | 411 | SQD  | 5       | 0            |
| 25  | c     | 502 | CLA  | 12      | 0            |
| 25  | y     | 304 | CLA  | 20      | 0            |
| 33  | a     | 414 | BCT  | 1       | 0            |
| 25  | R     | 609 | CLA  | 5       | 0            |
| 26  | R     | 618 | LHG  | 14      | 0            |
| 24  | N     | 606 | CHL  | 18      | 0            |
| 24  | G     | 607 | CHL  | 11      | 0            |
| 25  | A     | 402 | CLA  | 13      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | c     | 509 | CLA  | 9       | 0            |
| 27  | a     | 404 | PHO  | 14      | 0            |
| 32  | y     | 321 | AJP  | 2       | 0            |
| 31  | D     | 405 | PL9  | 6       | 0            |
| 25  | b     | 613 | CLA  | 14      | 0            |
| 25  | D     | 401 | CLA  | 8       | 0            |
| 25  | B     | 604 | CLA  | 14      | 0            |
| 28  | t     | 101 | BCR  | 21      | 0            |
| 41  | r     | 616 | XAT  | 22      | 0            |
| 39  | S     | 315 | LUT  | 7       | 0            |
| 31  | A     | 409 | PL9  | 2       | 0            |
| 25  | g     | 614 | CLA  | 4       | 0            |
| 24  | N     | 601 | CHL  | 18      | 0            |
| 26  | B     | 625 | LHG  | 7       | 0            |
| 24  | g     | 608 | CHL  | 20      | 0            |
| 25  | B     | 602 | CLA  | 8       | 0            |
| 39  | N     | 615 | LUT  | 12      | 0            |
| 40  | r     | 617 | NEX  | 10      | 0            |
| 30  | B     | 620 | LMG  | 5       | 0            |
| 25  | S     | 310 | CLA  | 14      | 0            |
| 29  | l     | 102 | SQD  | 20      | 0            |
| 39  | y     | 316 | LUT  | 13      | 0            |
| 25  | g     | 602 | CLA  | 11      | 0            |
| 24  | Y     | 310 | CHL  | 17      | 0            |
| 26  | 2     | 606 | LHG  | 14      | 0            |
| 25  | Y     | 305 | CLA  | 4       | 0            |
| 25  | C     | 513 | CLA  | 15      | 0            |
| 25  | r     | 609 | CLA  | 7       | 0            |
| 29  | a     | 412 | SQD  | 6       | 0            |
| 24  | S     | 302 | CHL  | 4       | 0            |
| 25  | A     | 405 | CLA  | 9       | 0            |
| 24  | S     | 308 | CHL  | 9       | 0            |
| 24  | 6     | 603 | CHL  | 20      | 0            |
| 25  | B     | 615 | CLA  | 15      | 0            |
| 41  | R     | 616 | XAT  | 20      | 0            |
| 25  | c     | 512 | CLA  | 12      | 0            |
| 24  | s     | 302 | CHL  | 7       | 0            |
| 25  | S     | 309 | CLA  | 3       | 0            |
| 25  | S     | 314 | CLA  | 10      | 0            |
| 32  | S     | 319 | AJP  | 2       | 0            |
| 24  | Y     | 306 | CHL  | 6       | 0            |
| 25  | C     | 509 | CLA  | 7       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | g     | 607 | CHL  | 11      | 0            |
| 24  | Y     | 309 | CHL  | 14      | 0            |
| 24  | G     | 601 | CHL  | 17      | 0            |
| 39  | y     | 317 | LUT  | 12      | 0            |
| 24  | R     | 613 | CHL  | 4       | 0            |
| 25  | Y     | 312 | CLA  | 10      | 0            |
| 25  | g     | 604 | CLA  | 12      | 0            |
| 25  | N     | 612 | CLA  | 10      | 0            |
| 28  | k     | 101 | BCR  | 9       | 0            |
| 24  | g     | 605 | CHL  | 4       | 0            |
| 29  | A     | 407 | SQD  | 8       | 0            |
| 25  | G     | 610 | CLA  | 37      | 0            |
| 25  | Y     | 311 | CLA  | 25      | 0            |
| 31  | d     | 405 | PL9  | 6       | 0            |
| 39  | s     | 315 | LUT  | 7       | 0            |
| 40  | n     | 617 | NEX  | 13      | 0            |
| 27  | a     | 405 | PHO  | 14      | 0            |
| 28  | d     | 404 | BCR  | 3       | 0            |
| 25  | B     | 606 | CLA  | 15      | 0            |
| 29  | l     | 101 | SQD  | 5       | 0            |
| 39  | s     | 316 | LUT  | 22      | 0            |
| 25  | G     | 611 | CLA  | 12      | 0            |
| 24  | n     | 607 | CHL  | 50      | 0            |
| 25  | c     | 507 | CLA  | 7       | 0            |
| 26  | b     | 625 | LHG  | 7       | 0            |
| 30  | D     | 407 | LMG  | 3       | 0            |
| 24  | R     | 606 | CHL  | 2       | 0            |
| 40  | N     | 617 | NEX  | 15      | 0            |
| 39  | G     | 615 | LUT  | 15      | 0            |
| 35  | C     | 515 | DGD  | 8       | 0            |
| 25  | N     | 614 | CLA  | 6       | 0            |
| 29  | L     | 103 | SQD  | 6       | 0            |
| 26  | r     | 618 | LHG  | 16      | 0            |
| 24  | S     | 306 | CHL  | 10      | 0            |
| 25  | B     | 601 | CLA  | 10      | 0            |
| 24  | 6     | 601 | CHL  | 10      | 0            |
| 24  | r     | 613 | CHL  | 4       | 0            |
| 25  | S     | 312 | CLA  | 9       | 0            |
| 25  | B     | 616 | CLA  | 14      | 0            |
| 25  | Y     | 304 | CLA  | 23      | 0            |
| 25  | s     | 305 | CLA  | 15      | 0            |
| 24  | s     | 306 | CHL  | 11      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | y     | 308 | CHL  | 14      | 0            |
| 40  | Y     | 318 | NEX  | 7       | 0            |
| 25  | g     | 603 | CLA  | 14      | 0            |
| 25  | r     | 610 | CLA  | 11      | 0            |
| 26  | C     | 518 | LHG  | 3       | 0            |
| 28  | K     | 101 | BCR  | 7       | 0            |
| 30  | B     | 623 | LMG  | 5       | 0            |
| 25  | G     | 612 | CLA  | 8       | 0            |
| 35  | c     | 516 | DGD  | 10      | 0            |
| 25  | S     | 311 | CLA  | 8       | 0            |
| 32  | n     | 620 | AJP  | 1       | 0            |
| 38  | F     | 101 | HEM  | 7       | 0            |
| 25  | c     | 504 | CLA  | 15      | 0            |
| 25  | d     | 401 | CLA  | 9       | 0            |
| 25  | C     | 503 | CLA  | 4       | 0            |
| 25  | b     | 610 | CLA  | 14      | 0            |
| 40  | G     | 617 | NEX  | 15      | 0            |
| 28  | A     | 406 | BCR  | 4       | 0            |
| 25  | N     | 602 | CLA  | 22      | 0            |
| 25  | 6     | 604 | CLA  | 19      | 0            |
| 24  | g     | 609 | CHL  | 10      | 0            |
| 25  | n     | 613 | CLA  | 28      | 0            |
| 25  | b     | 606 | CLA  | 16      | 0            |
| 25  | B     | 614 | CLA  | 12      | 0            |
| 24  | s     | 307 | CHL  | 7       | 0            |
| 25  | r     | 611 | CLA  | 4       | 0            |
| 29  | a     | 408 | SQD  | 6       | 0            |
| 25  | a     | 406 | CLA  | 9       | 0            |
| 35  | C     | 516 | DGD  | 10      | 0            |
| 26  | y     | 319 | LHG  | 8       | 0            |
| 30  | c     | 520 | LMG  | 4       | 0            |
| 25  | c     | 508 | CLA  | 12      | 0            |
| 25  | g     | 611 | CLA  | 14      | 0            |
| 25  | Y     | 314 | CLA  | 15      | 0            |
| 38  | f     | 101 | HEM  | 8       | 0            |
| 25  | C     | 512 | CLA  | 12      | 0            |
| 25  | C     | 506 | CLA  | 8       | 0            |
| 25  | B     | 613 | CLA  | 16      | 0            |
| 32  | N     | 620 | AJP  | 1       | 0            |
| 24  | N     | 607 | CHL  | 48      | 0            |
| 39  | n     | 615 | LUT  | 12      | 0            |
| 32  | Y     | 322 | AJP  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | D     | 406 | LHG  | 10      | 0            |
| 25  | S     | 304 | CLA  | 12      | 0            |
| 24  | Y     | 308 | CHL  | 17      | 0            |
| 24  | n     | 601 | CHL  | 16      | 0            |
| 25  | C     | 501 | CLA  | 18      | 0            |
| 28  | i     | 101 | BCR  | 20      | 0            |
| 25  | n     | 610 | CLA  | 33      | 0            |
| 28  | C     | 514 | BCR  | 7       | 0            |
| 25  | a     | 402 | CLA  | 19      | 0            |
| 24  | G     | 609 | CHL  | 10      | 0            |
| 25  | C     | 505 | CLA  | 10      | 0            |
| 25  | c     | 503 | CLA  | 5       | 0            |
| 25  | R     | 611 | CLA  | 3       | 0            |
| 25  | b     | 609 | CLA  | 11      | 0            |
| 25  | b     | 603 | CLA  | 6       | 0            |
| 25  | b     | 612 | CLA  | 7       | 0            |
| 39  | Y     | 316 | LUT  | 12      | 0            |
| 24  | r     | 606 | CHL  | 2       | 0            |
| 25  | d     | 403 | CLA  | 15      | 0            |
| 25  | n     | 611 | CLA  | 7       | 0            |
| 30  | b     | 620 | LMG  | 5       | 0            |
| 25  | s     | 313 | CLA  | 9       | 0            |
| 25  | G     | 613 | CLA  | 18      | 0            |
| 26  | n     | 618 | LHG  | 10      | 0            |
| 28  | I     | 101 | BCR  | 20      | 0            |
| 25  | r     | 601 | CLA  | 17      | 0            |
| 33  | A     | 413 | BCT  | 2       | 0            |
| 25  | y     | 315 | CLA  | 17      | 0            |
| 35  | b     | 626 | DGD  | 6       | 0            |
| 25  | N     | 611 | CLA  | 7       | 0            |
| 25  | s     | 304 | CLA  | 12      | 0            |
| 24  | y     | 310 | CHL  | 18      | 0            |
| 26  | y     | 301 | LHG  | 12      | 0            |
| 28  | B     | 619 | BCR  | 4       | 0            |
| 28  | B     | 618 | BCR  | 7       | 0            |
| 25  | g     | 613 | CLA  | 17      | 0            |
| 26  | s     | 318 | LHG  | 6       | 0            |
| 24  | r     | 607 | CHL  | 9       | 0            |
| 25  | 6     | 605 | CLA  | 8       | 0            |
| 25  | y     | 314 | CLA  | 17      | 0            |
| 25  | y     | 305 | CLA  | 4       | 0            |
| 25  | C     | 502 | CLA  | 12      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | r     | 605 | CHL  | 9       | 0            |
| 28  | T     | 101 | BCR  | 20      | 0            |
| 25  | B     | 605 | CLA  | 7       | 0            |
| 26  | C     | 517 | LHG  | 3       | 0            |
| 25  | c     | 510 | CLA  | 24      | 0            |
| 25  | N     | 603 | CLA  | 33      | 0            |
| 39  | R     | 615 | LUT  | 6       | 0            |
| 25  | c     | 506 | CLA  | 10      | 0            |
| 24  | l     | 301 | CHL  | 9       | 0            |
| 24  | 5     | 301 | CHL  | 9       | 0            |
| 25  | d     | 402 | CLA  | 19      | 0            |
| 26  | c     | 518 | LHG  | 3       | 0            |
| 25  | b     | 601 | CLA  | 9       | 0            |
| 24  | y     | 302 | CHL  | 31      | 0            |
| 25  | R     | 610 | CLA  | 11      | 0            |
| 24  | y     | 306 | CHL  | 5       | 0            |
| 25  | r     | 603 | CLA  | 17      | 0            |
| 25  | c     | 501 | CLA  | 19      | 0            |
| 25  | s     | 309 | CLA  | 3       | 0            |
| 32  | s     | 319 | AJP  | 2       | 0            |
| 25  | A     | 401 | CLA  | 19      | 0            |
| 28  | b     | 617 | BCR  | 7       | 0            |
| 25  | D     | 403 | CLA  | 15      | 0            |
| 25  | c     | 513 | CLA  | 17      | 0            |
| 24  | y     | 309 | CHL  | 14      | 0            |
| 28  | c     | 514 | BCR  | 7       | 0            |
| 24  | R     | 607 | CHL  | 9       | 0            |
| 26  | B     | 621 | LHG  | 3       | 0            |
| 25  | y     | 311 | CLA  | 24      | 0            |
| 25  | s     | 310 | CLA  | 15      | 0            |
| 25  | y     | 303 | CLA  | 24      | 0            |
| 39  | Y     | 317 | LUT  | 13      | 0            |
| 25  | b     | 615 | CLA  | 16      | 0            |
| 24  | G     | 606 | CHL  | 19      | 0            |
| 25  | N     | 610 | CLA  | 34      | 0            |
| 24  | g     | 606 | CHL  | 19      | 0            |
| 24  | 5     | 302 | CHL  | 8       | 0            |
| 35  | c     | 515 | DGD  | 7       | 0            |
| 26  | C     | 519 | LHG  | 4       | 0            |
| 26  | Y     | 319 | LHG  | 7       | 0            |
| 25  | G     | 614 | CLA  | 5       | 0            |
| 25  | R     | 601 | CLA  | 15      | 0            |

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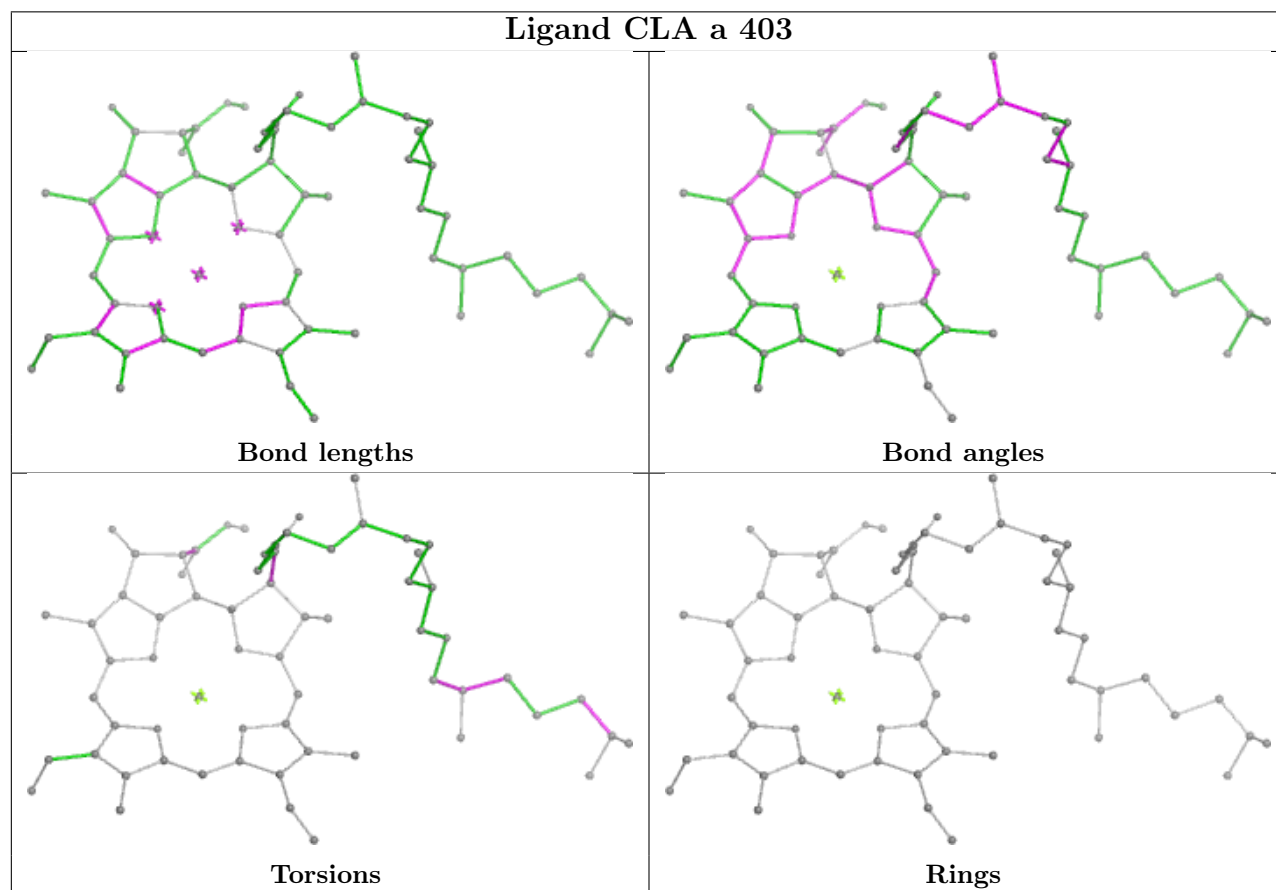
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | B     | 607 | CLA  | 15      | 0            |
| 39  | n     | 616 | LUT  | 15      | 0            |
| 32  | y     | 320 | AJP  | 3       | 0            |
| 40  | s     | 317 | NEX  | 5       | 0            |
| 28  | D     | 404 | BCR  | 3       | 0            |
| 26  | N     | 618 | LHG  | 11      | 0            |
| 25  | C     | 504 | CLA  | 14      | 0            |
| 24  | G     | 608 | CHL  | 19      | 0            |
| 24  | g     | 601 | CHL  | 15      | 0            |
| 28  | z     | 101 | BCR  | 5       | 0            |
| 24  | y     | 307 | CHL  | 15      | 0            |
| 25  | r     | 612 | CLA  | 19      | 0            |
| 25  | b     | 608 | CLA  | 9       | 0            |
| 28  | h     | 101 | BCR  | 8       | 0            |
| 25  | b     | 614 | CLA  | 10      | 0            |
| 24  | G     | 605 | CHL  | 4       | 0            |
| 28  | H     | 101 | BCR  | 6       | 0            |
| 39  | G     | 616 | LUT  | 15      | 0            |
| 26  | c     | 517 | LHG  | 3       | 0            |
| 25  | s     | 311 | CLA  | 9       | 0            |
| 25  | r     | 602 | CLA  | 14      | 0            |
| 39  | g     | 616 | LUT  | 15      | 0            |
| 26  | b     | 621 | LHG  | 3       | 0            |
| 25  | s     | 312 | CLA  | 10      | 0            |
| 25  | Y     | 303 | CLA  | 26      | 0            |
| 25  | 6     | 602 | CLA  | 10      | 0            |
| 24  | 2     | 603 | CHL  | 21      | 0            |
| 25  | N     | 613 | CLA  | 30      | 0            |
| 25  | b     | 602 | CLA  | 9       | 0            |
| 25  | r     | 604 | CLA  | 10      | 0            |
| 26  | Y     | 301 | LHG  | 13      | 0            |
| 25  | R     | 603 | CLA  | 17      | 0            |
| 25  | B     | 603 | CLA  | 6       | 0            |
| 30  | a     | 409 | LMG  | 3       | 0            |
| 25  | R     | 608 | CLA  | 18      | 0            |
| 25  | S     | 305 | CLA  | 14      | 0            |
| 25  | r     | 614 | CLA  | 13      | 0            |
| 25  | G     | 604 | CLA  | 12      | 0            |
| 25  | b     | 604 | CLA  | 14      | 0            |
| 25  | b     | 607 | CLA  | 14      | 0            |
| 25  | y     | 312 | CLA  | 11      | 0            |
| 26  | S     | 301 | LHG  | 8       | 0            |

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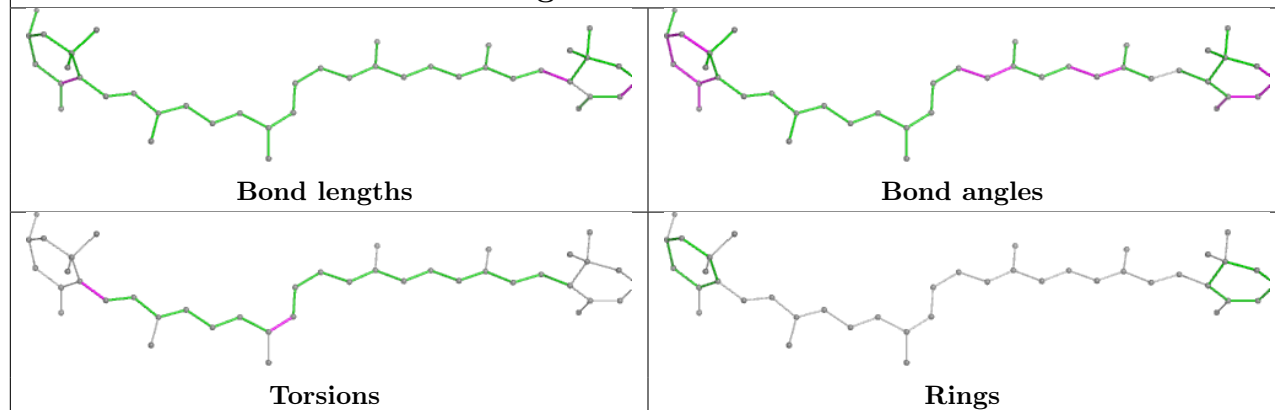
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27  | A     | 403 | PHO  | 13      | 0            |
| 32  | Y     | 321 | AJP  | 2       | 0            |
| 25  | b     | 605 | CLA  | 9       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

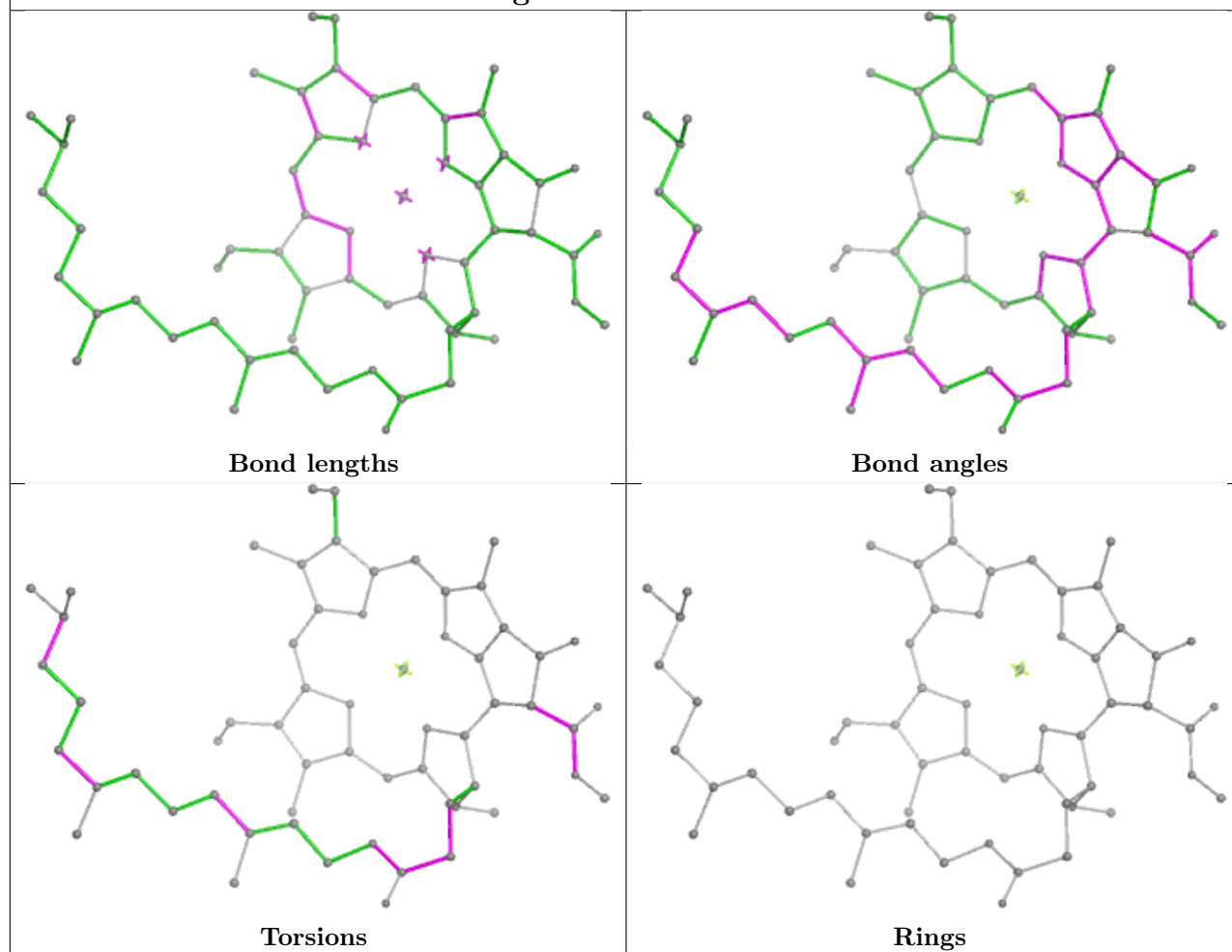




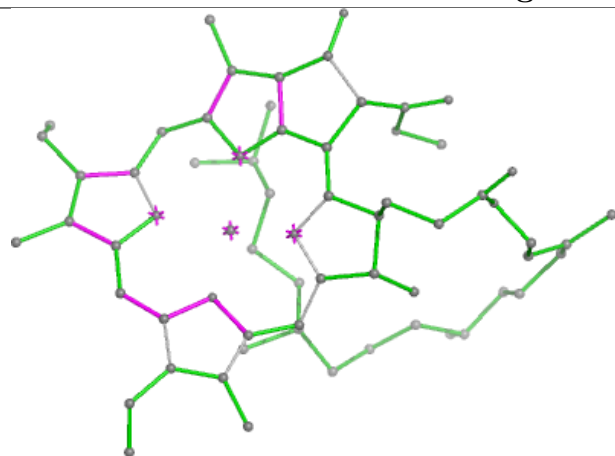
## Ligand LUT r 615



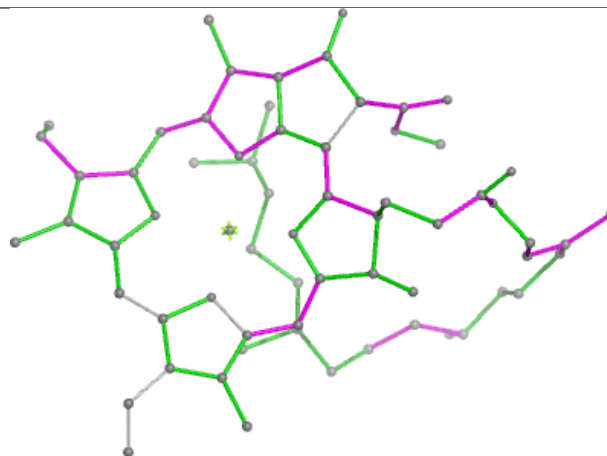
## Ligand CLA R 602



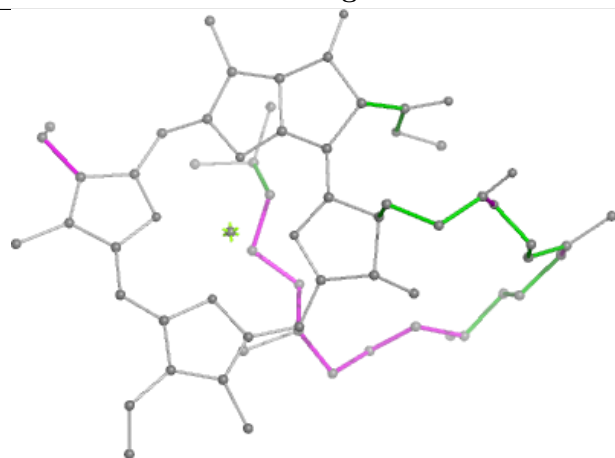
## Ligand CLA C 510



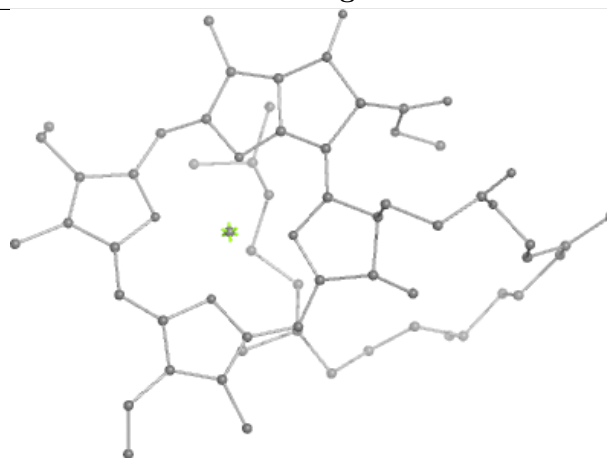
Bond lengths



Bond angles

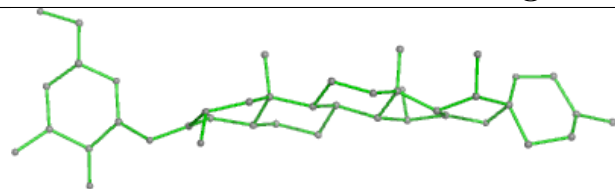


Torsions

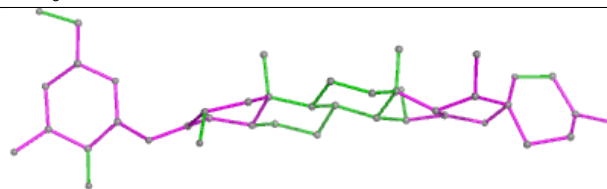


Rings

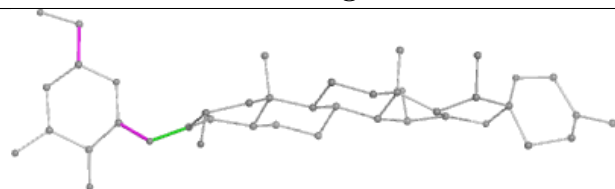
## Ligand AJP y 322



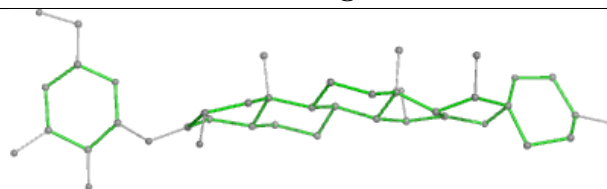
Bond lengths



Bond angles

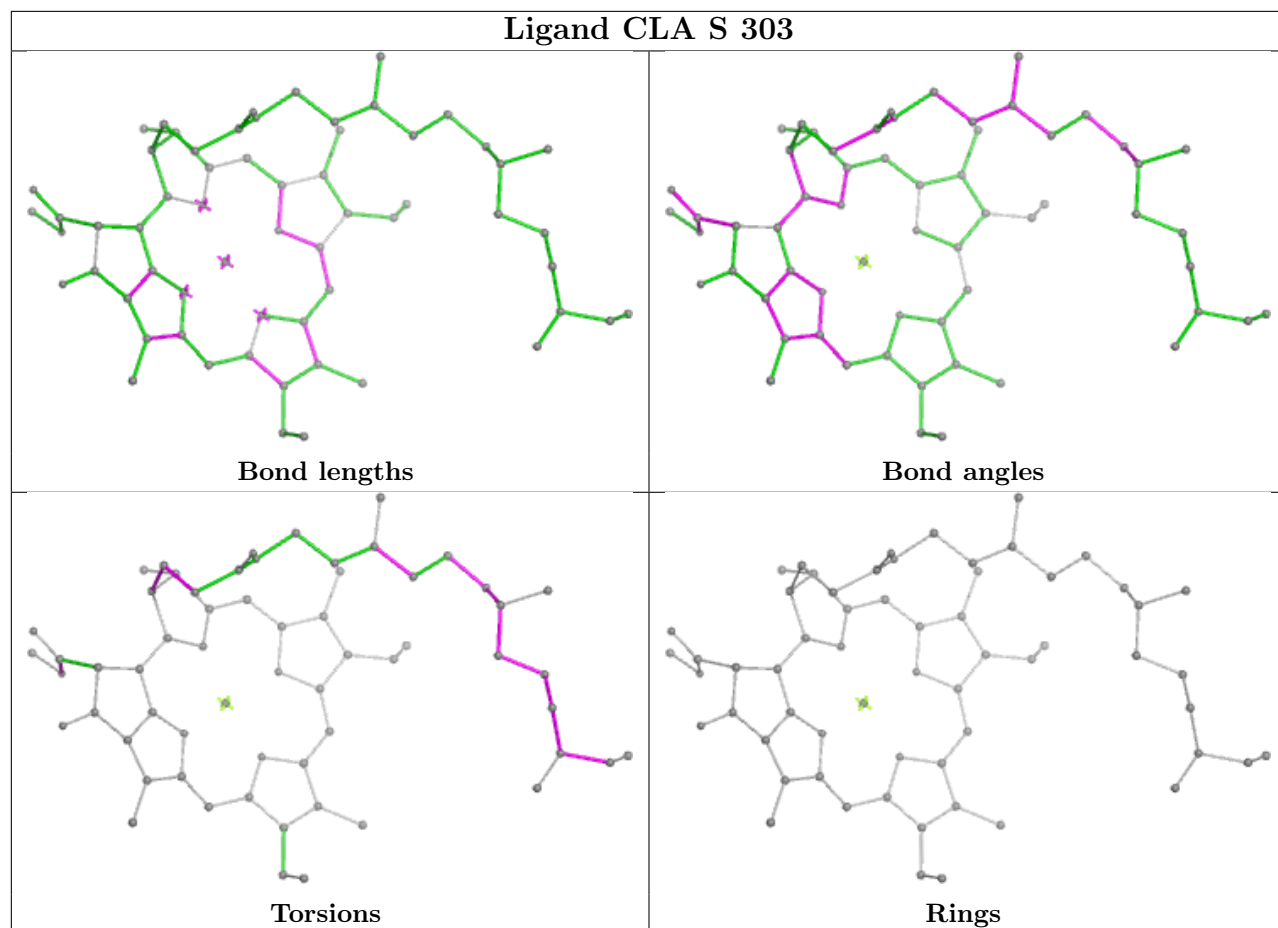


Torsions

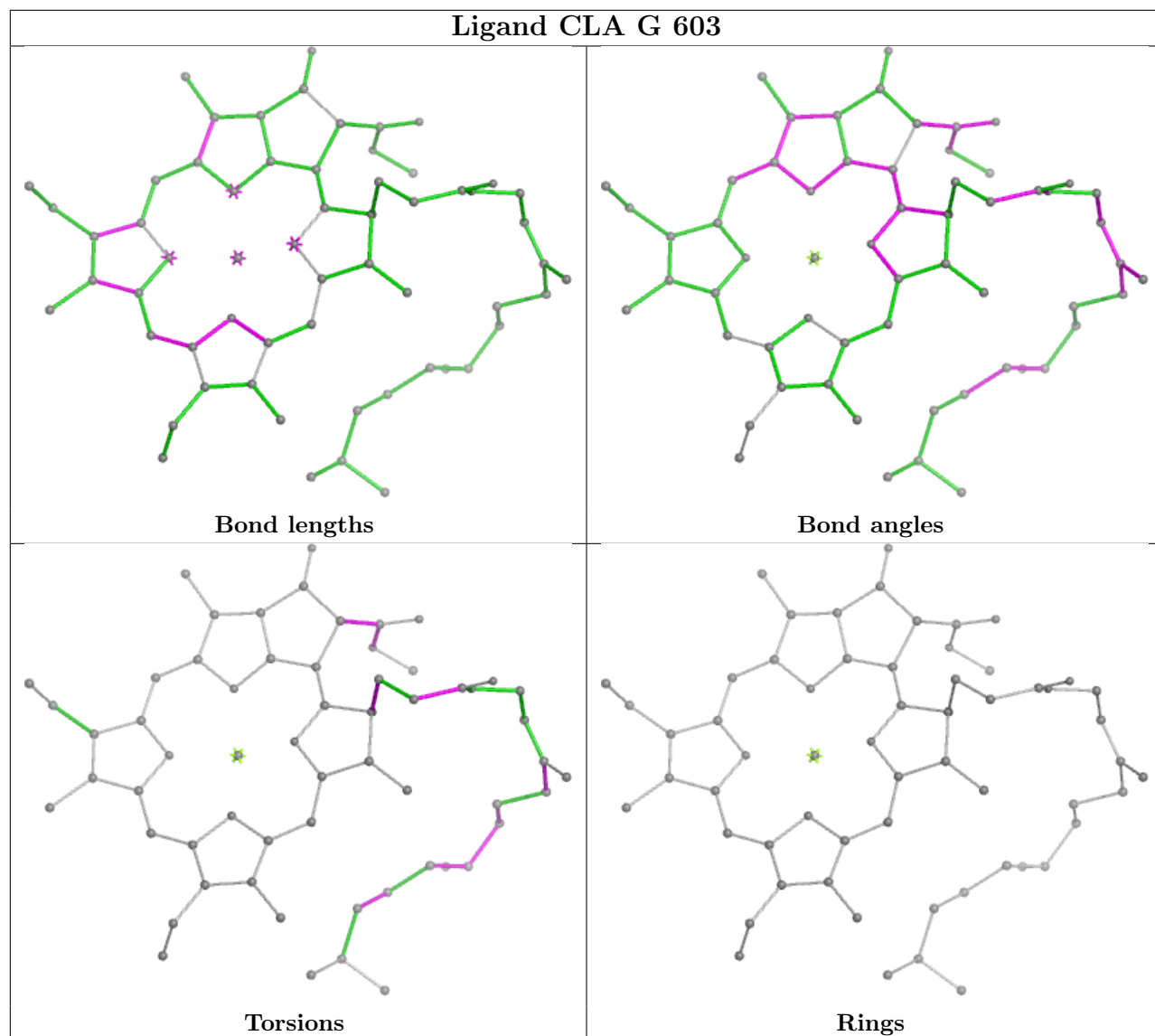


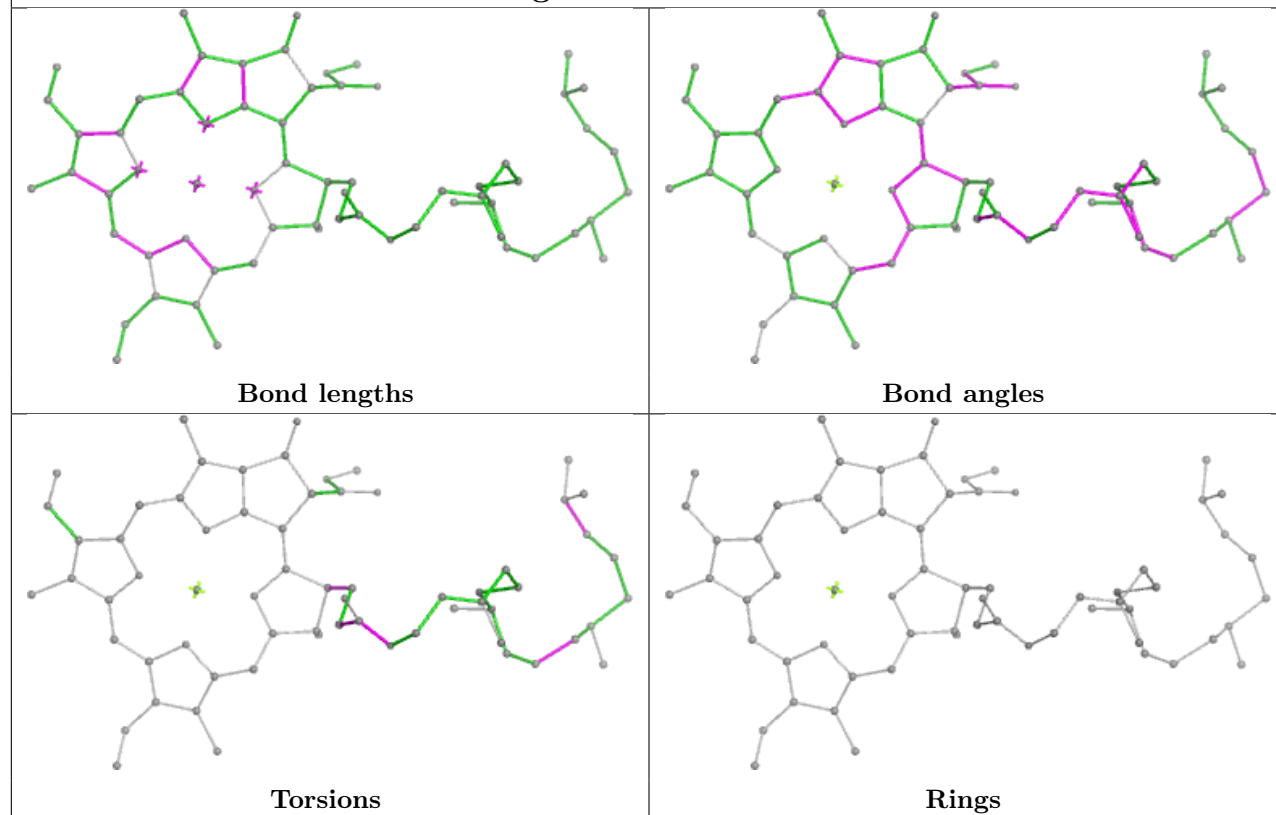
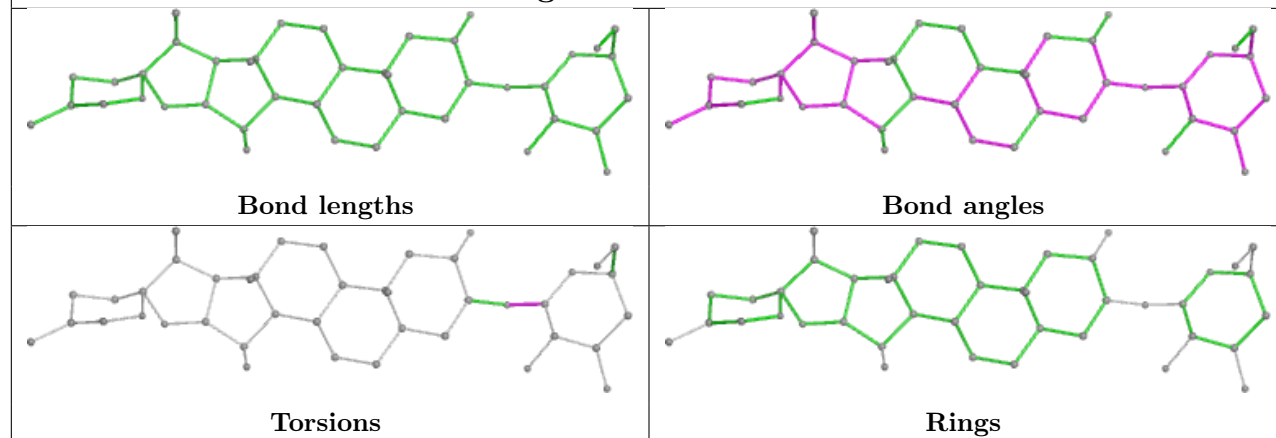
Rings

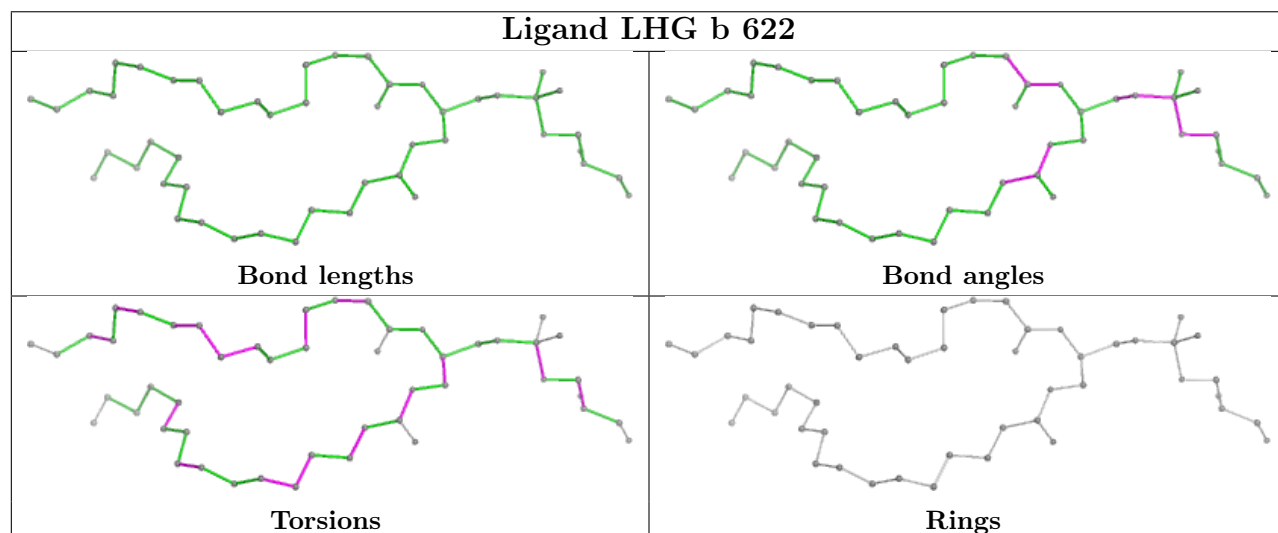
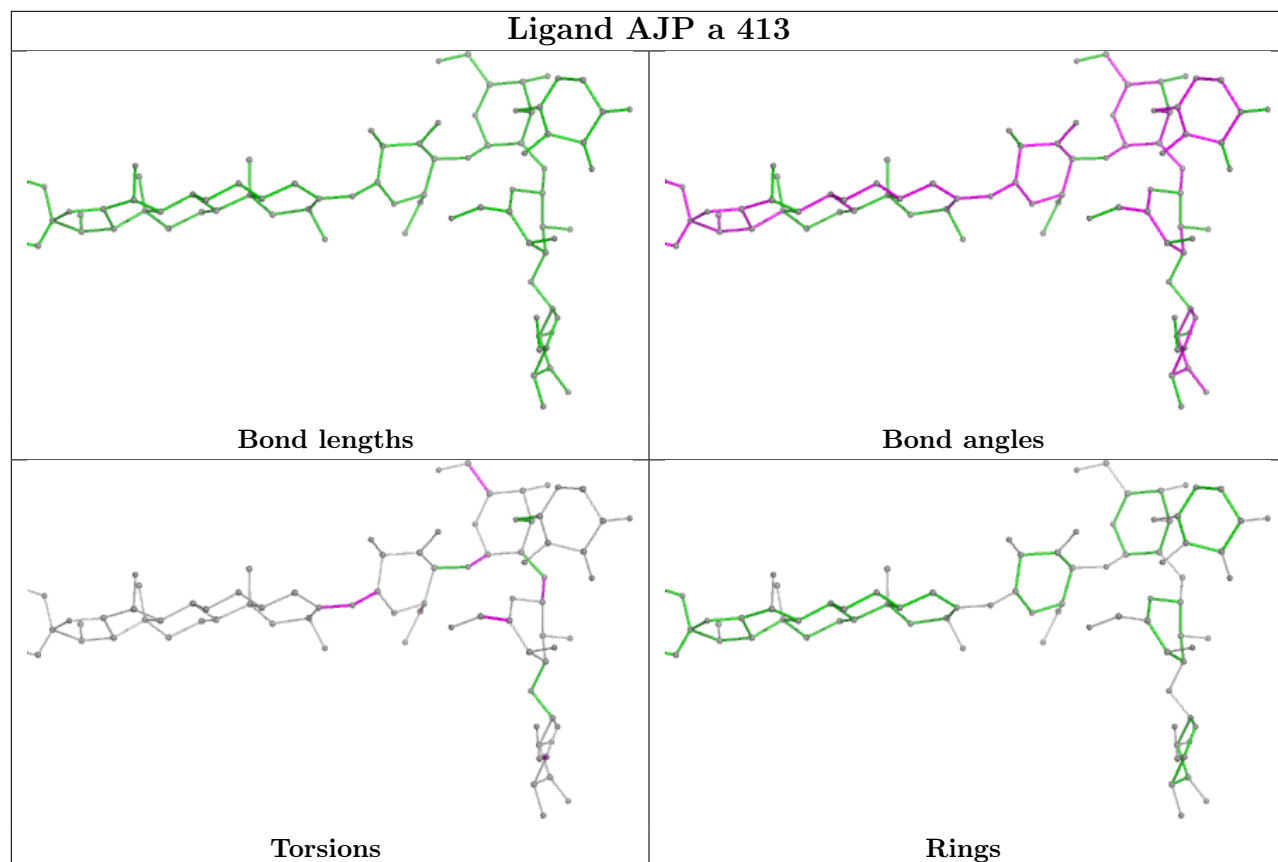
## Ligand CLA S 303

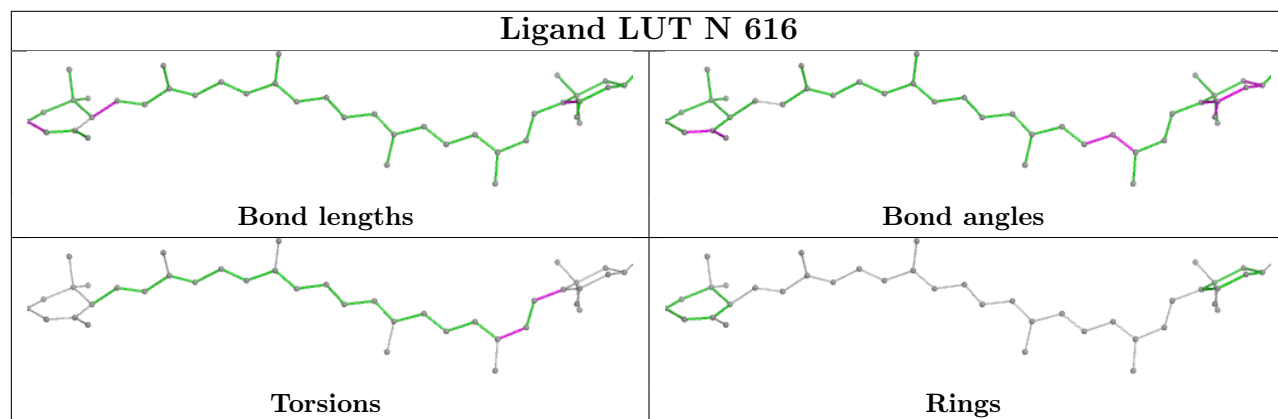
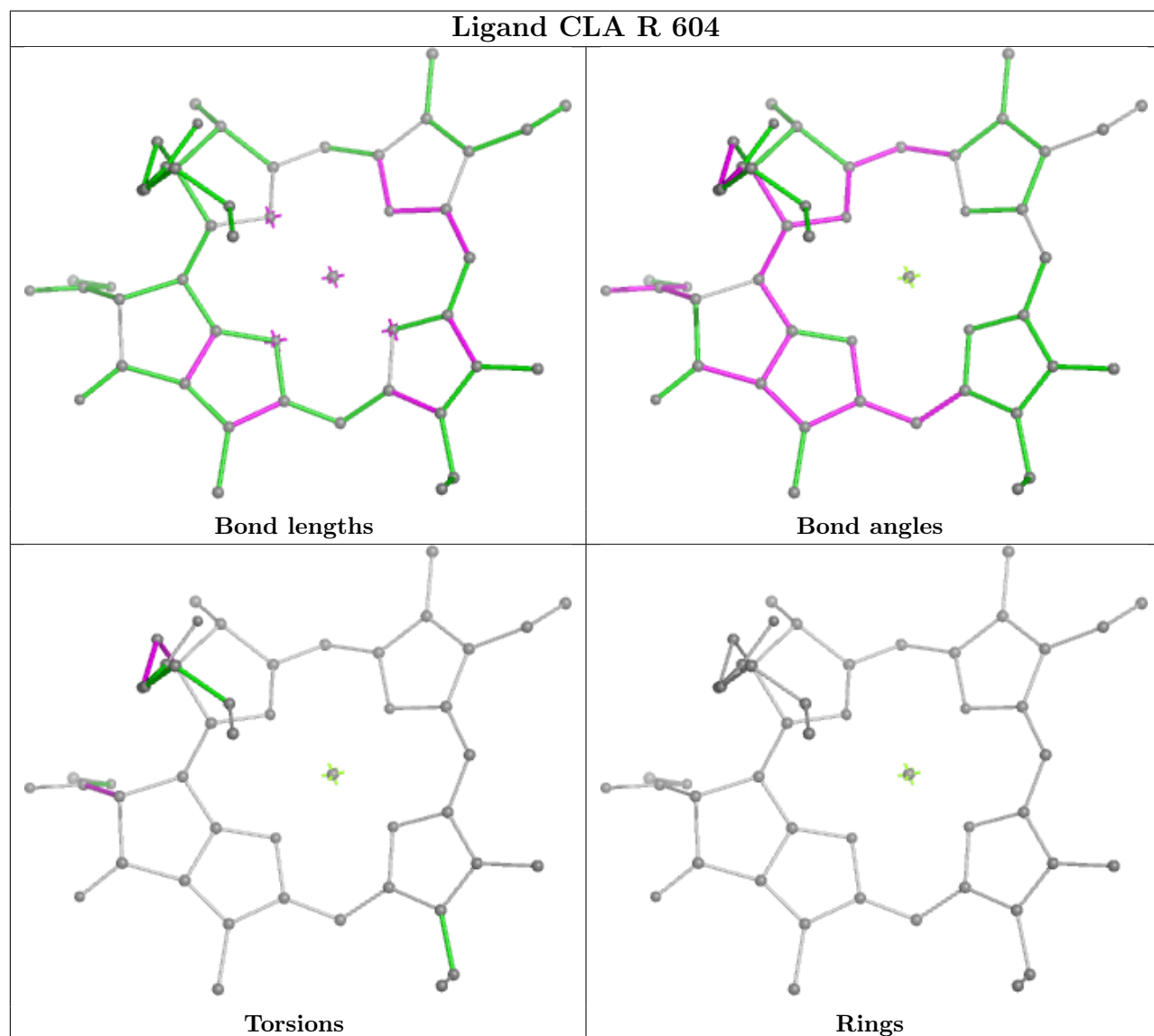


## Ligand CLA G 603

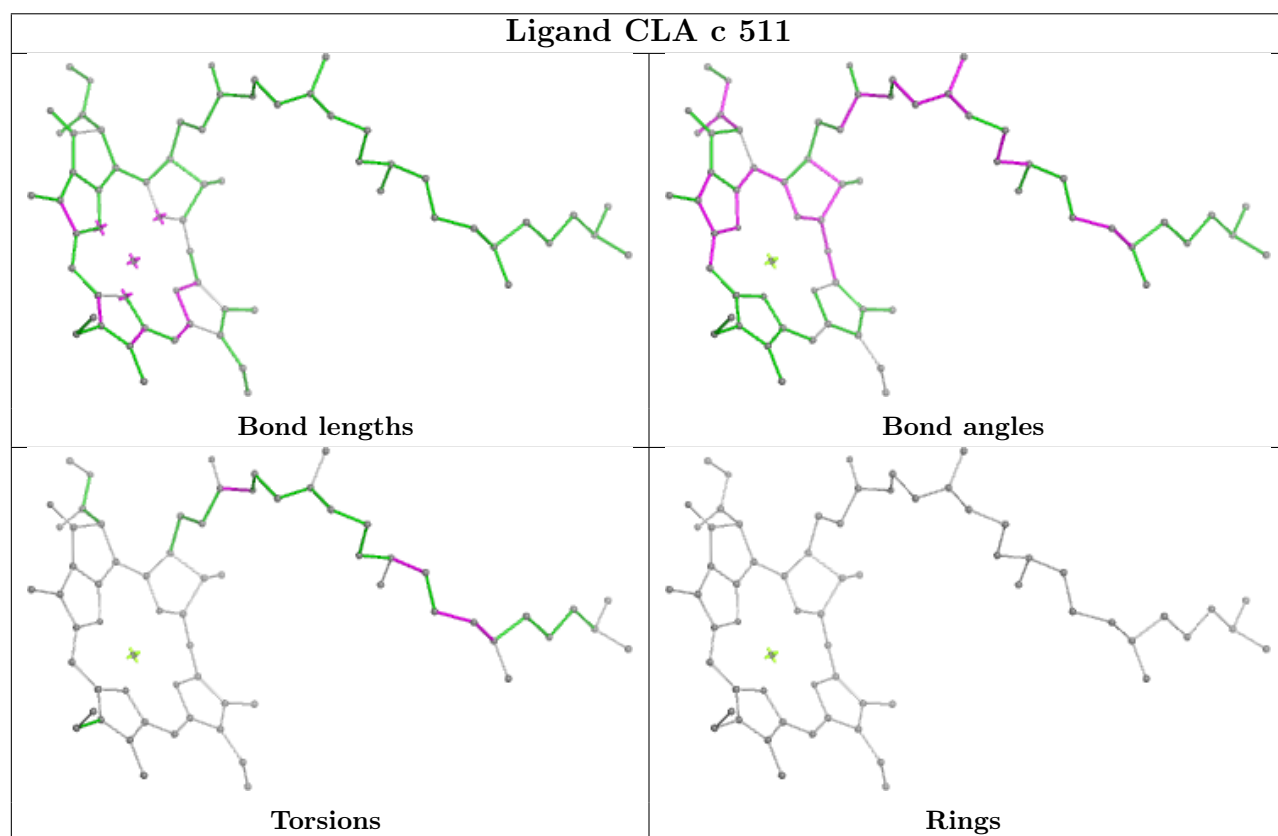
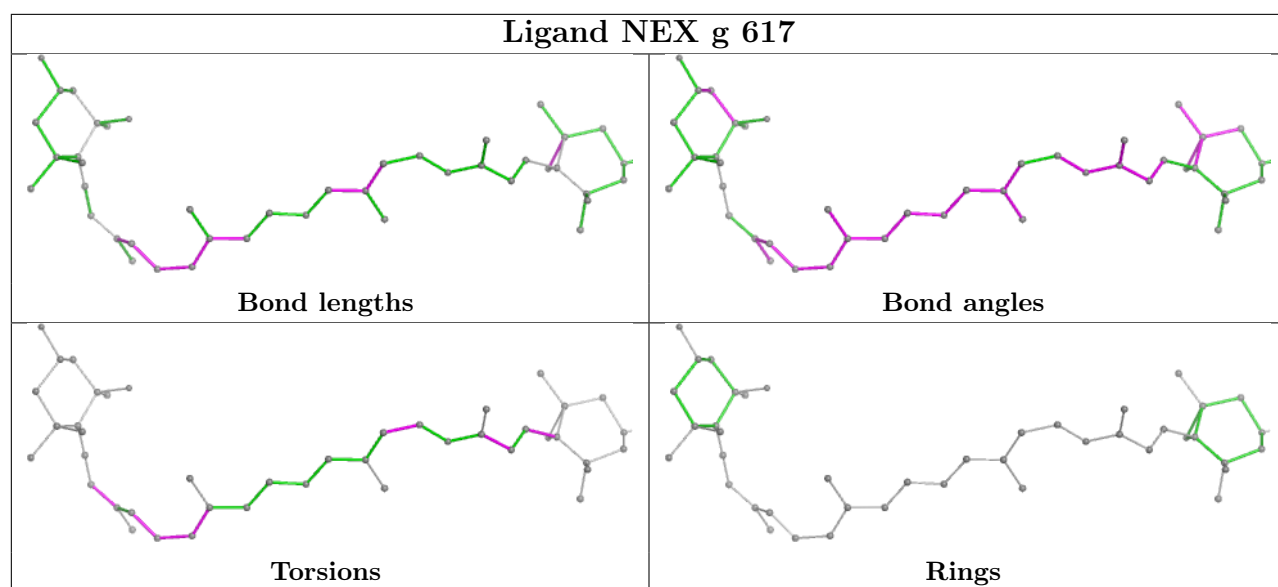


**Ligand CLA B 612****Ligand AJP n 619**

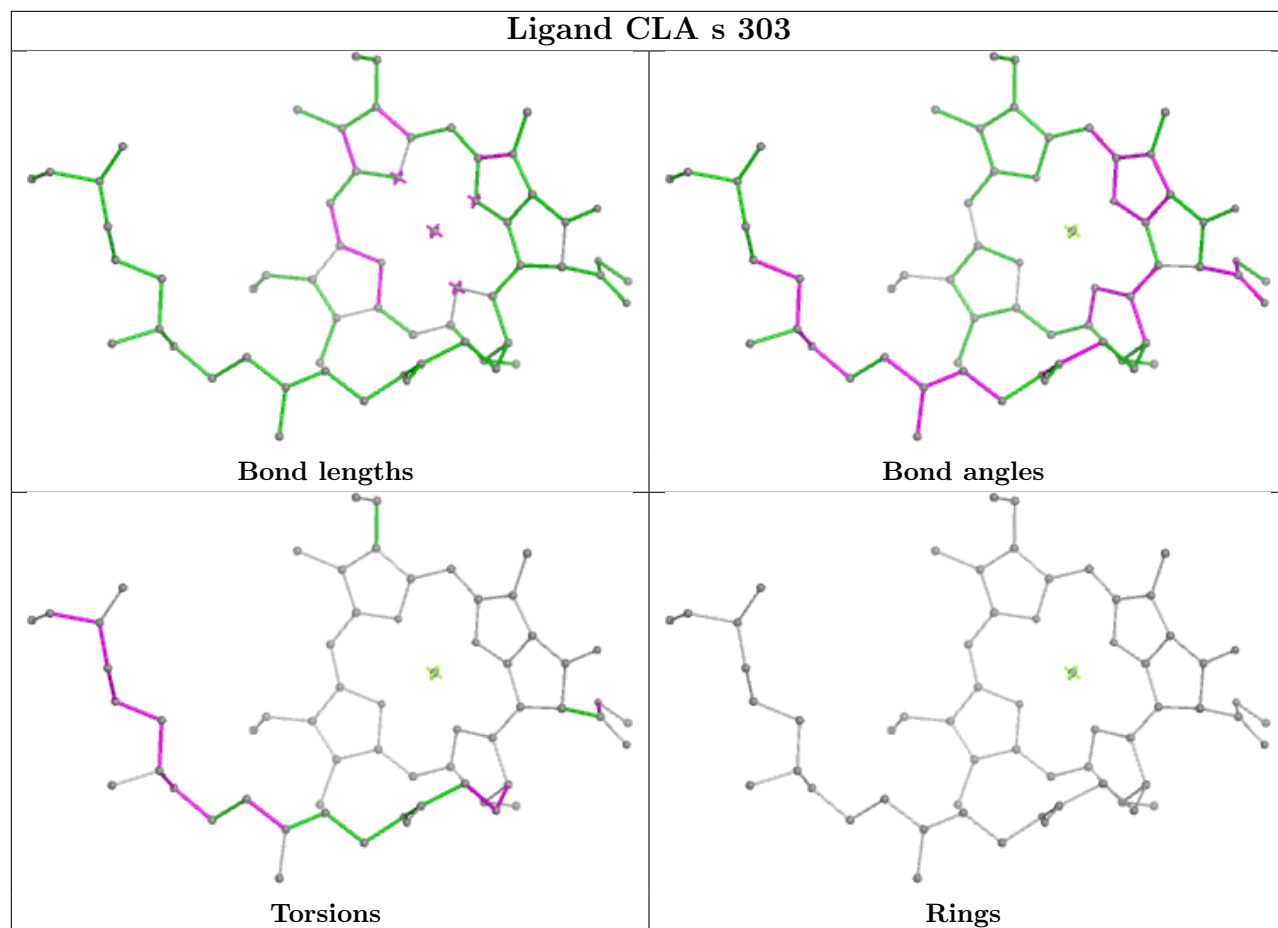


**Ligand LUT N 616****Ligand CLA R 604**

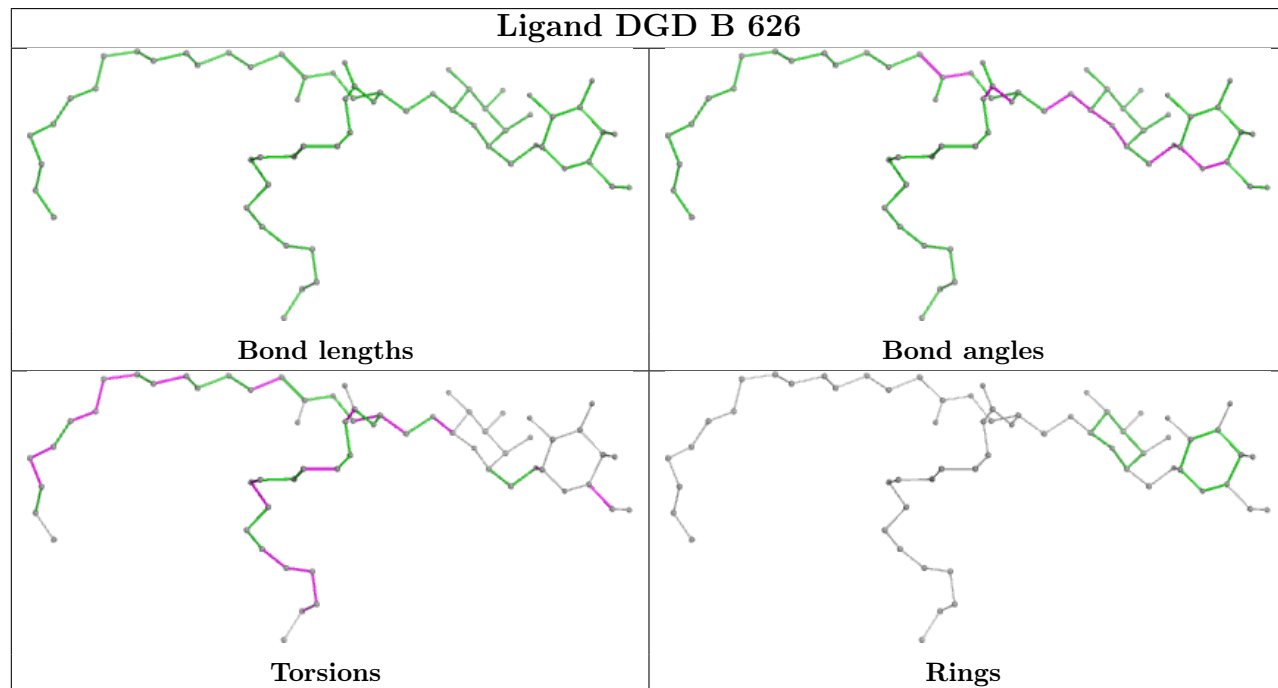


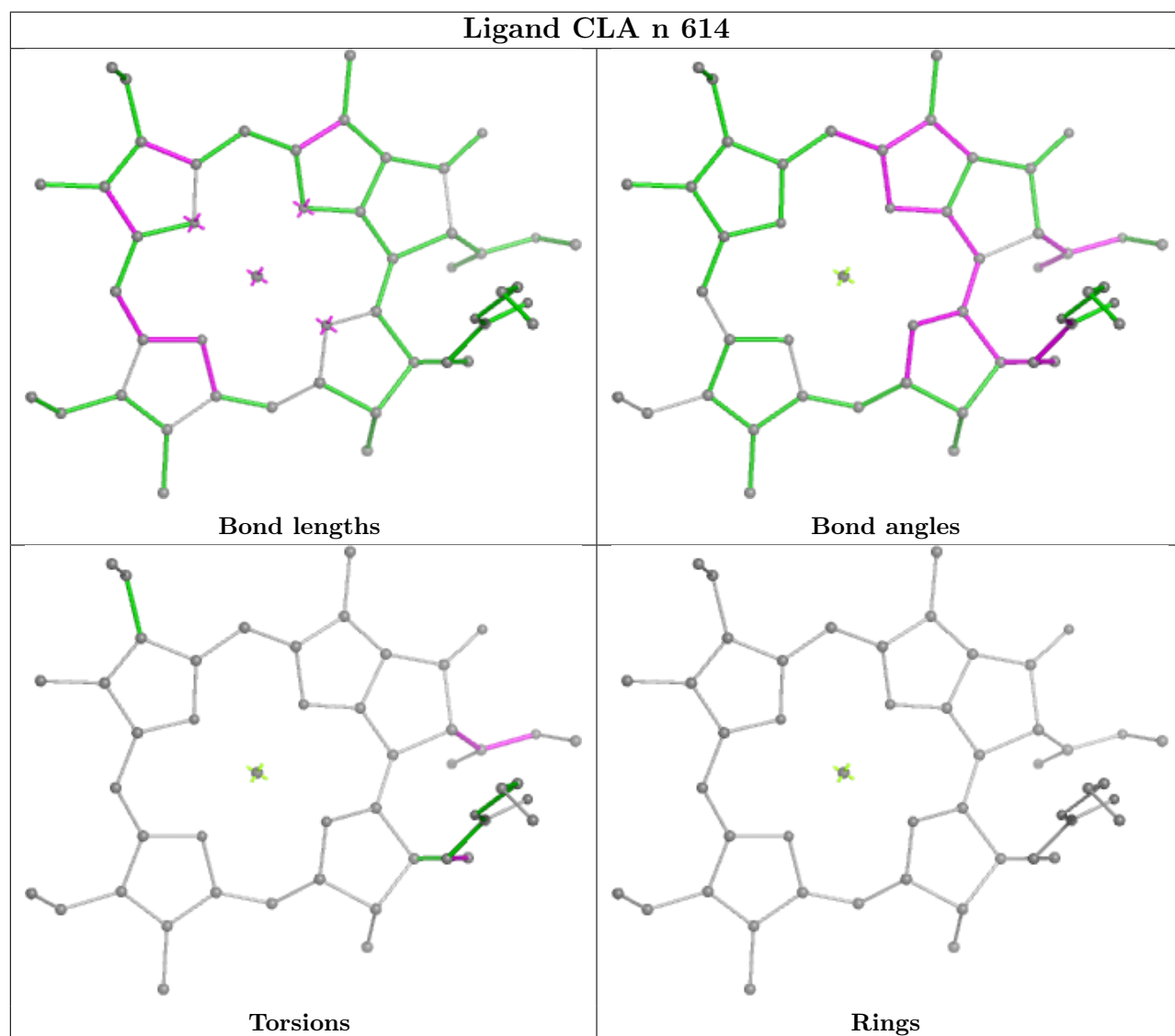
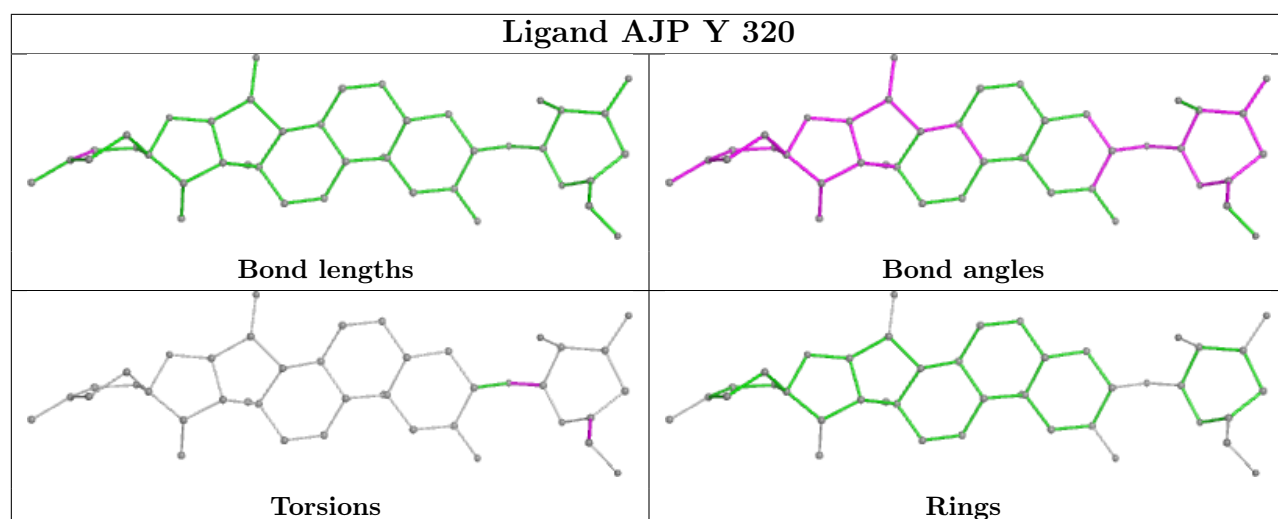


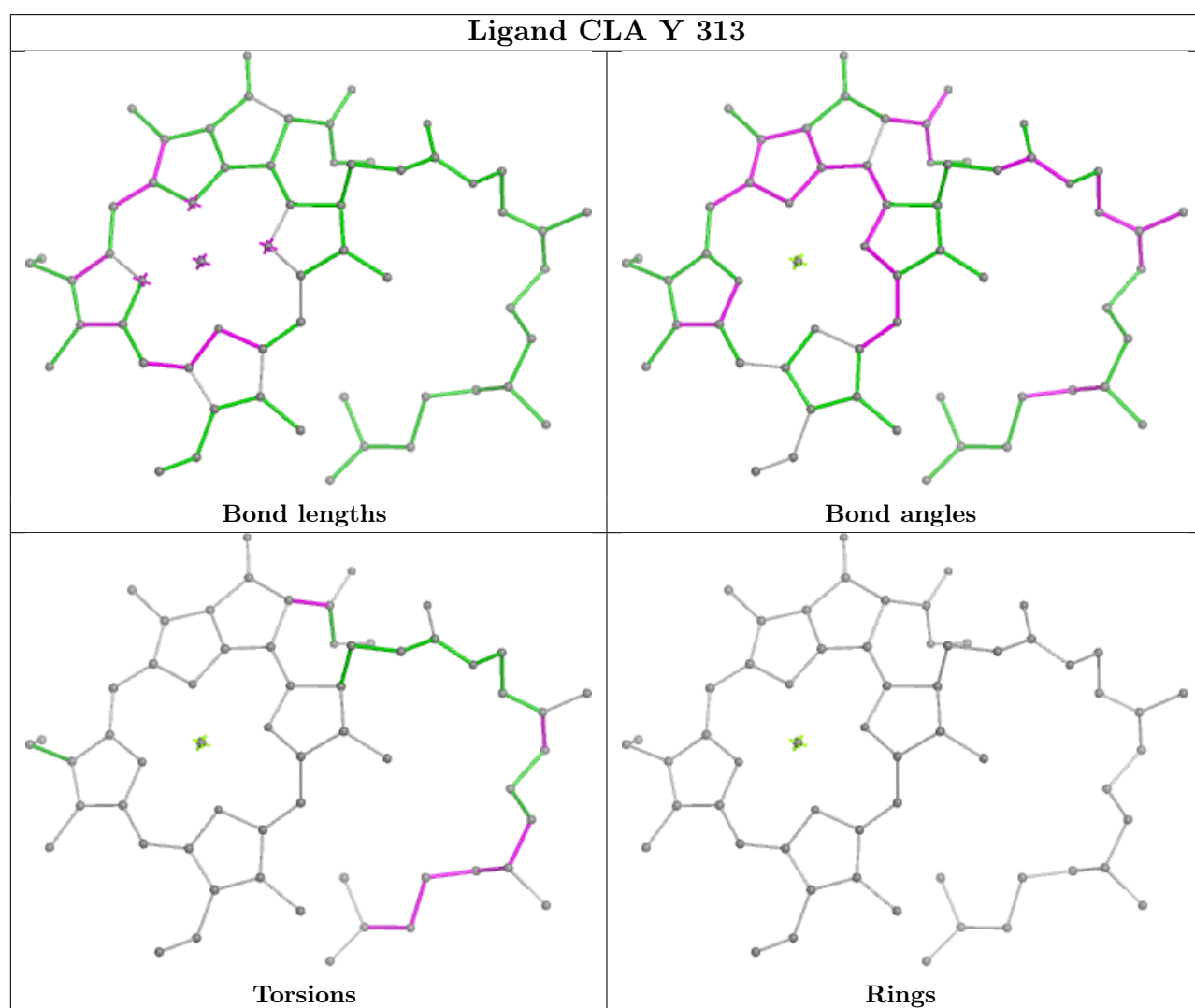
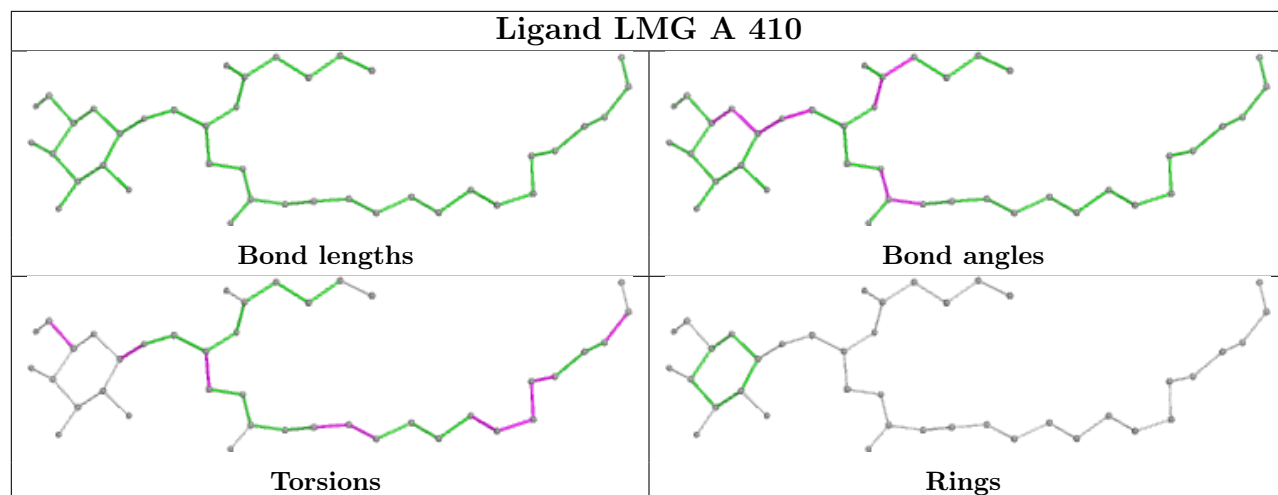
## Ligand CLA s 303

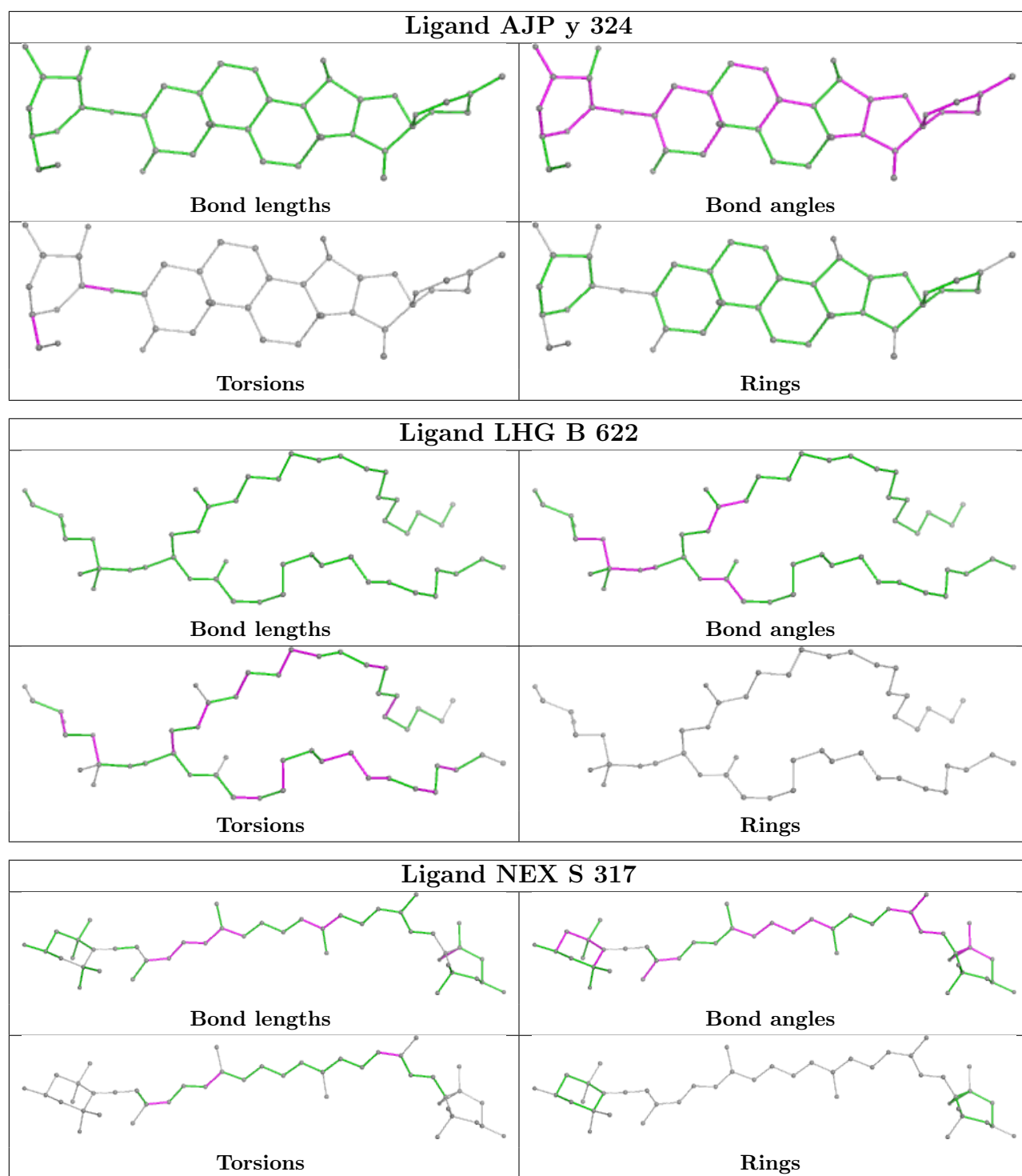


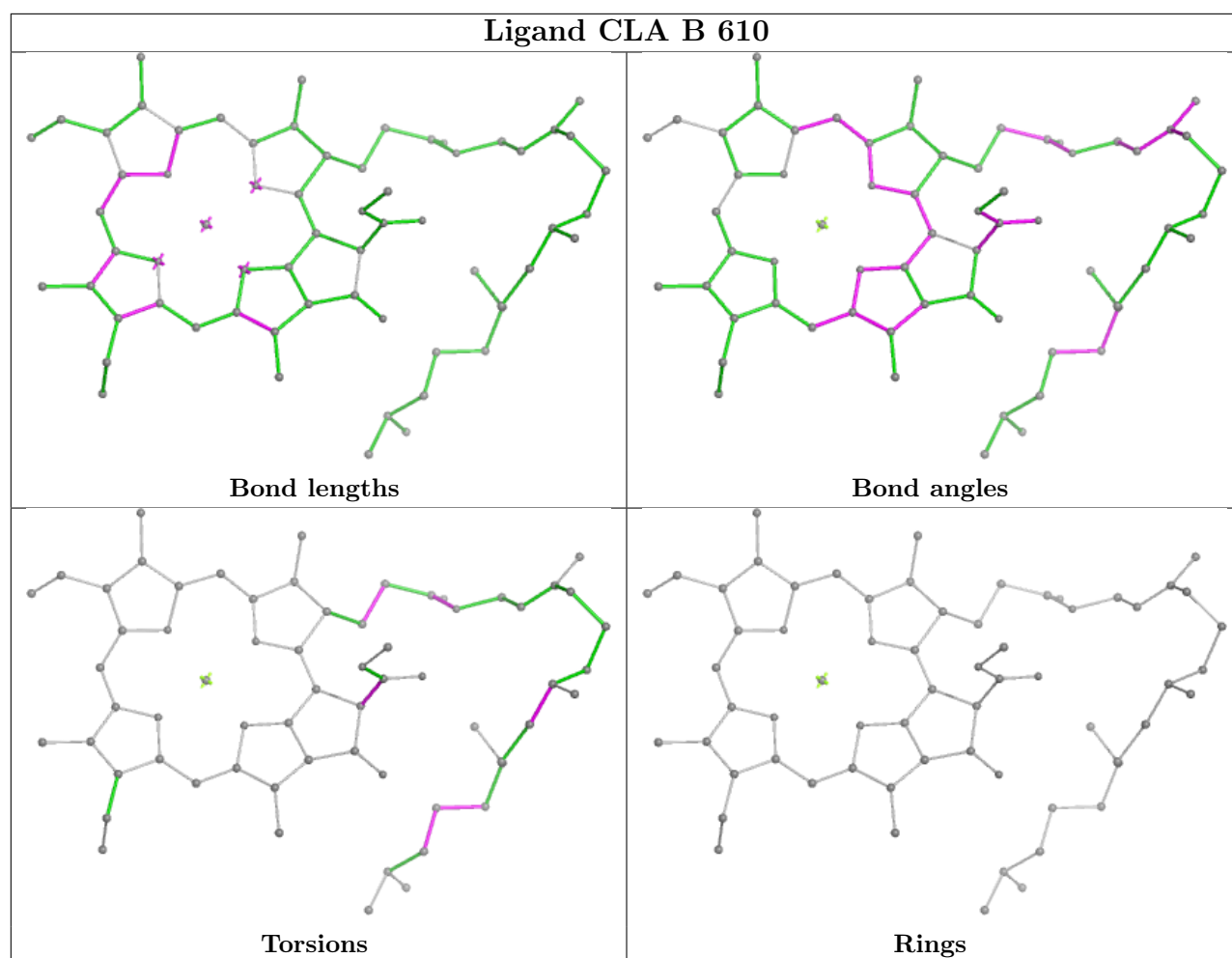
## Ligand DGD B 626

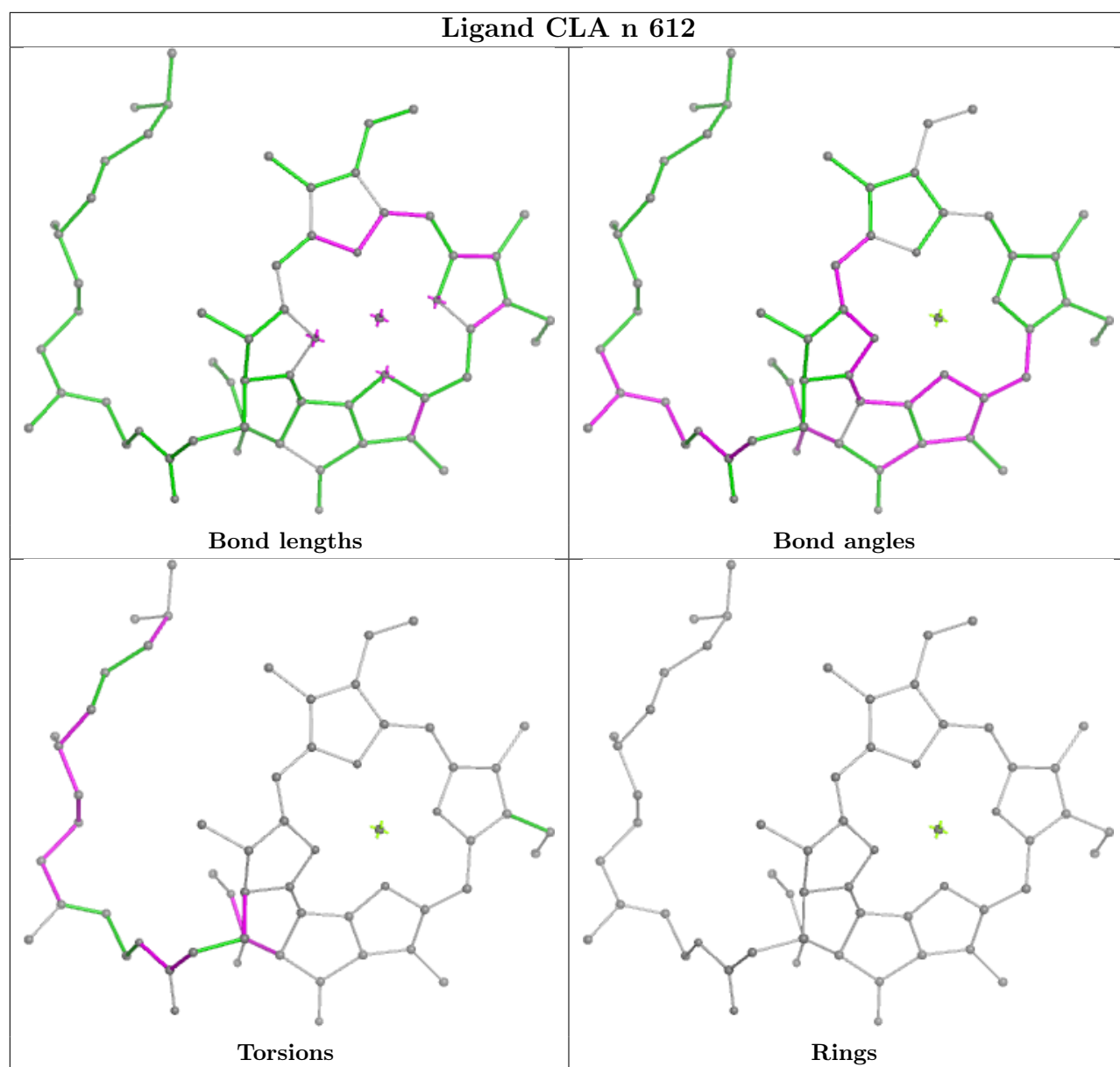




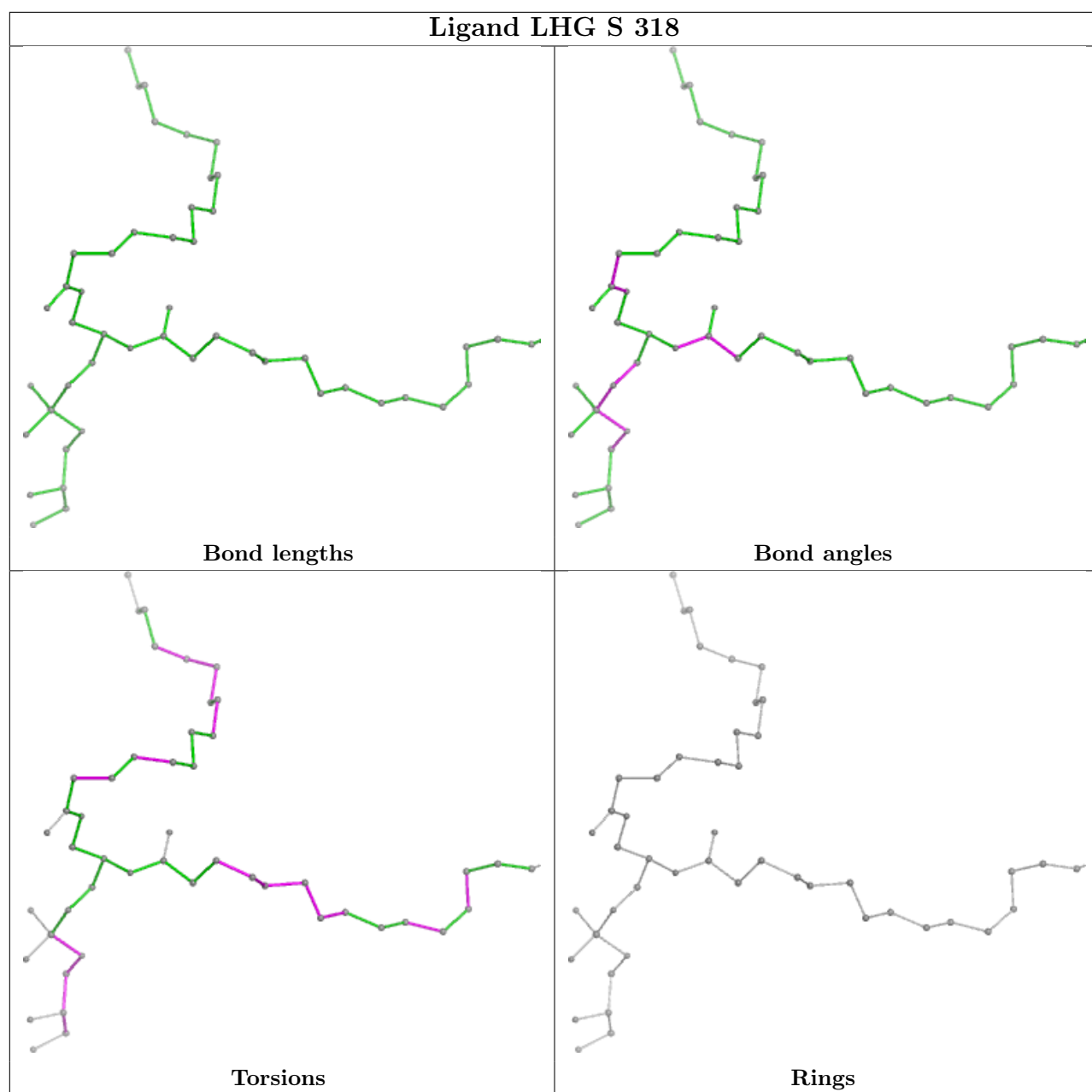


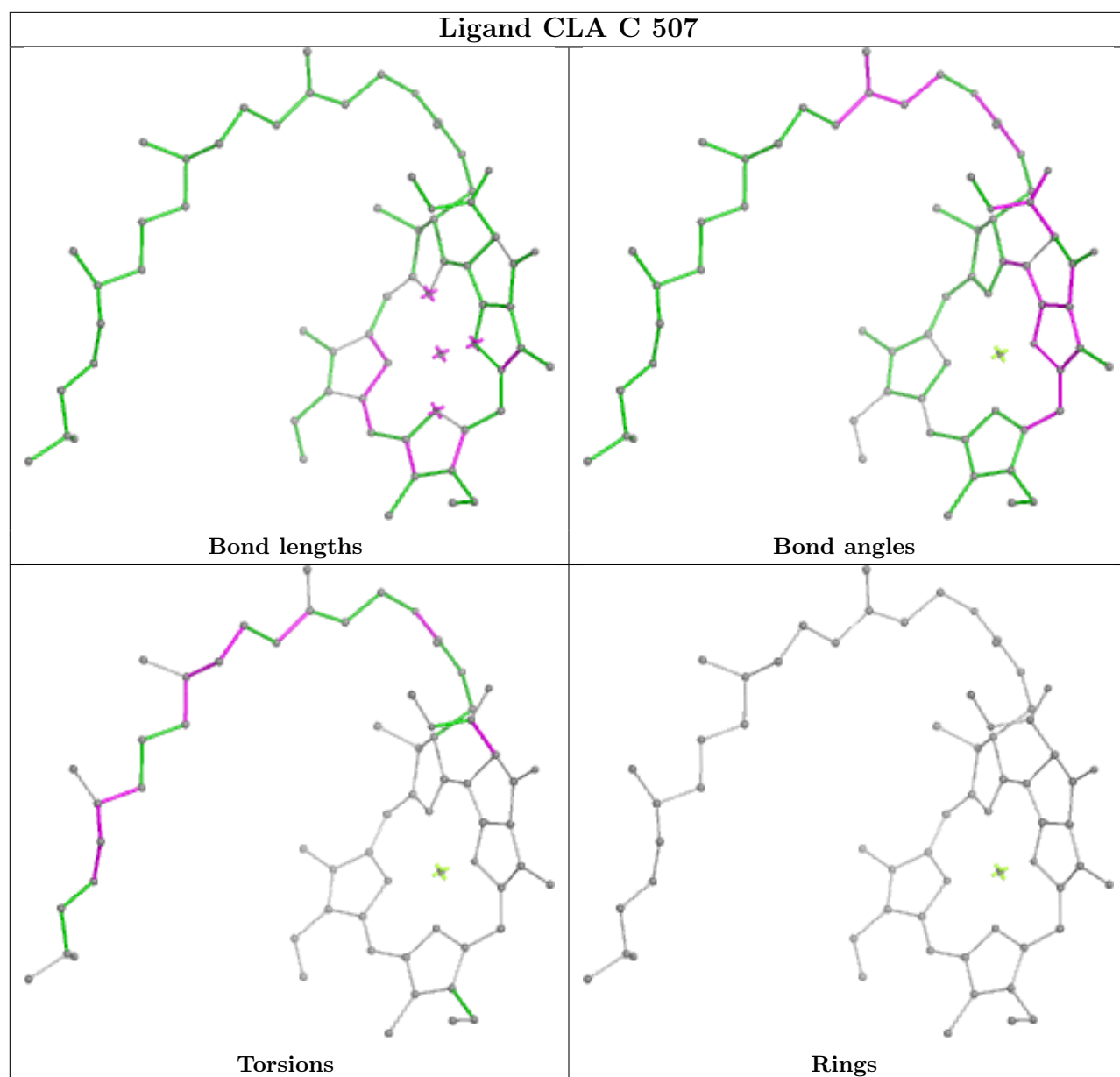


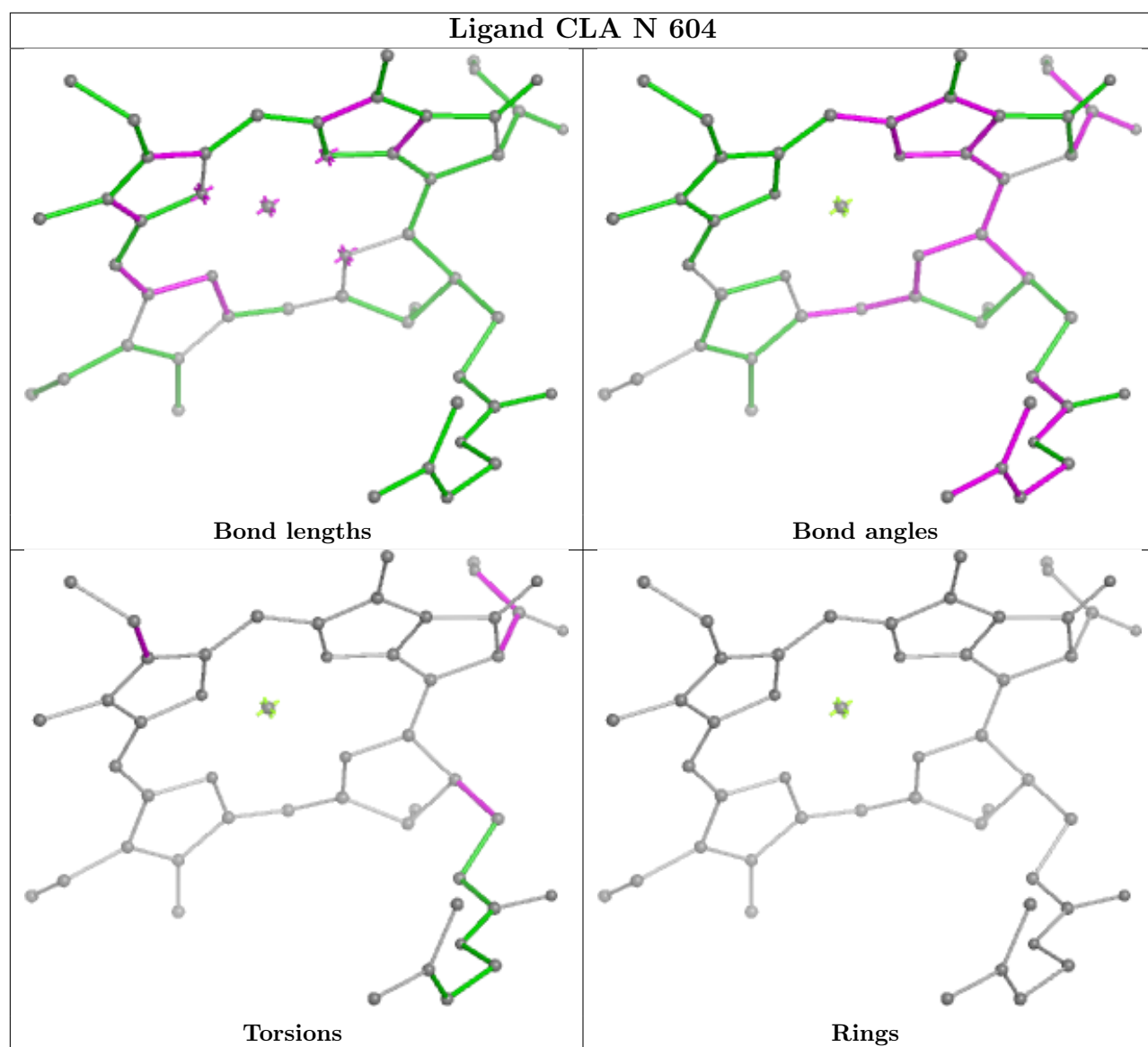


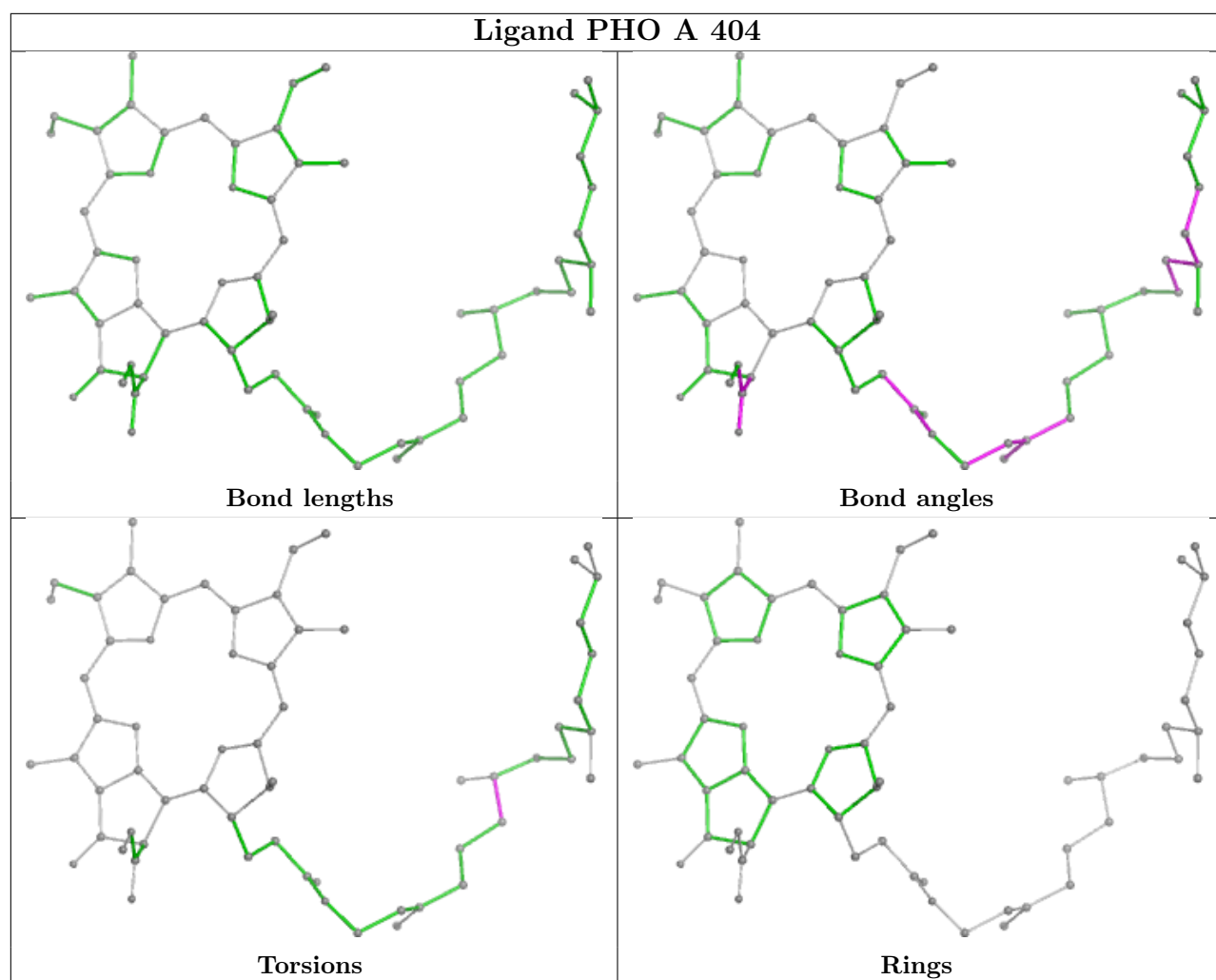


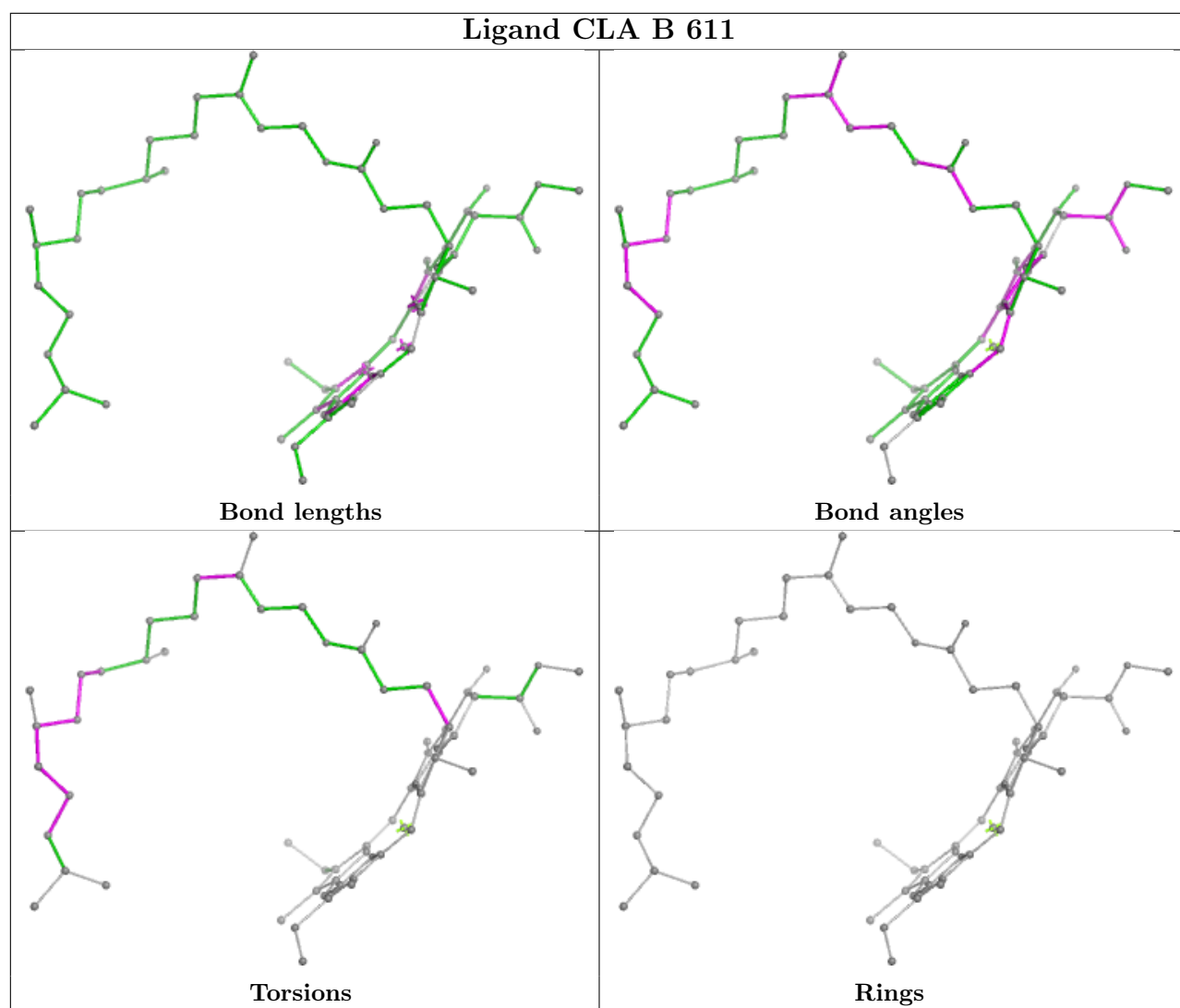




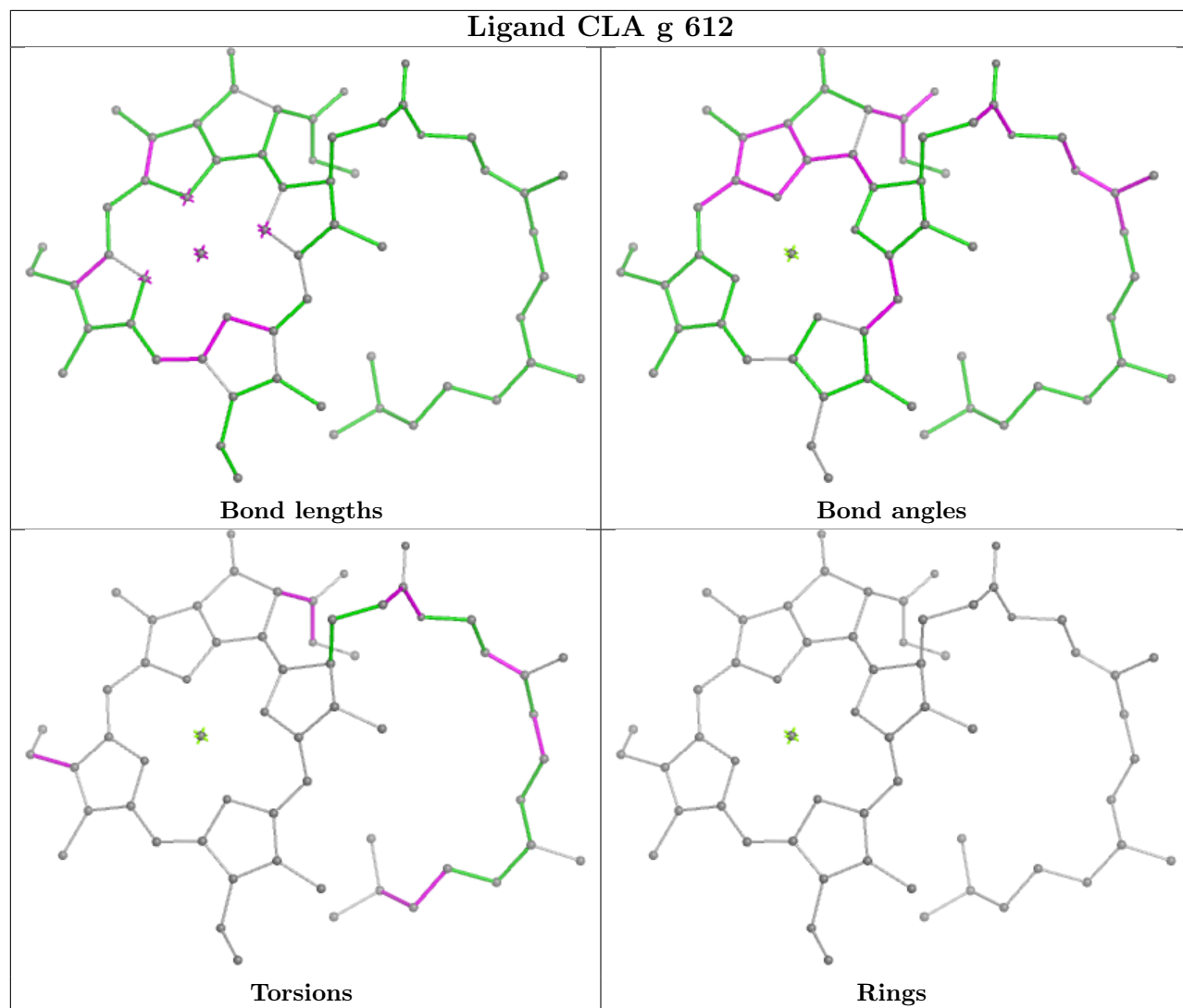


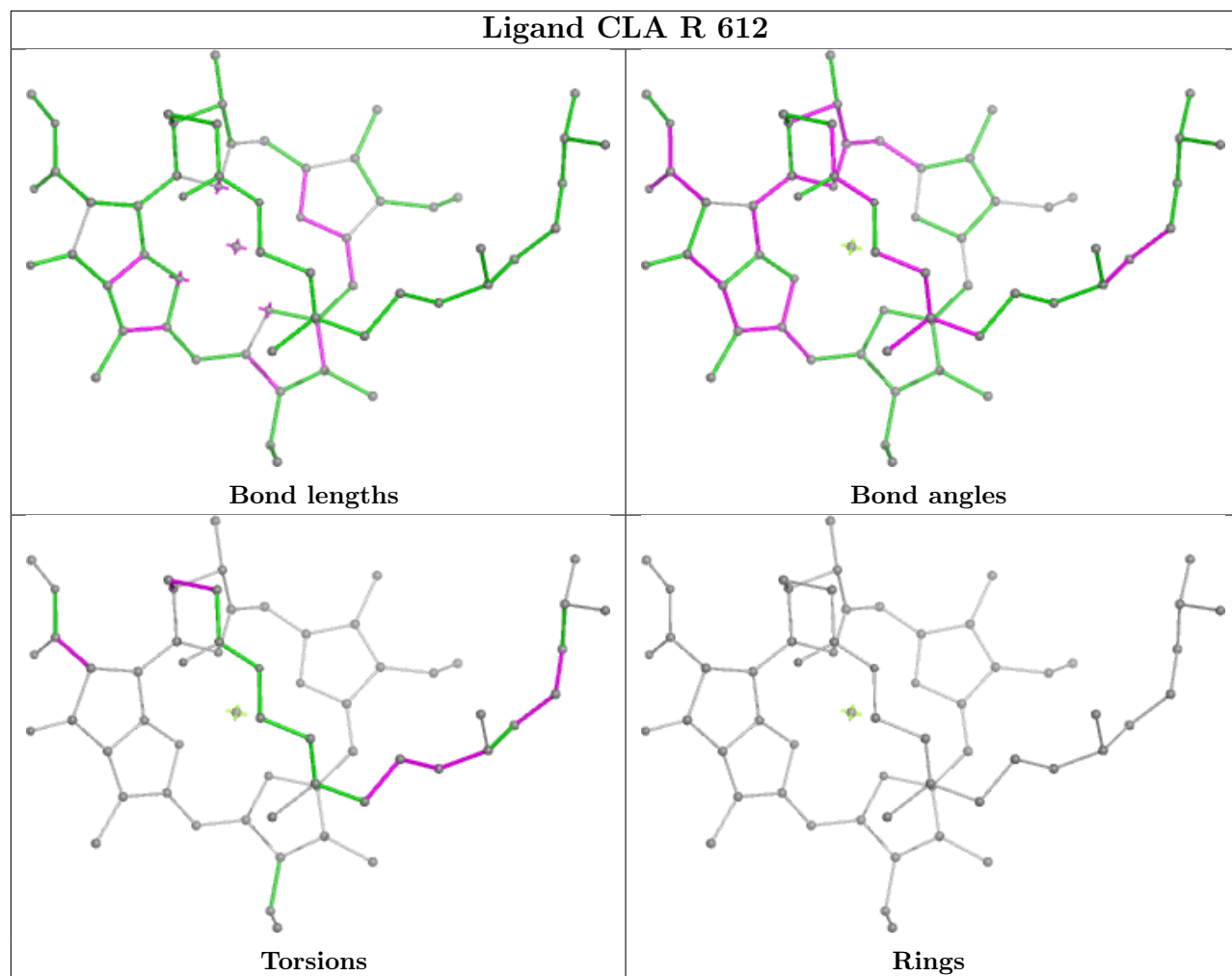




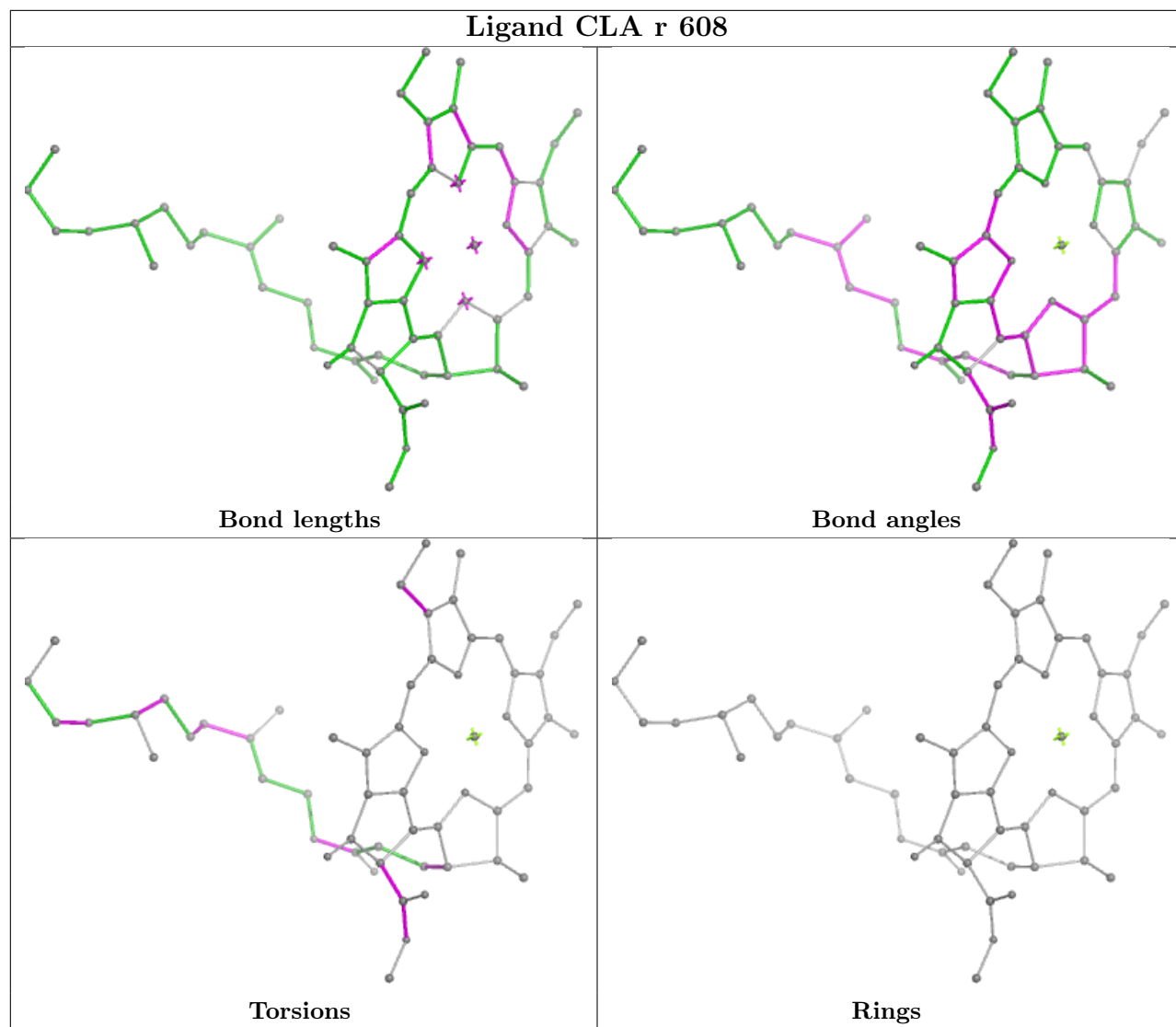


## Ligand CLA g 612

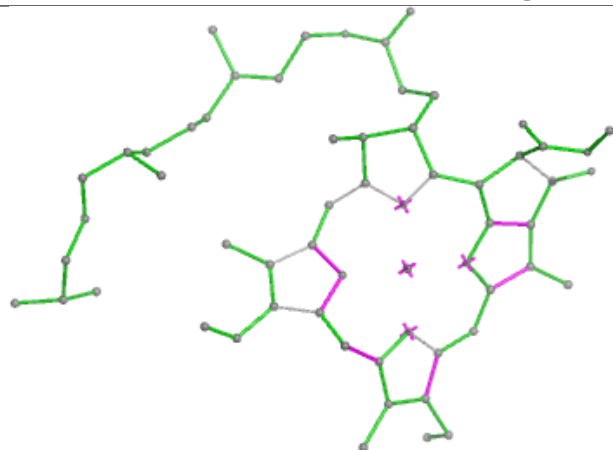




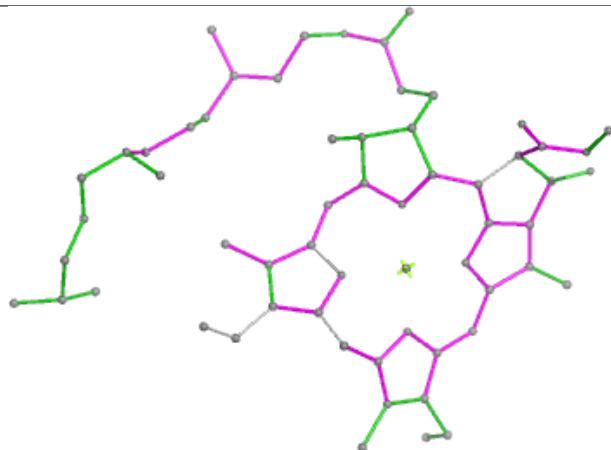




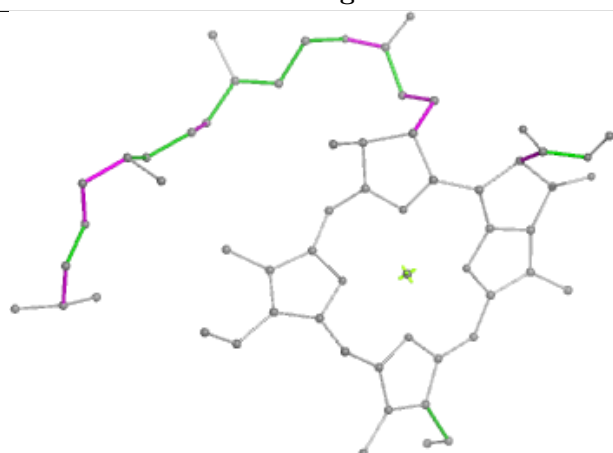
## Ligand CLA 2 602



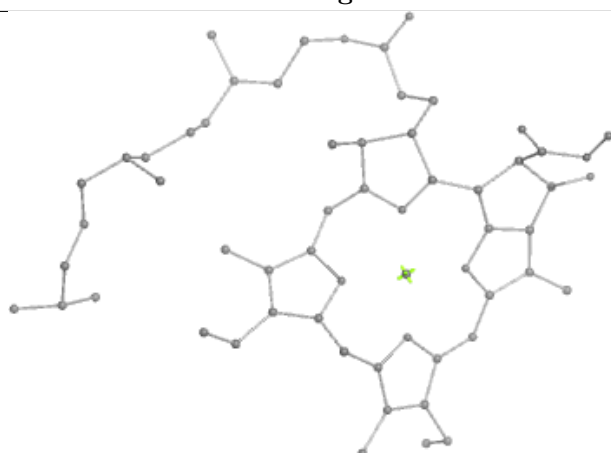
Bond lengths



Bond angles

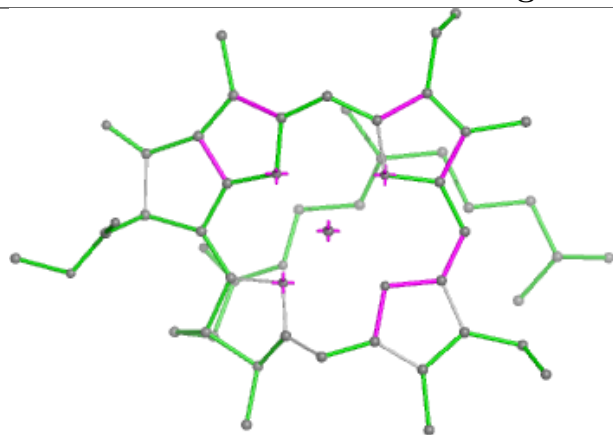


Torsions

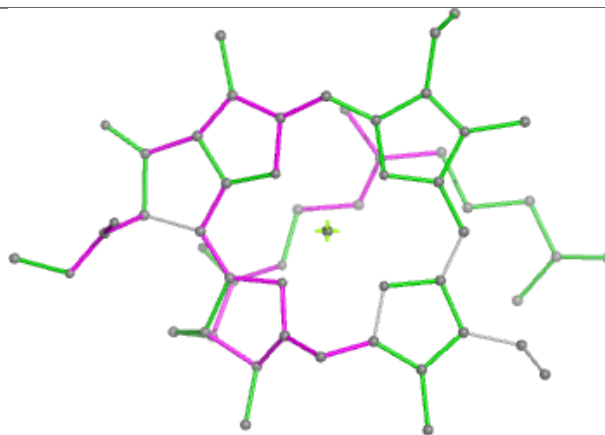


Rings

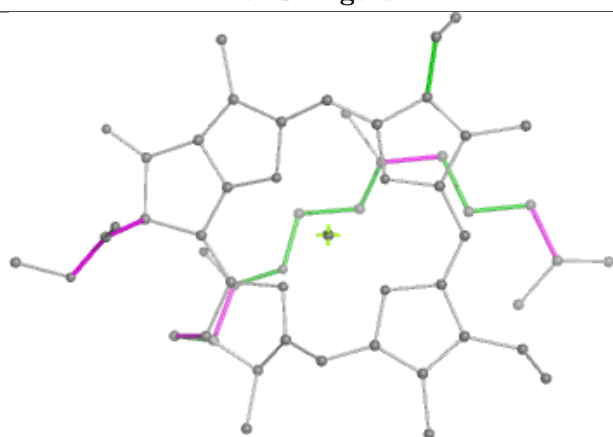
## Ligand CLA S 313



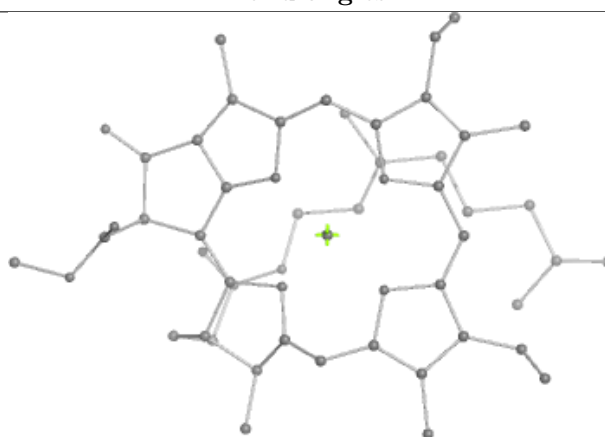
Bond lengths



Bond angles

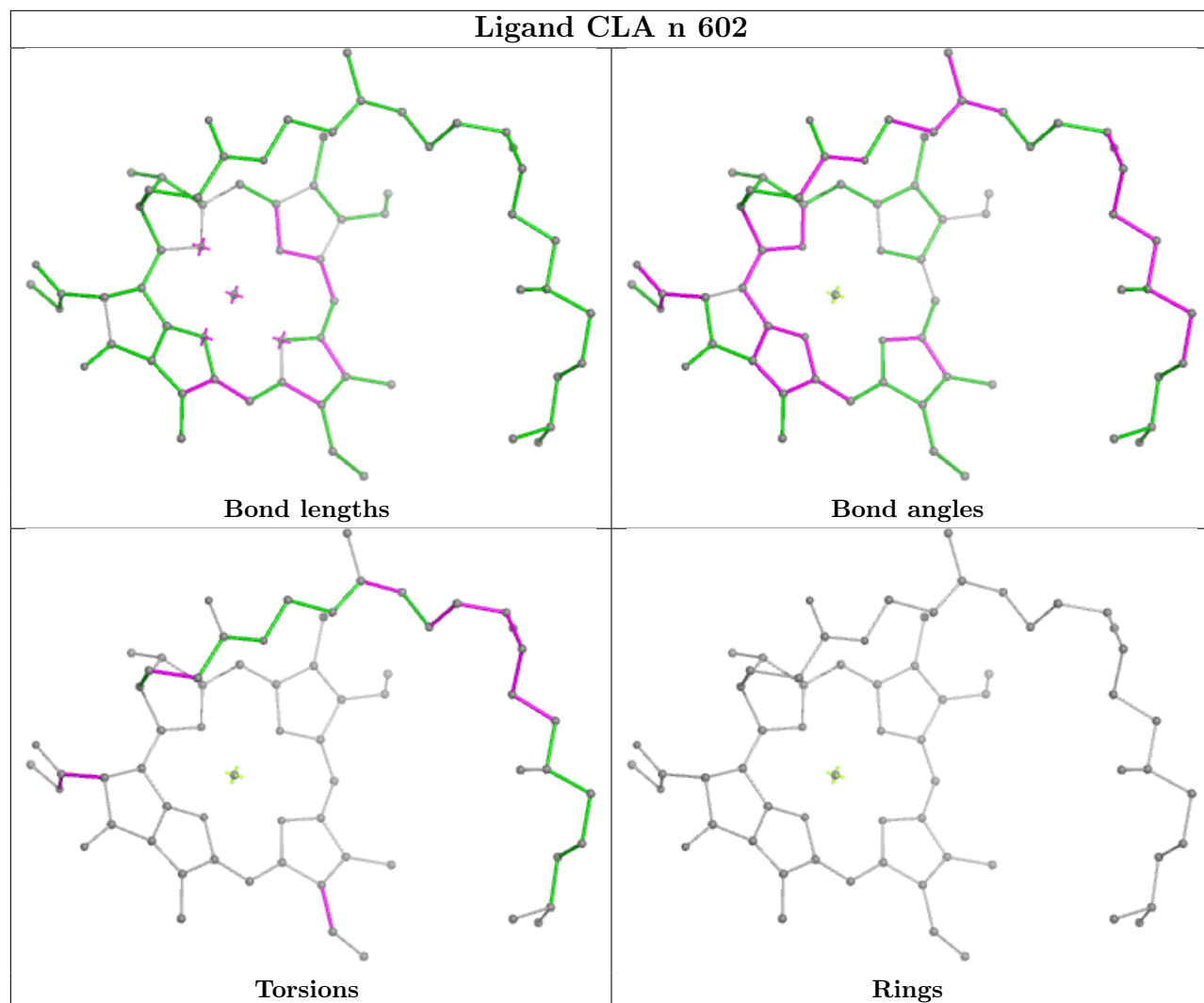


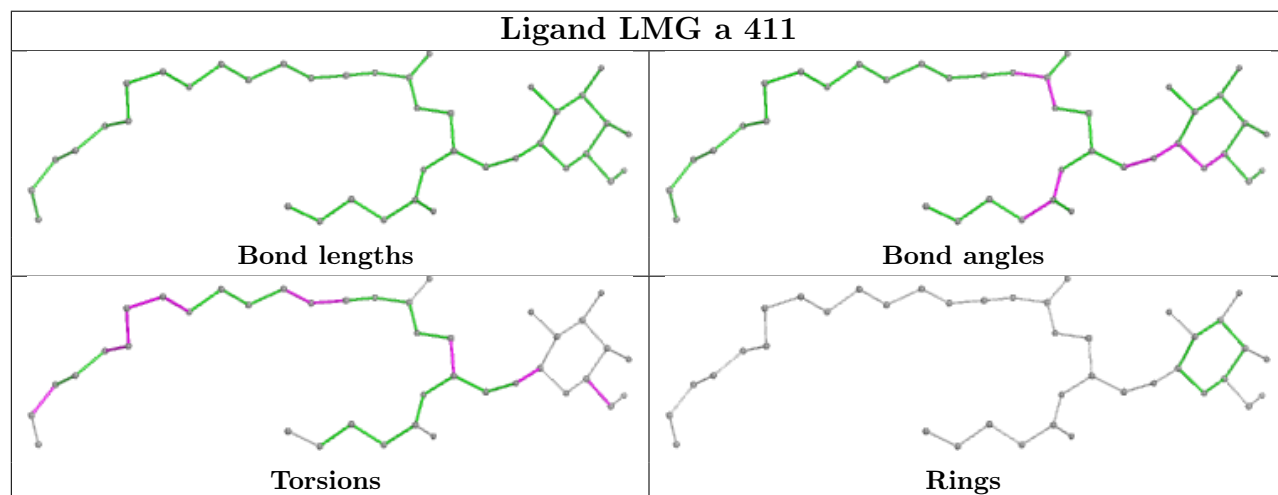
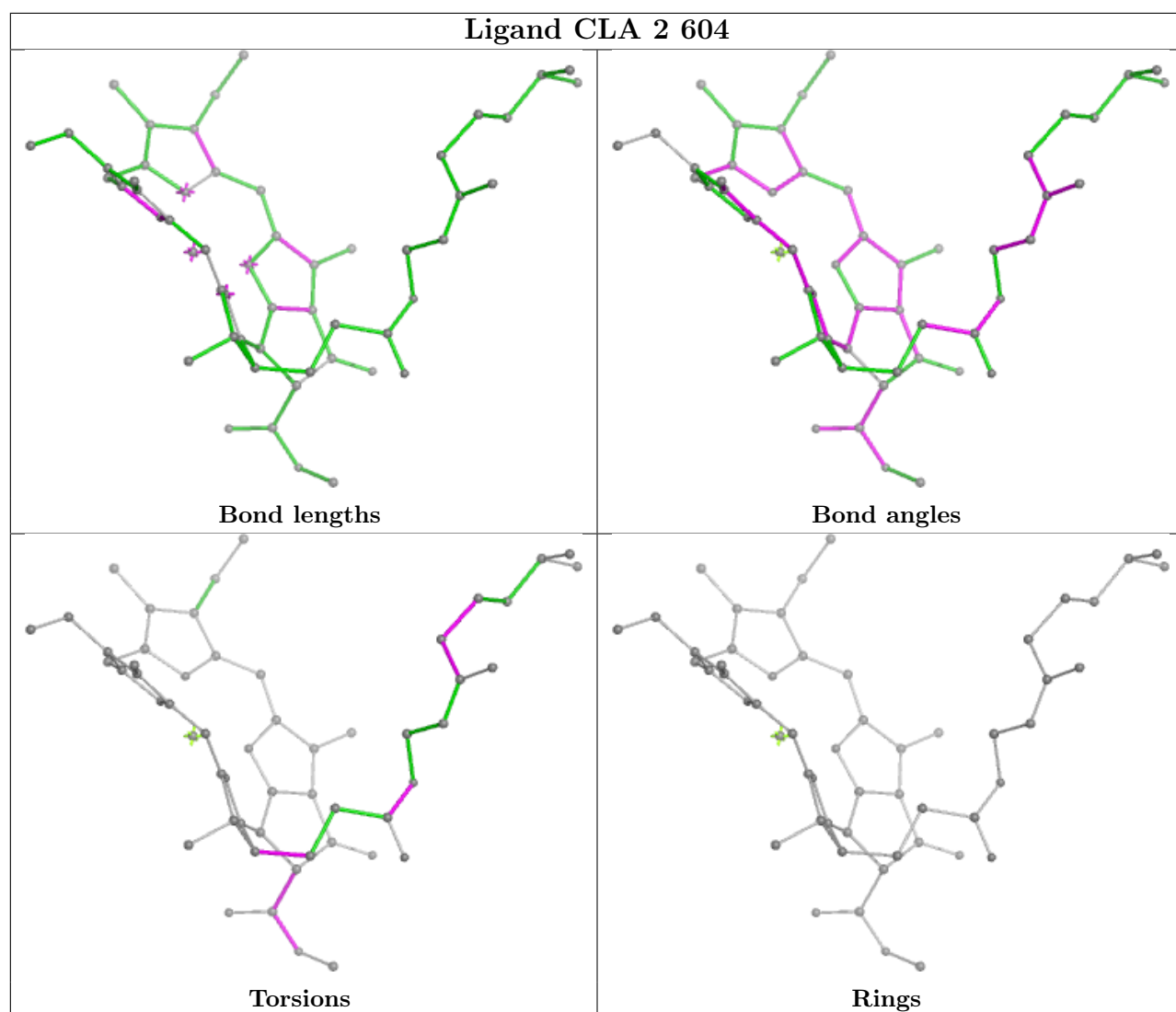
Torsions

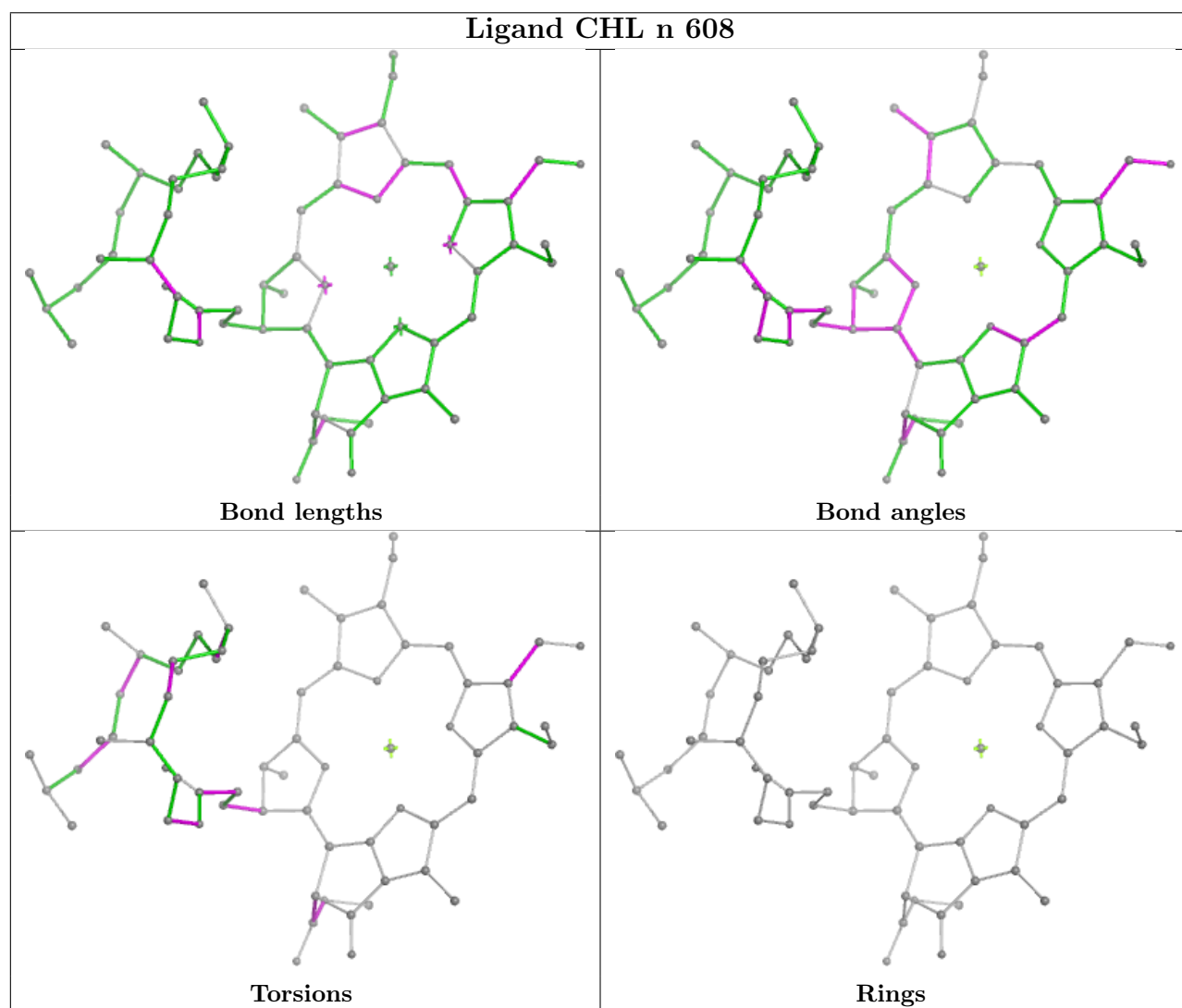
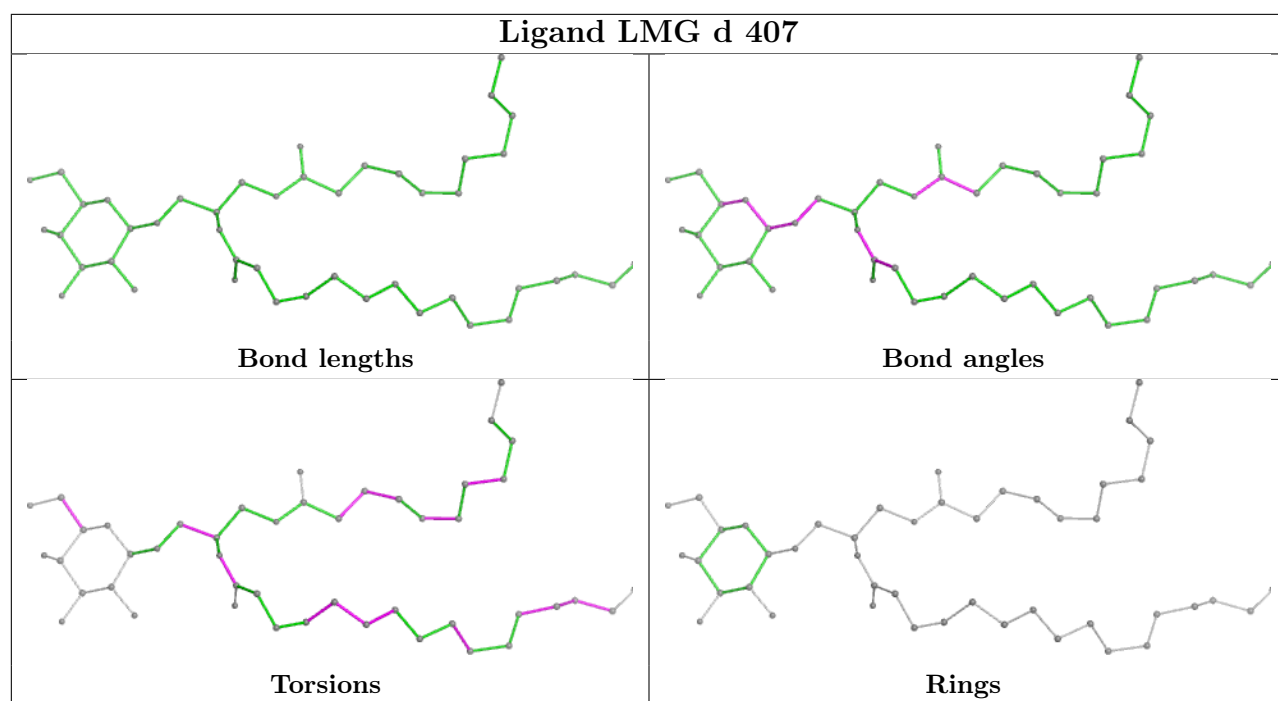


Rings

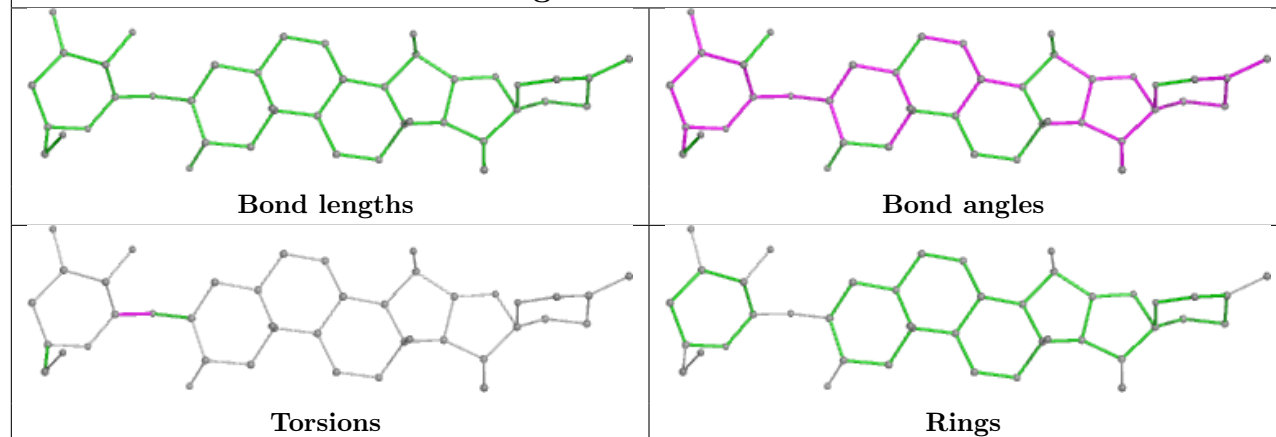
## Ligand CLA n 602



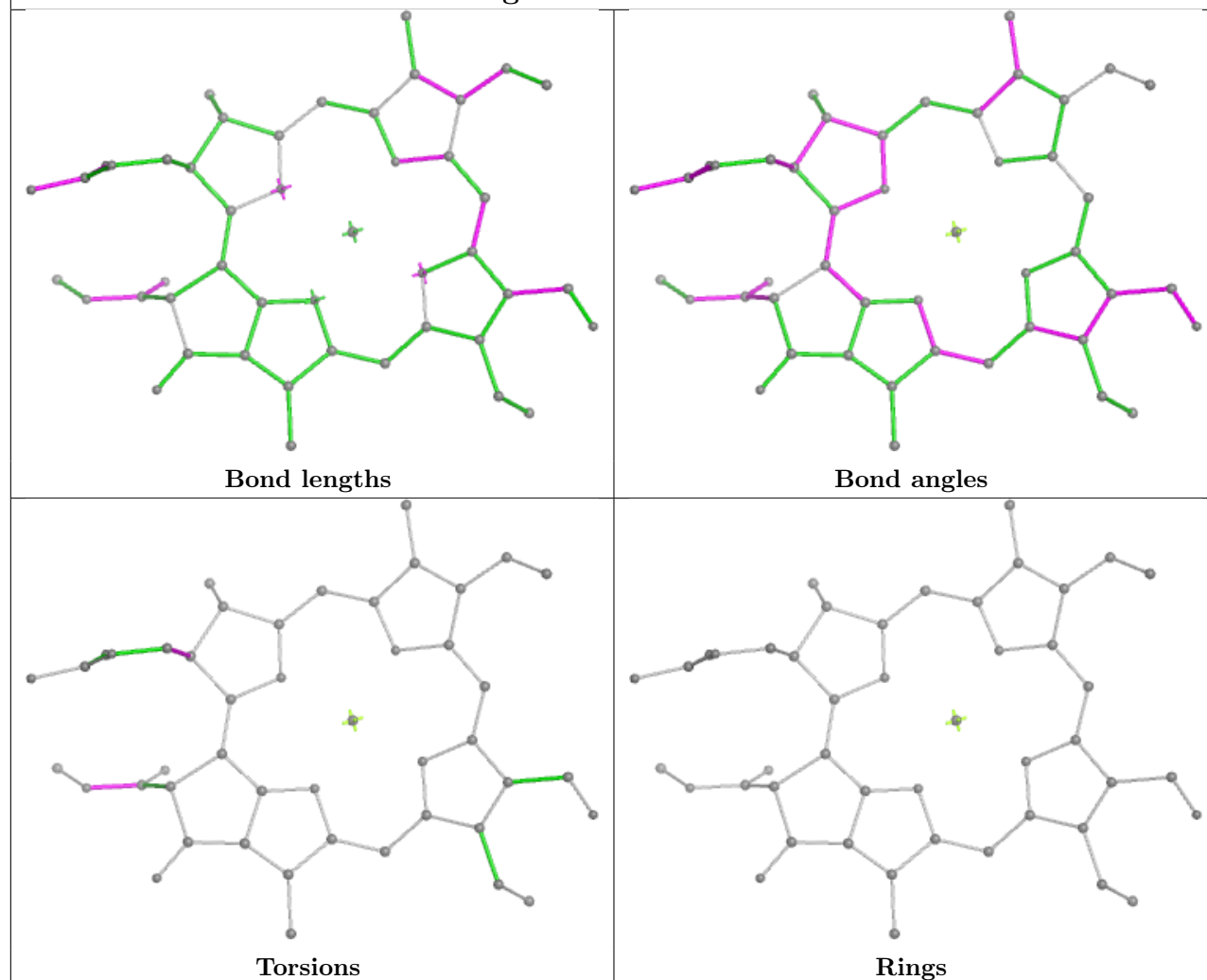




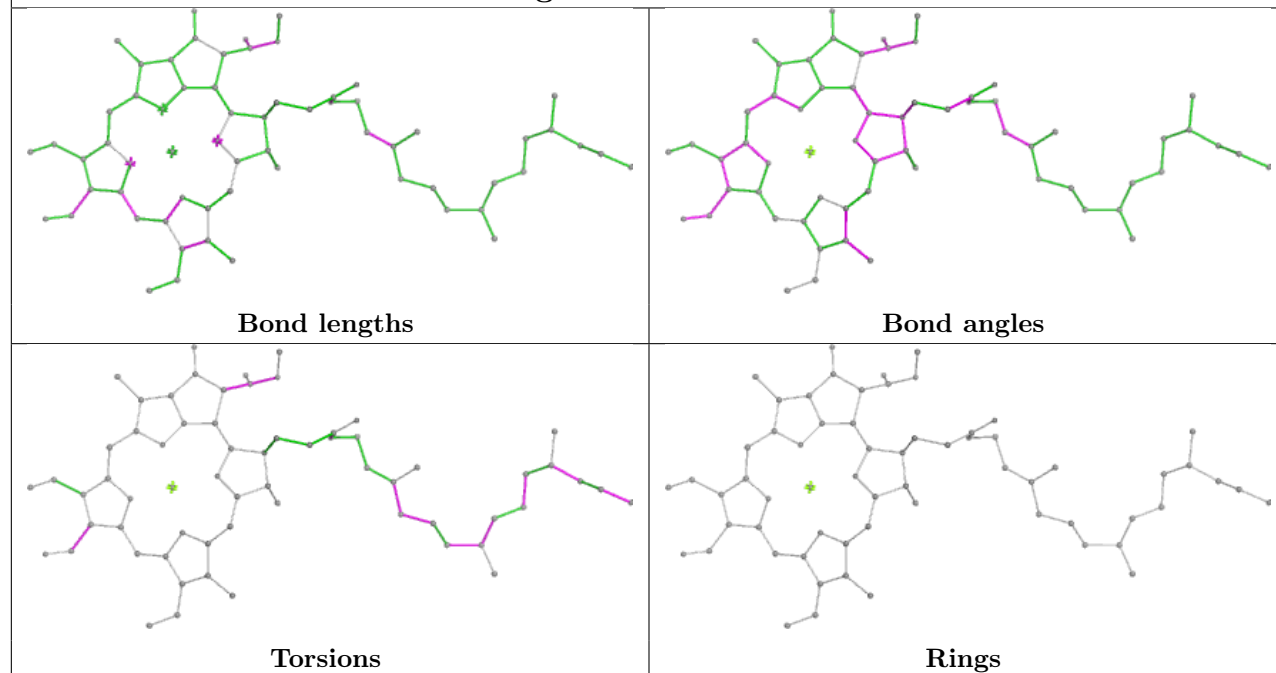
## Ligand AJP N 619



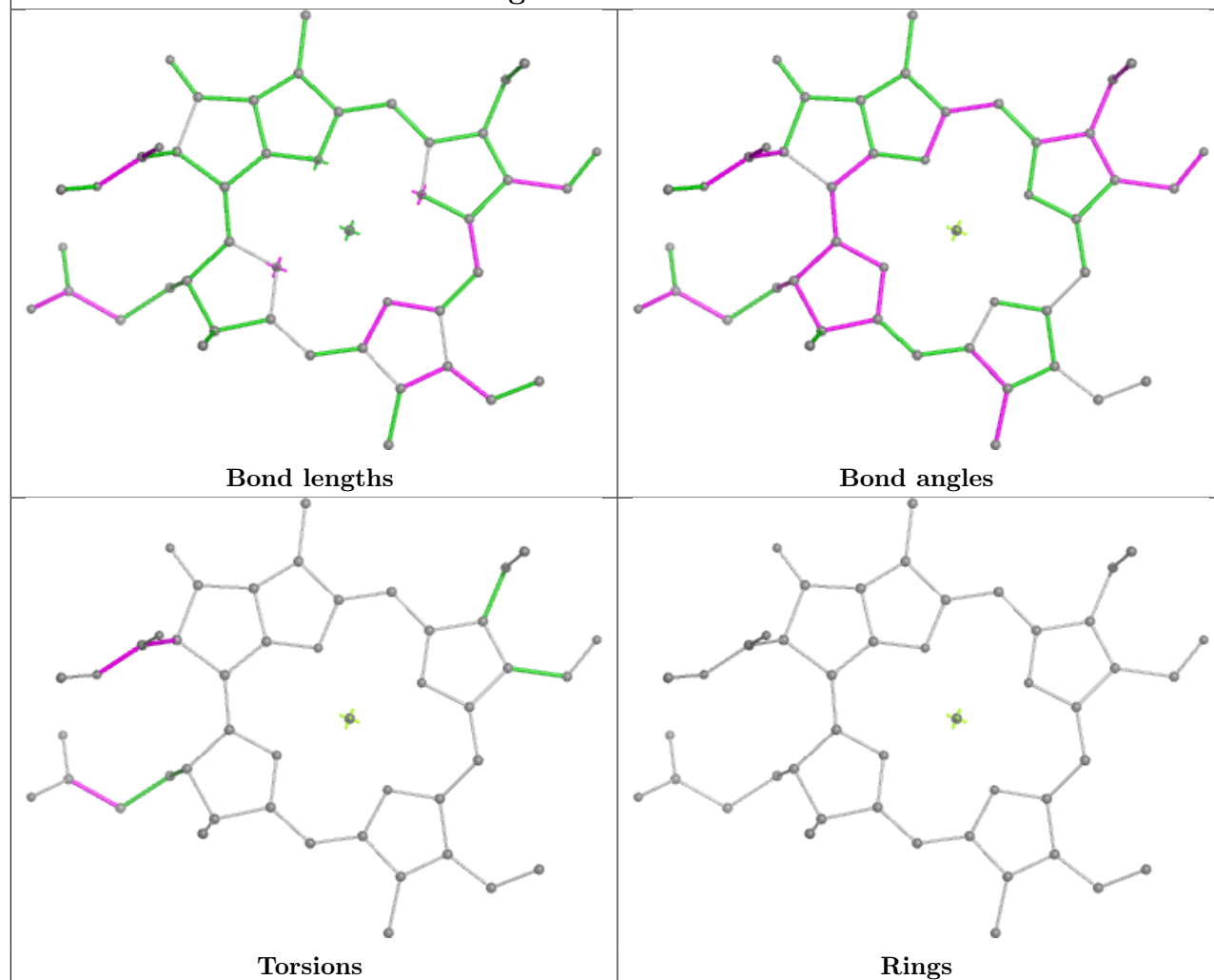
## Ligand CHL R 605



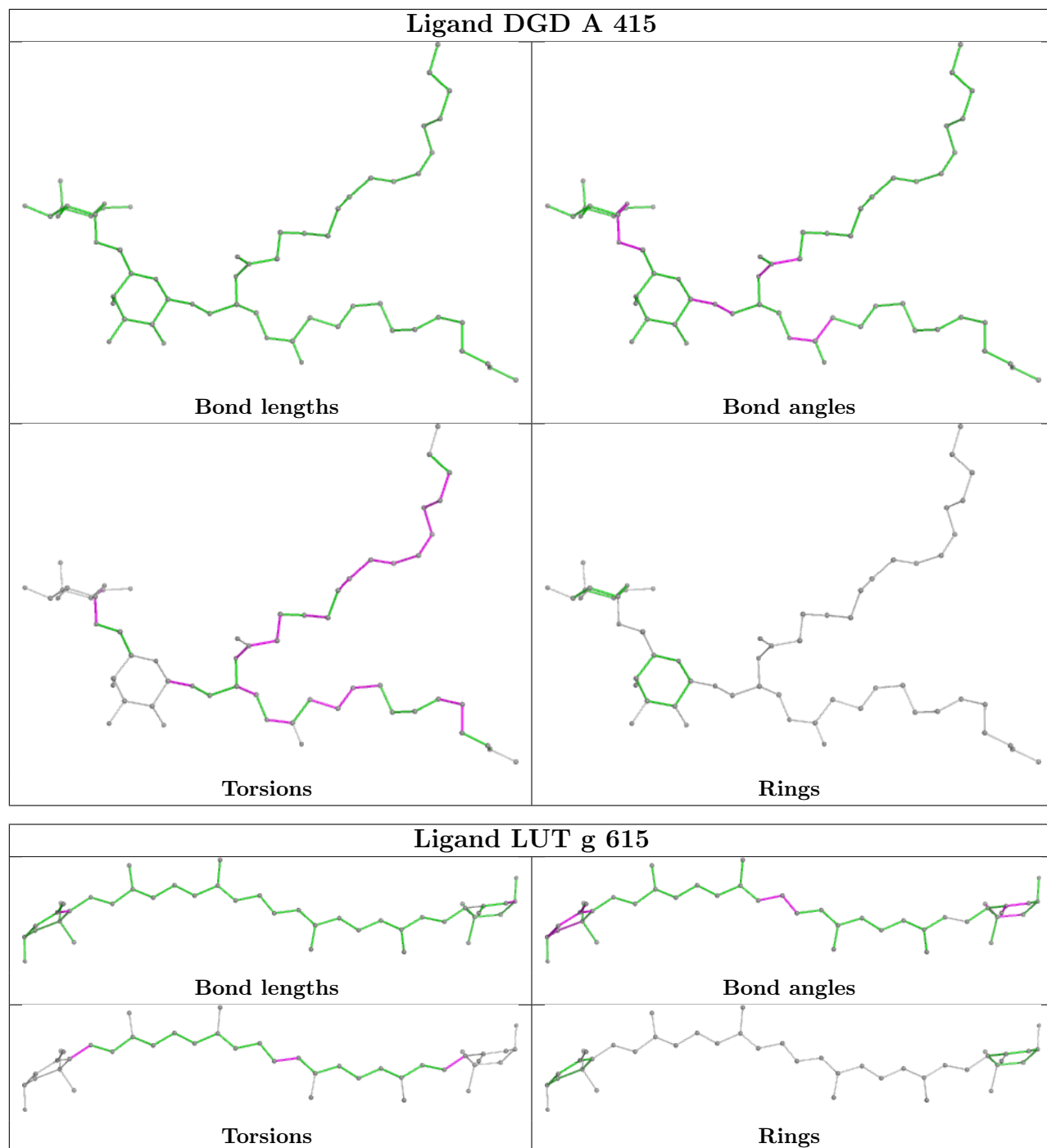
## Ligand CHL 2 601

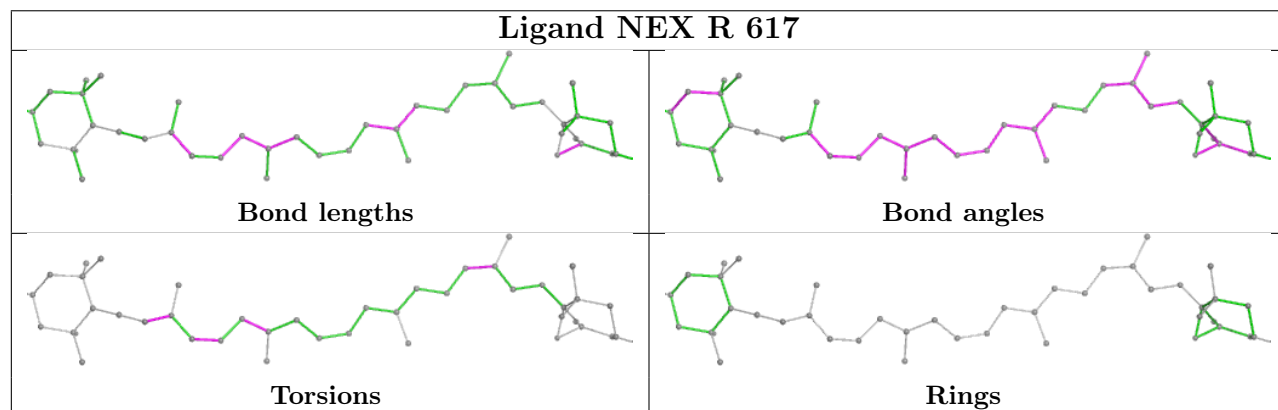
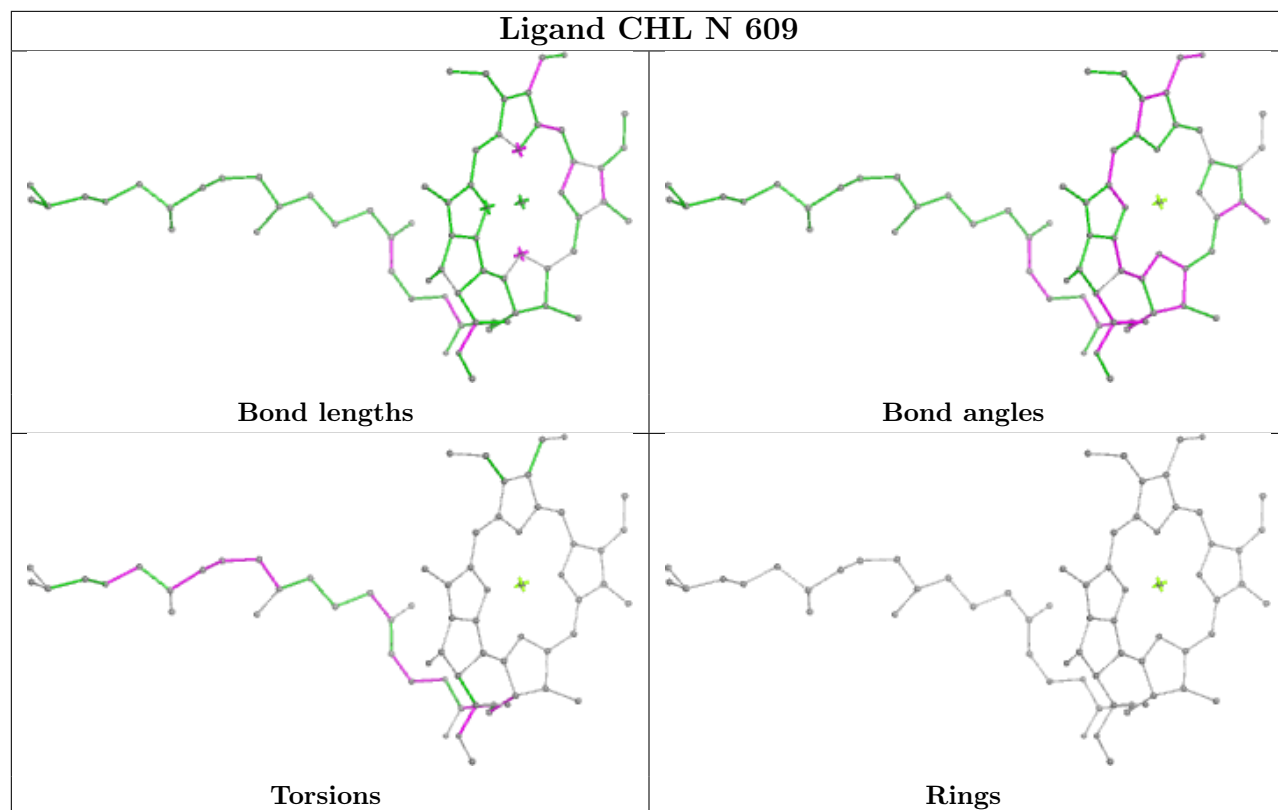


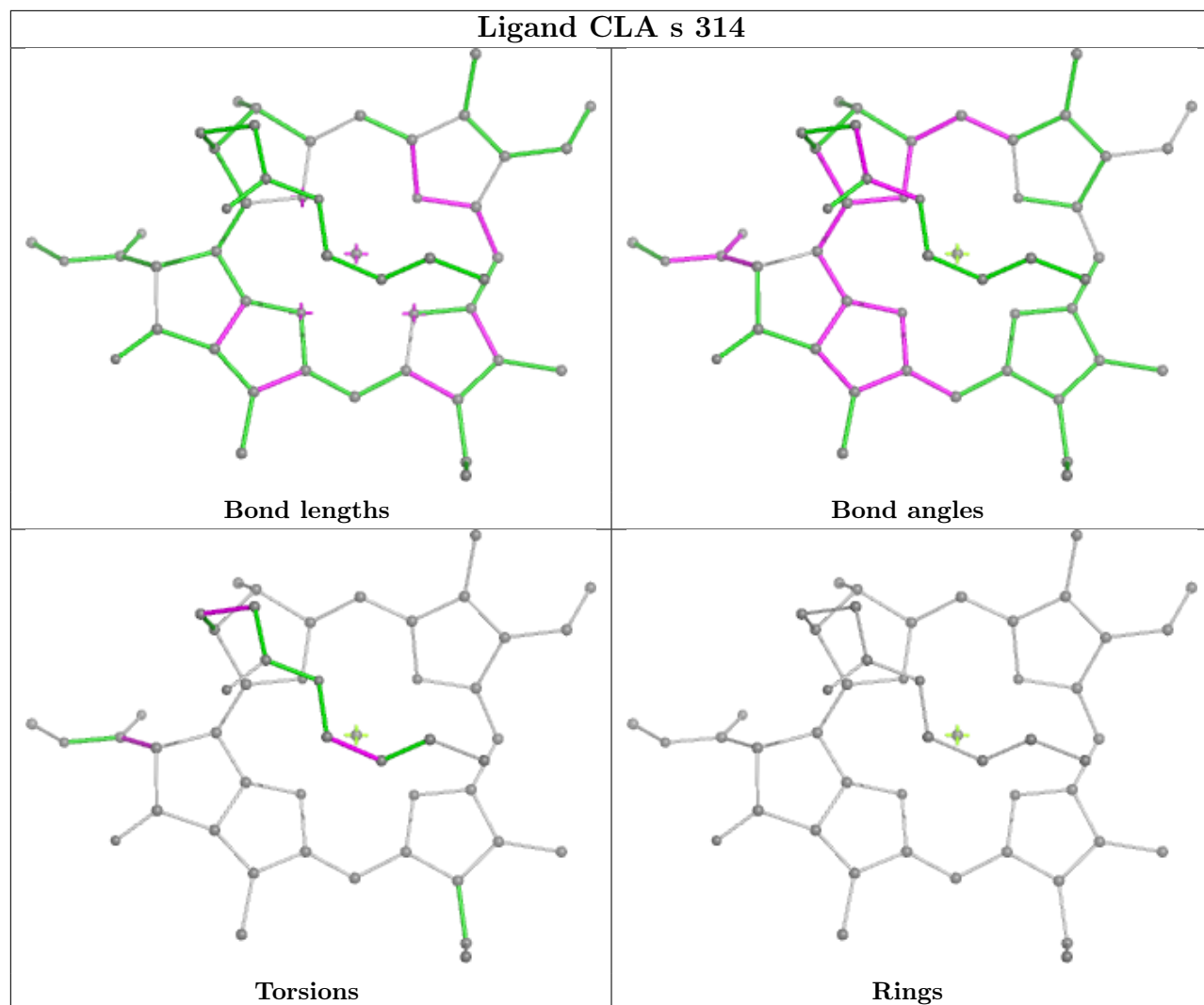
## Ligand CHL n 606



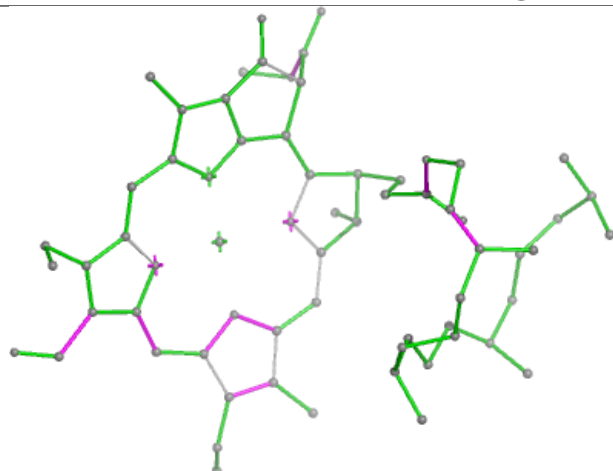




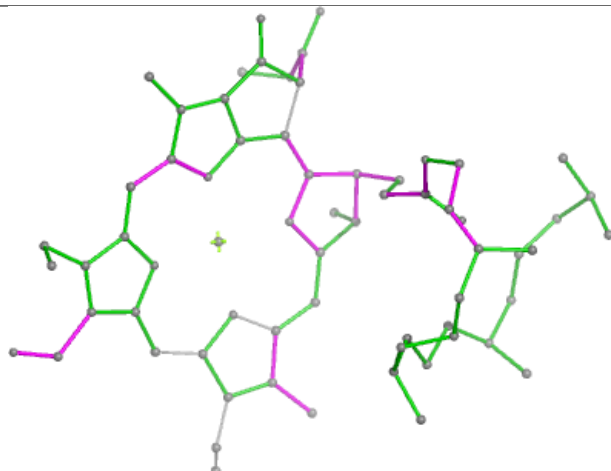




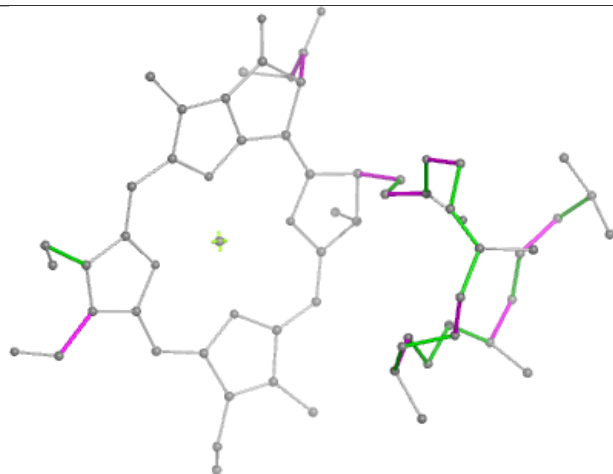
## Ligand CHL N 608



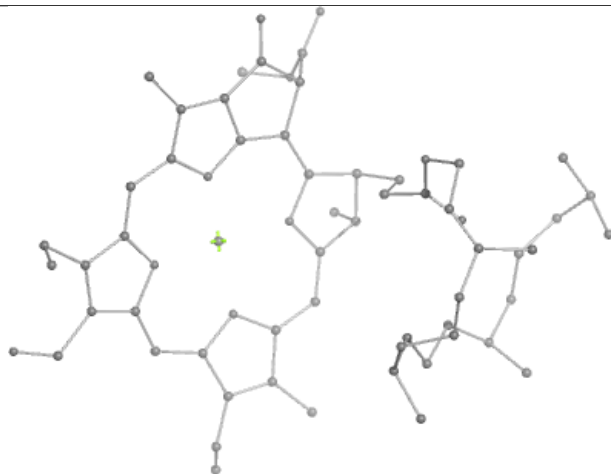
Bond lengths



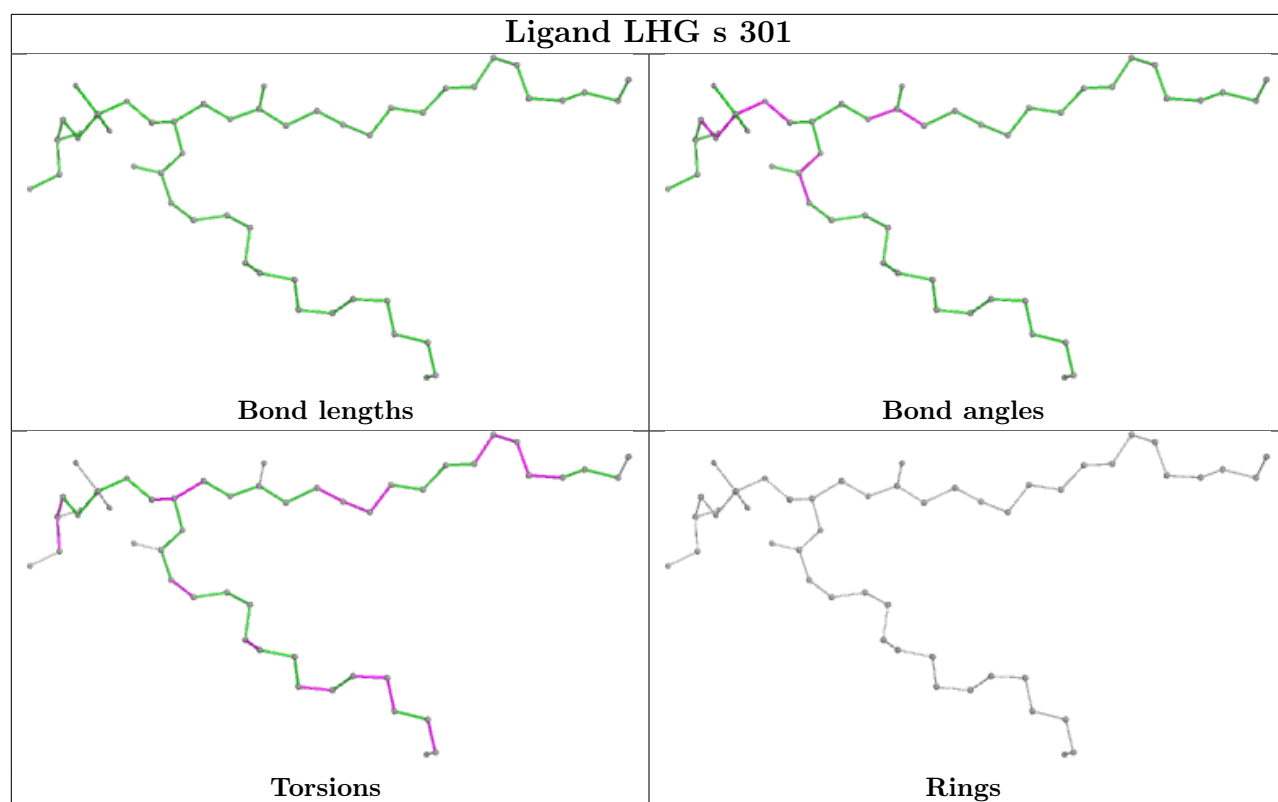
Bond angles

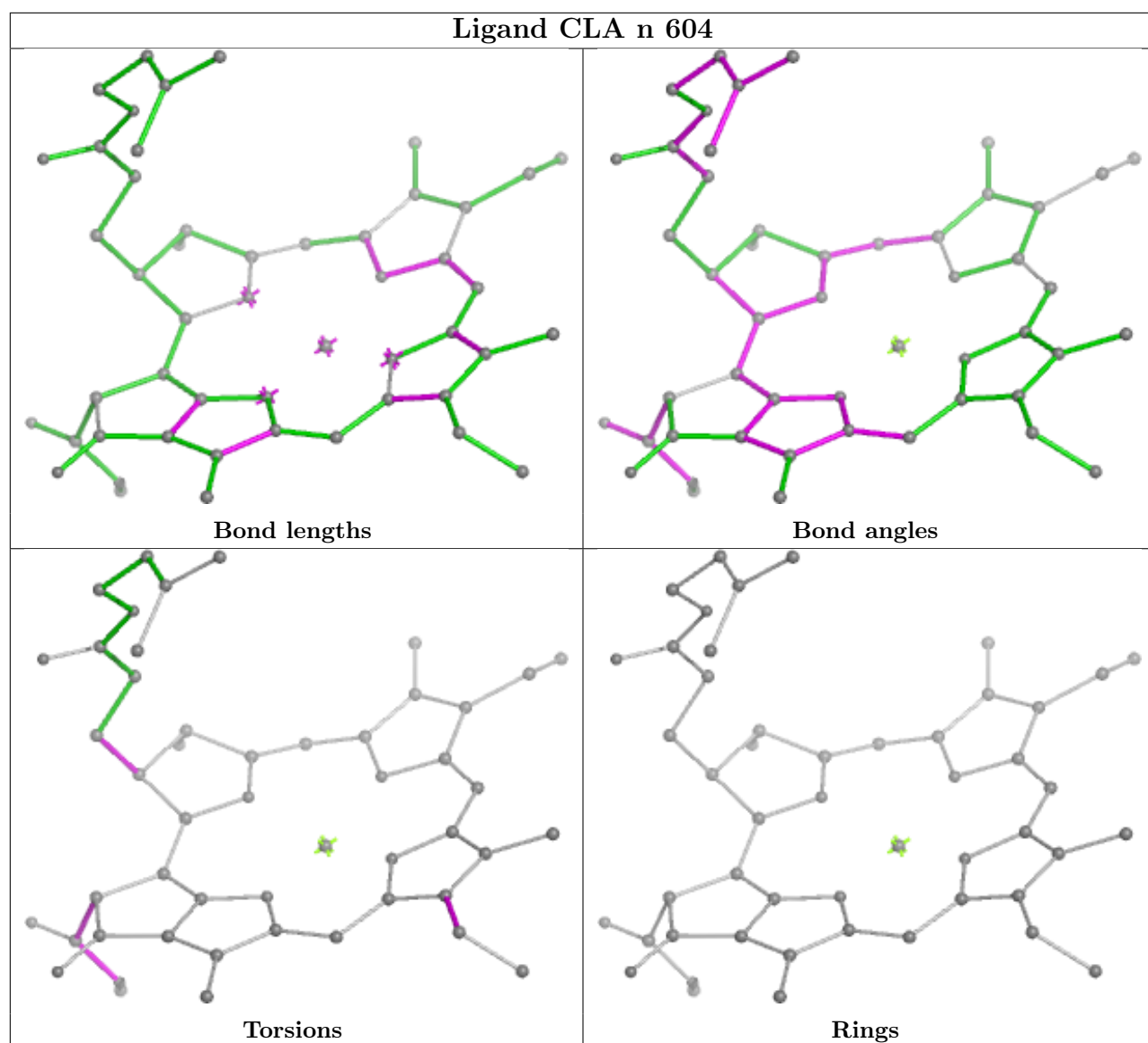


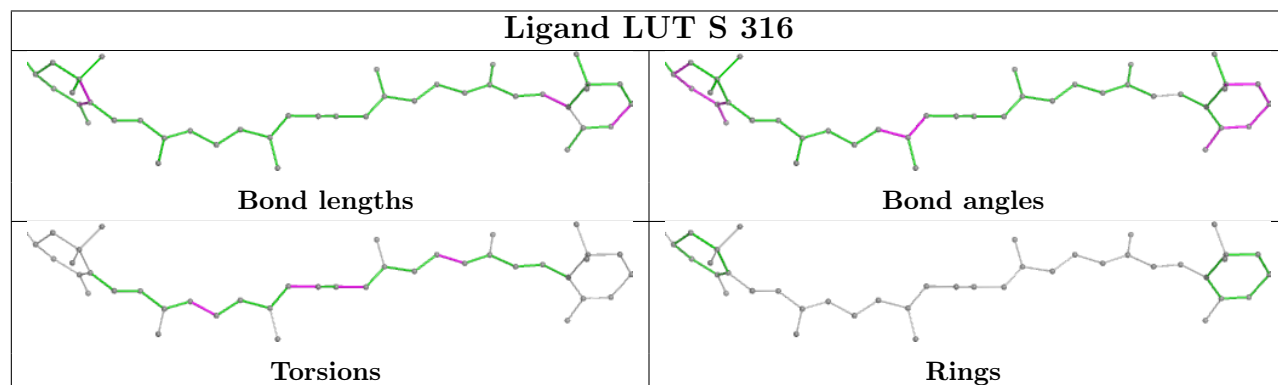
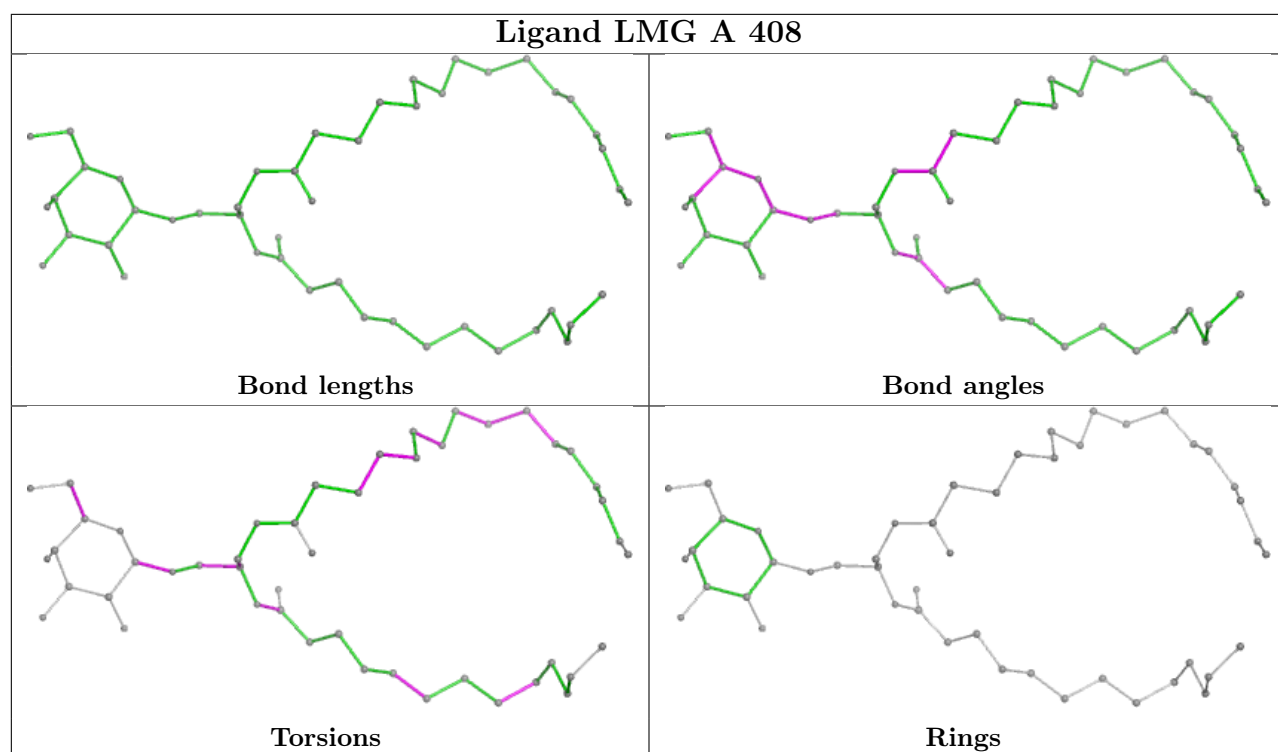
Torsions



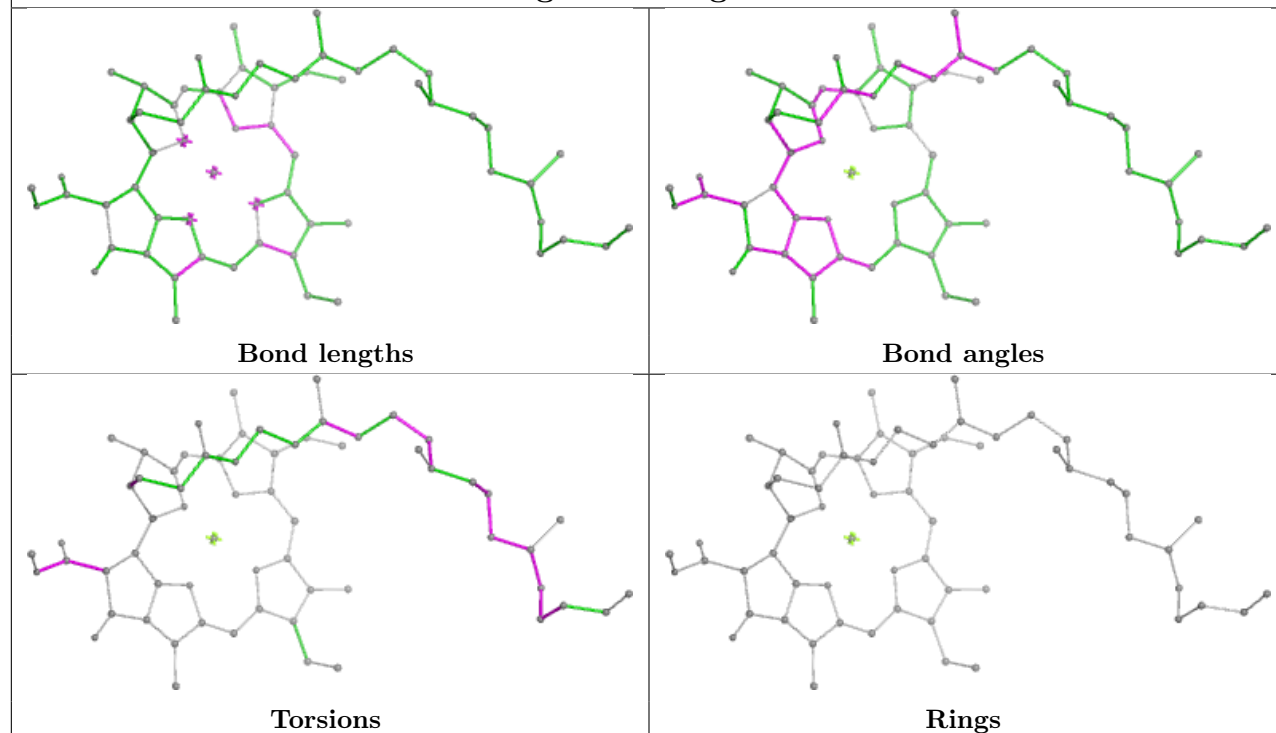
Rings



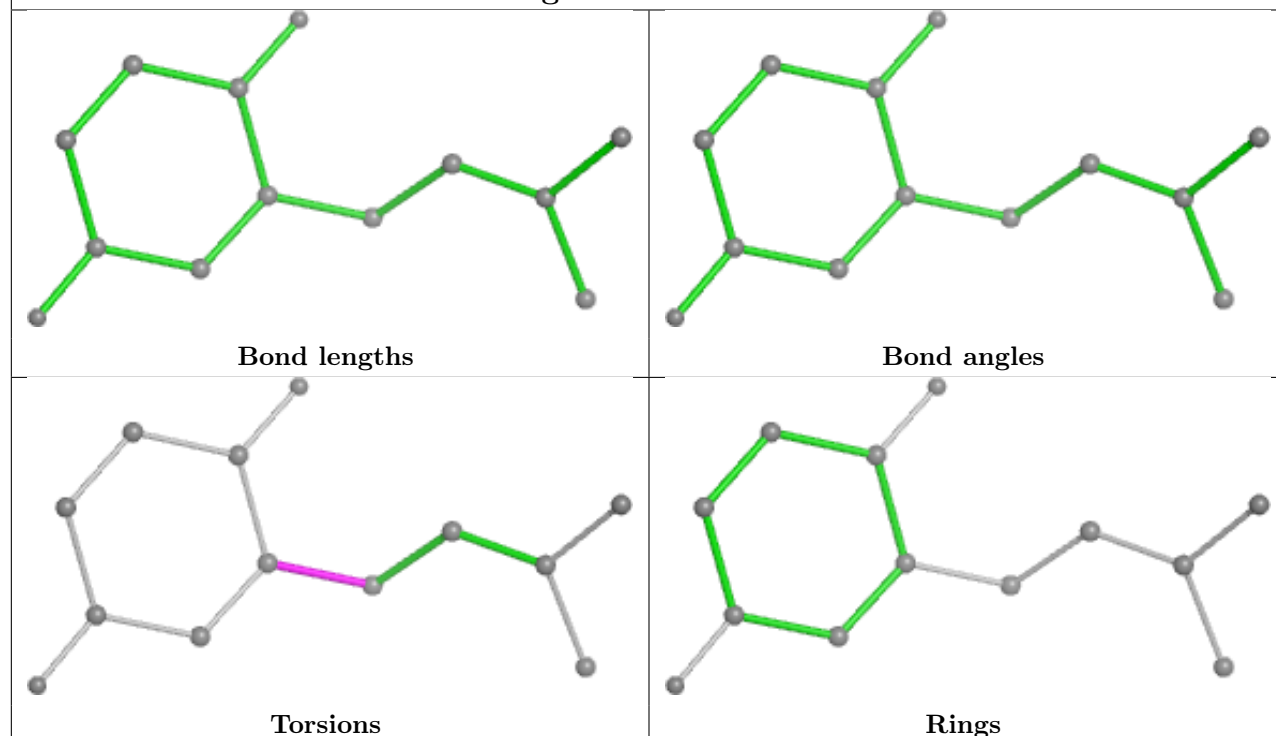




## Ligand CLA g 610

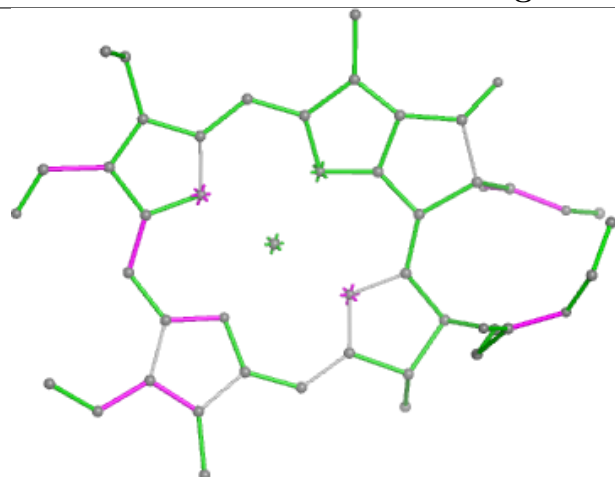


## Ligand PL9 a 410

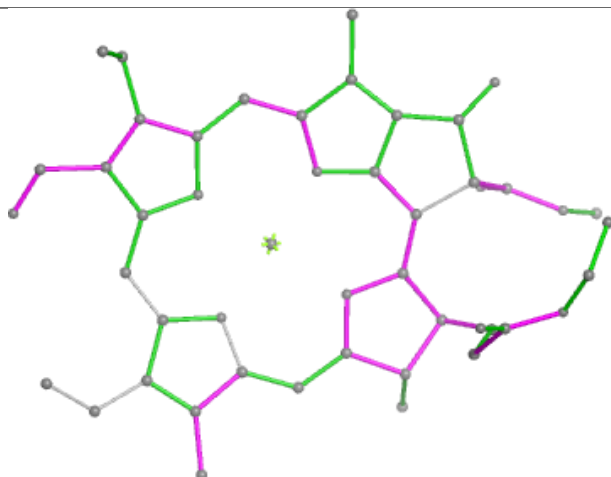




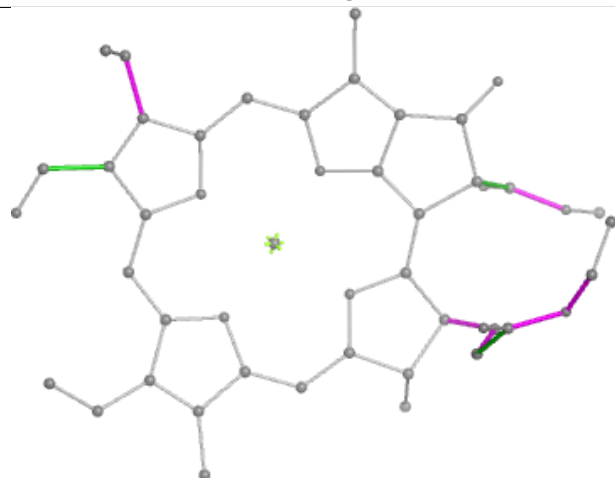
## Ligand CHL N 605



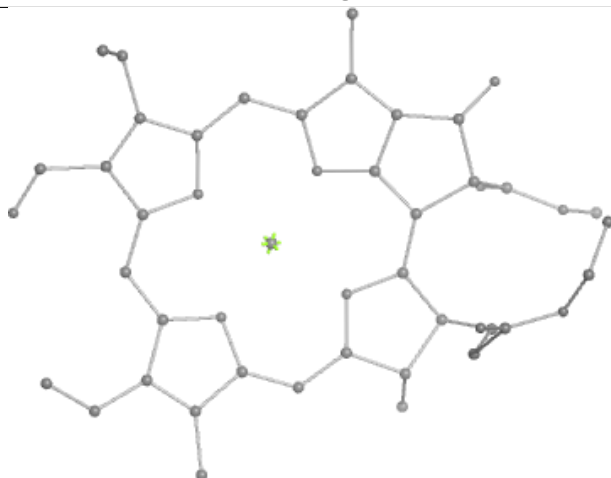
Bond lengths



Bond angles



Torsions



Rings

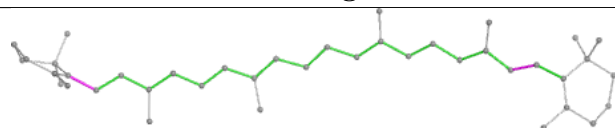
## Ligand BCR B 617



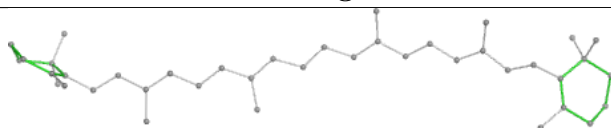
Bond lengths



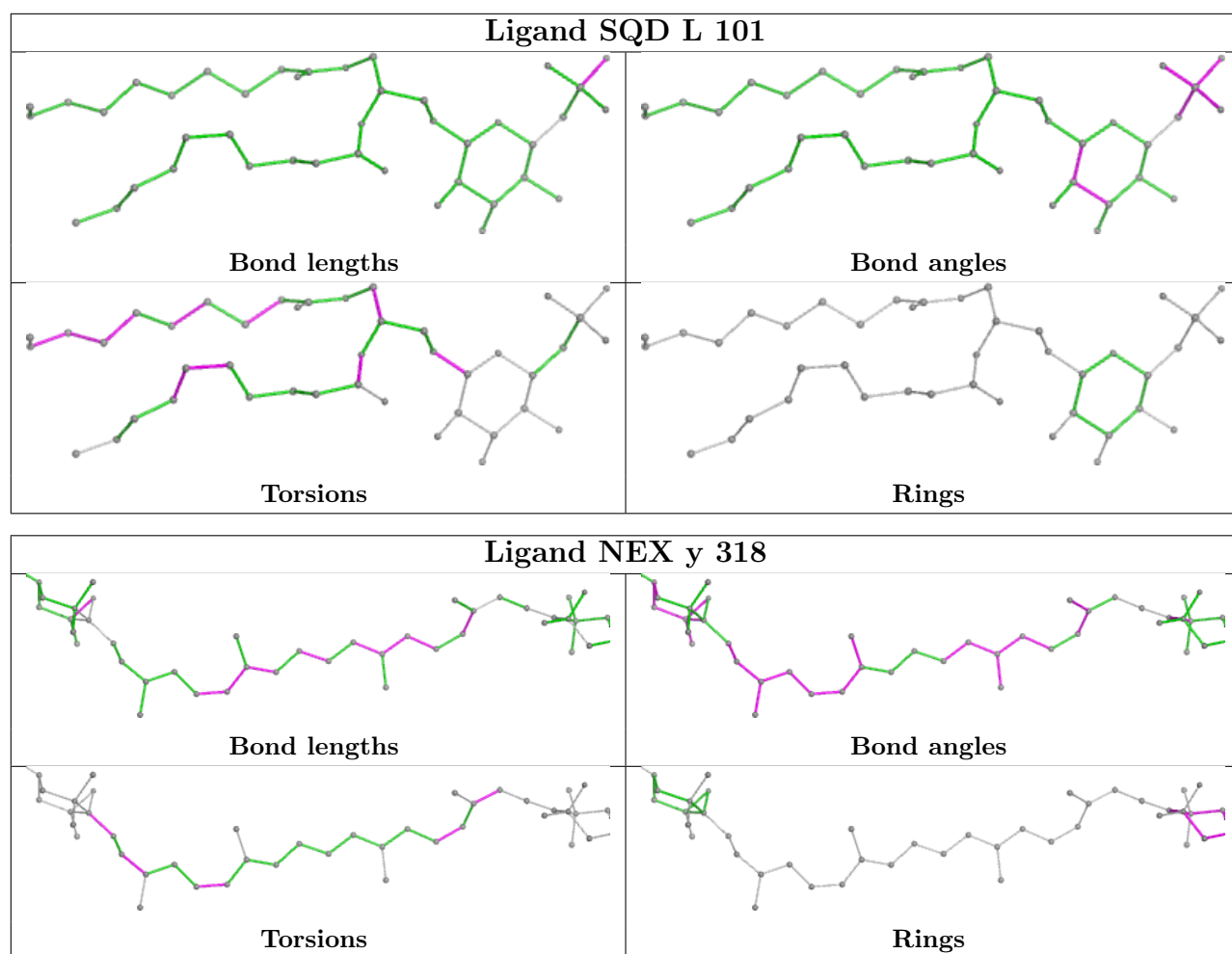
Bond angles



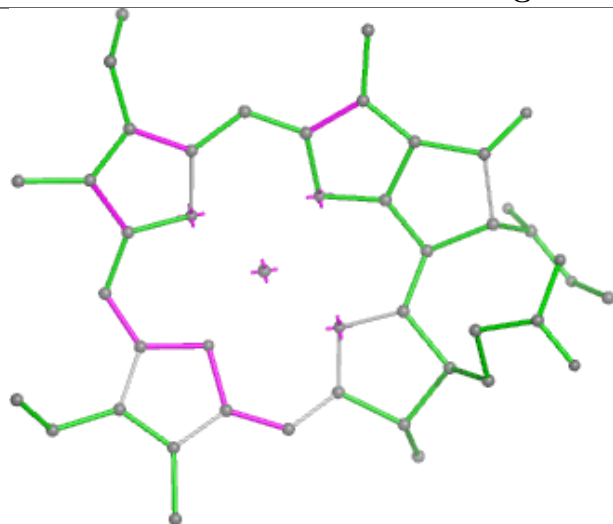
Torsions



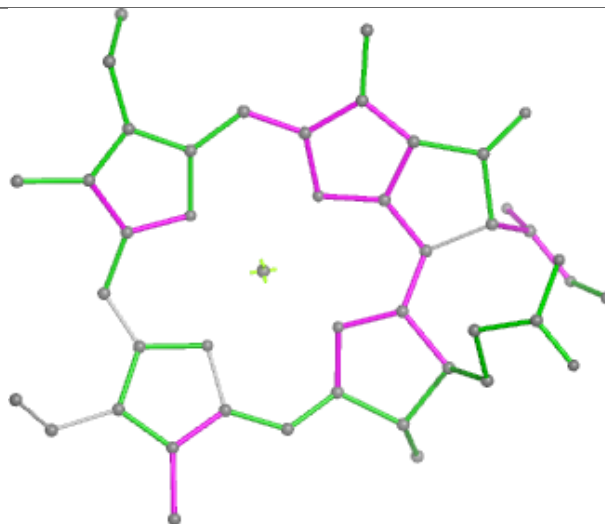
Rings



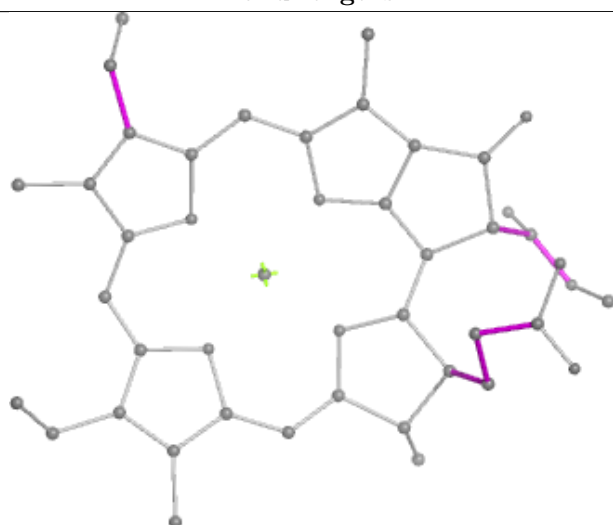
## Ligand CLA Y 315



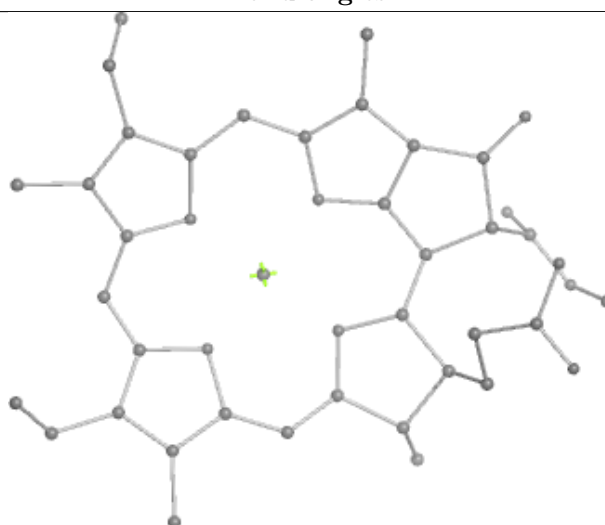
Bond lengths



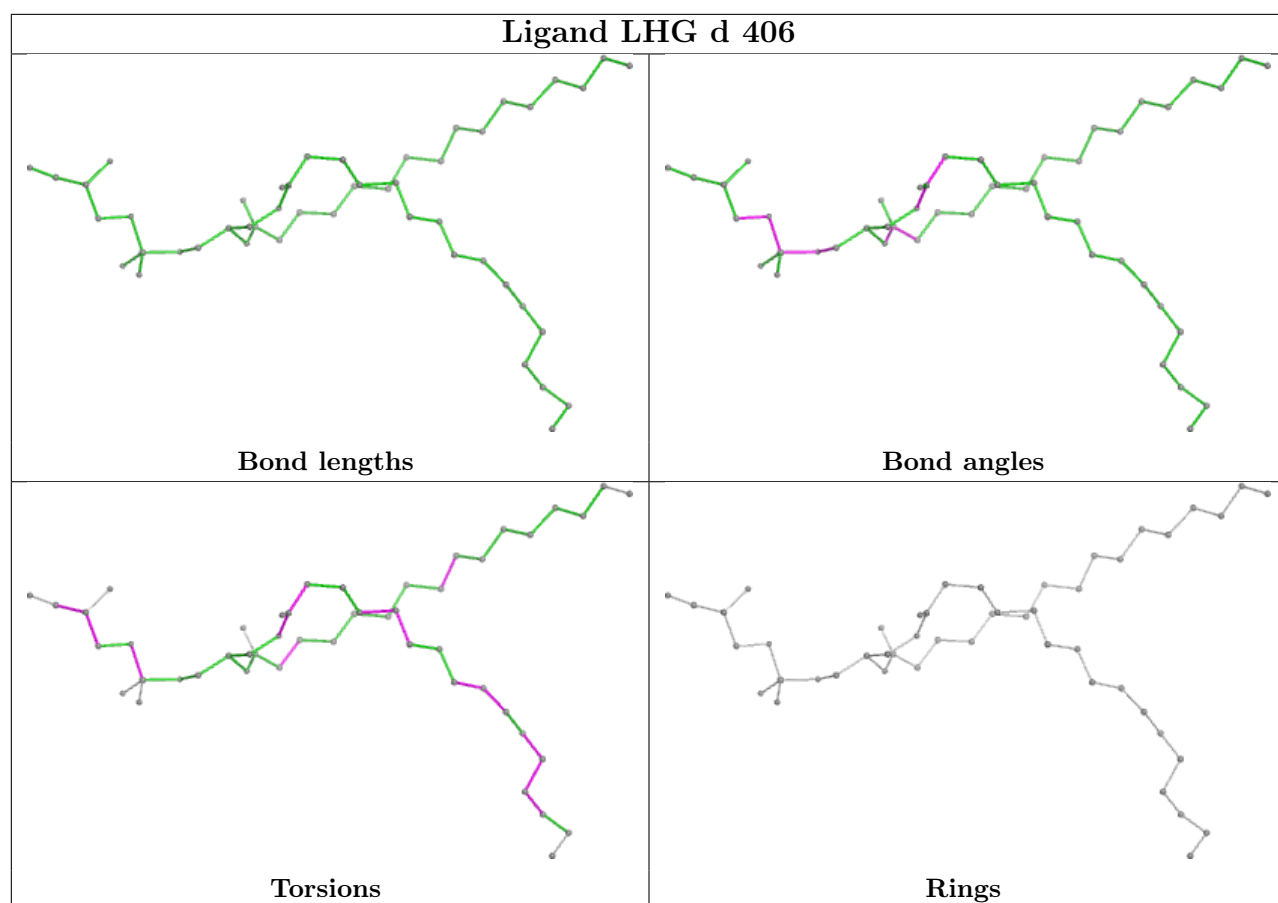
Bond angles



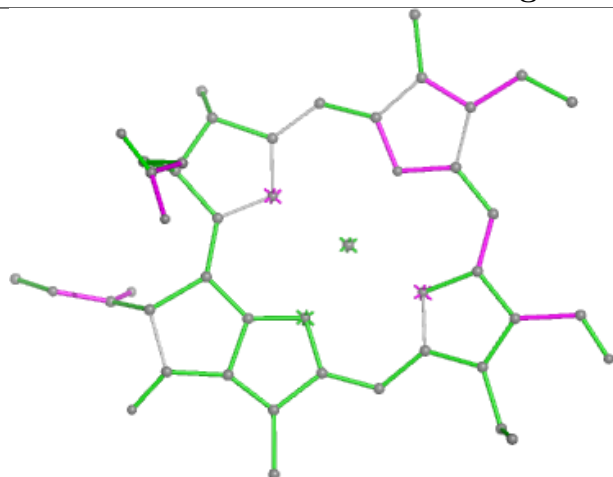
Torsions



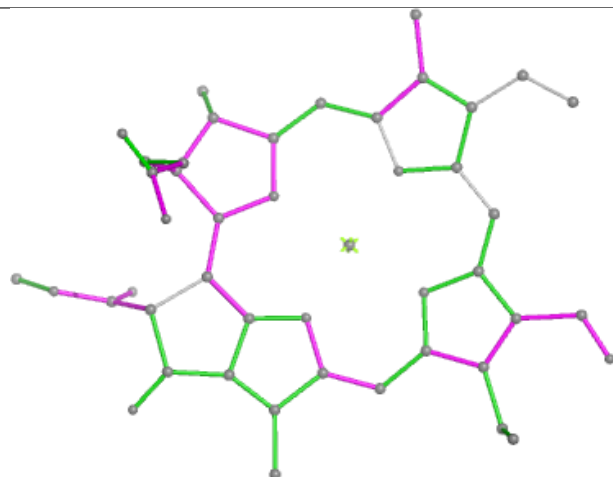
Rings



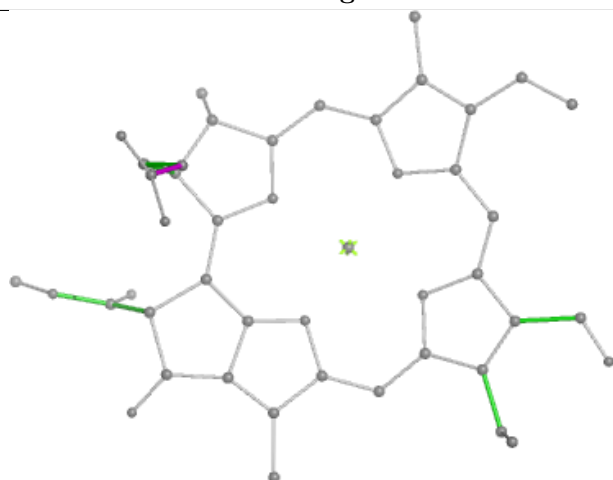
## Ligand CHL s 308



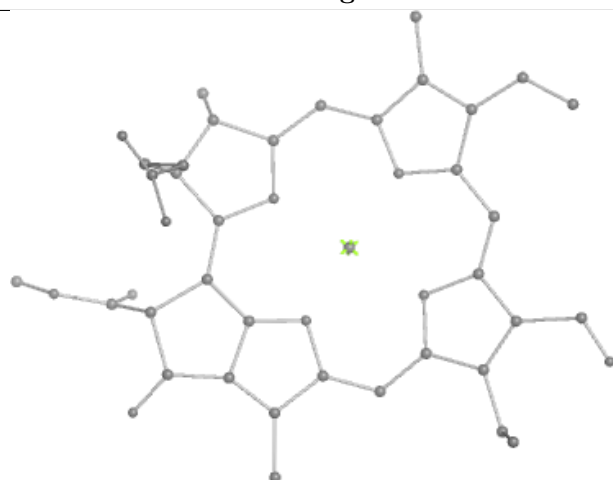
Bond lengths



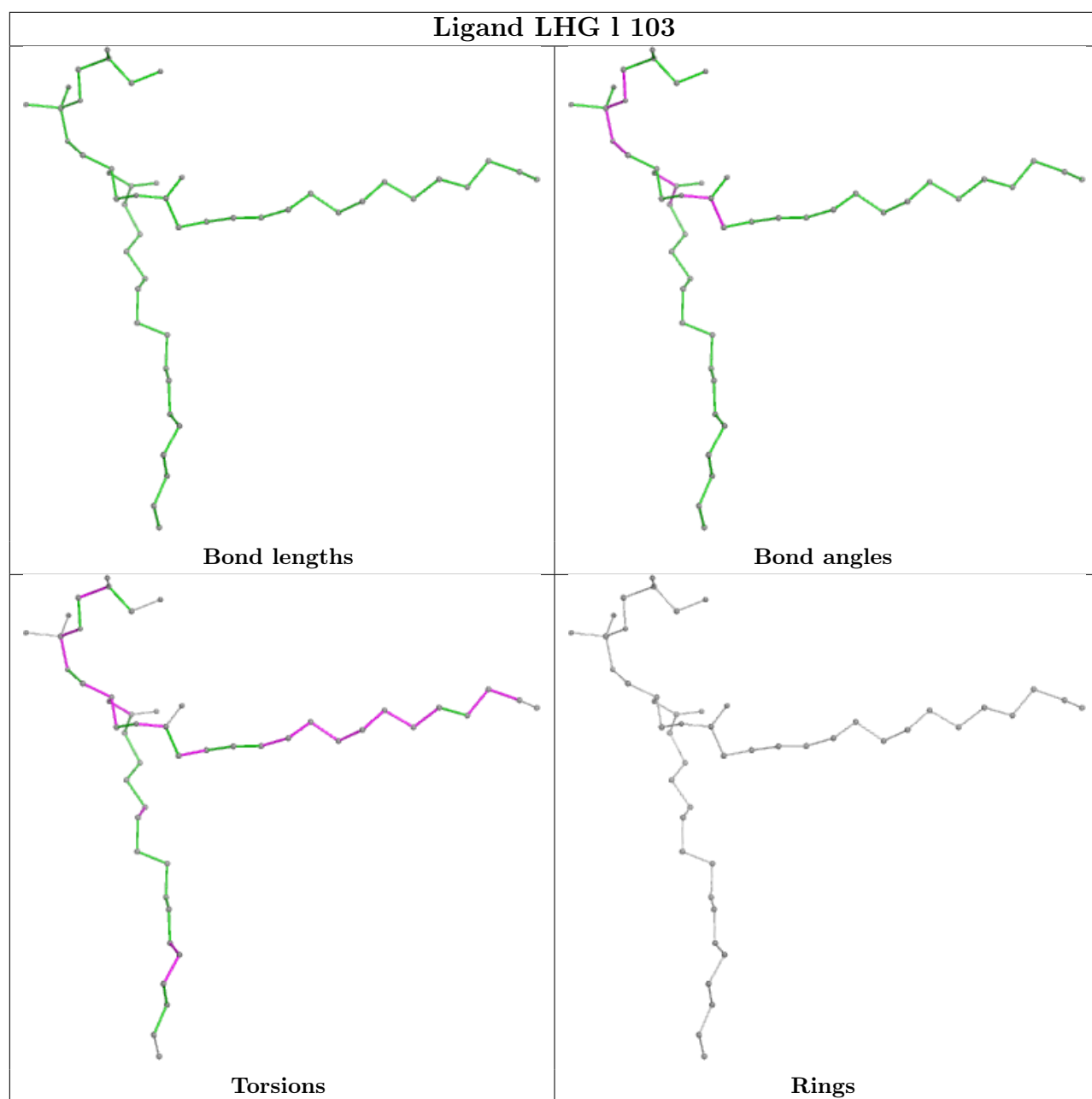
Bond angles



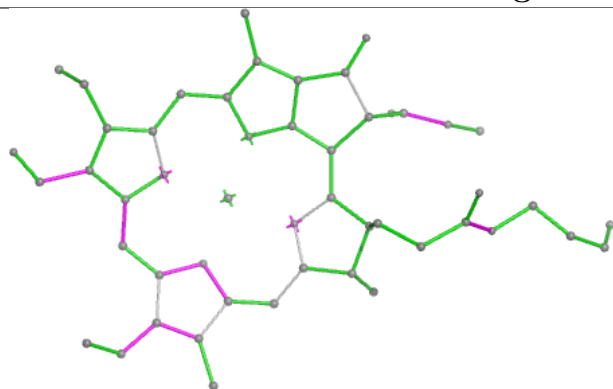
Torsions



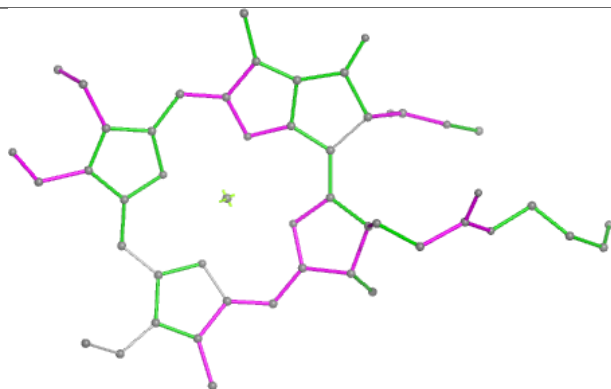
Rings



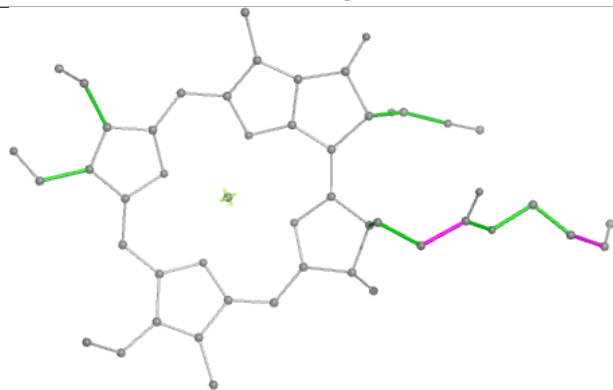
## Ligand CHL Y 307



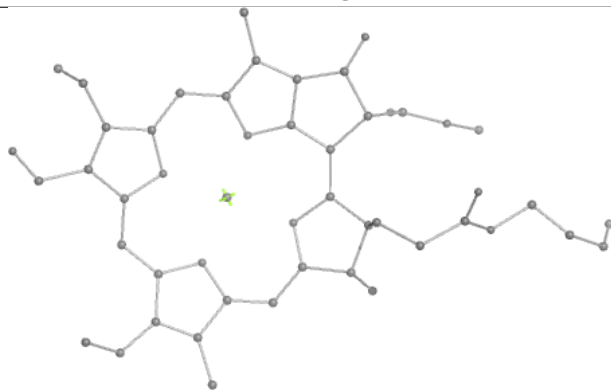
Bond lengths



Bond angles

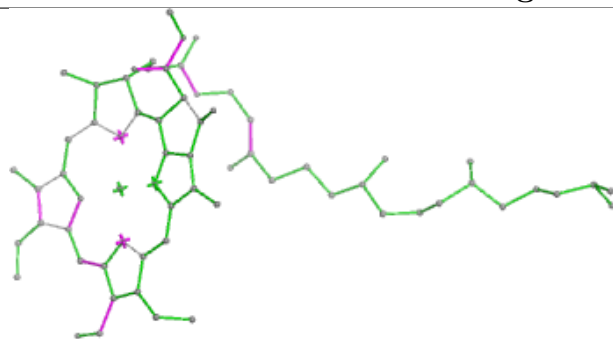


Torsions

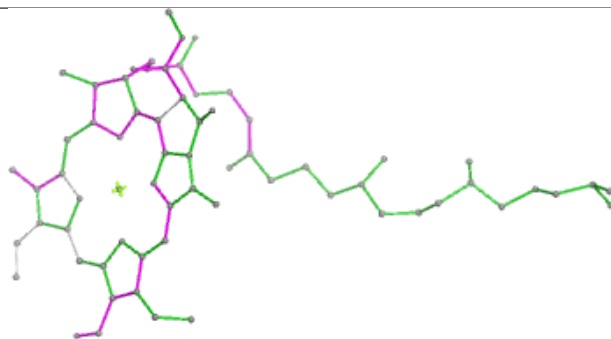


Rings

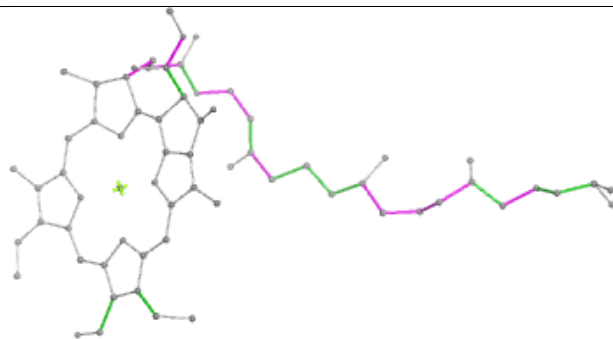
## Ligand CHL n 609



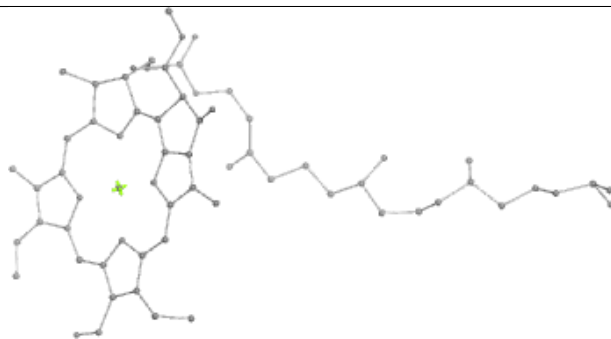
Bond lengths



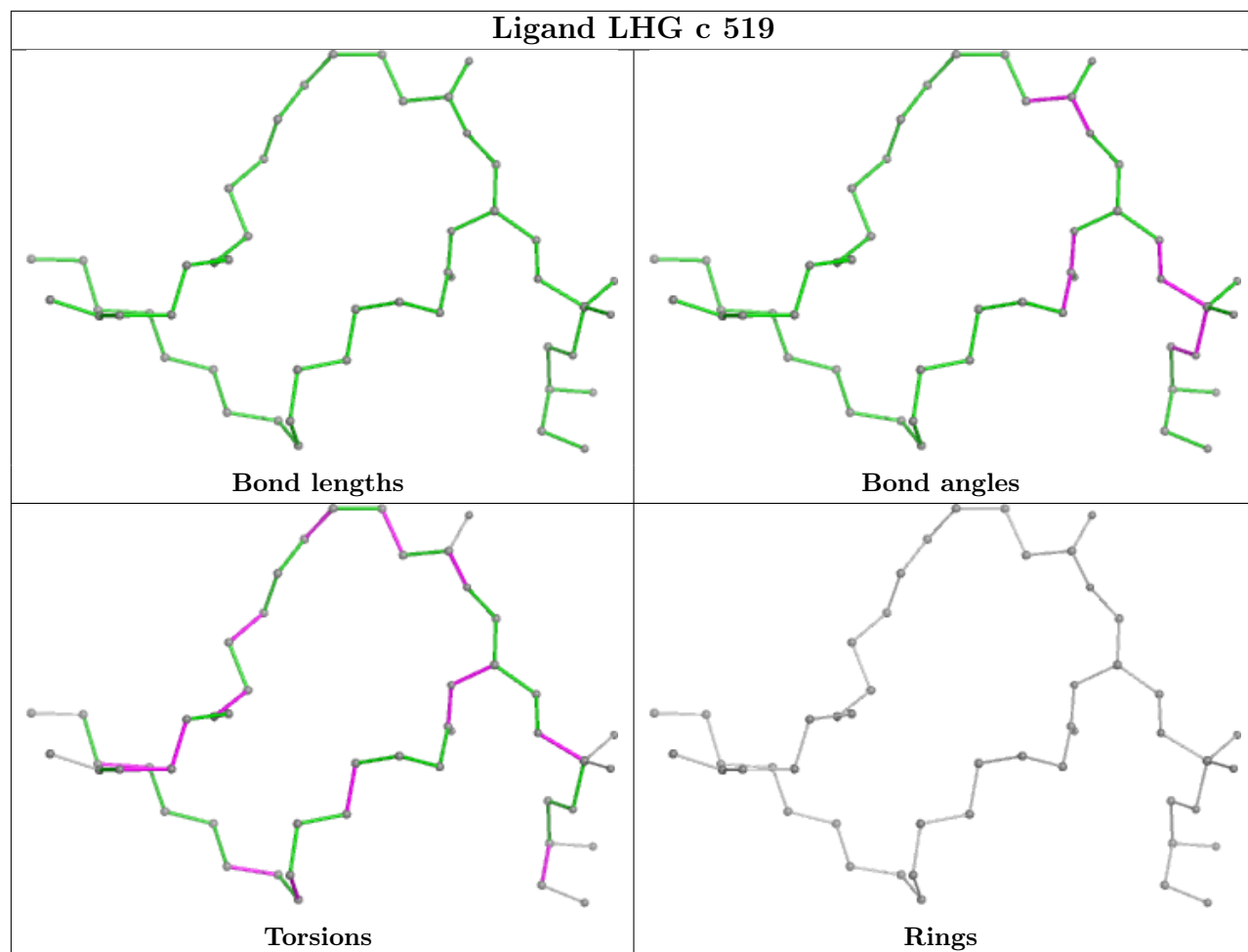
Bond angles



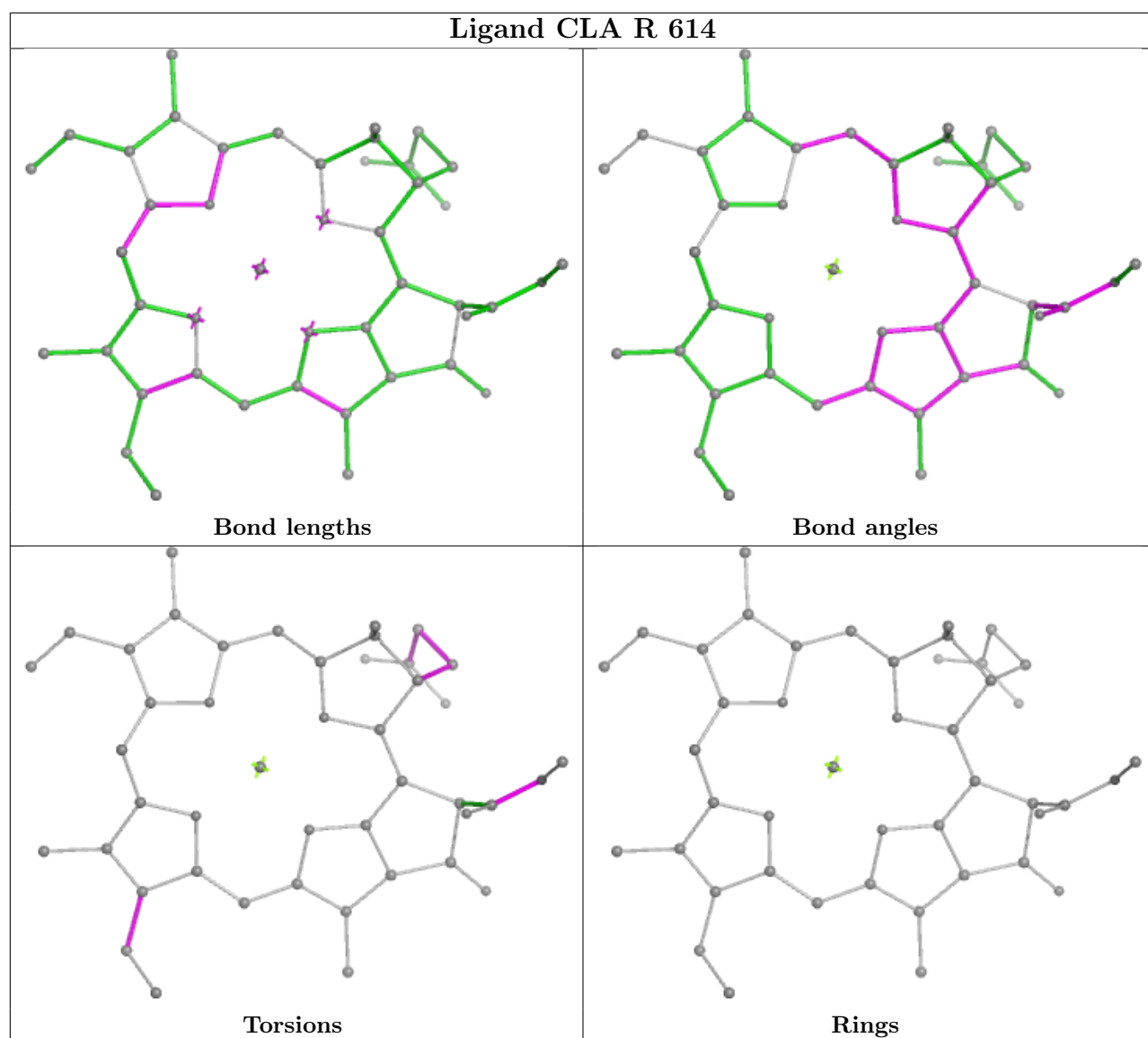
Torsions



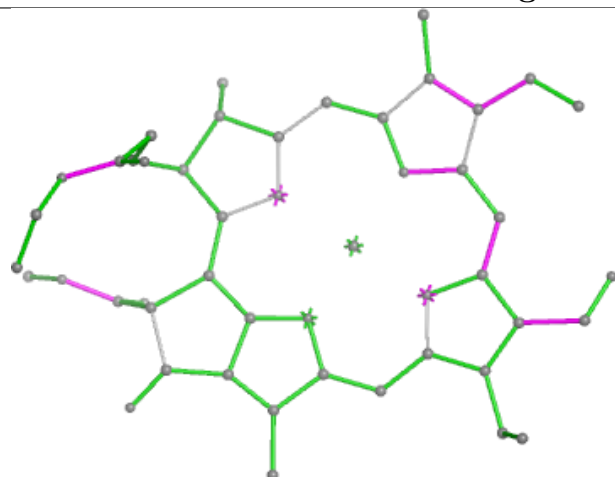
Rings



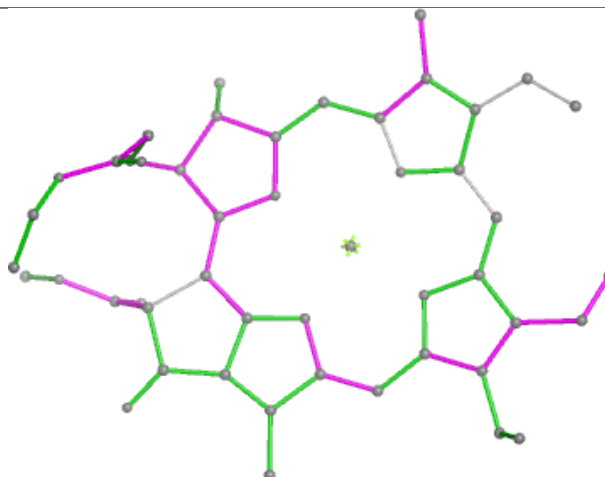




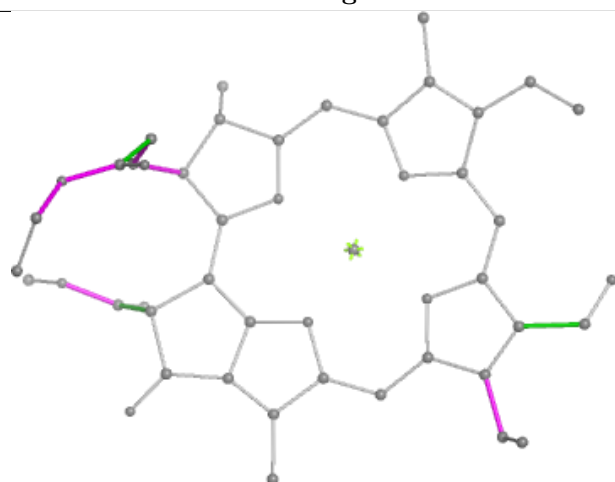
## Ligand CHL n 605



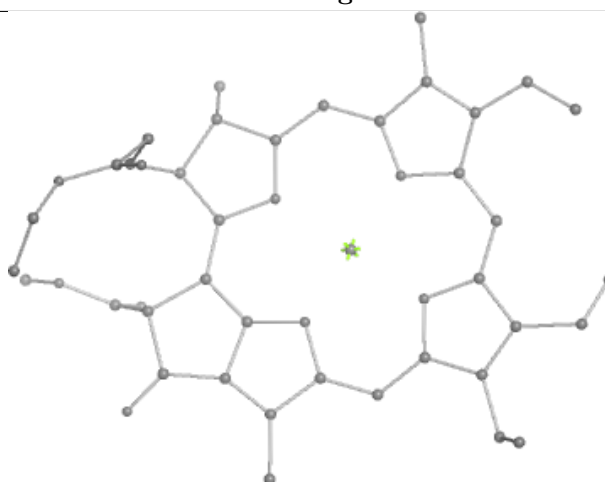
Bond lengths



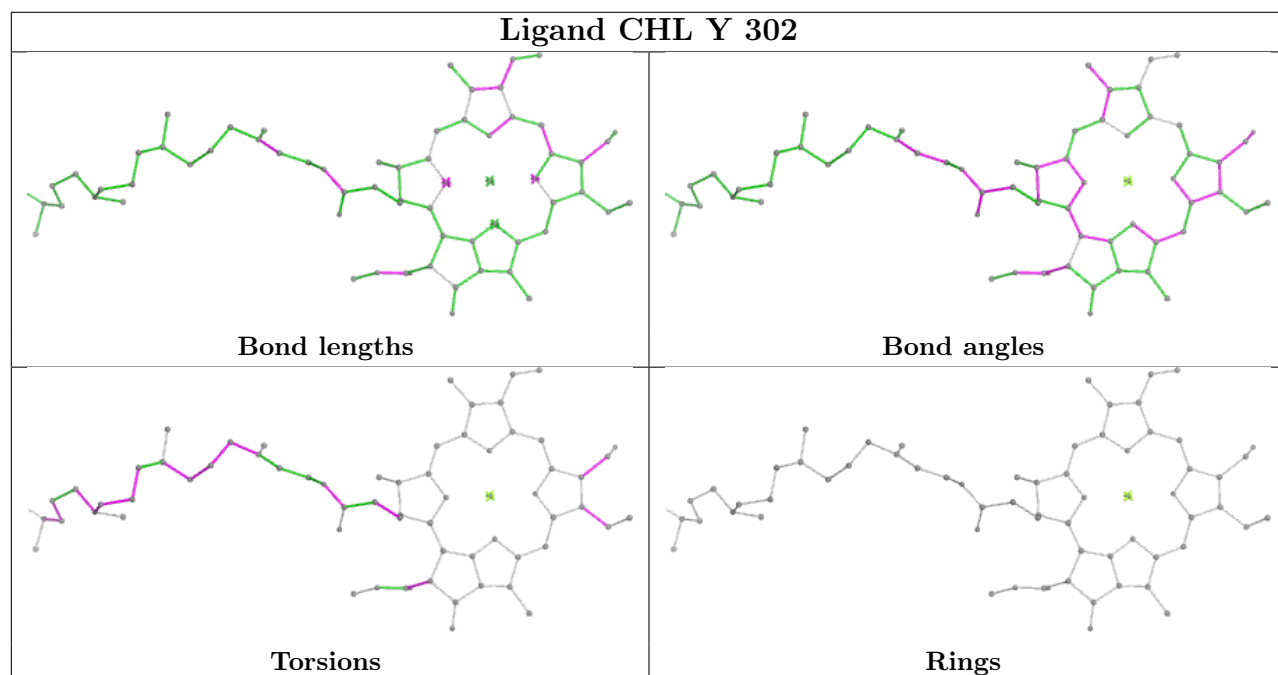
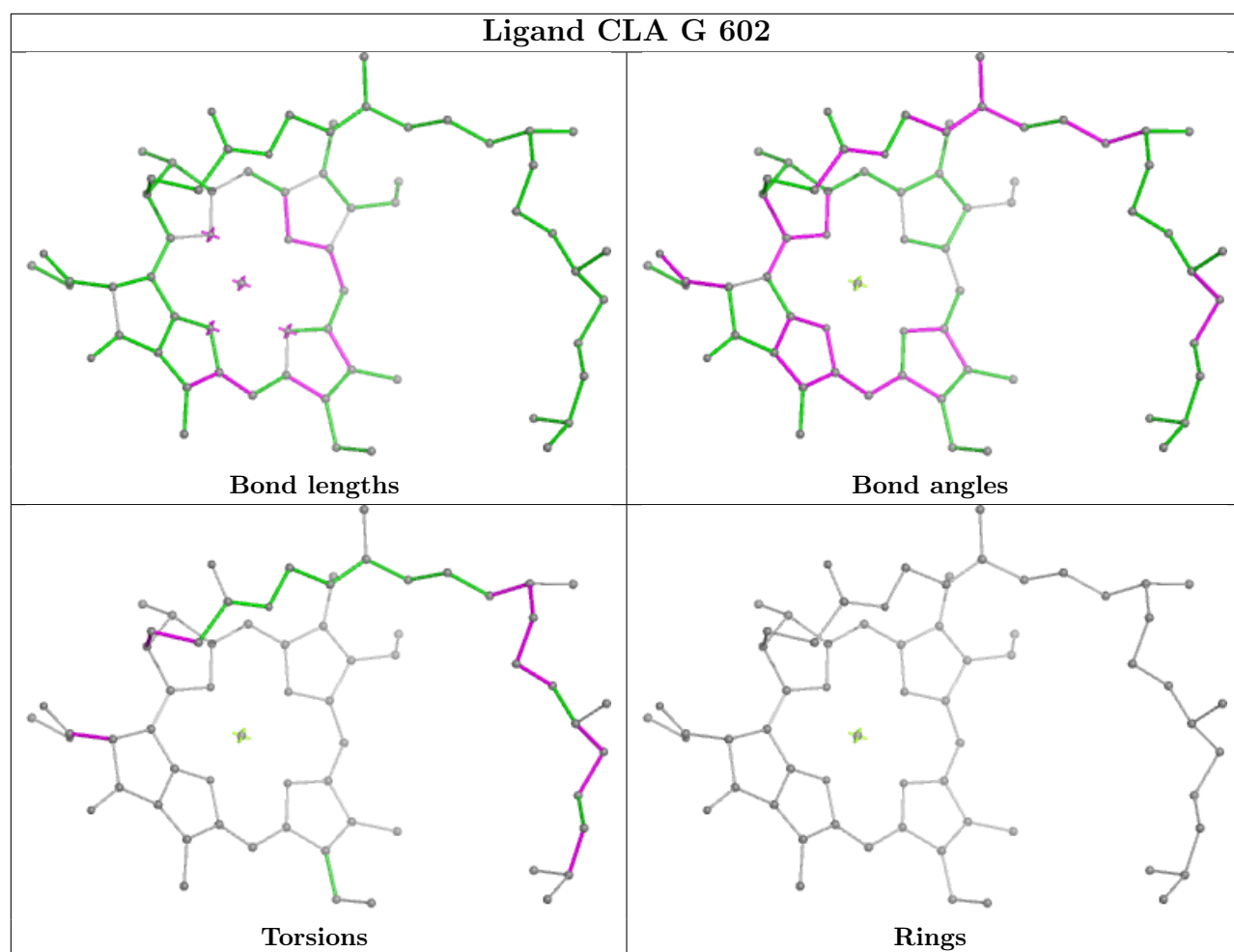
Bond angles

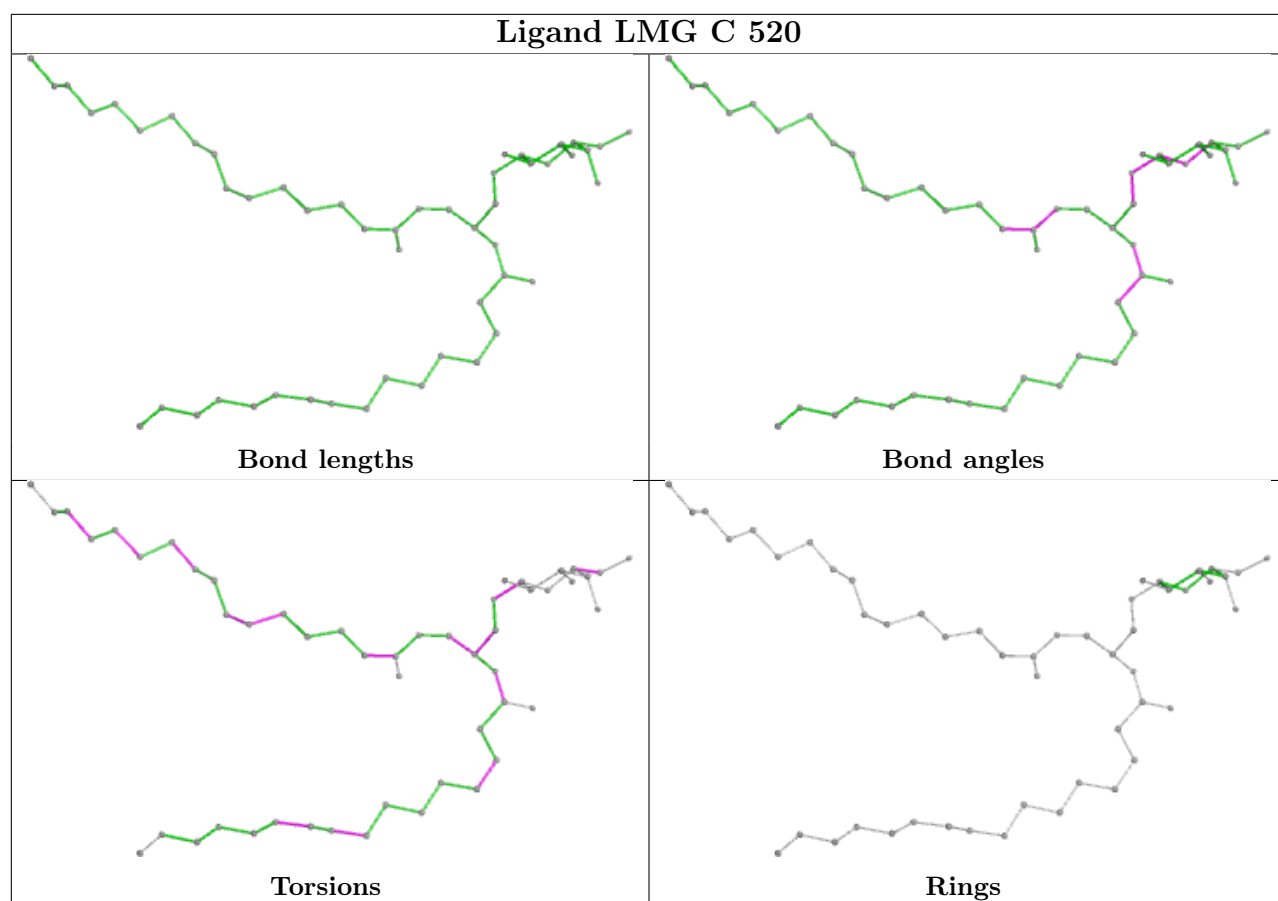


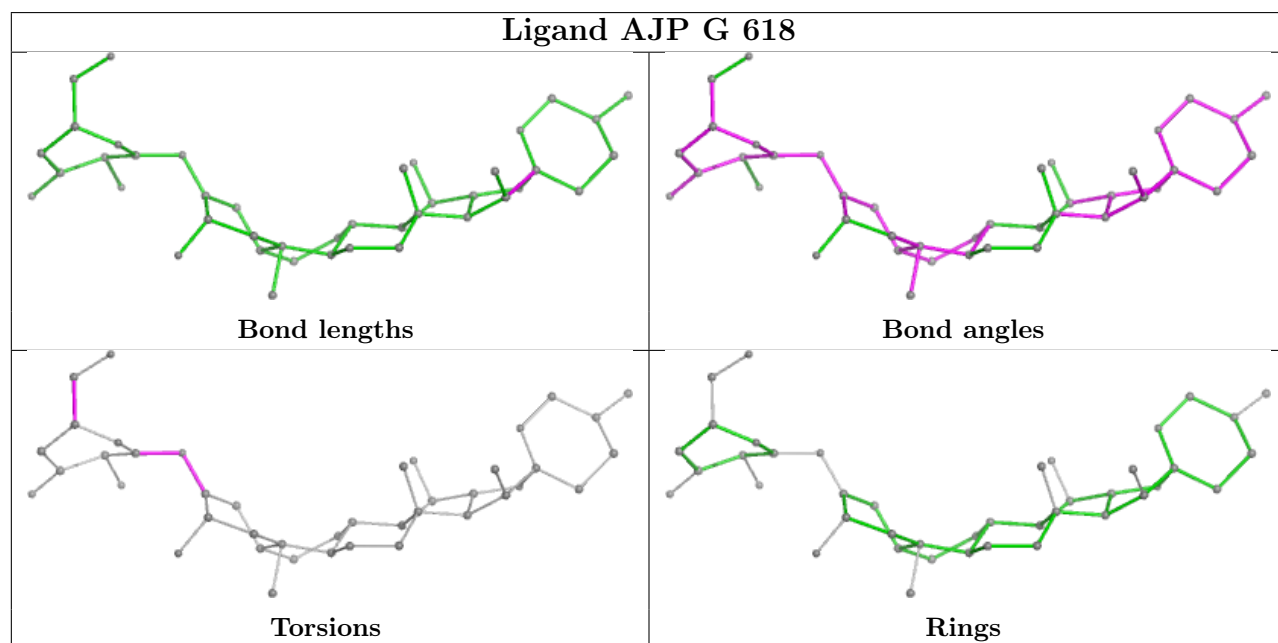
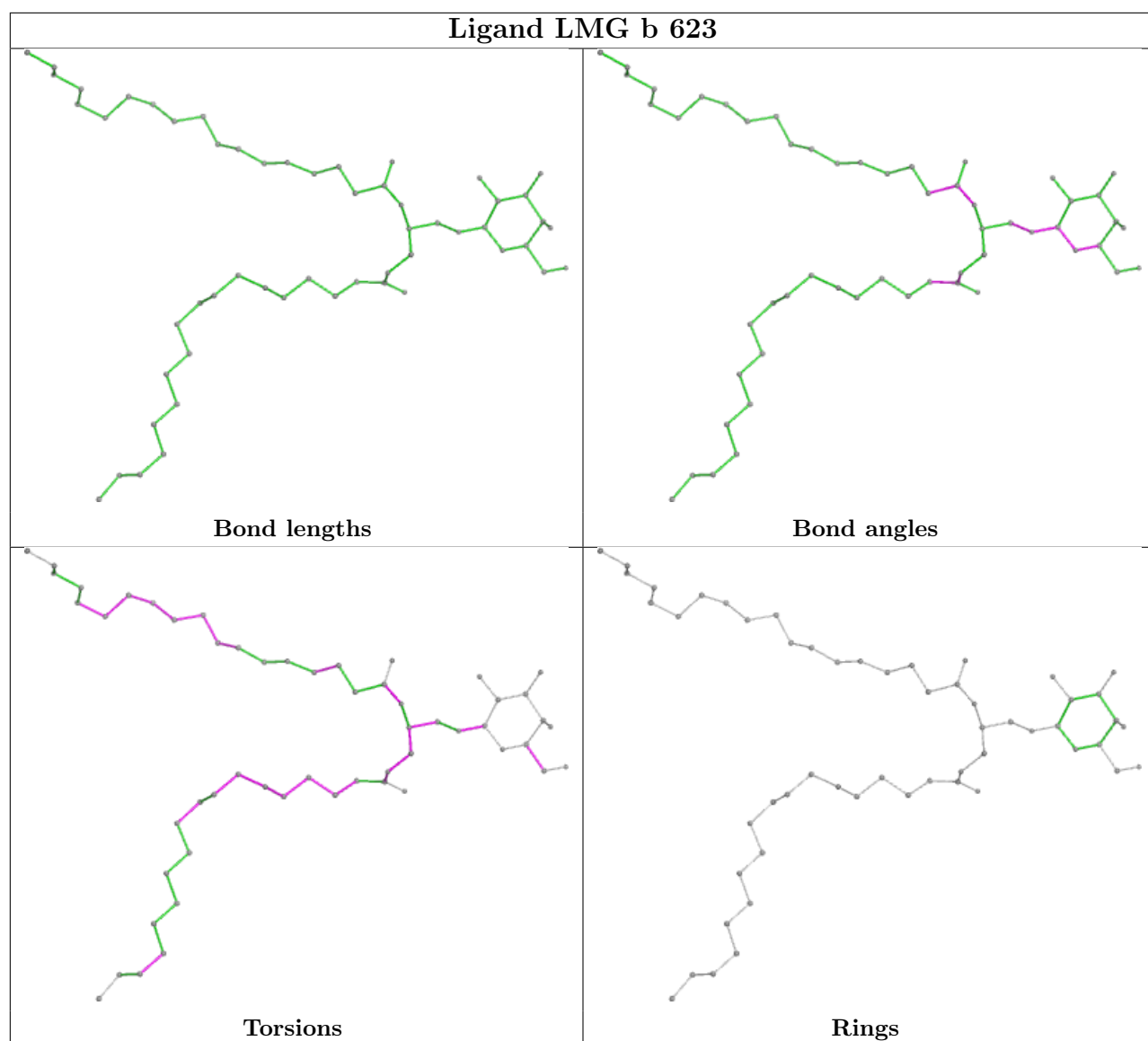
Torsions

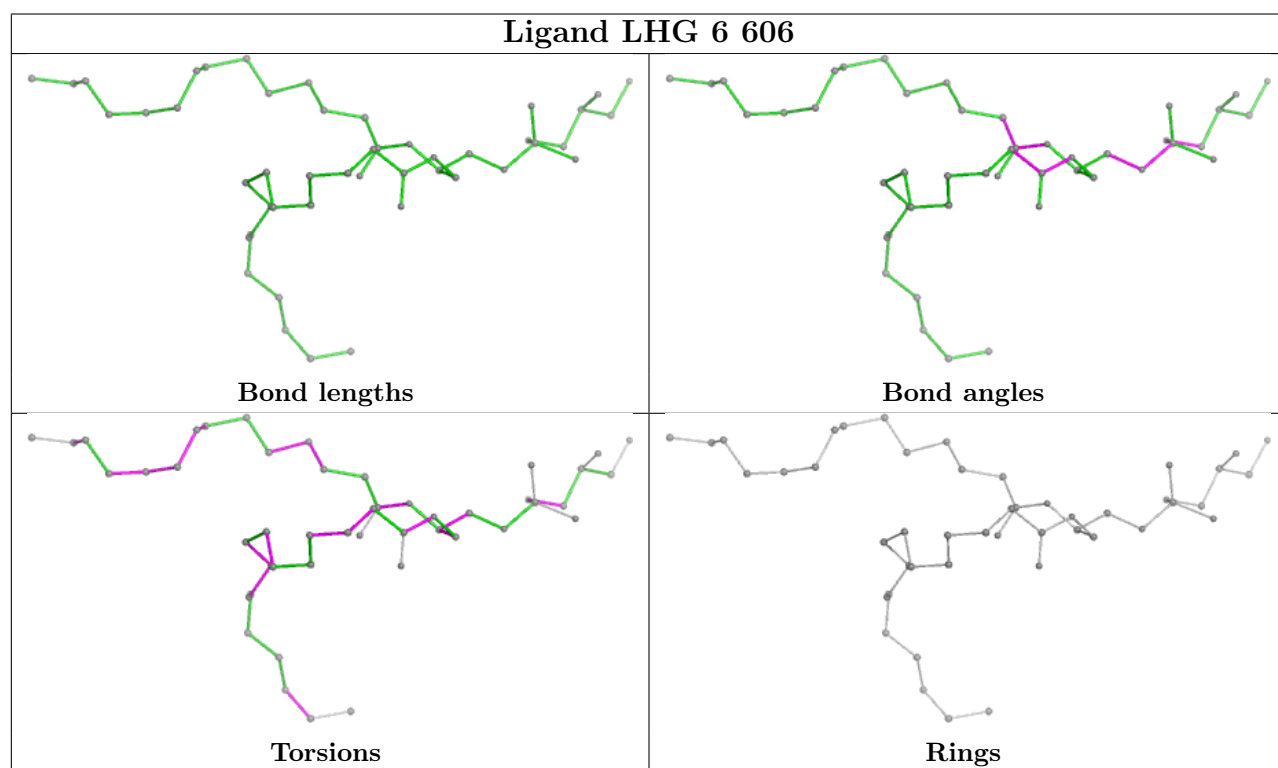
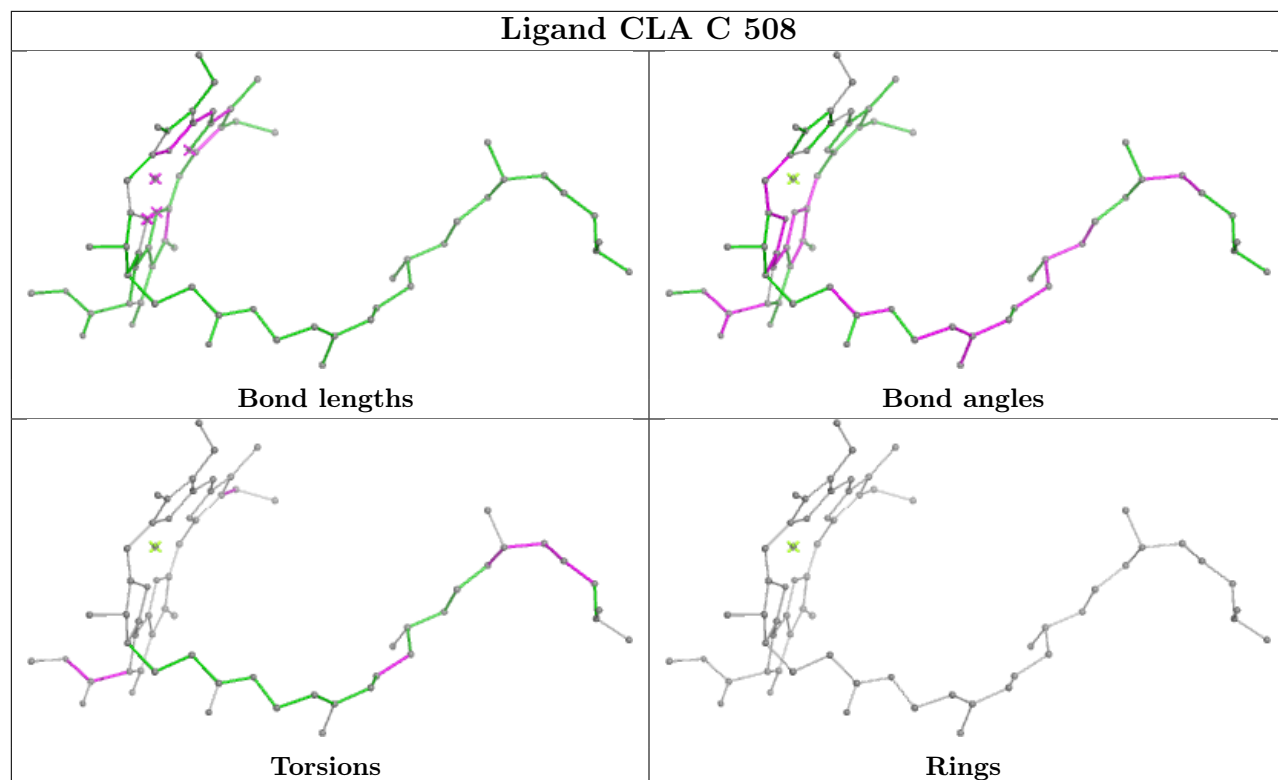


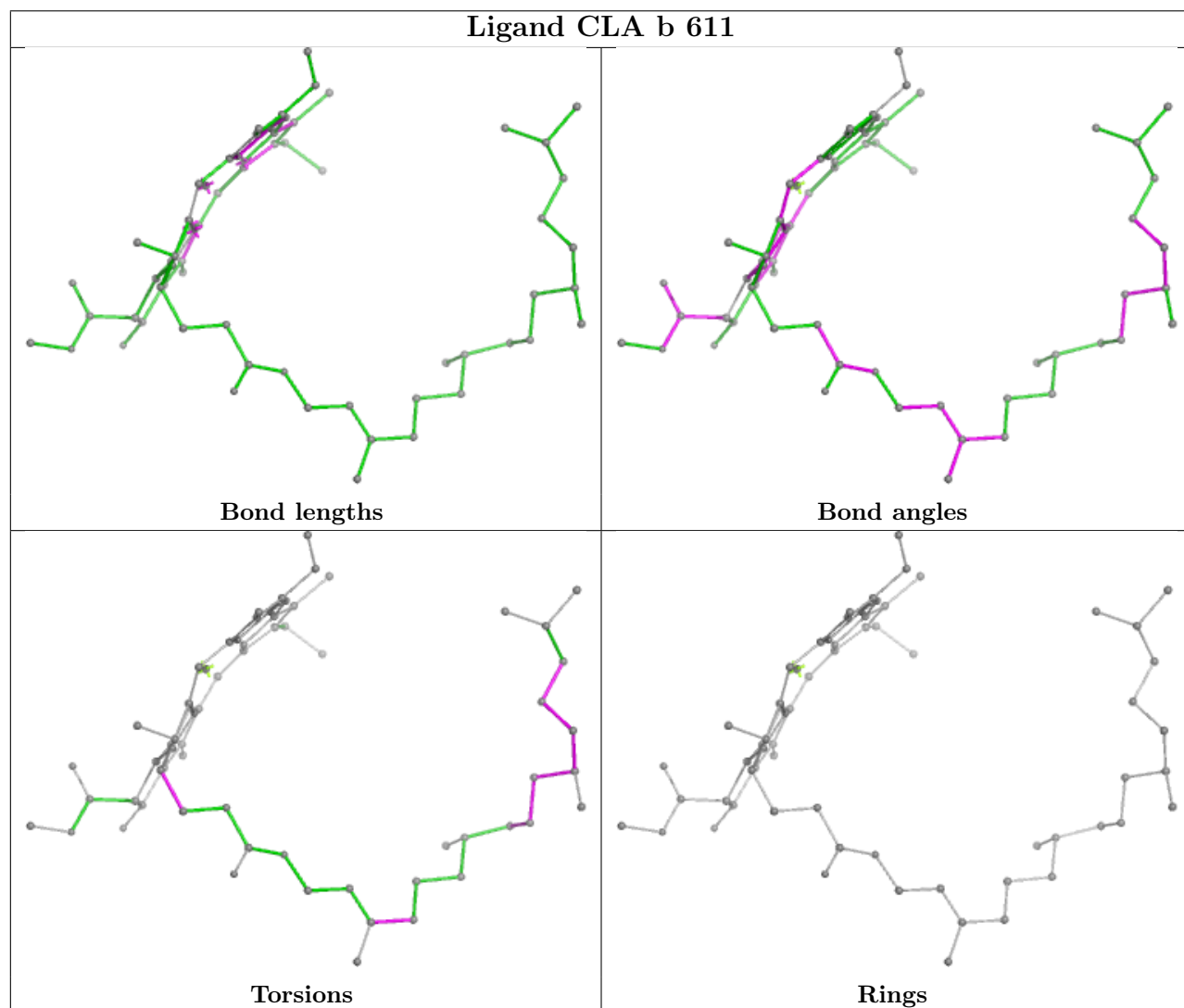
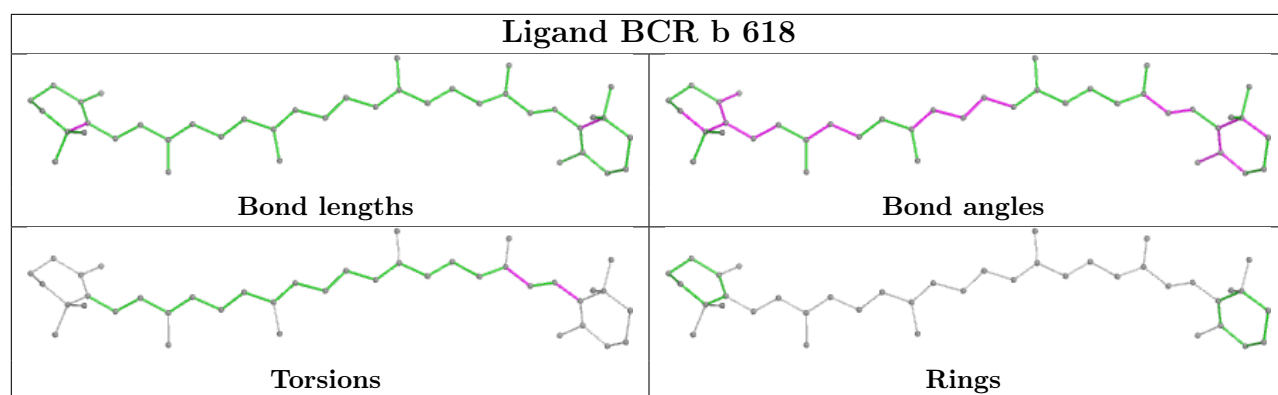
Rings

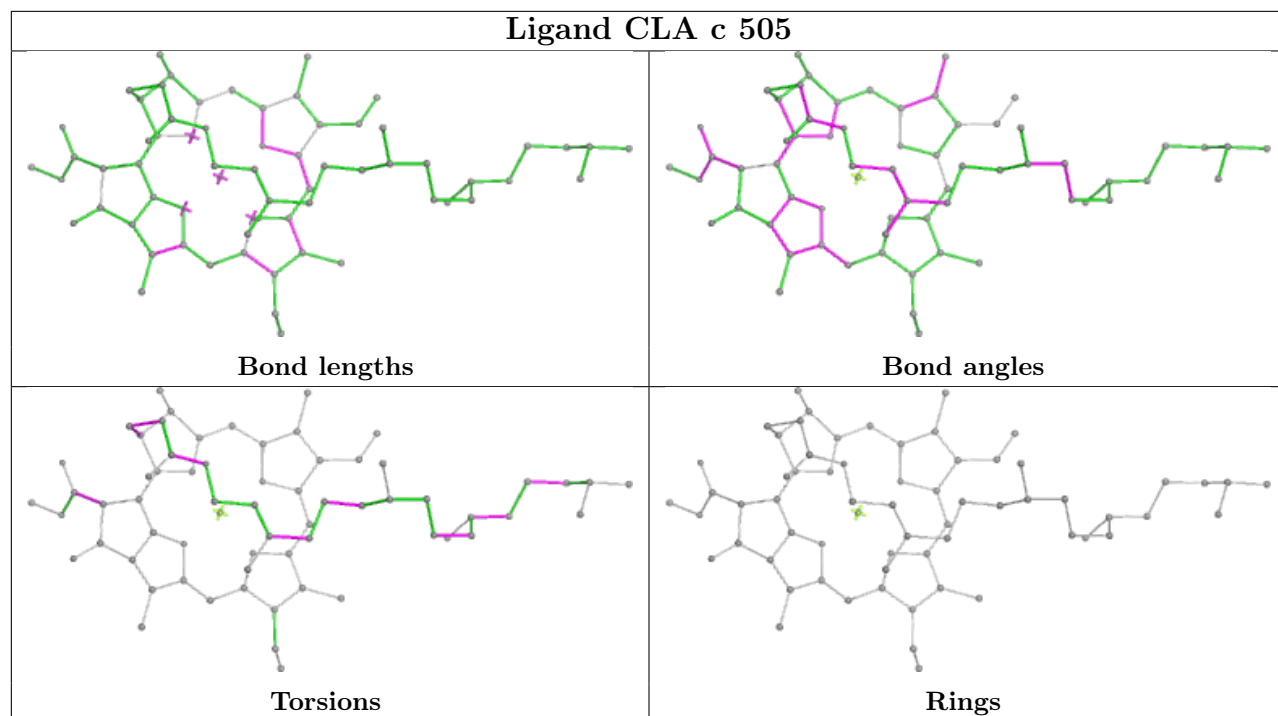
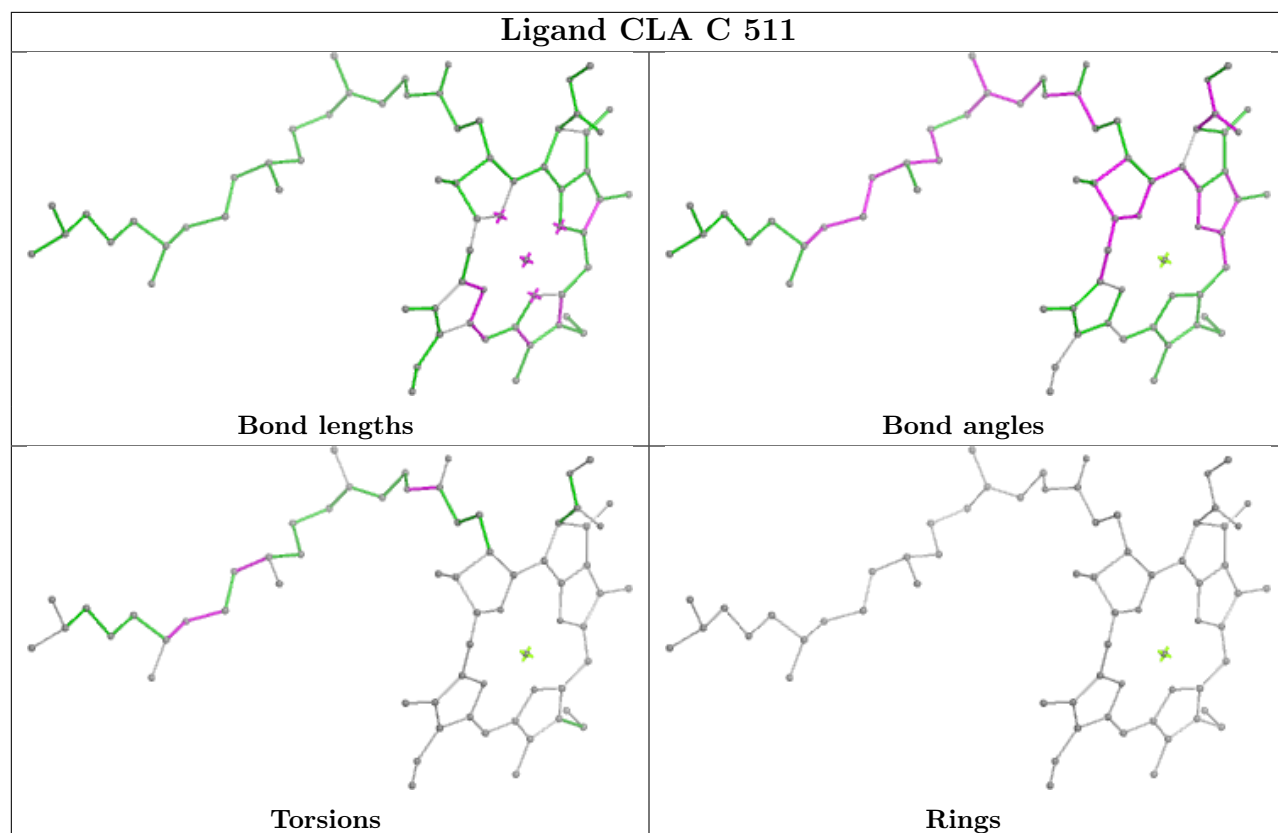




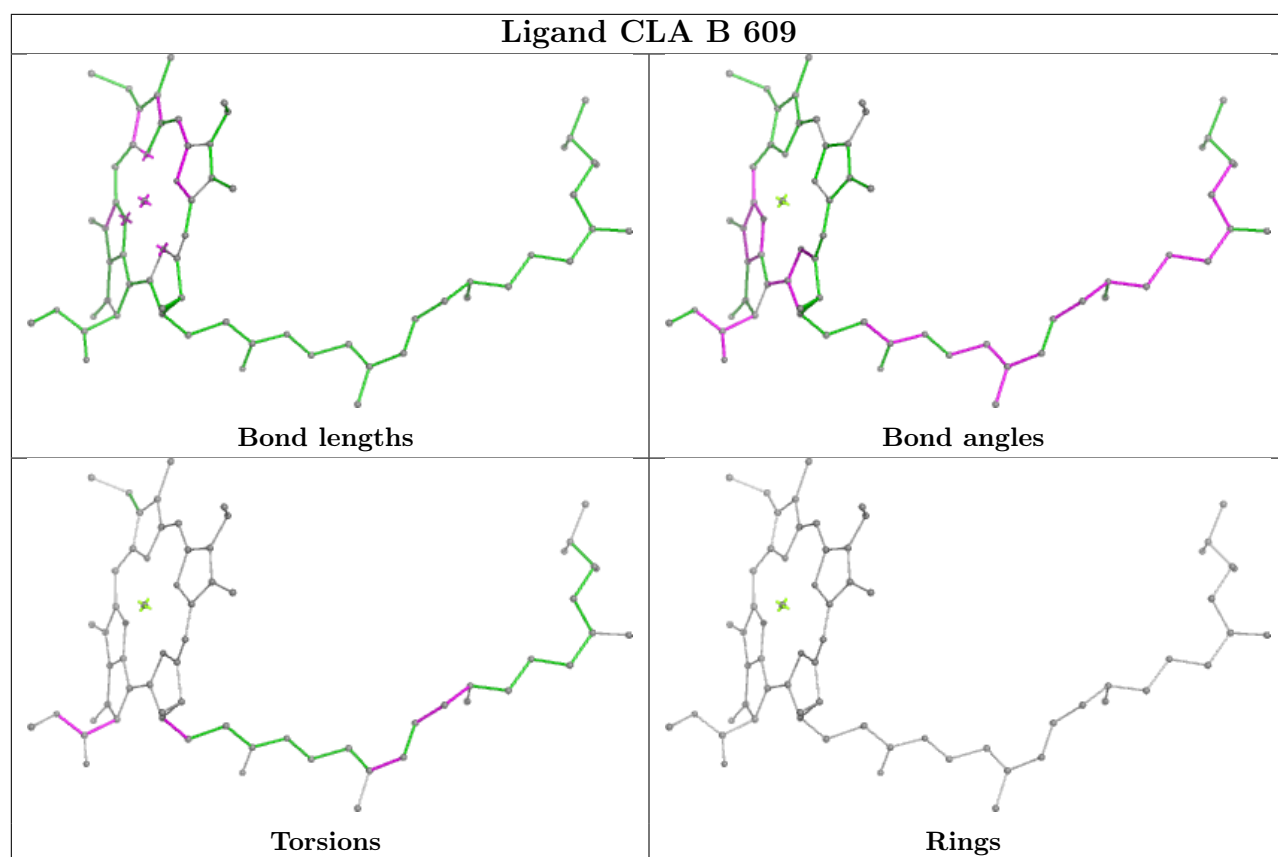


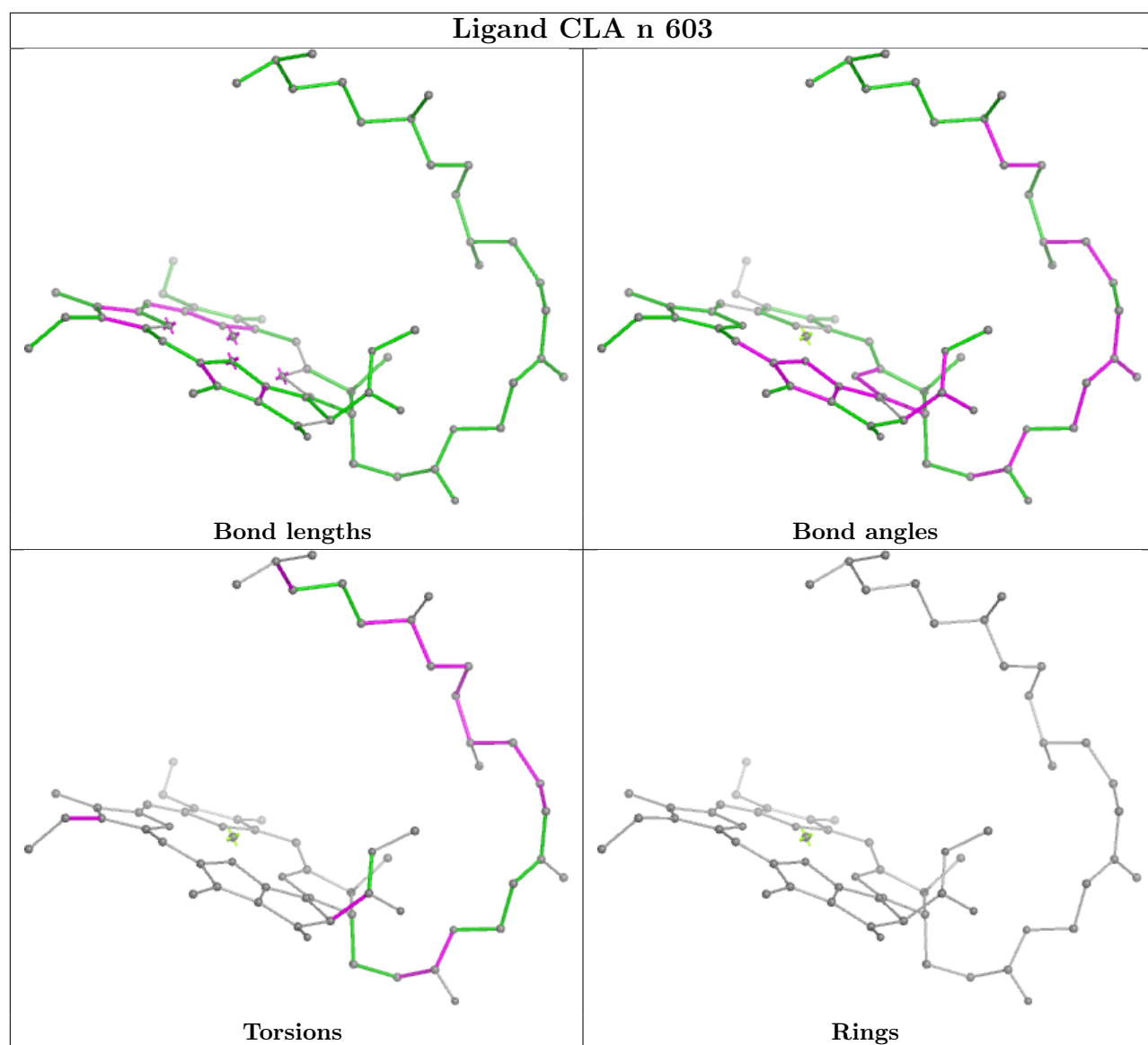




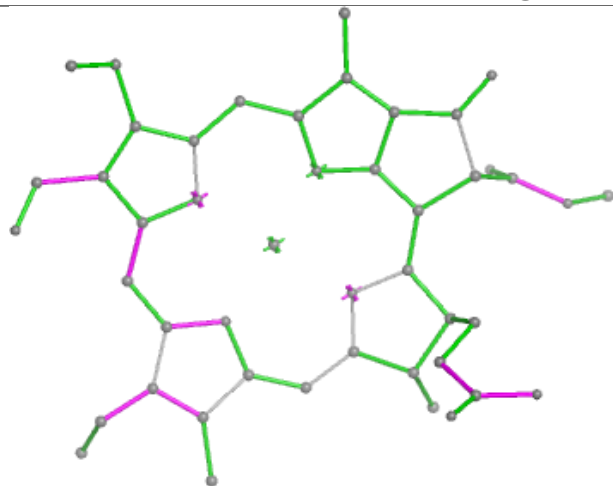
**Ligand CLA c 505****Ligand CLA C 511**



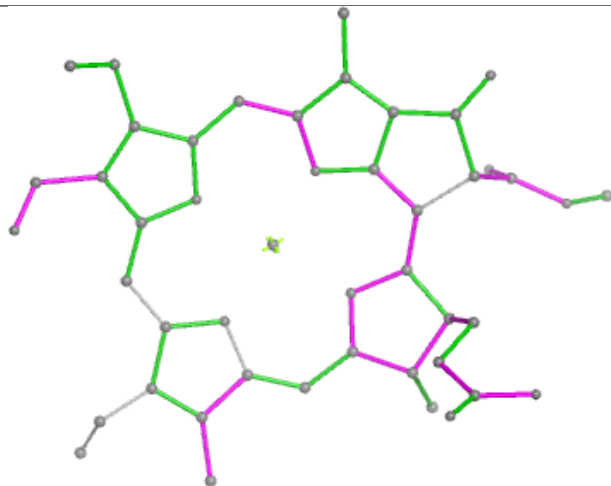




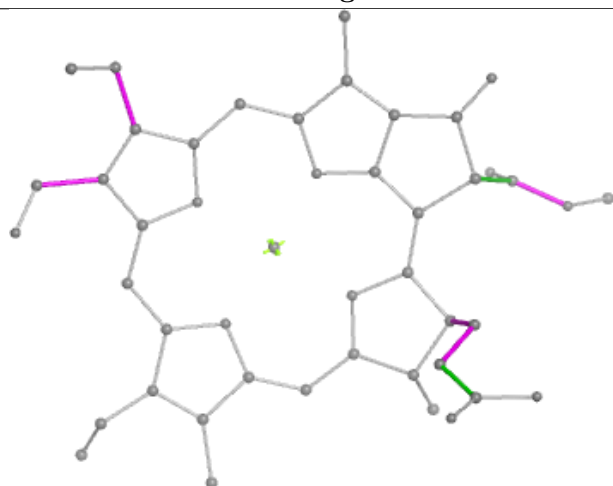
## Ligand CHL S 307



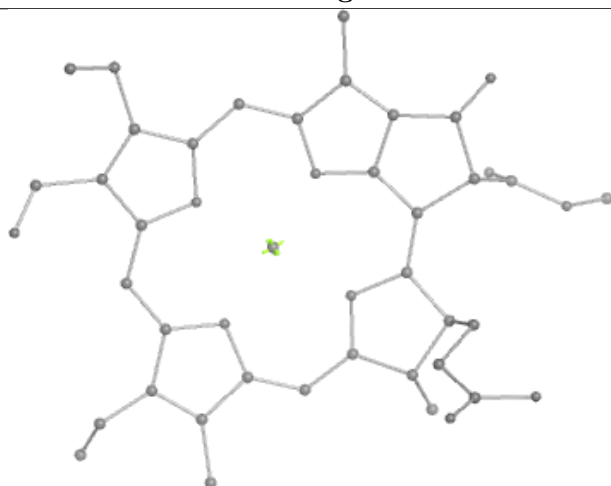
Bond lengths



Bond angles

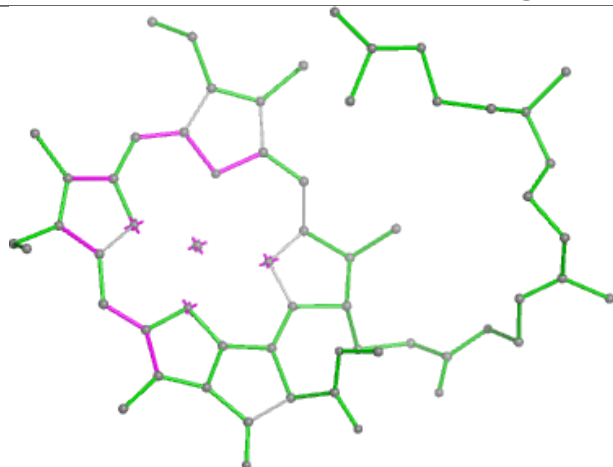


Torsions

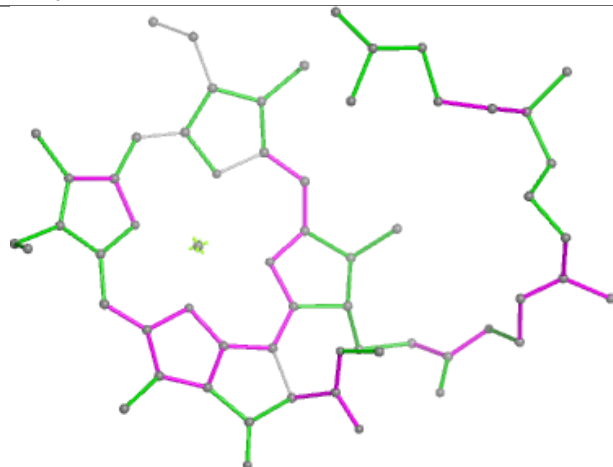


Rings

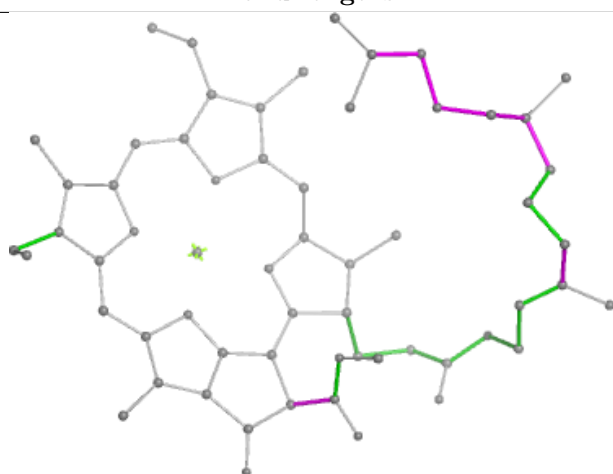
## Ligand CLA y 313



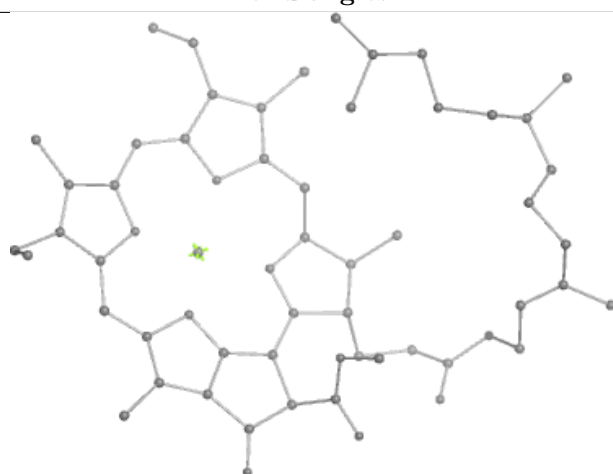
Bond lengths



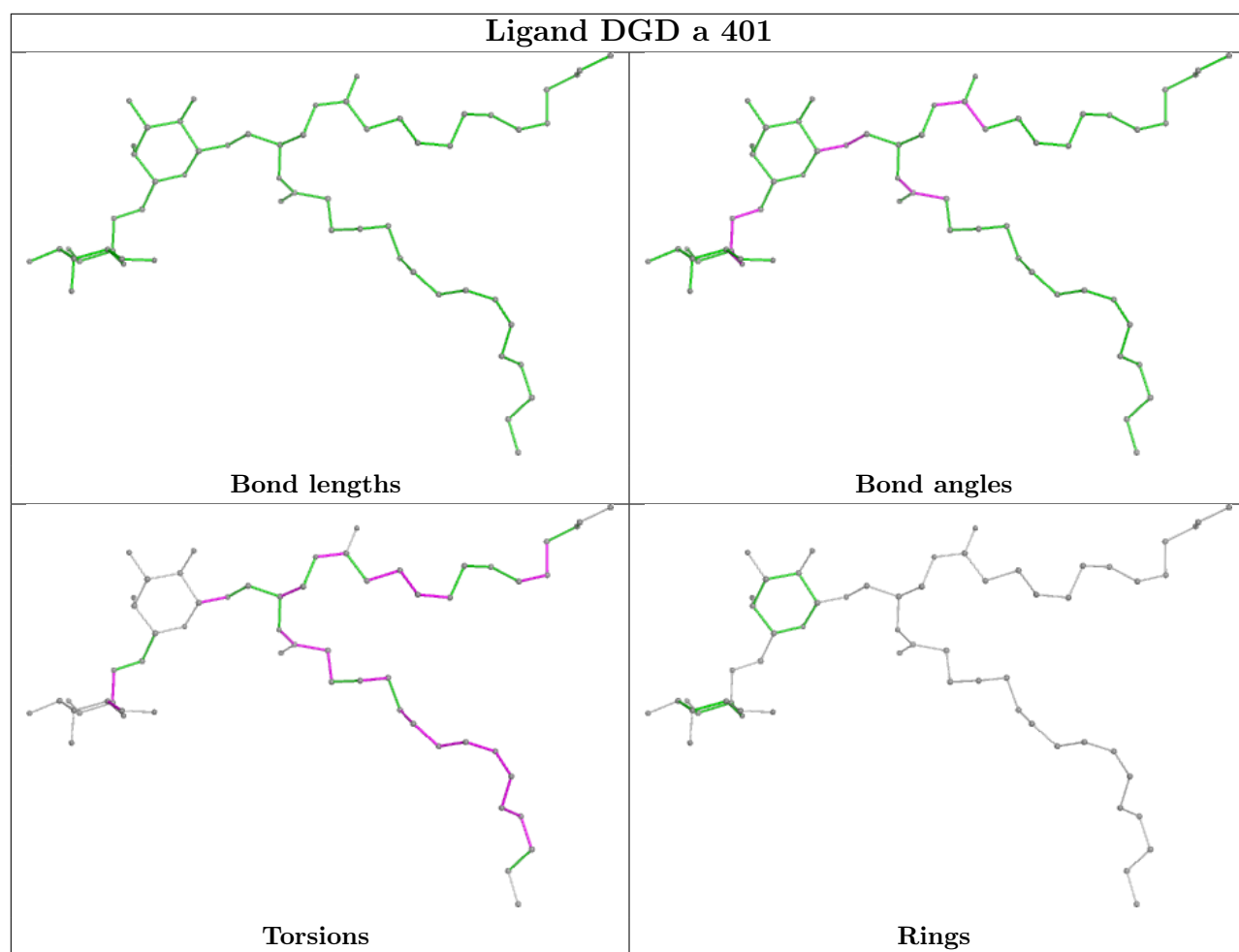
Bond angles



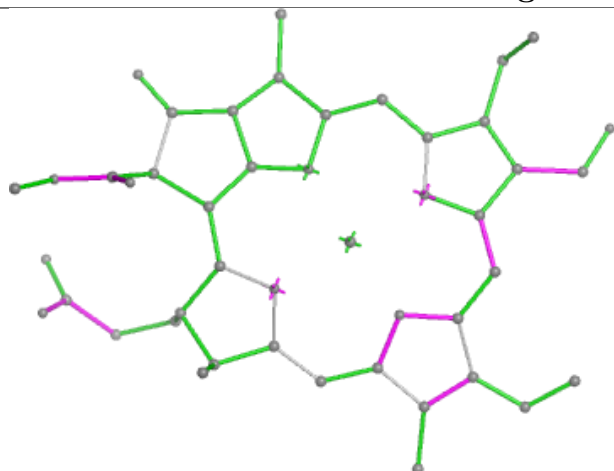
Torsions



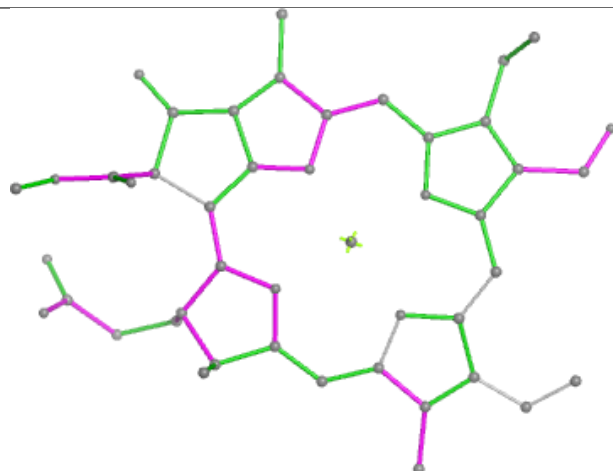
Rings



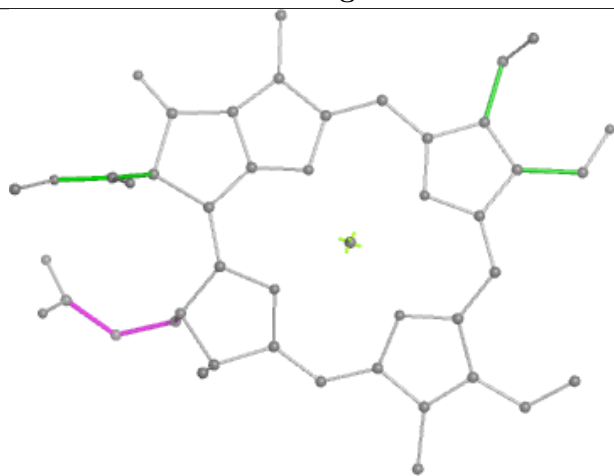
## Ligand CHL 1 302



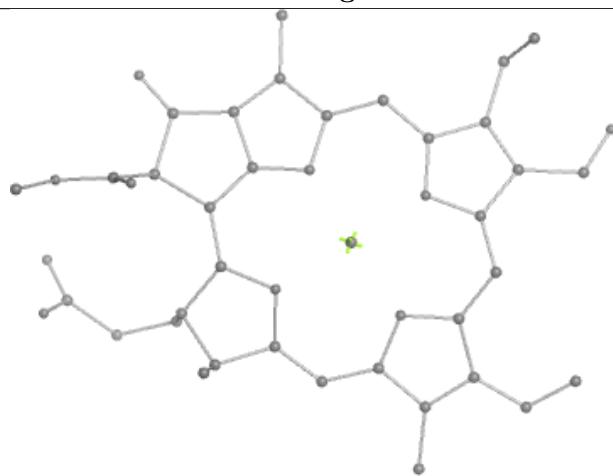
Bond lengths



Bond angles

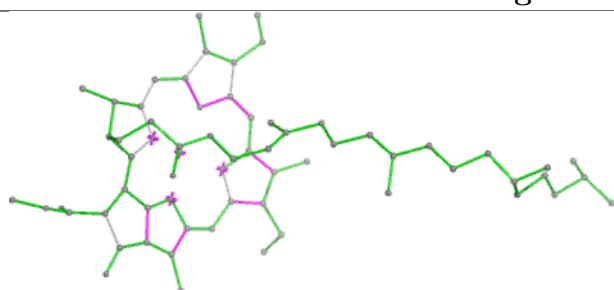


Torsions

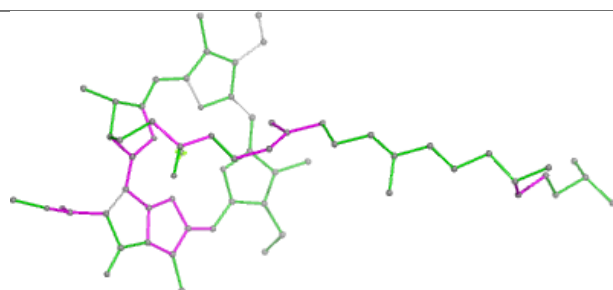


Rings

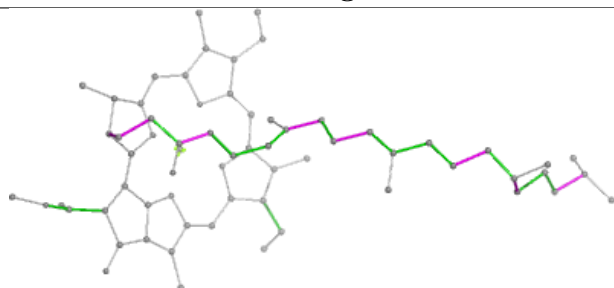
## Ligand CLA B 608



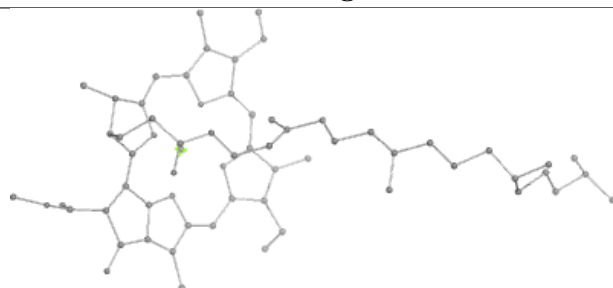
Bond lengths



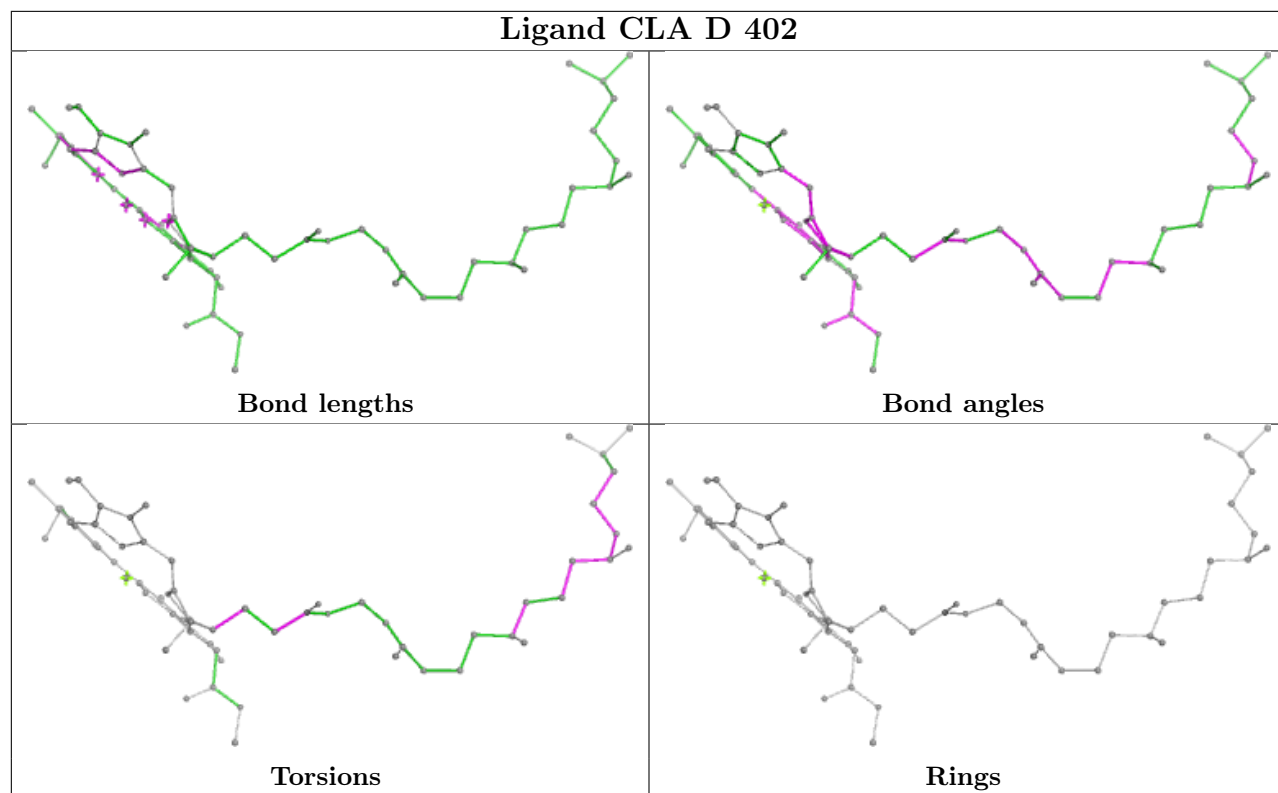
Bond angles

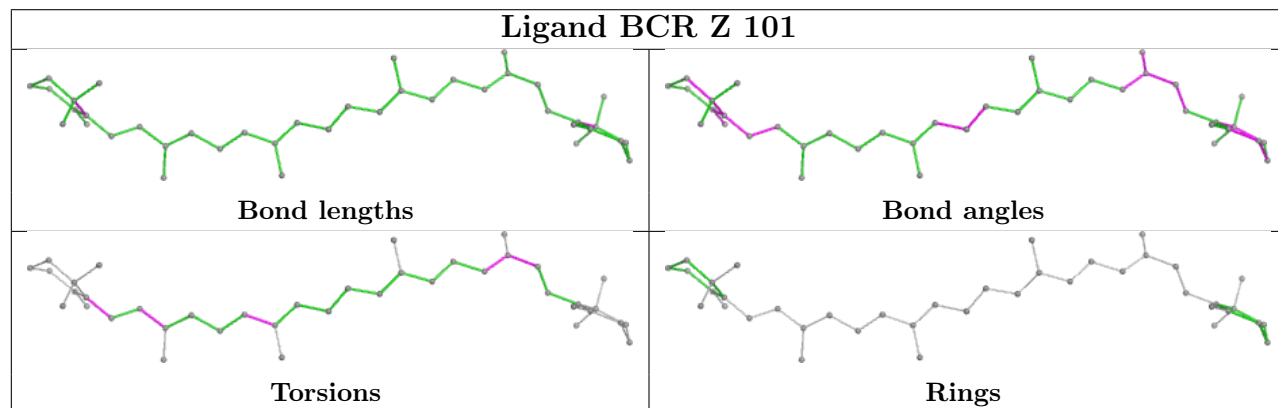
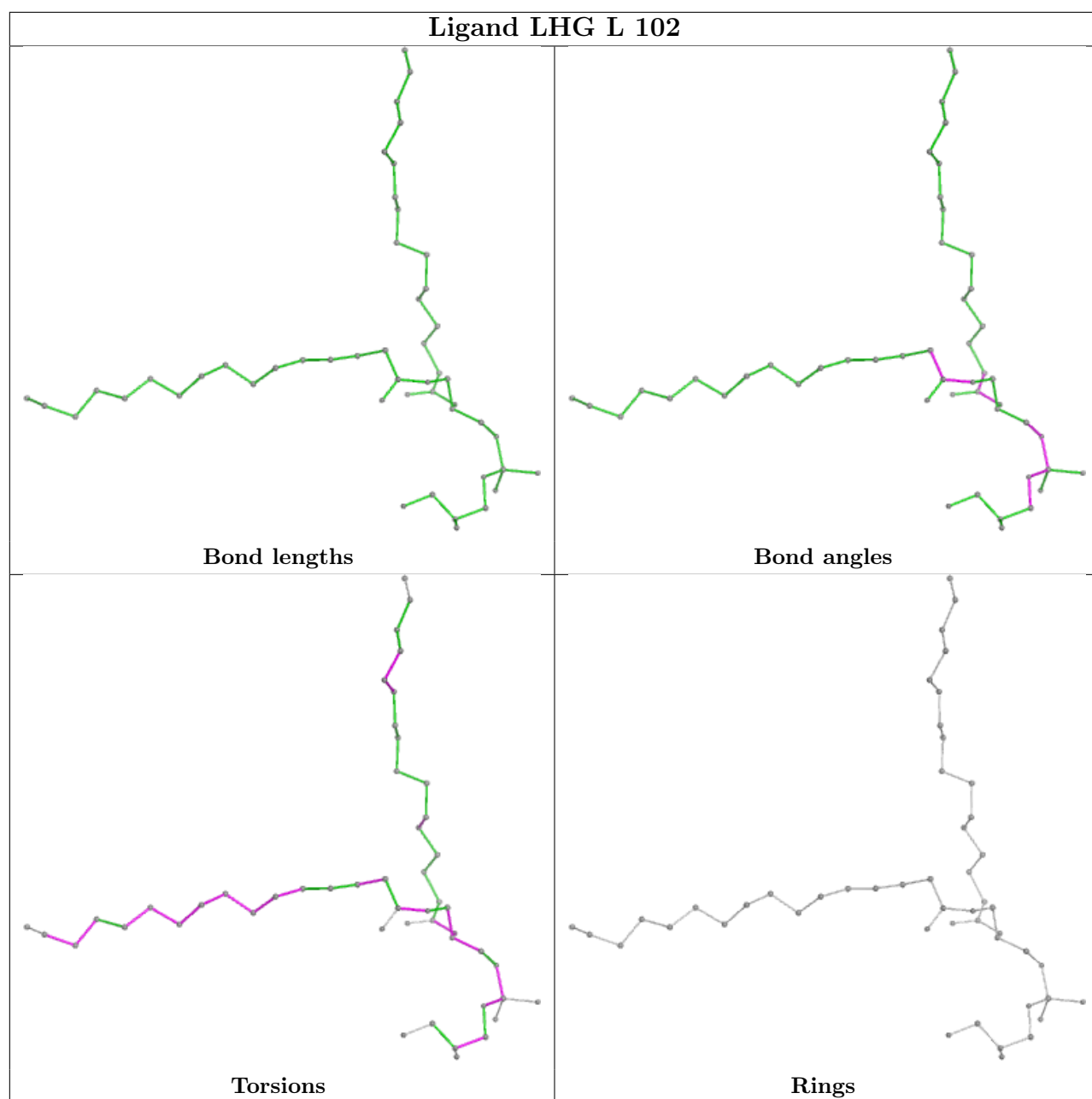


Torsions

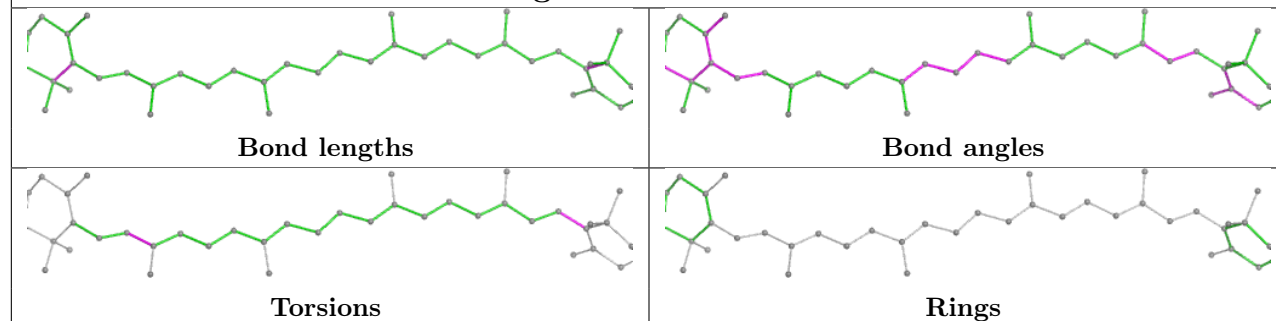
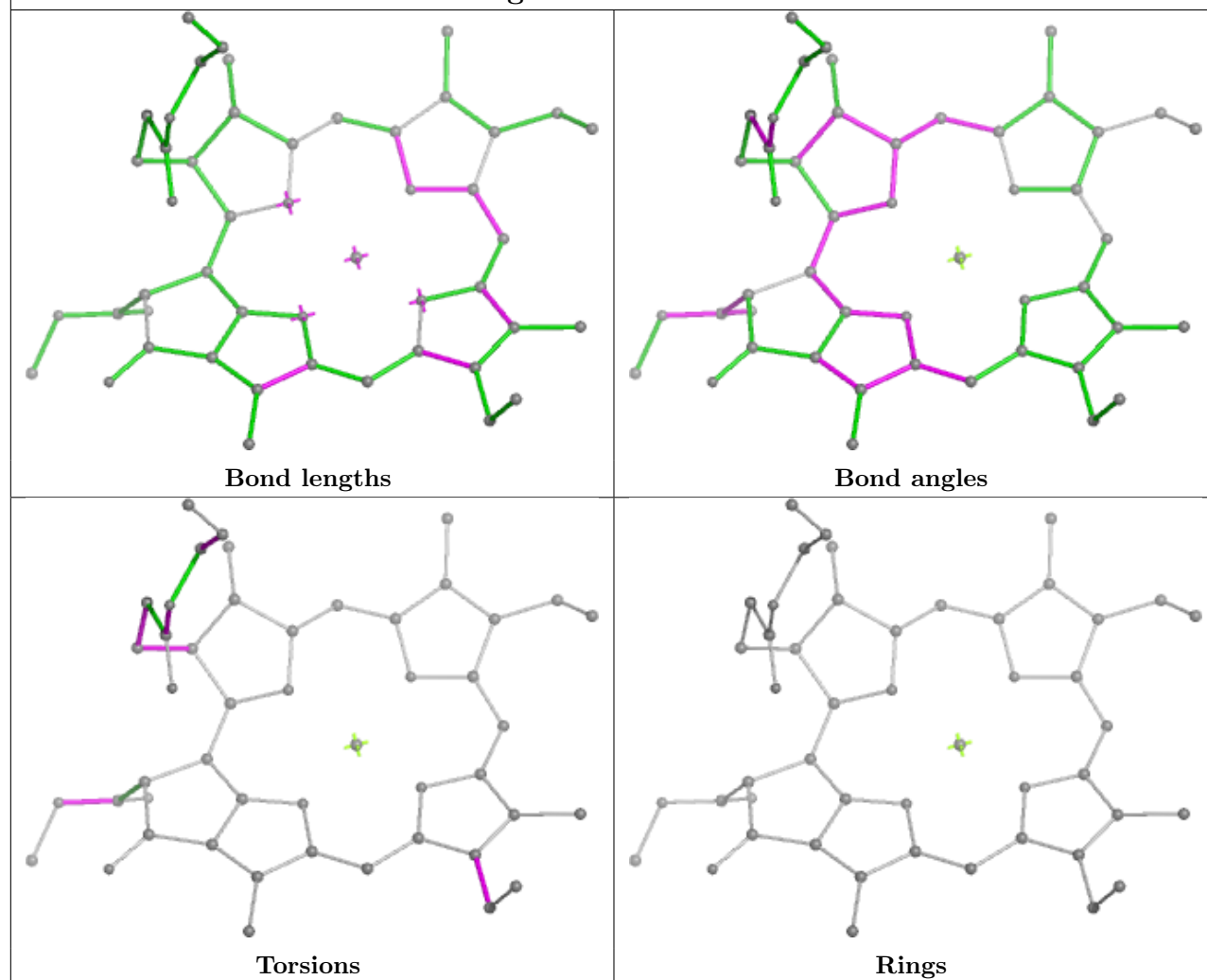


Rings

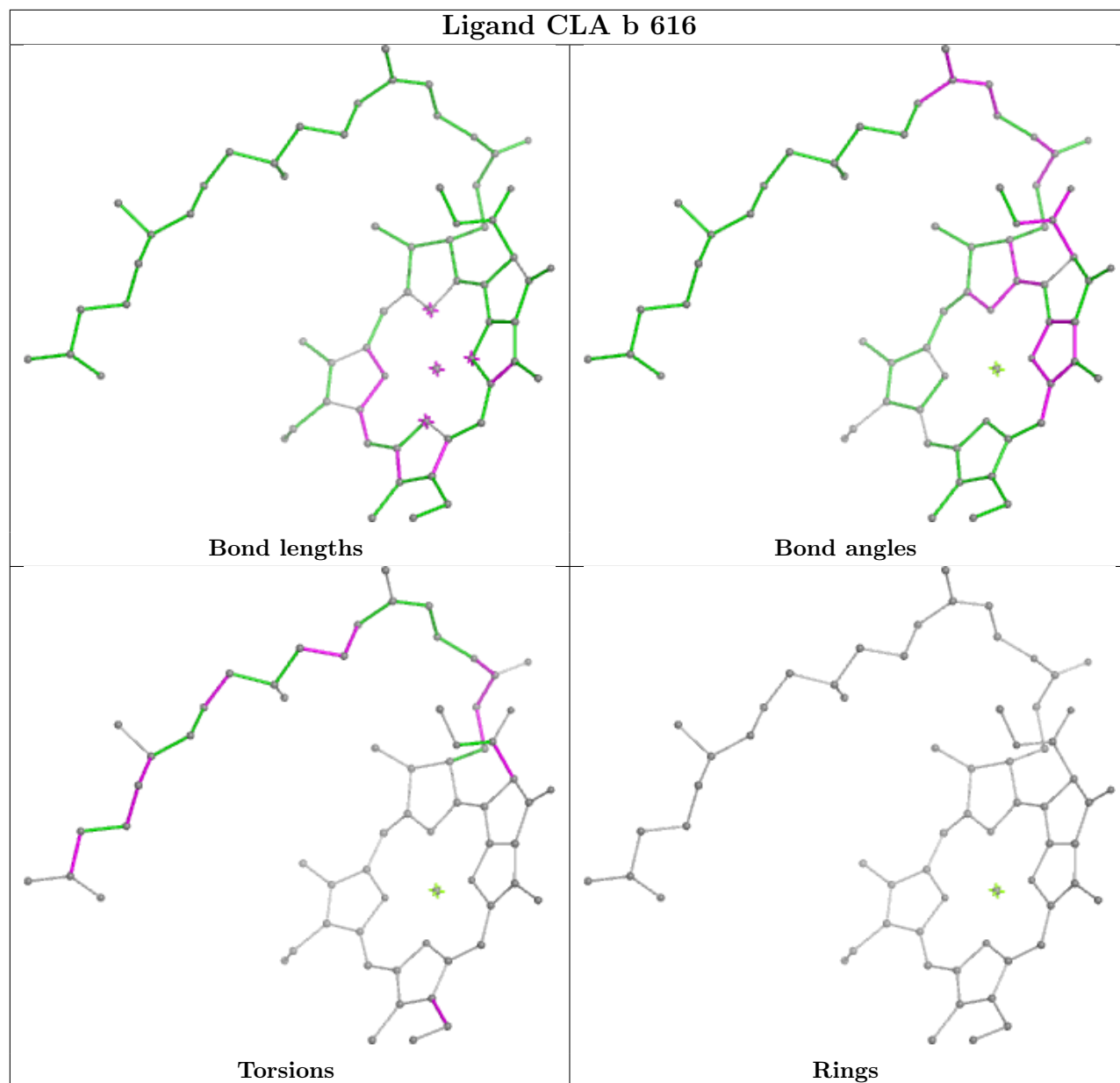




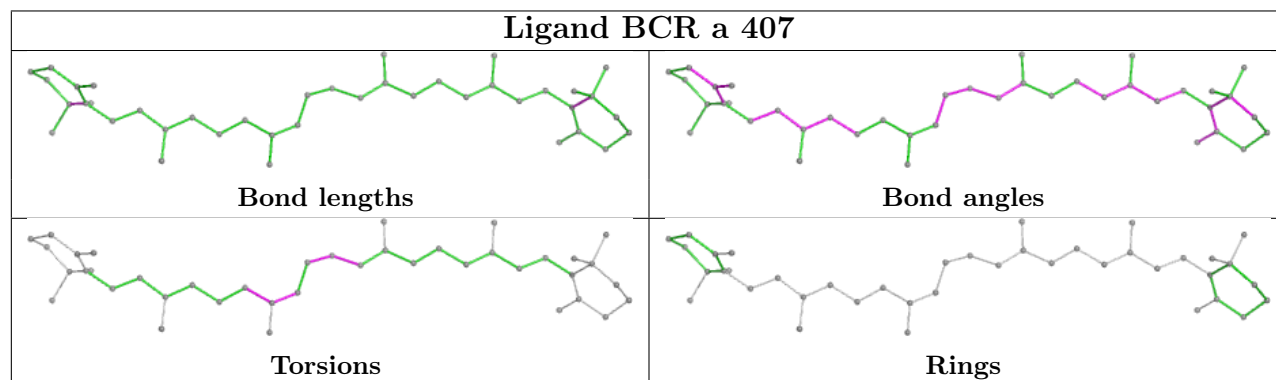


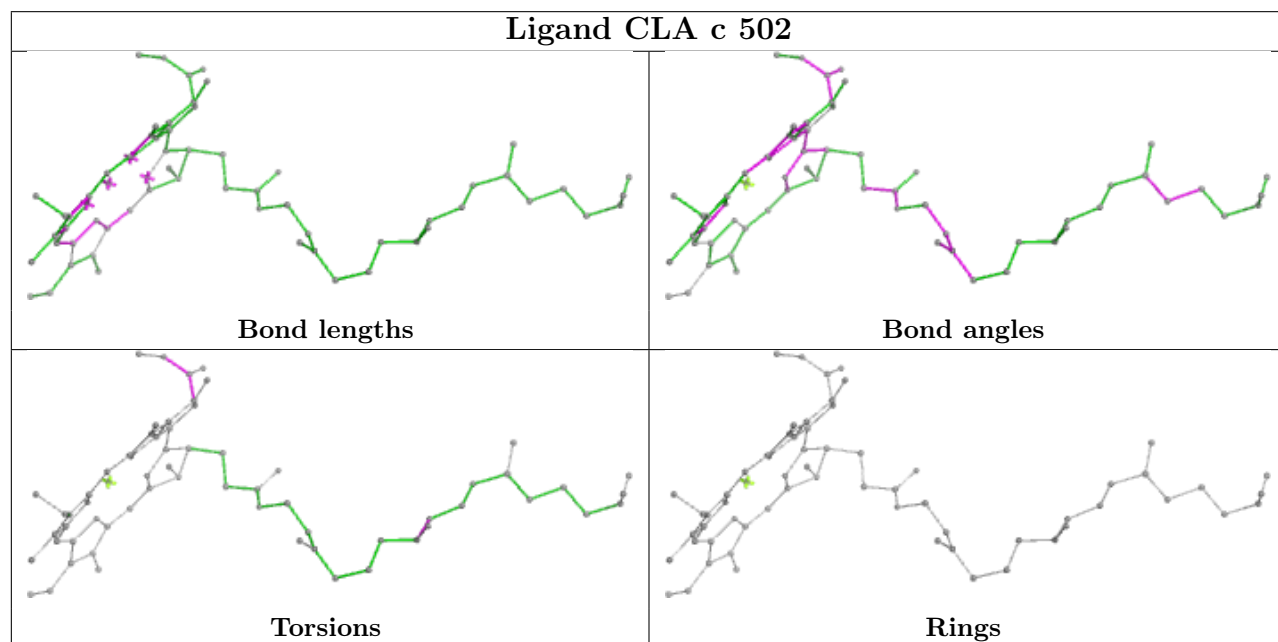
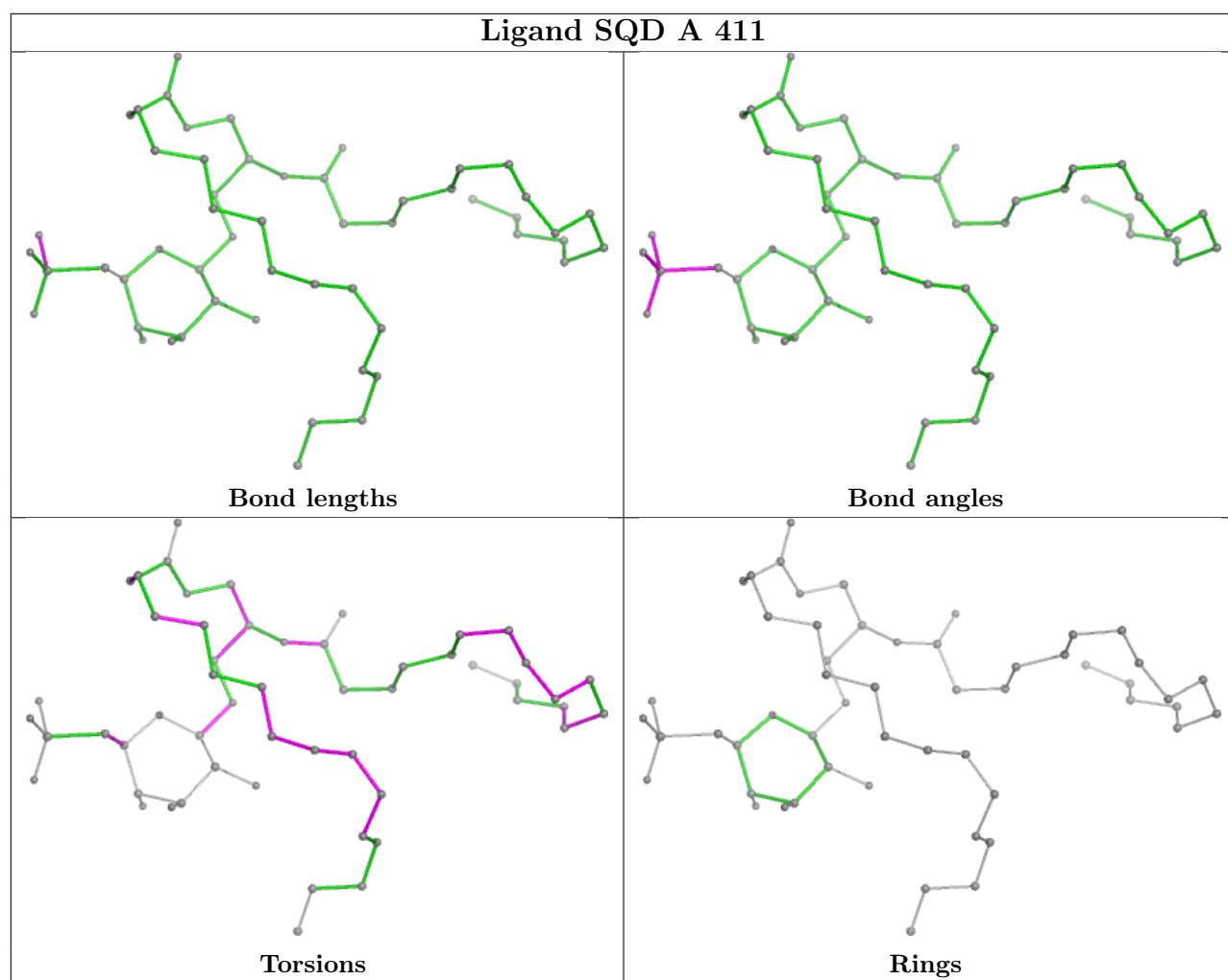
**Ligand BCR b 619****Ligand CLA 2 605**

## Ligand CLA b 616

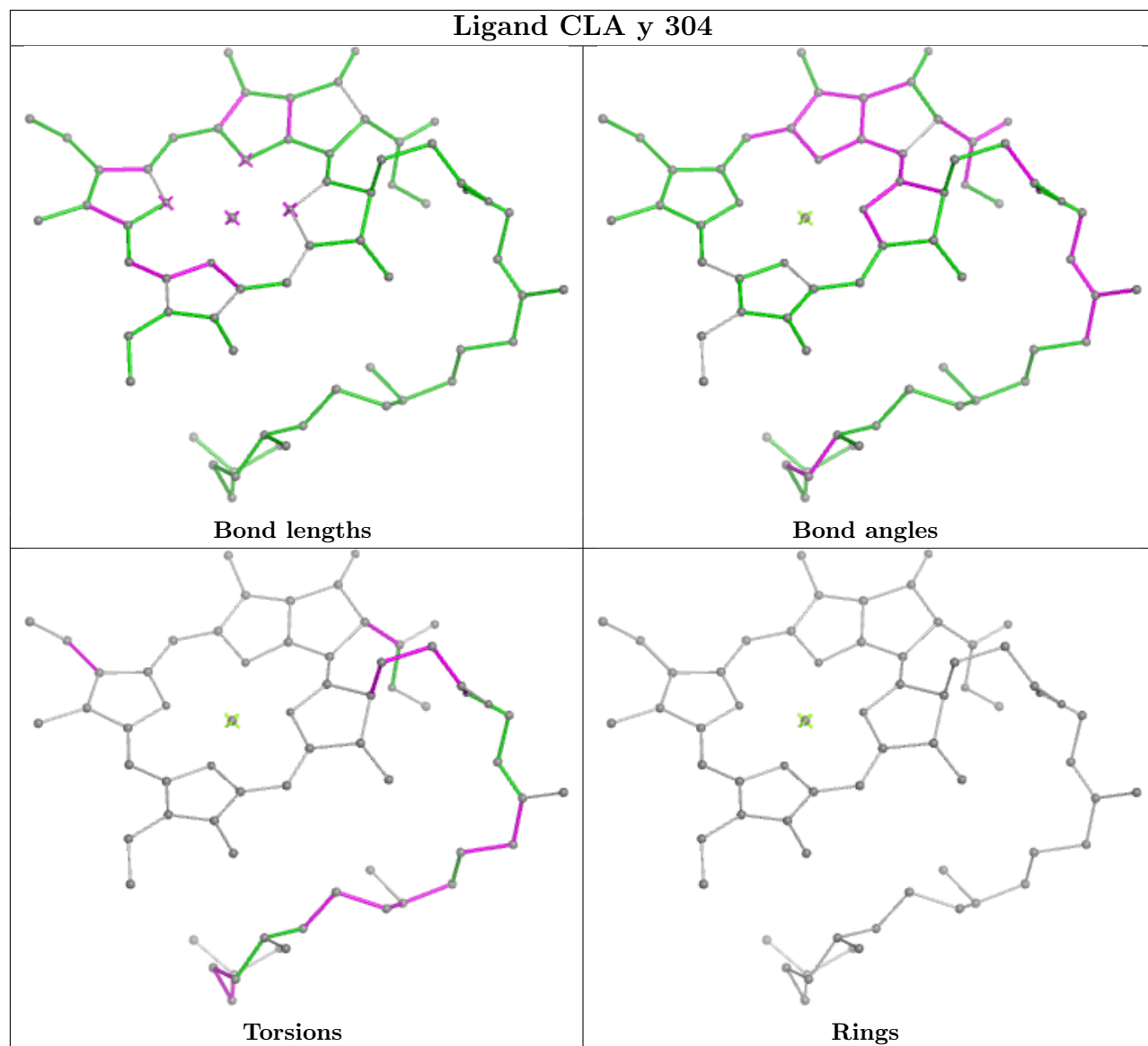


## Ligand BCR a 407

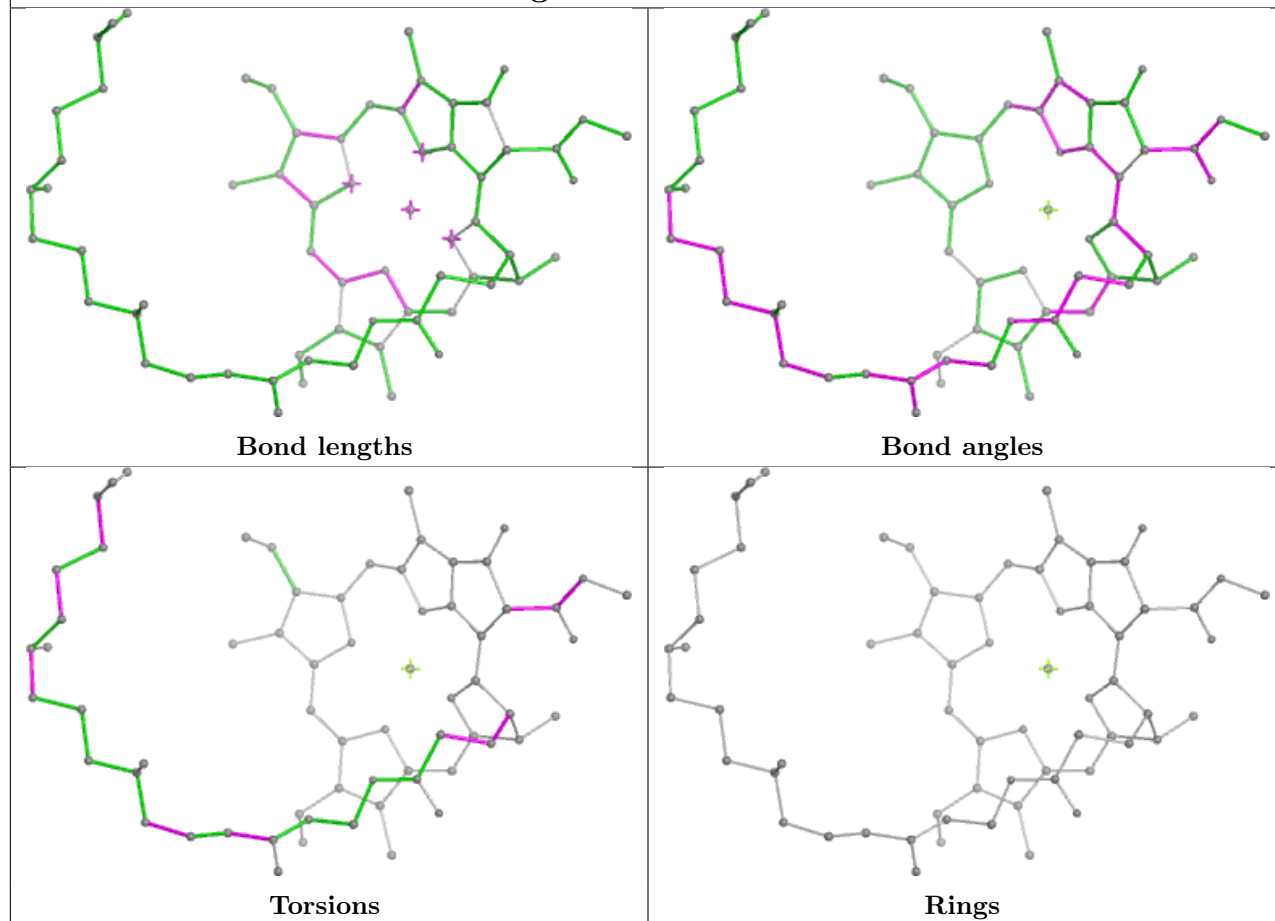




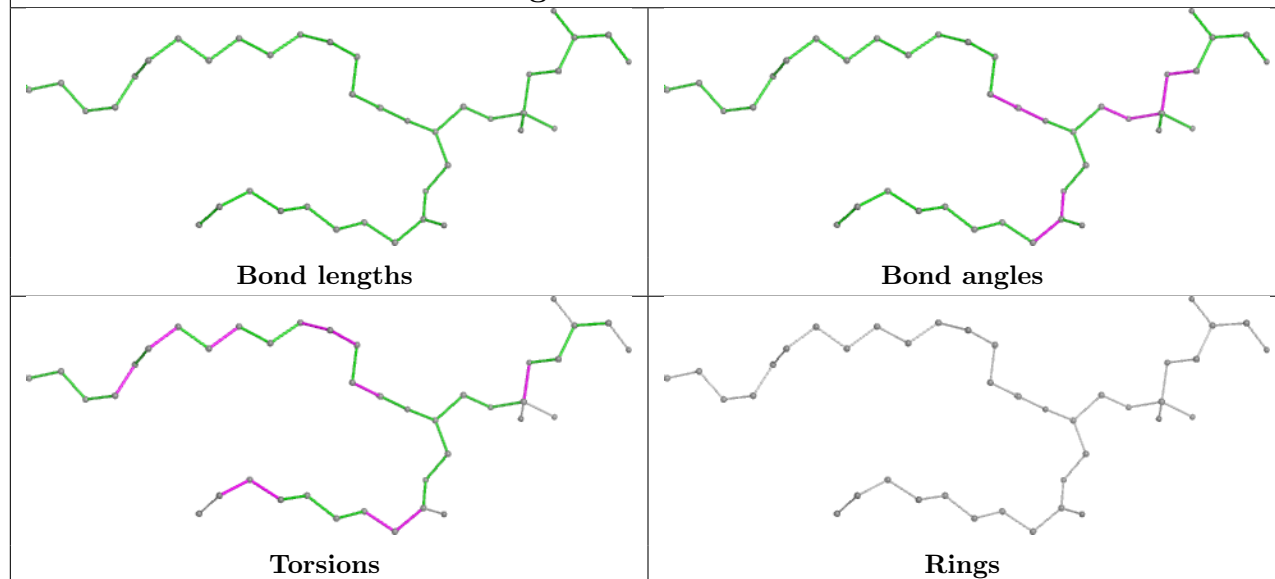
## Ligand CLA y 304

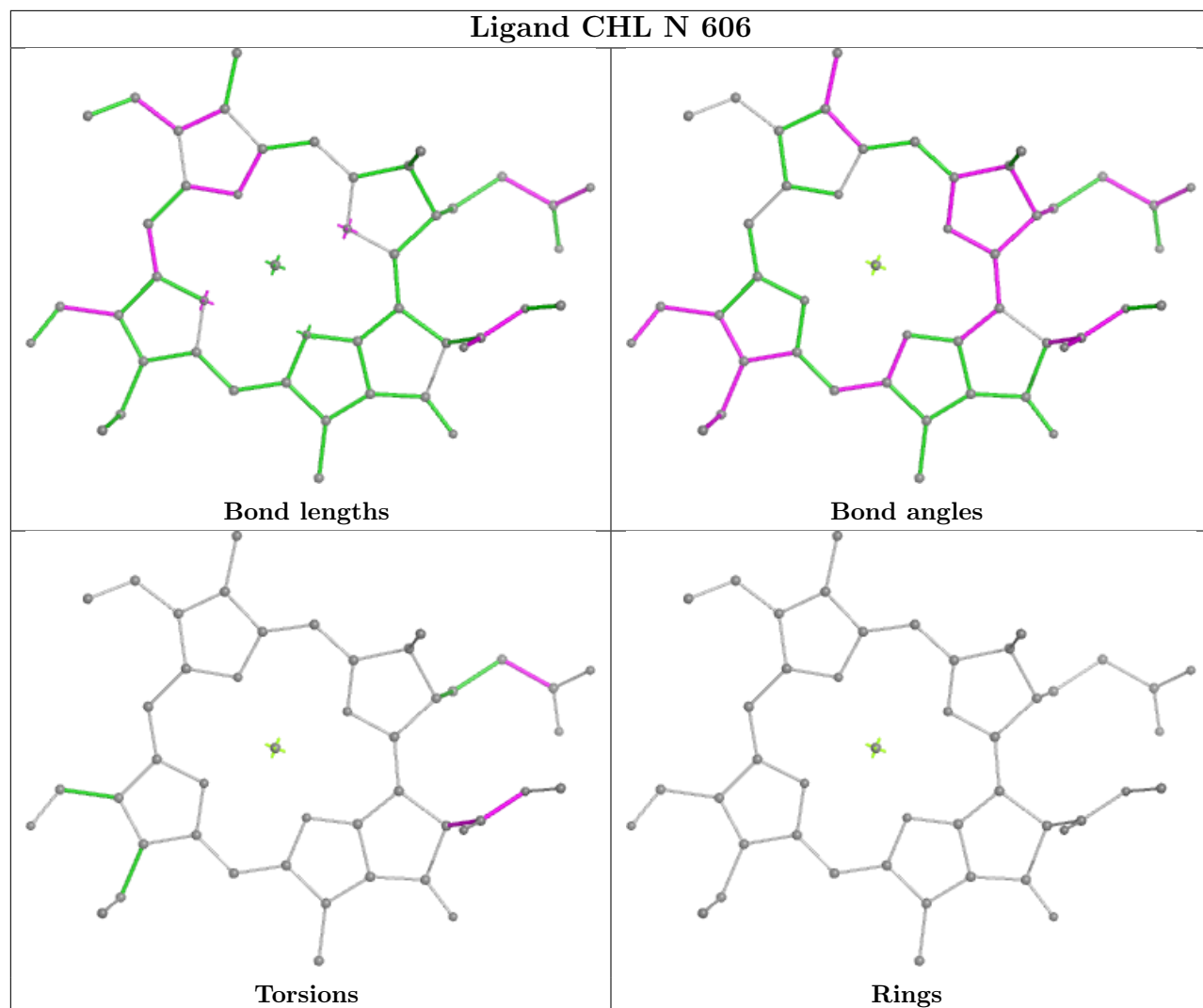


## Ligand CLA R 609

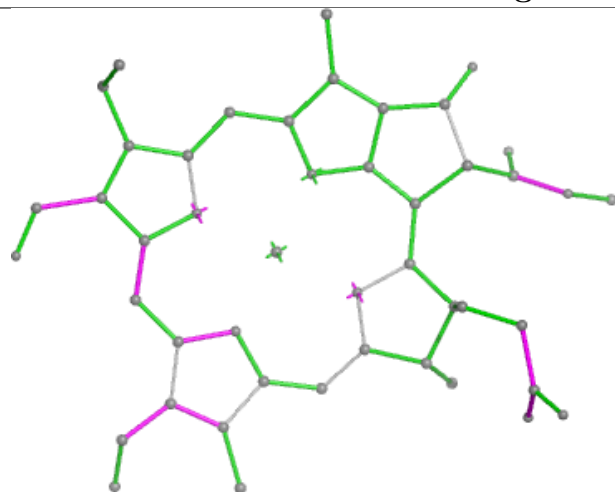


## Ligand LHG R 618

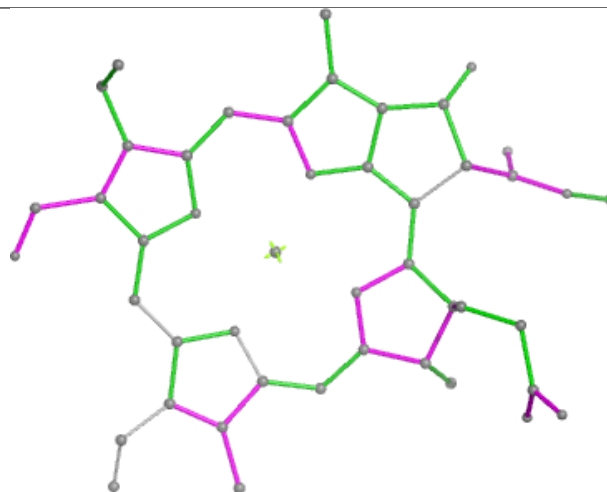




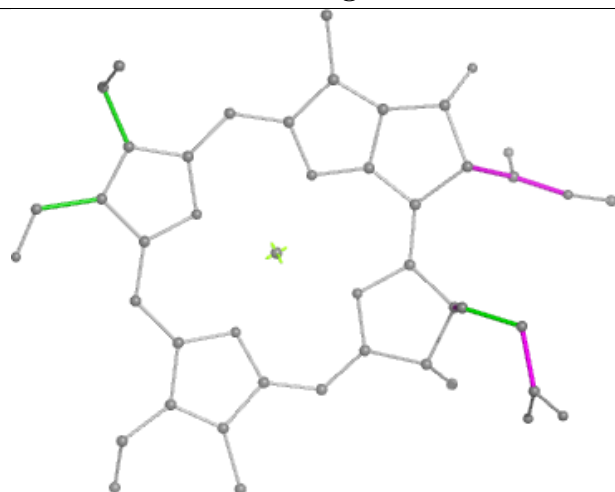
## Ligand CHL G 607



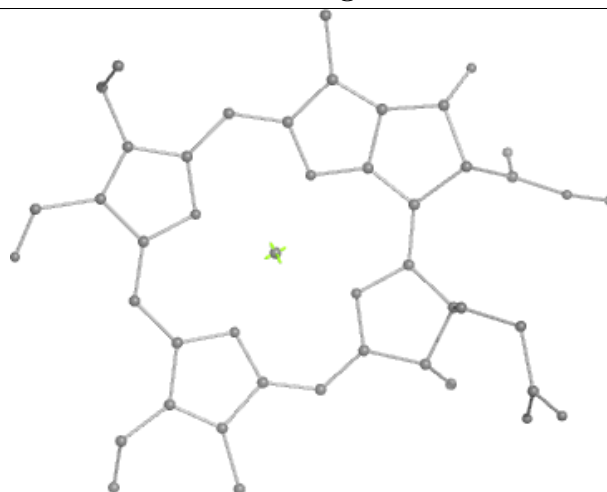
Bond lengths



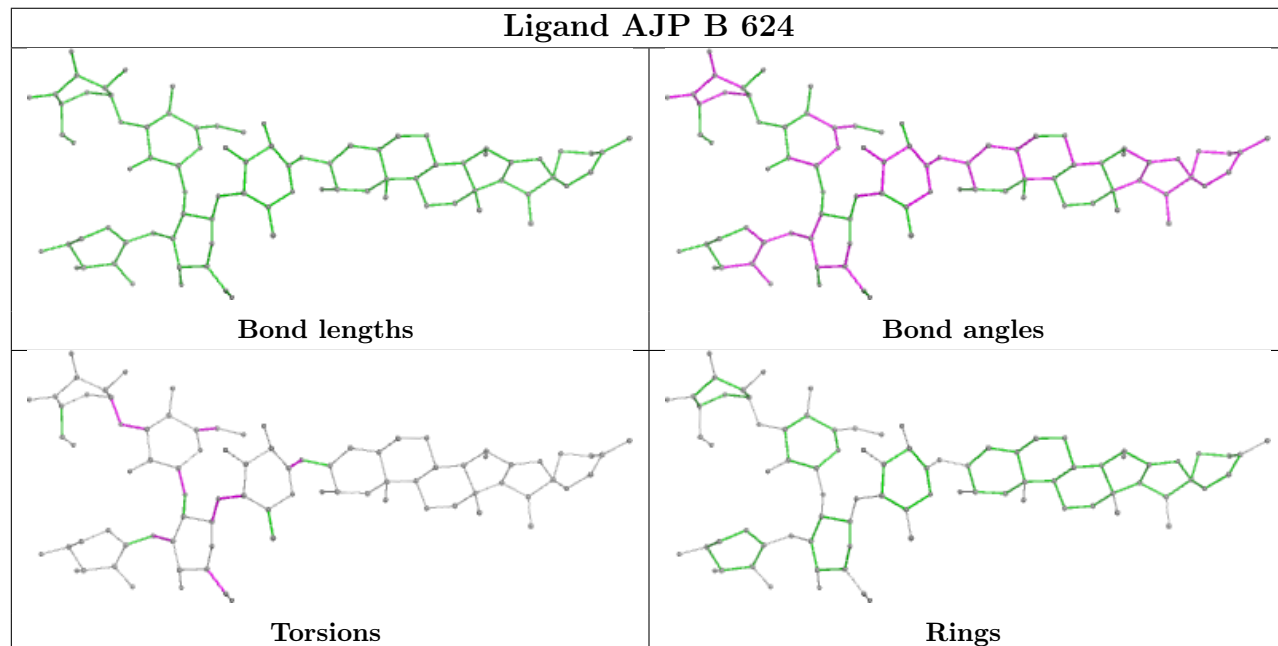
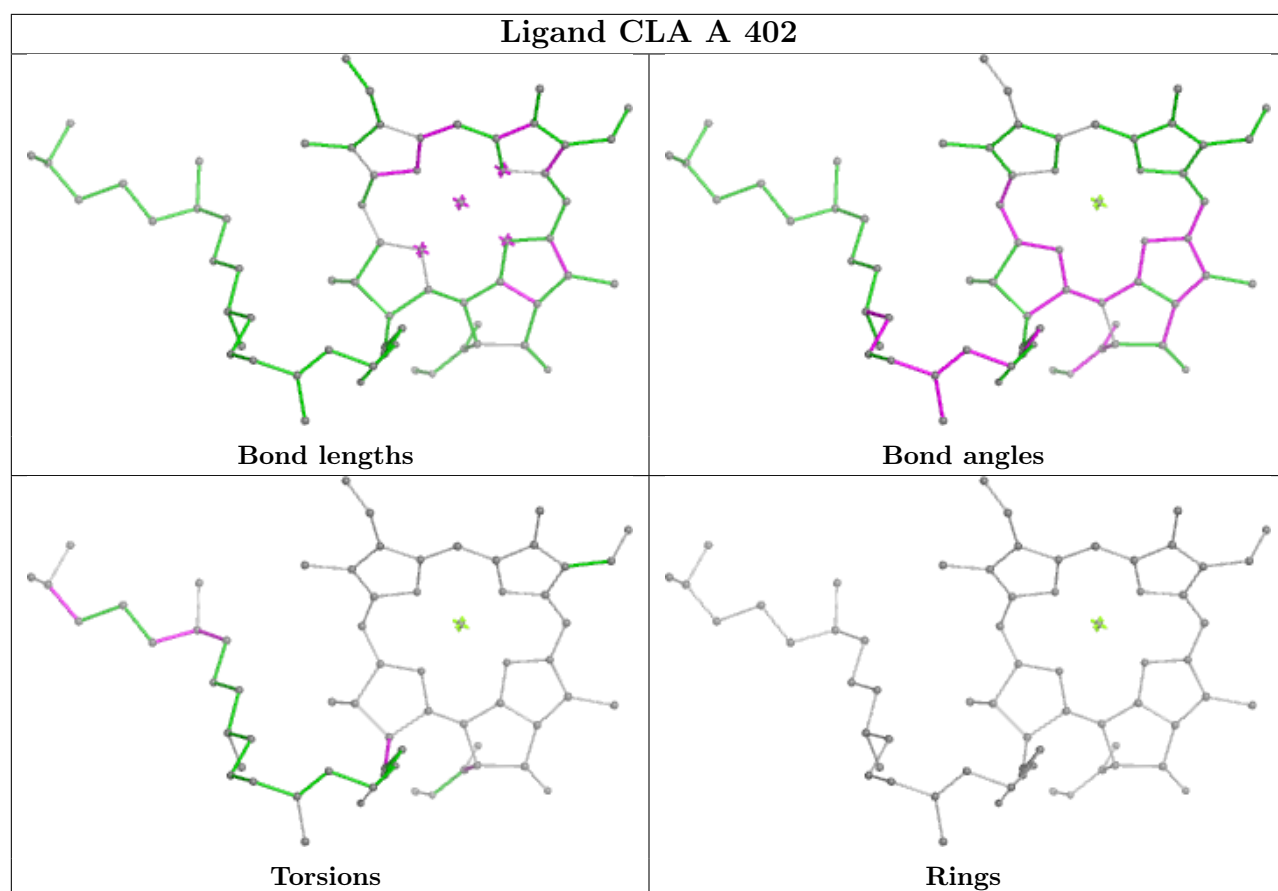
Bond angles



Torsions

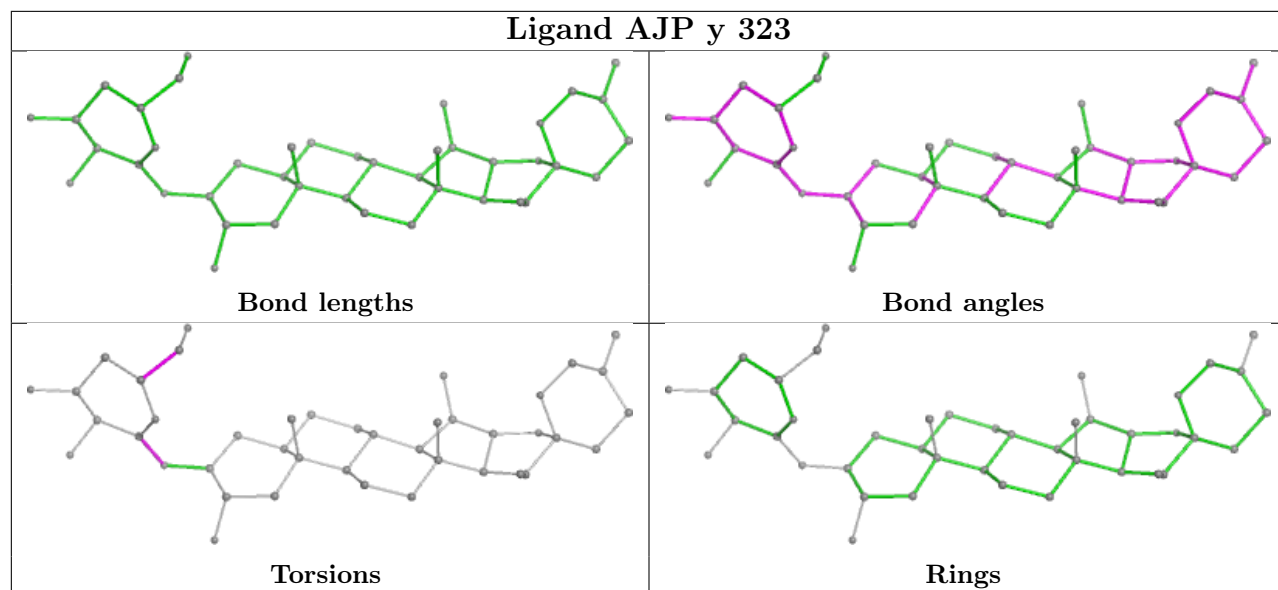


Rings

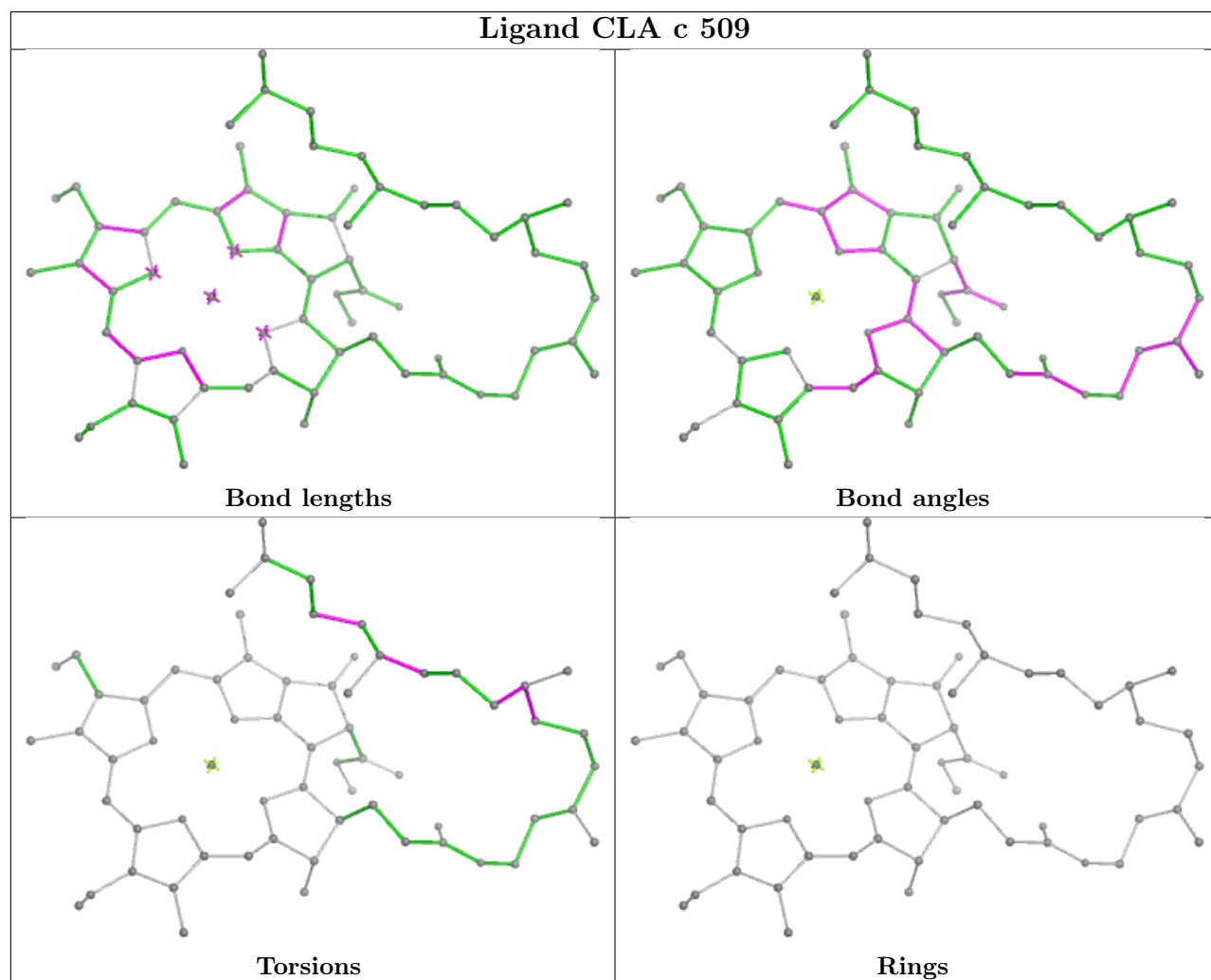




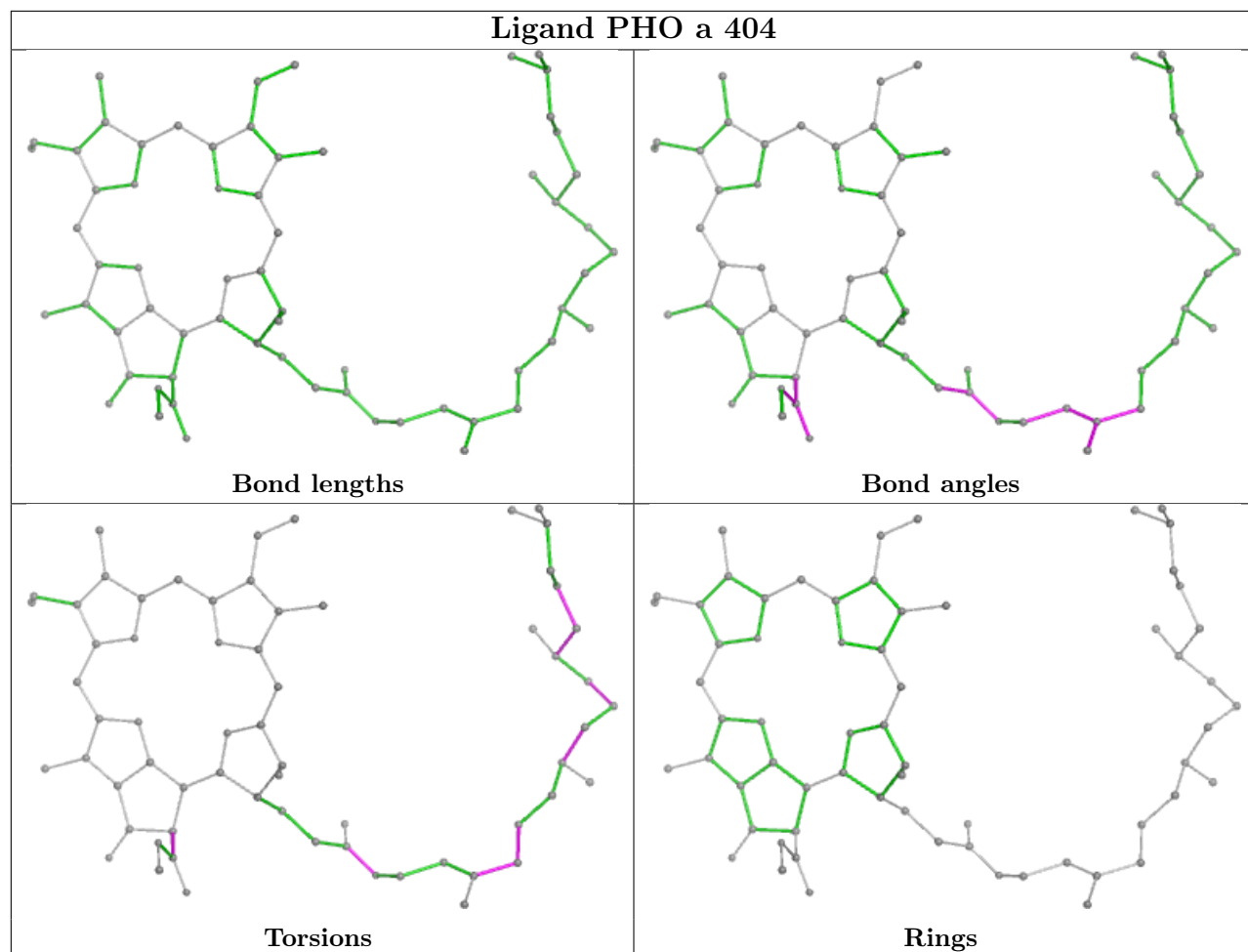
## Ligand AJP y 323



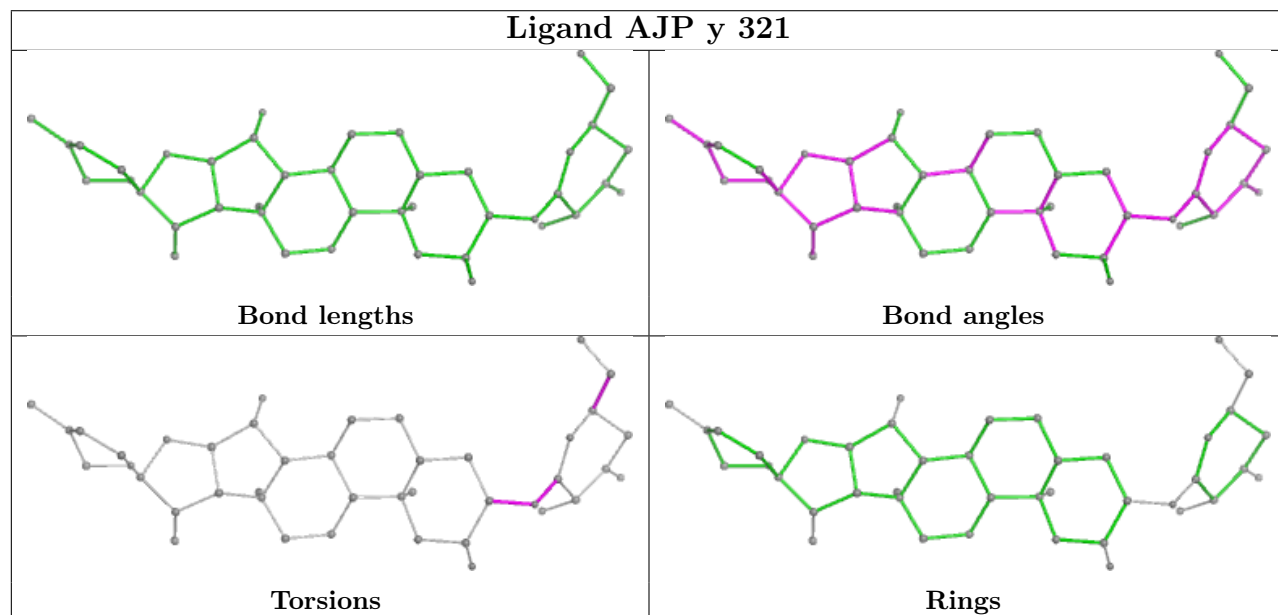
## Ligand CLA c 509

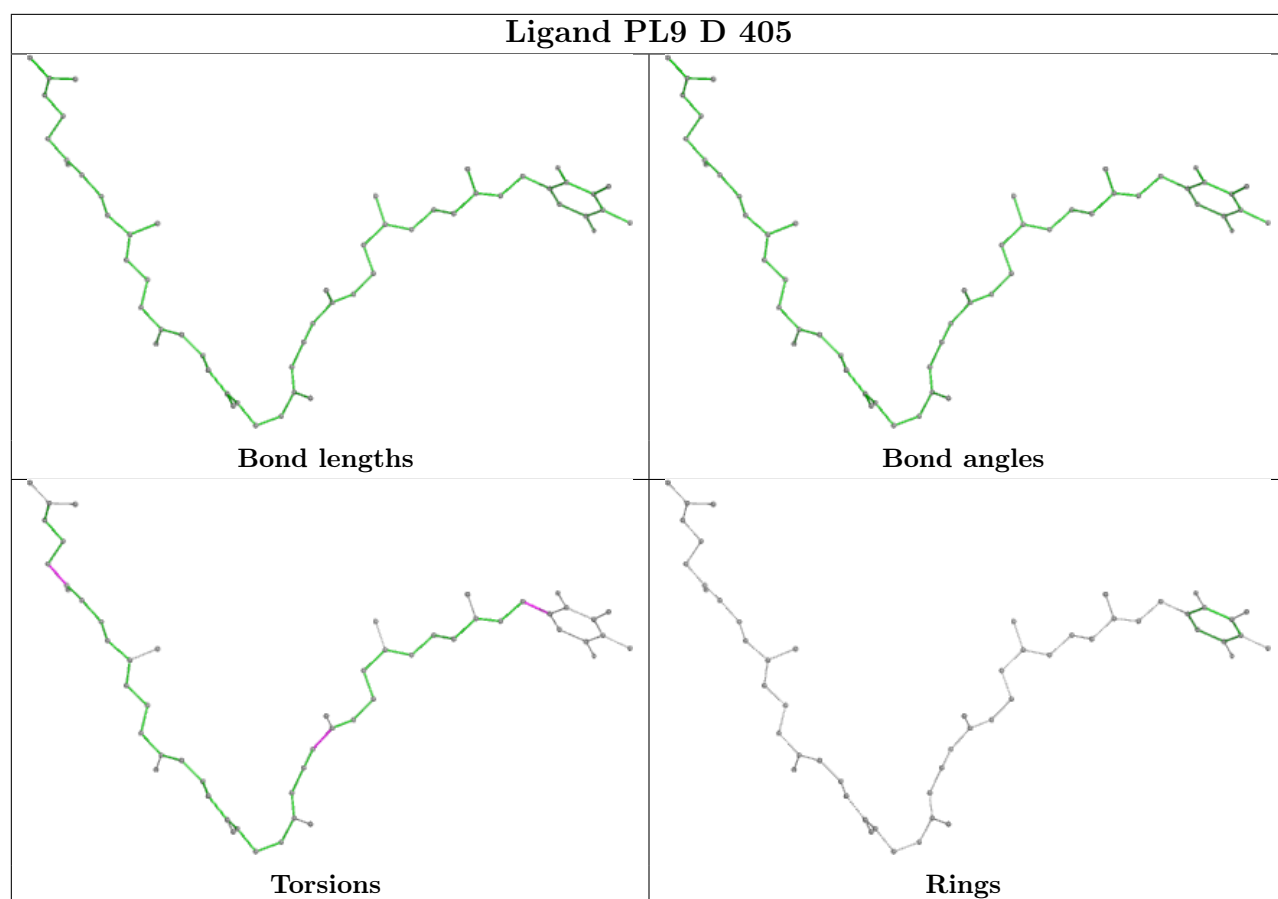


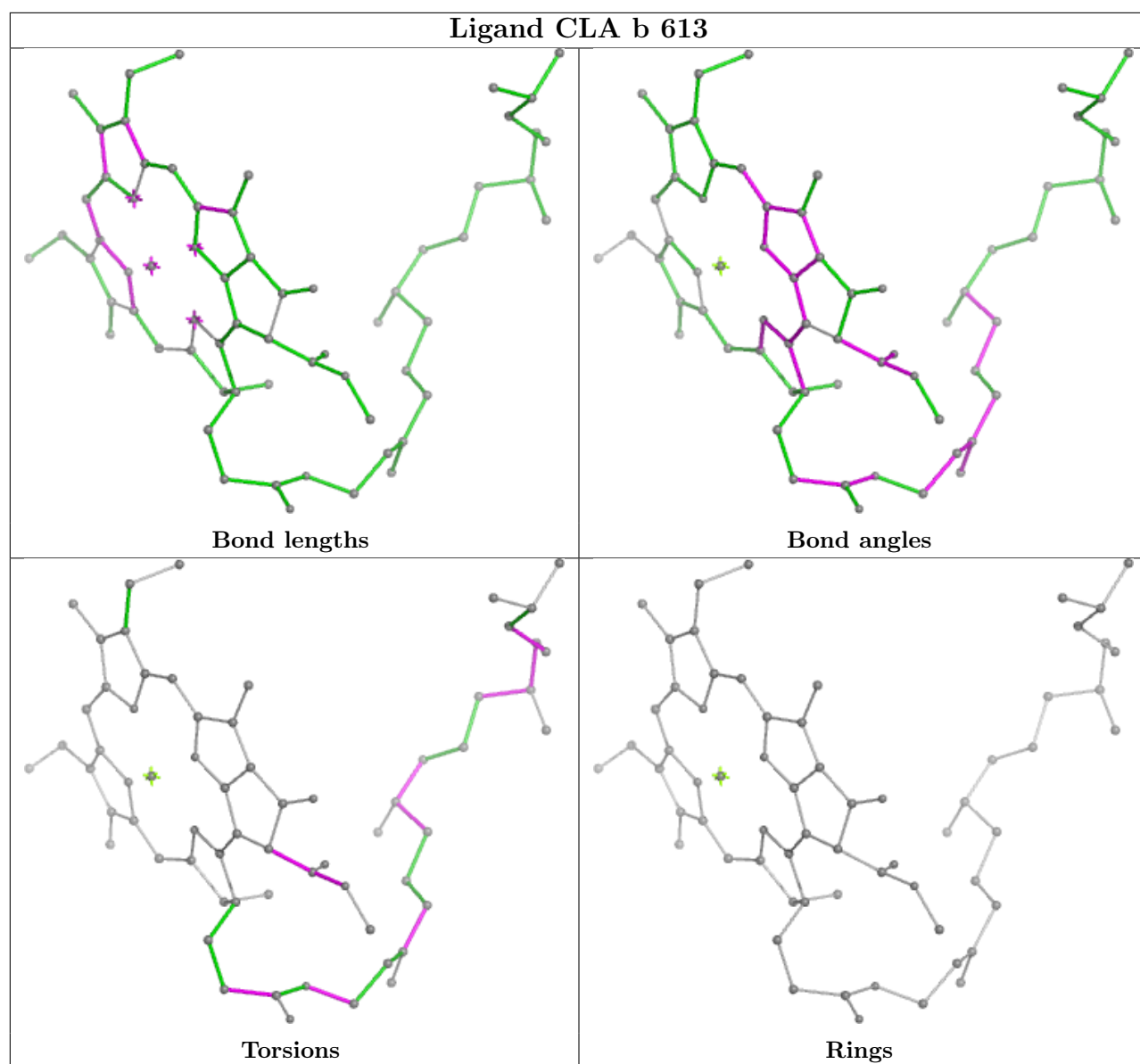
## Ligand PHO a 404

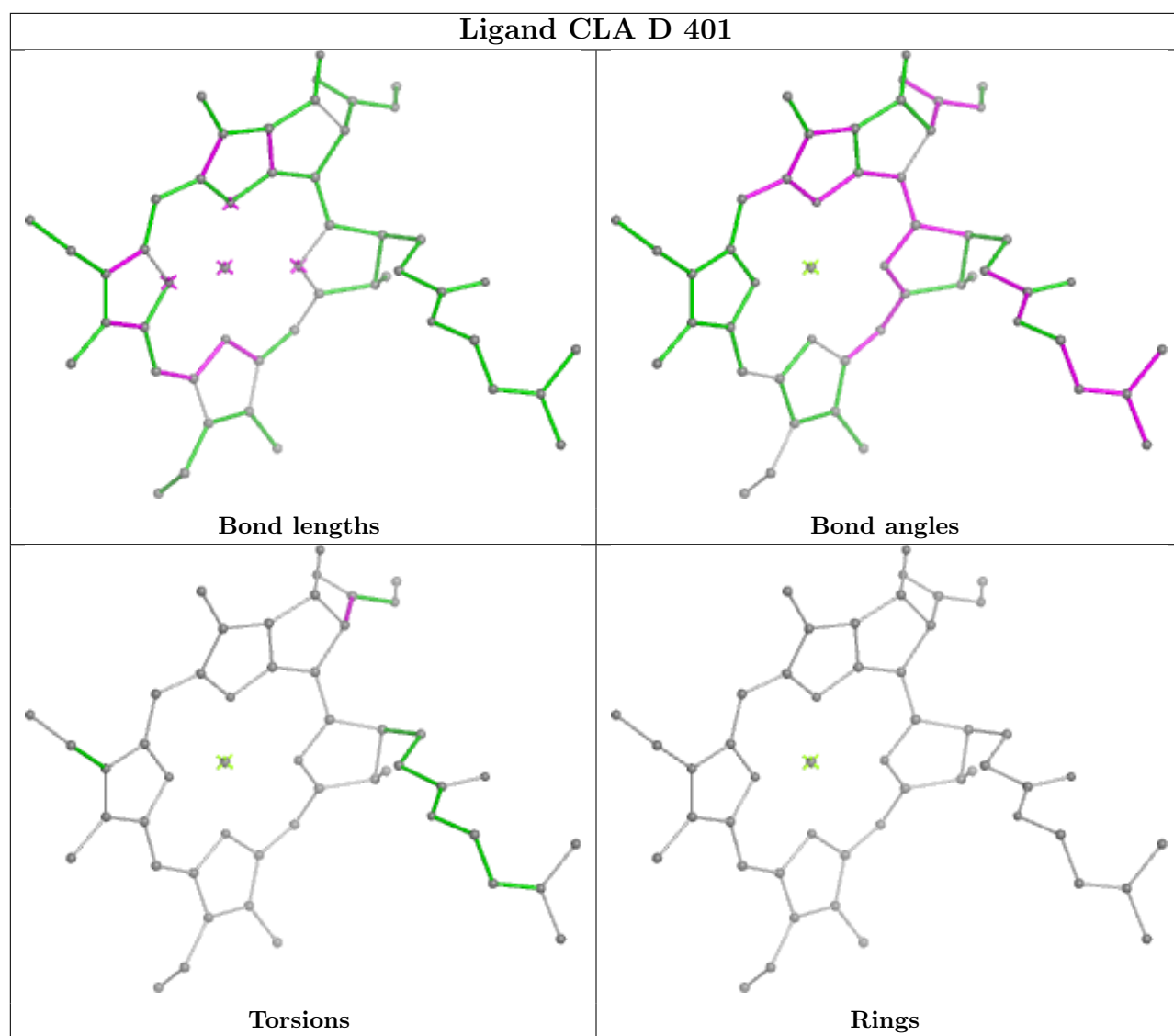


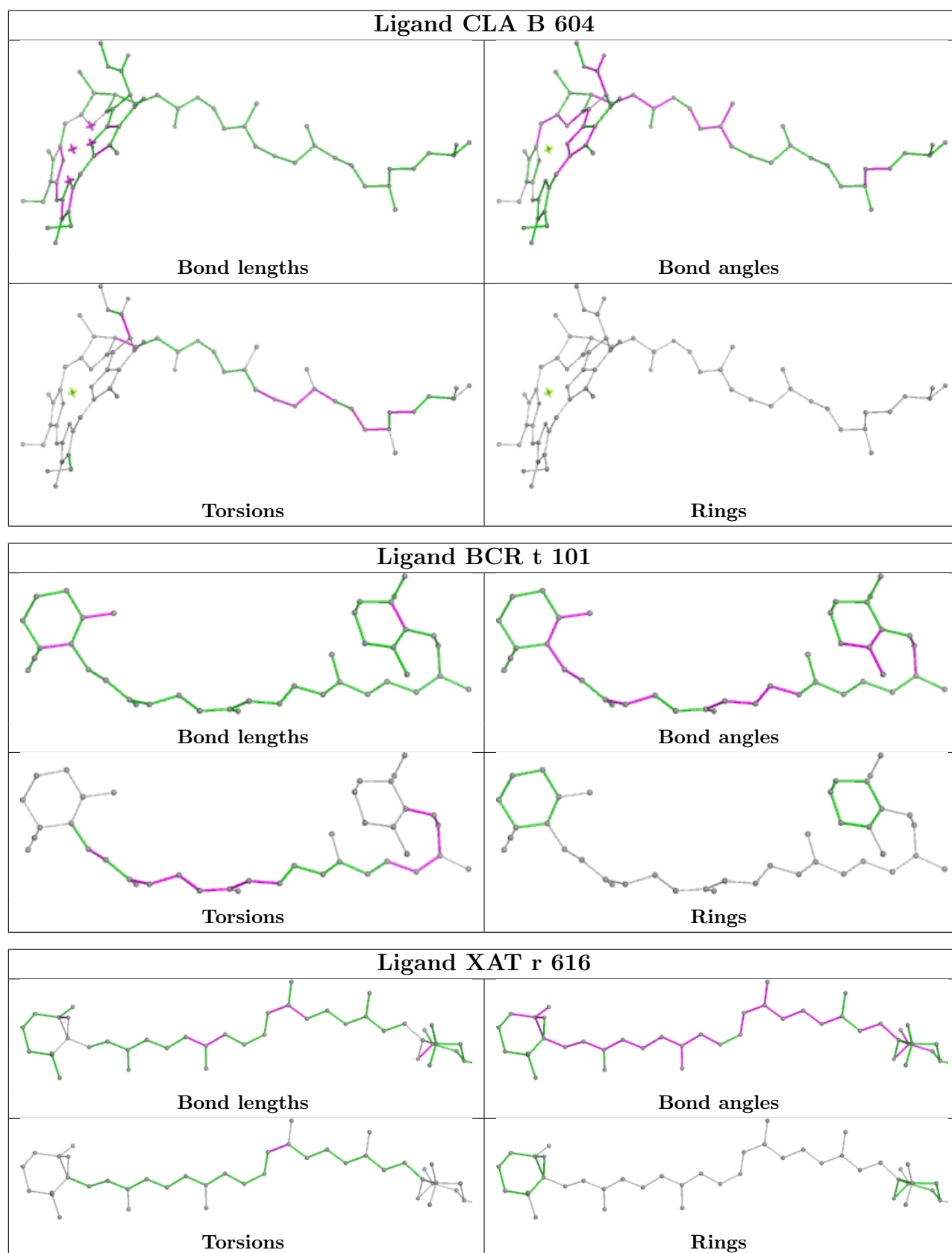
## Ligand AJP y 321



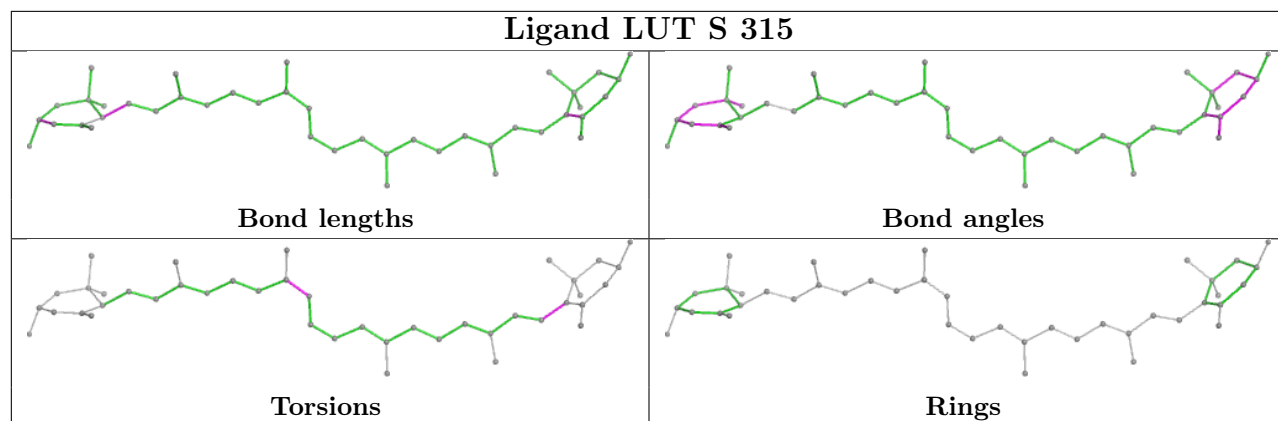




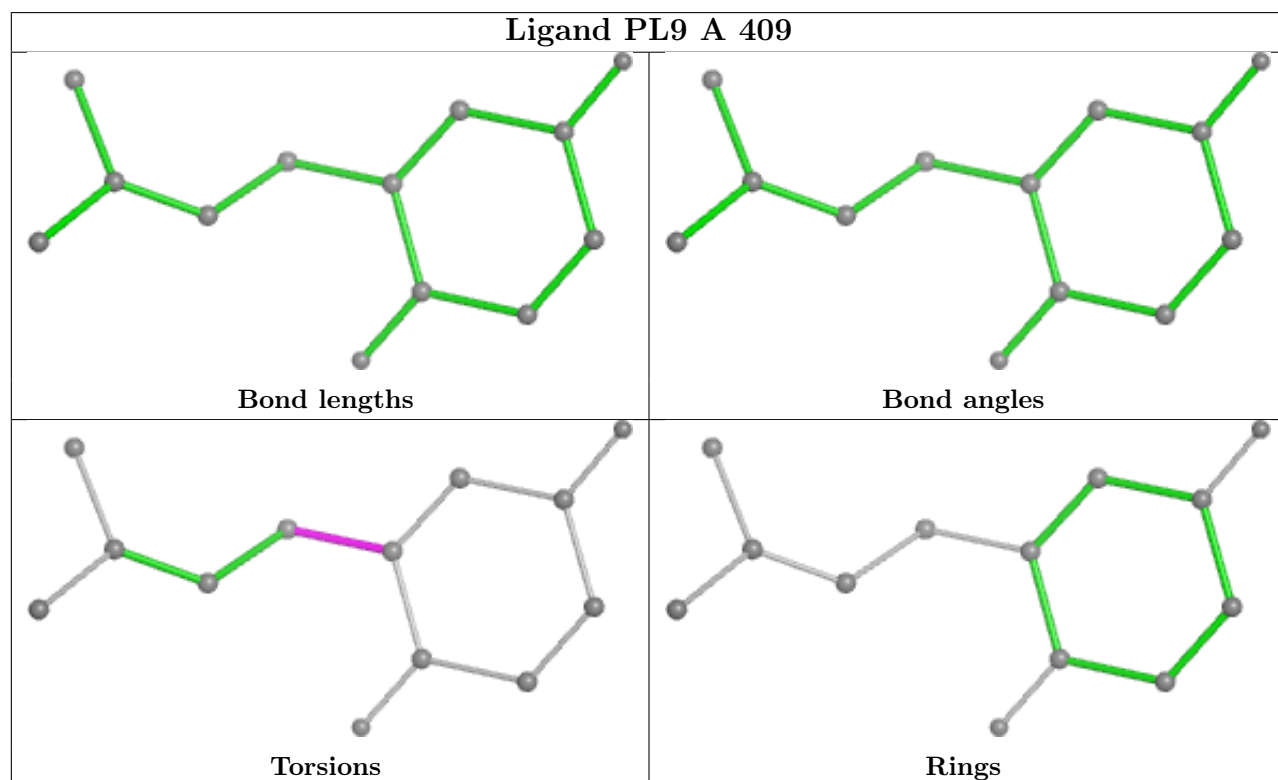




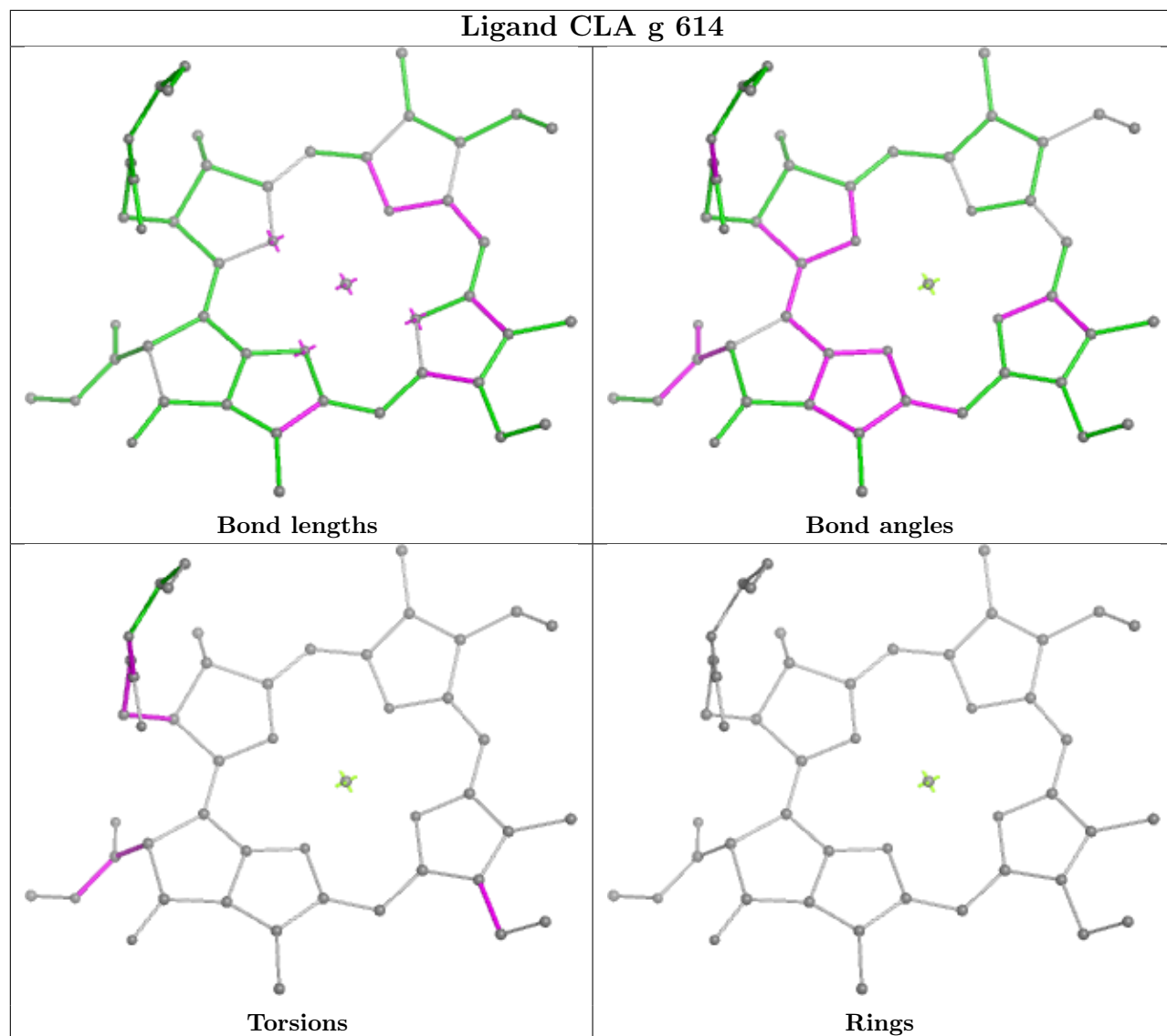
## Ligand LUT S 315



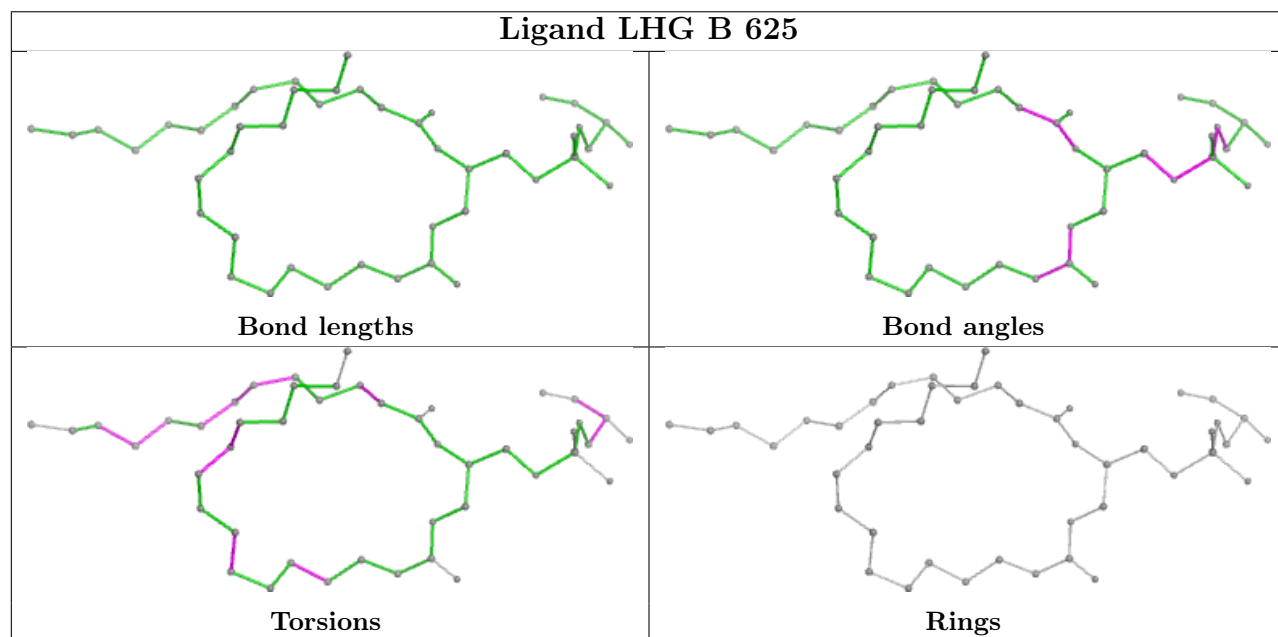
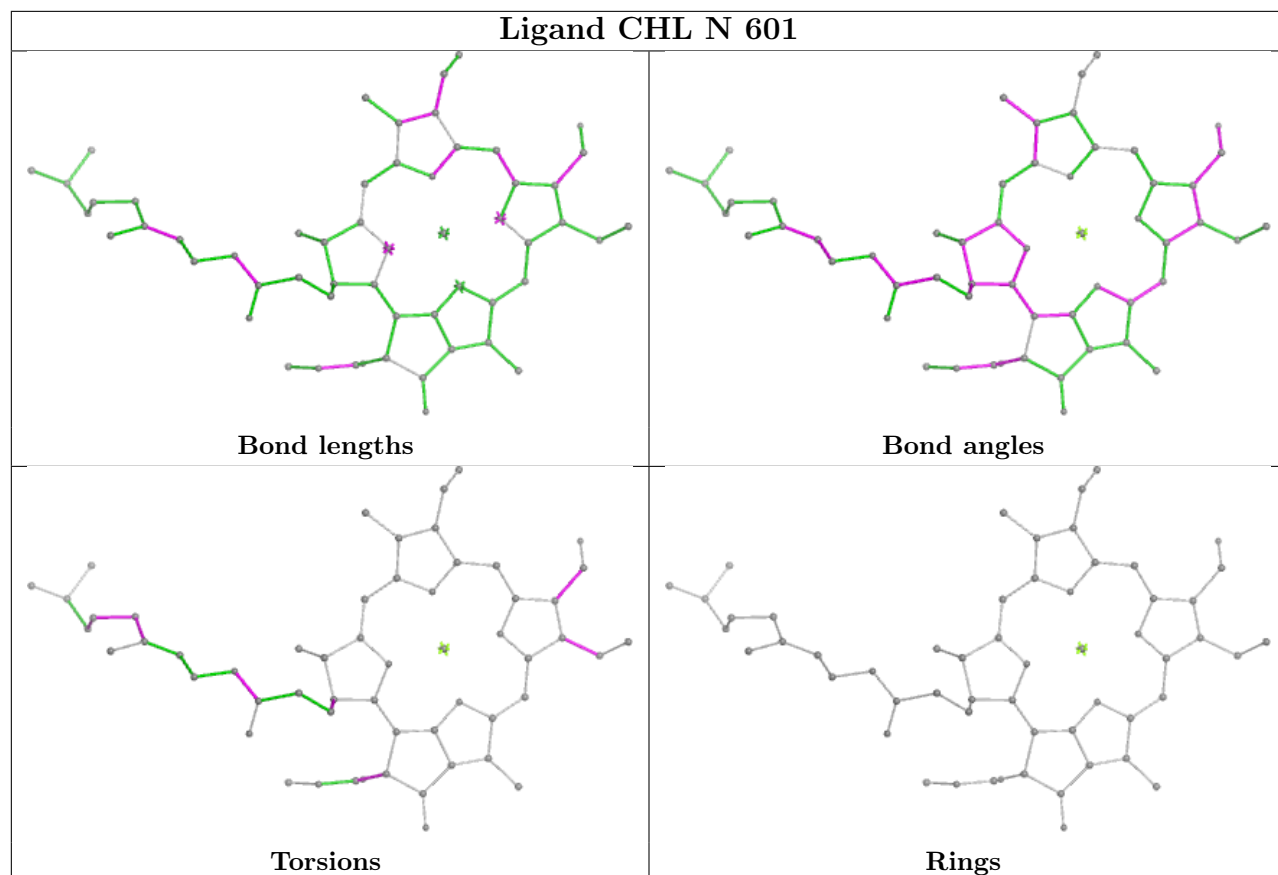
## Ligand PL9 A 409

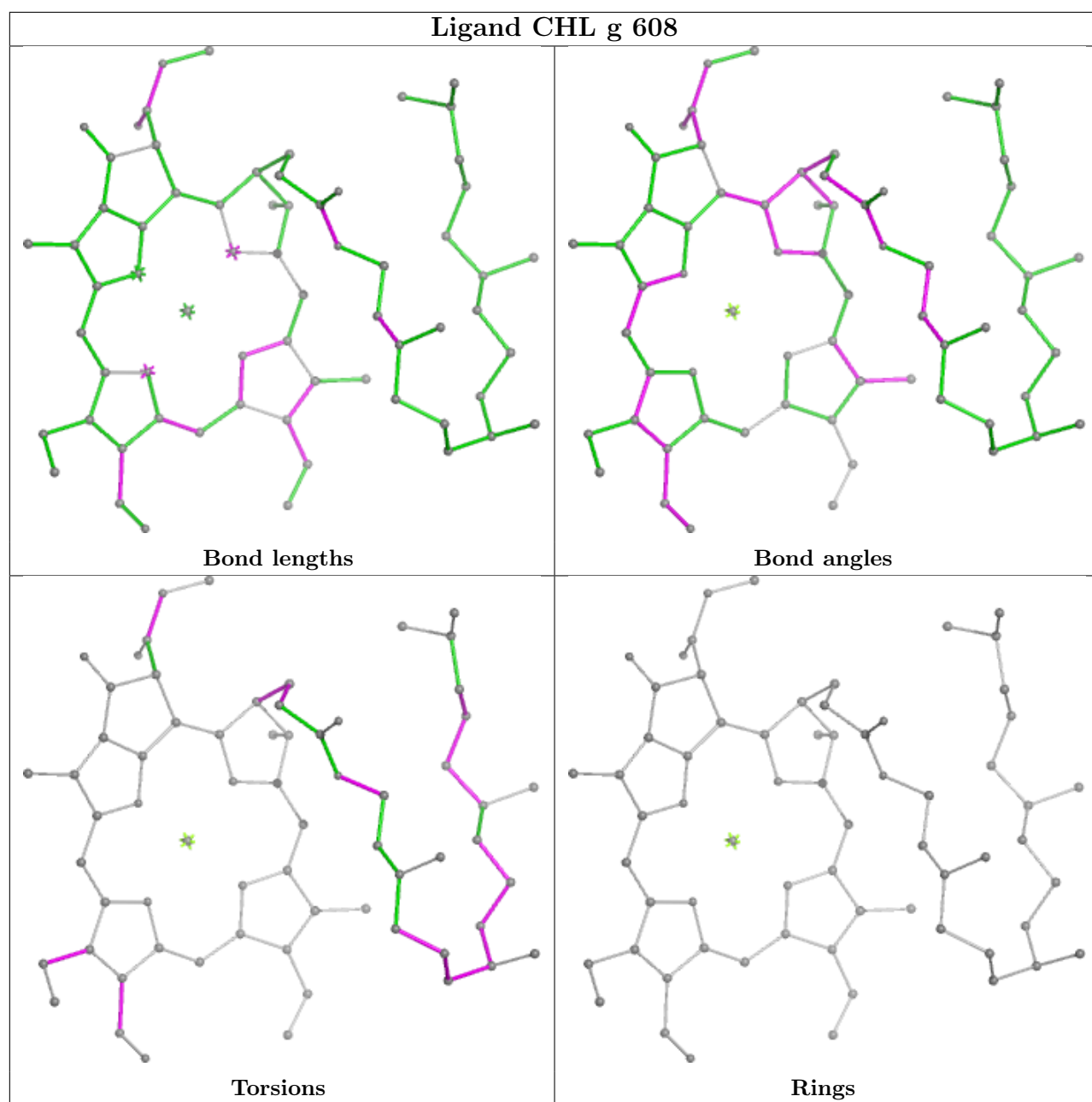


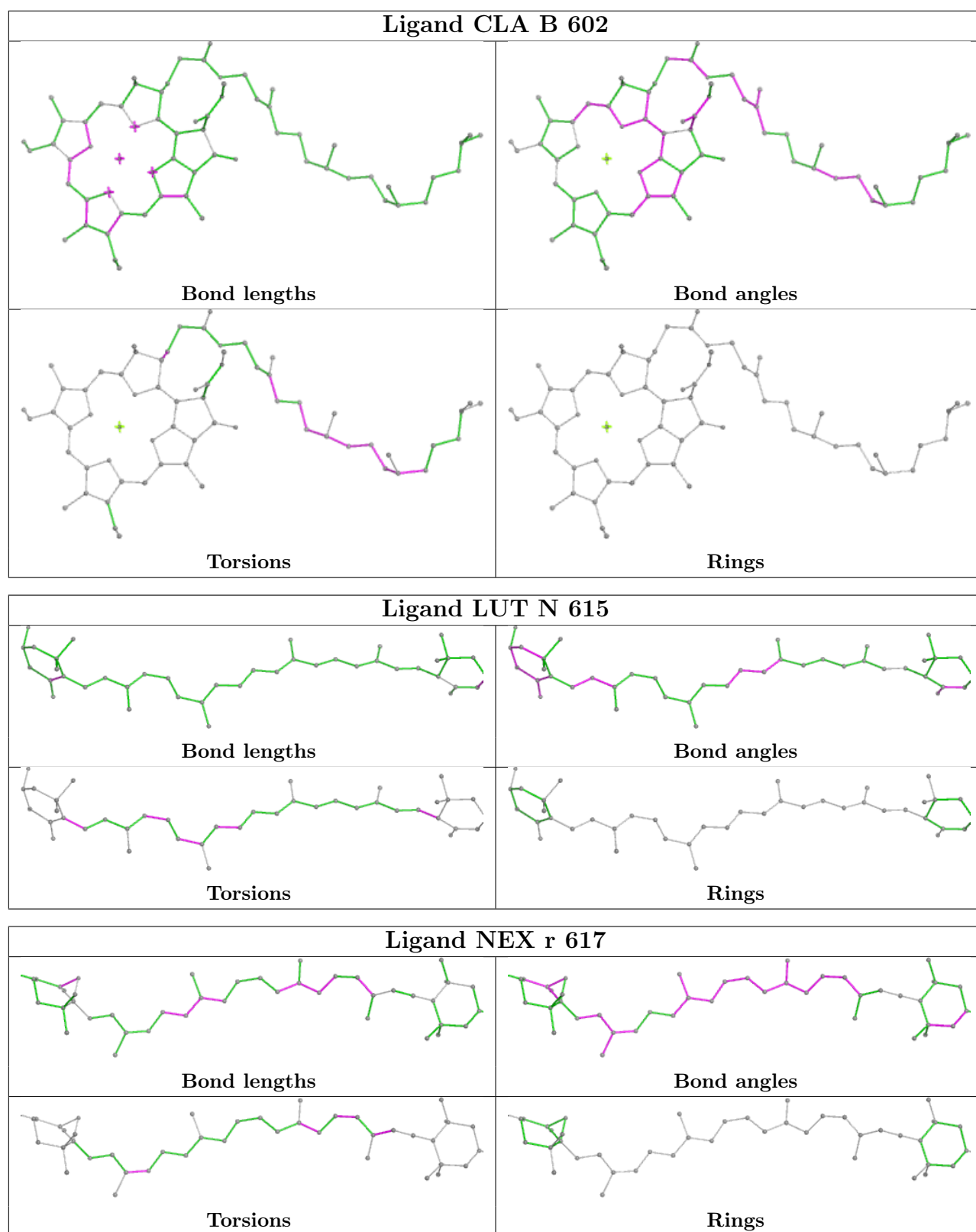
## Ligand CLA g 614

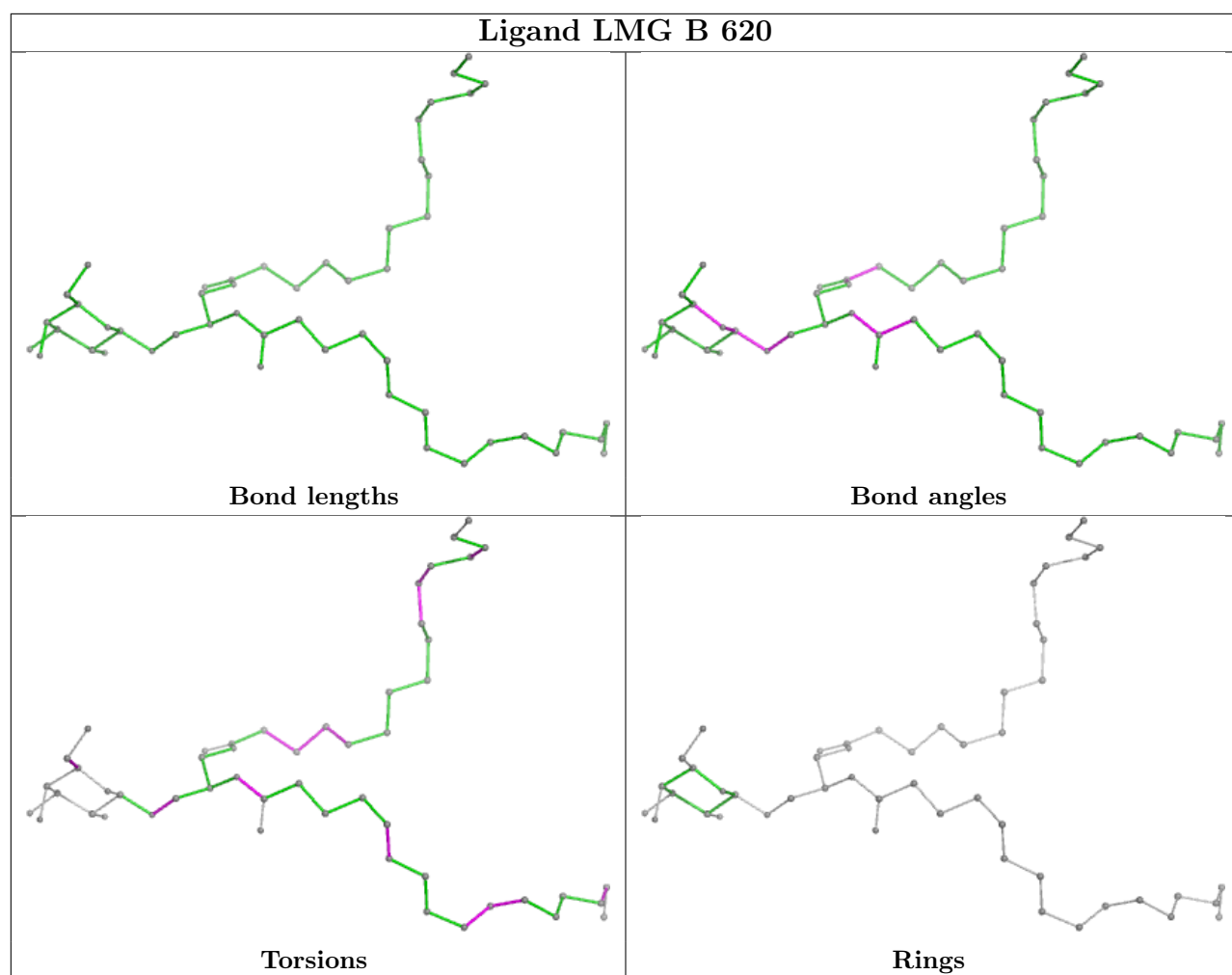




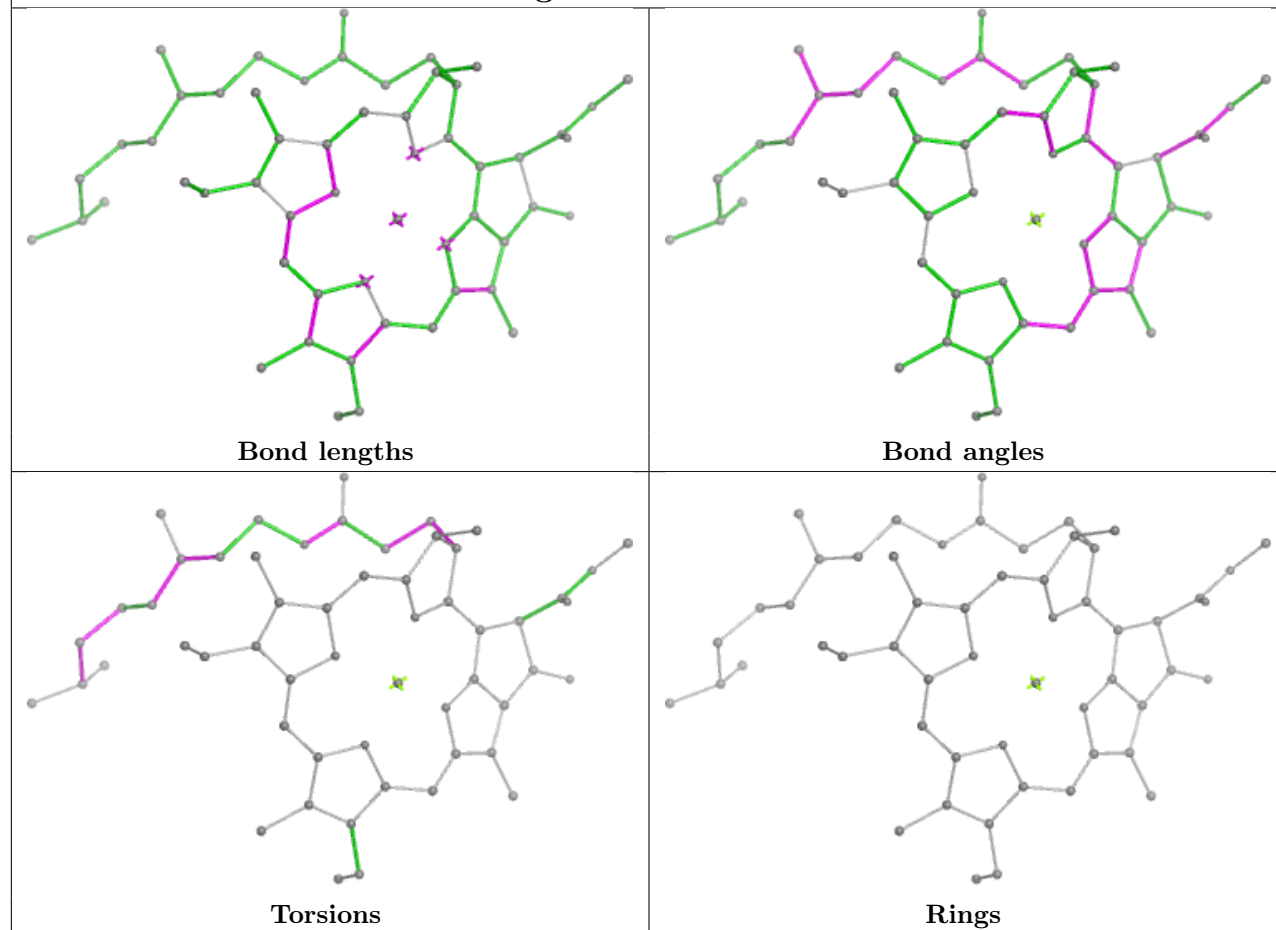




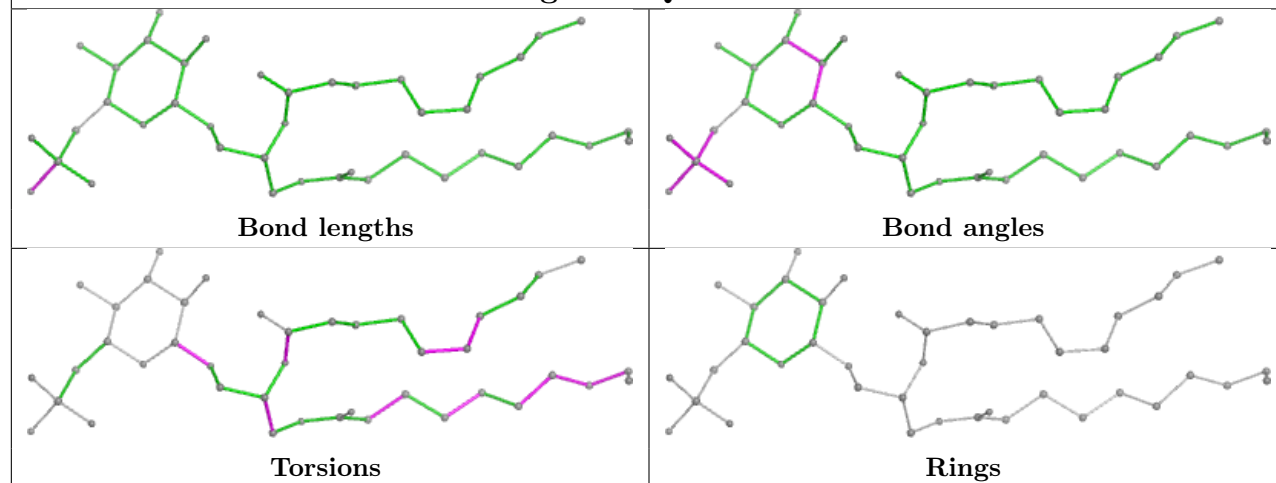


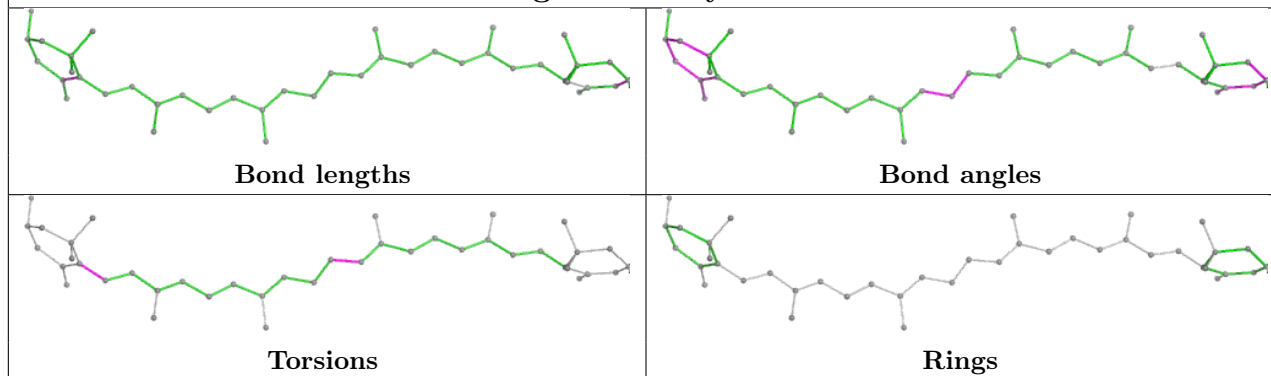
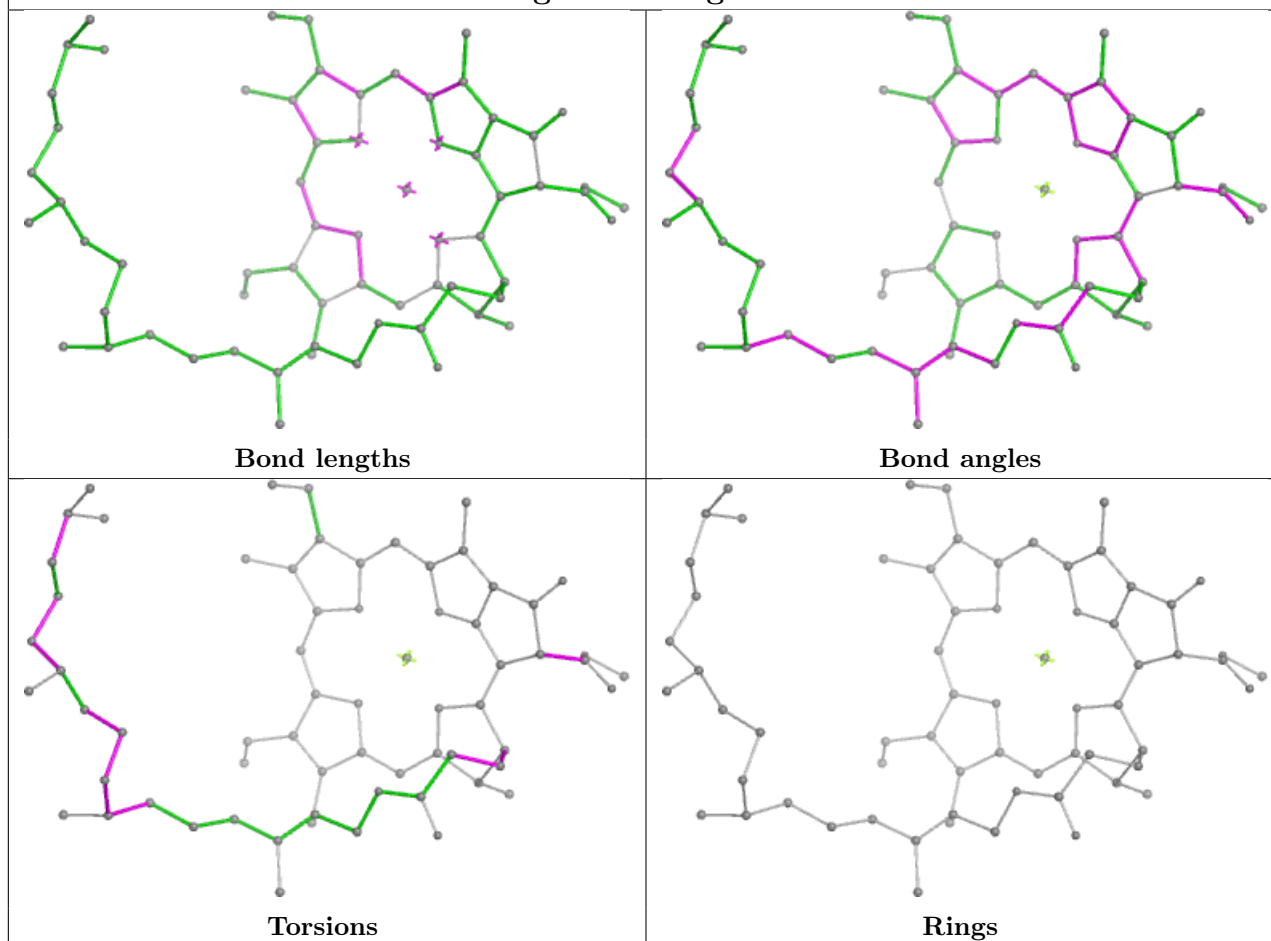


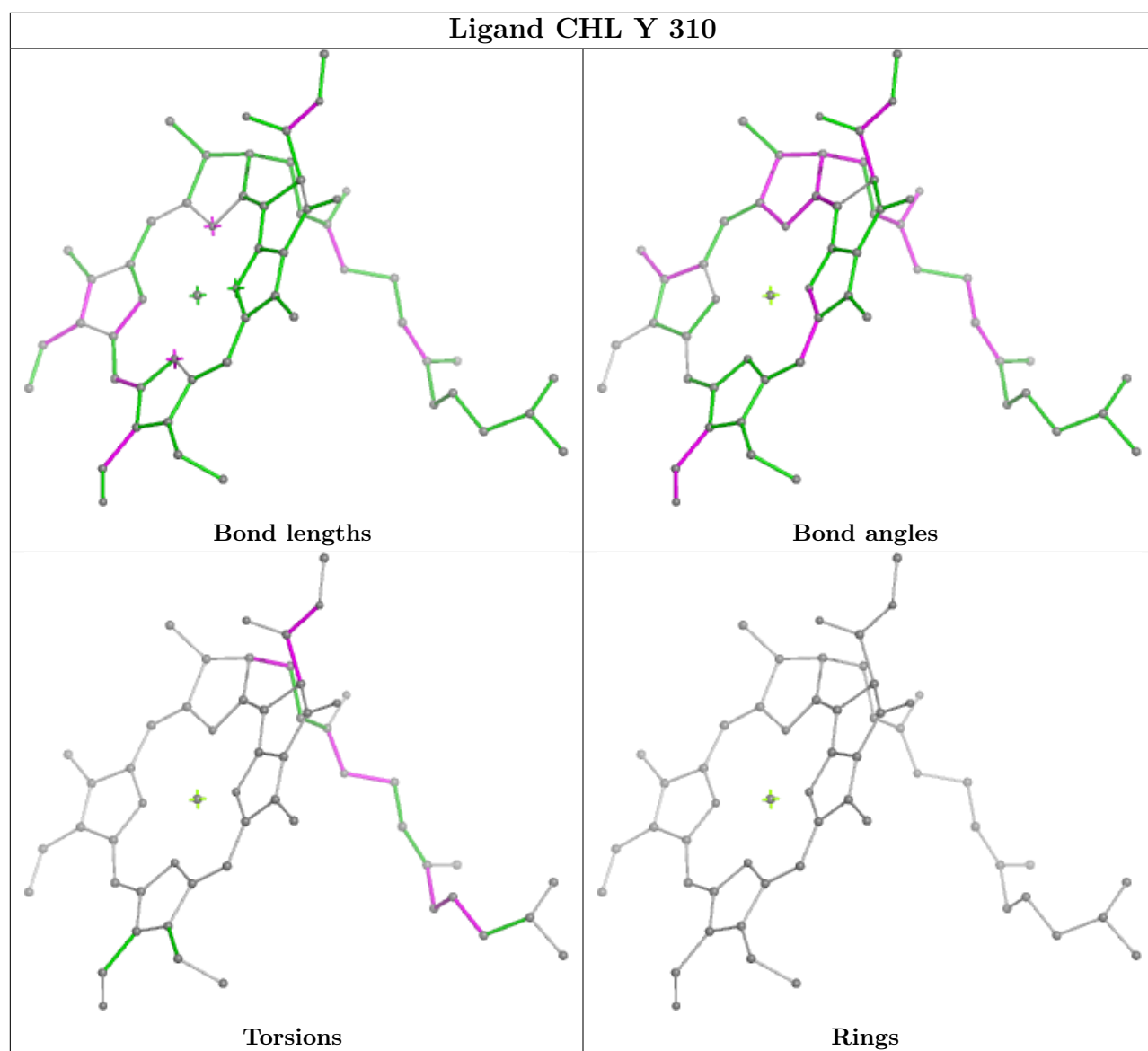
## Ligand CLA S 310

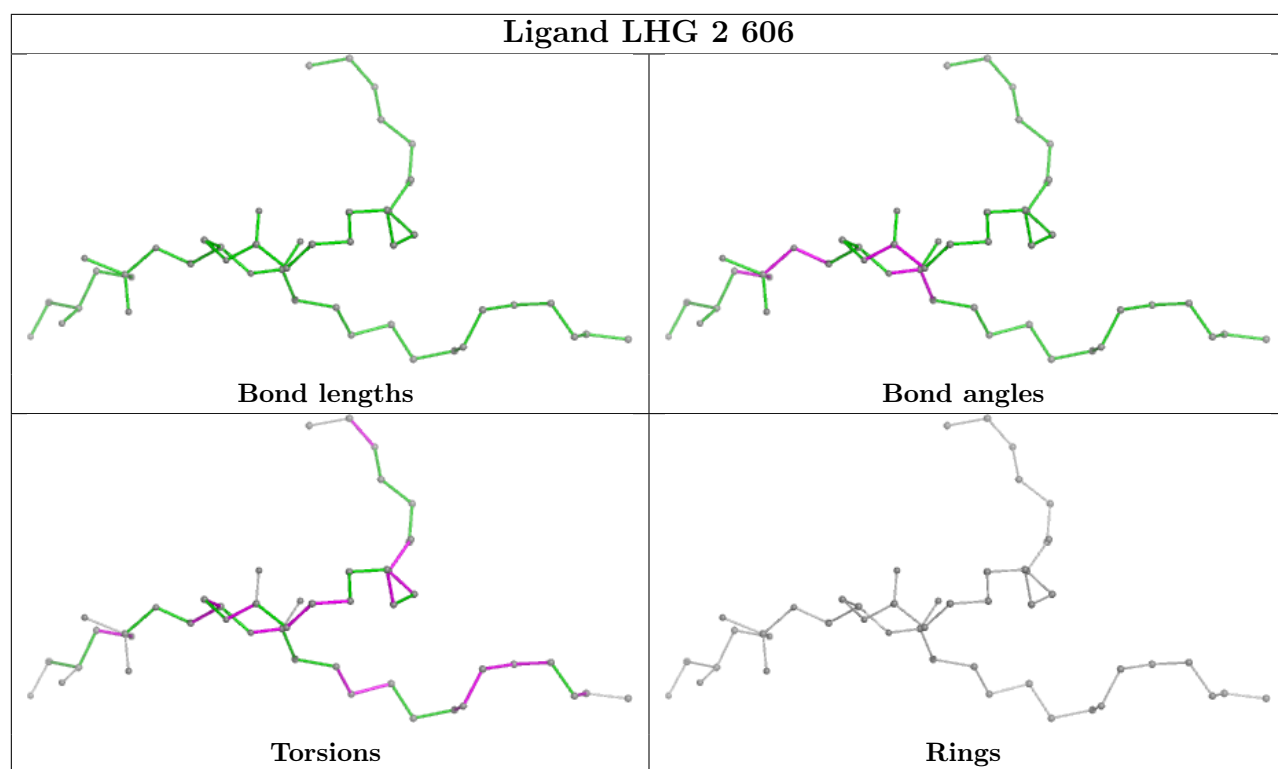


## Ligand SQD 1 102

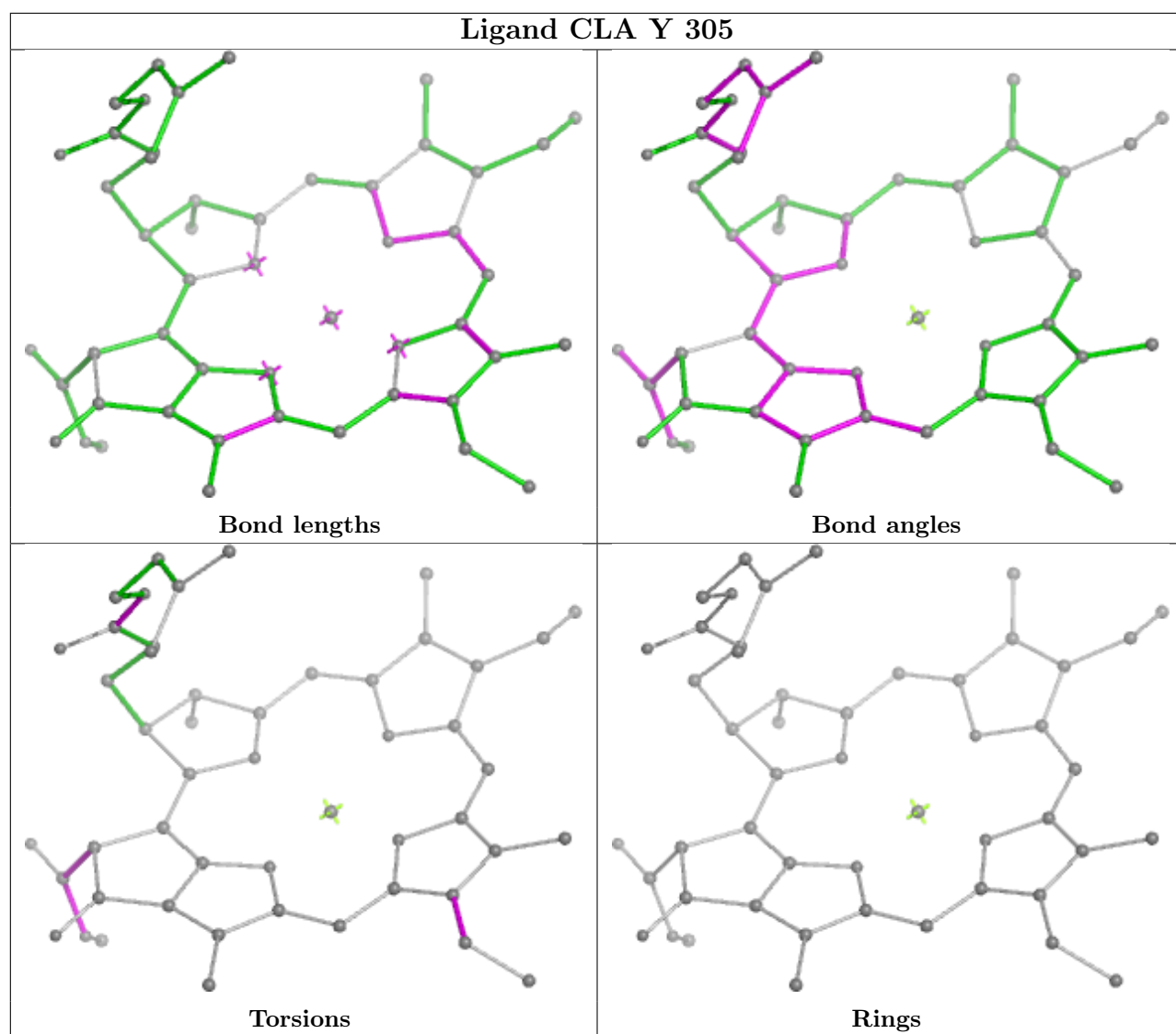


**Ligand LUT y 316****Ligand CLA g 602**

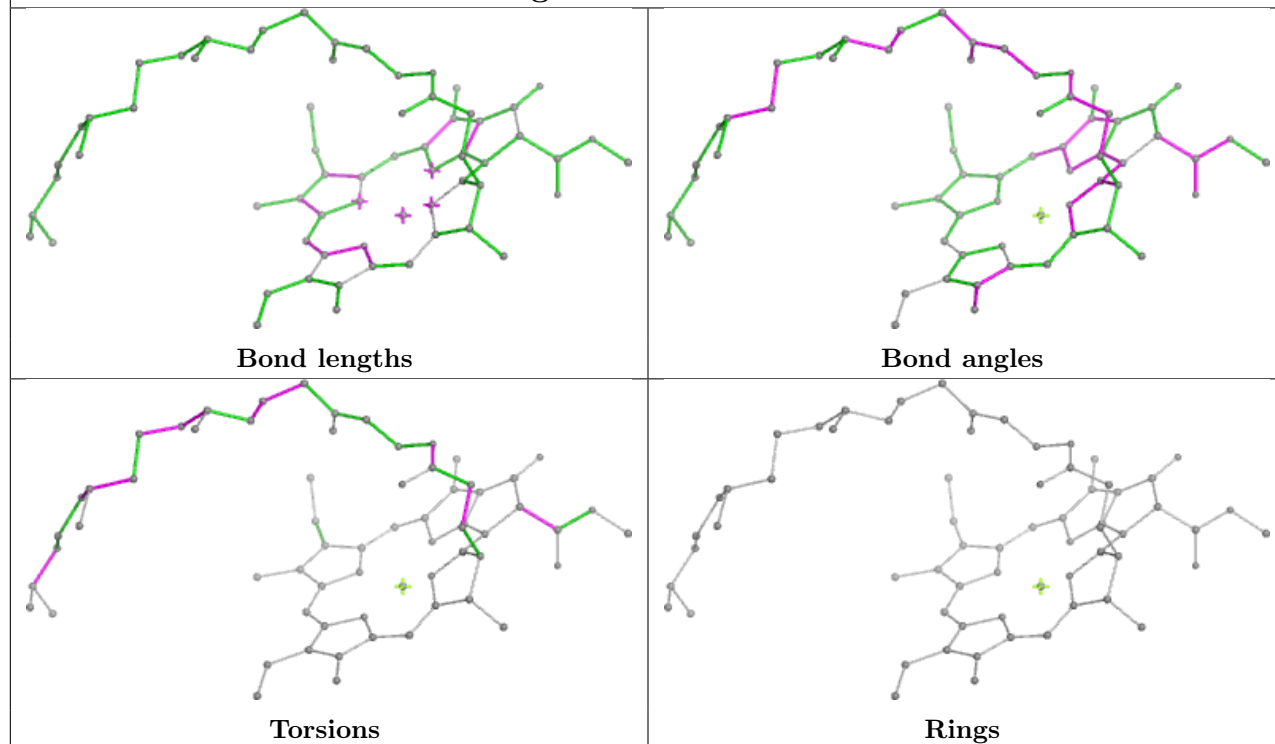




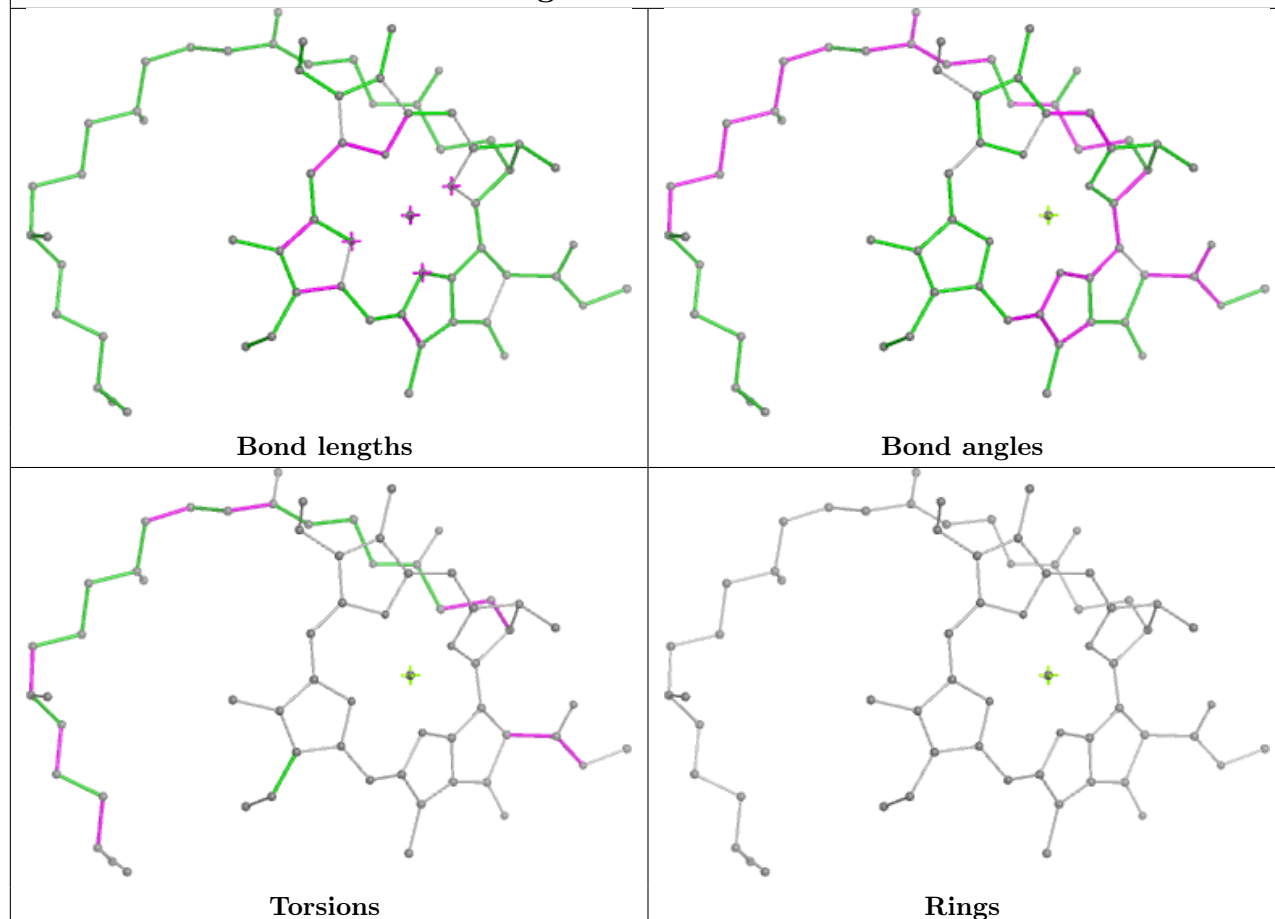


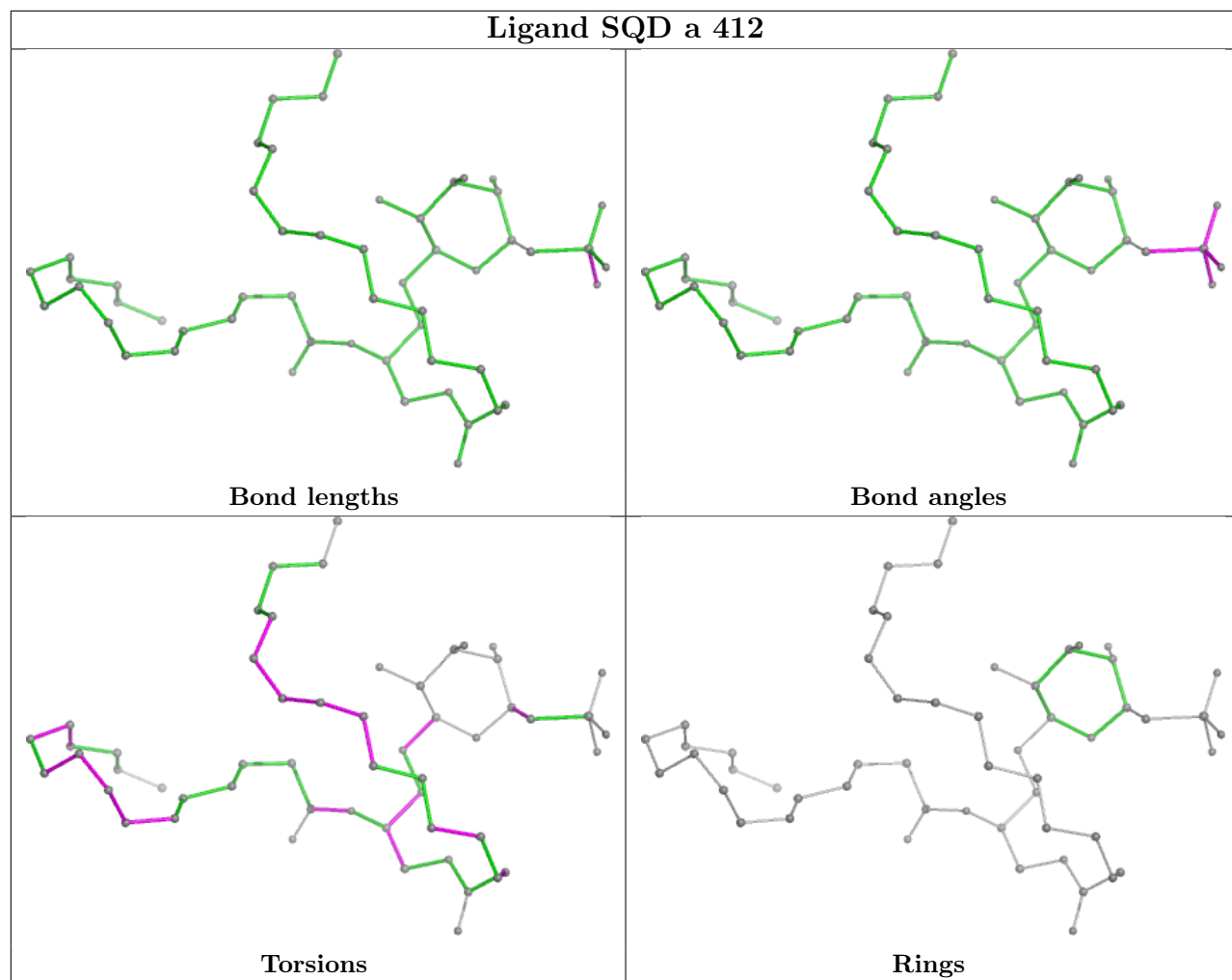


## Ligand CLA C 513

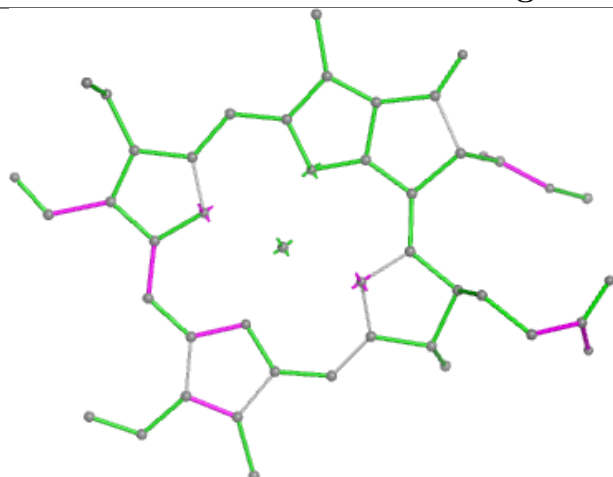


## Ligand CLA r 609

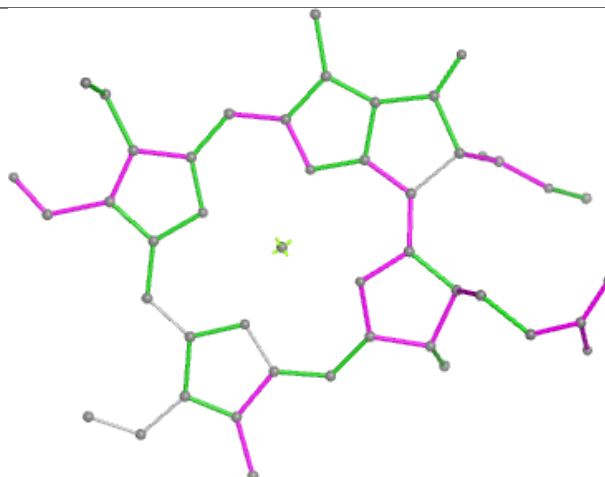




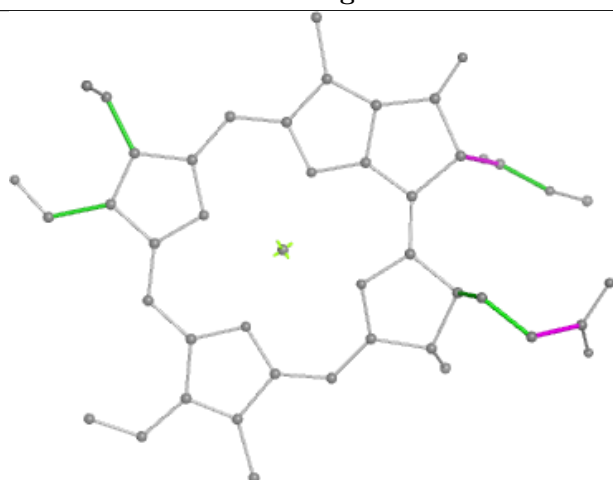
## Ligand CHL S 302



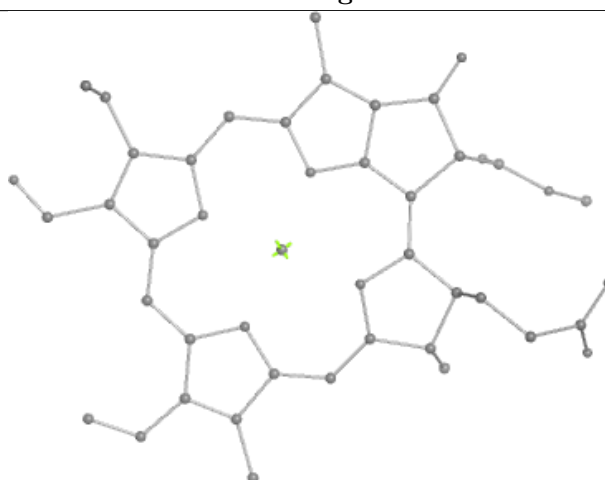
Bond lengths



Bond angles

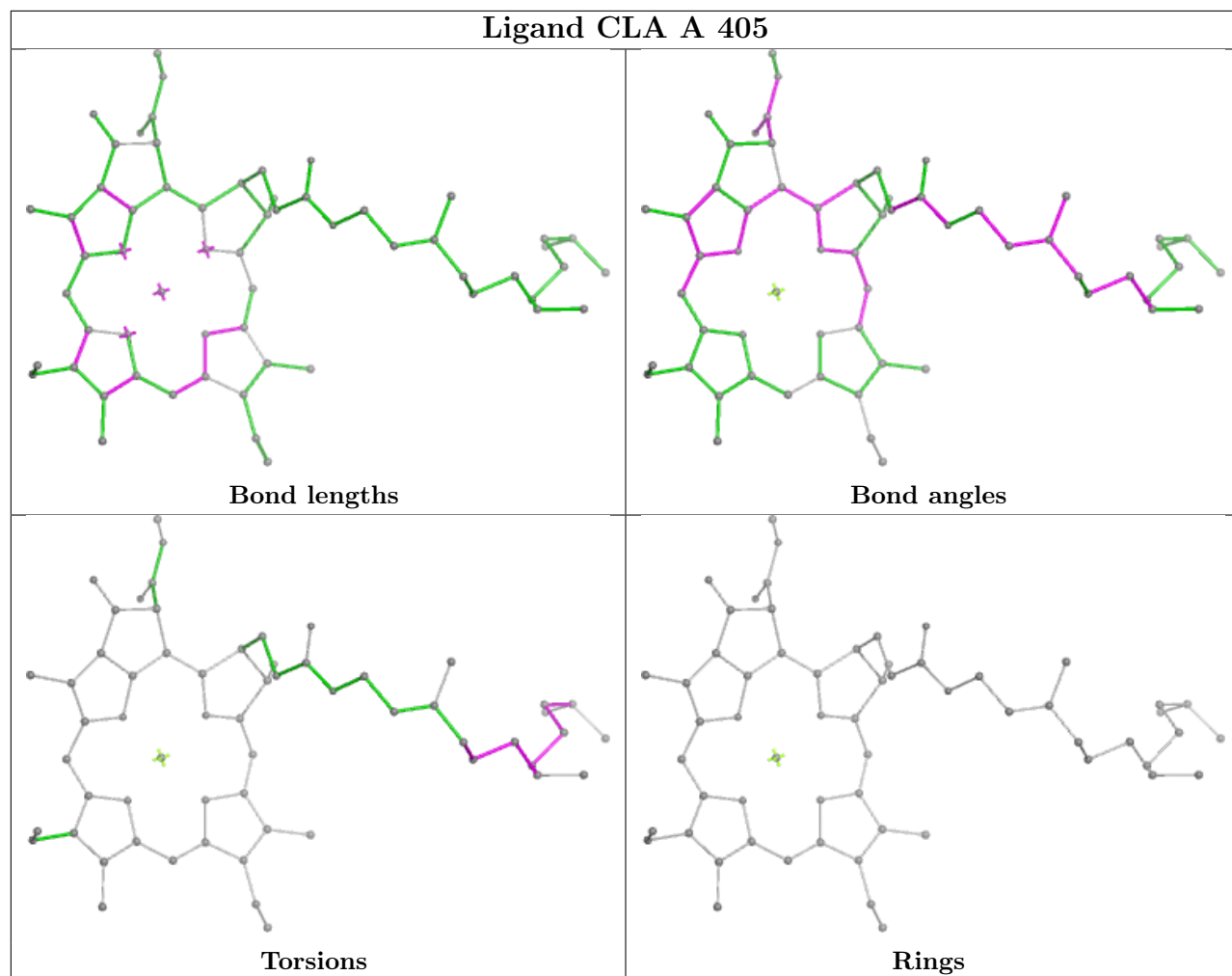


Torsions

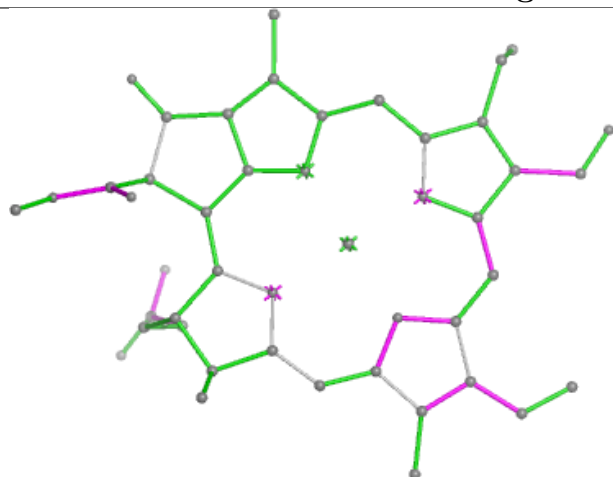


Rings

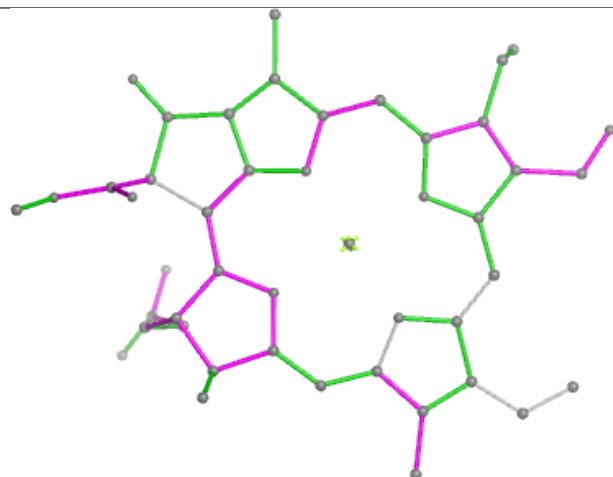
## Ligand CLA A 405



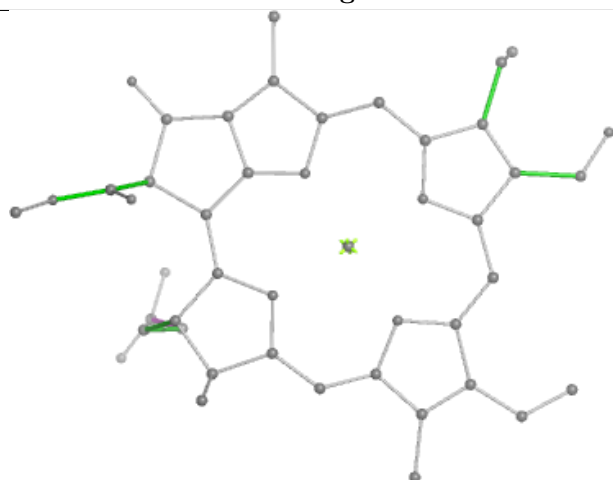
## Ligand CHL S 308



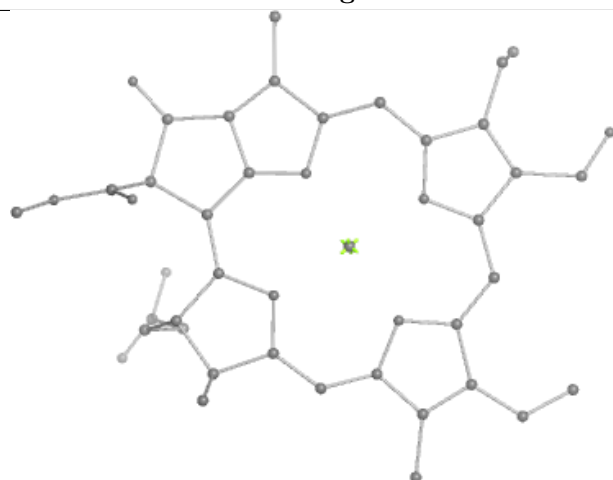
Bond lengths



Bond angles

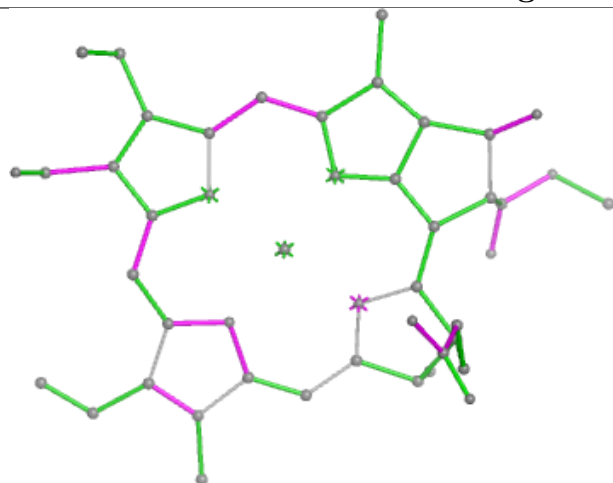


Torsions

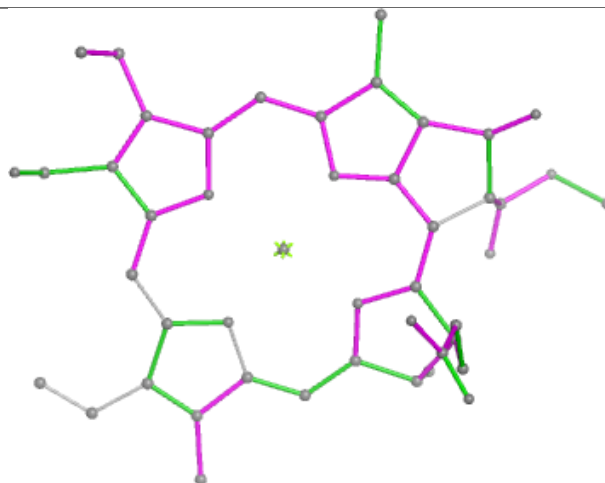


Rings

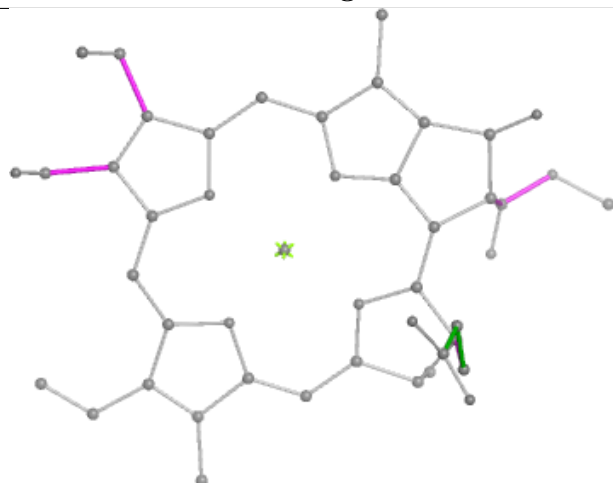
## Ligand CHL 6 603



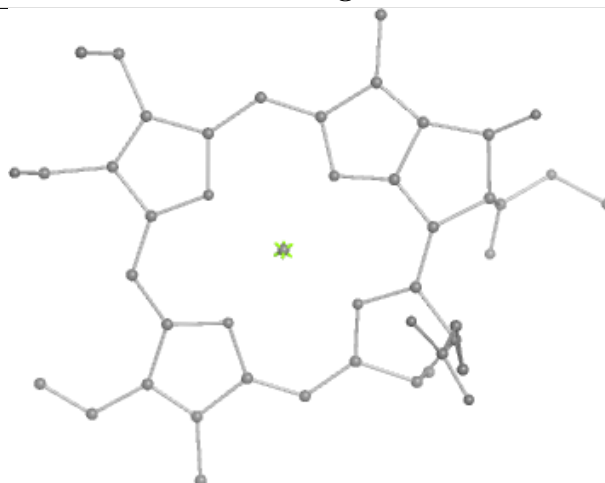
Bond lengths



Bond angles

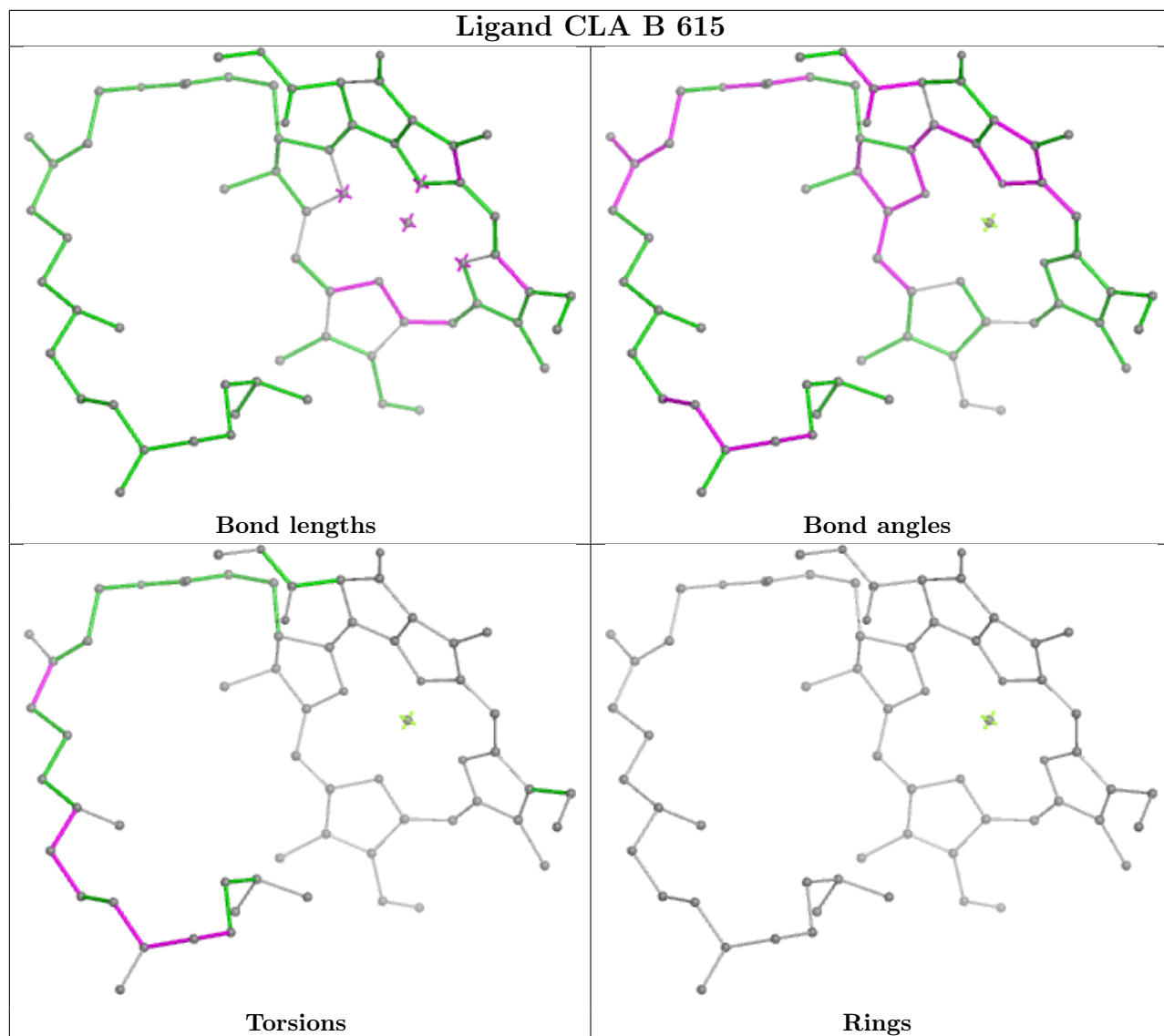


Torsions

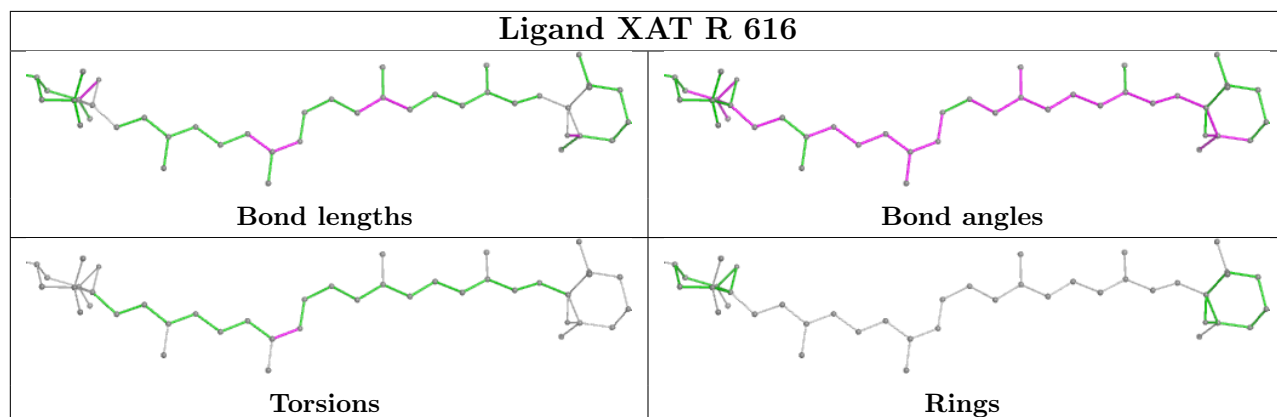


Rings

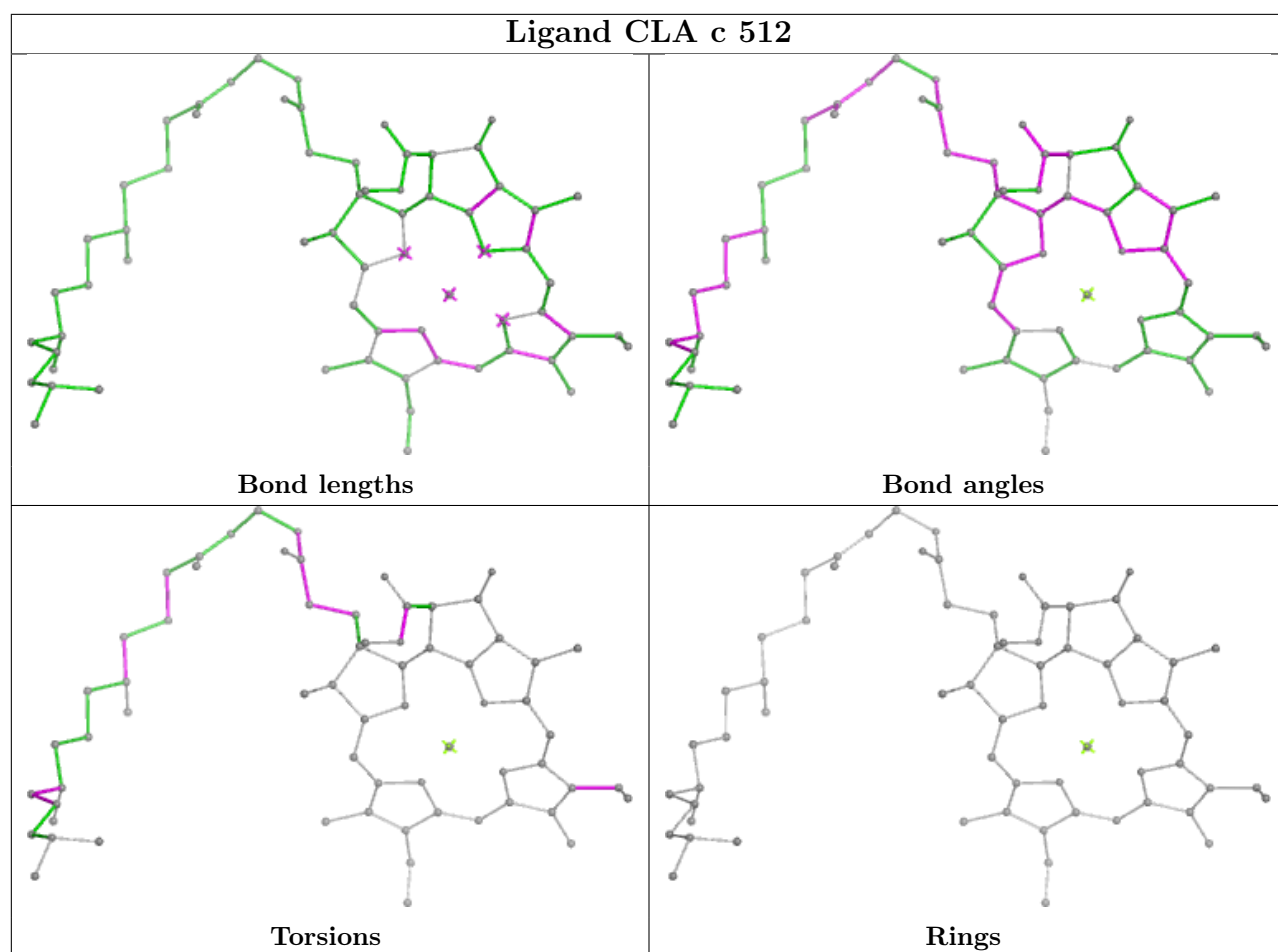
## Ligand CLA B 615



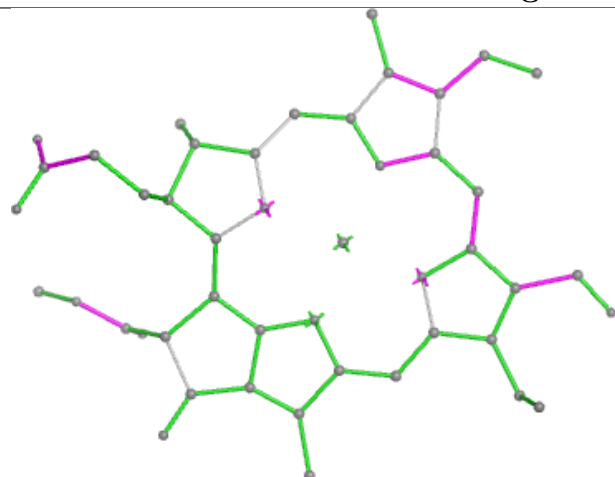
## Ligand XAT R 616



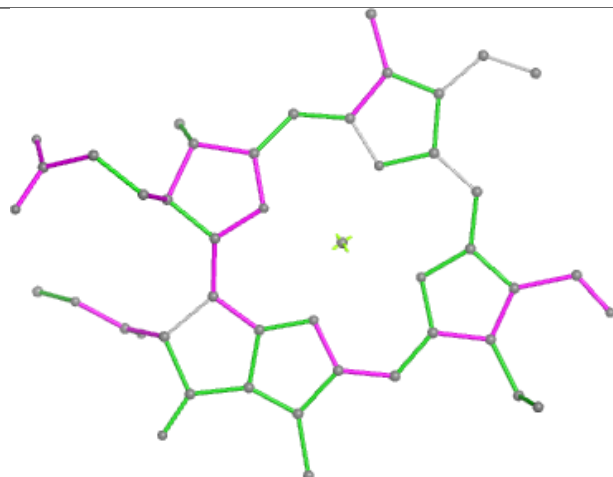




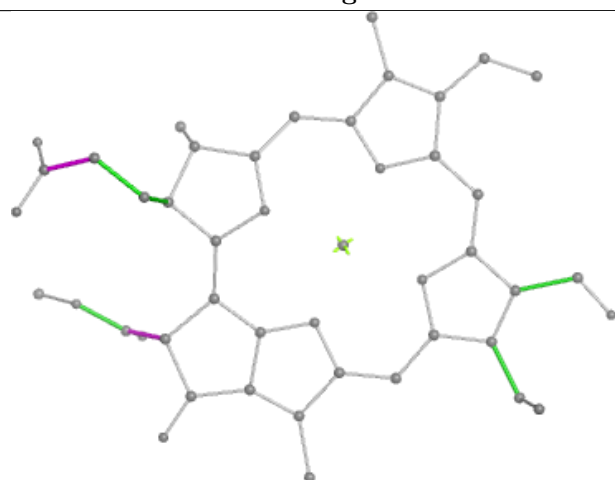
## Ligand CHL s 302



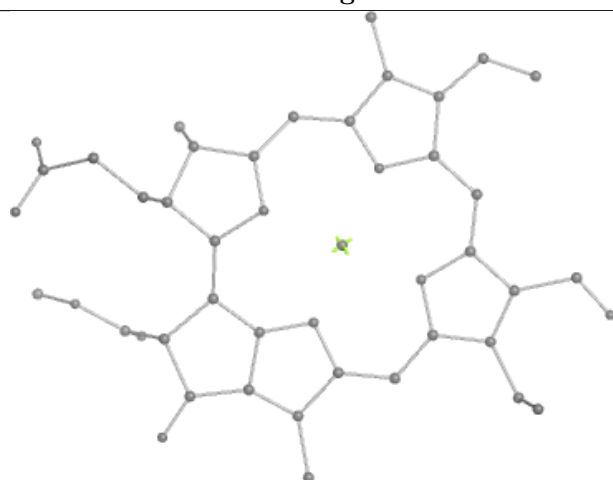
Bond lengths



Bond angles

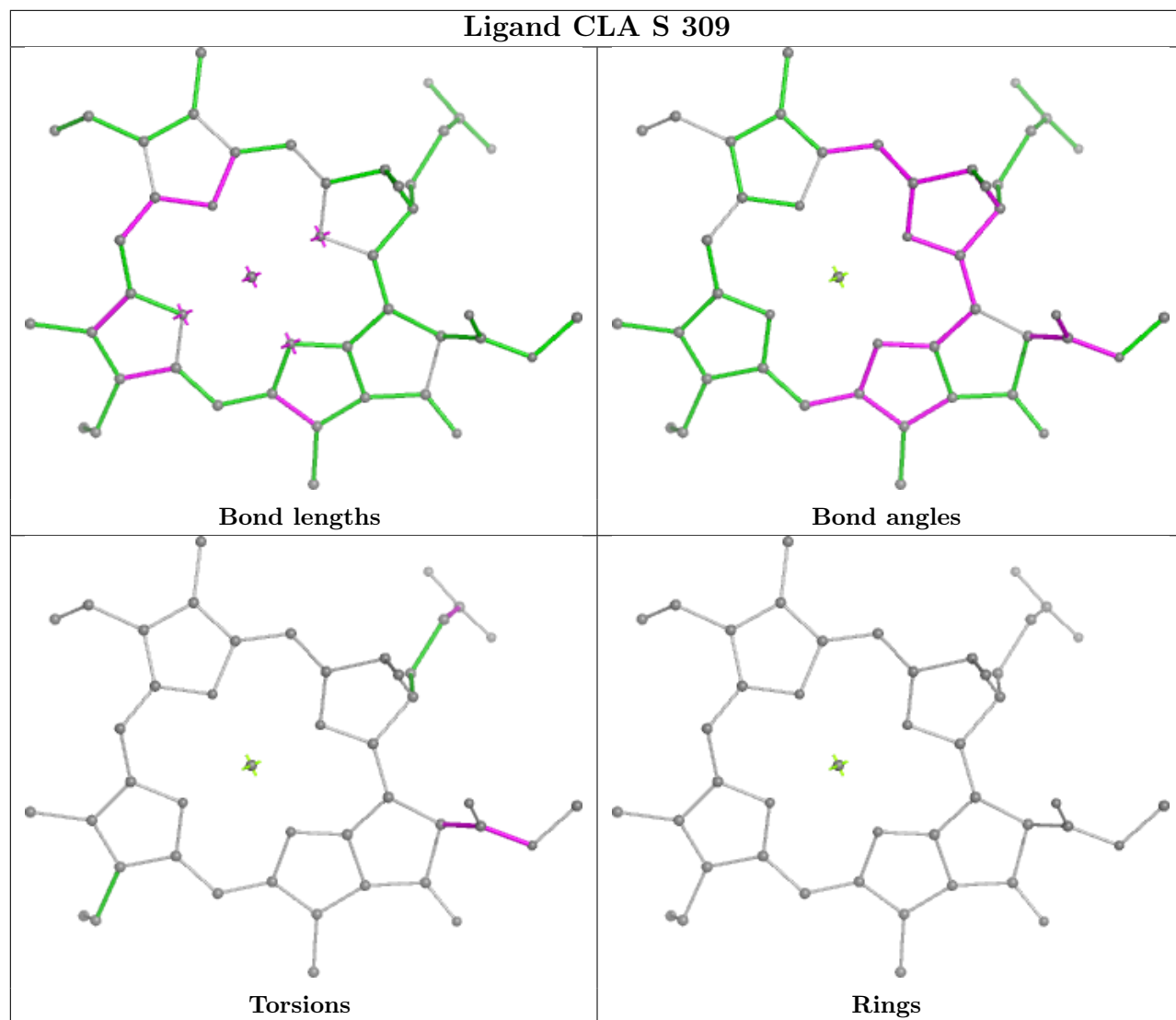


Torsions

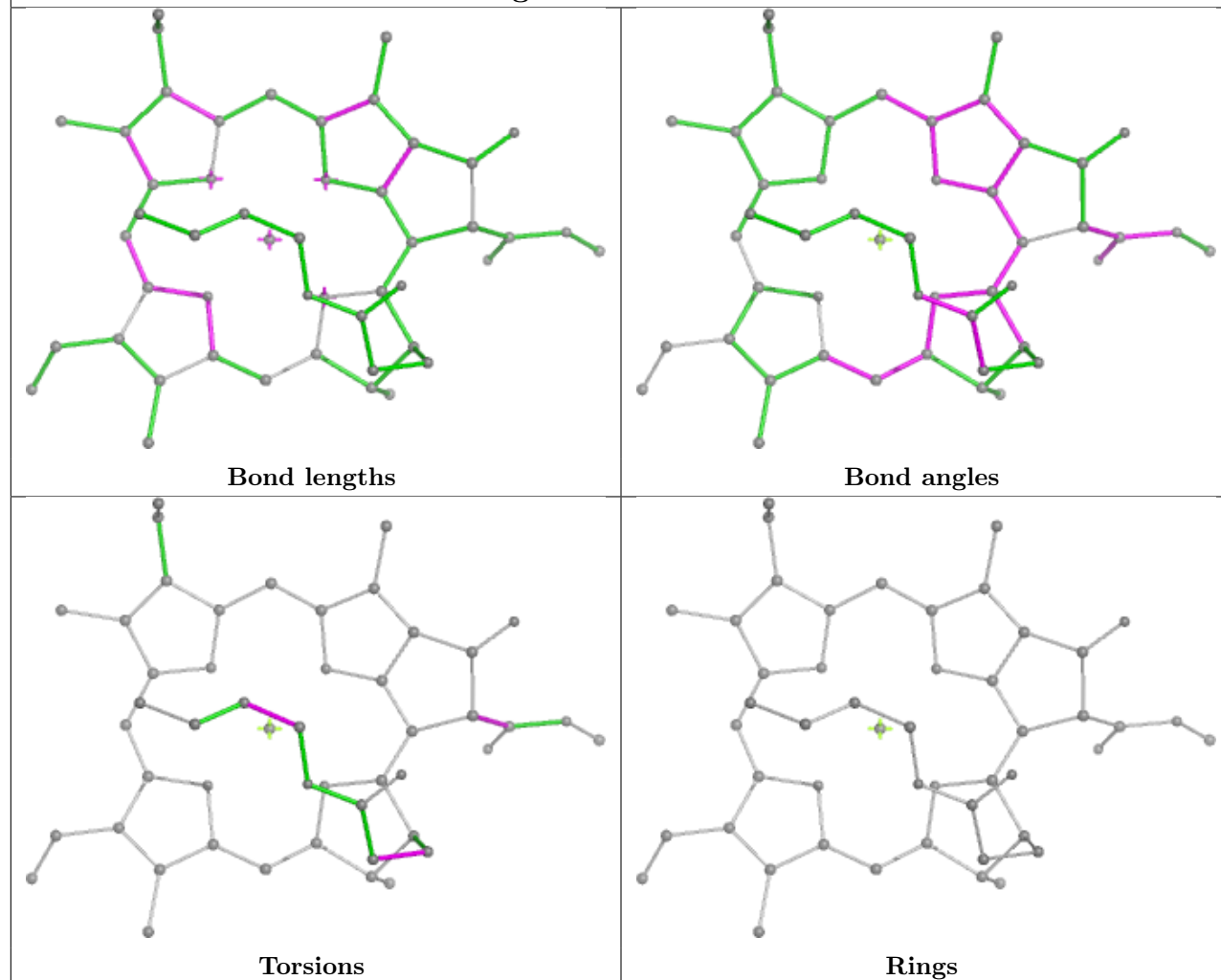


Rings

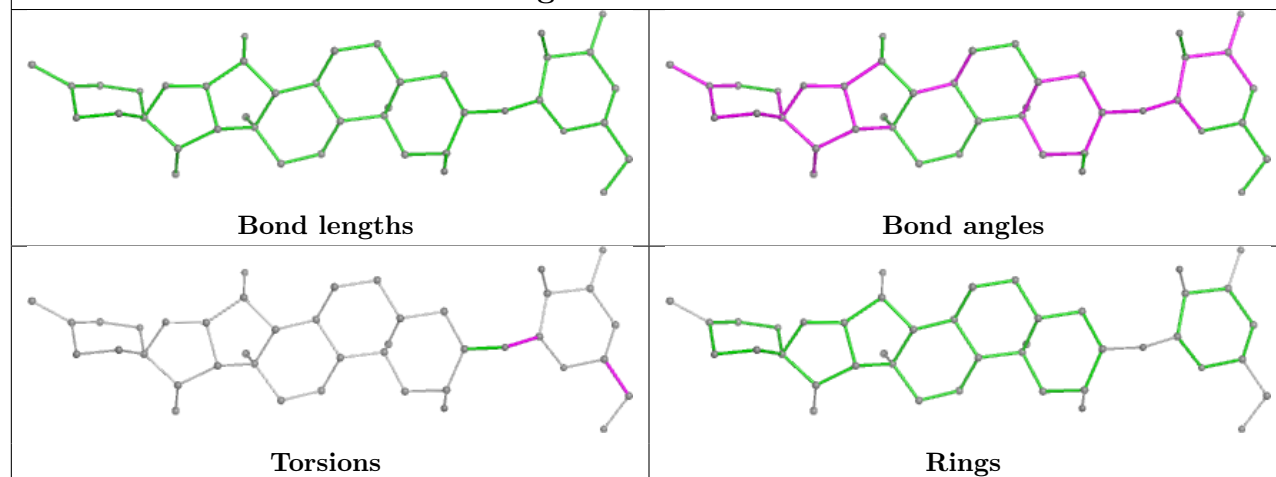
## Ligand CLA S 309



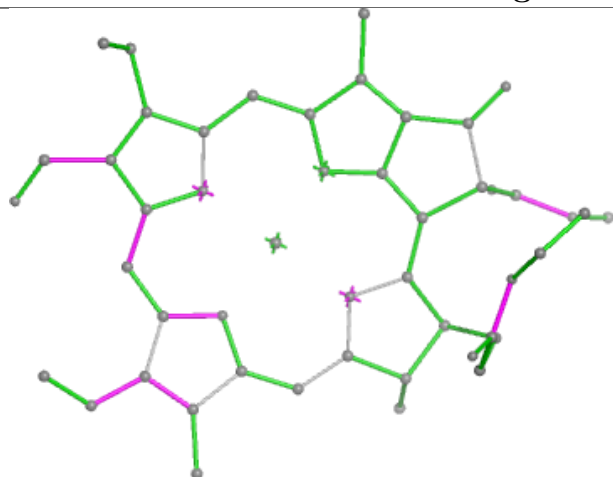
## Ligand CLA S 314



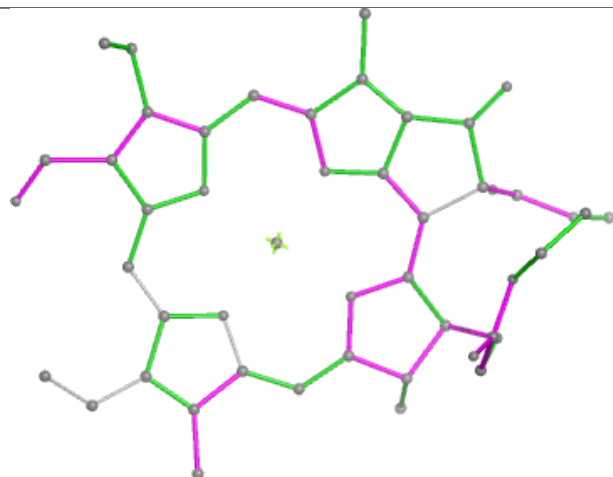
## Ligand AJP S 319



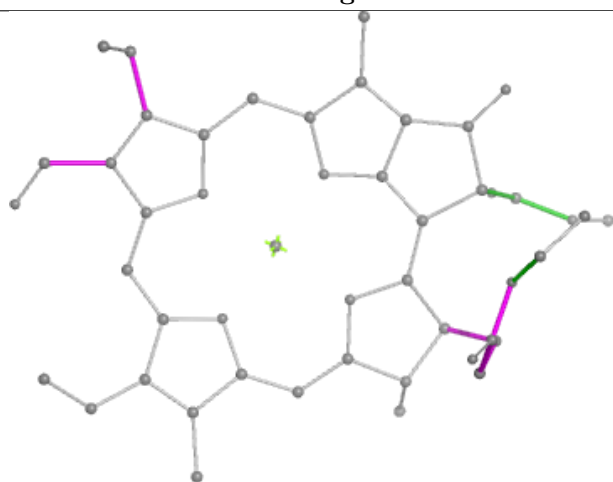
## Ligand CHL Y 306



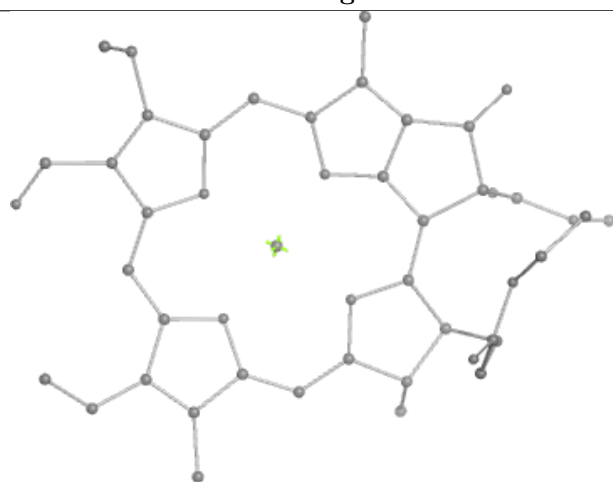
Bond lengths



Bond angles

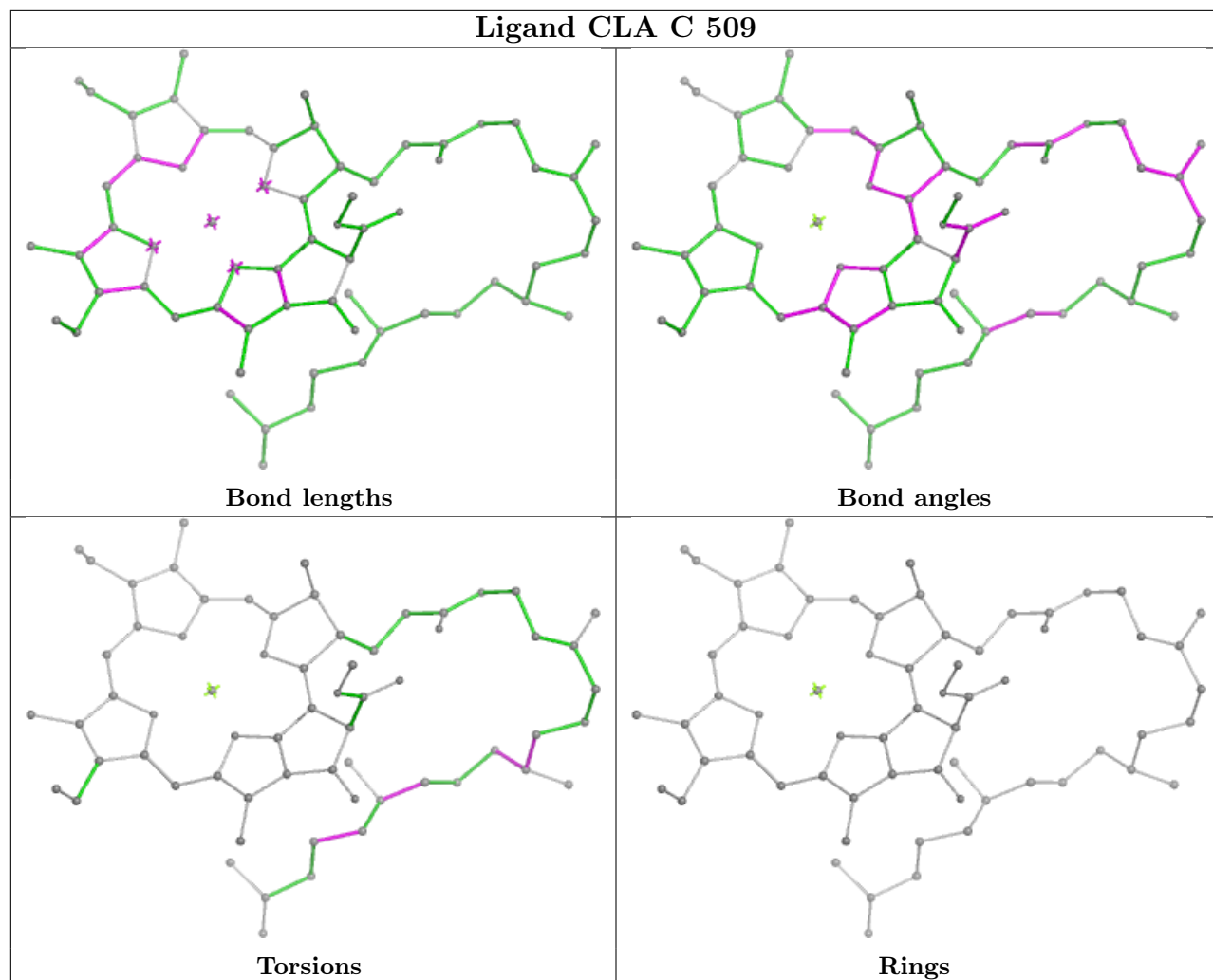


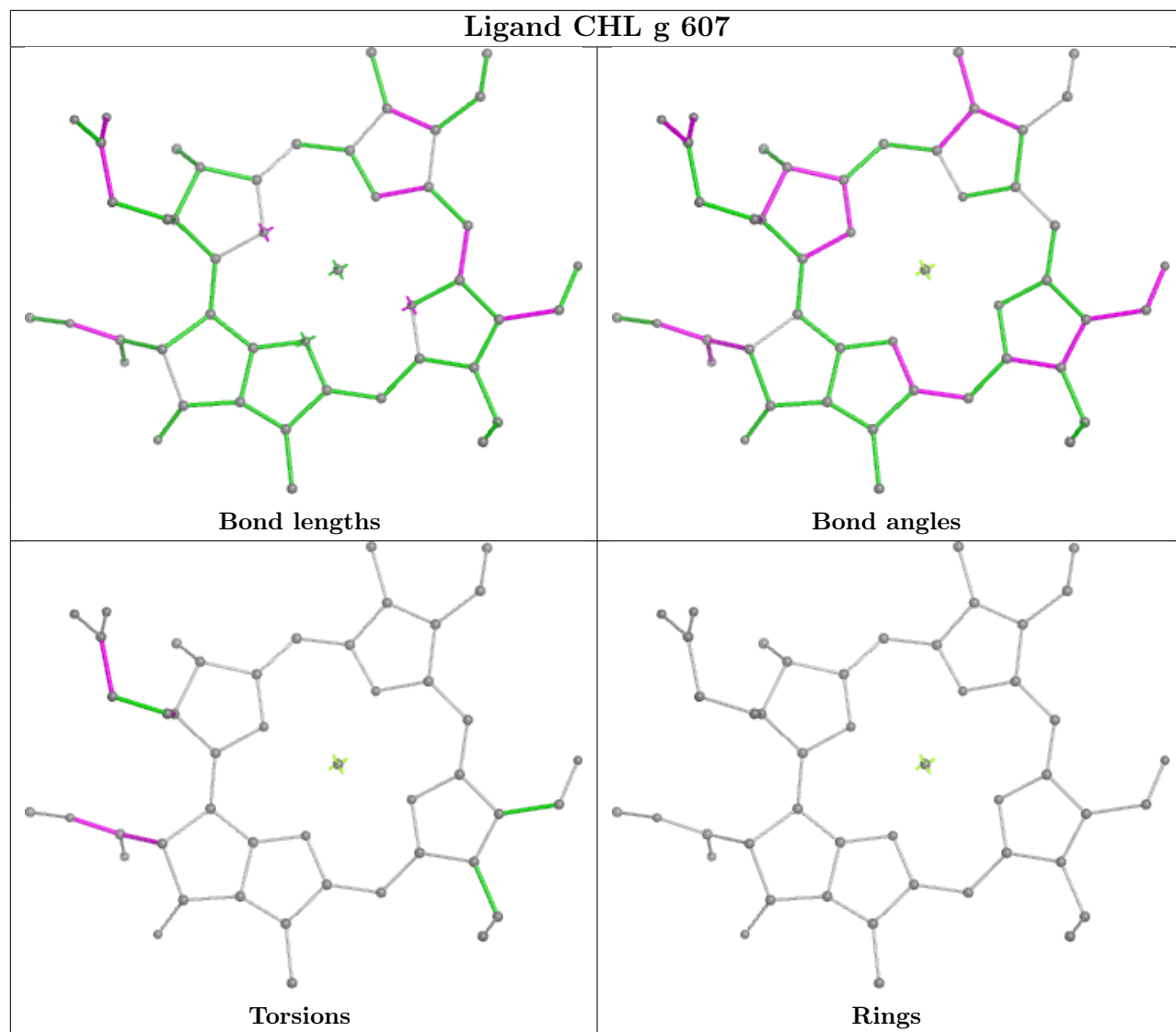
Torsions



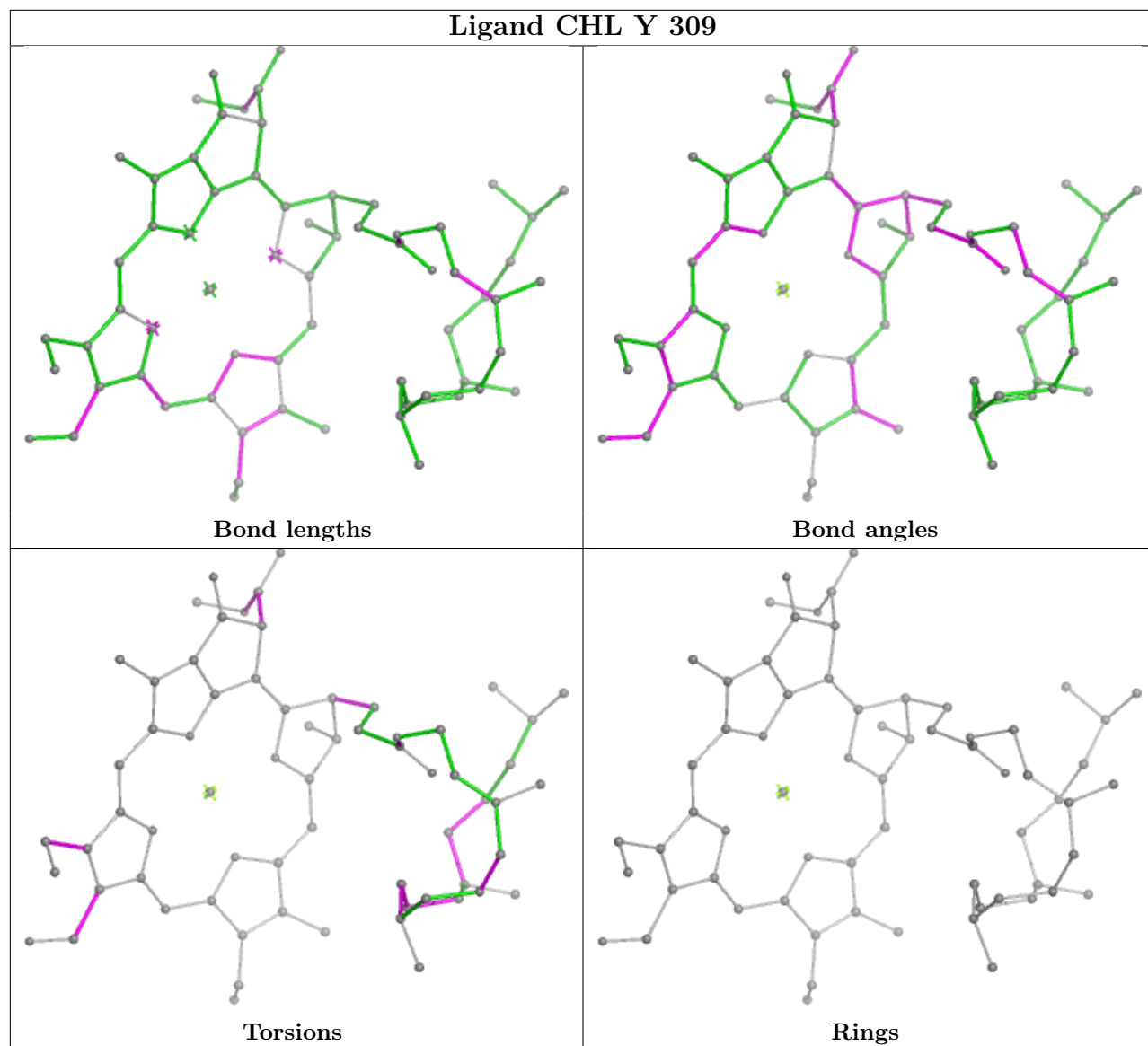
Rings

## Ligand CLA C 509

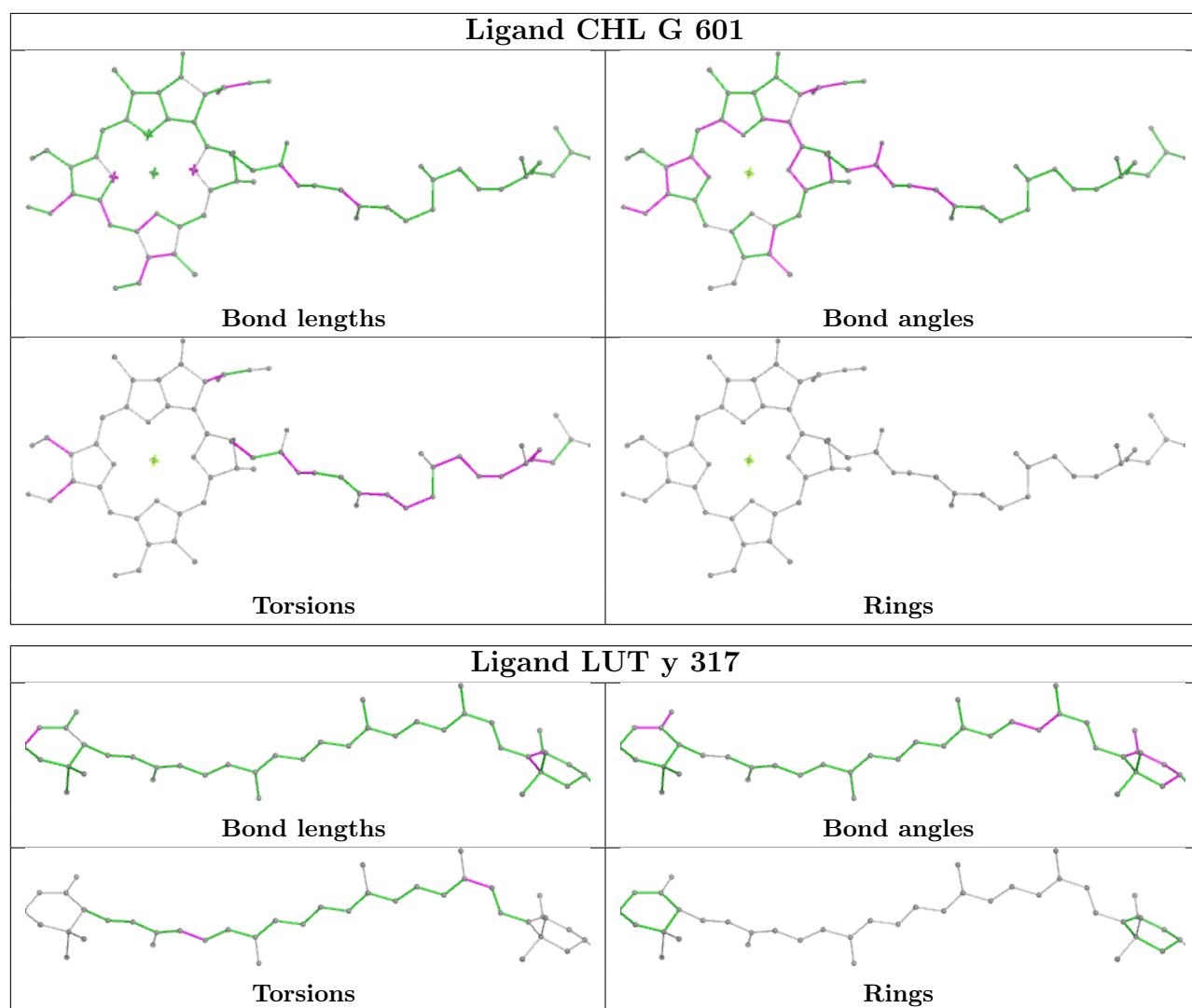




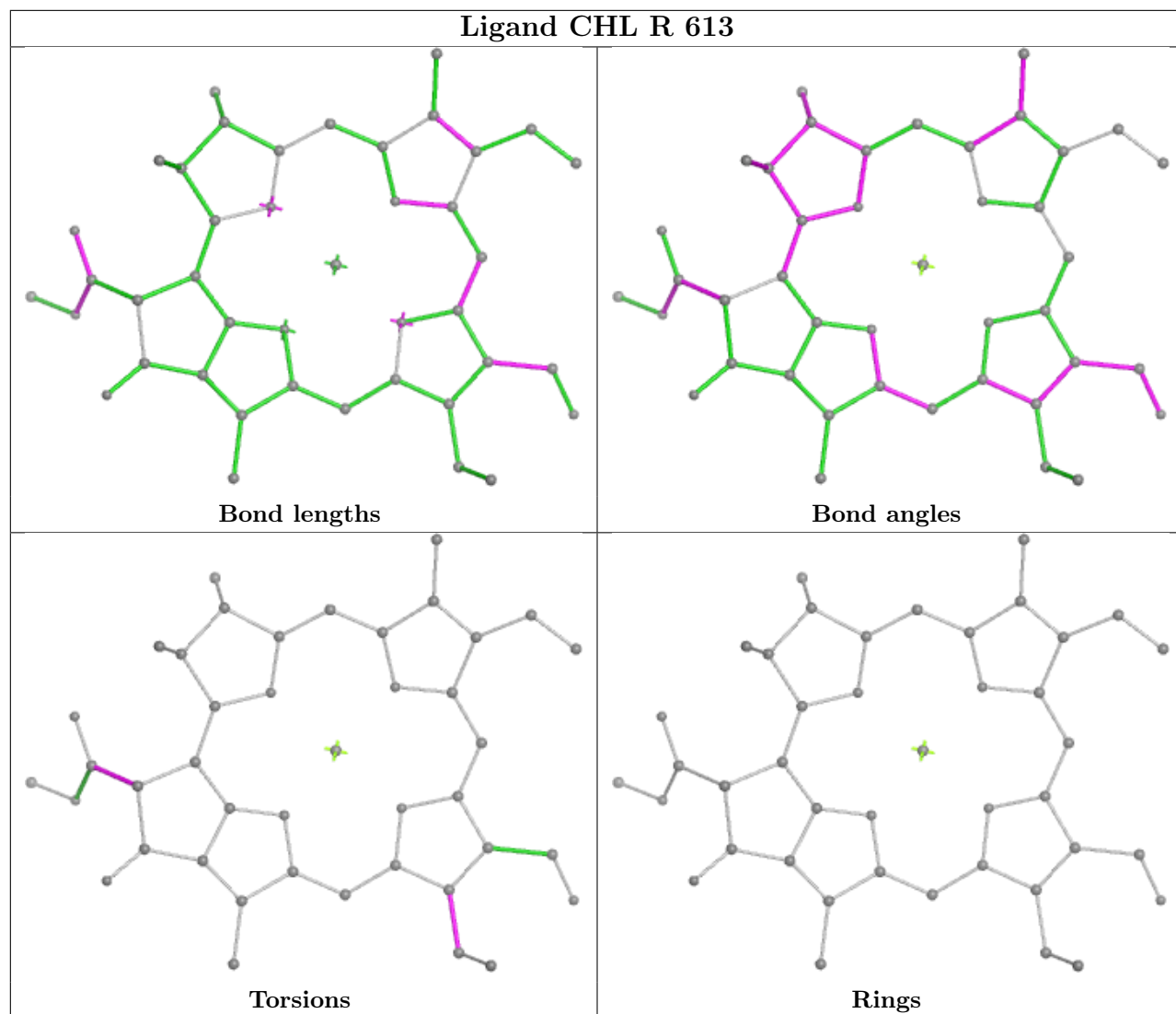
## Ligand CHL Y 309

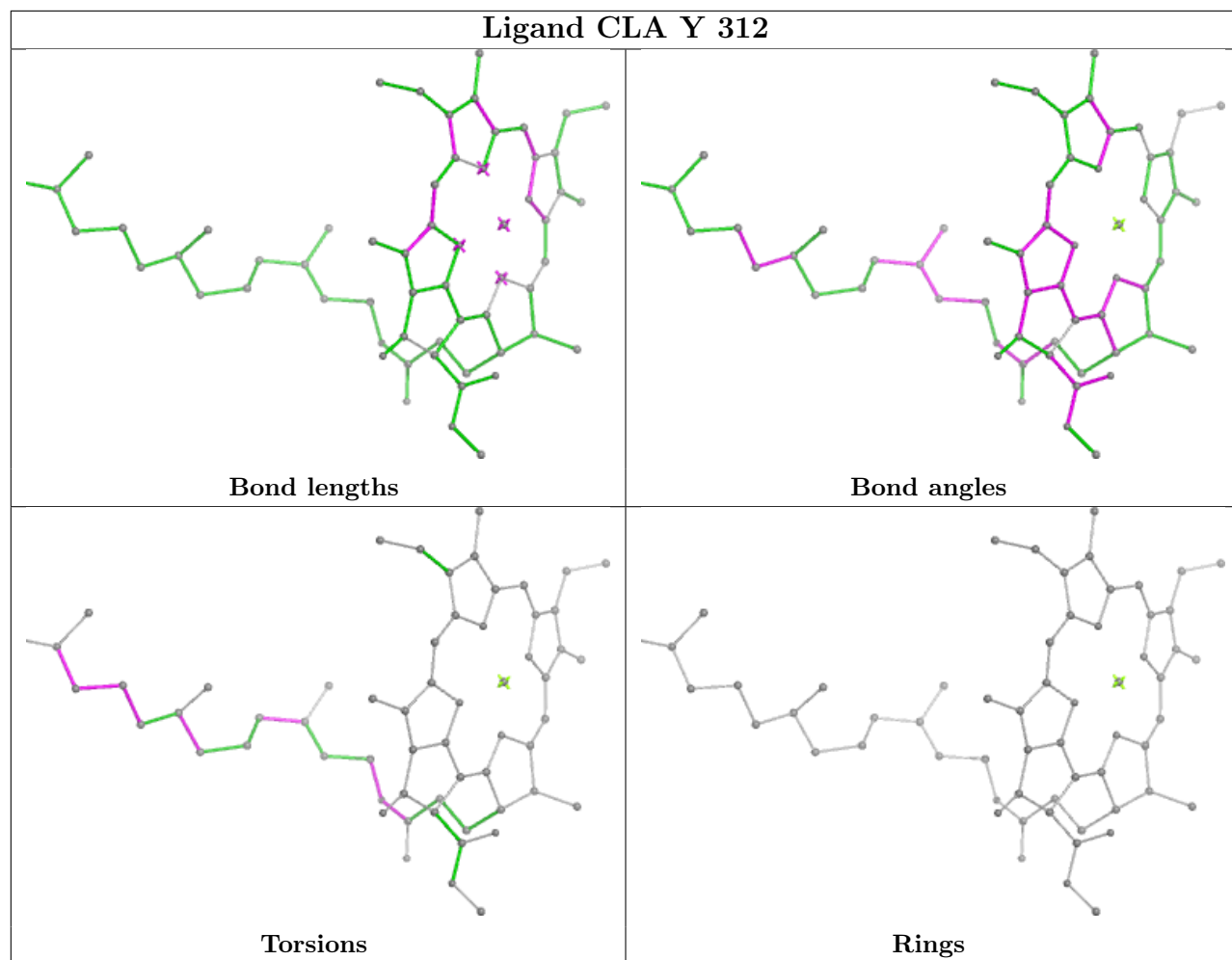




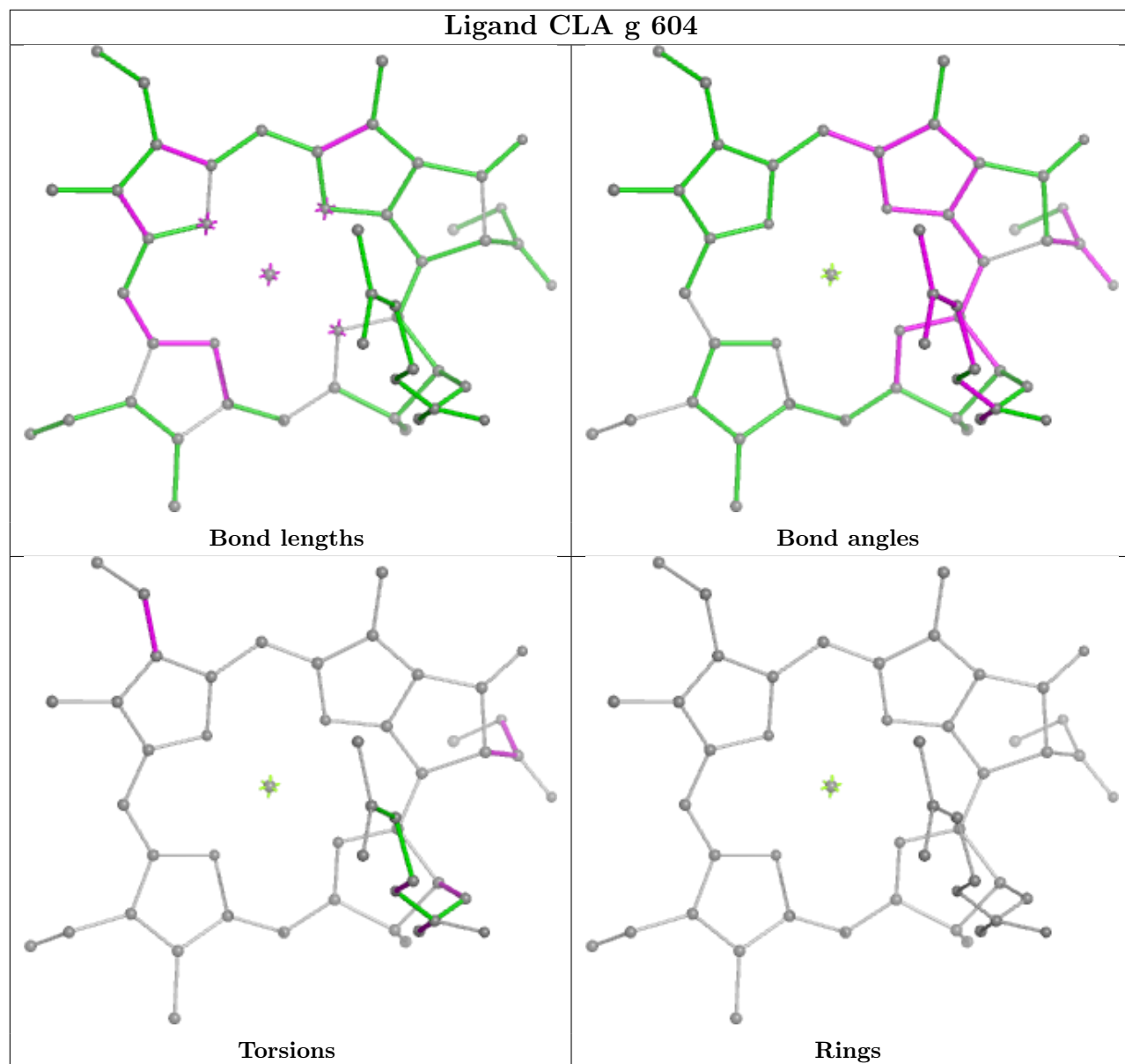


## Ligand CHL R 613

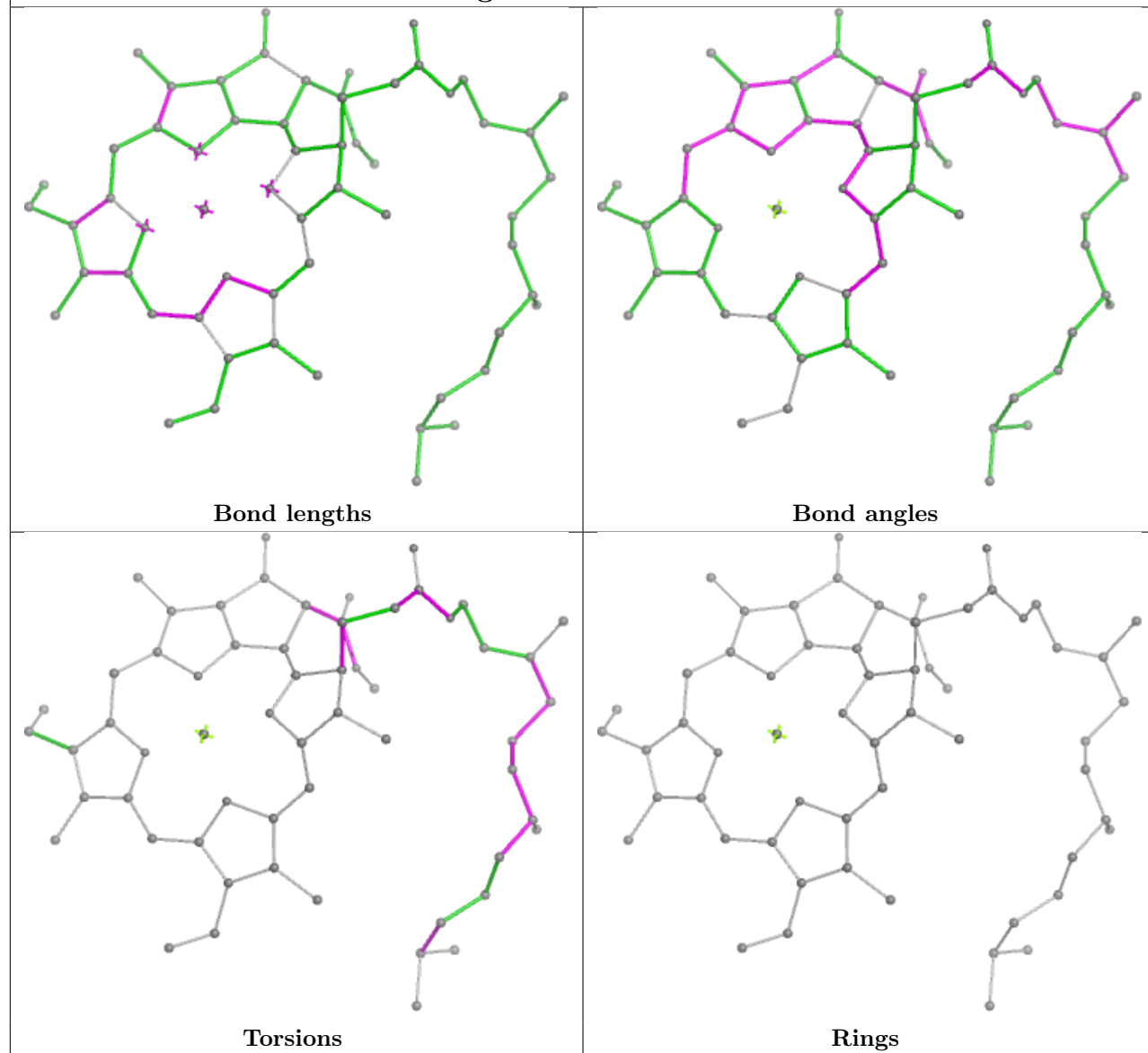




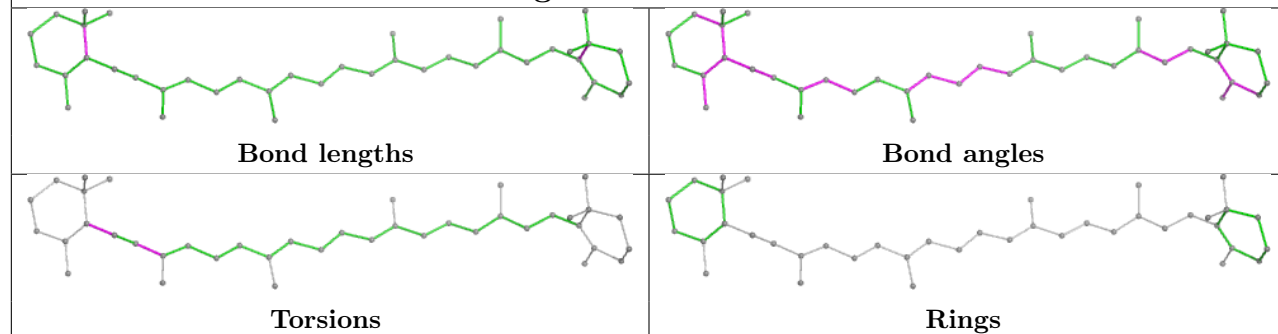
## Ligand CLA g 604



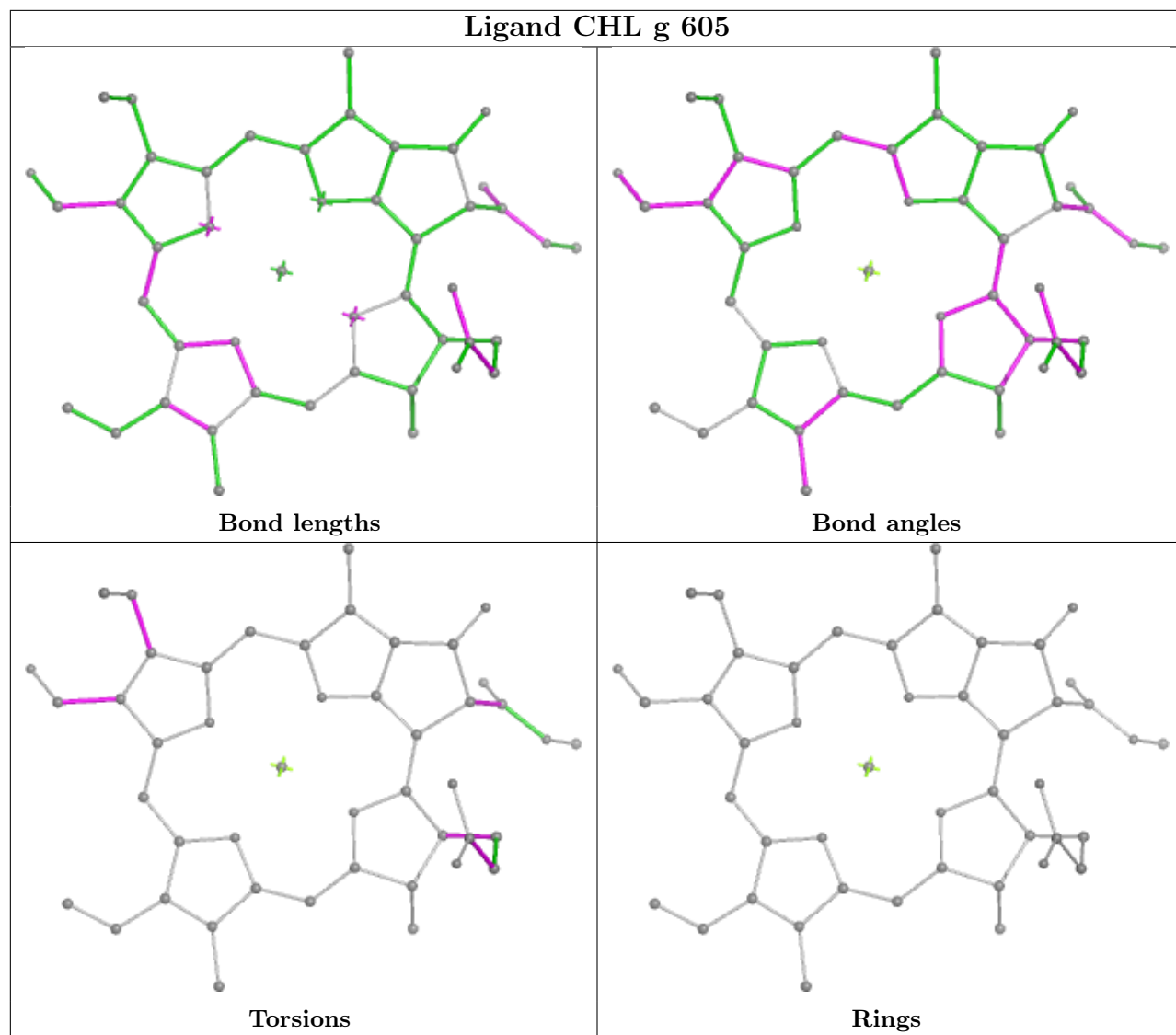
## Ligand CLA N 612

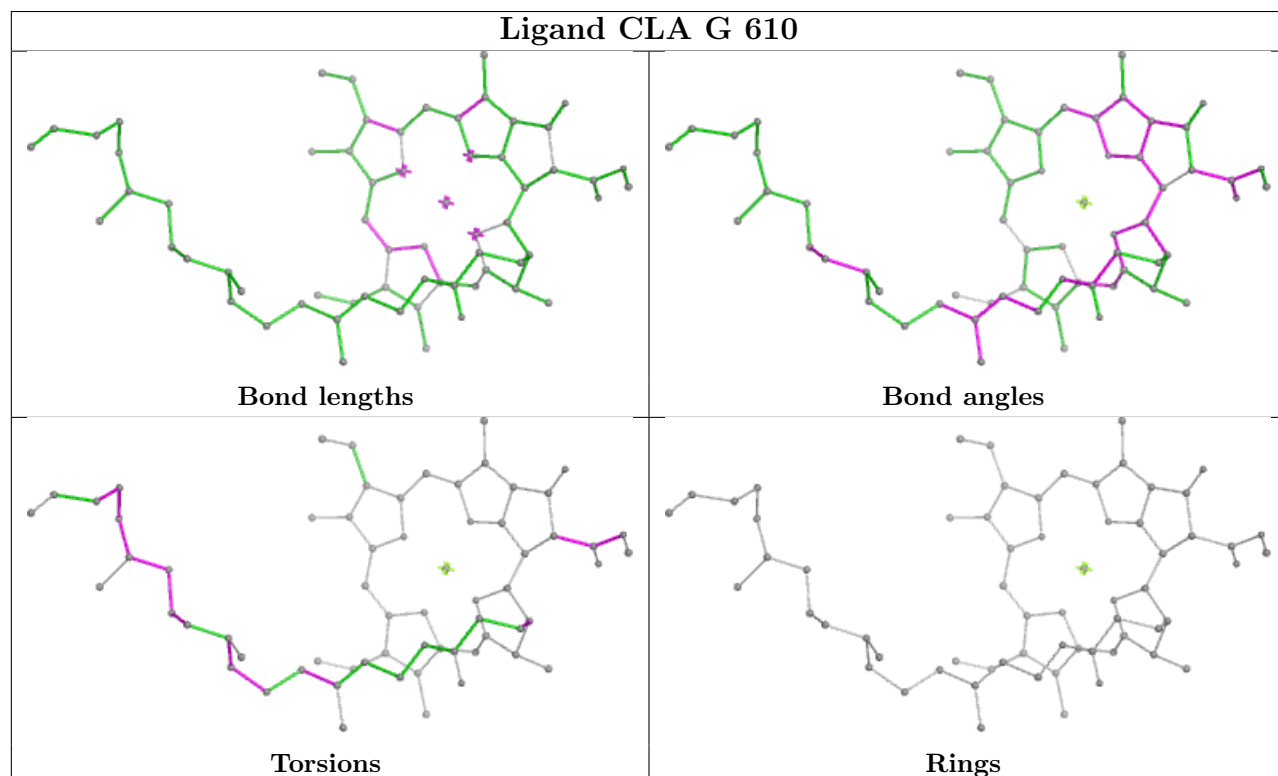
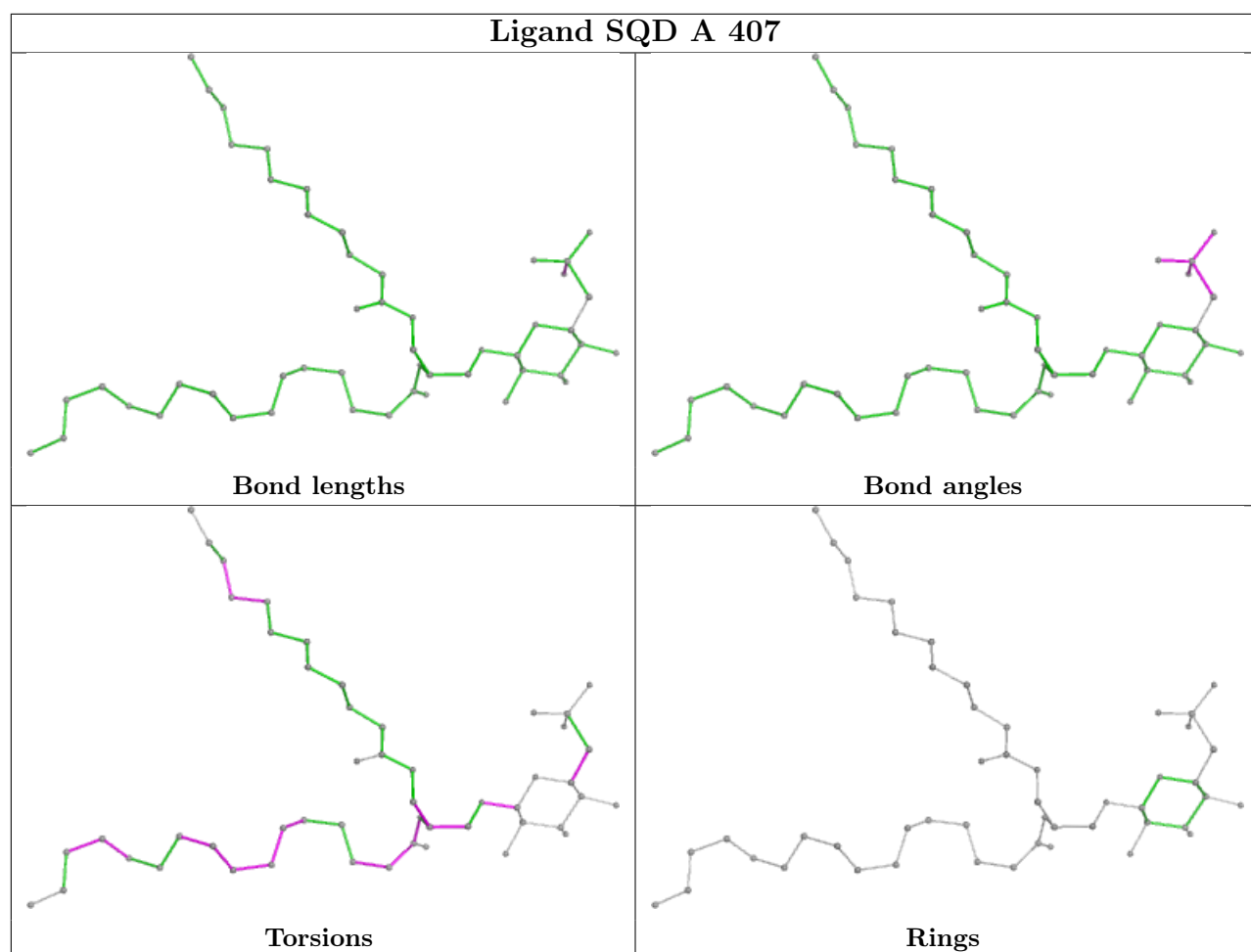


## Ligand BCR k 101

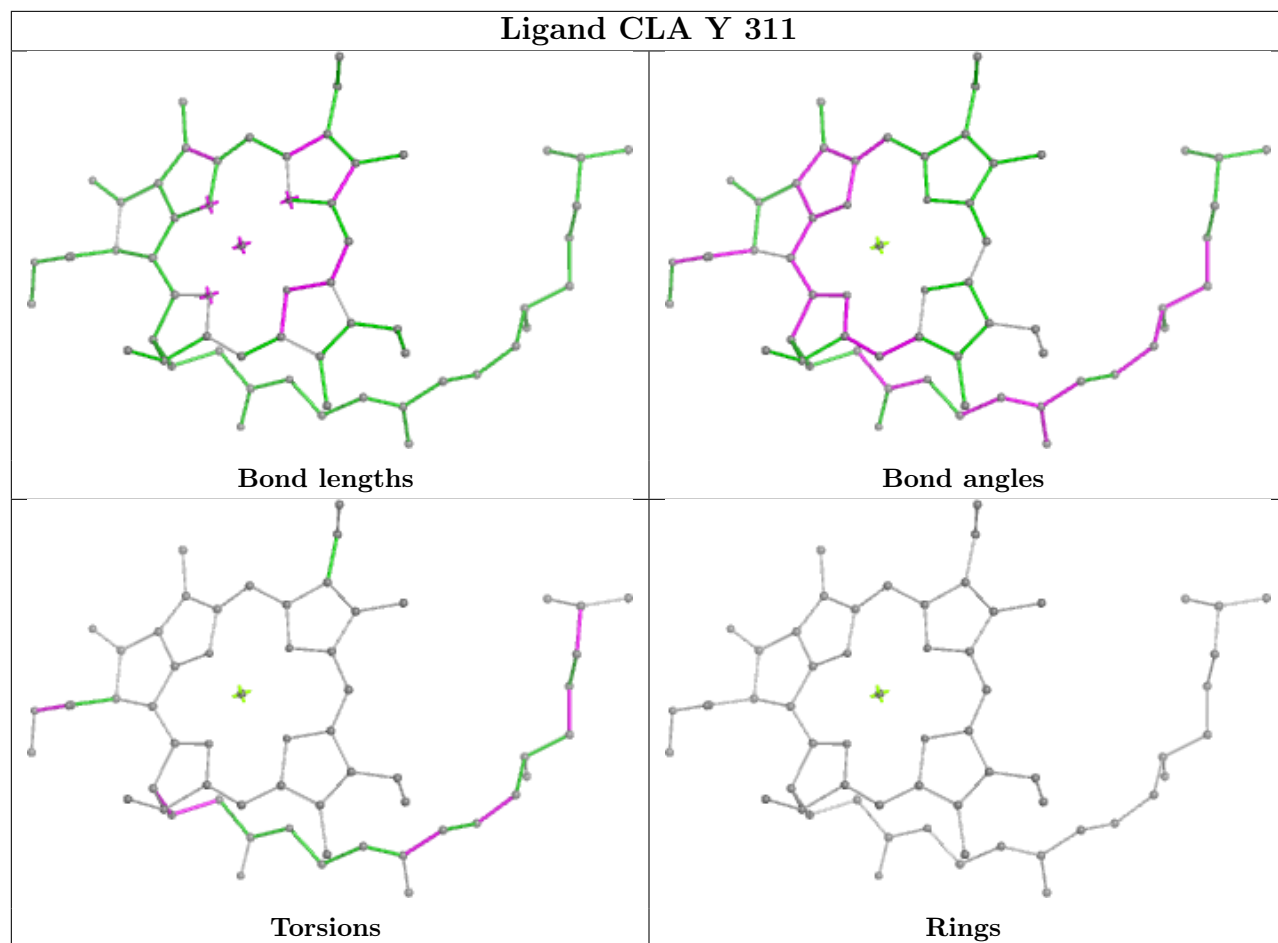


## Ligand CHL g 605

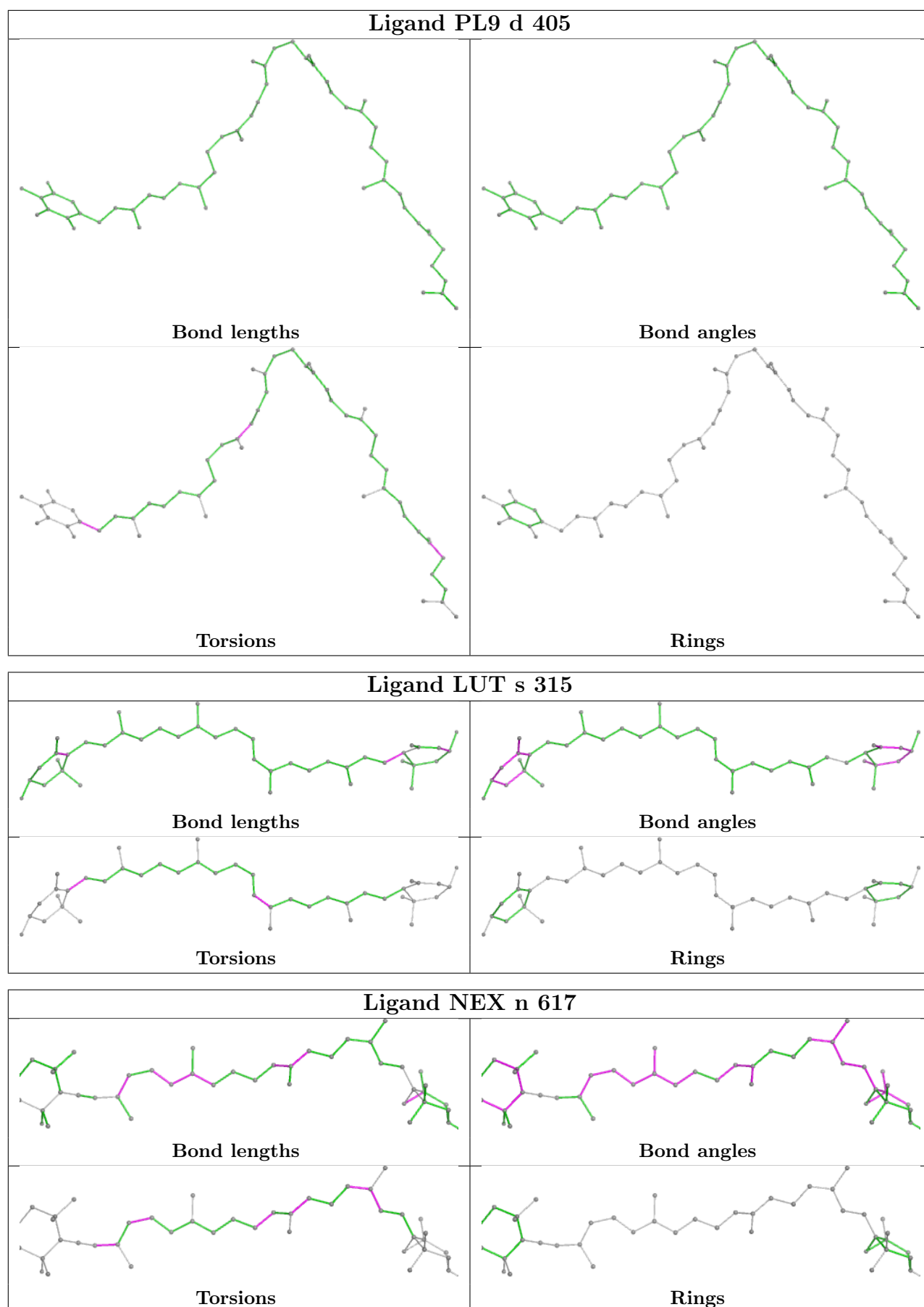




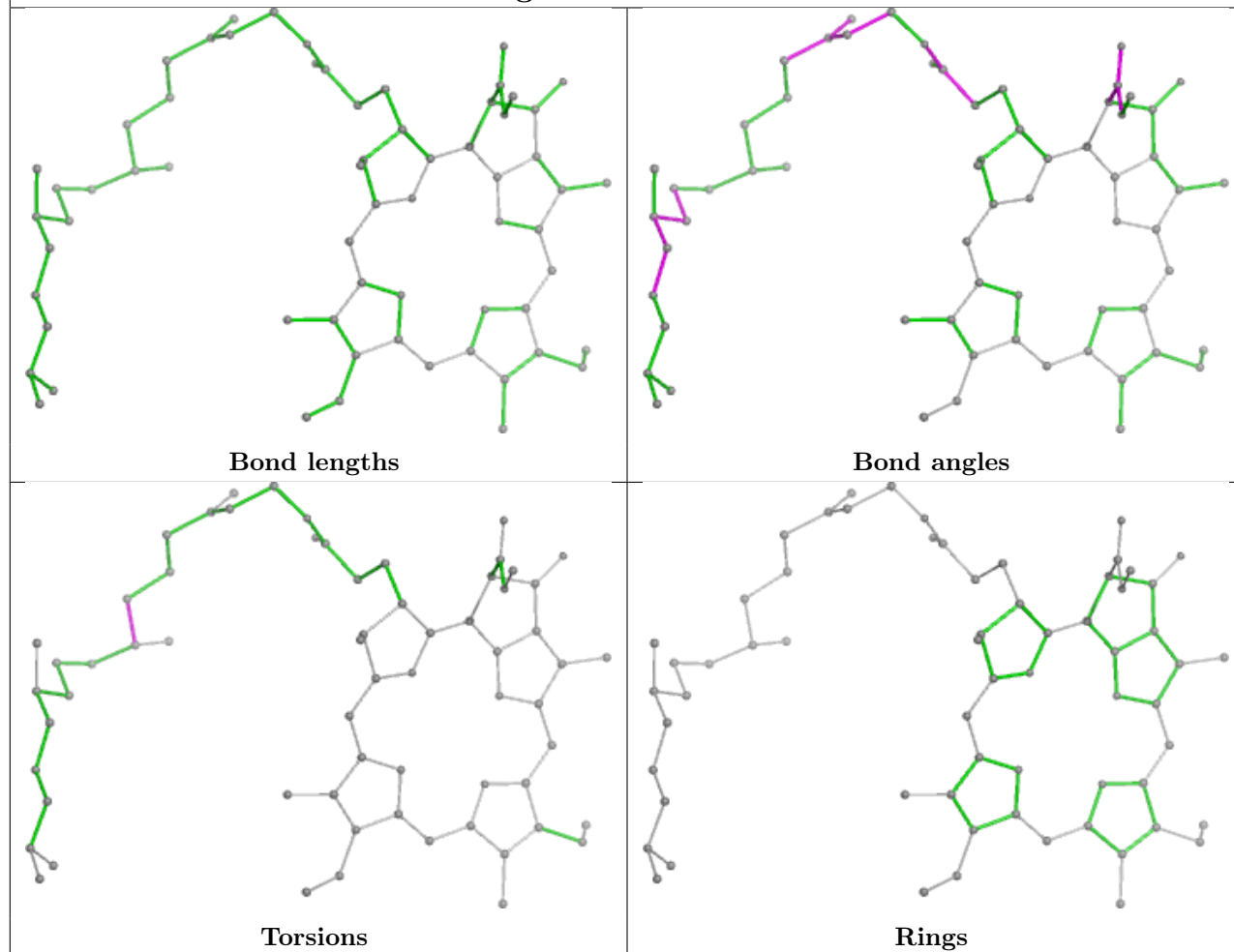
## Ligand CLA Y 311



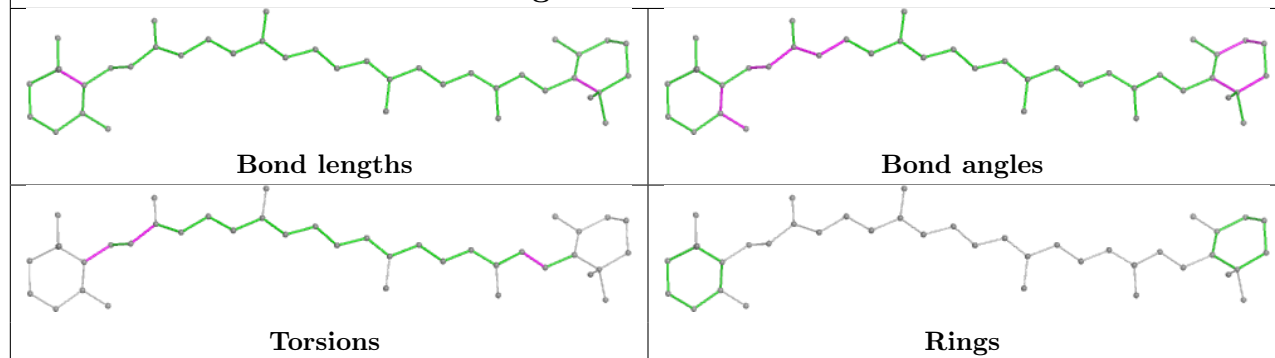


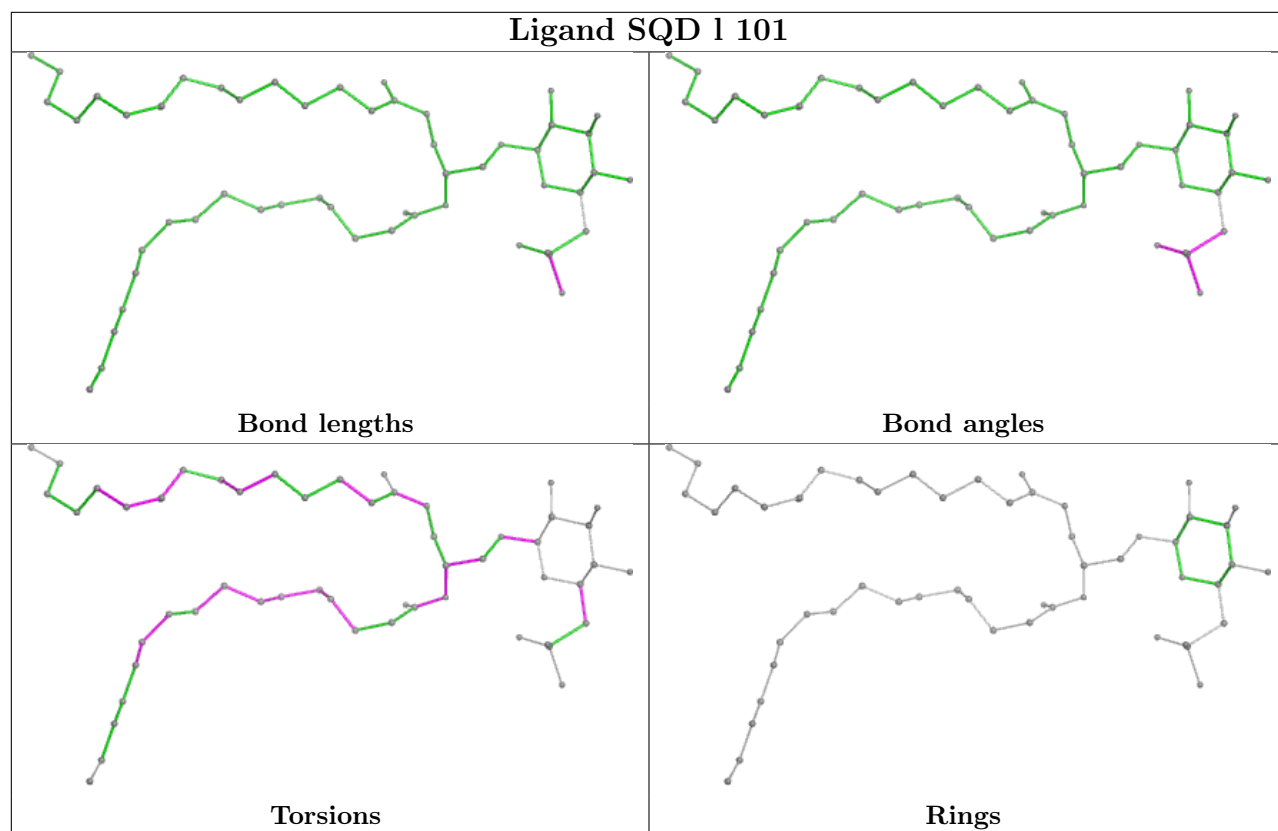
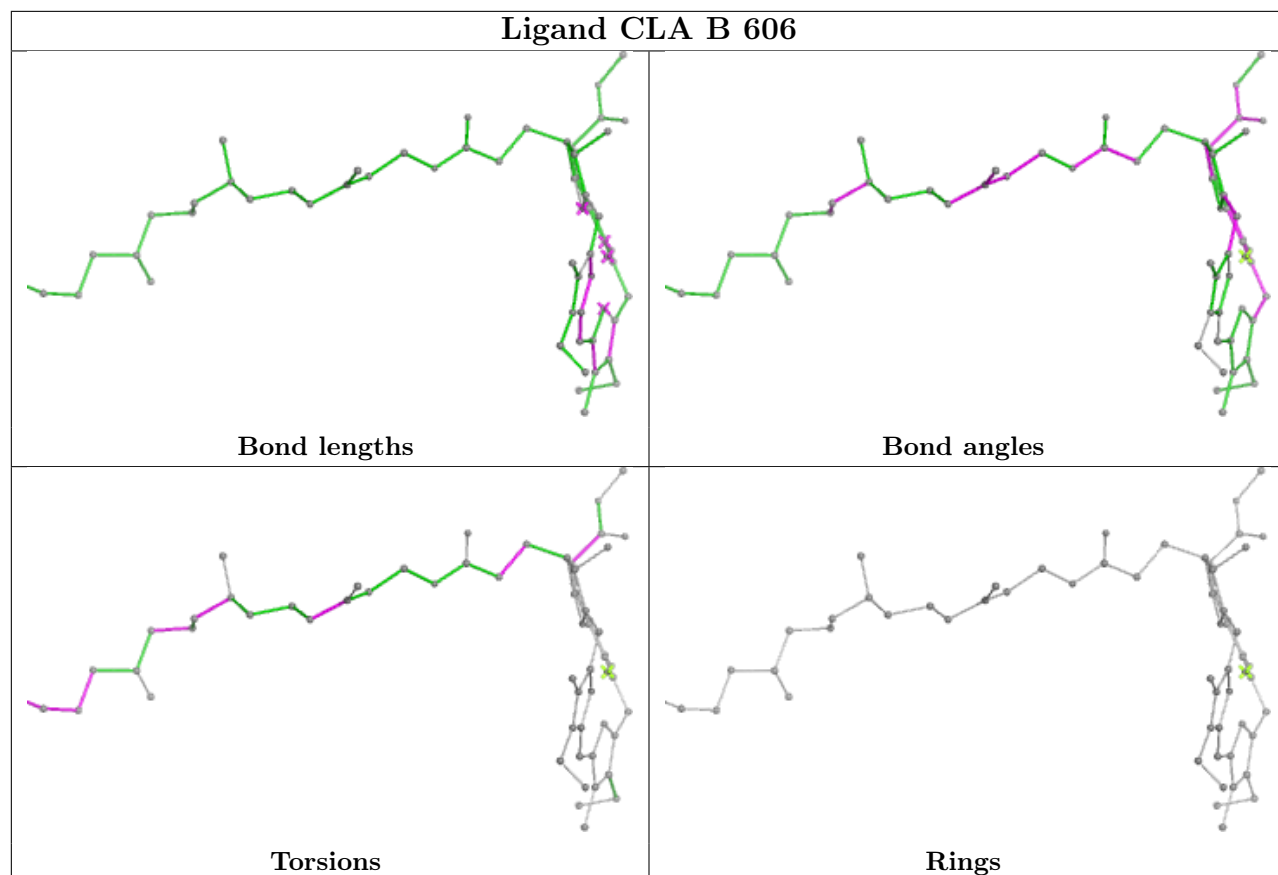


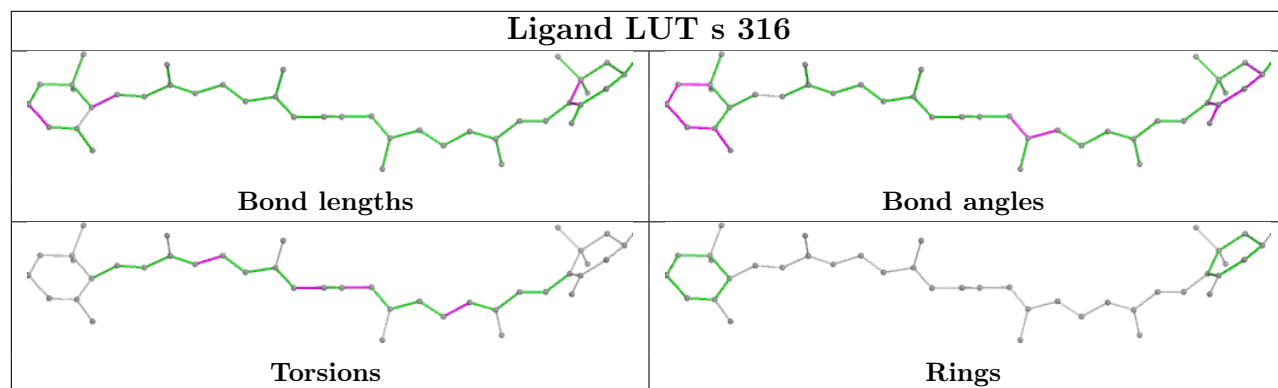
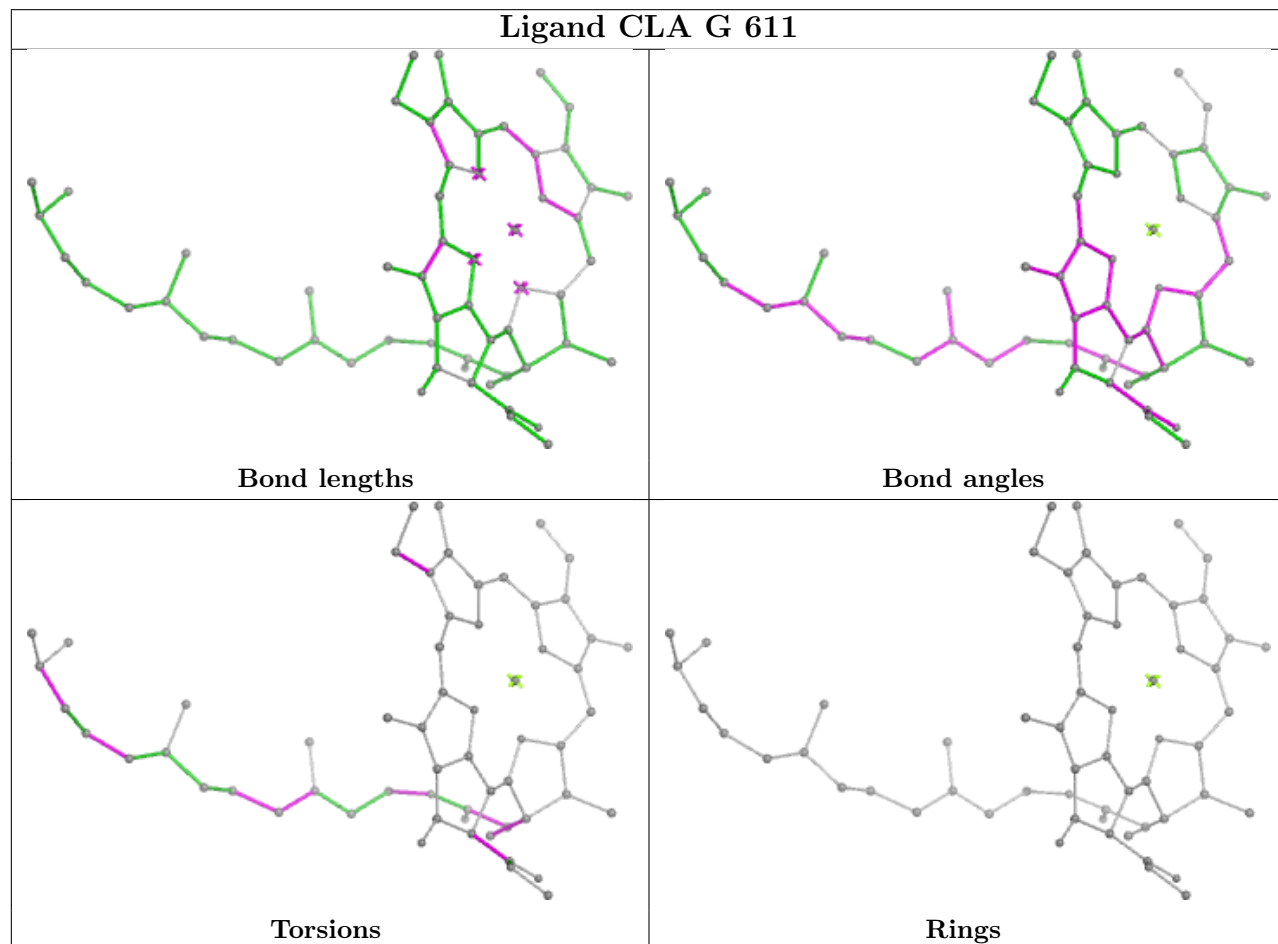
## Ligand PHO a 405



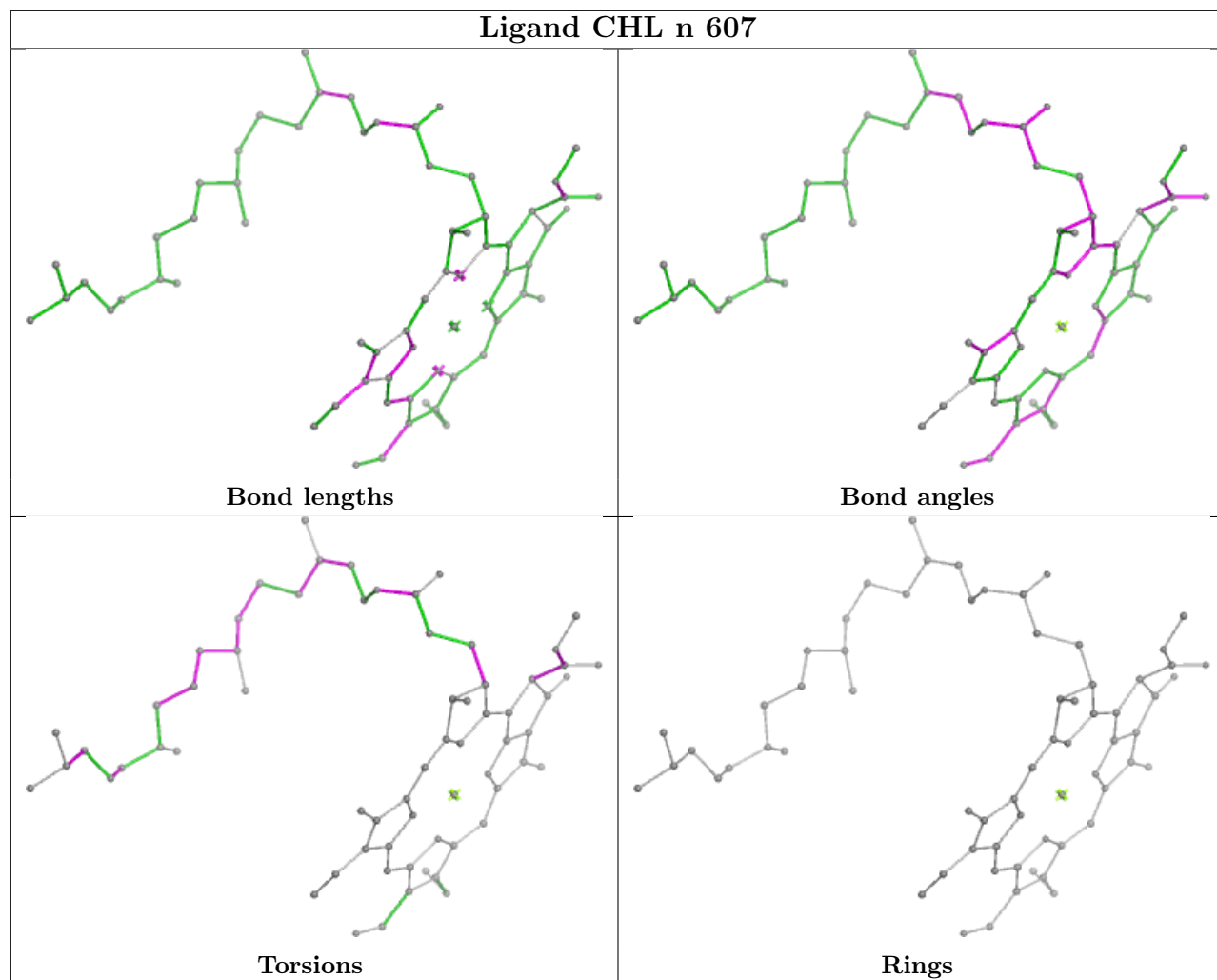
## Ligand BCR d 404



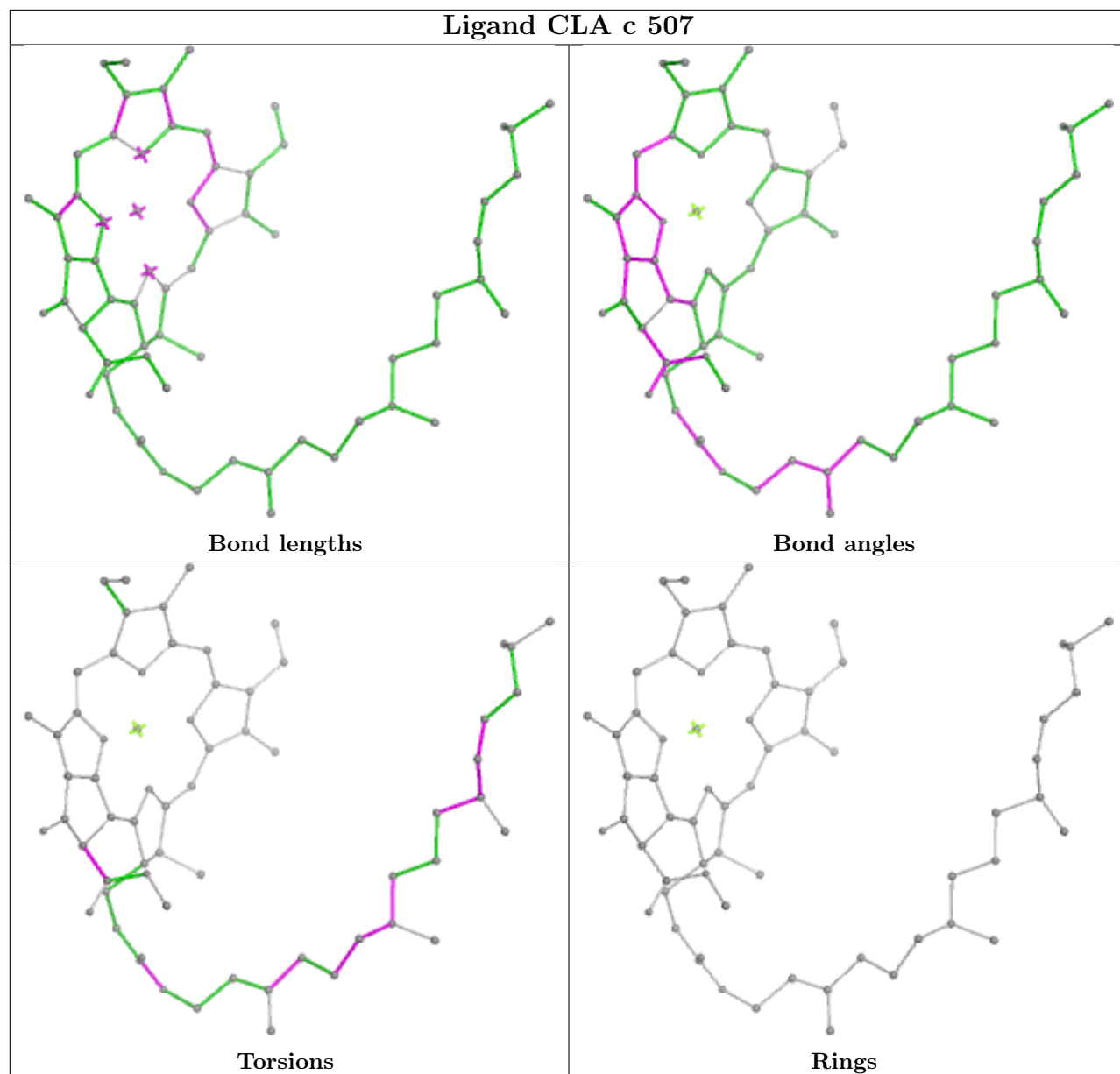


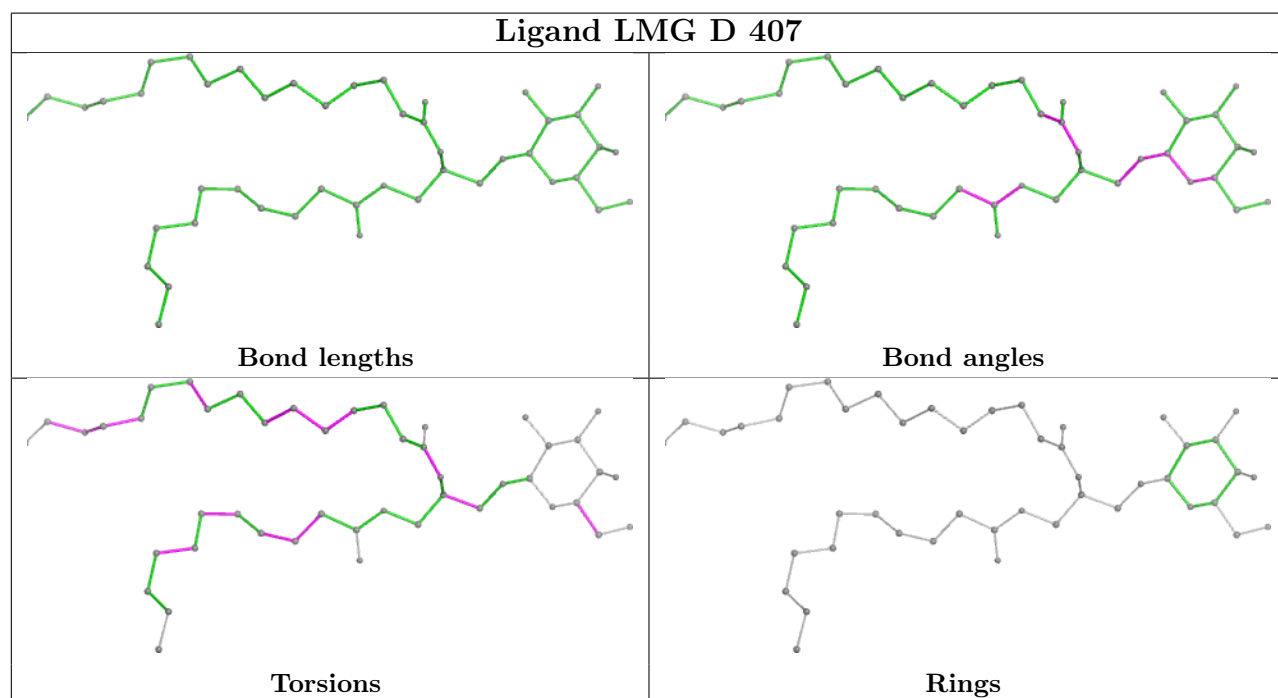
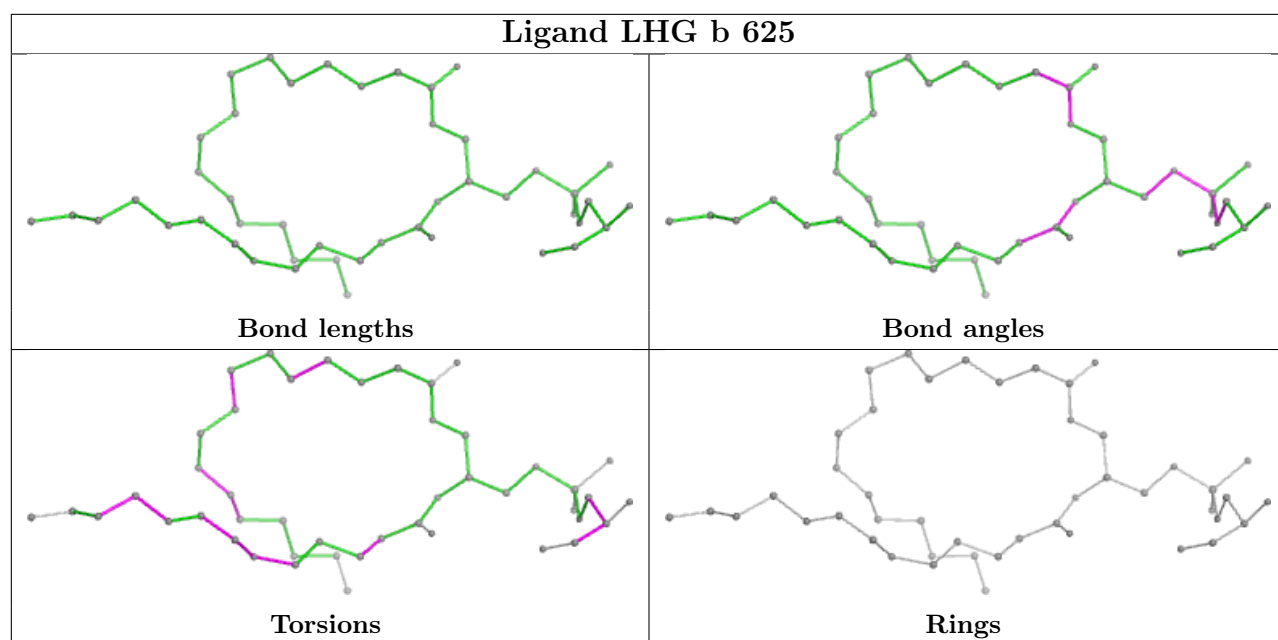
**Ligand LUT s 316****Ligand CLA G 611**

## Ligand CHL n 607

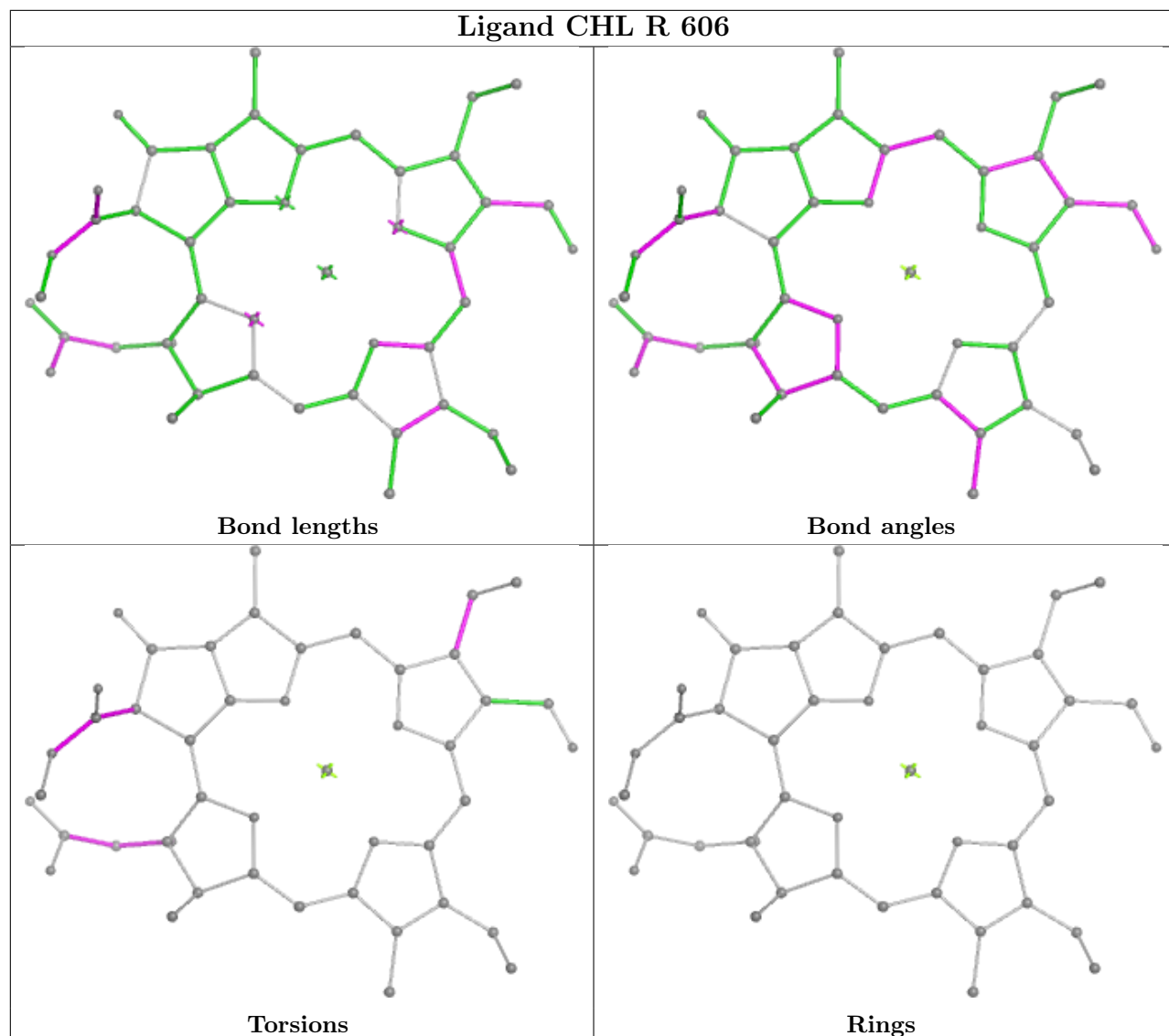


## Ligand CLA c 507

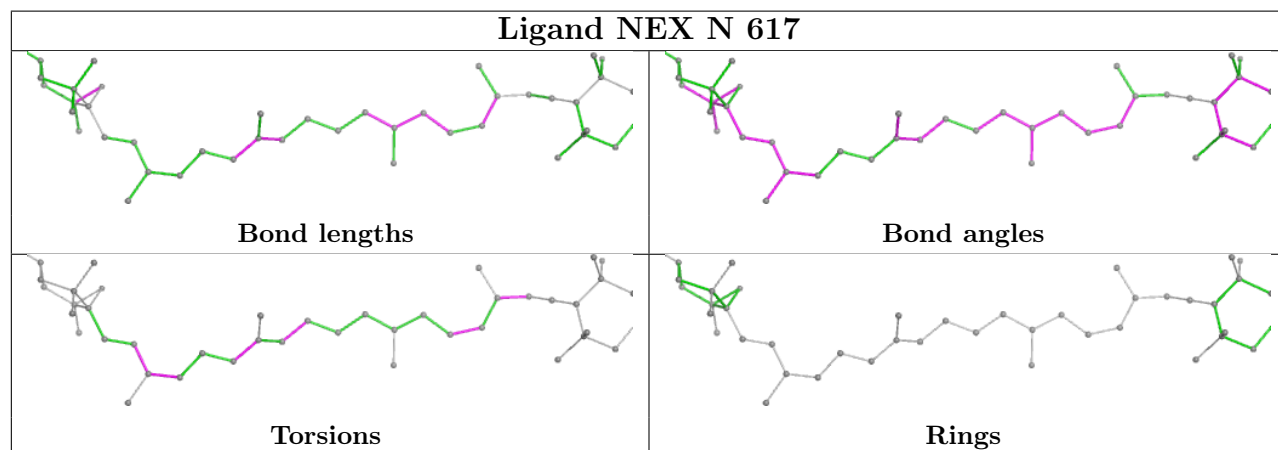




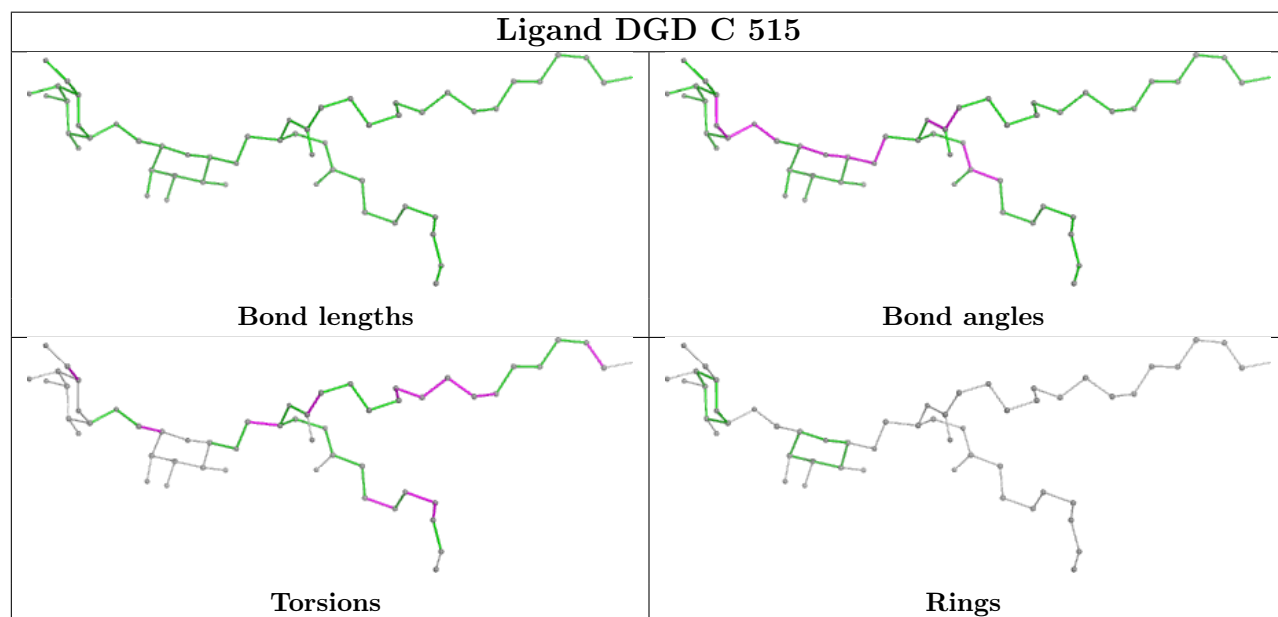
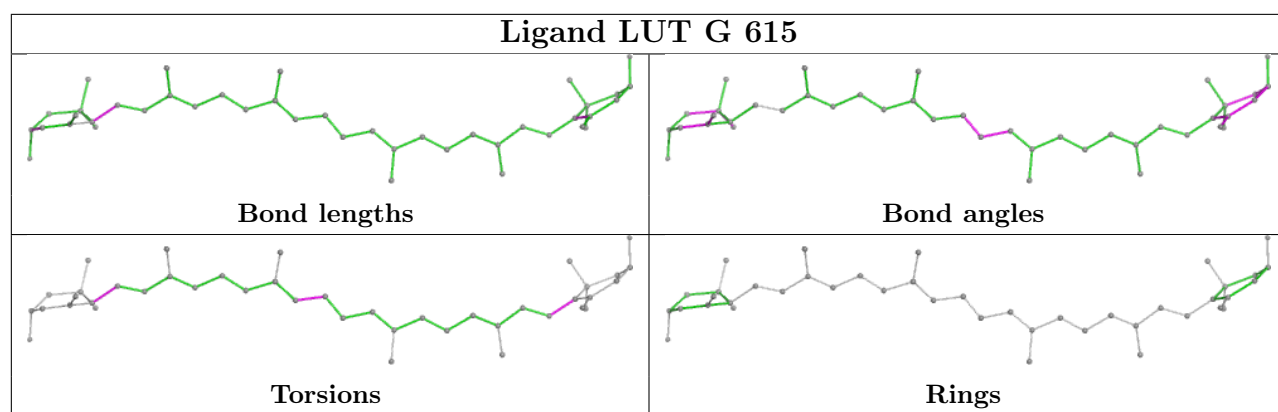
## Ligand CHL R 606



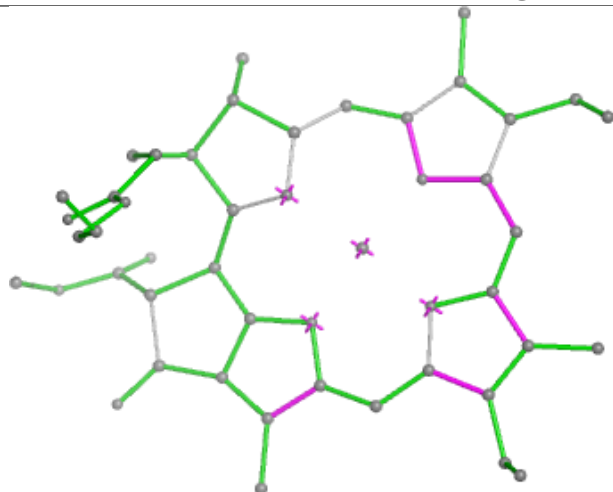
## Ligand NEX N 617



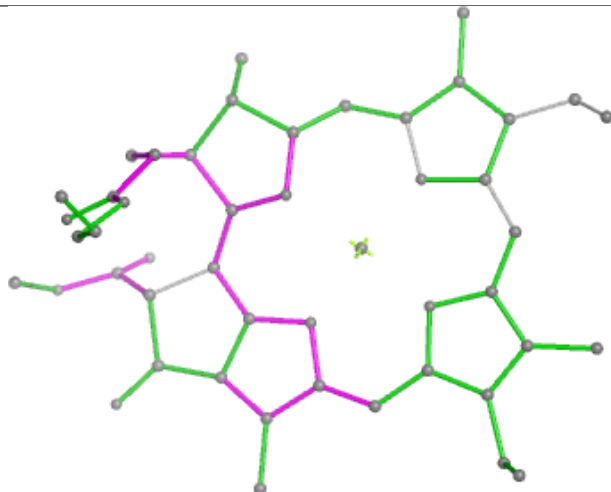




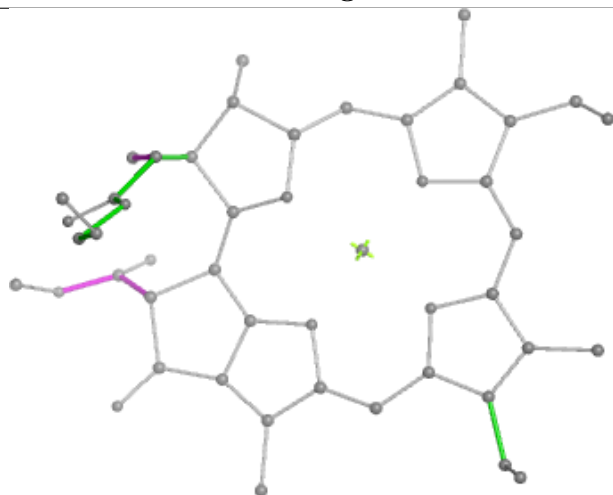
## Ligand CLA N 614



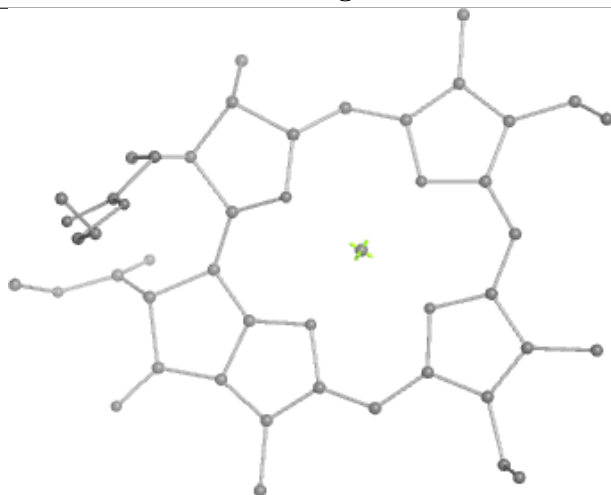
Bond lengths



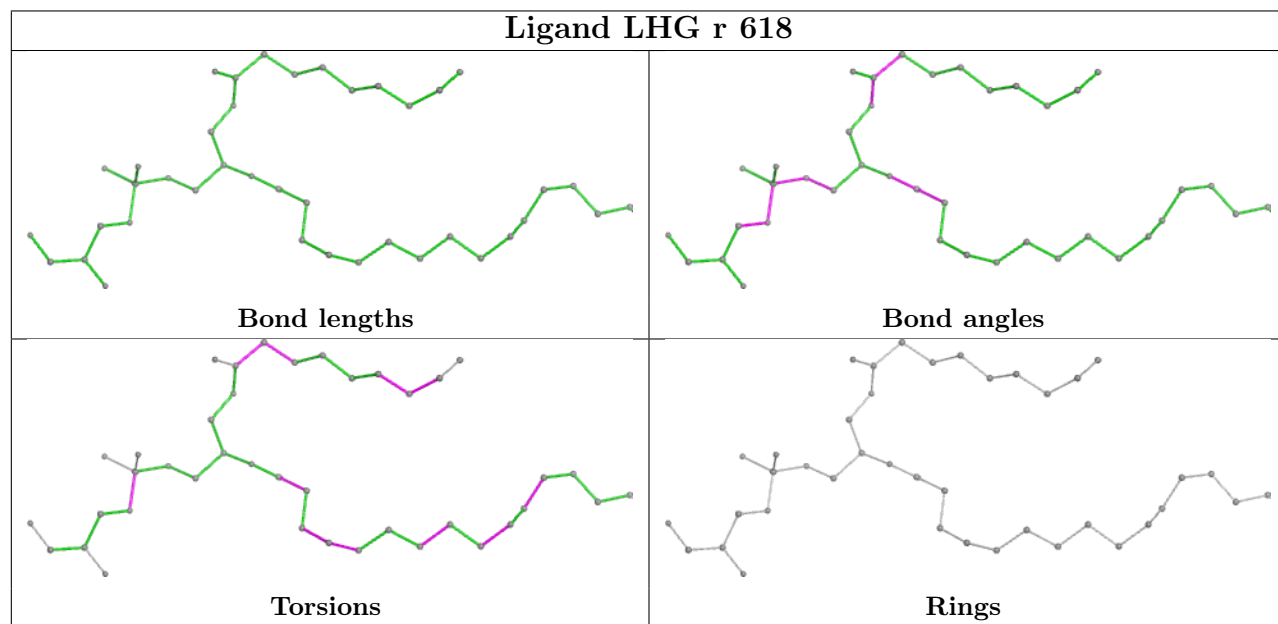
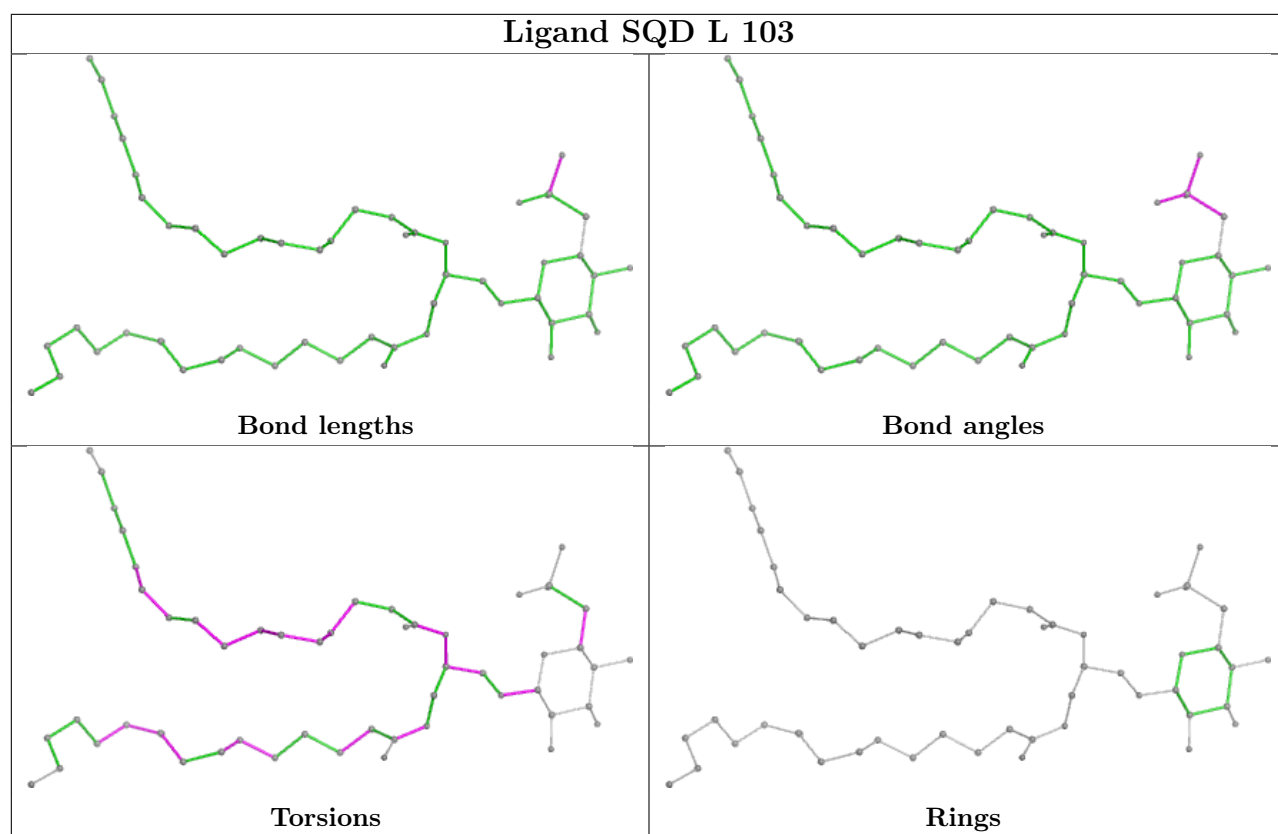
Bond angles



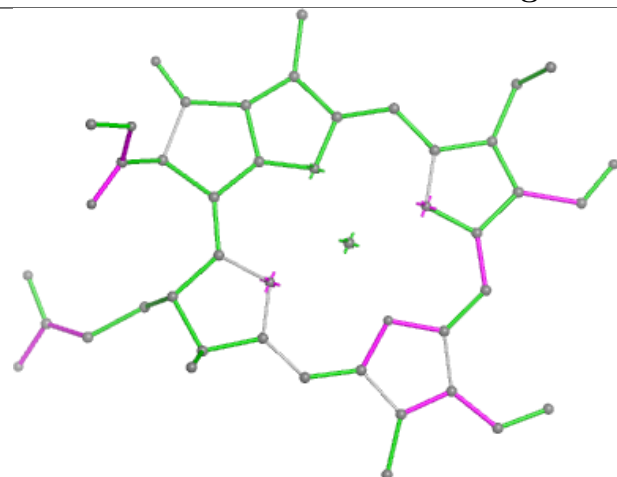
Torsions



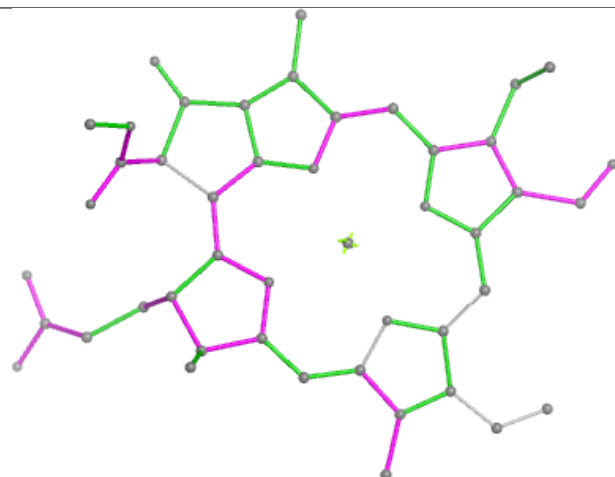
Rings



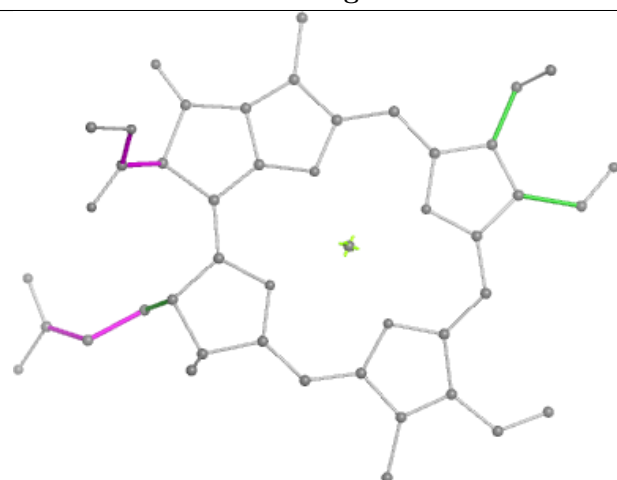
## Ligand CHL S 306



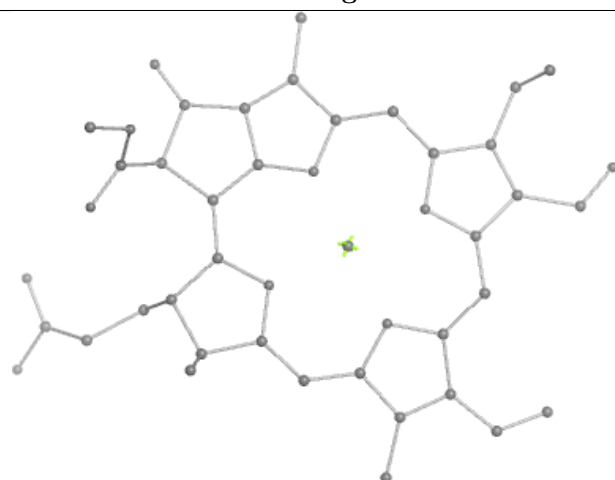
Bond lengths



Bond angles

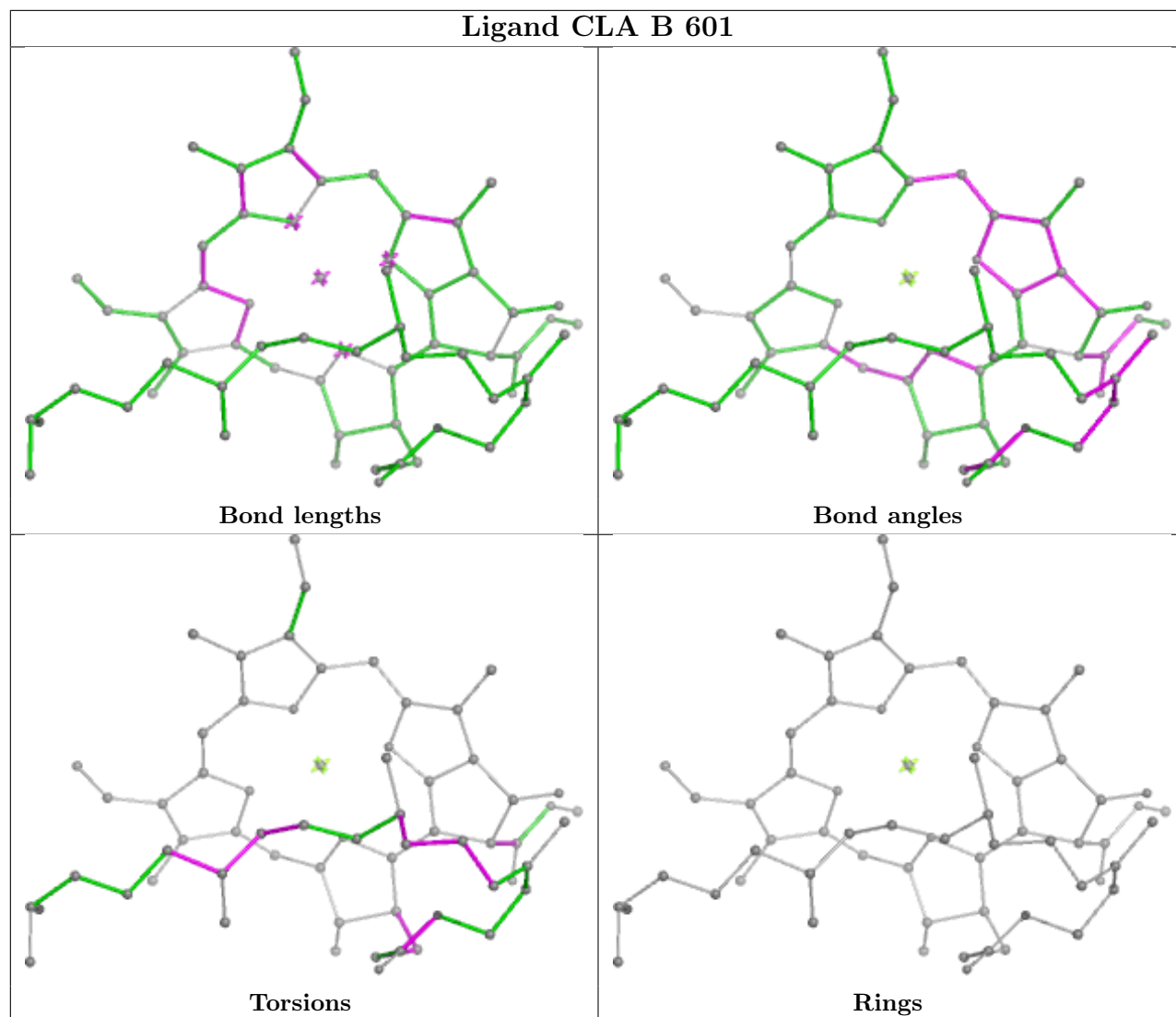


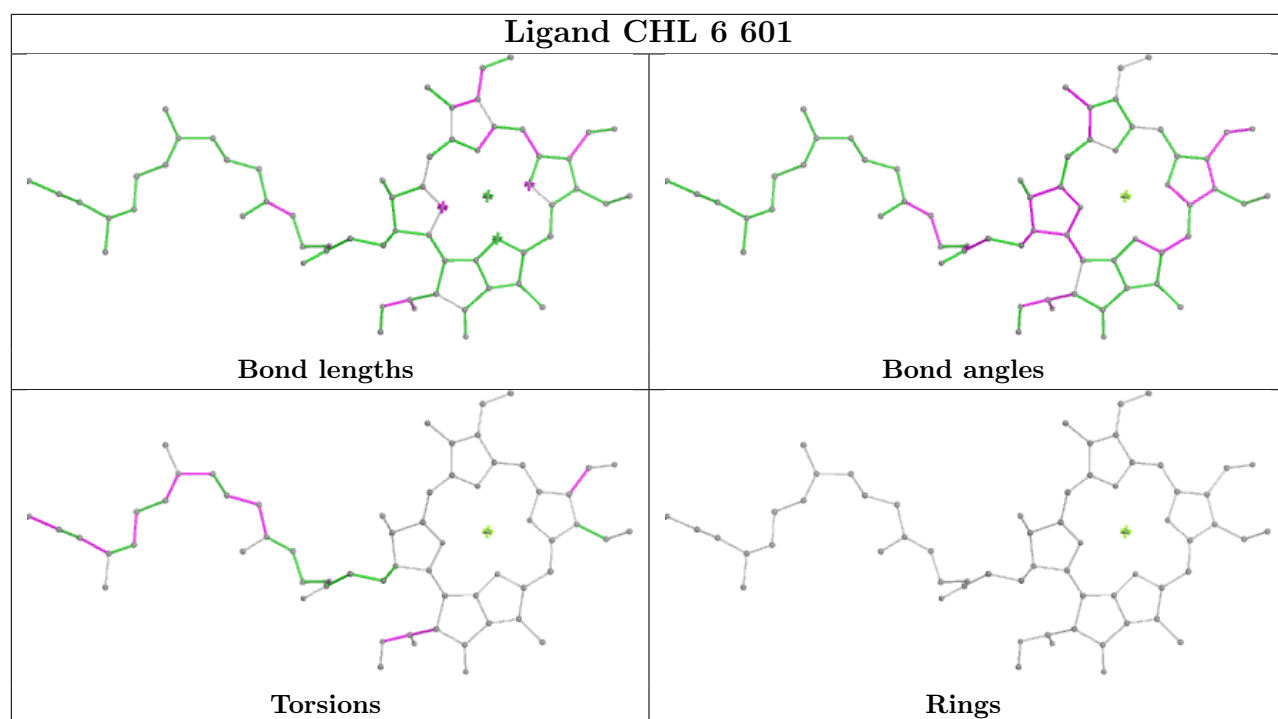
Torsions



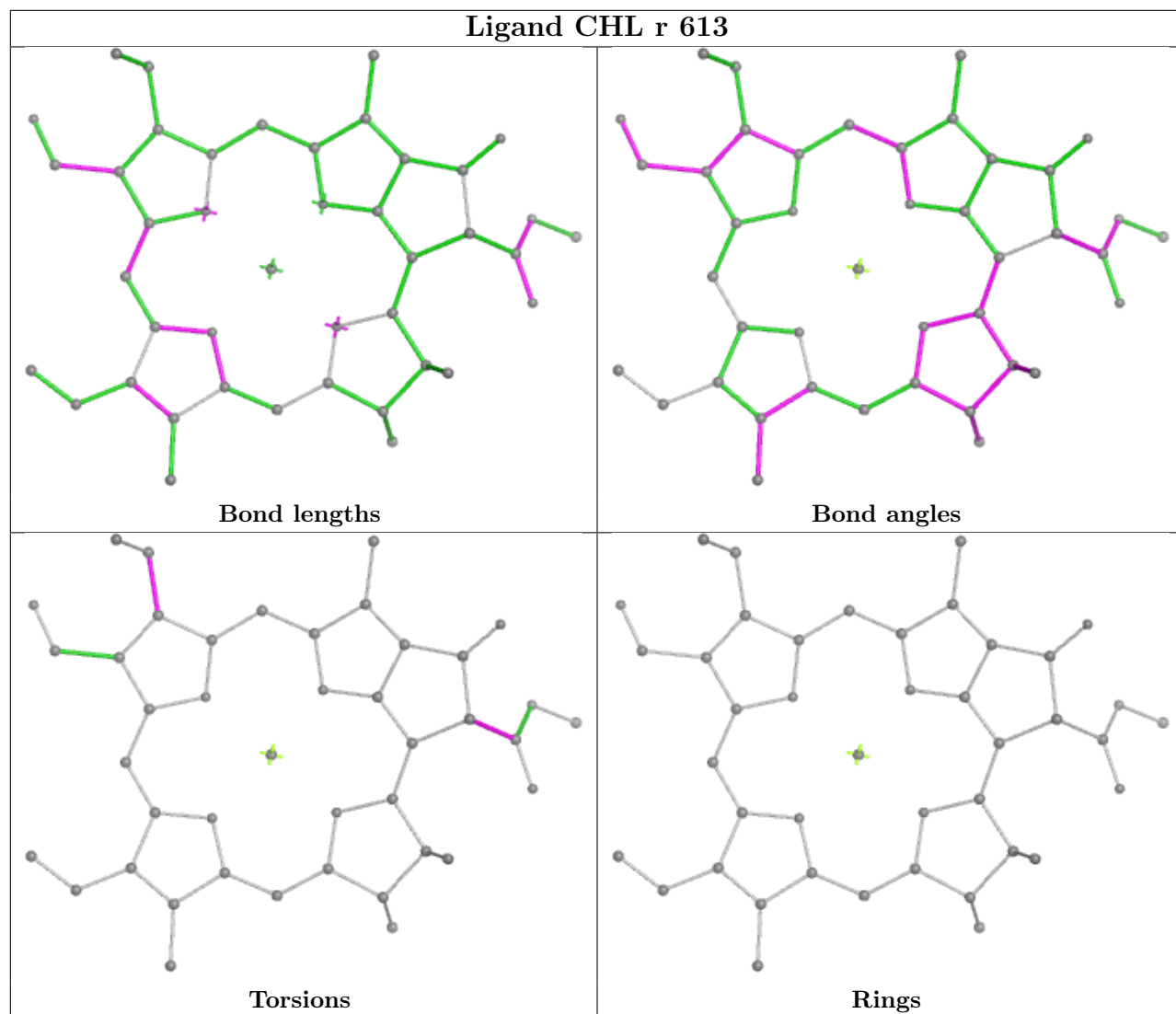
Rings

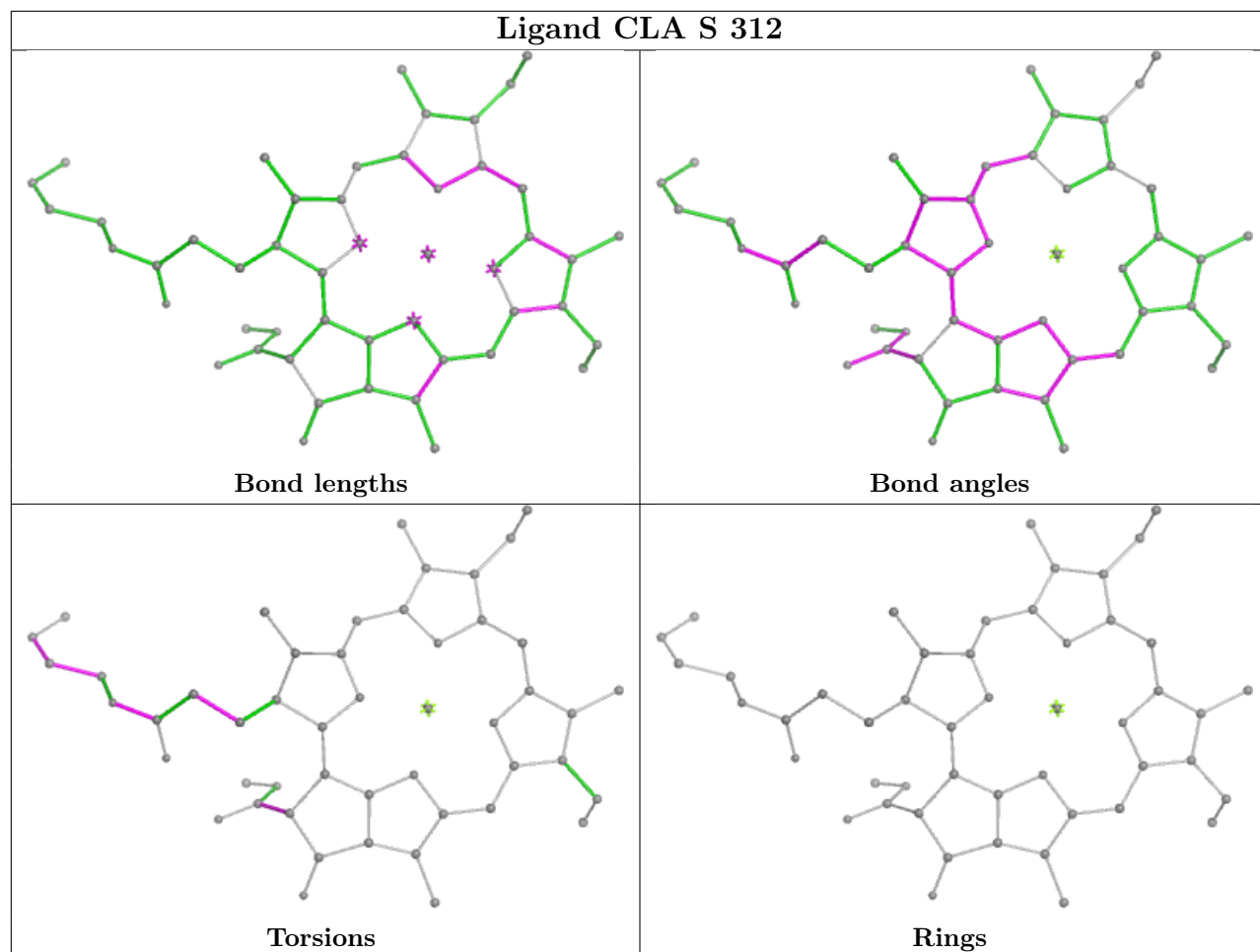
## Ligand CLA B 601



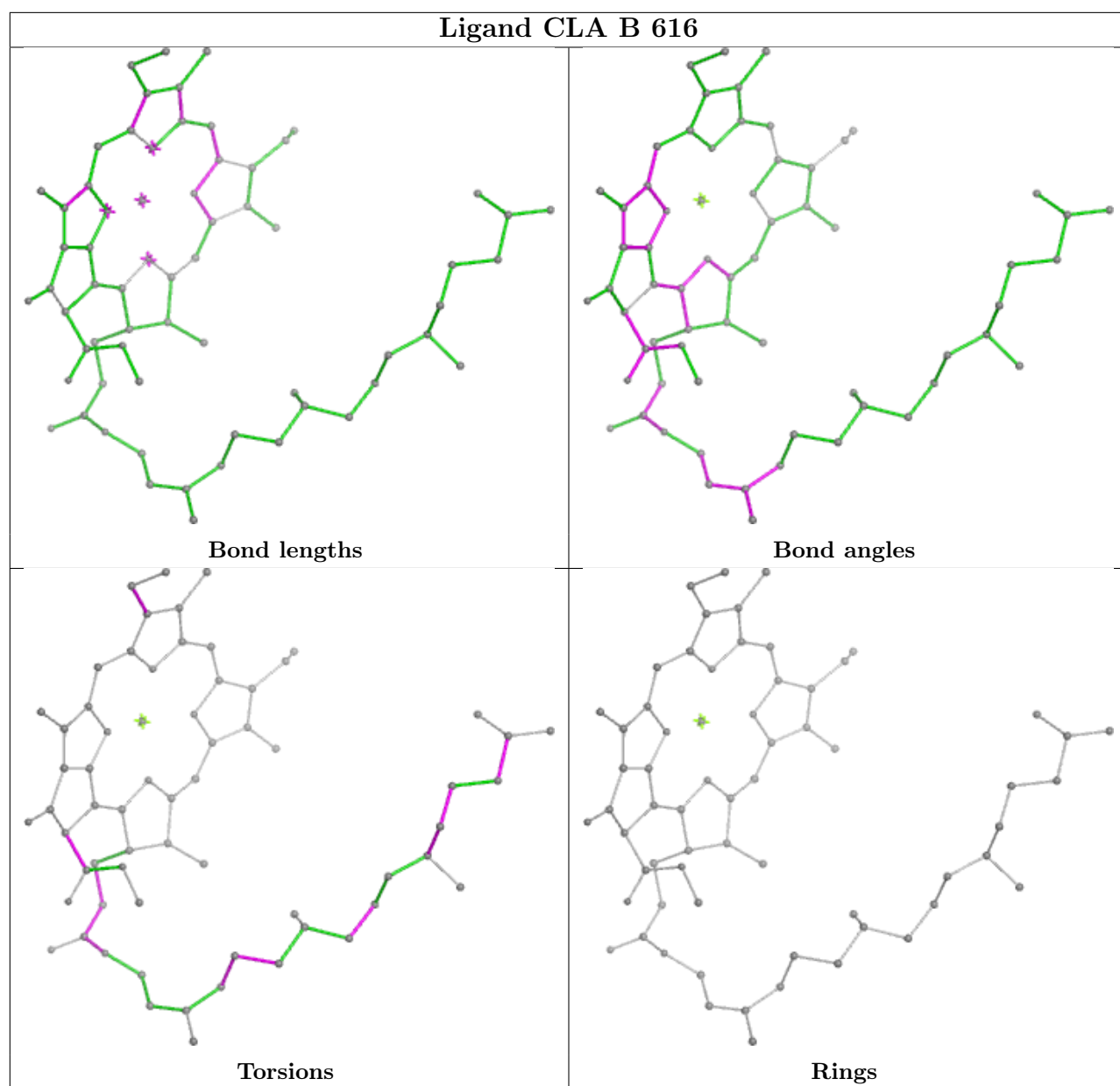


## Ligand CHL r 613

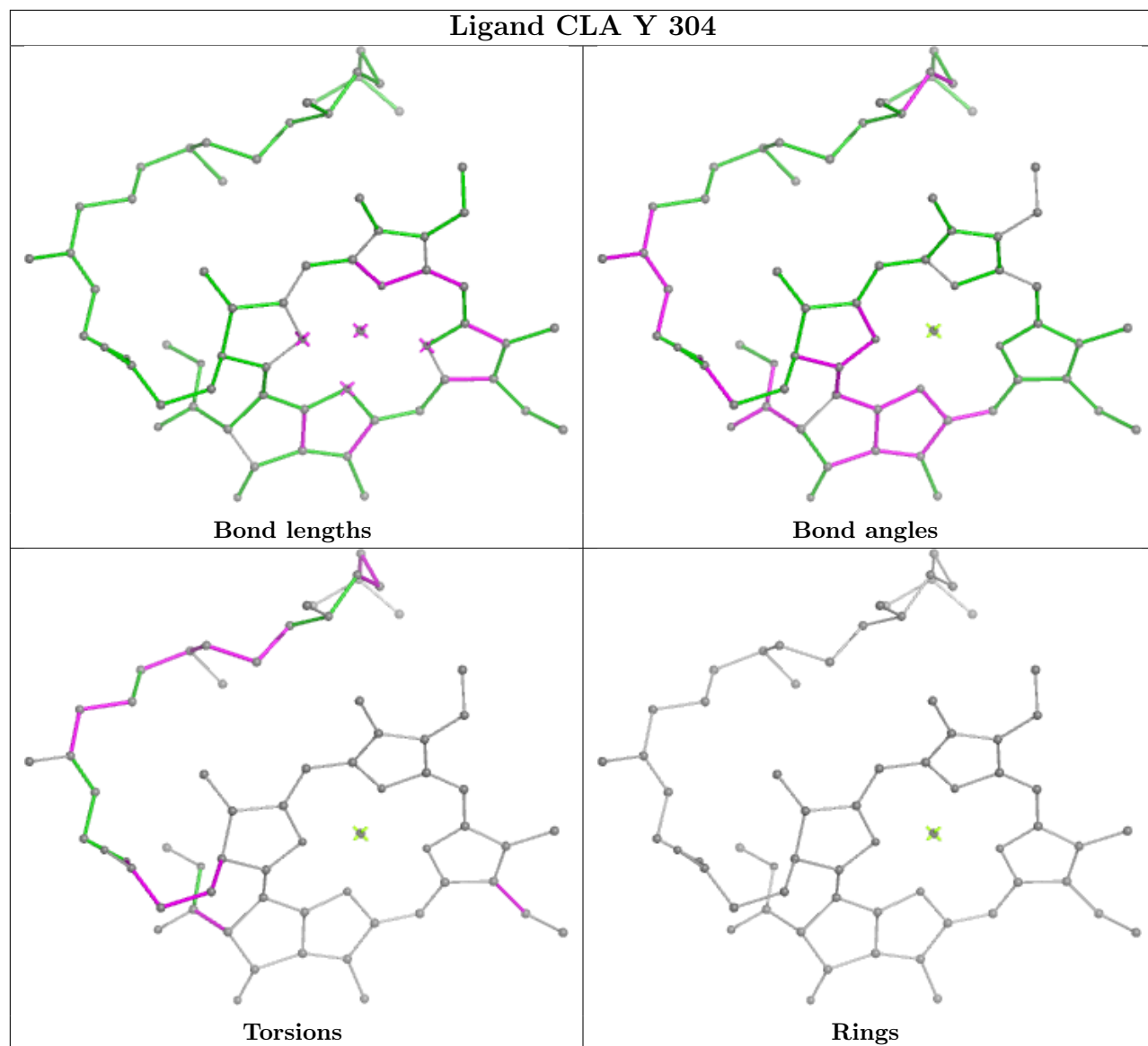




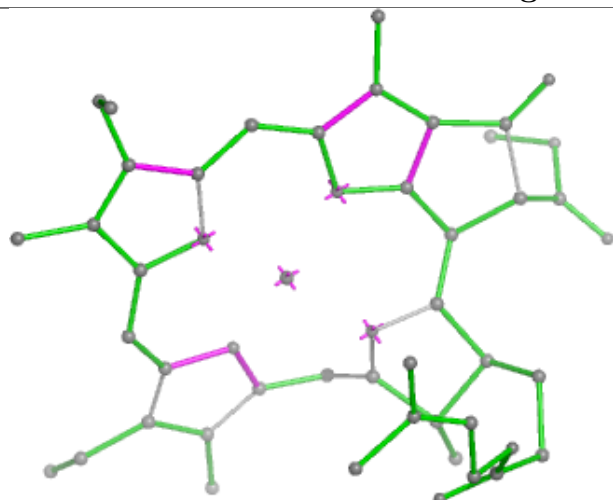




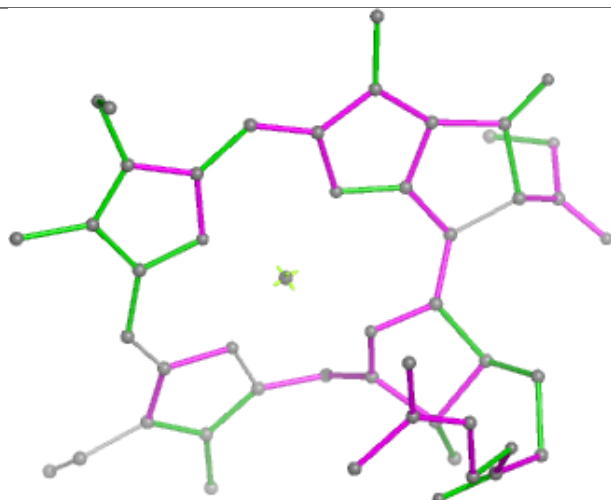
## Ligand CLA Y 304



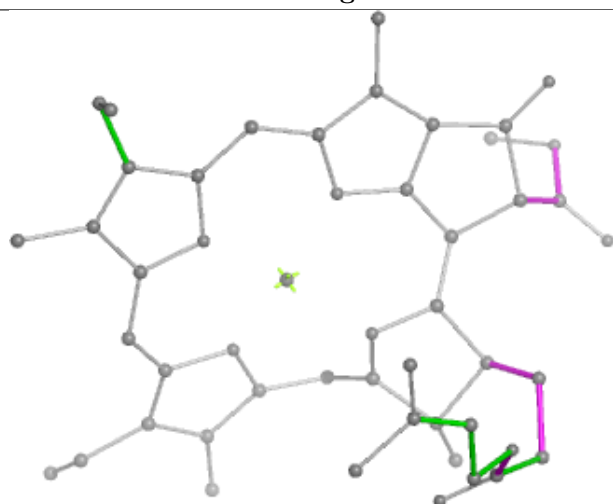
## Ligand CLA s 305



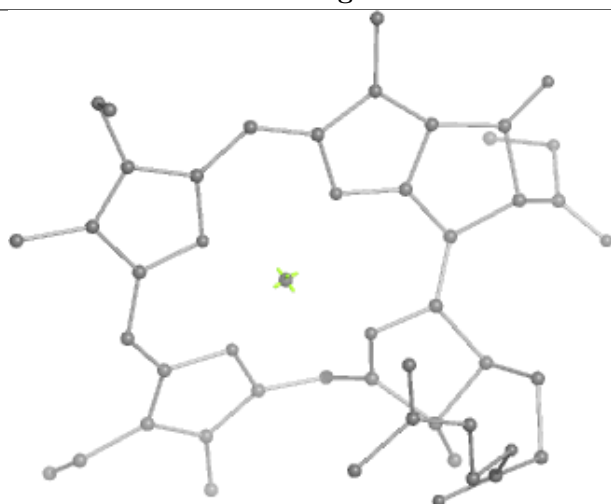
Bond lengths



Bond angles

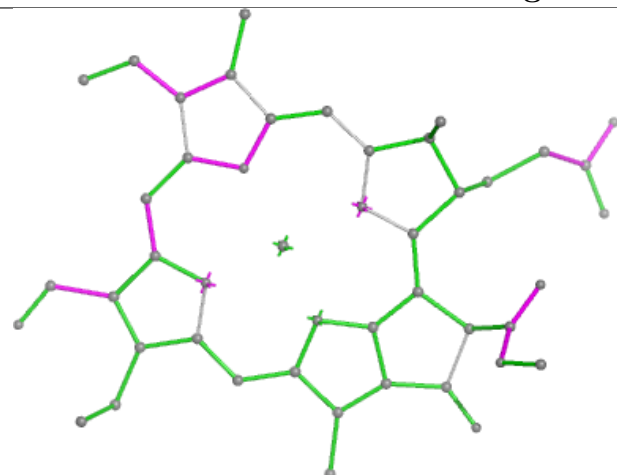


Torsions

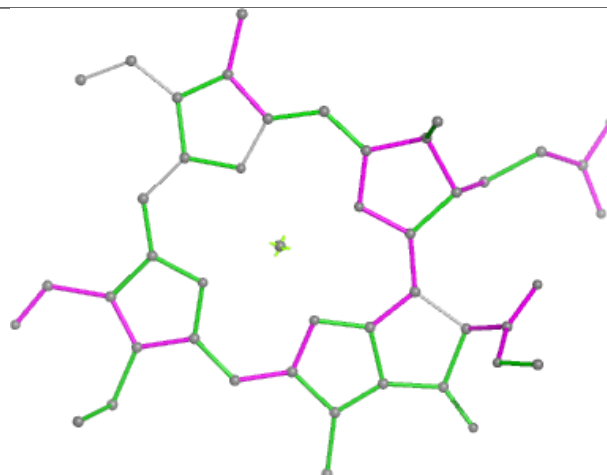


Rings

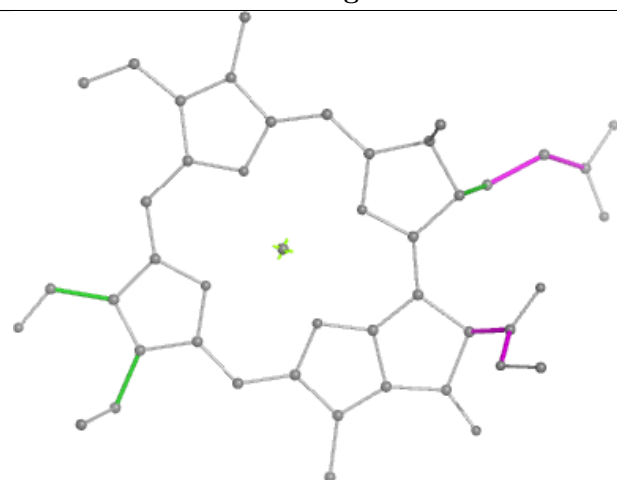
## Ligand CHL s 306



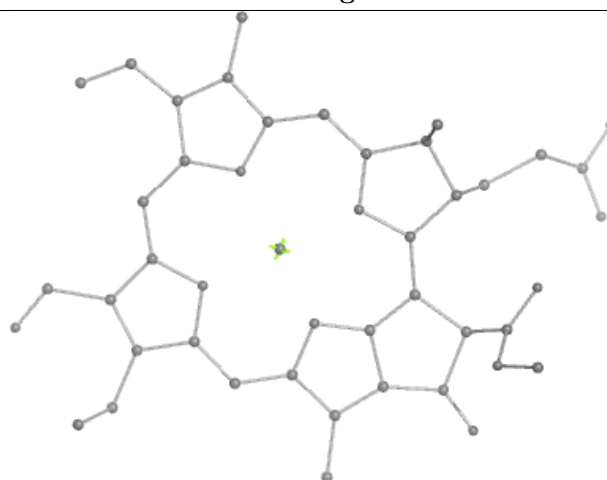
Bond lengths



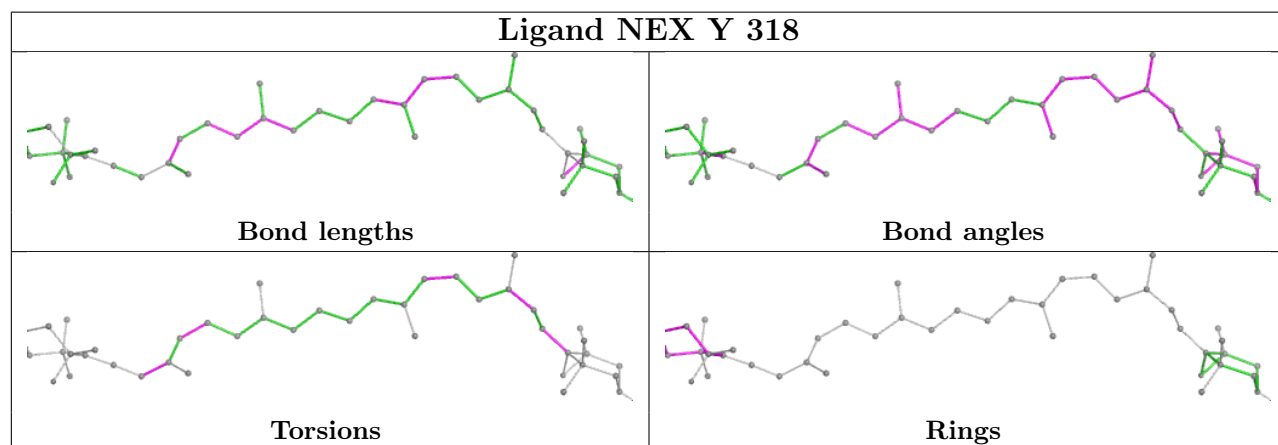
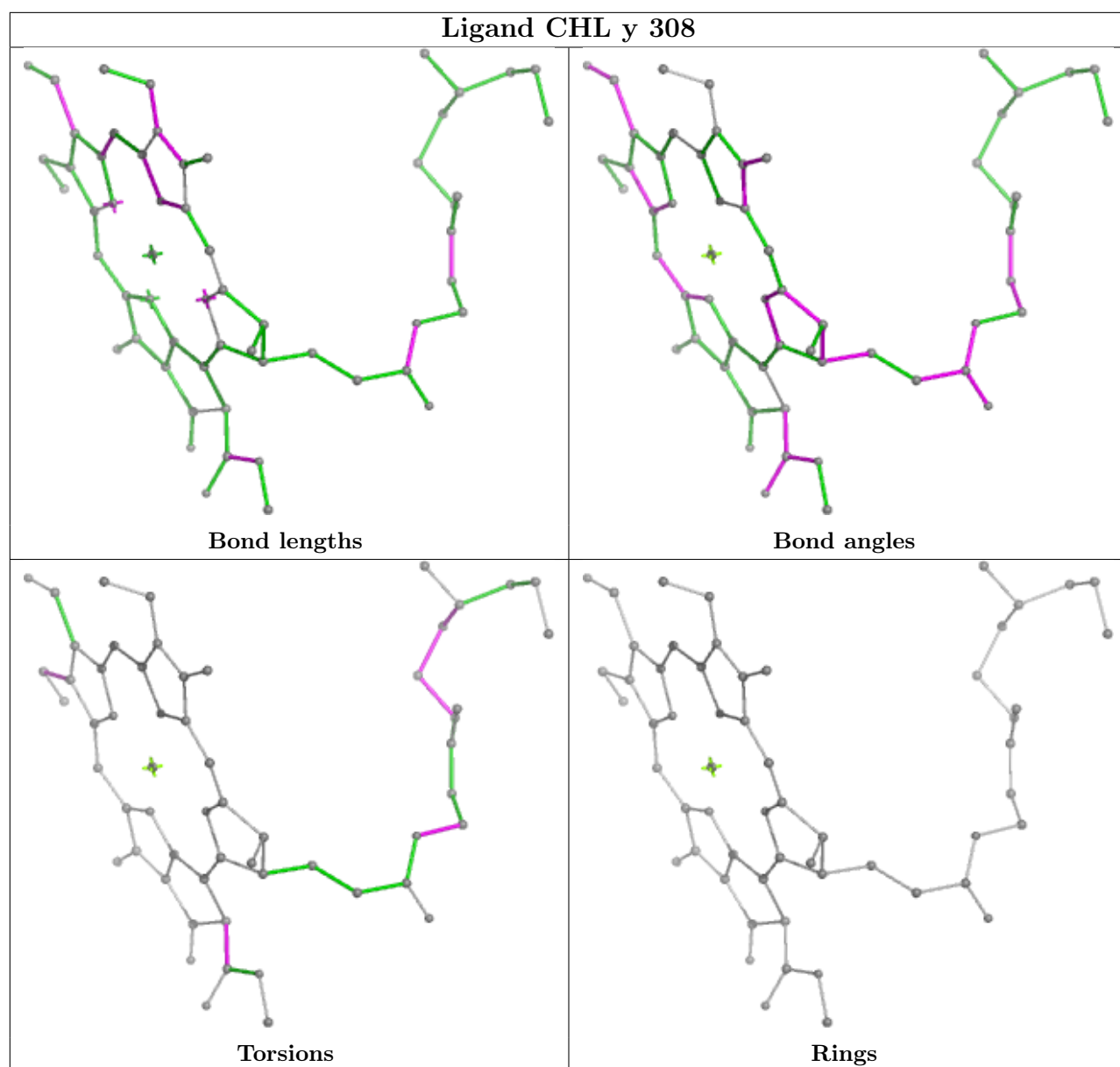
Bond angles



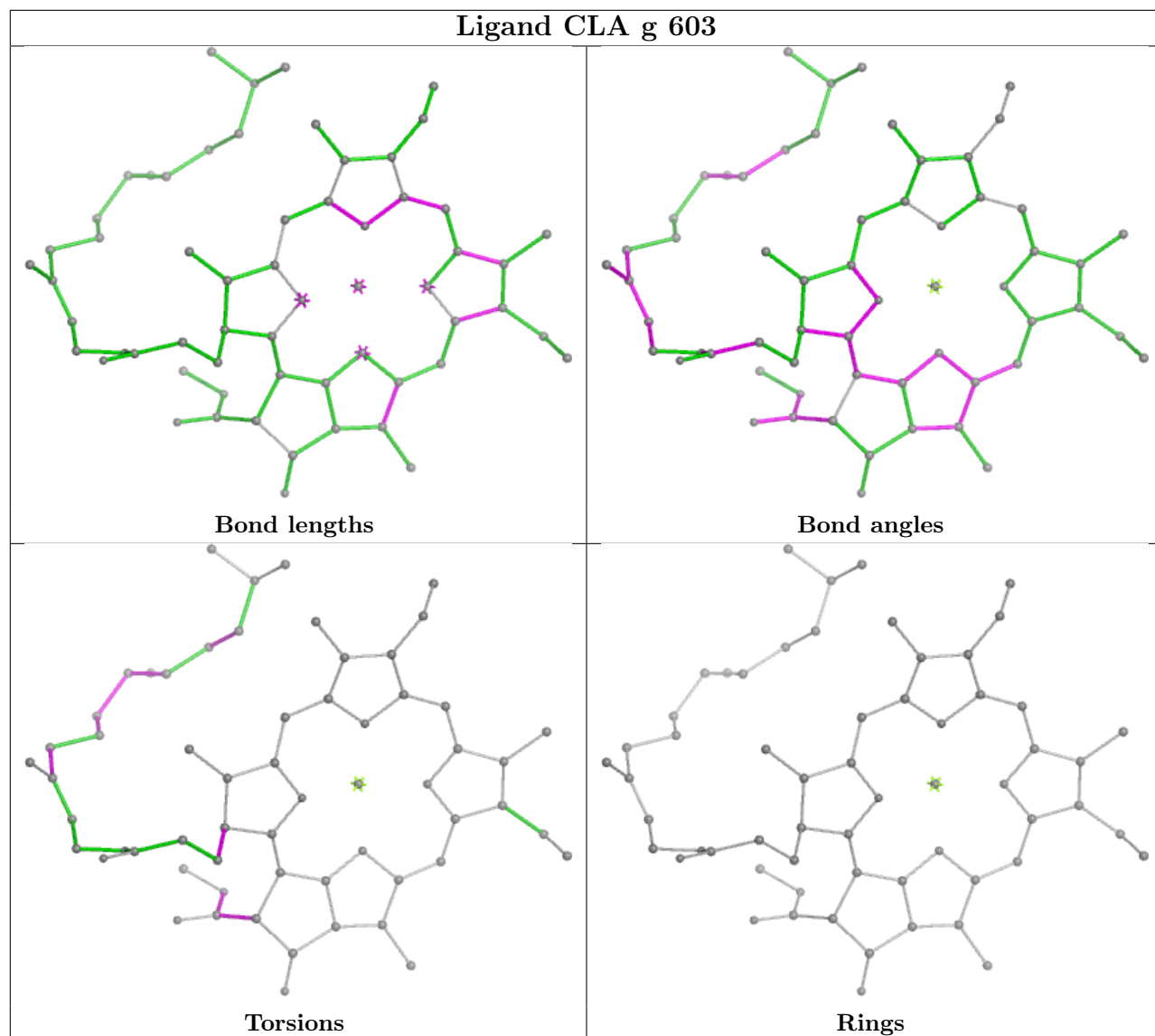
Torsions



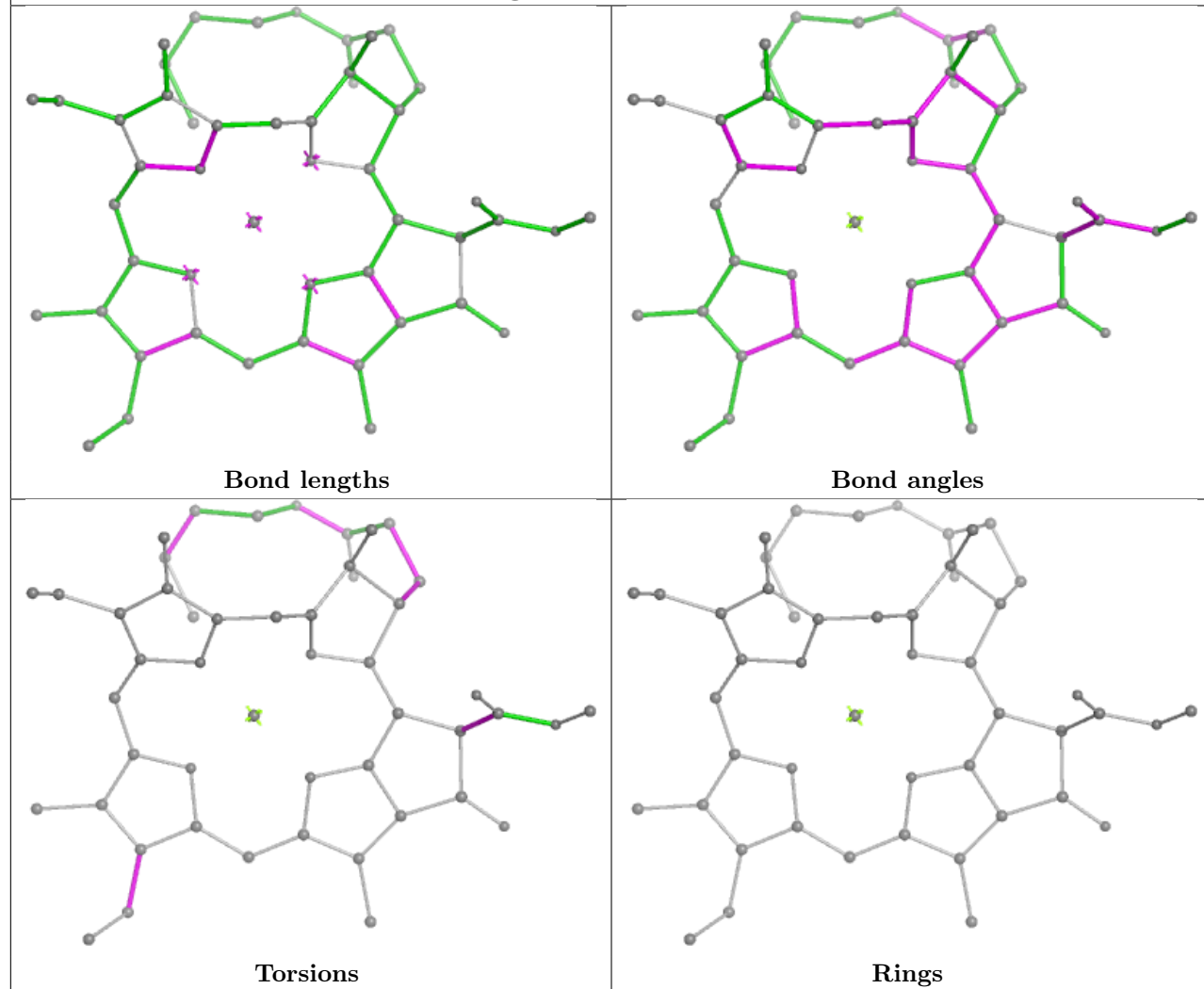
Rings

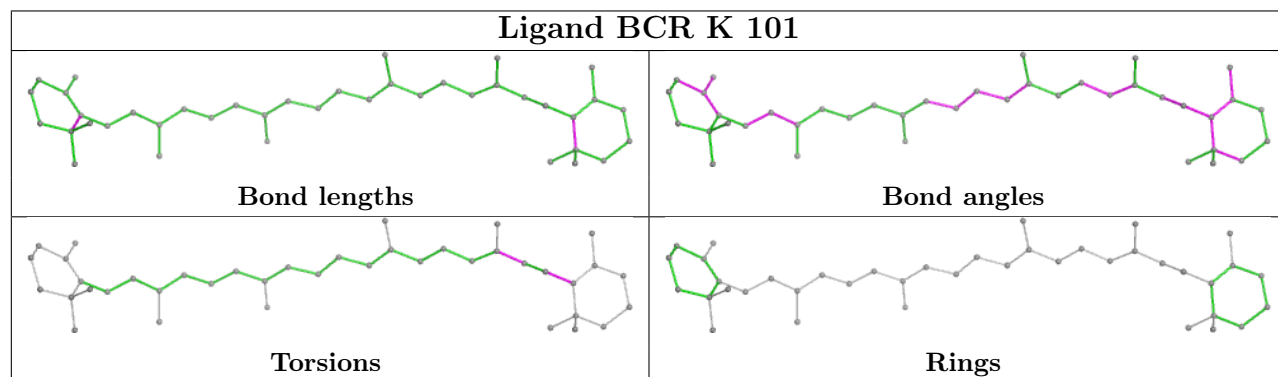
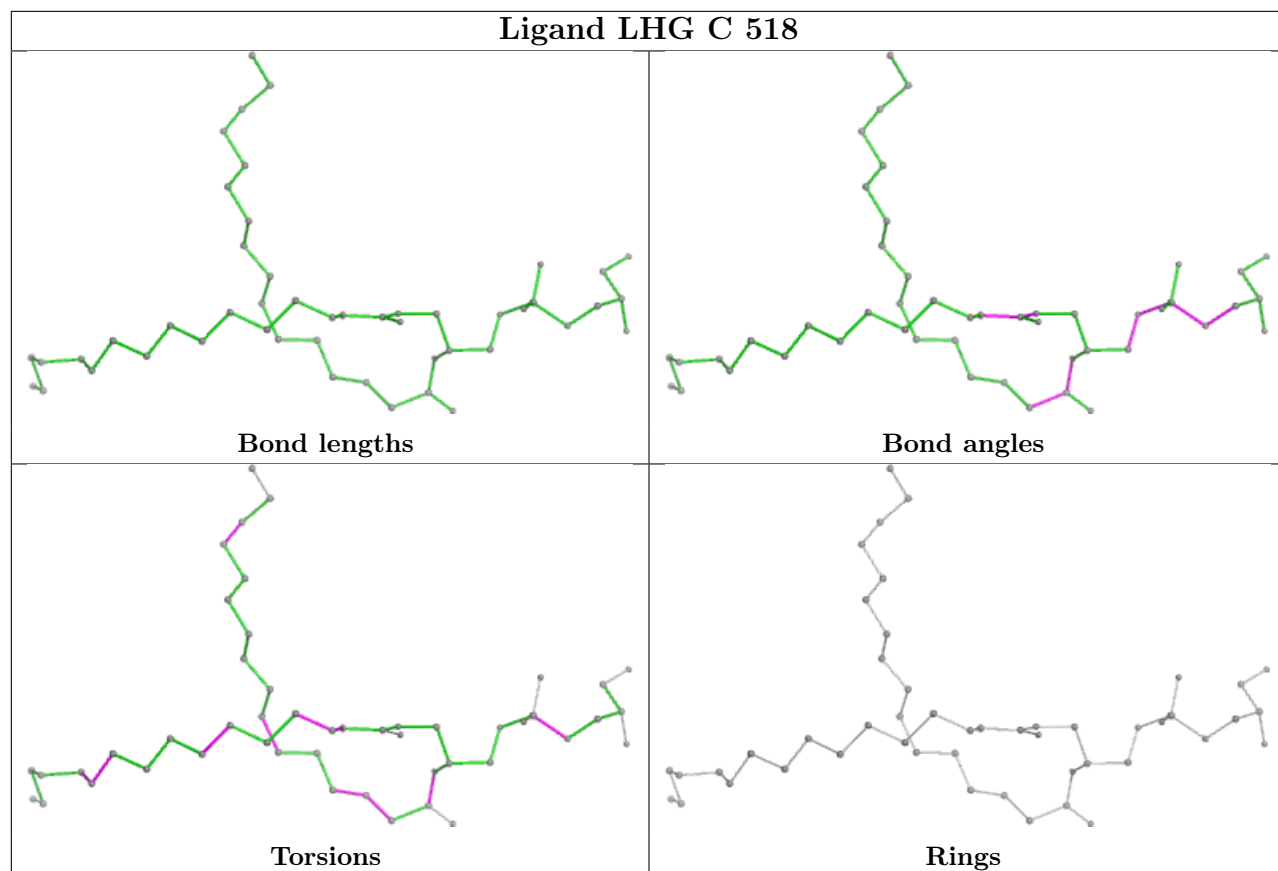


## Ligand CLA g 603

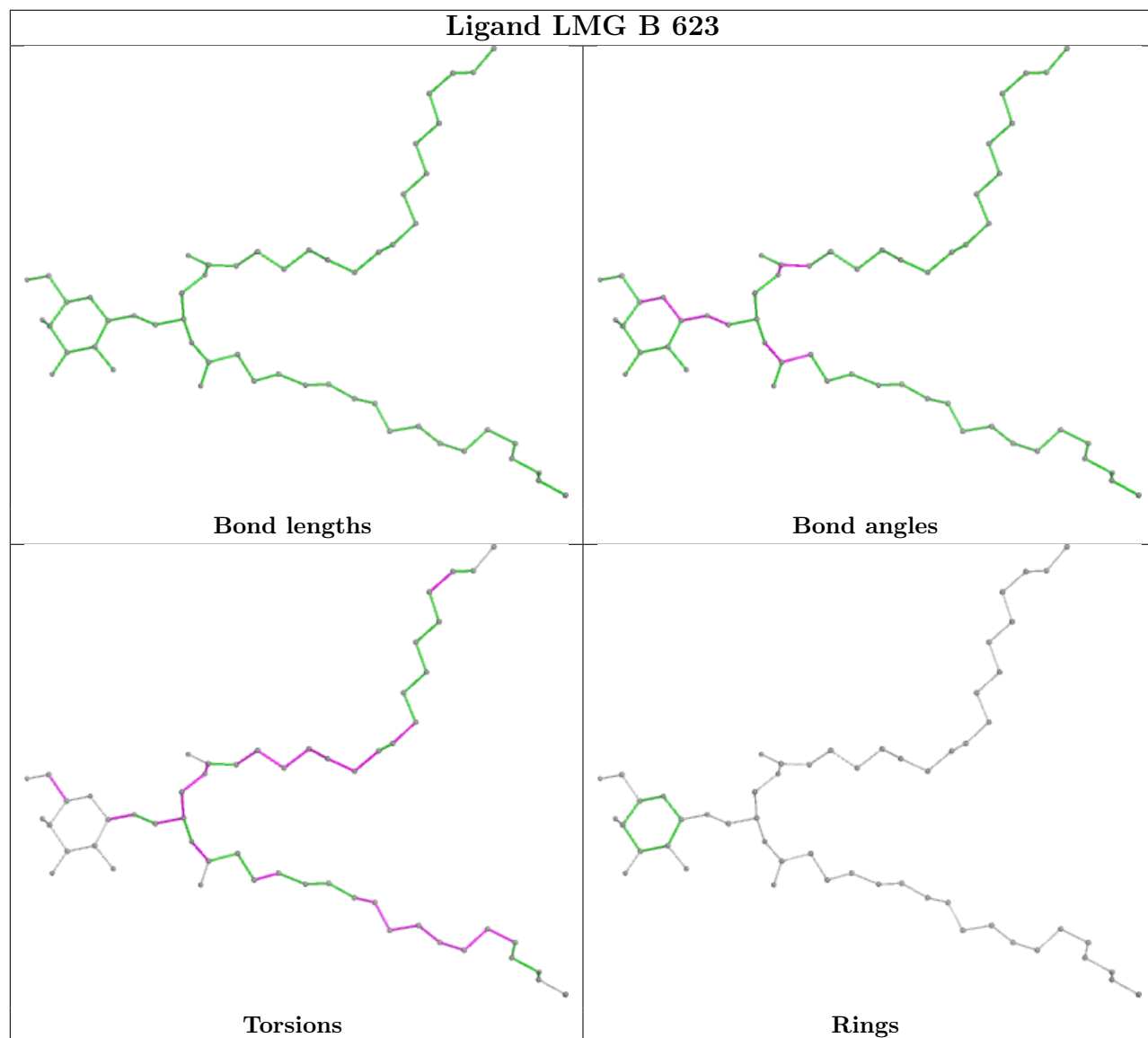


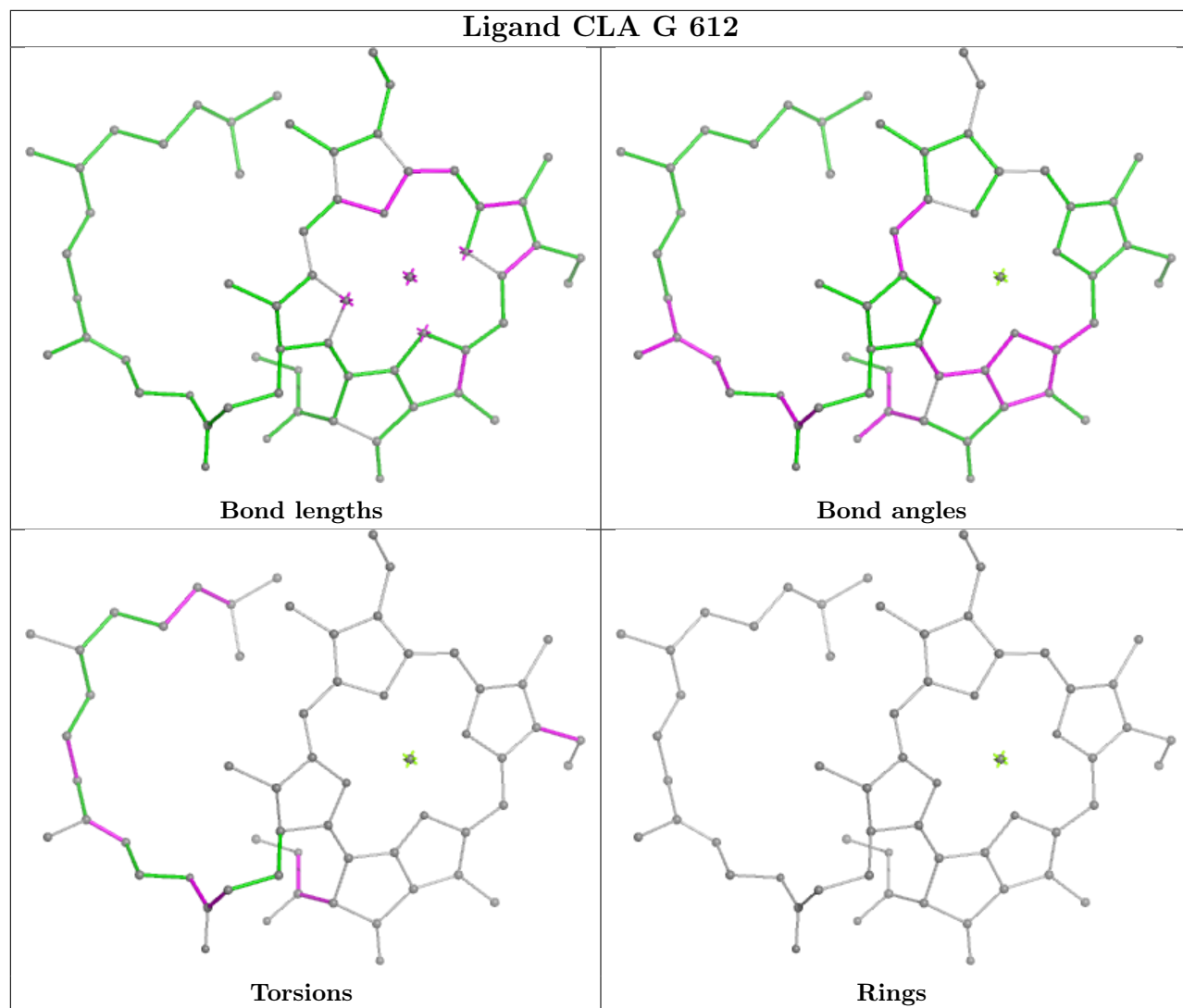
## Ligand CLA r 610

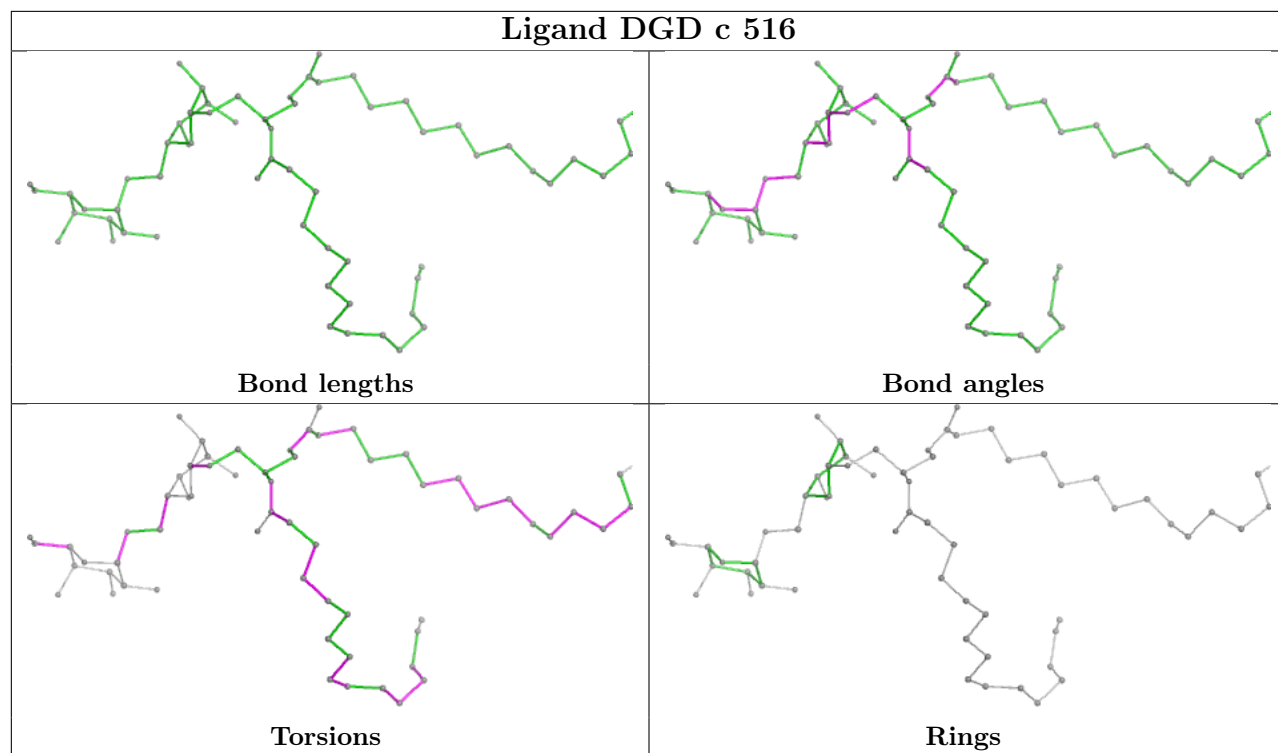




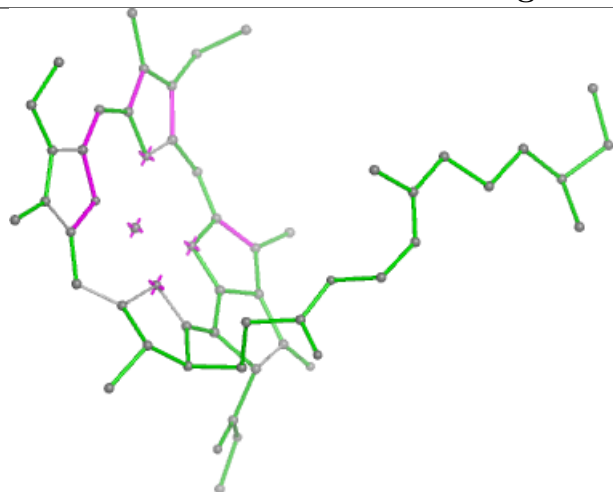




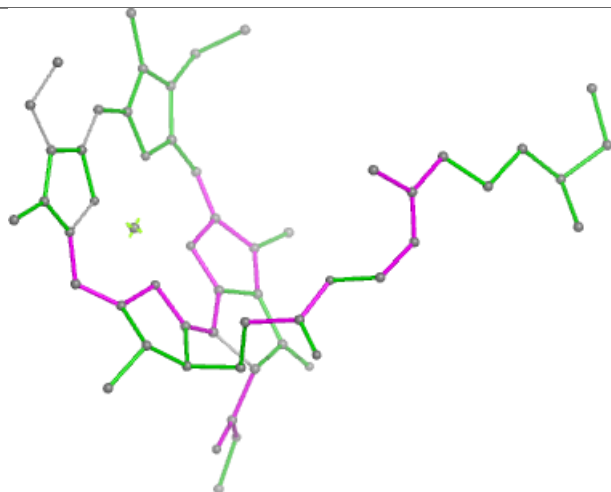




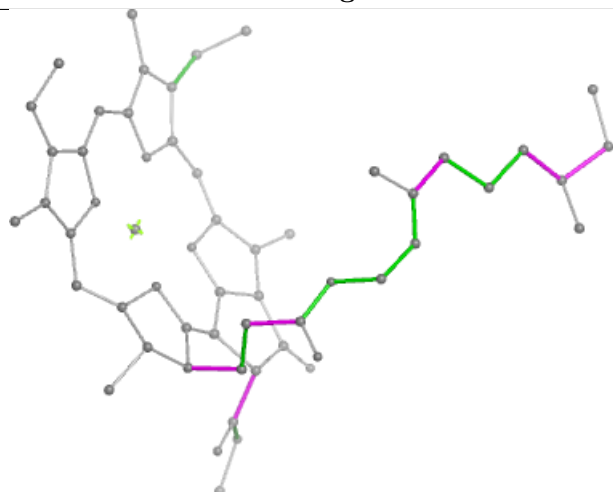
## Ligand CLA S 311



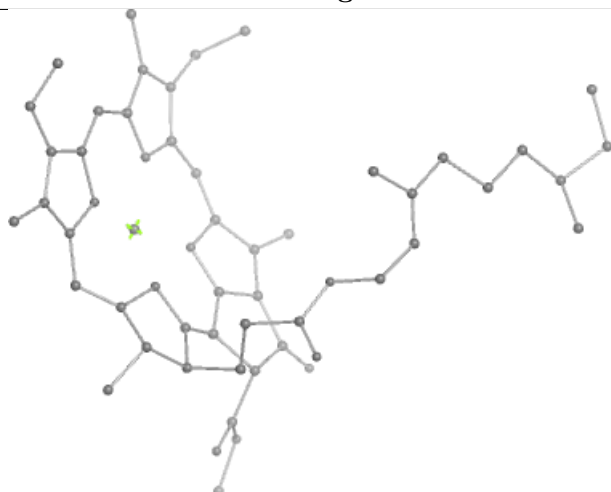
Bond lengths



Bond angles

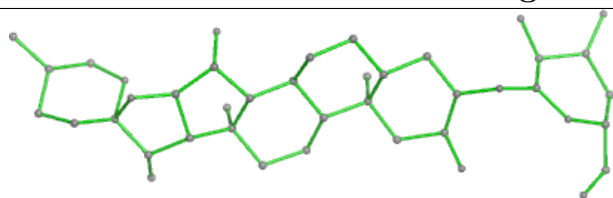


Torsions

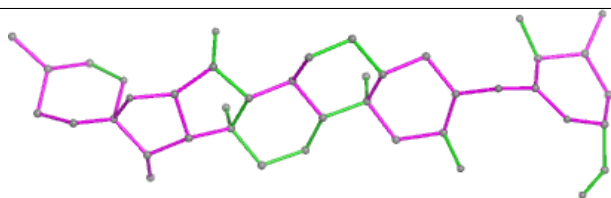


Rings

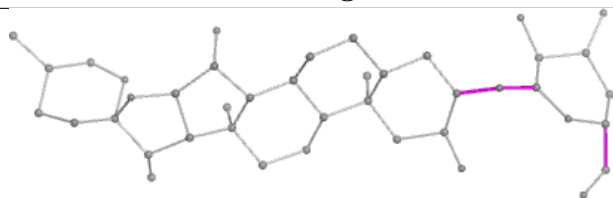
## Ligand AJP n 620



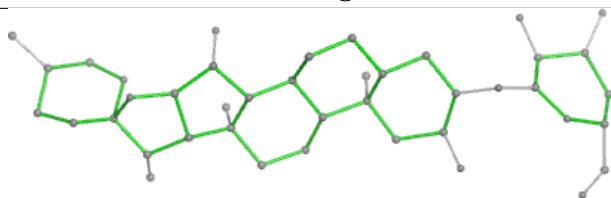
Bond lengths



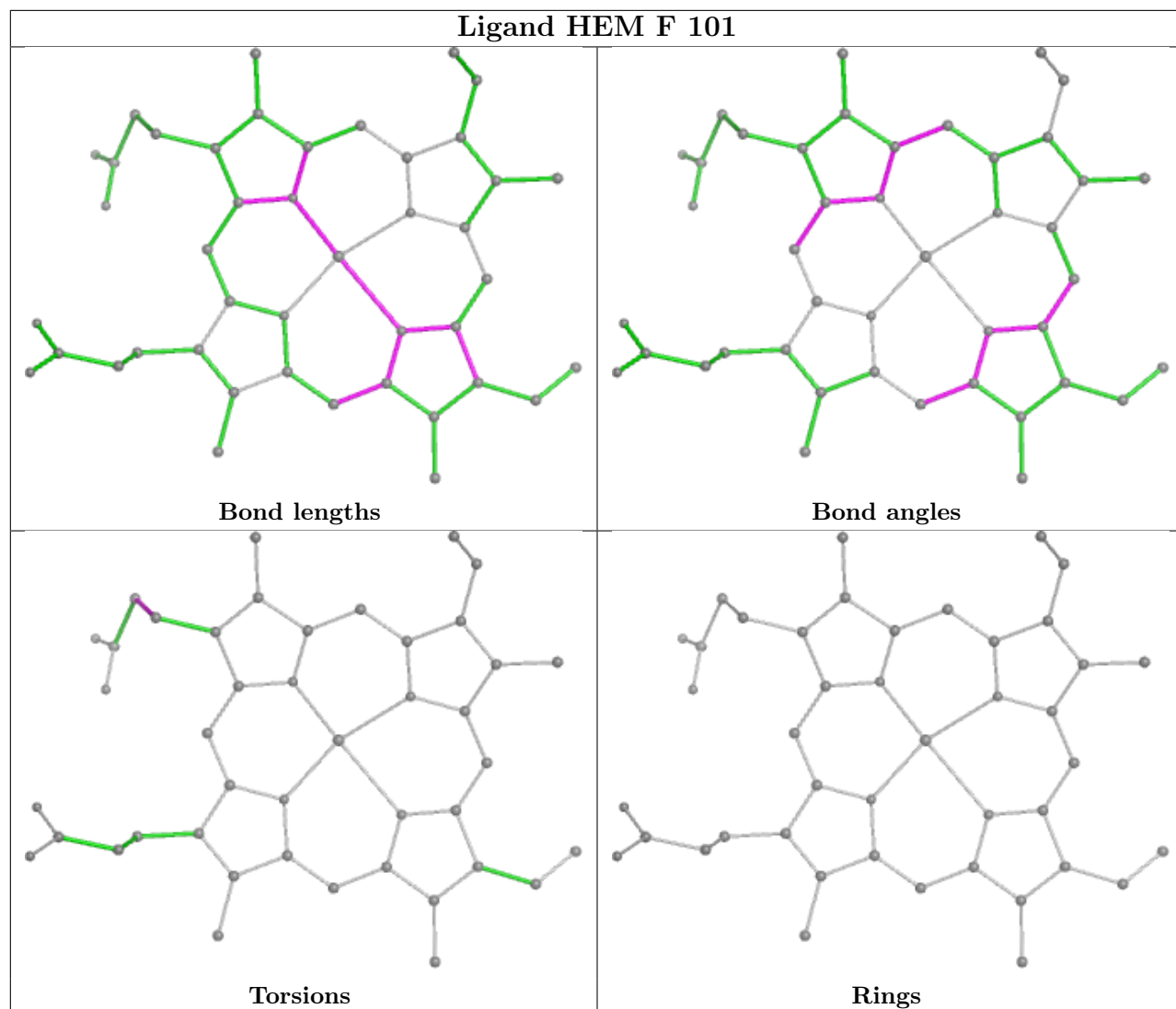
Bond angles

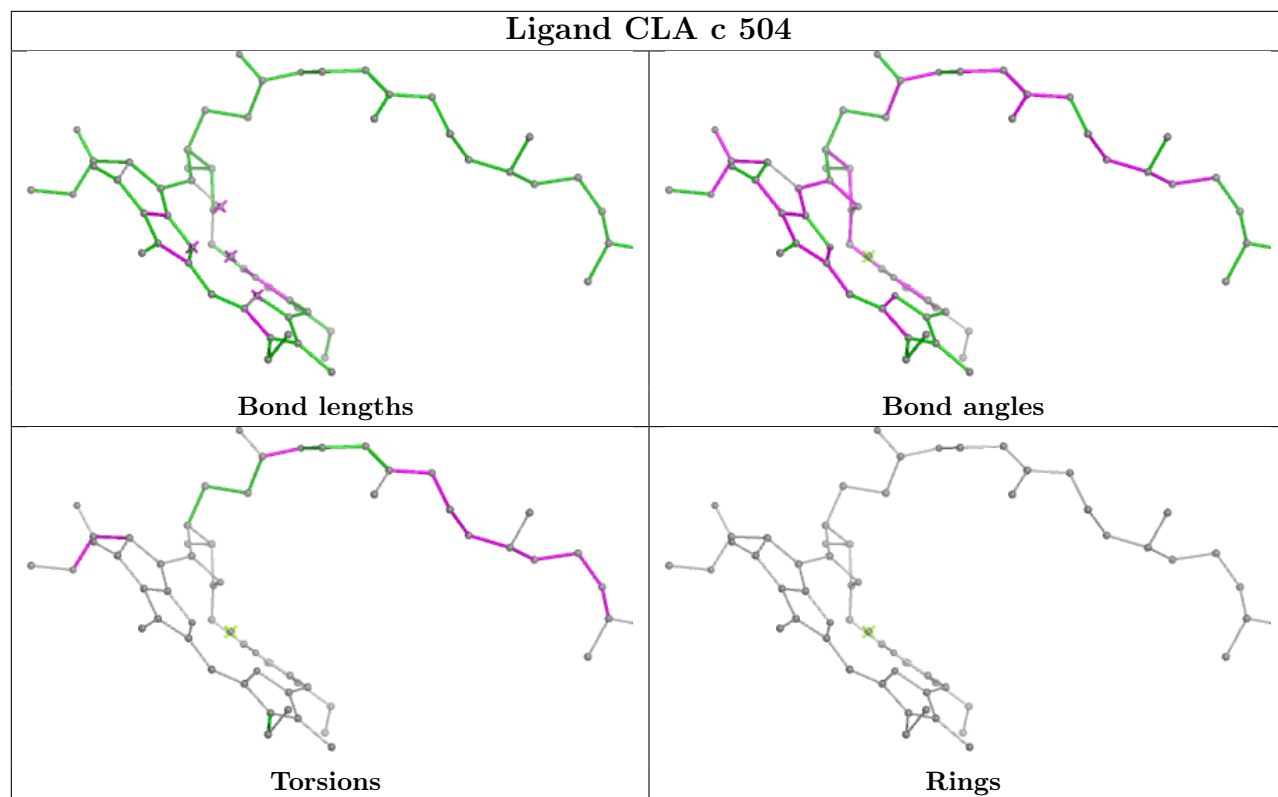


Torsions

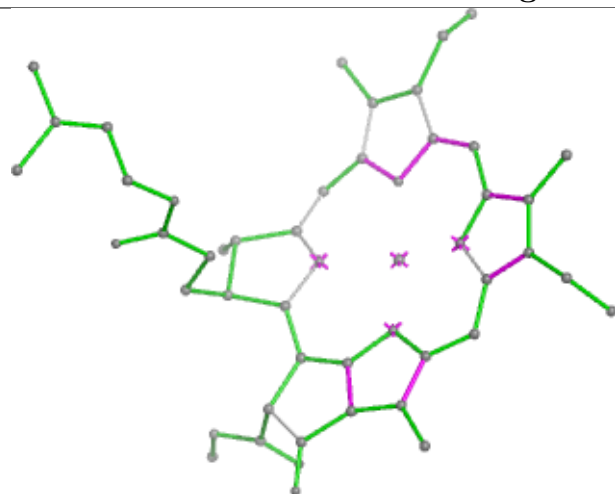


Rings

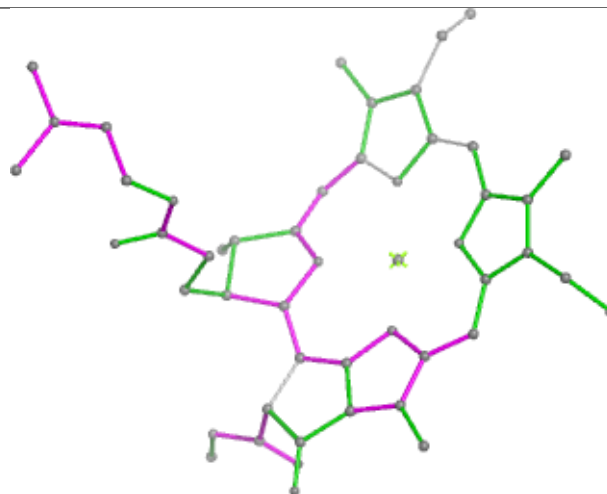




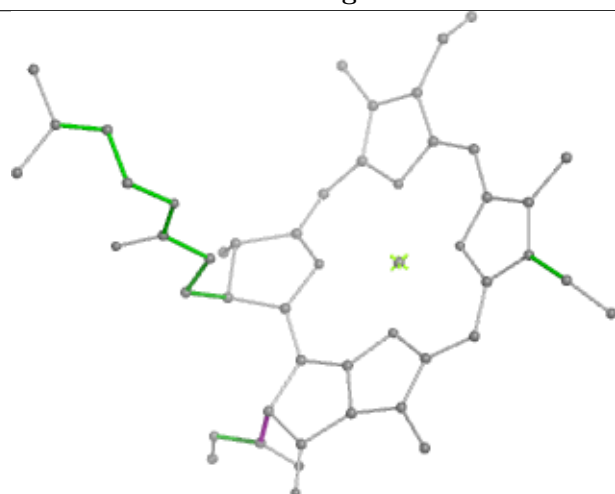
## Ligand CLA d 401



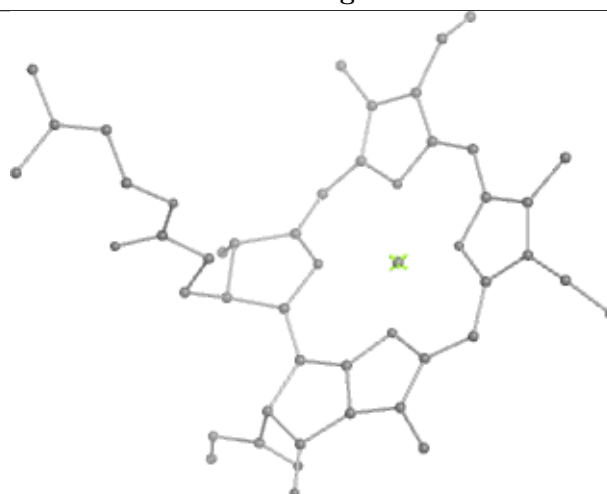
Bond lengths



Bond angles

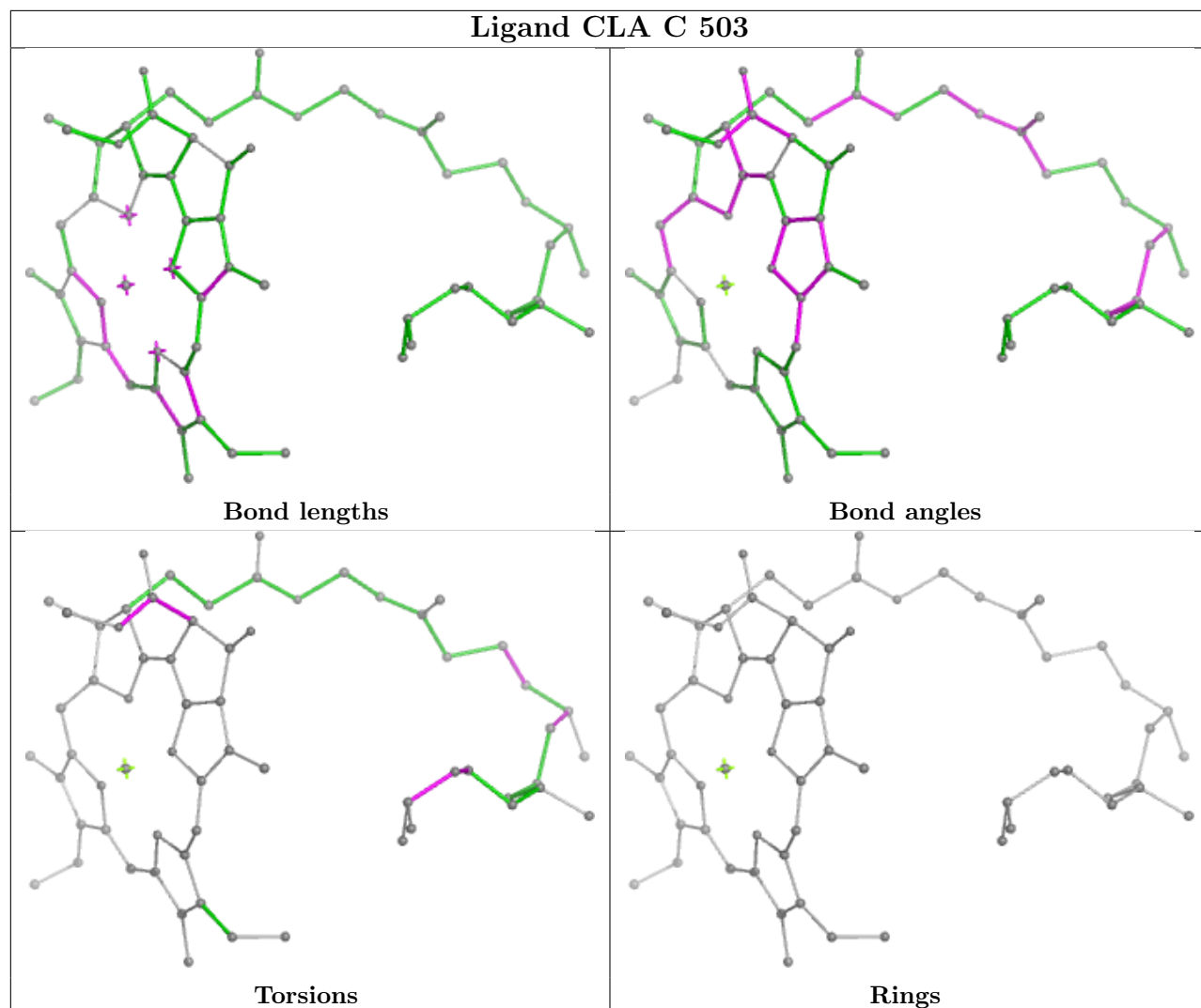


Torsions



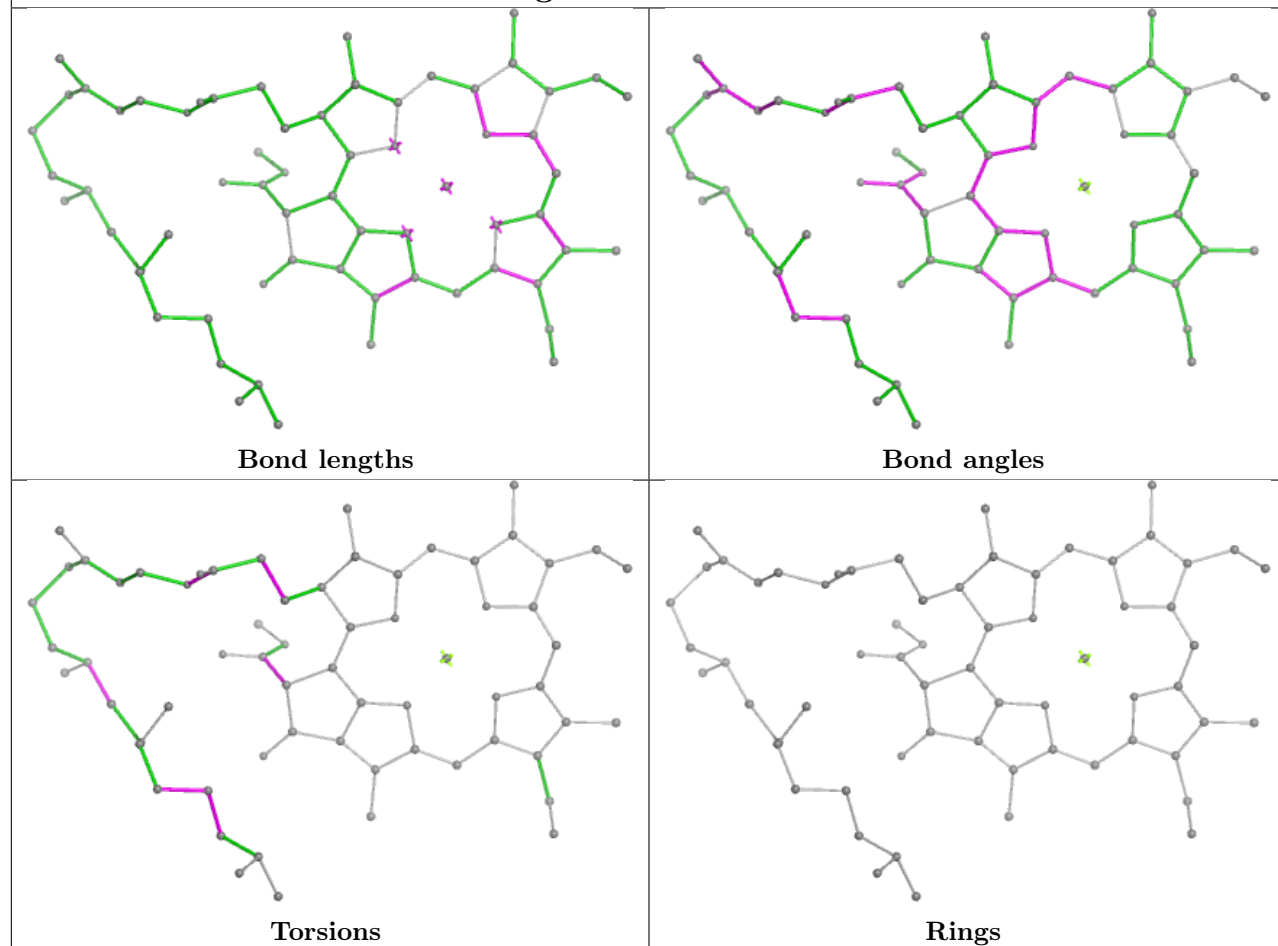
Rings

## Ligand CLA C 503

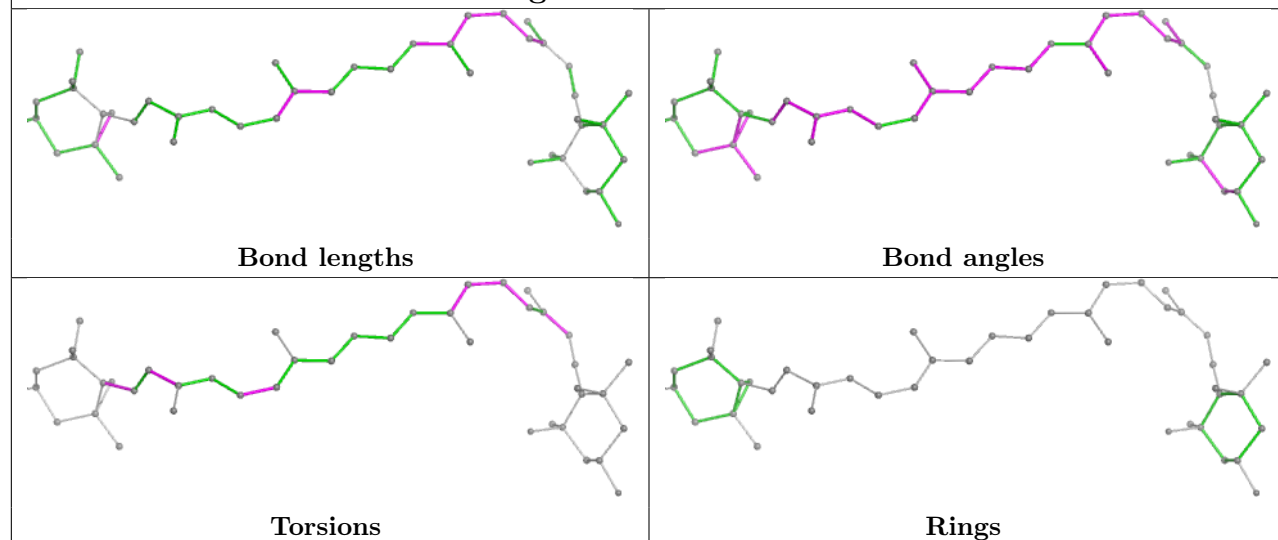


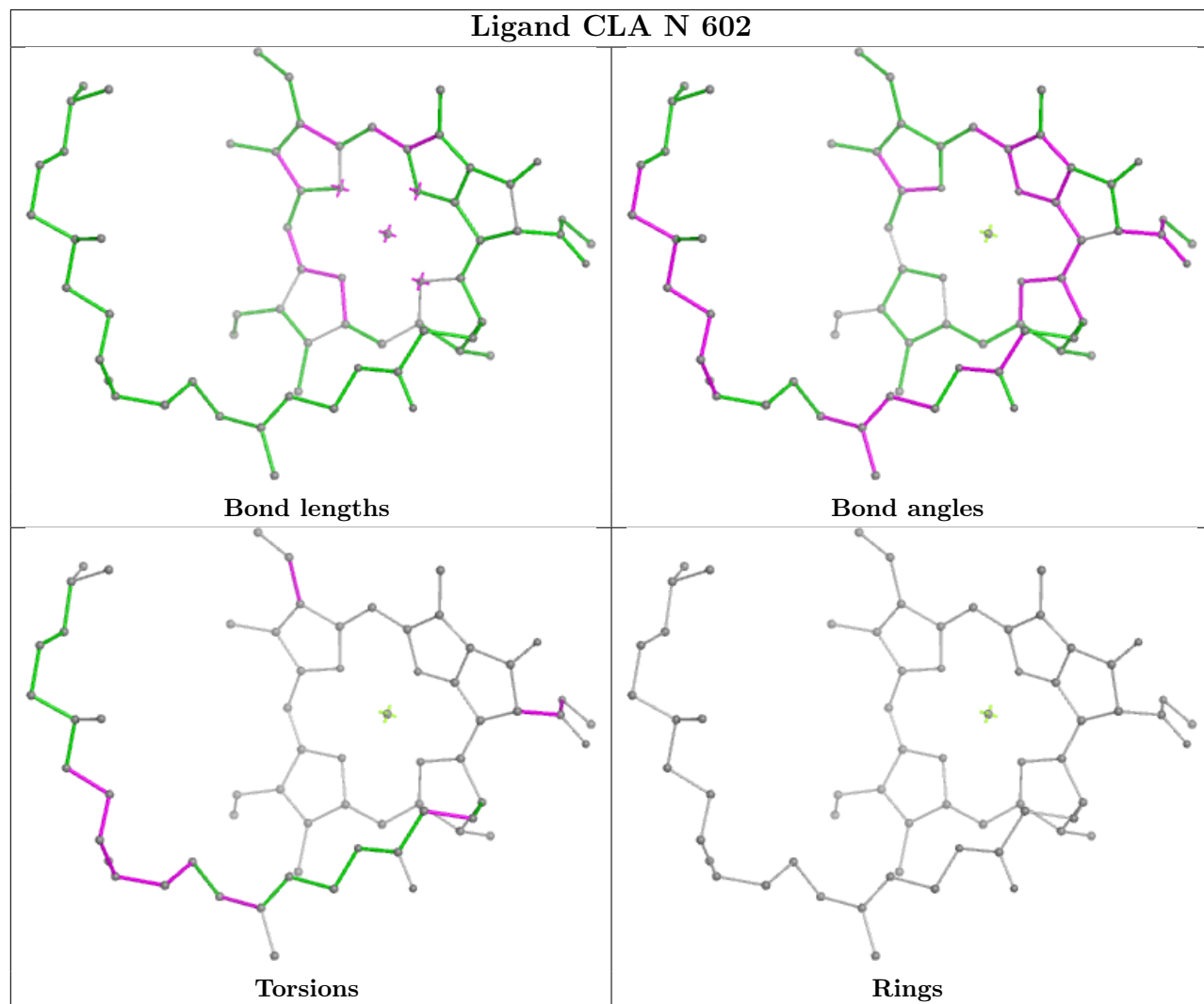
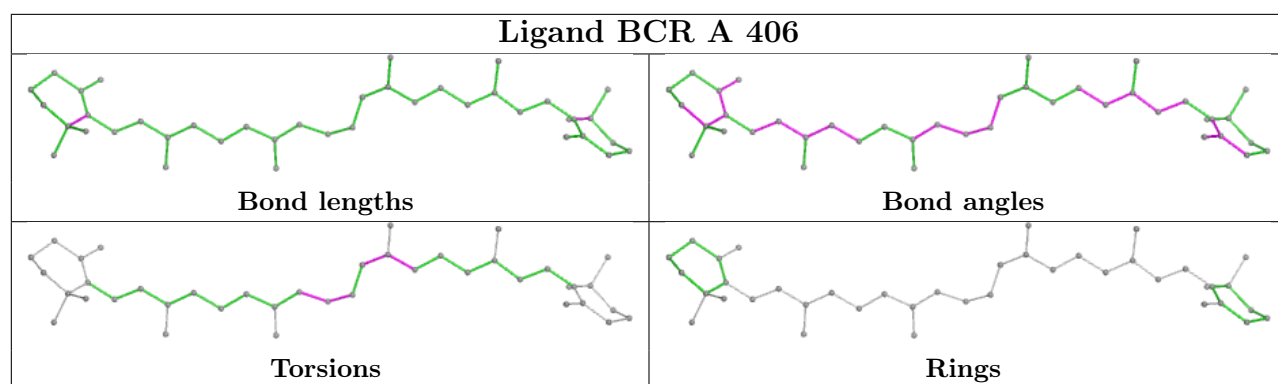


## Ligand CLA b 610

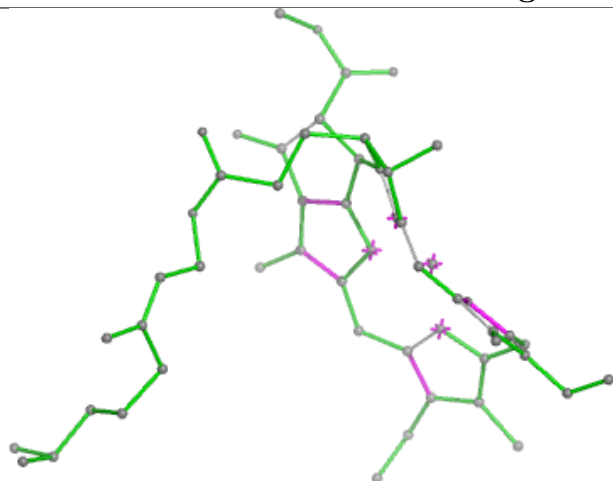


## Ligand NEX G 617

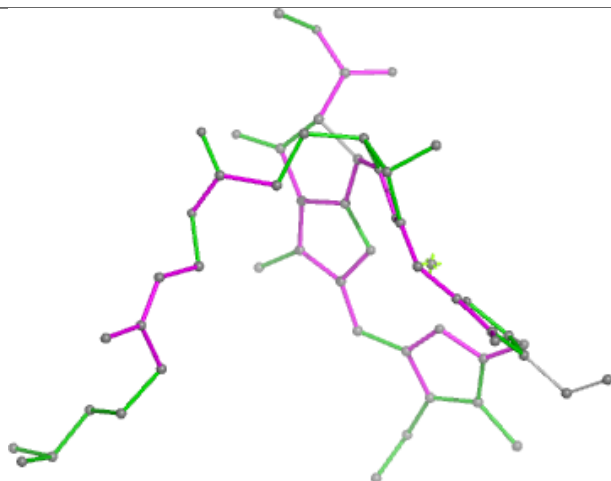




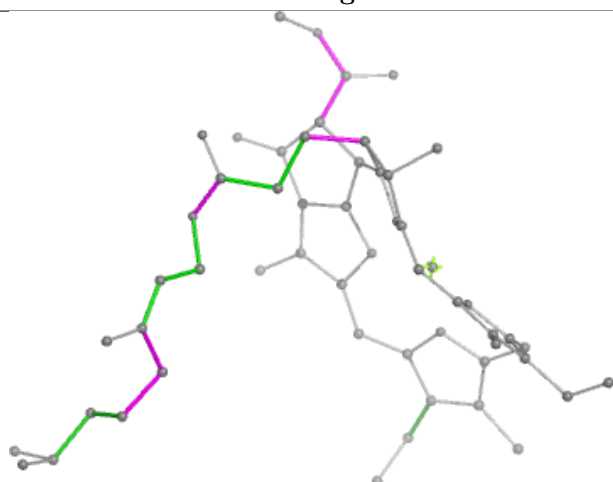
## Ligand CLA 6 604



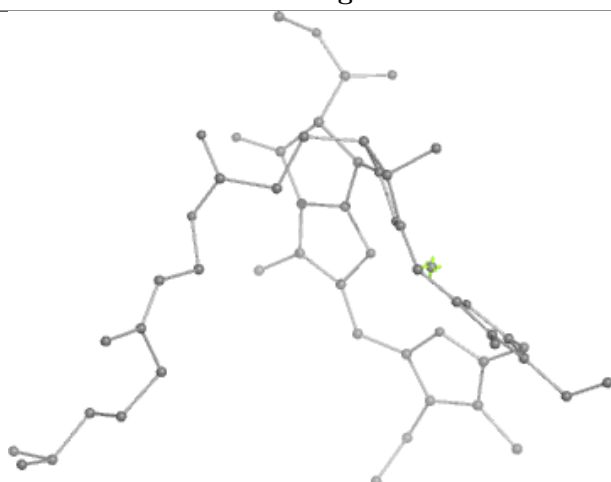
Bond lengths



Bond angles

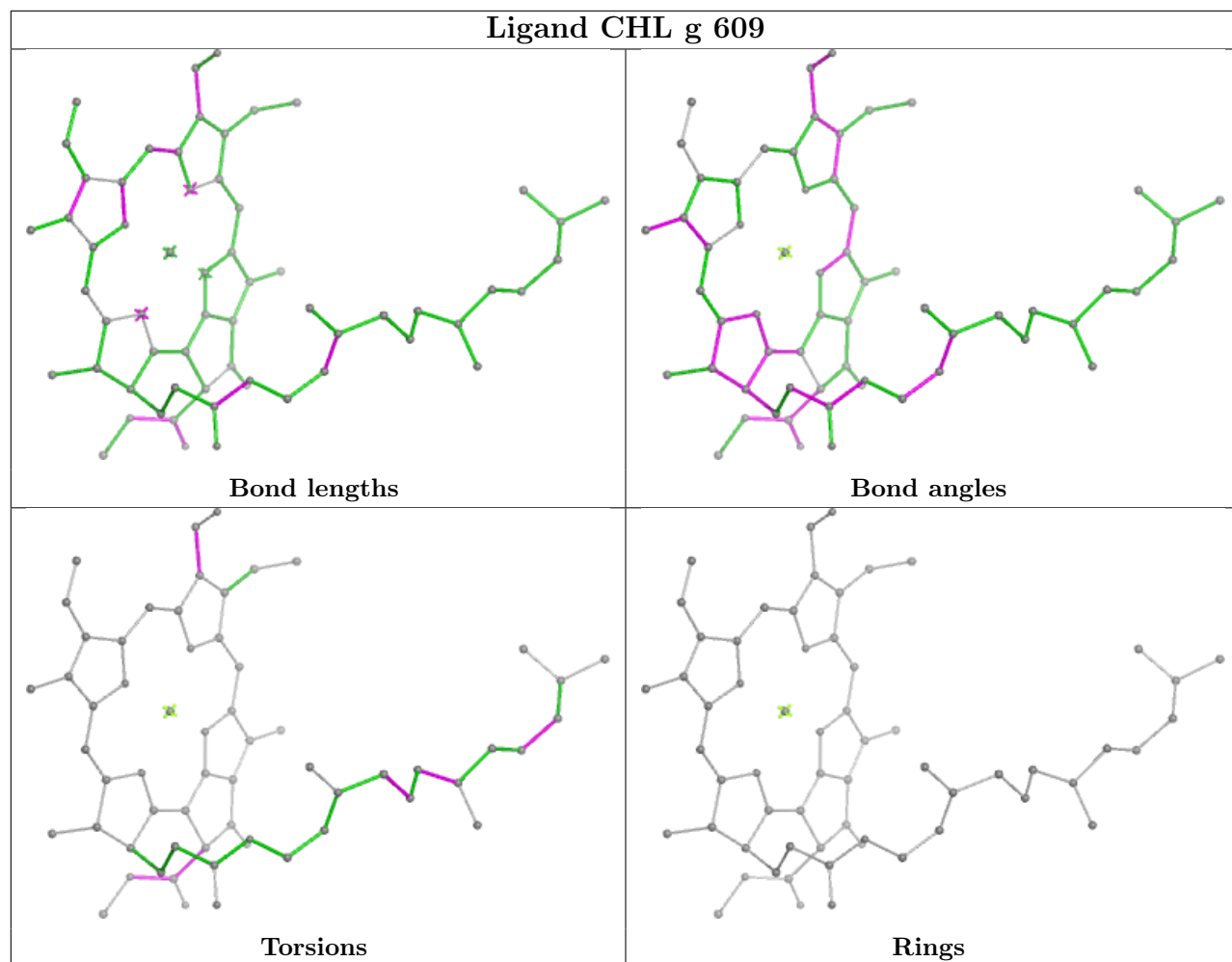


Torsions

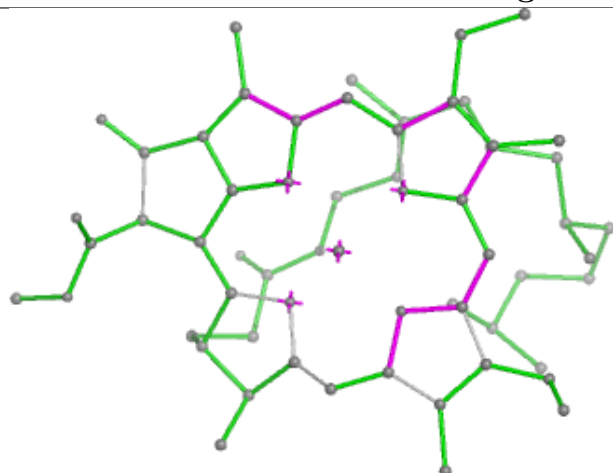


Rings

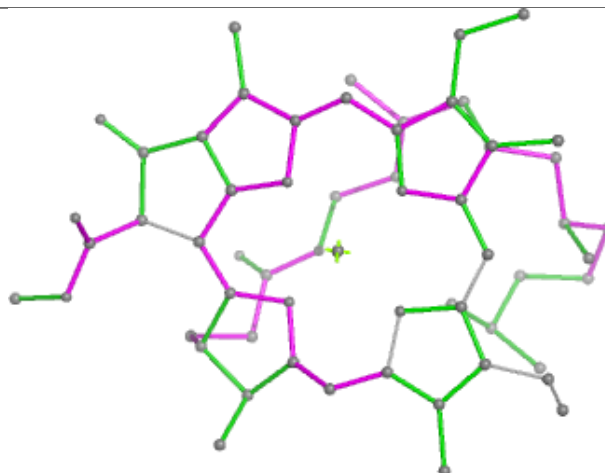
## Ligand CHL g 609



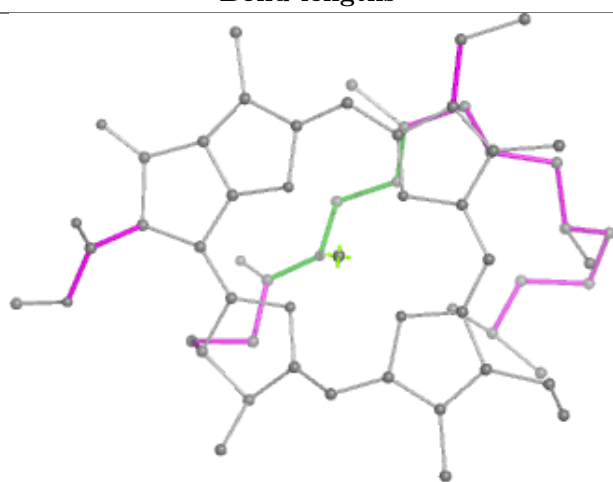
## Ligand CLA n 613



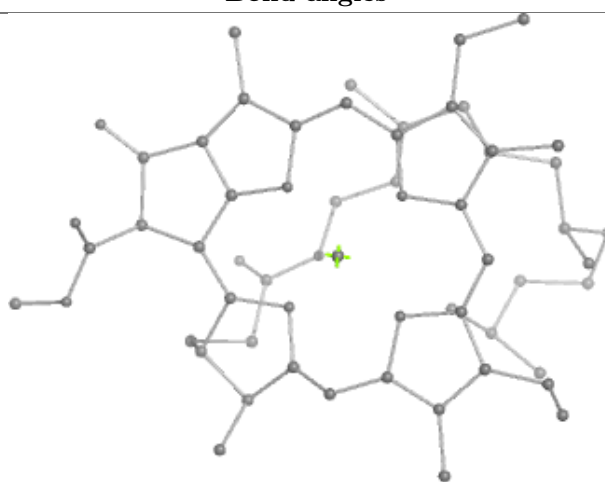
Bond lengths



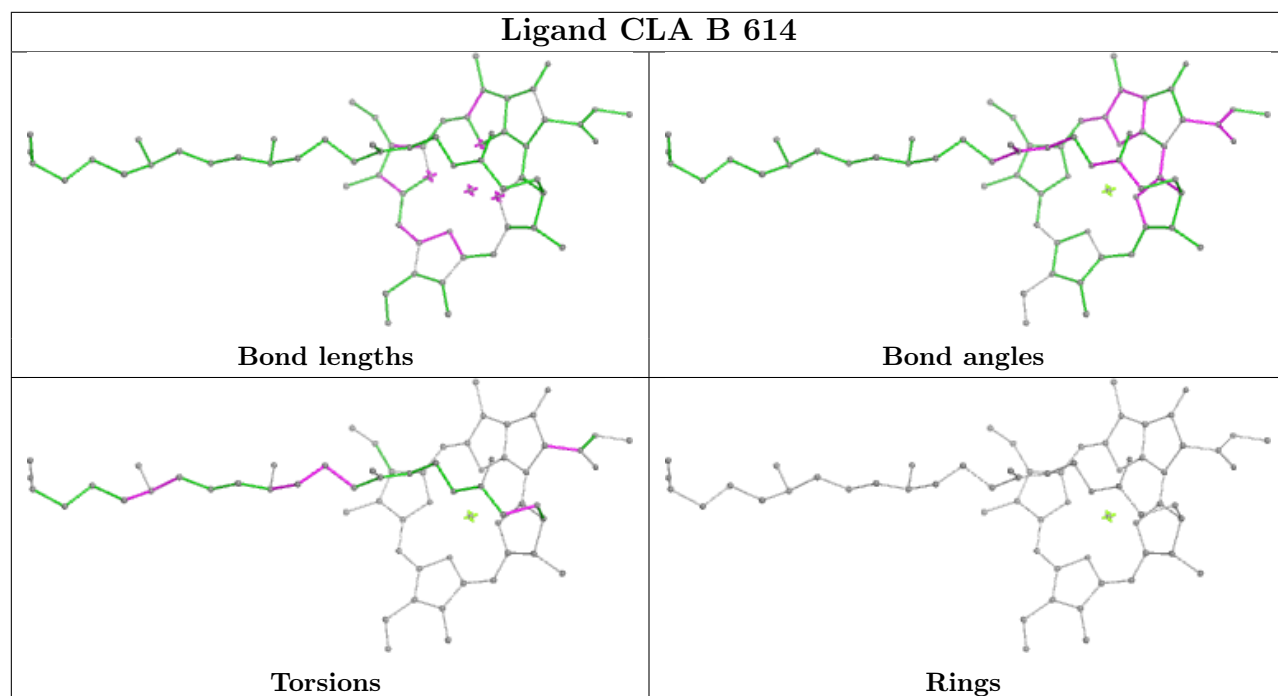
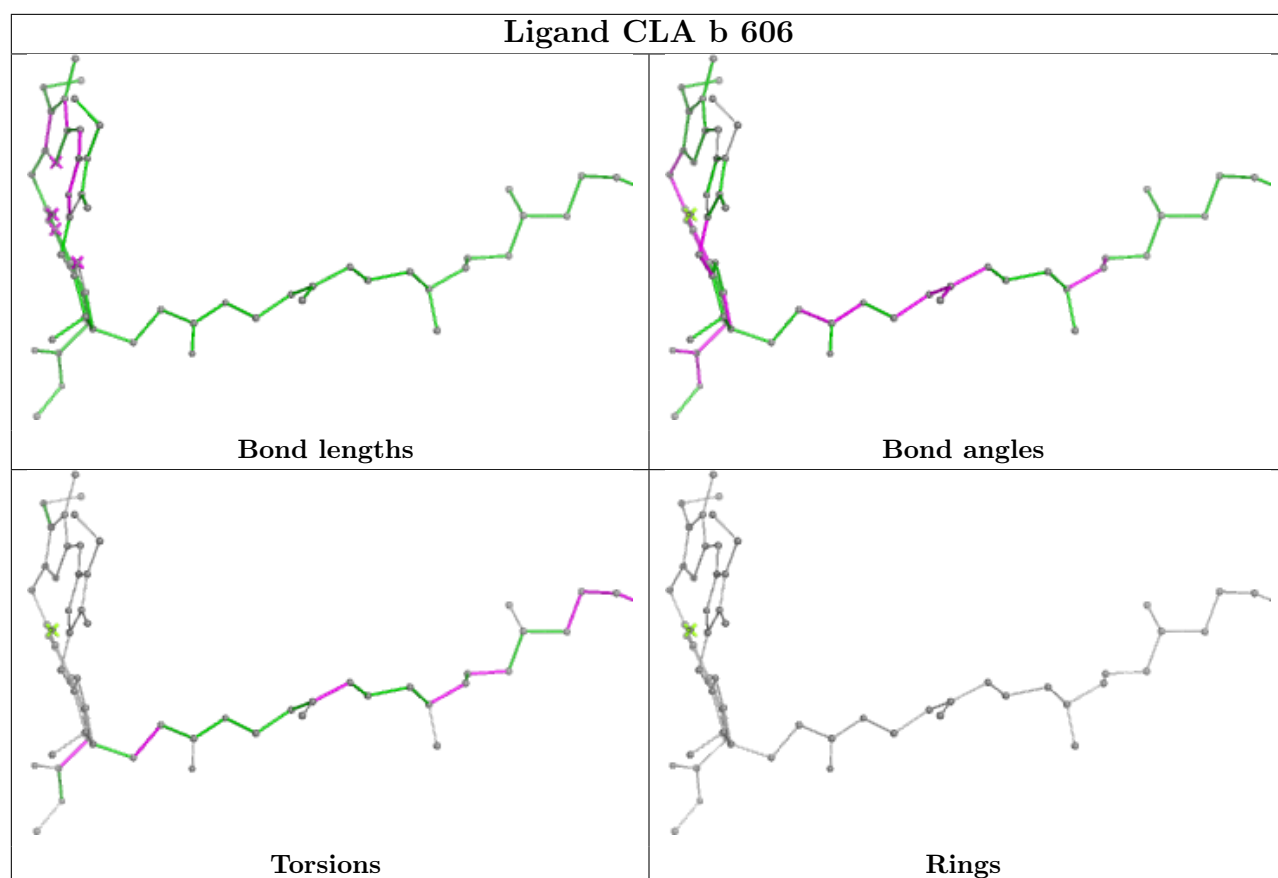
Bond angles



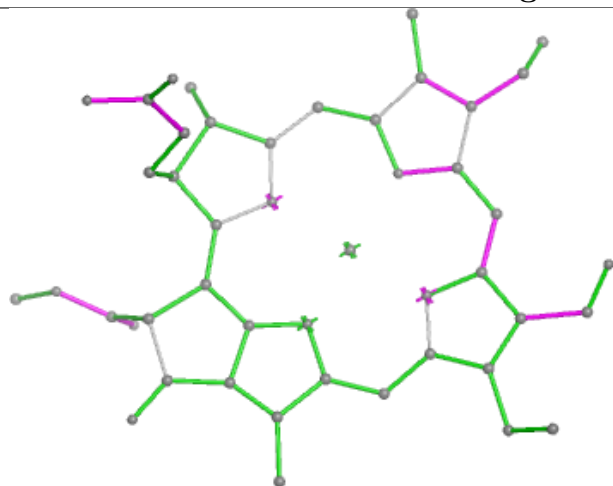
Torsions



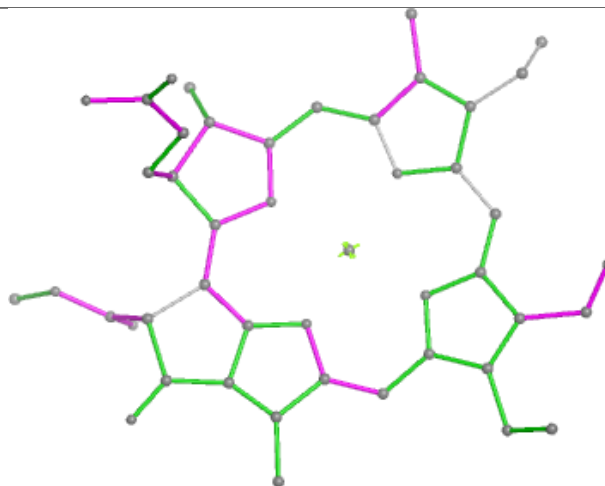
Rings



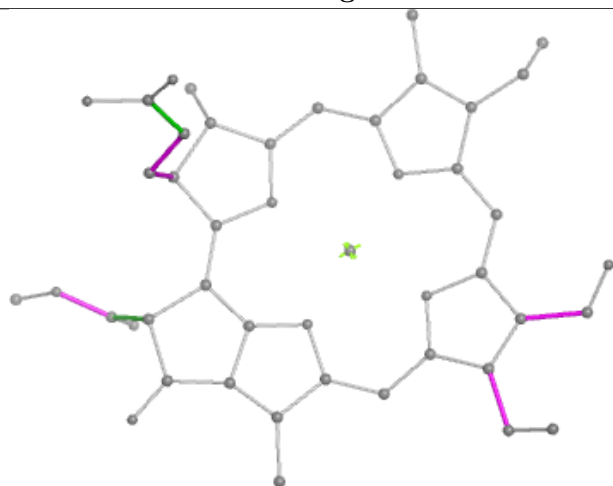
## Ligand CHL s 307



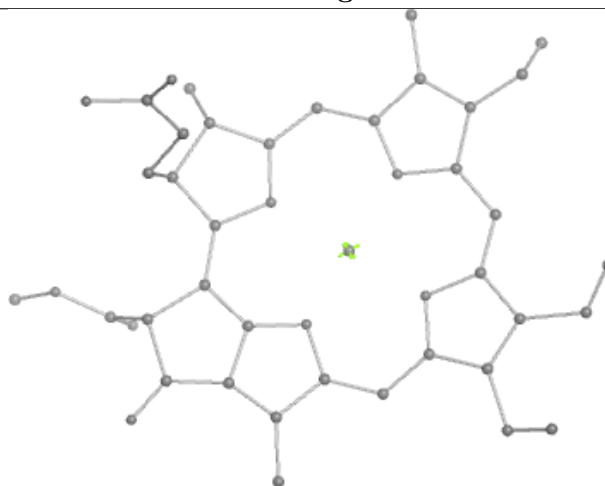
Bond lengths



Bond angles

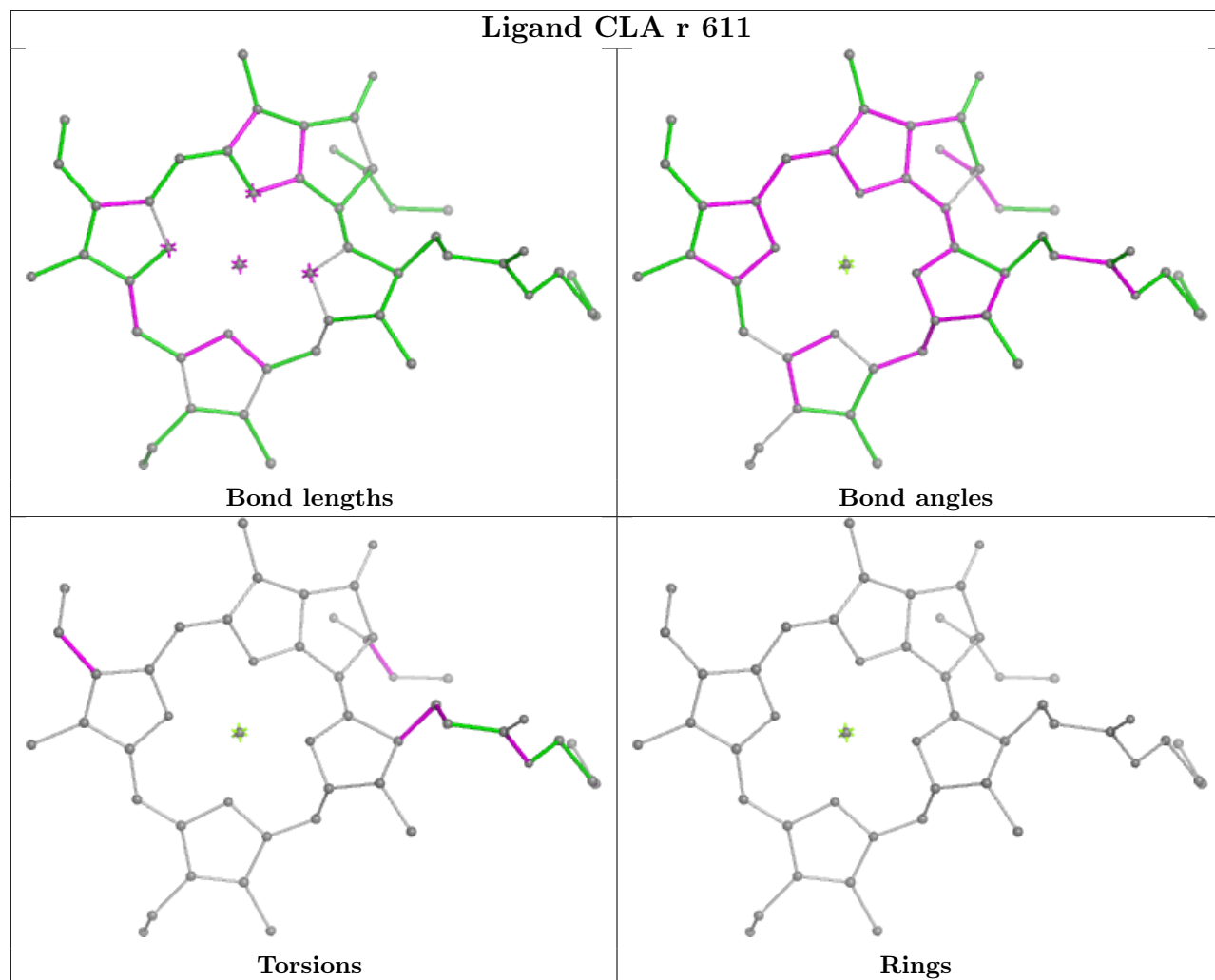


Torsions

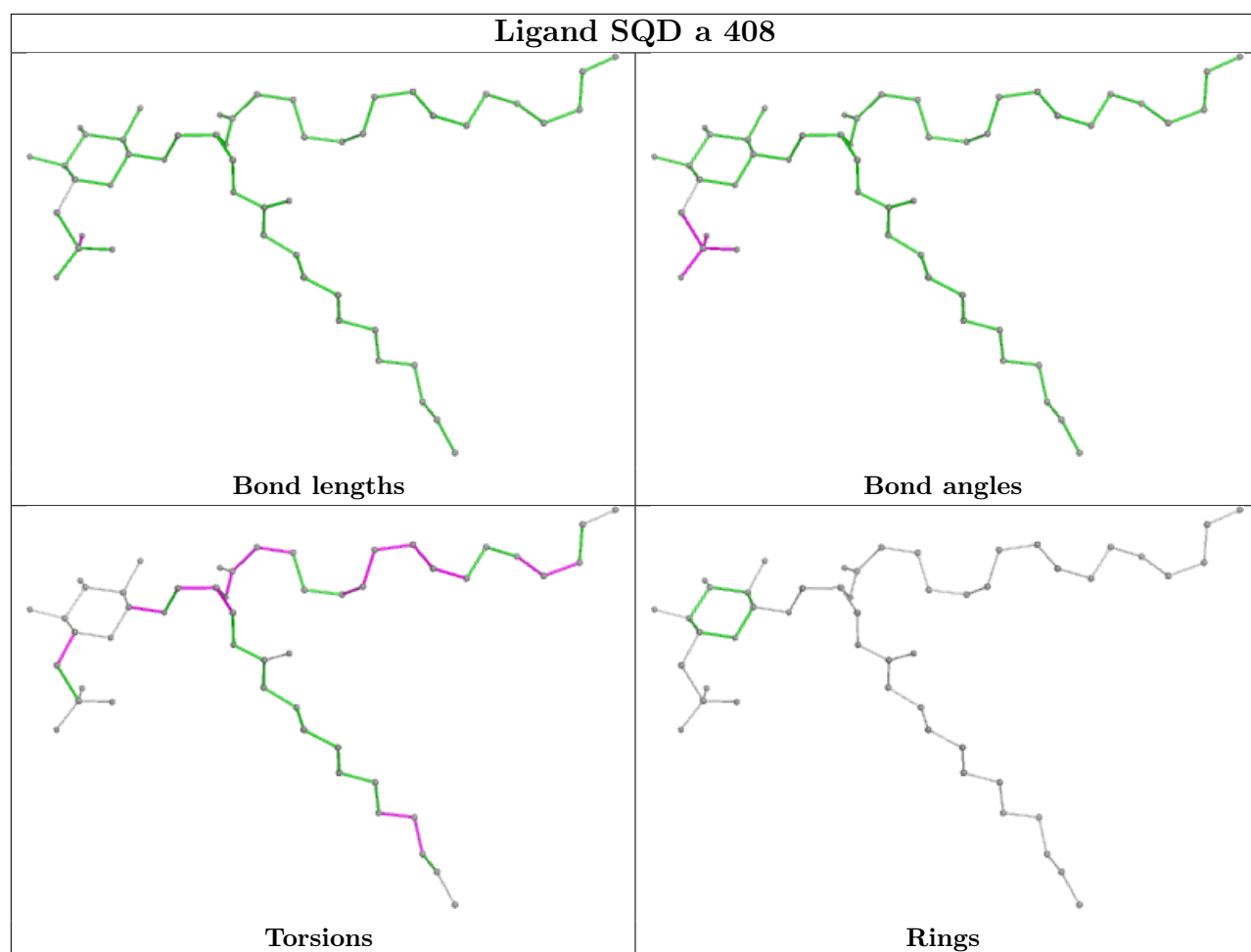


Rings

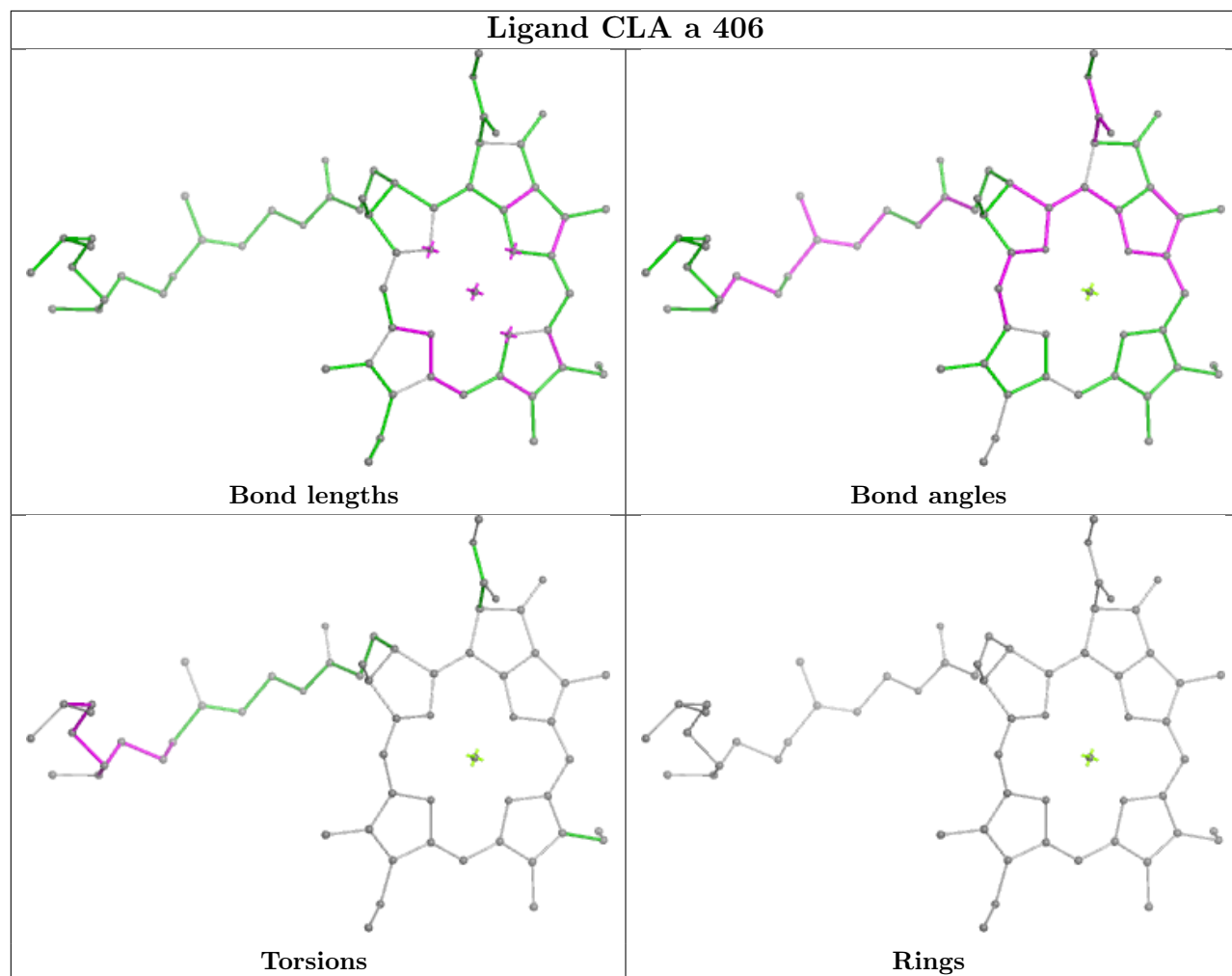
## Ligand CLA r 611



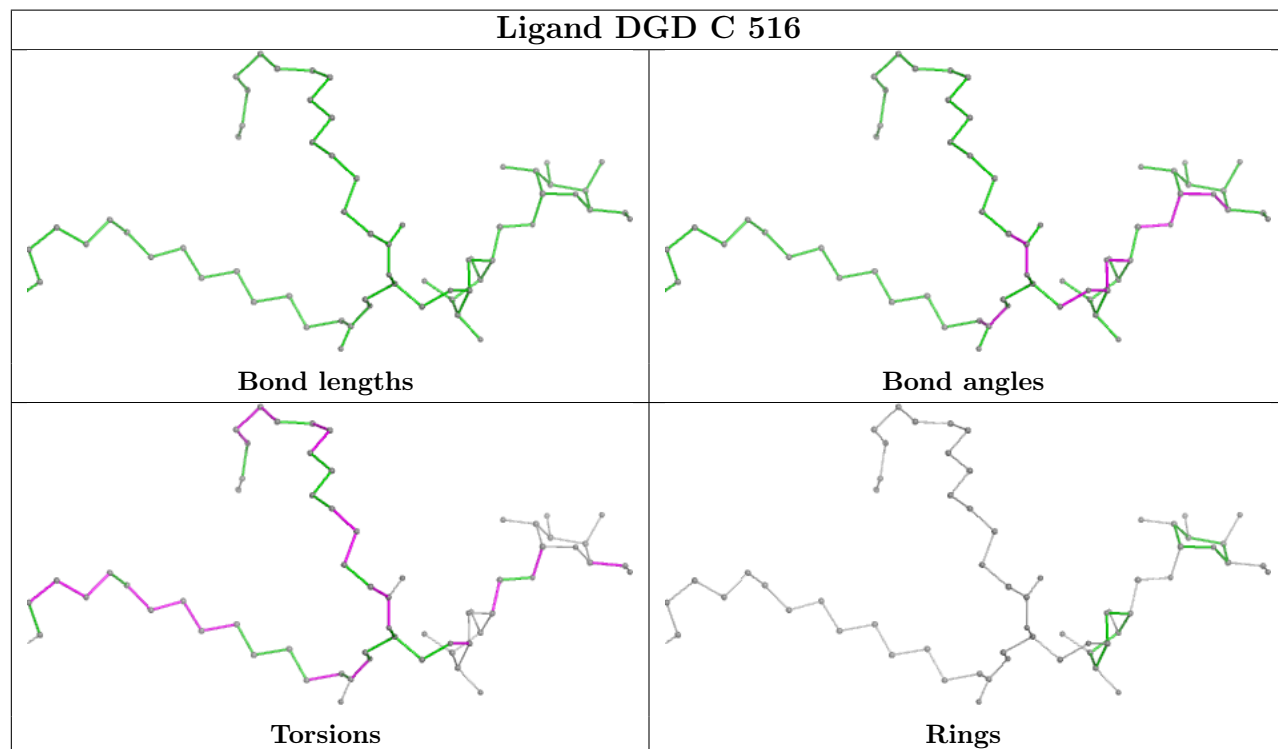


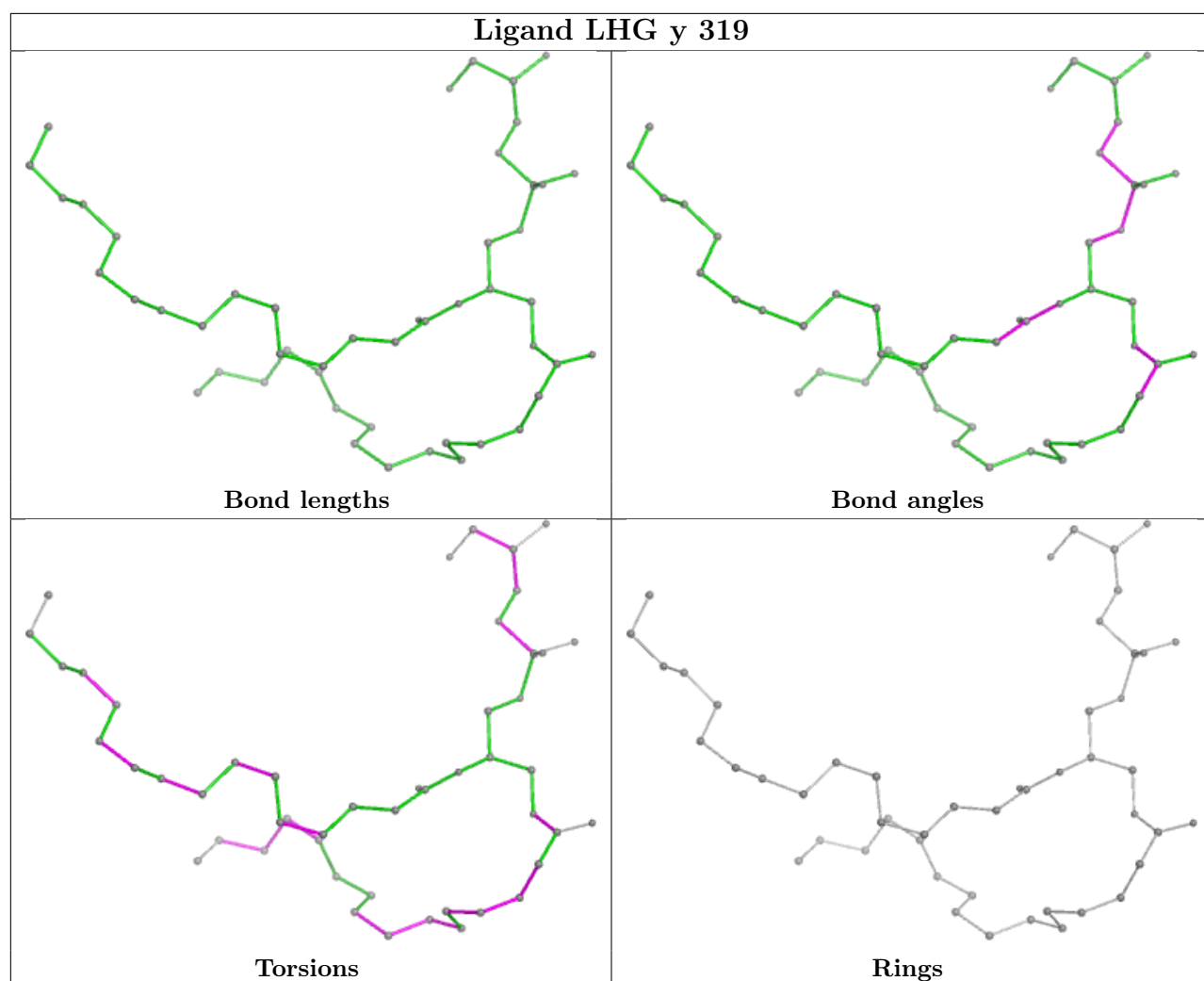


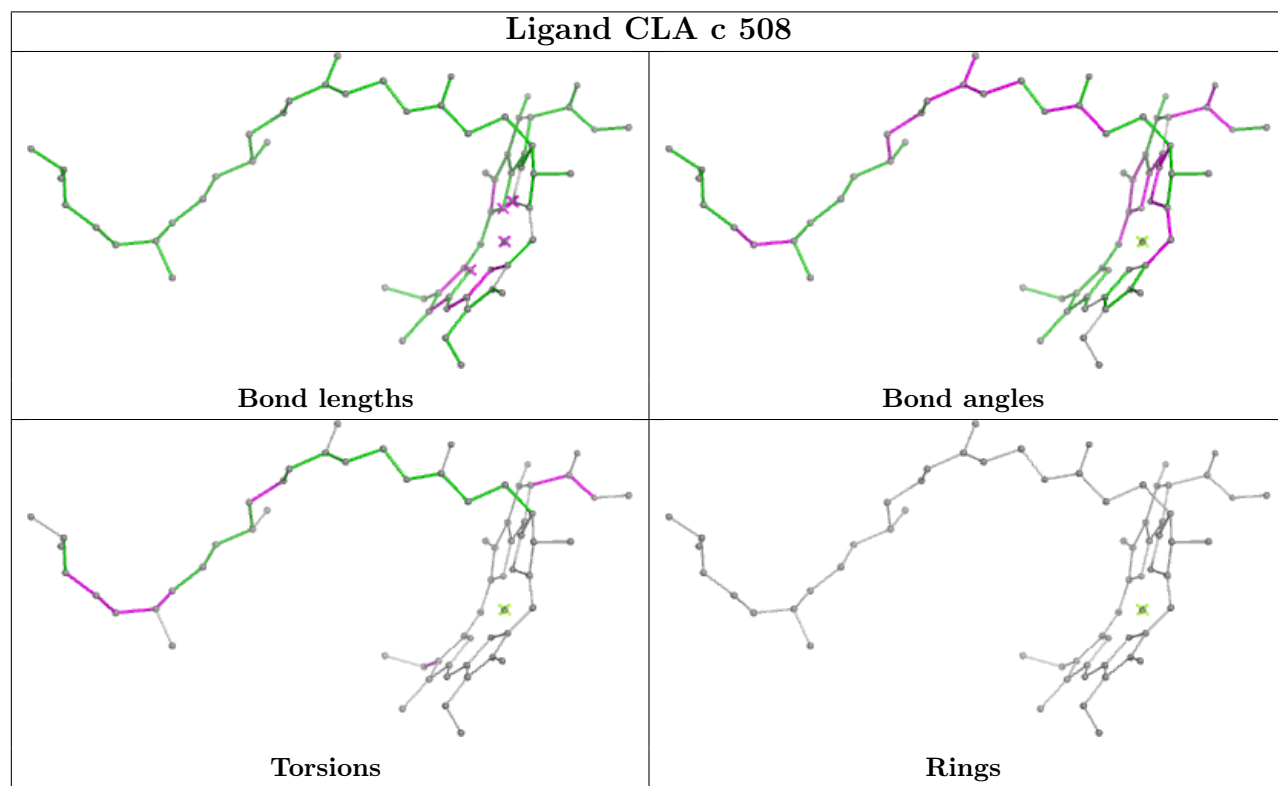
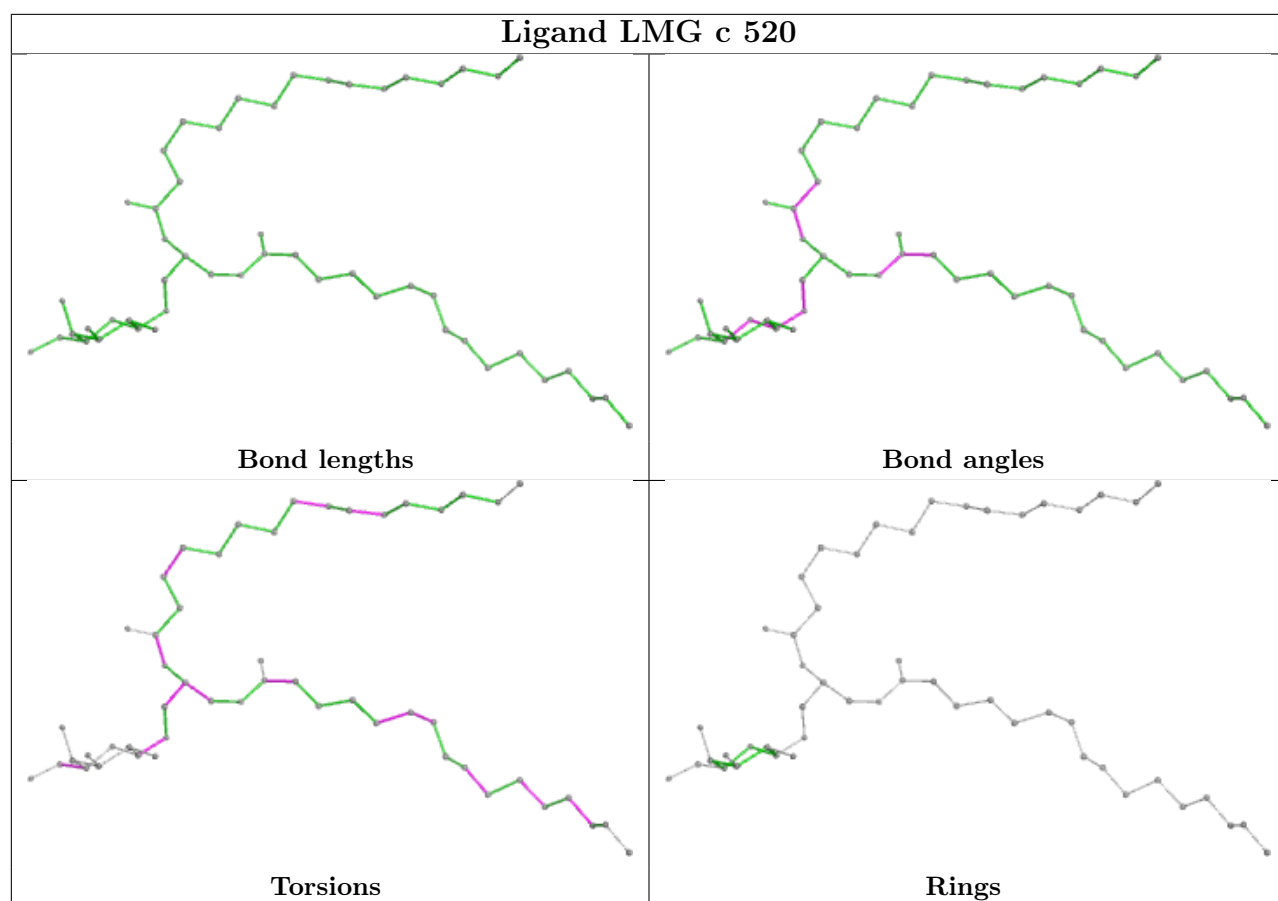
## Ligand CLA a 406



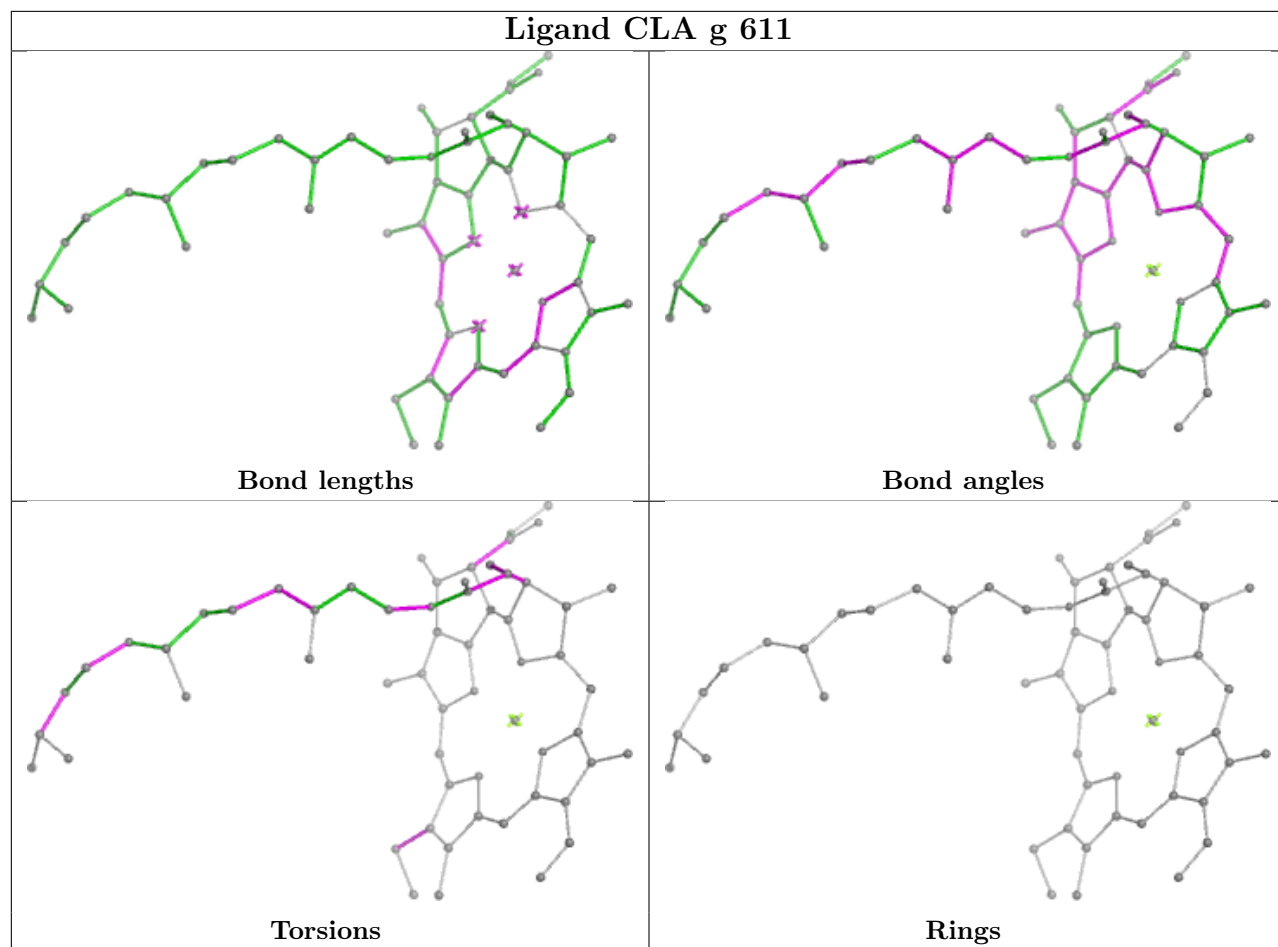
## Ligand DGD C 516



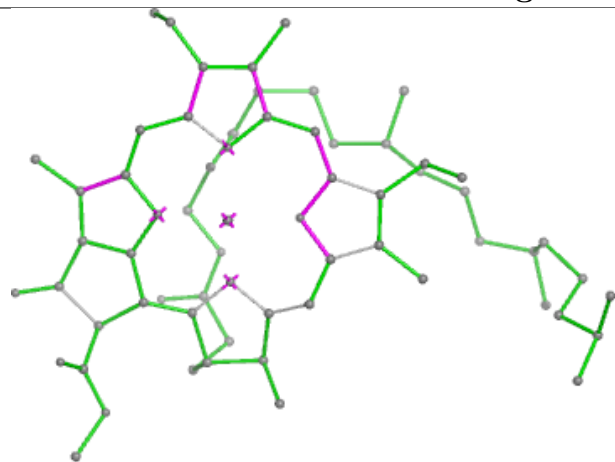




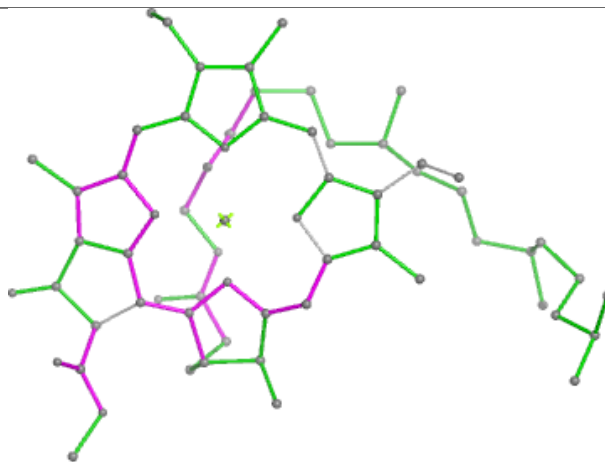
## Ligand CLA g 611



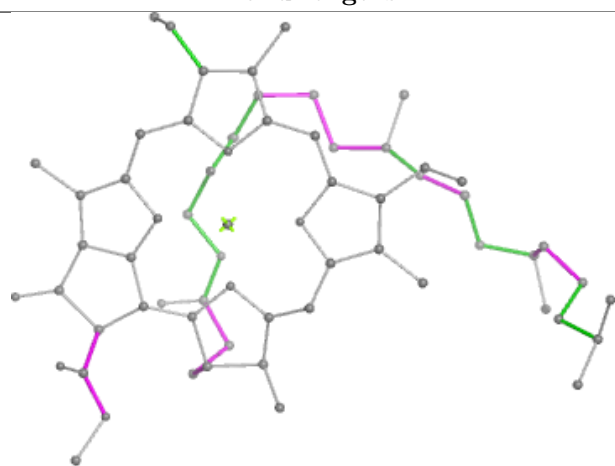
## Ligand CLA Y 314



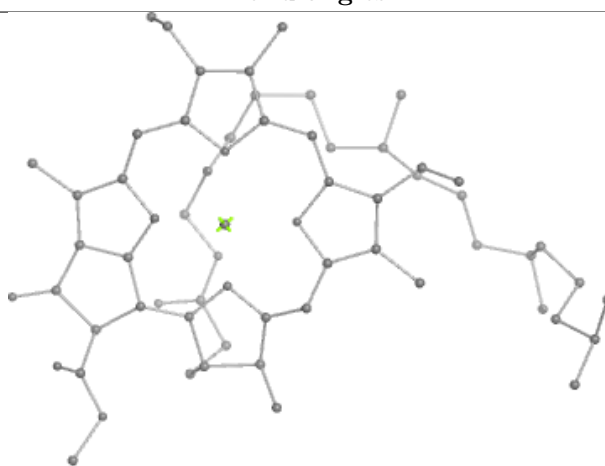
Bond lengths



Bond angles

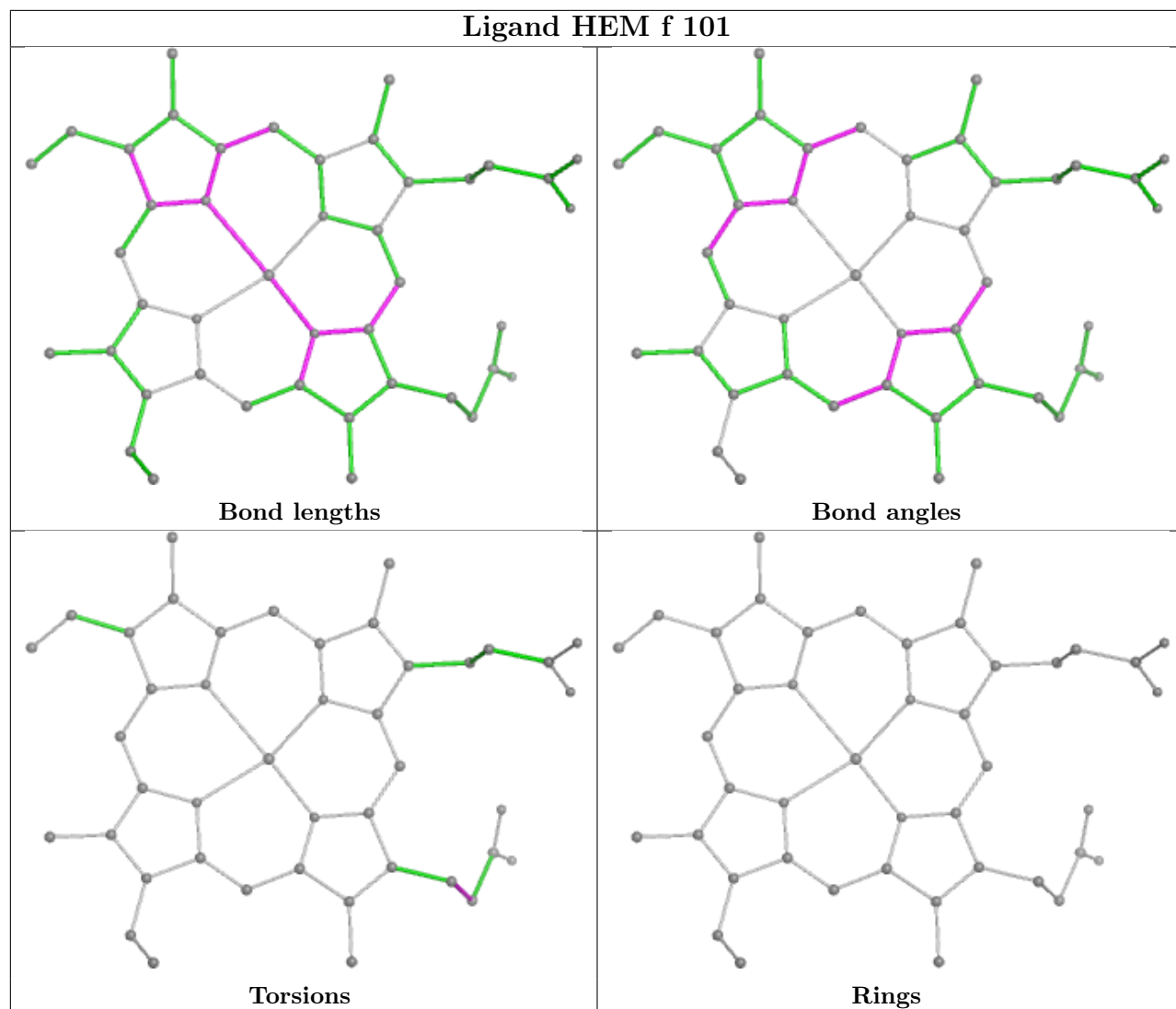


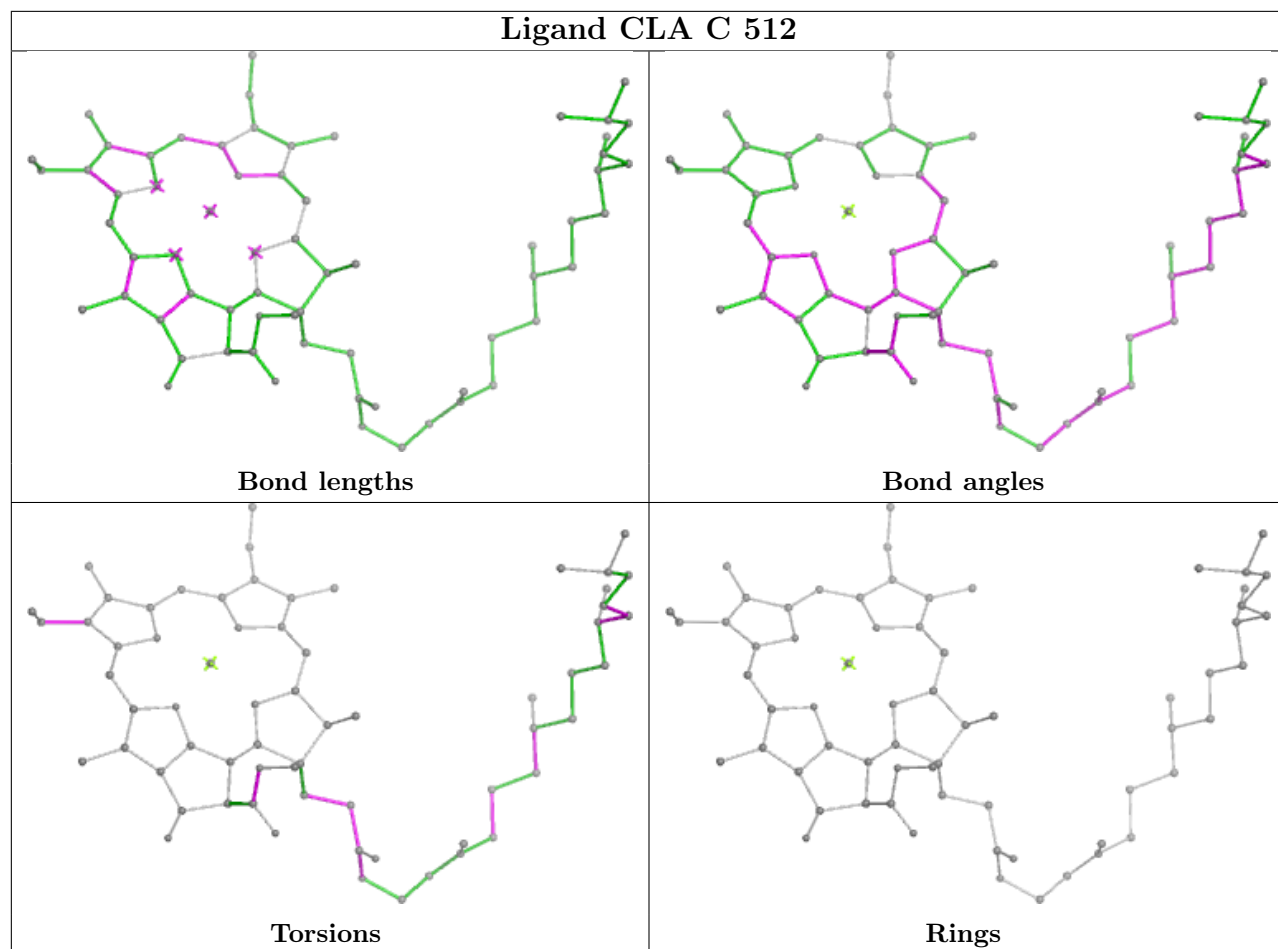
Torsions



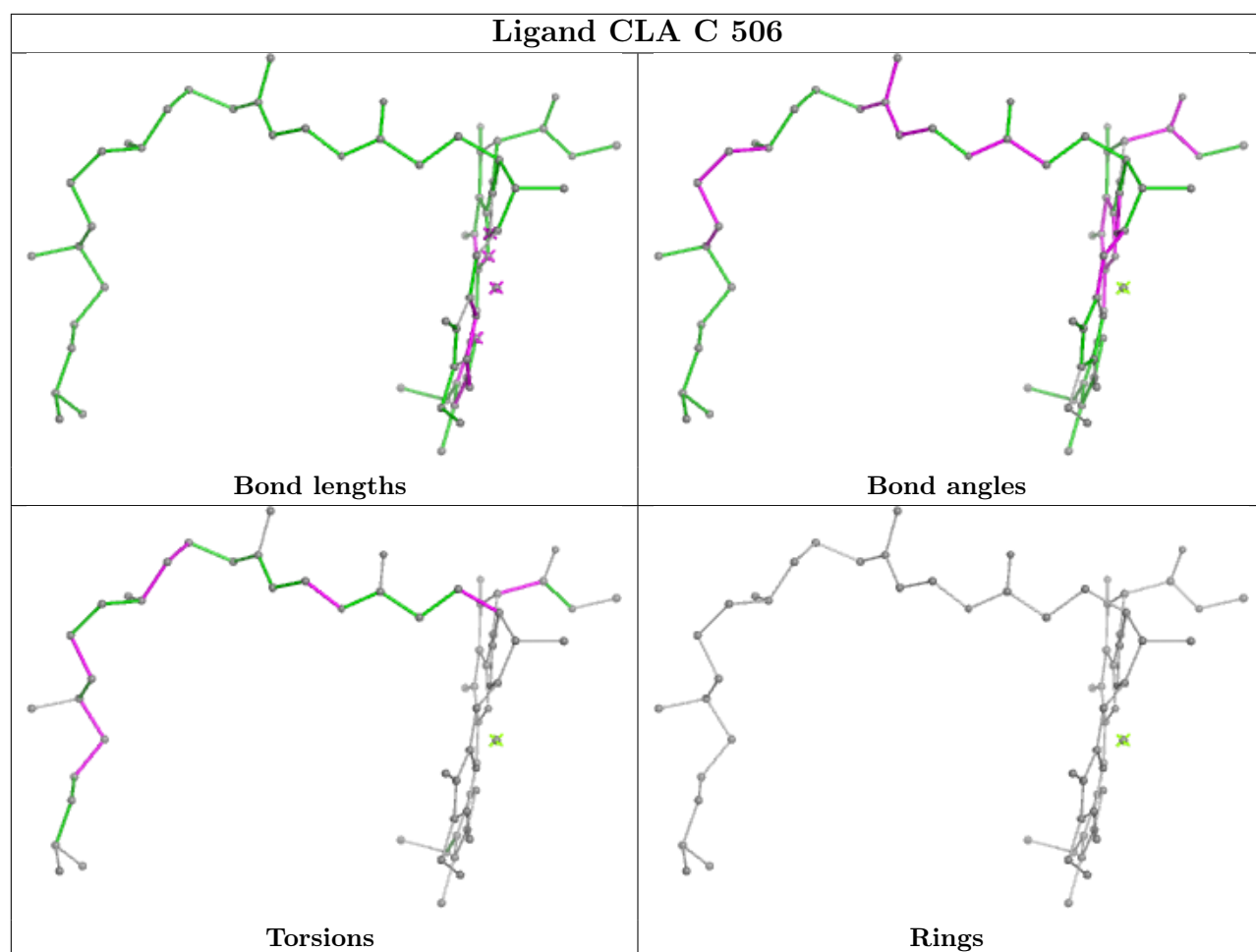
Rings

## Ligand HEM f 101

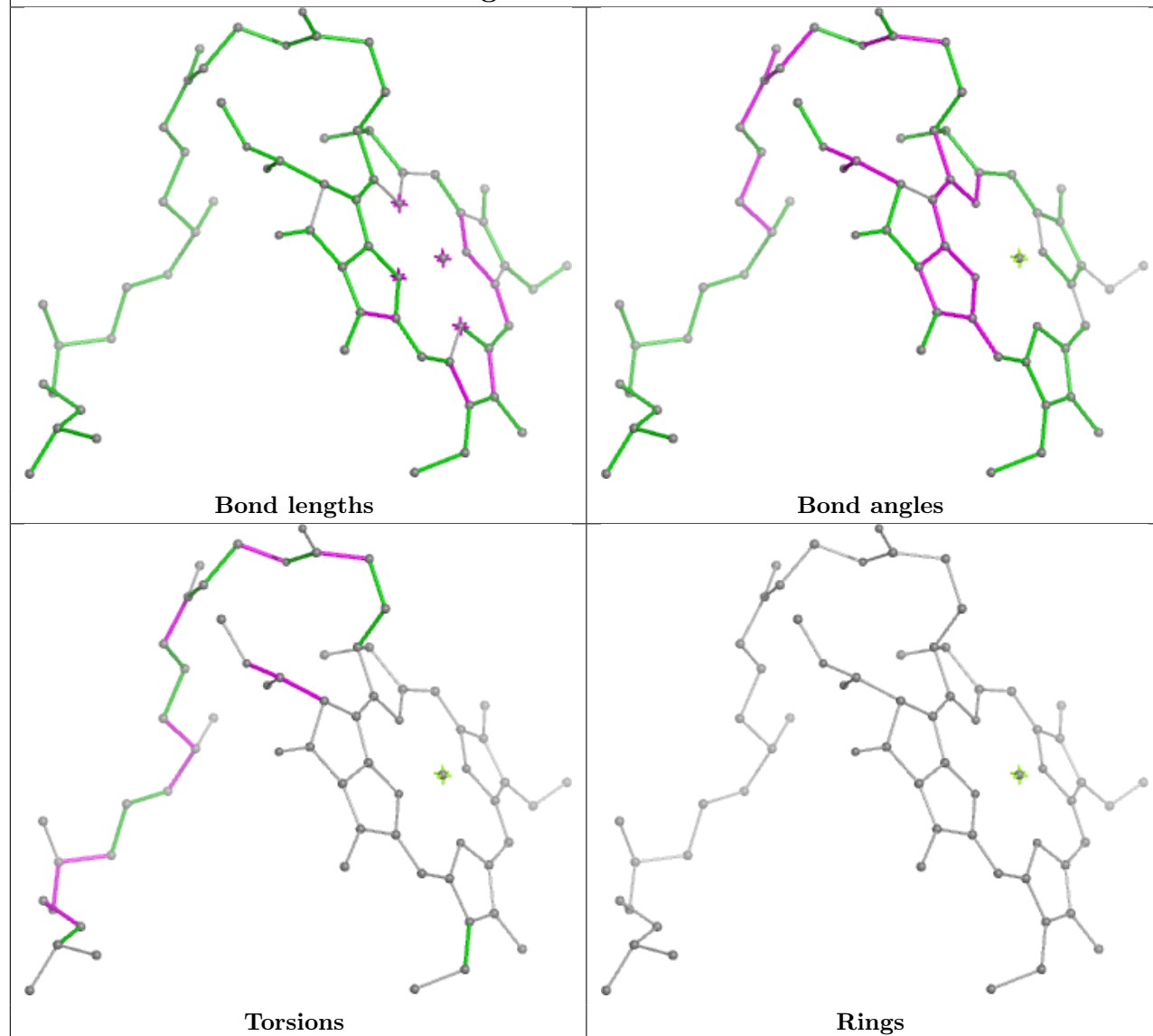




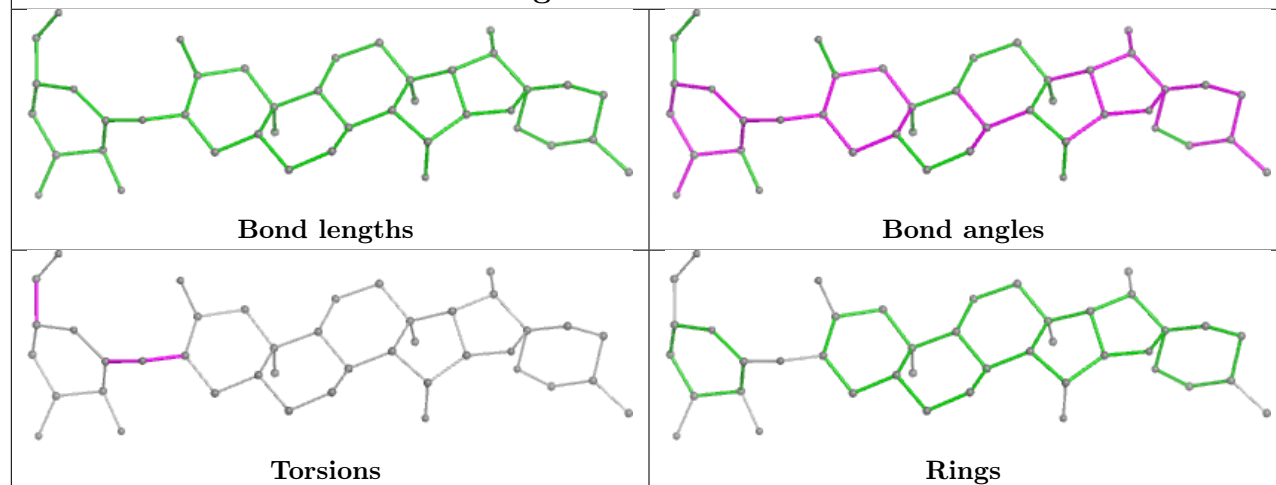


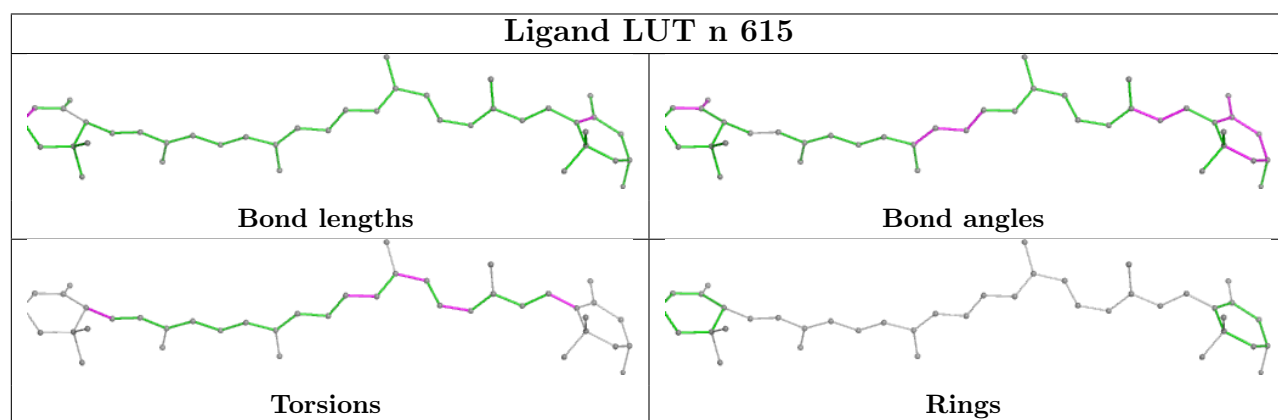
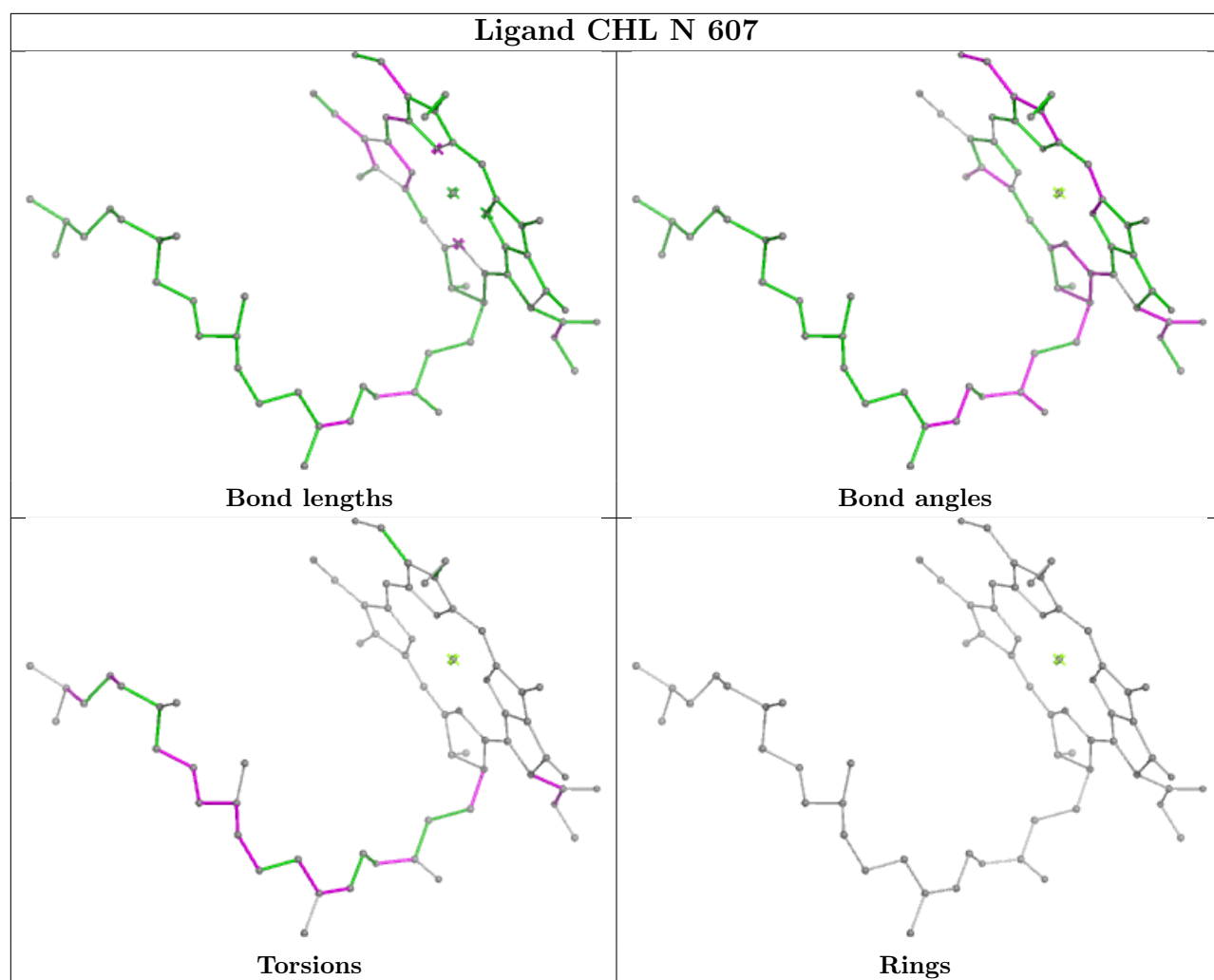


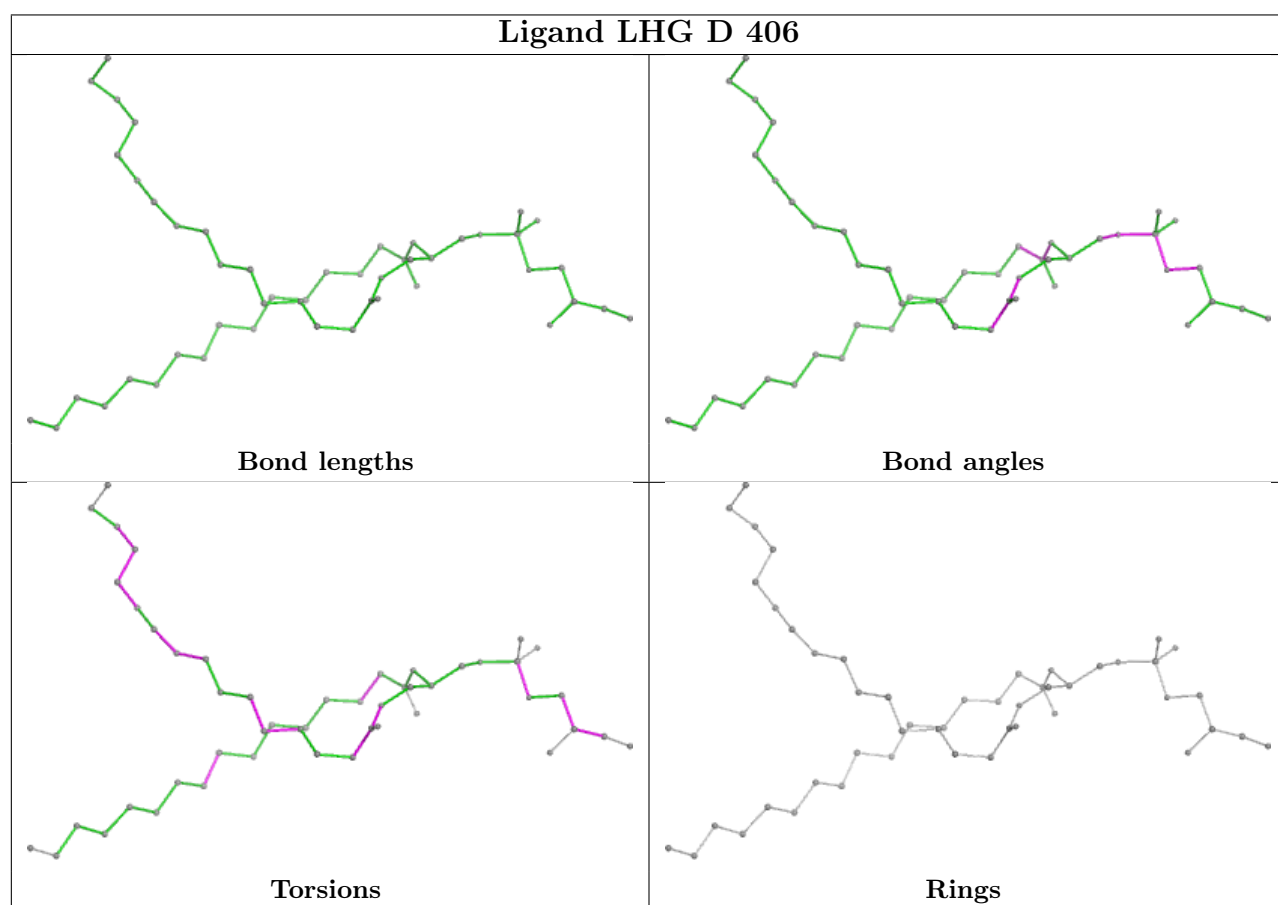
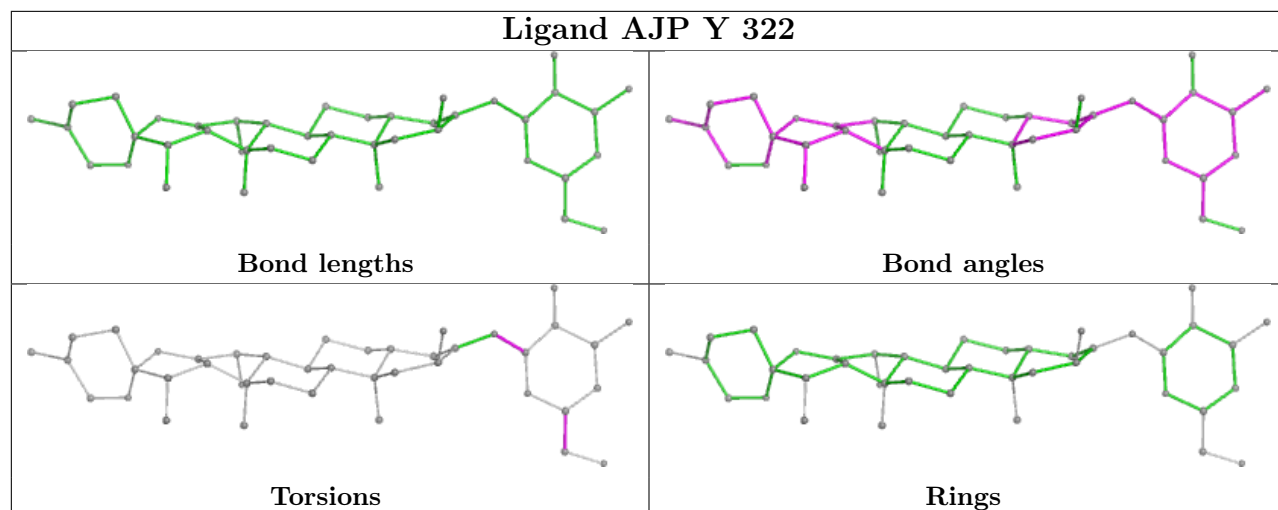
## Ligand CLA B 613



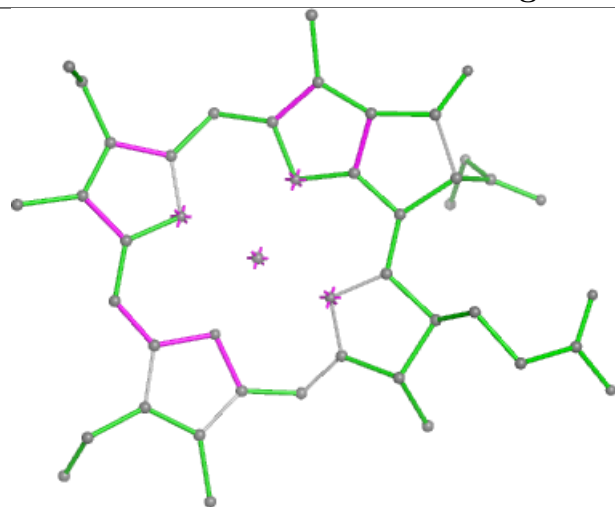
## Ligand AJP N 620



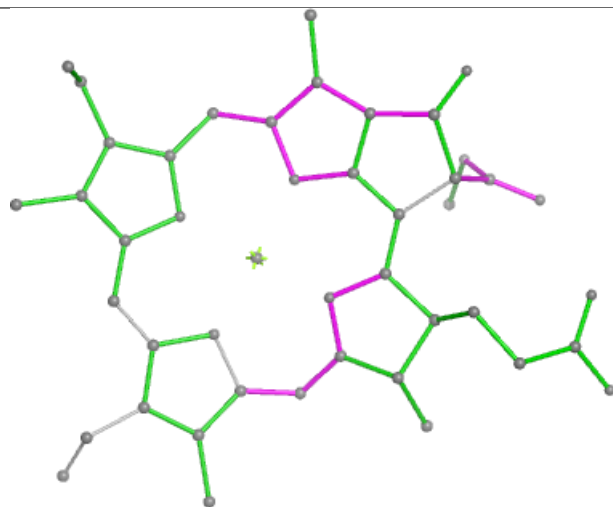




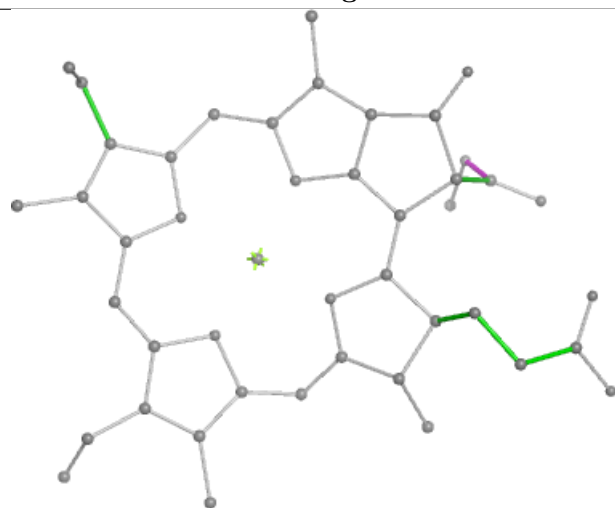
## Ligand CLA S 304



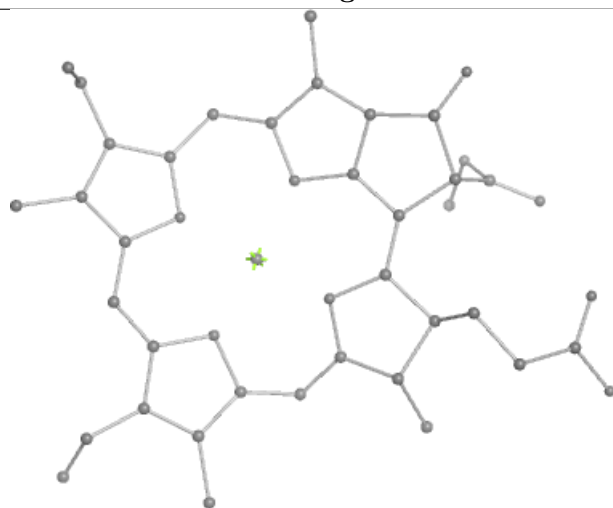
Bond lengths



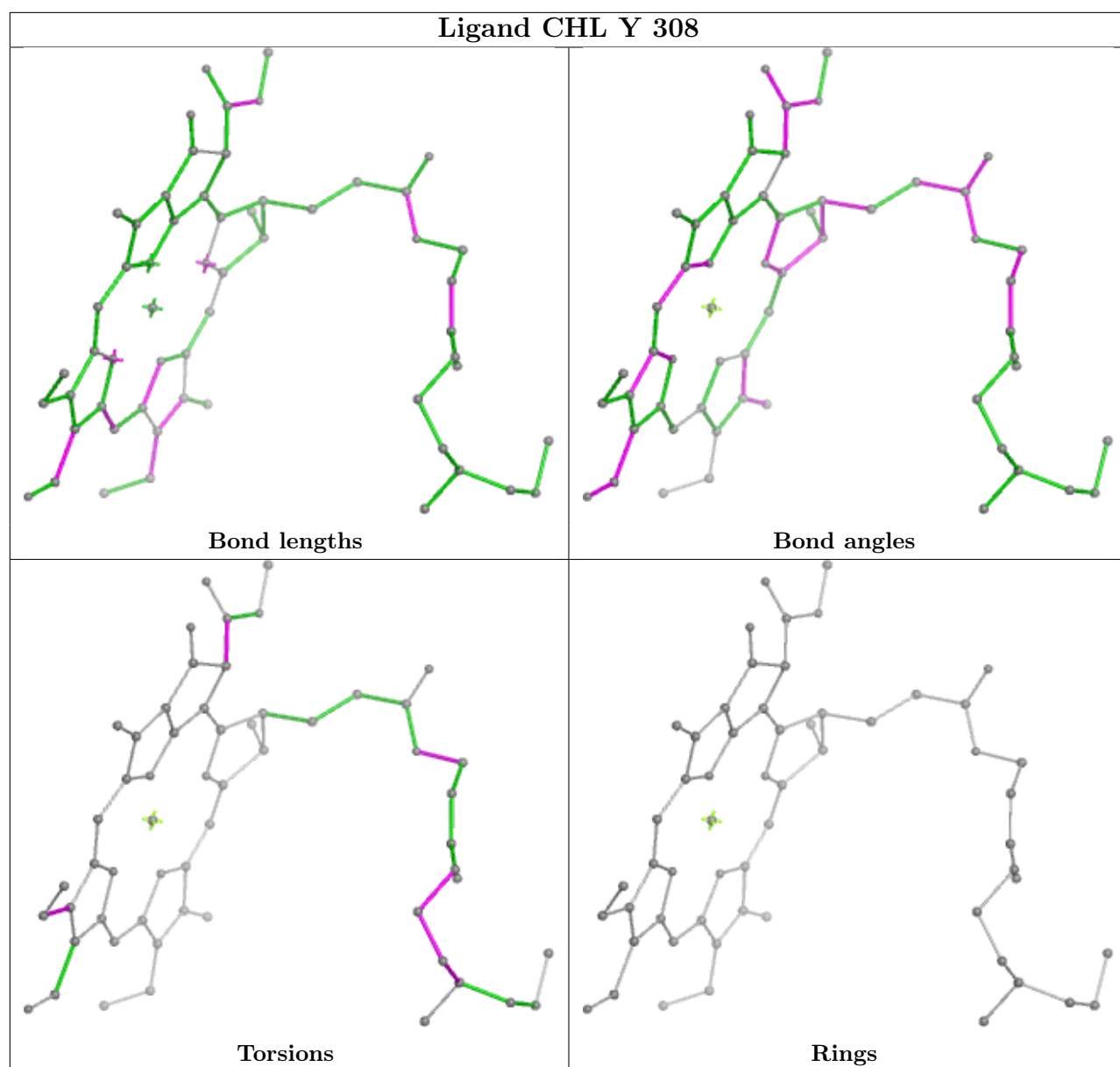
Bond angles



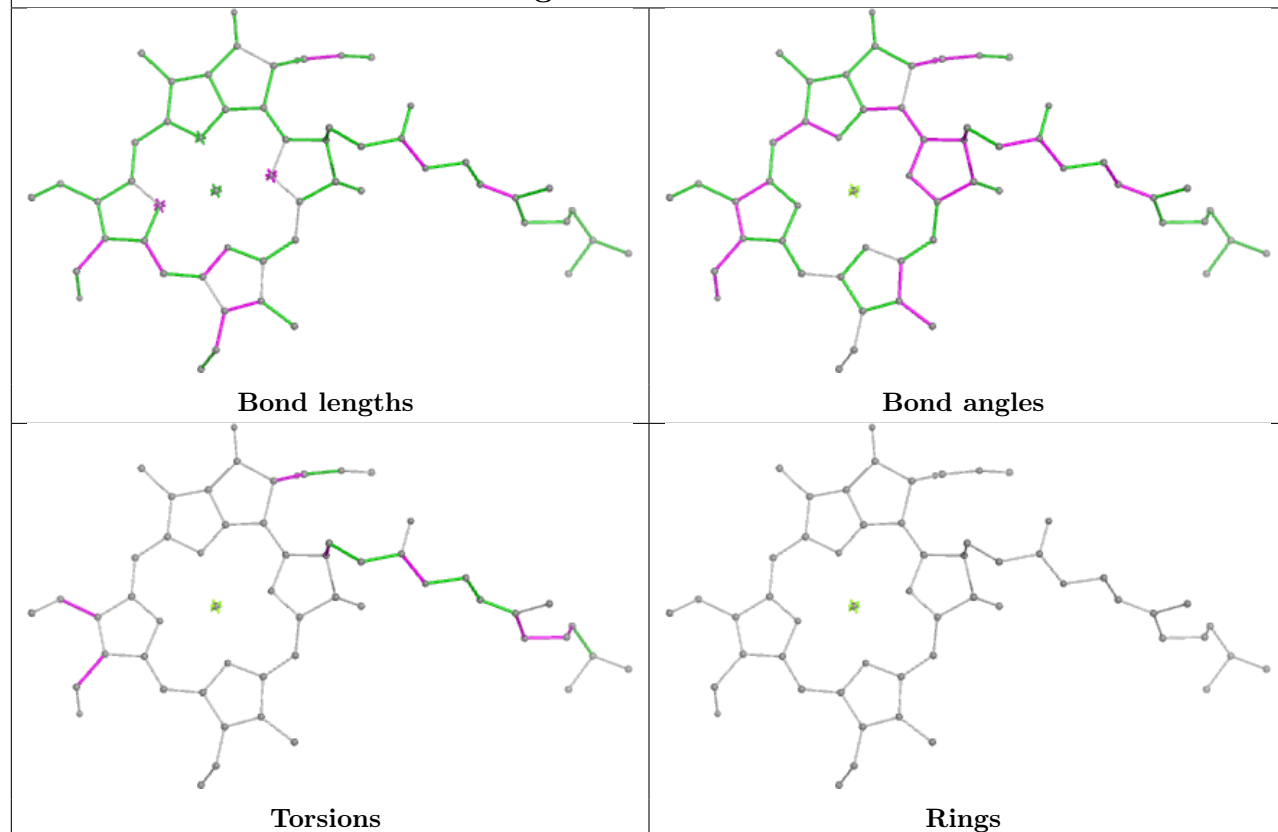
Torsions



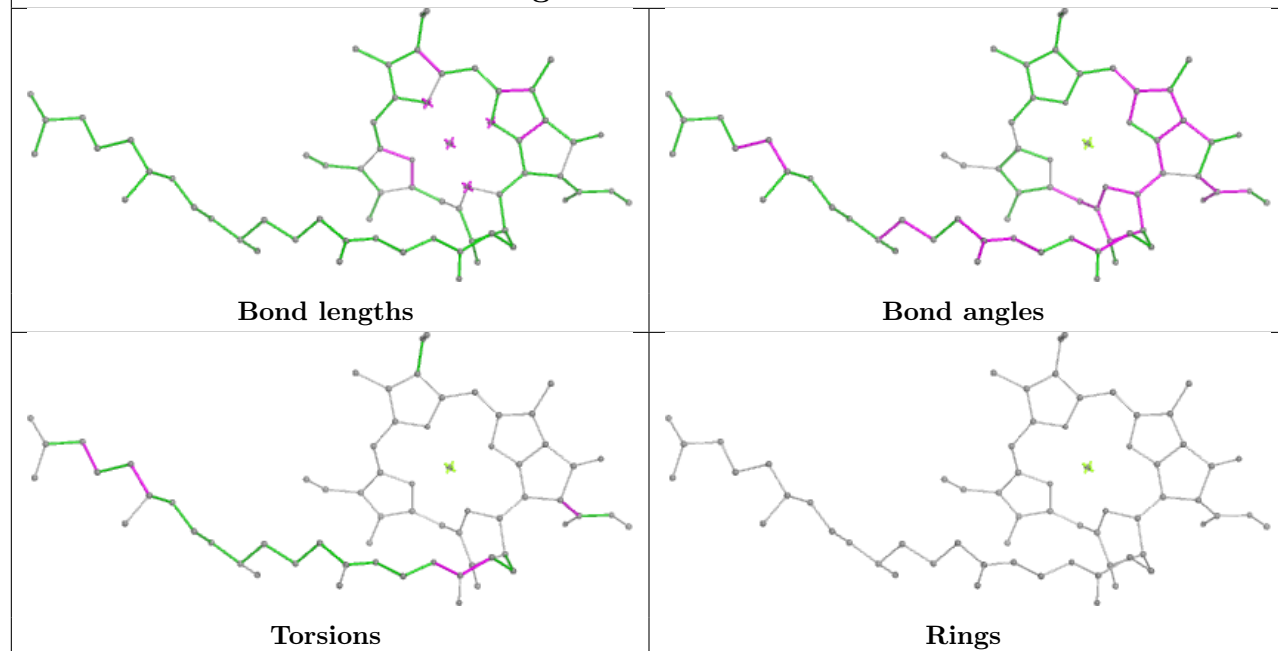
Rings

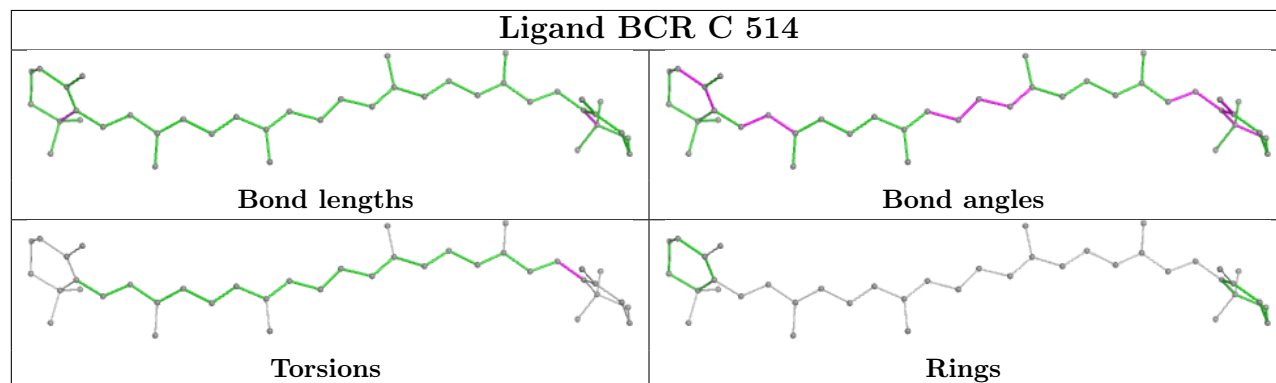
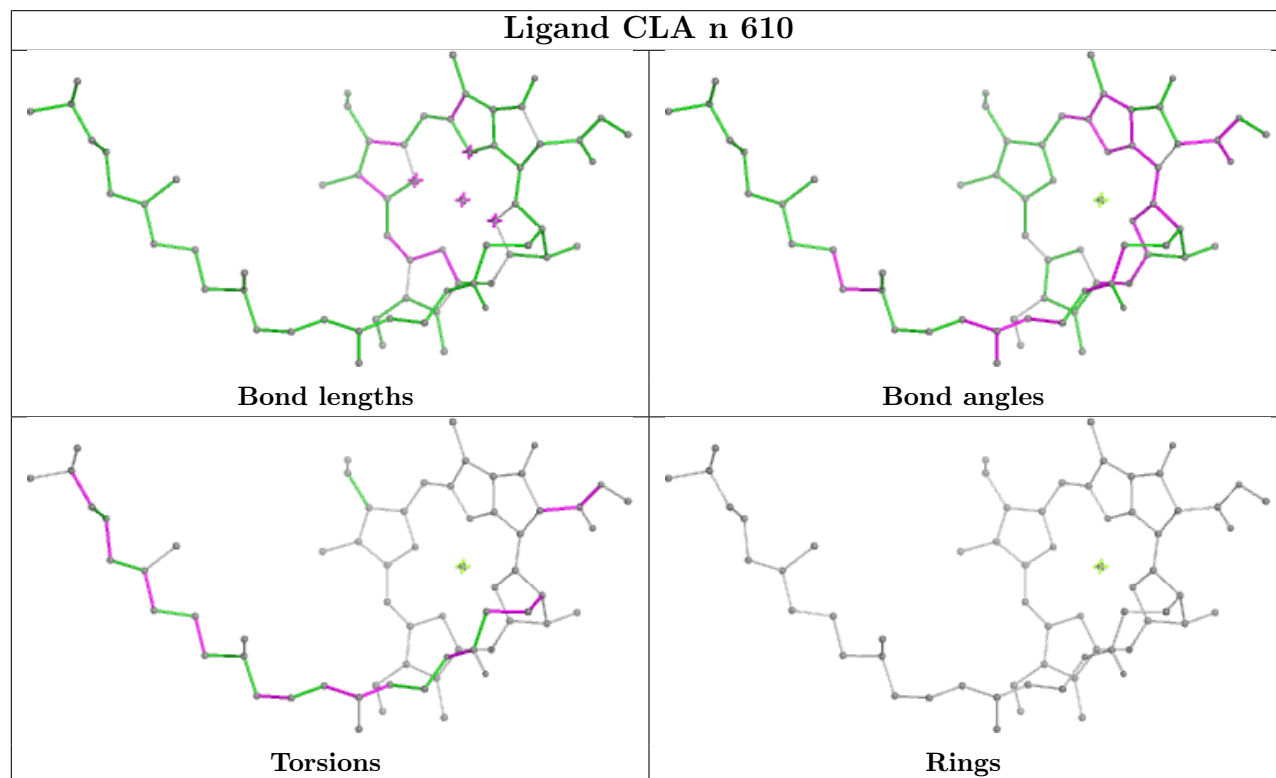
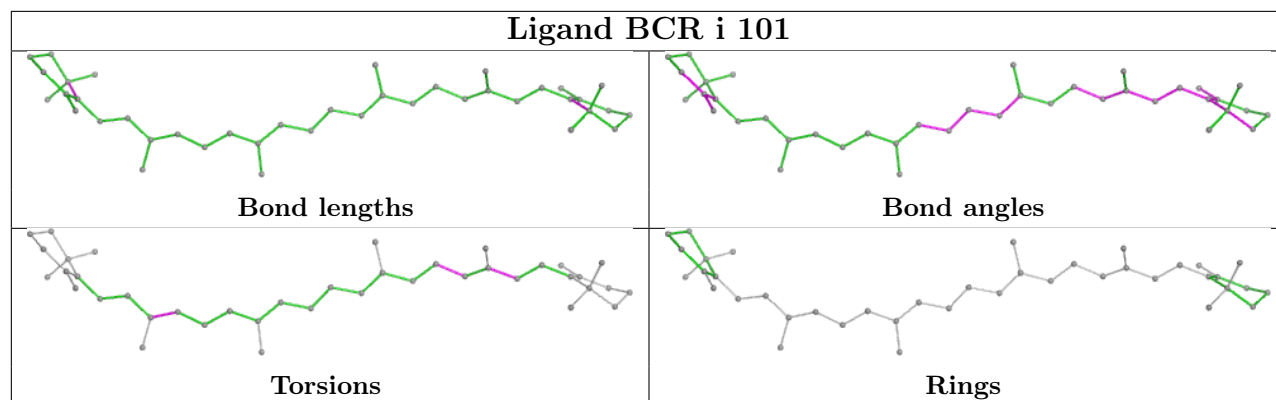


## Ligand CHL n 601



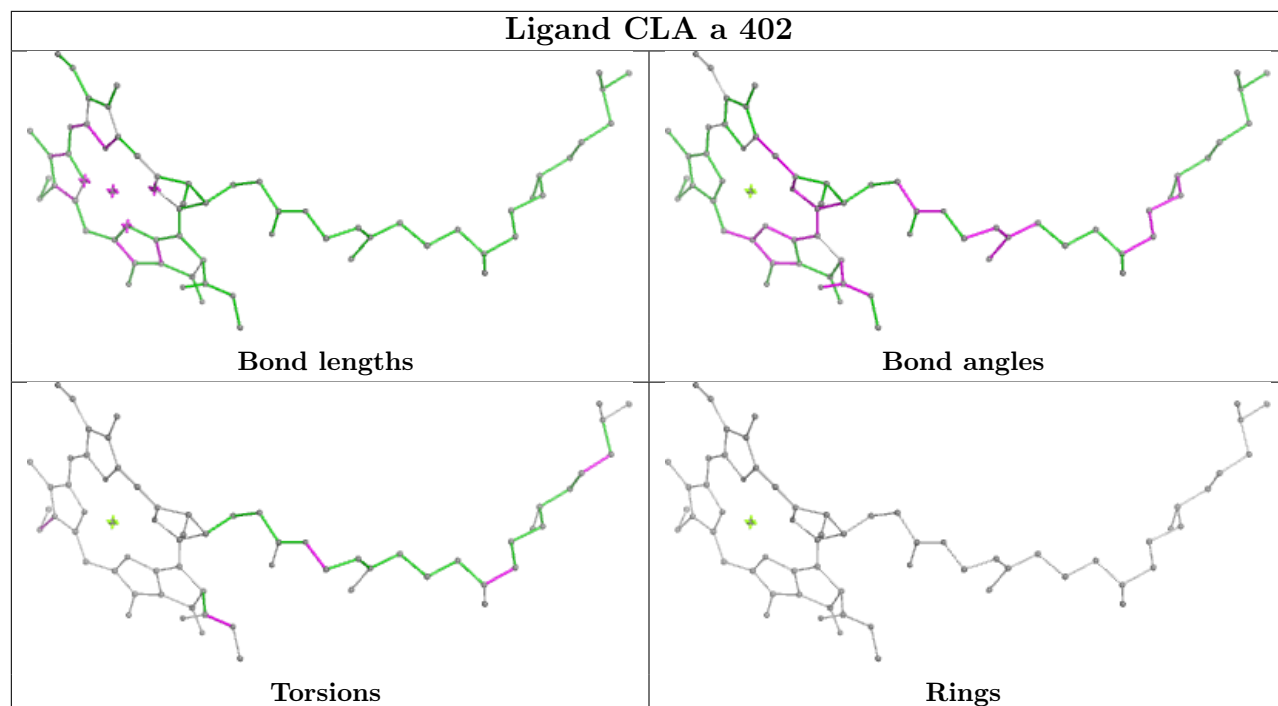
## Ligand CLA C 501



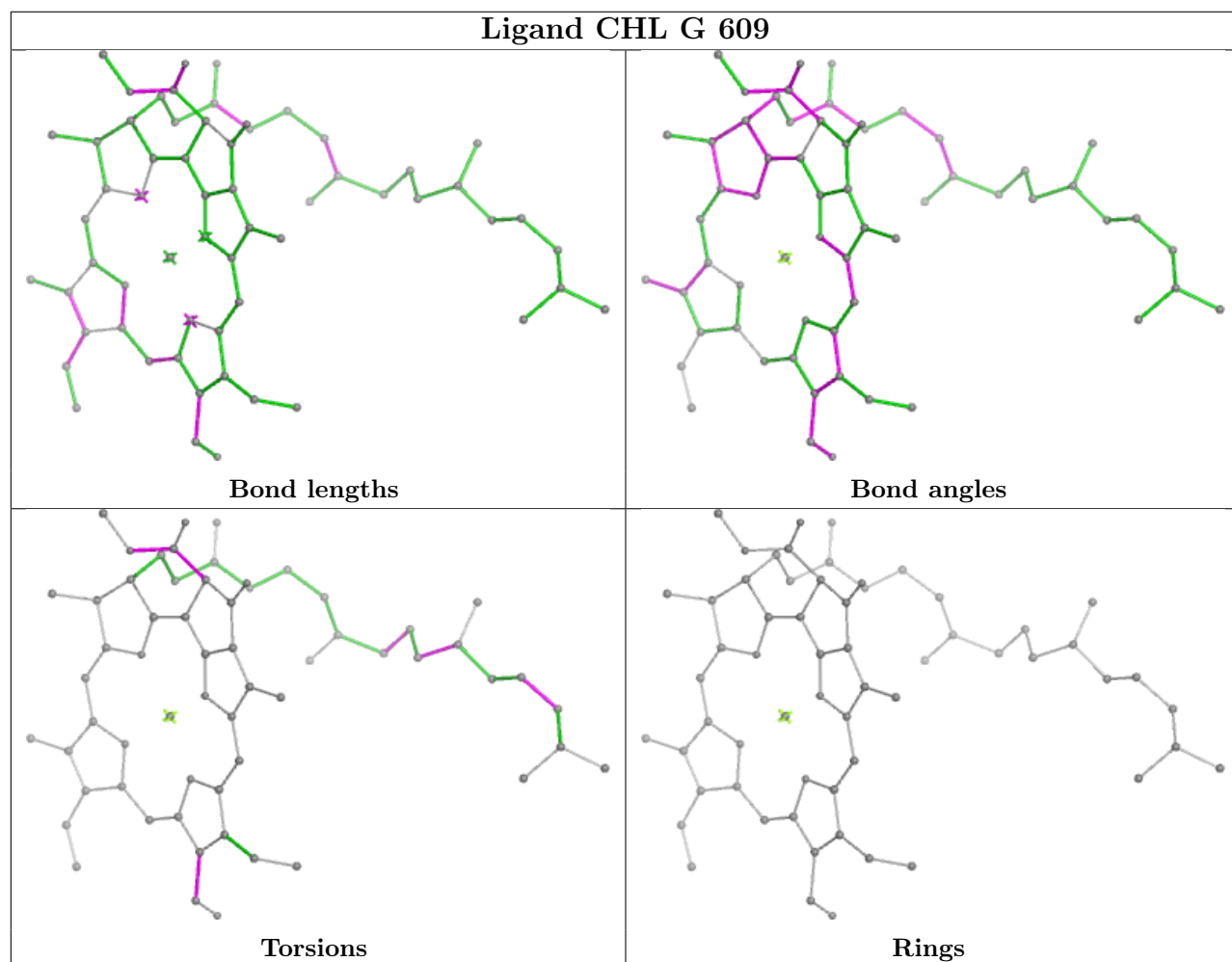




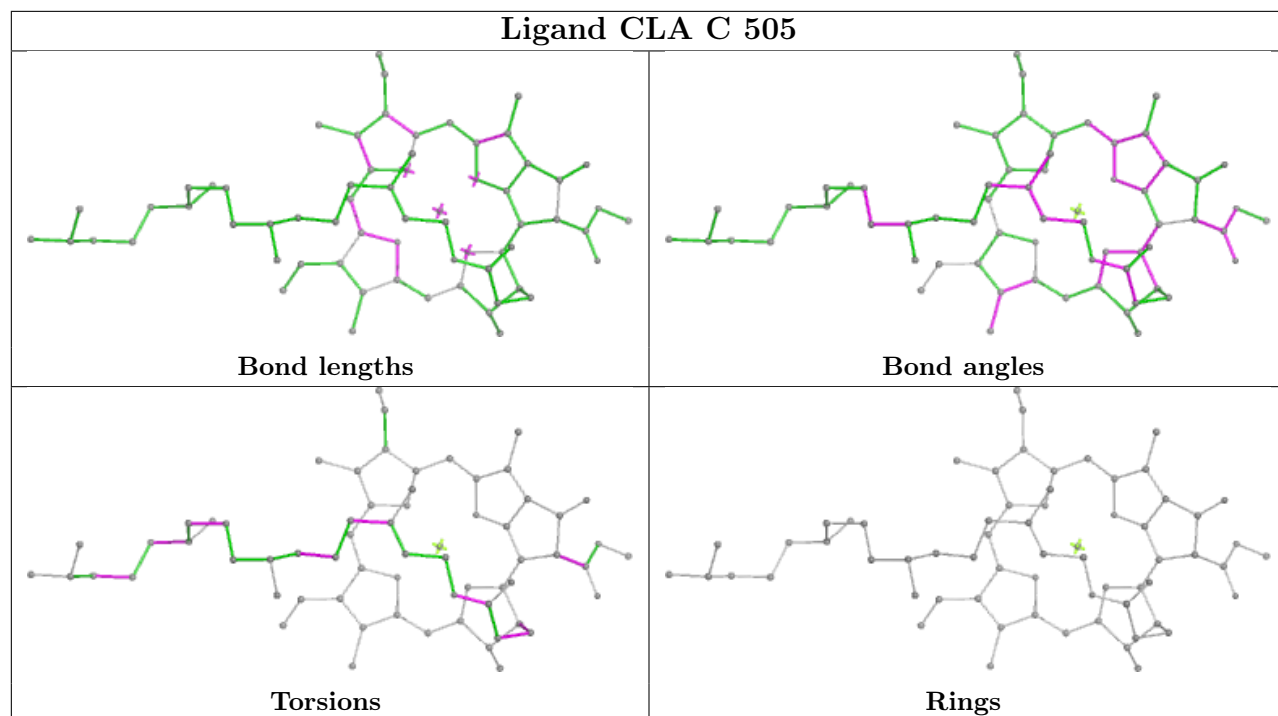
## Ligand CLA a 402



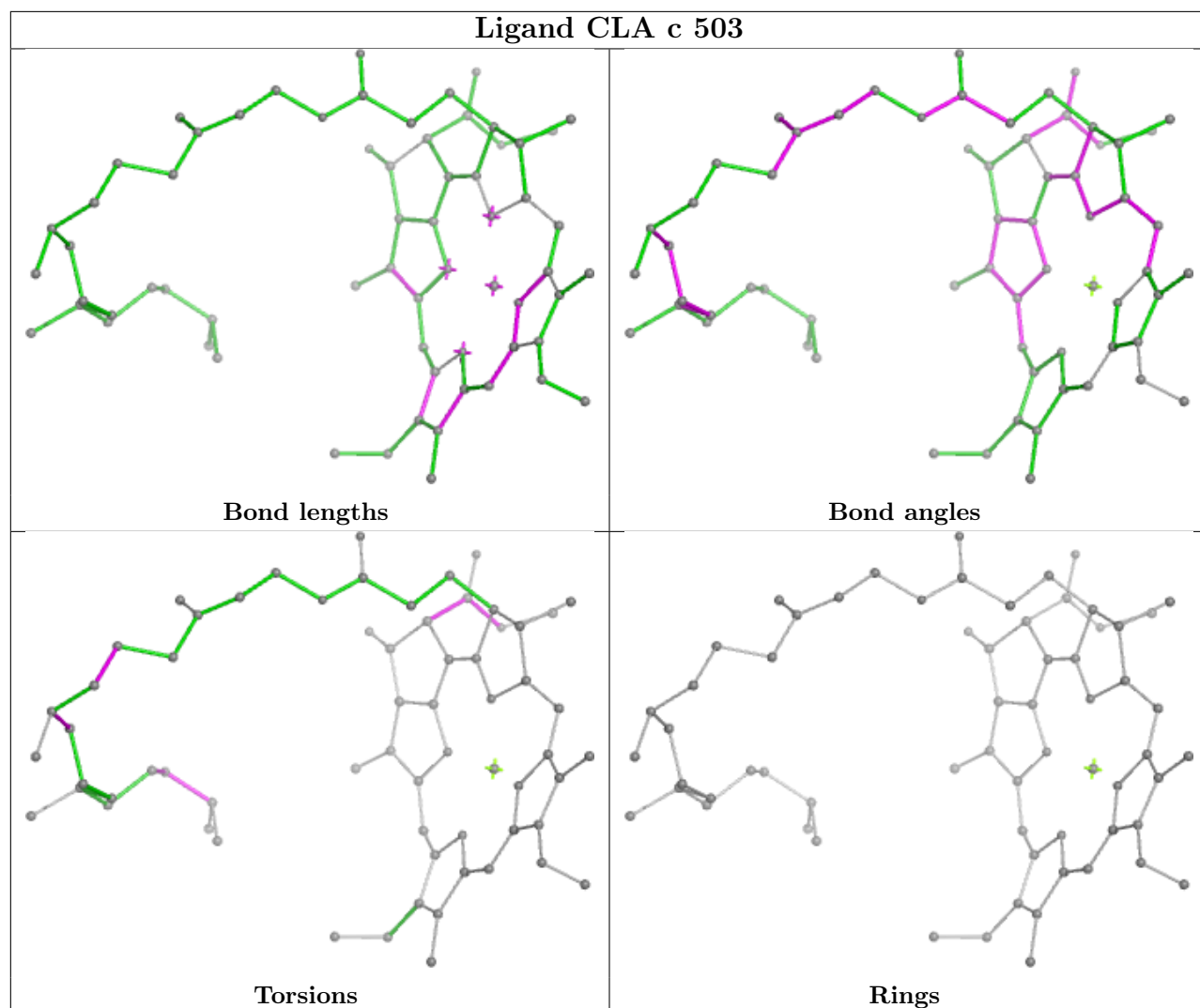
## Ligand CHL G 609



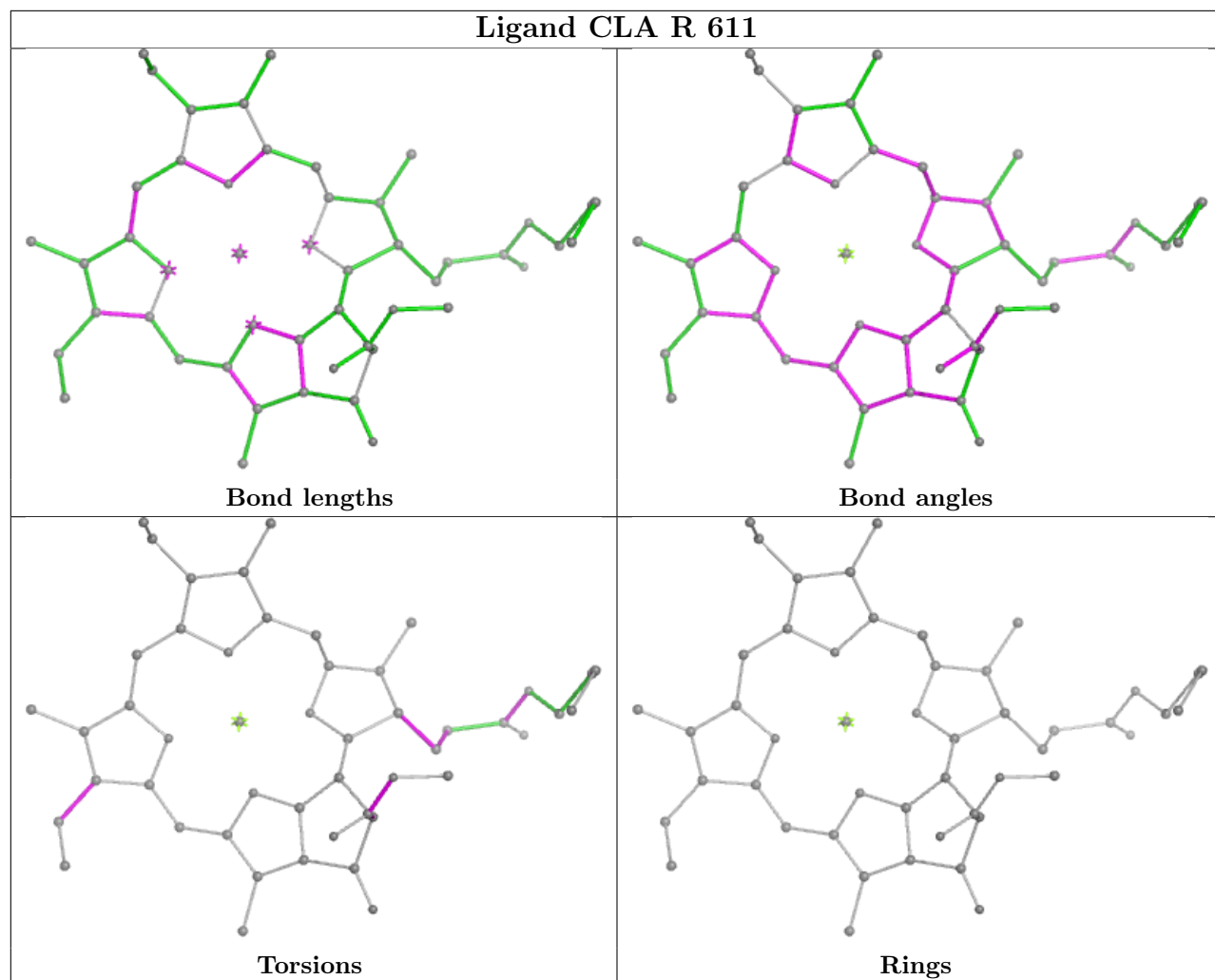
## Ligand CLA C 505



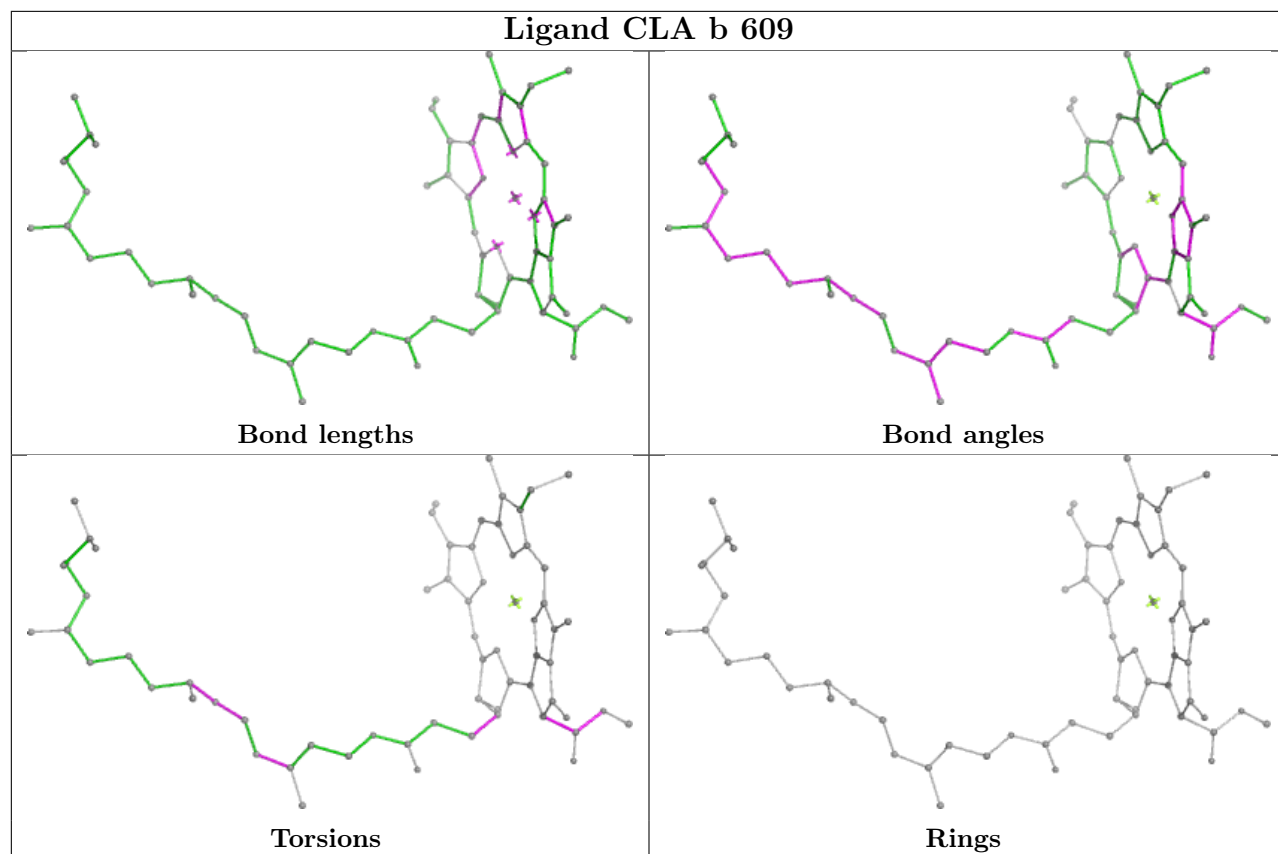
## Ligand CLA c 503



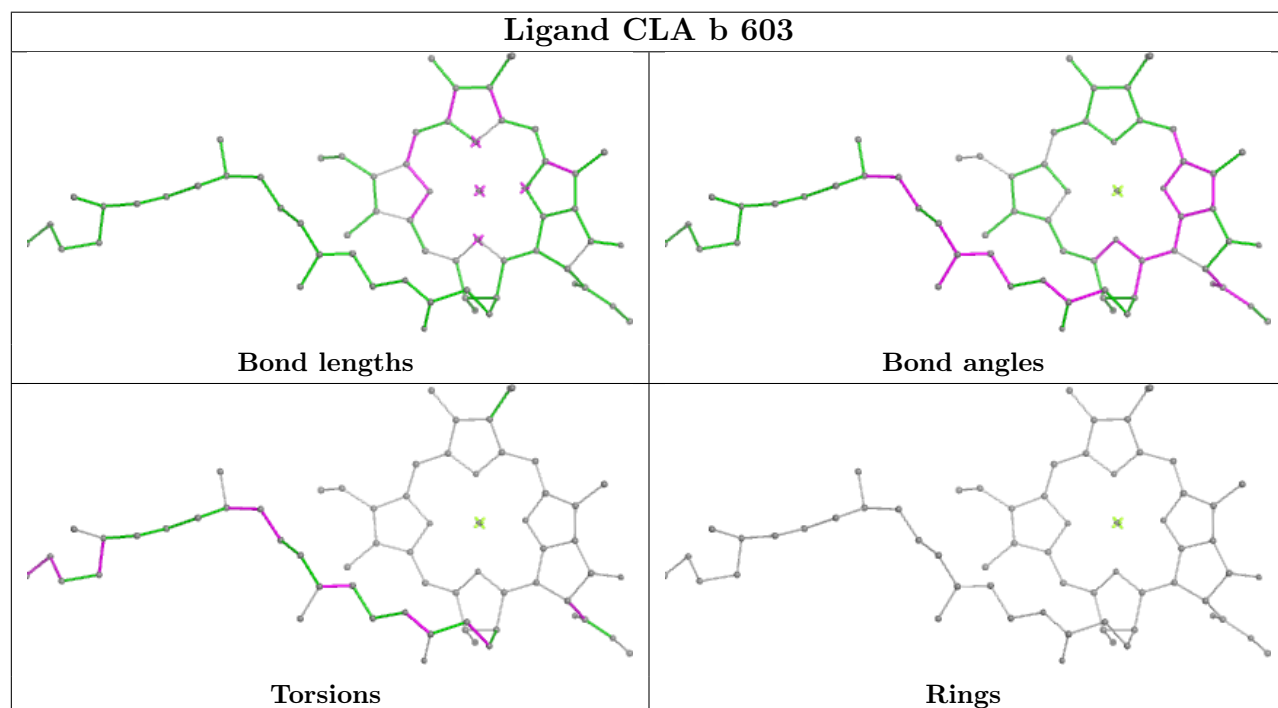
## Ligand CLA R 611

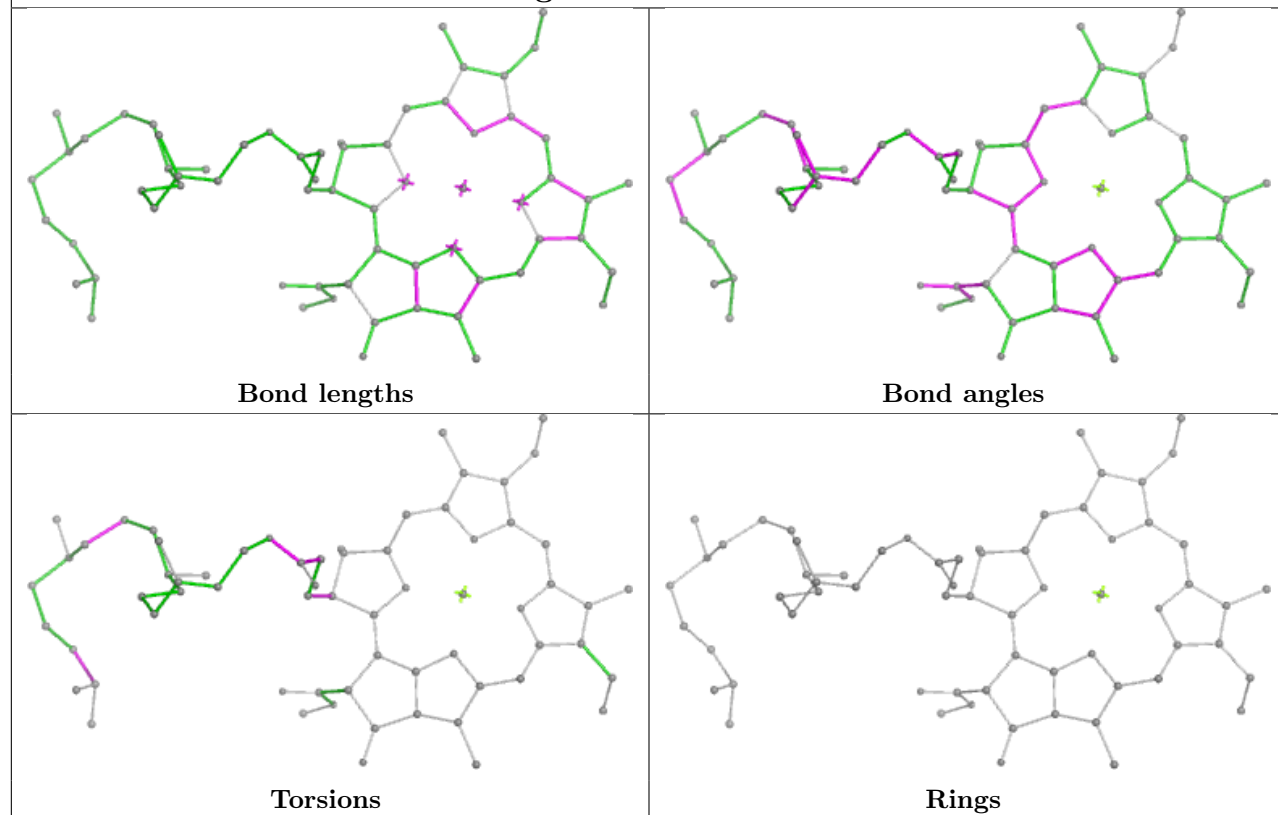
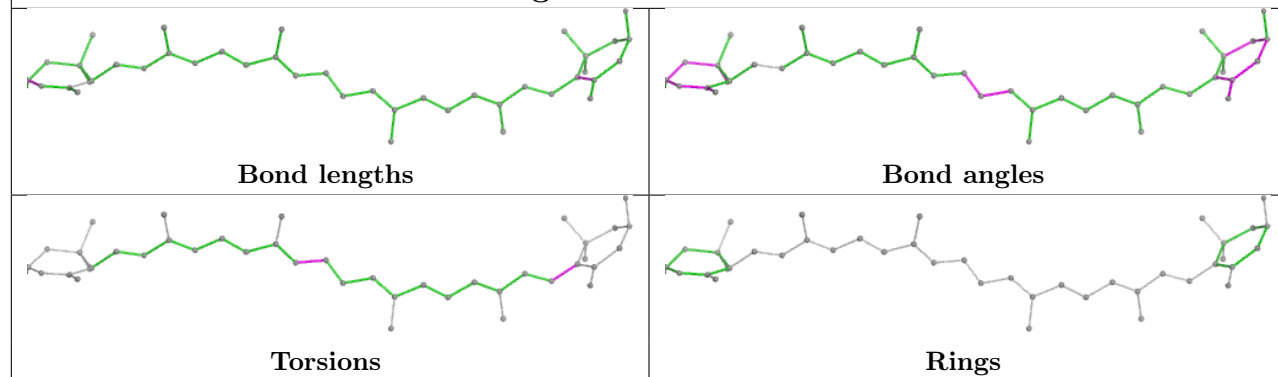


## Ligand CLA b 609

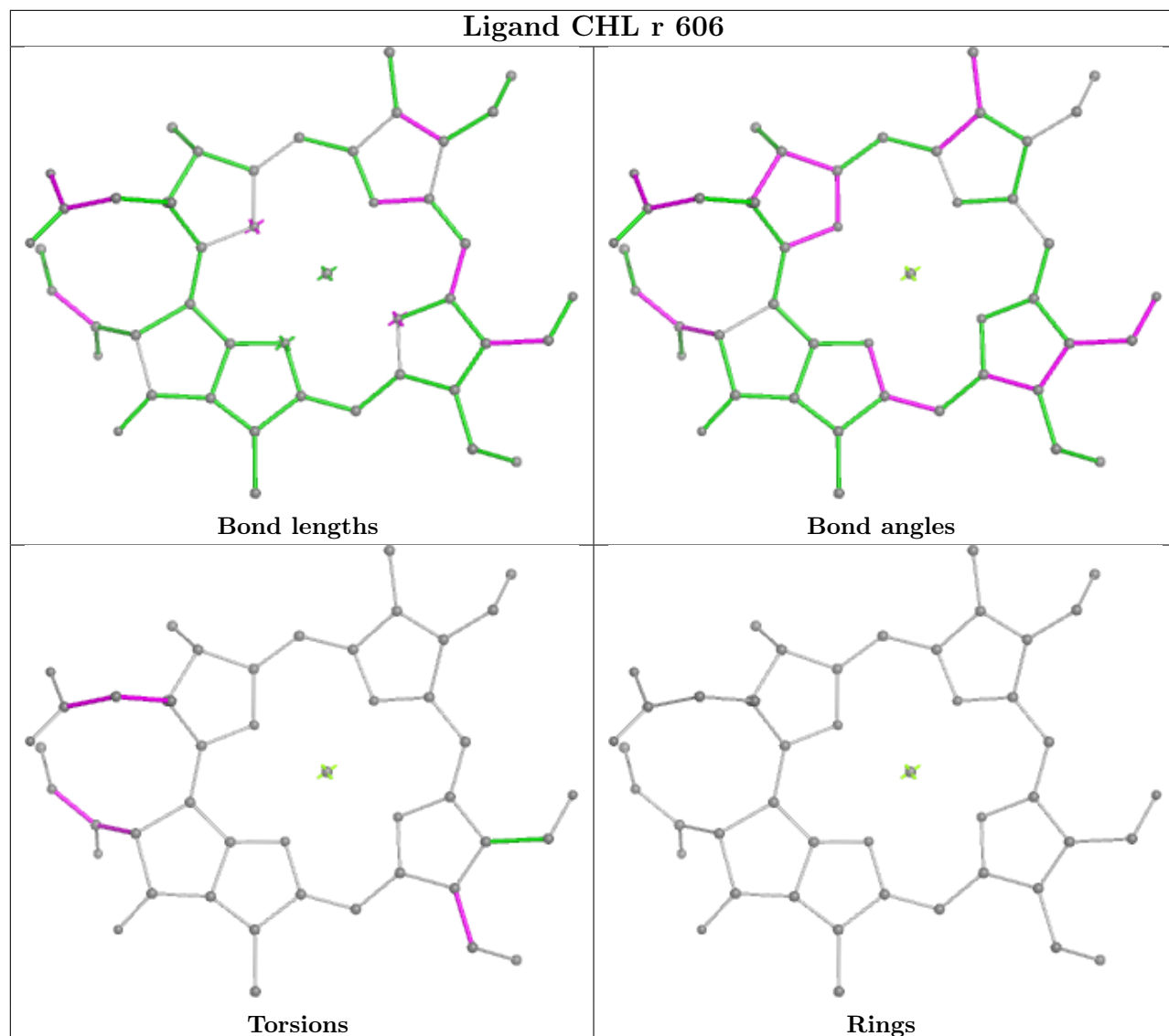


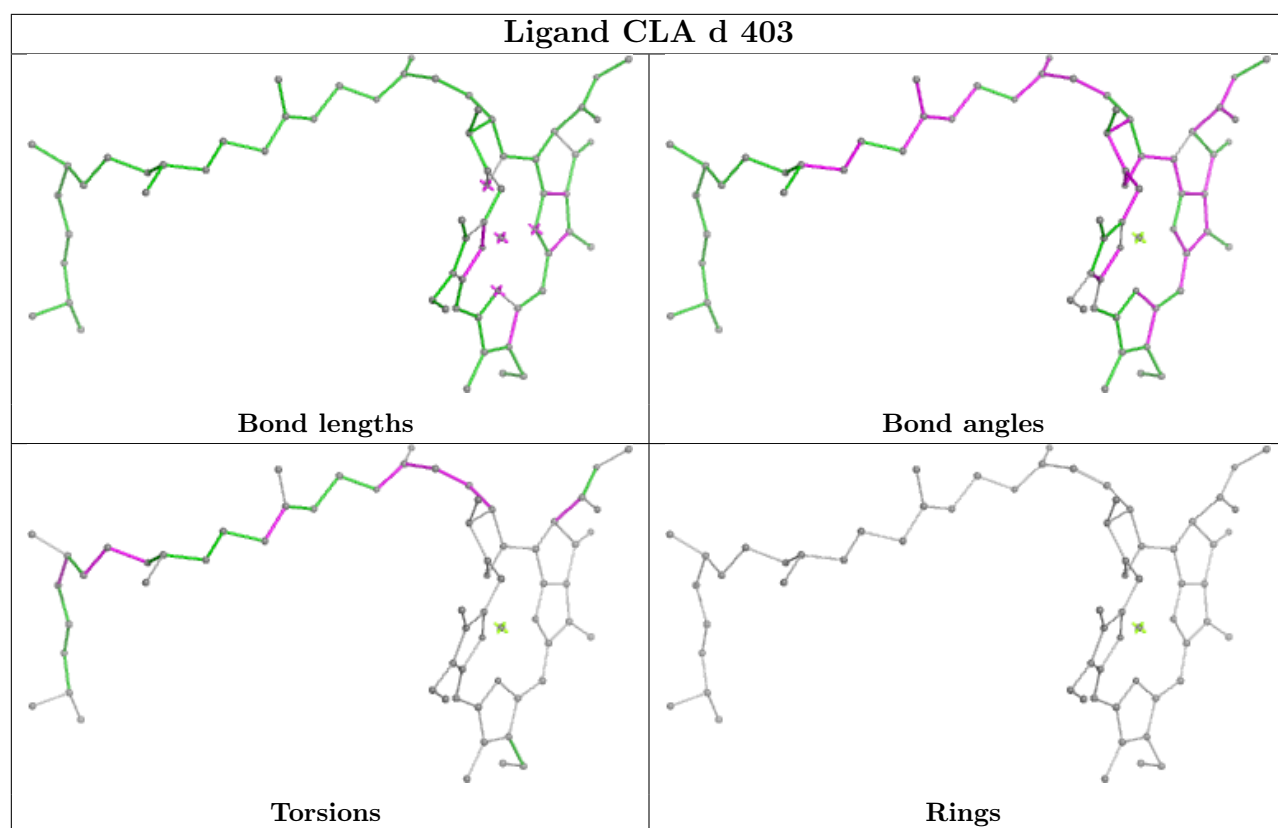
## Ligand CLA b 603

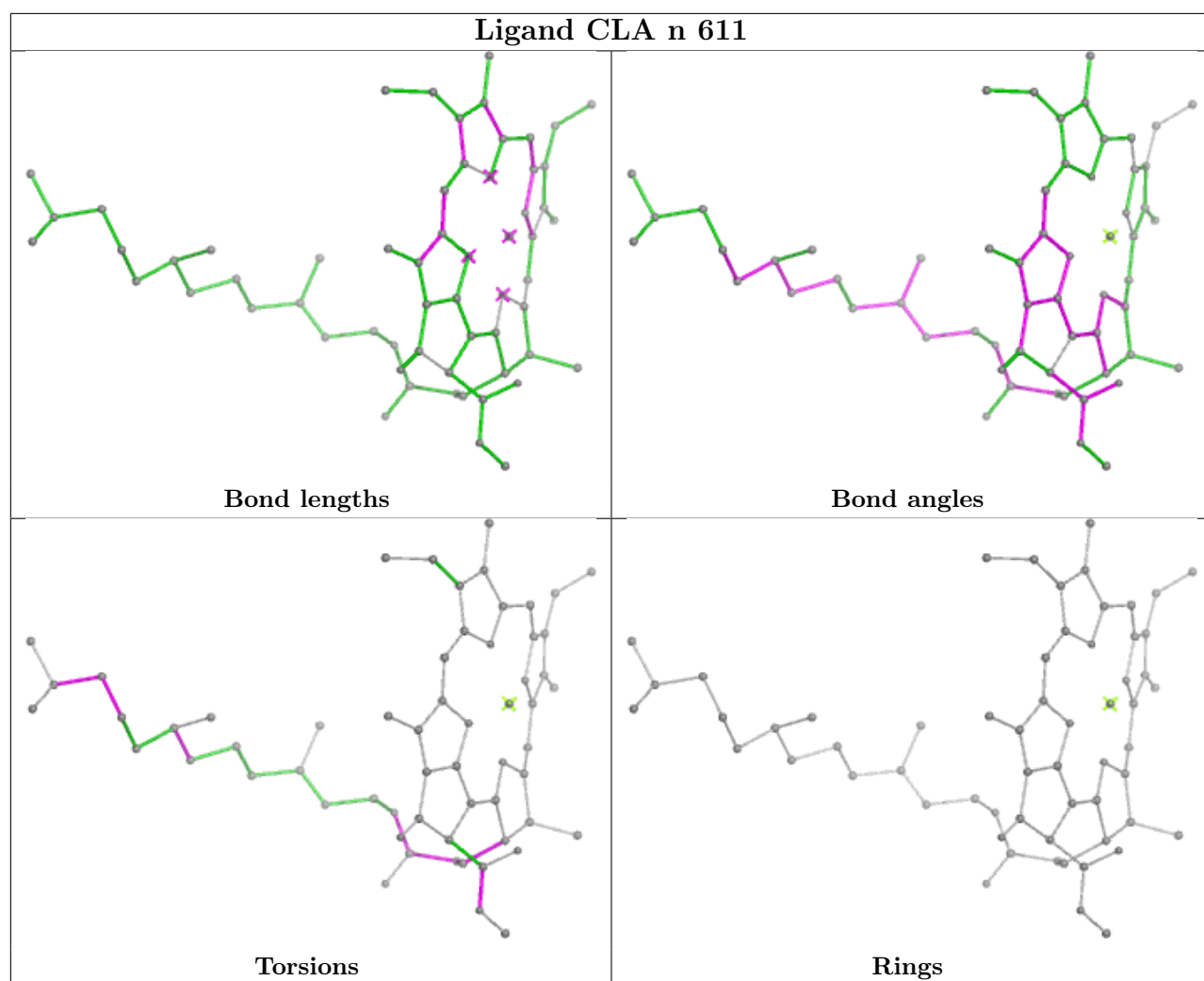


**Ligand CLA b 612****Ligand LUT Y 316**

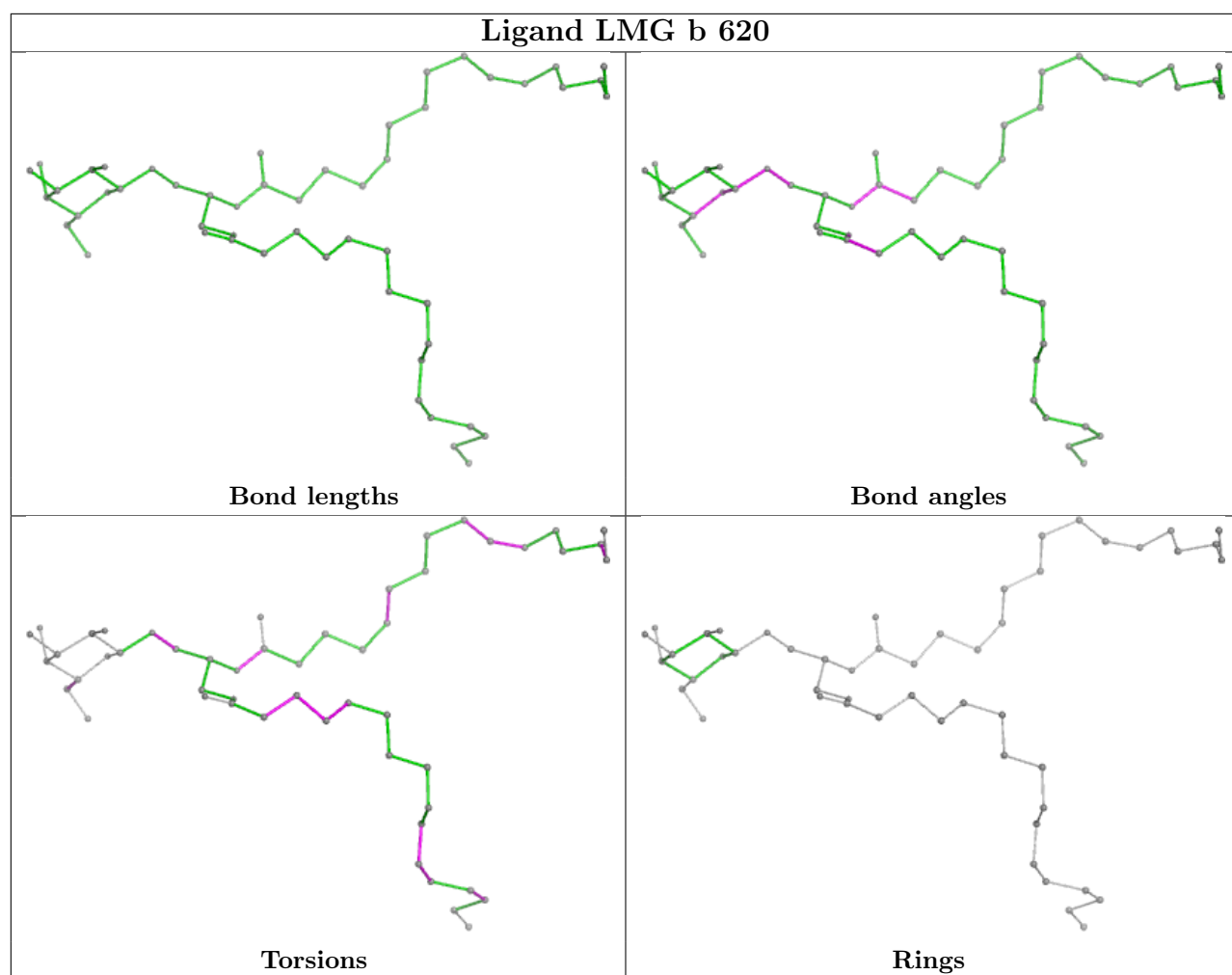
## Ligand CHL r 606



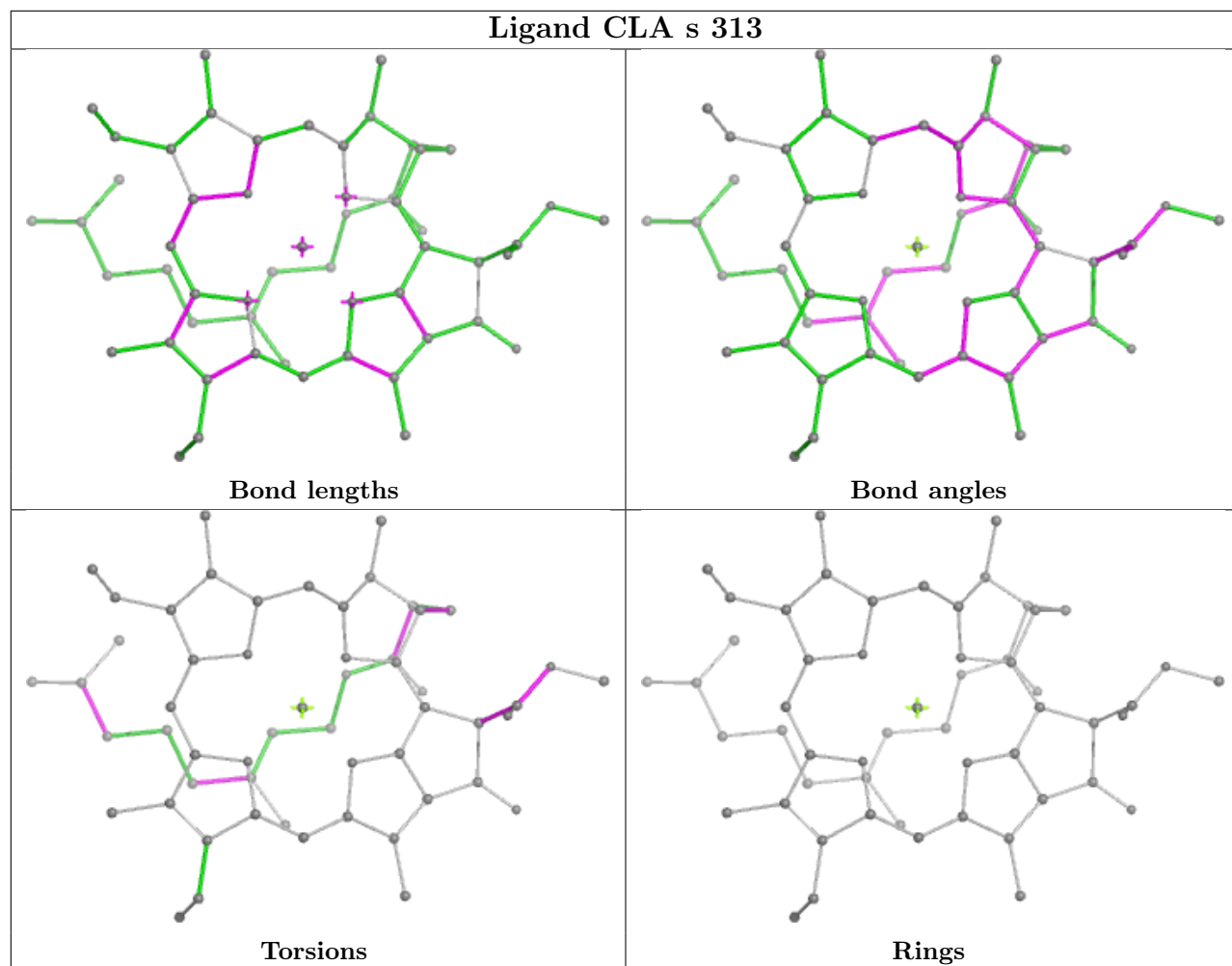


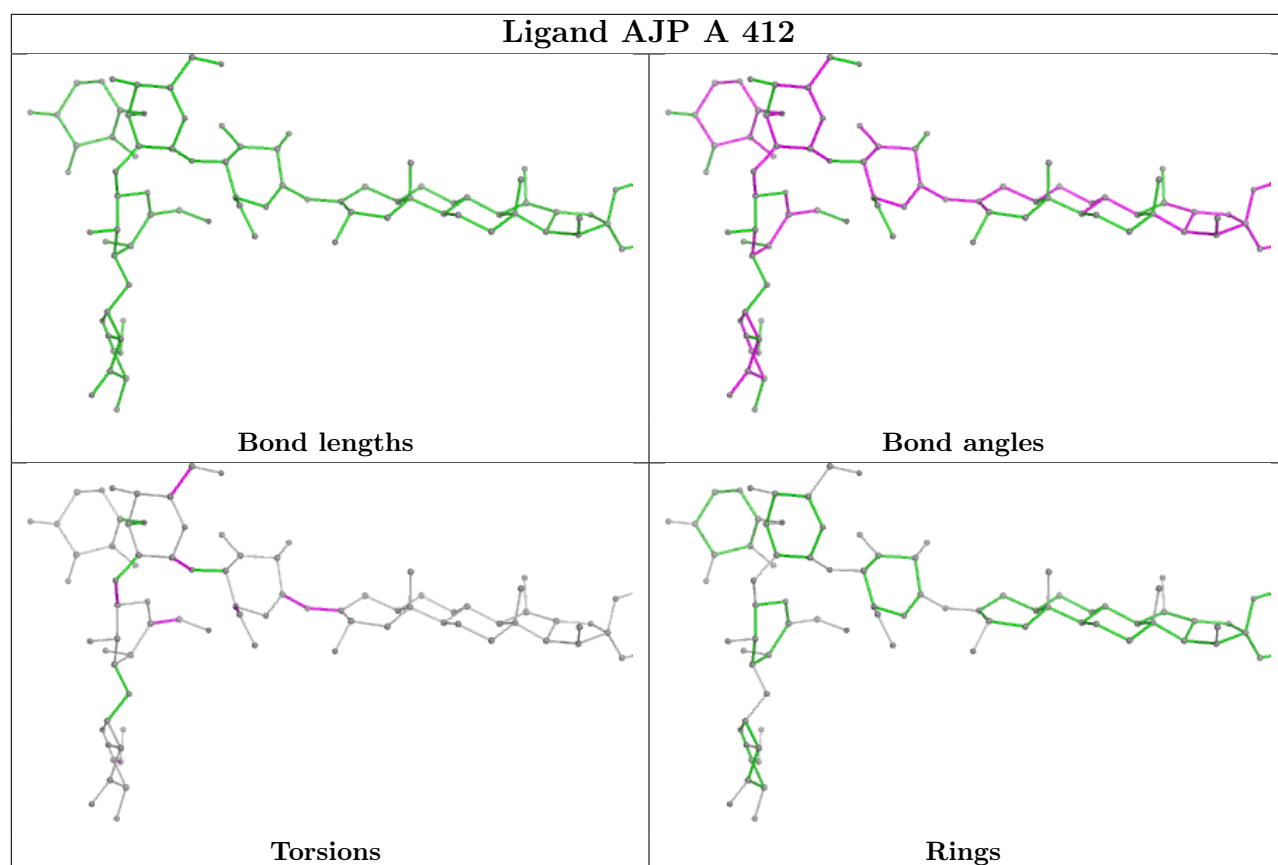


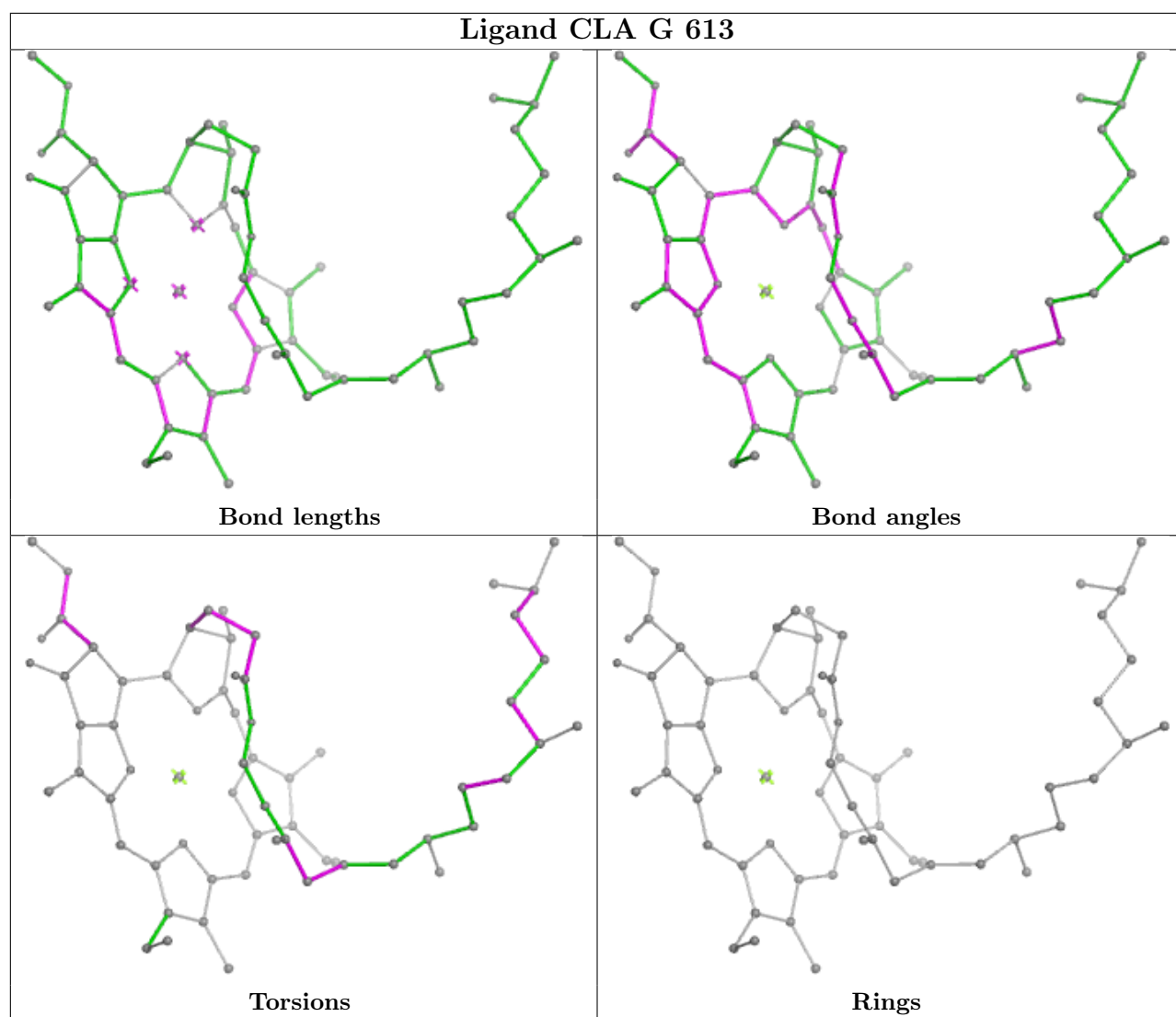


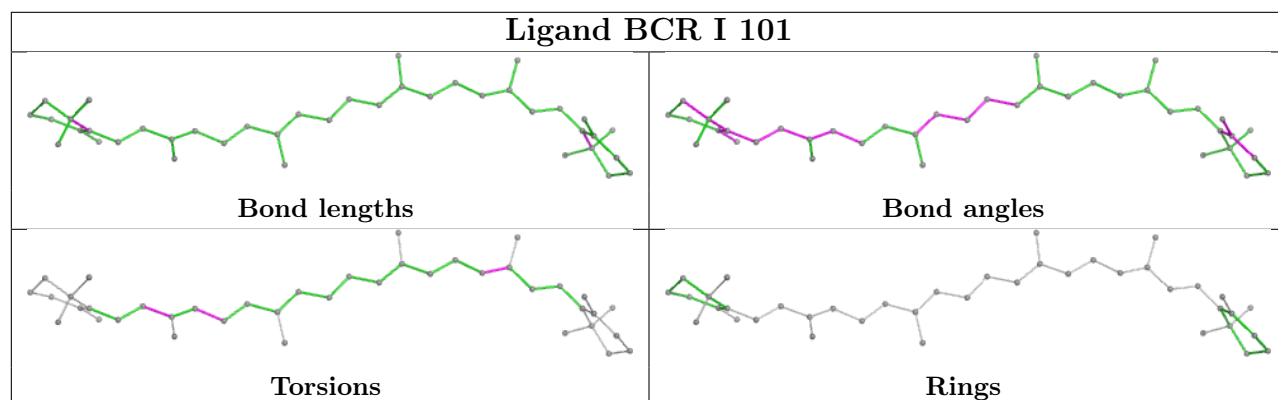
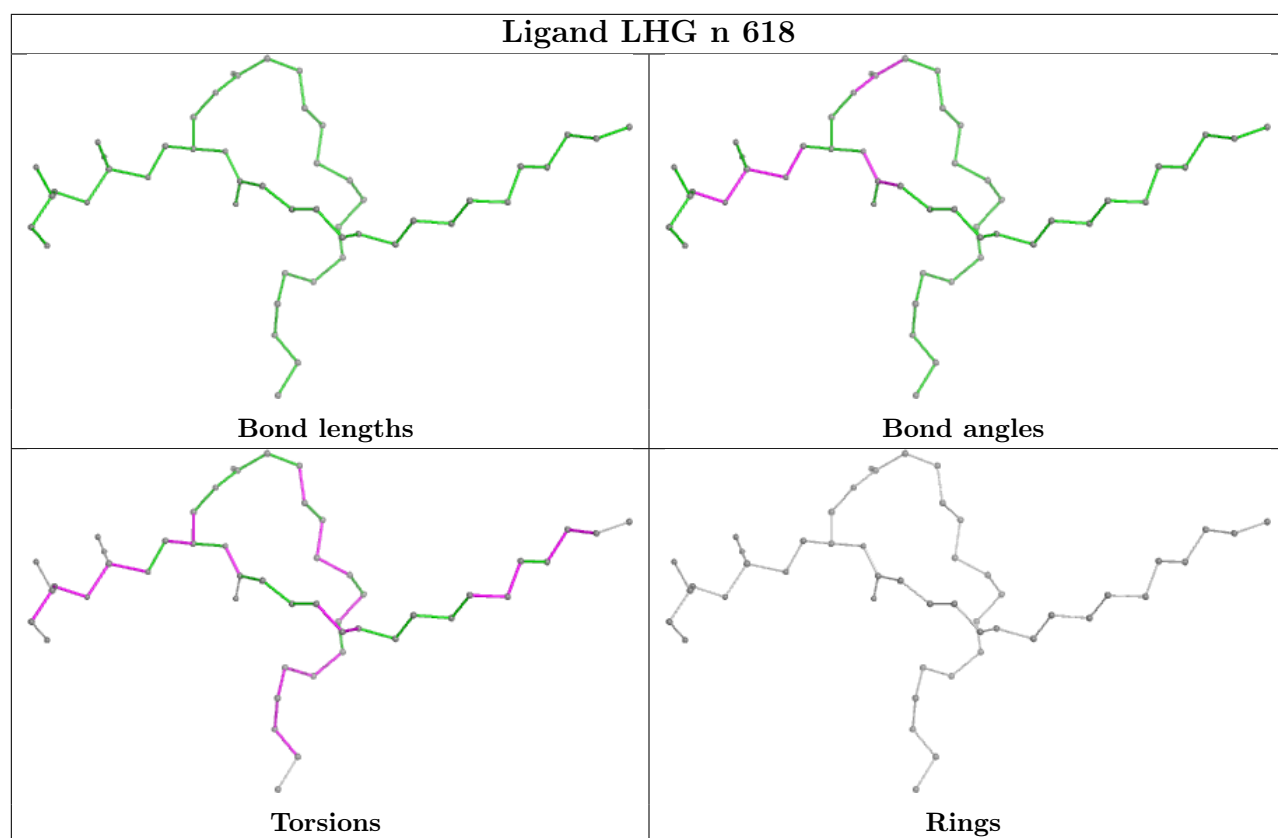


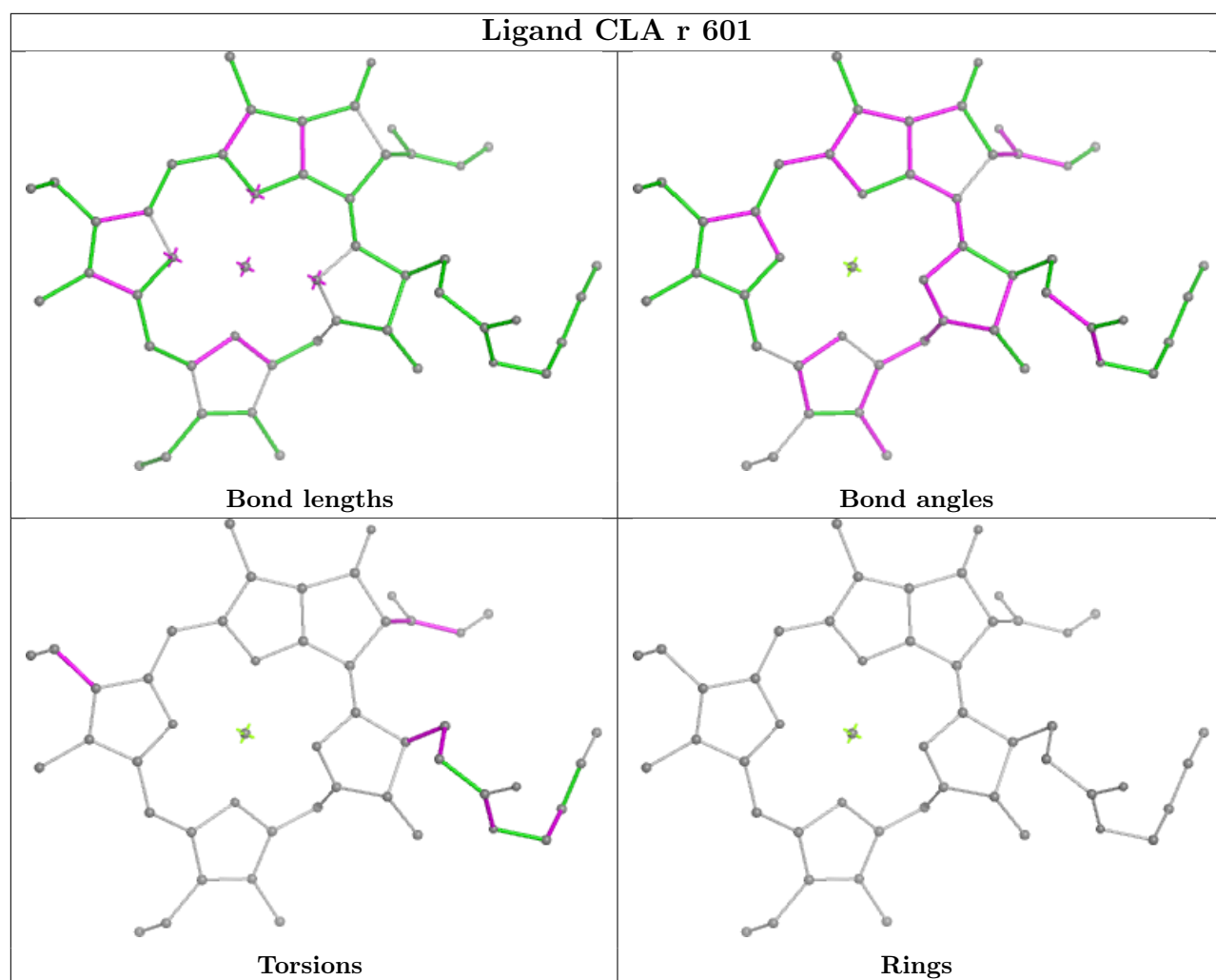
## Ligand CLA s 313



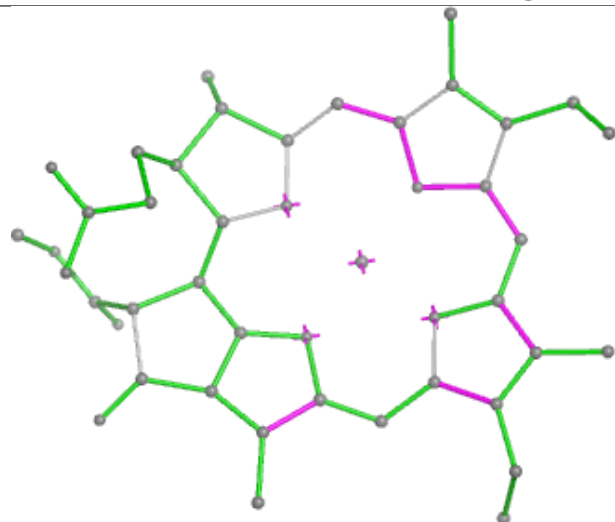




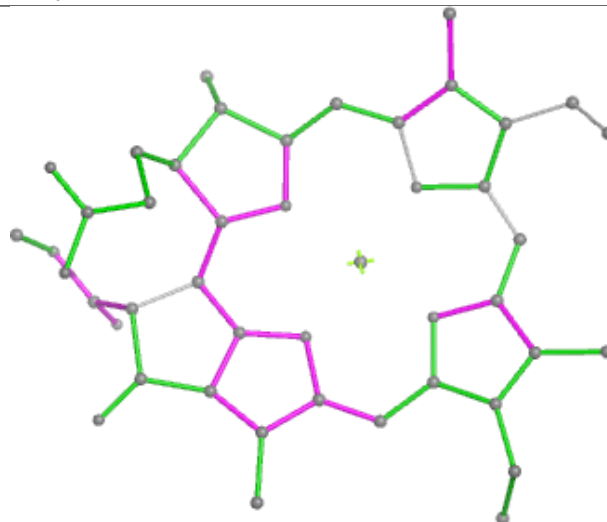




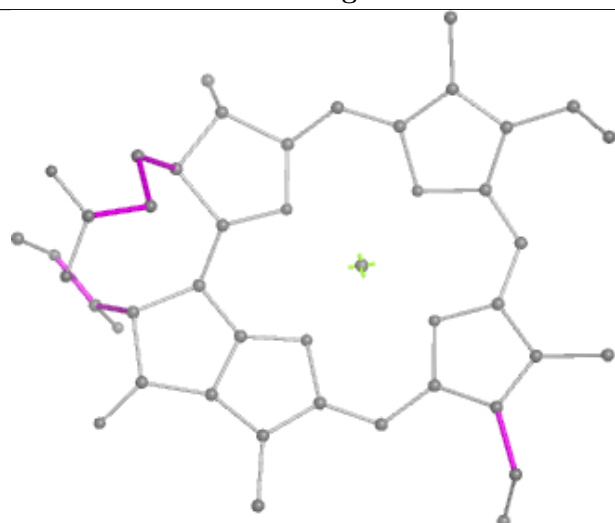
## Ligand CLA y 315



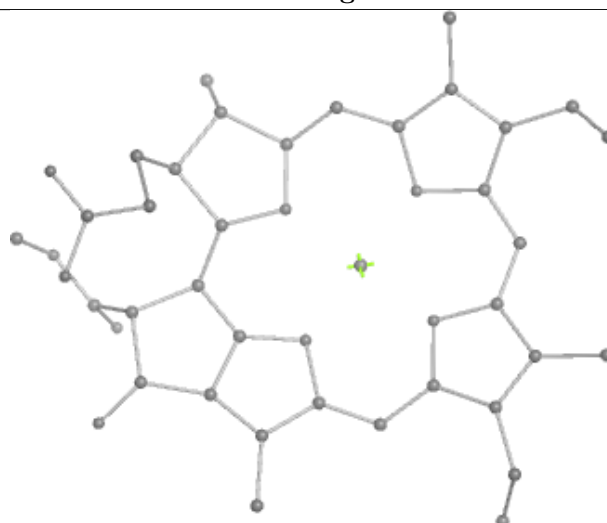
Bond lengths



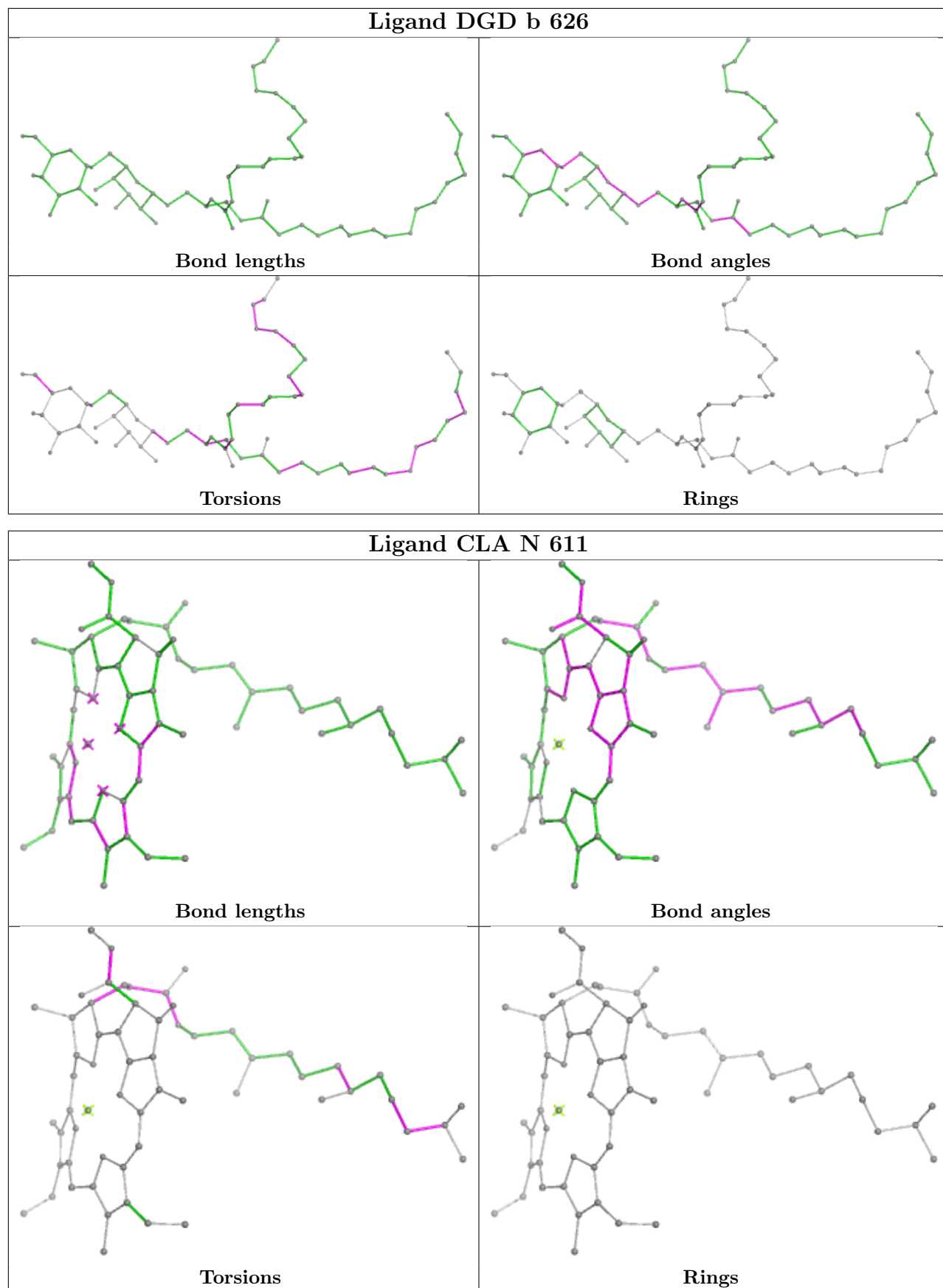
Bond angles



Torsions

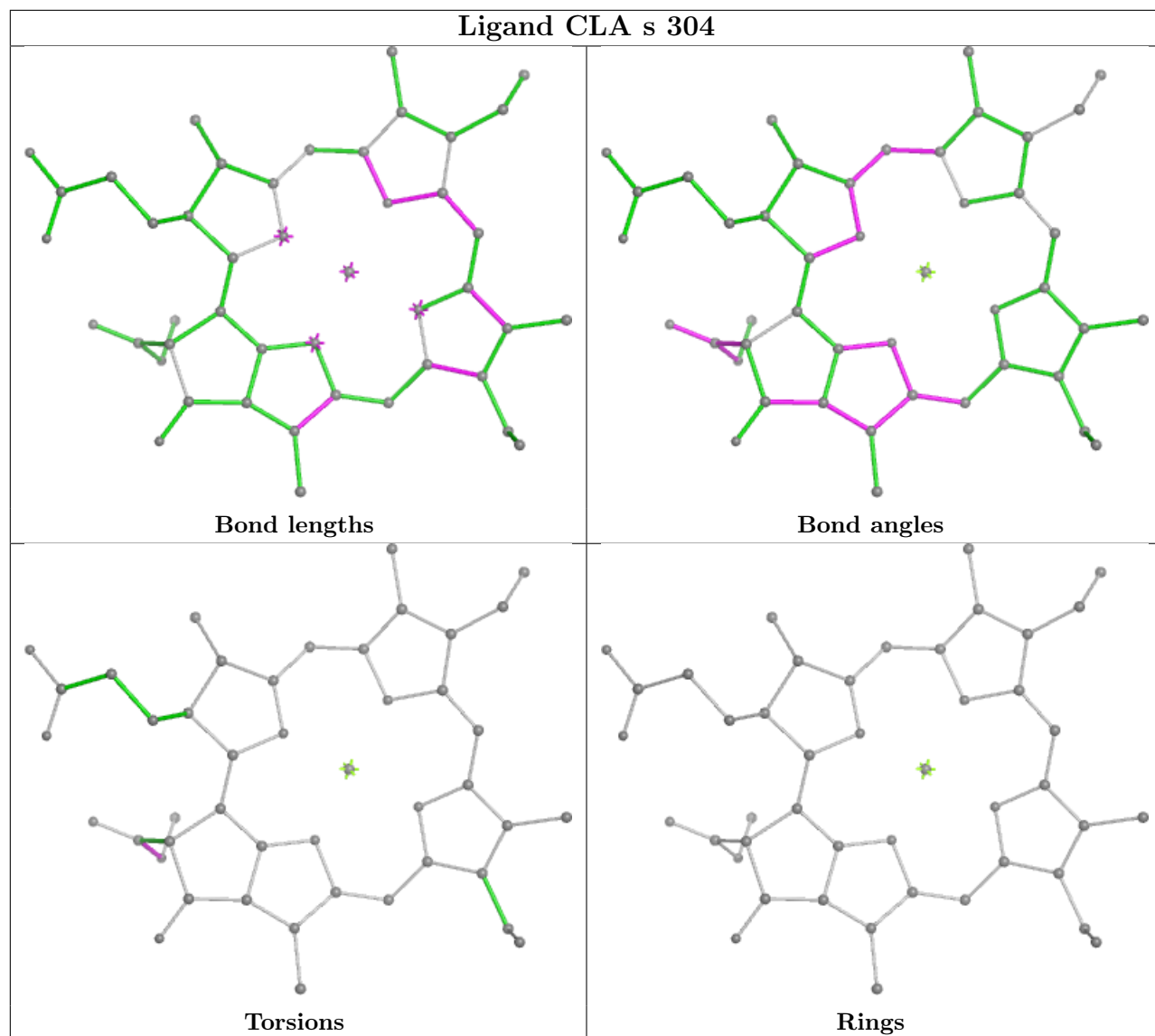


Rings

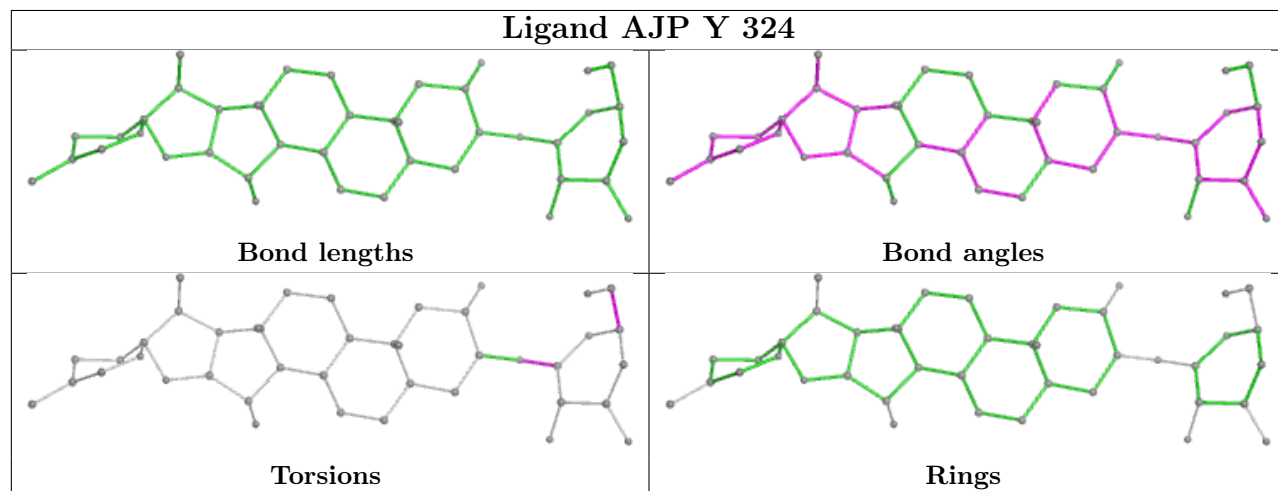


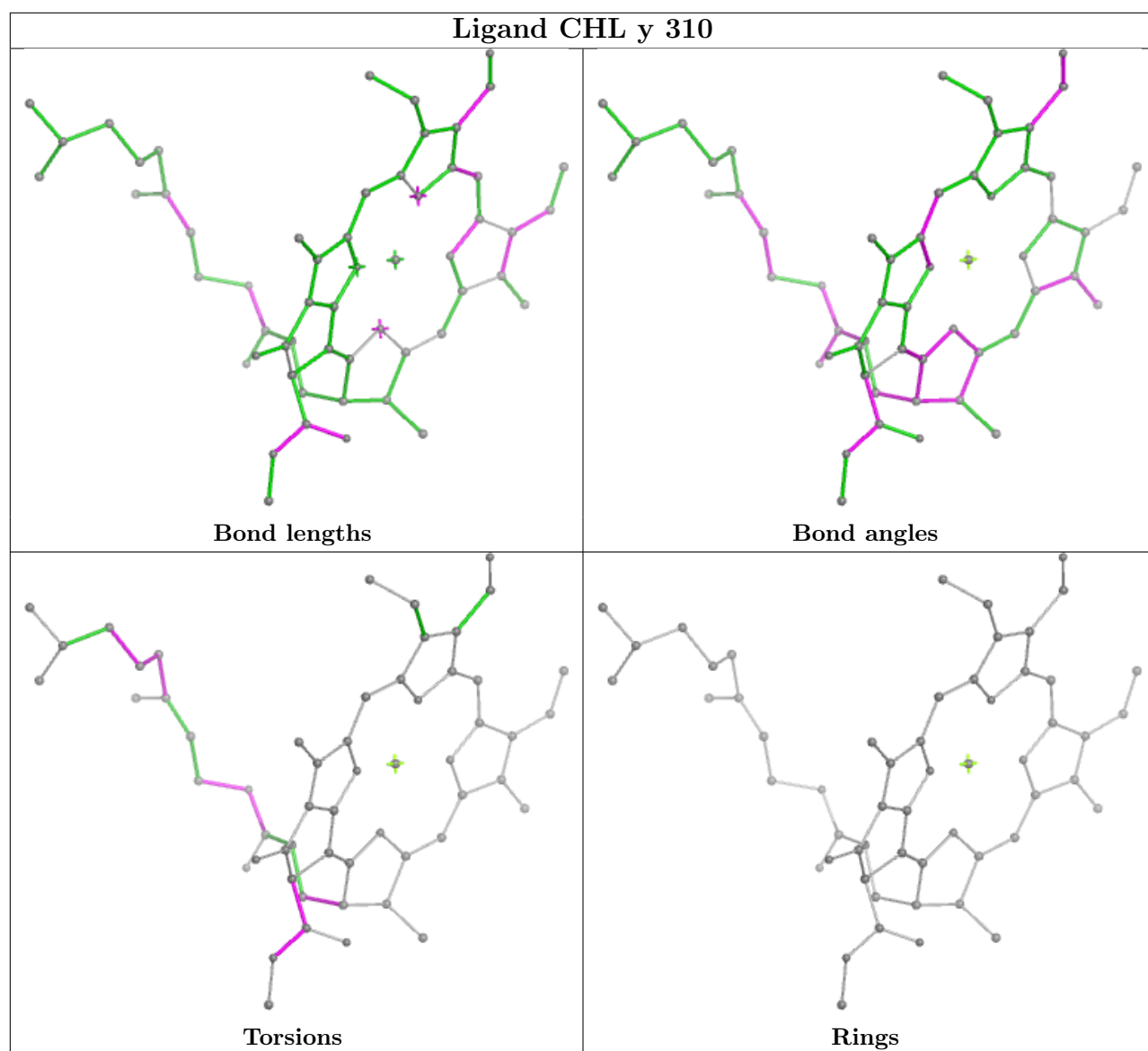


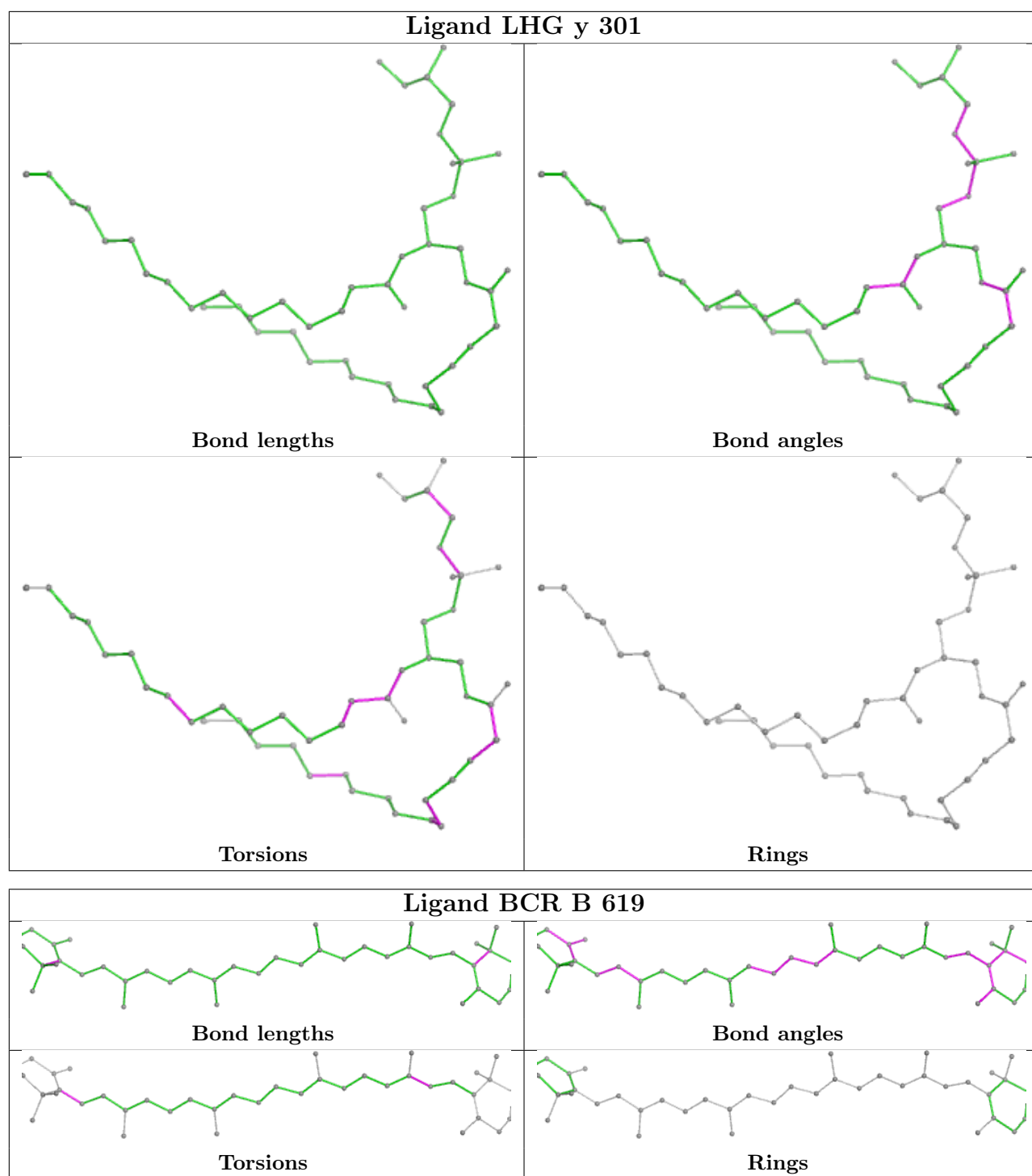
## Ligand CLA s 304

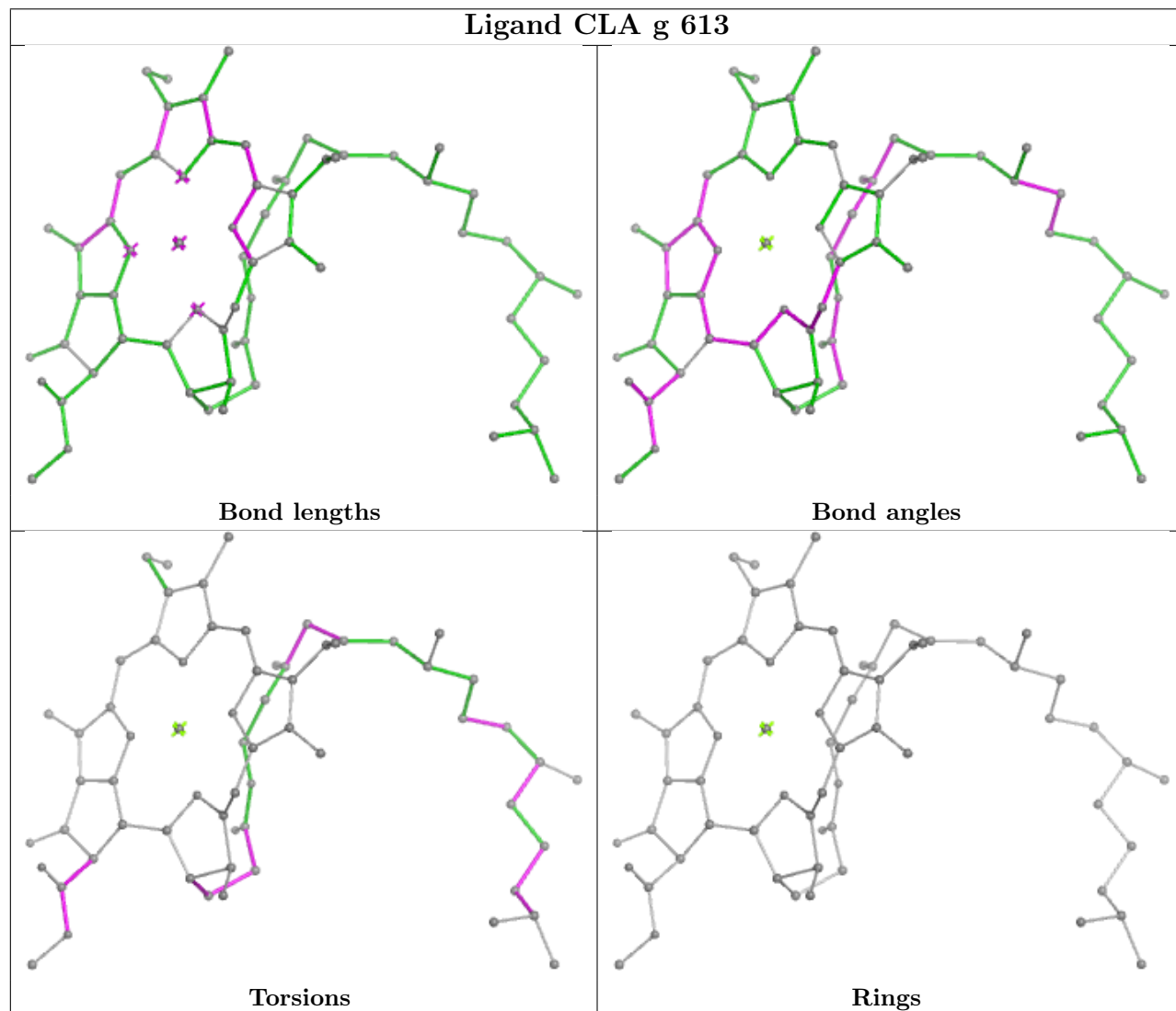
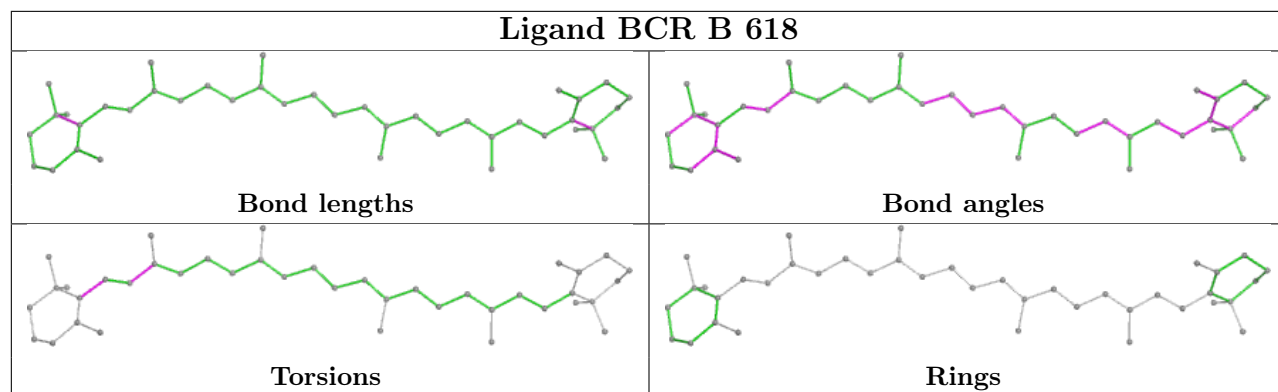


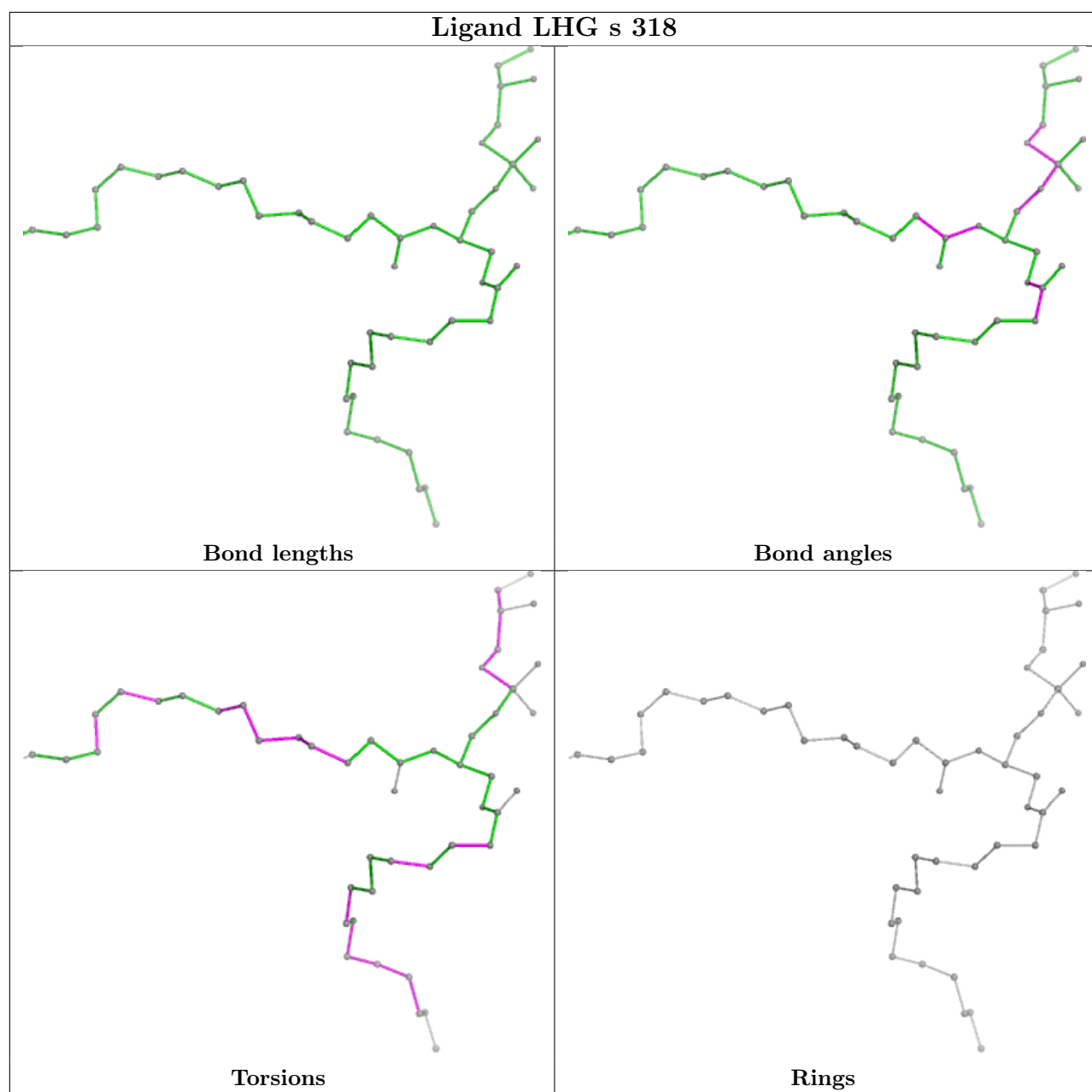
## Ligand AJP Y 324



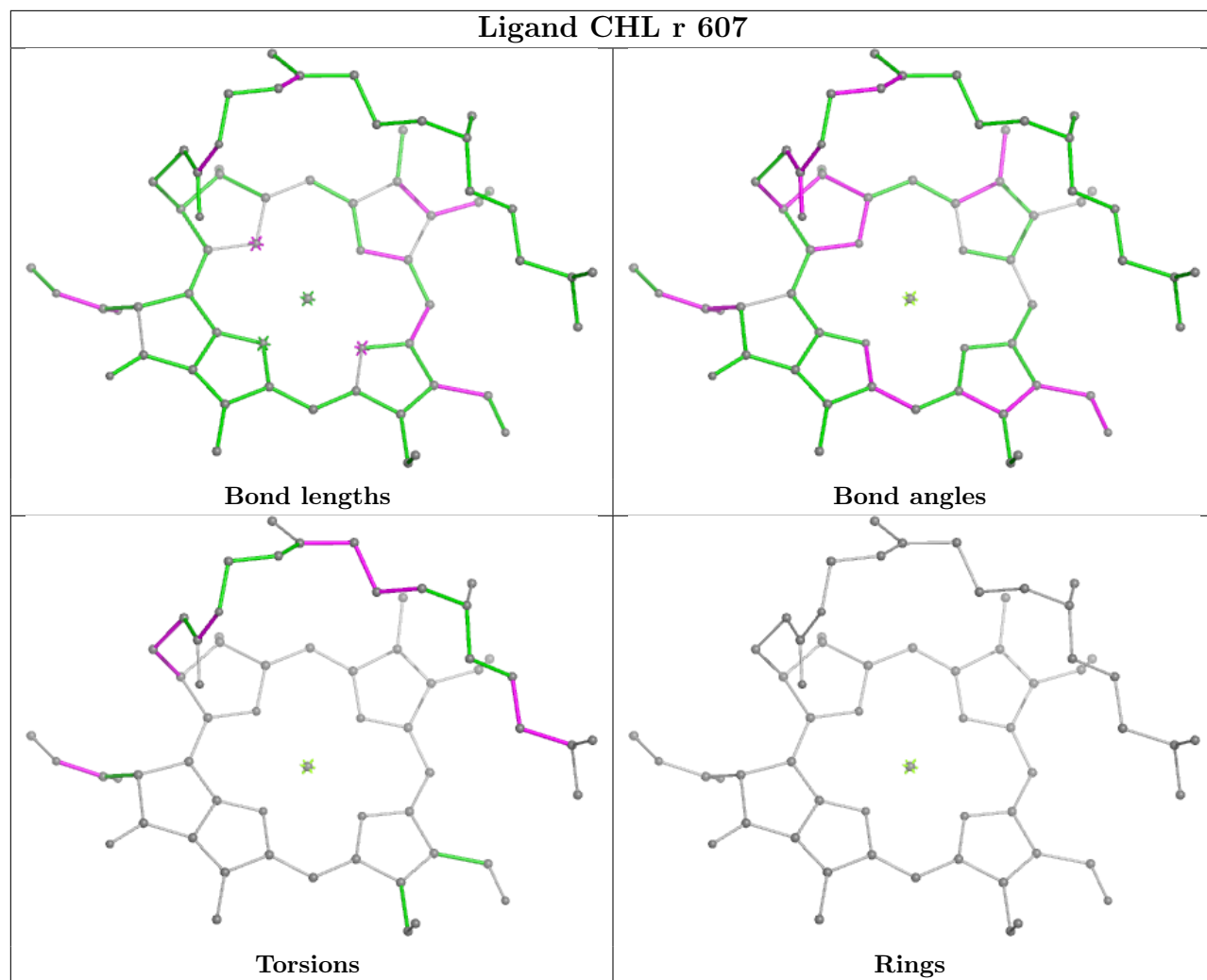




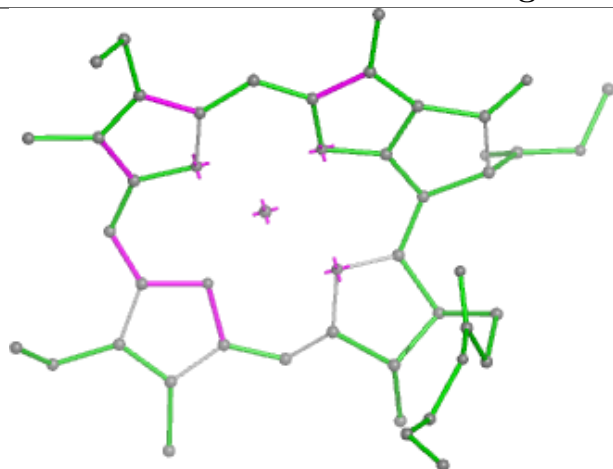




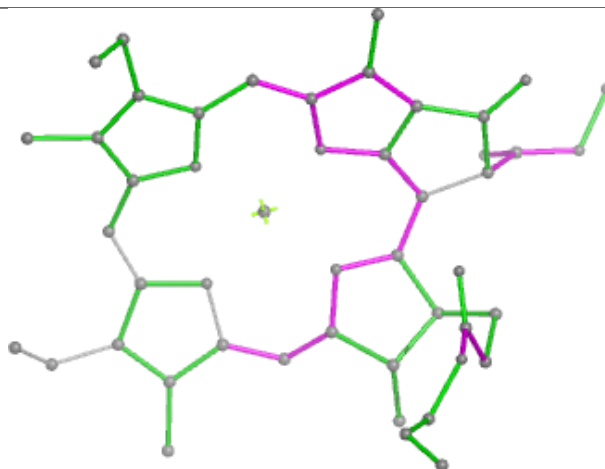
## Ligand CHL r 607



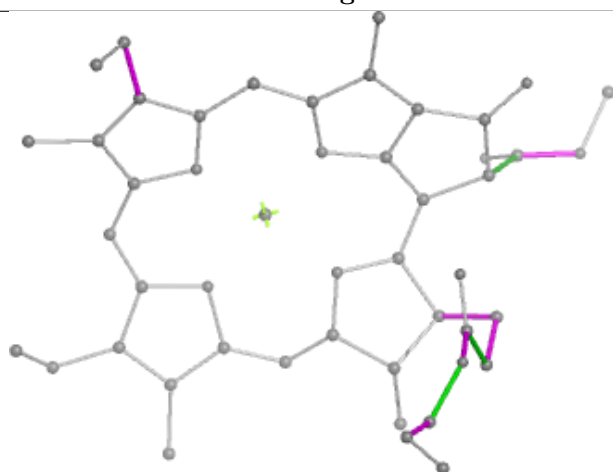
## Ligand CLA 6 605



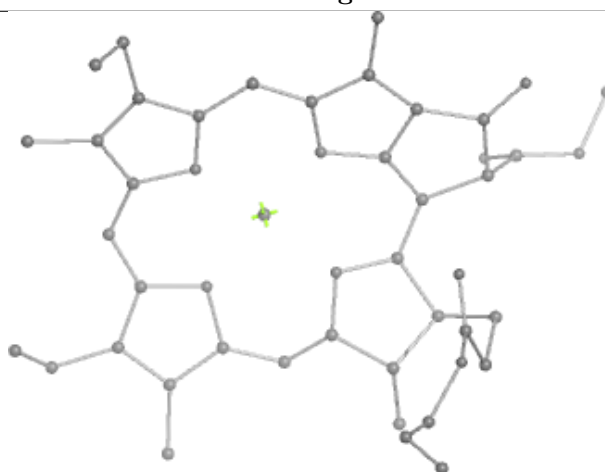
Bond lengths



Bond angles

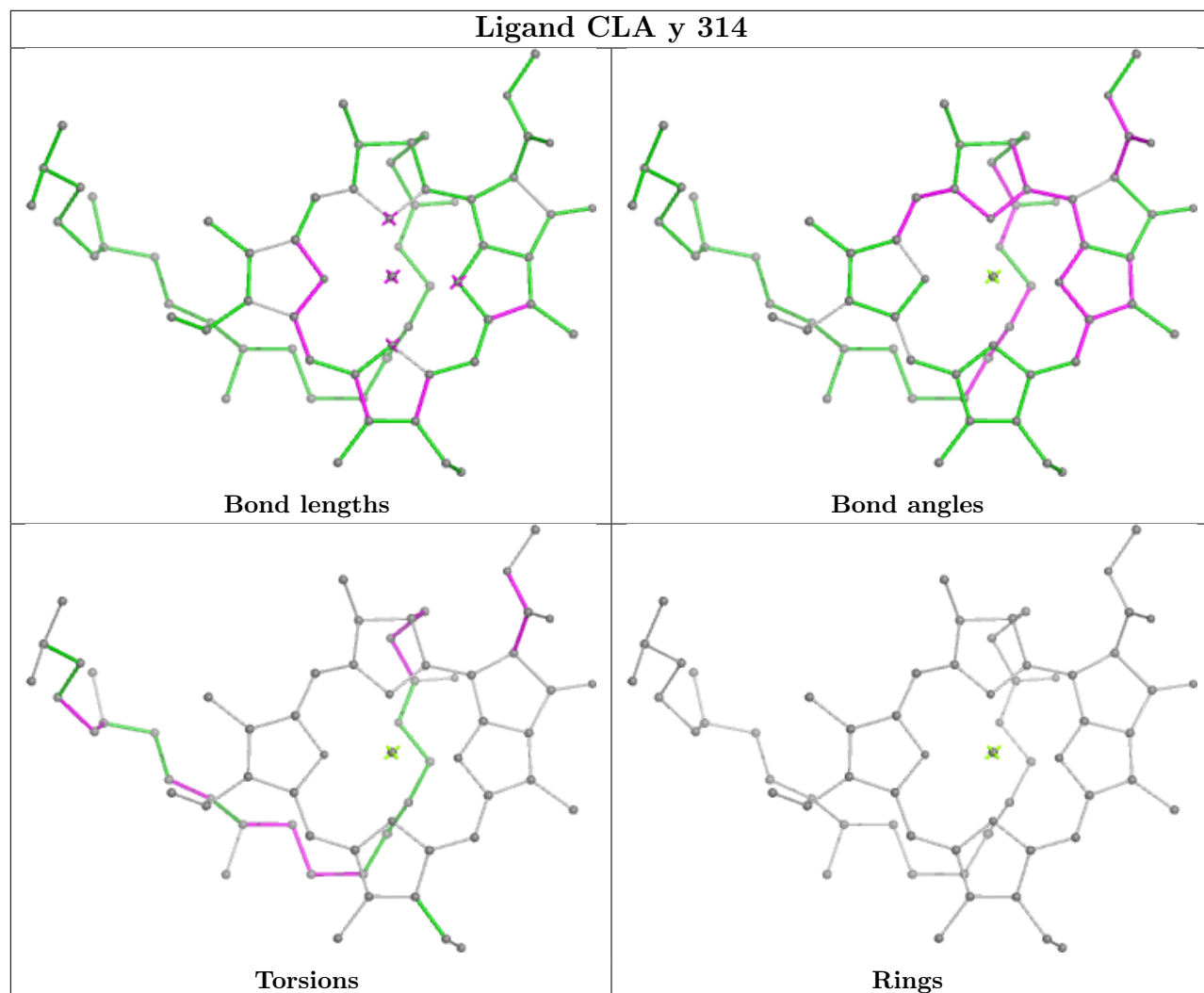


Torsions



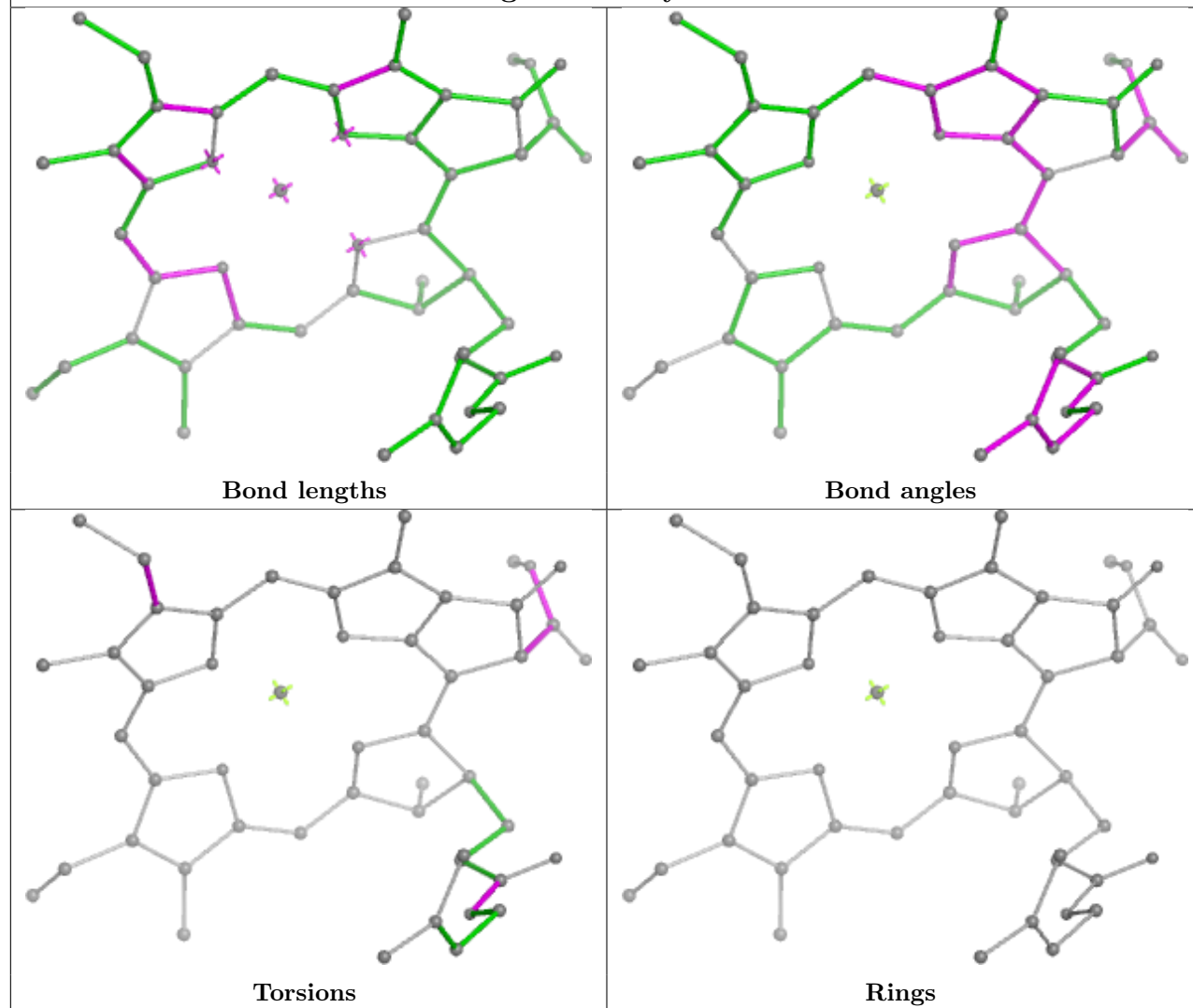
Rings

## Ligand CLA y 314

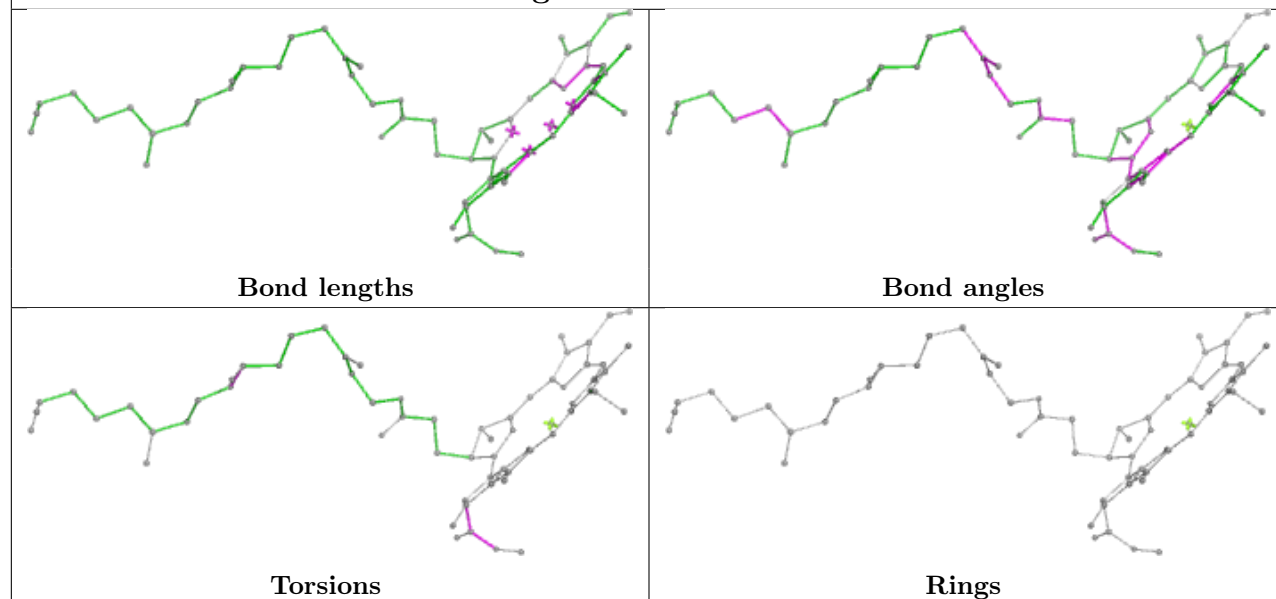




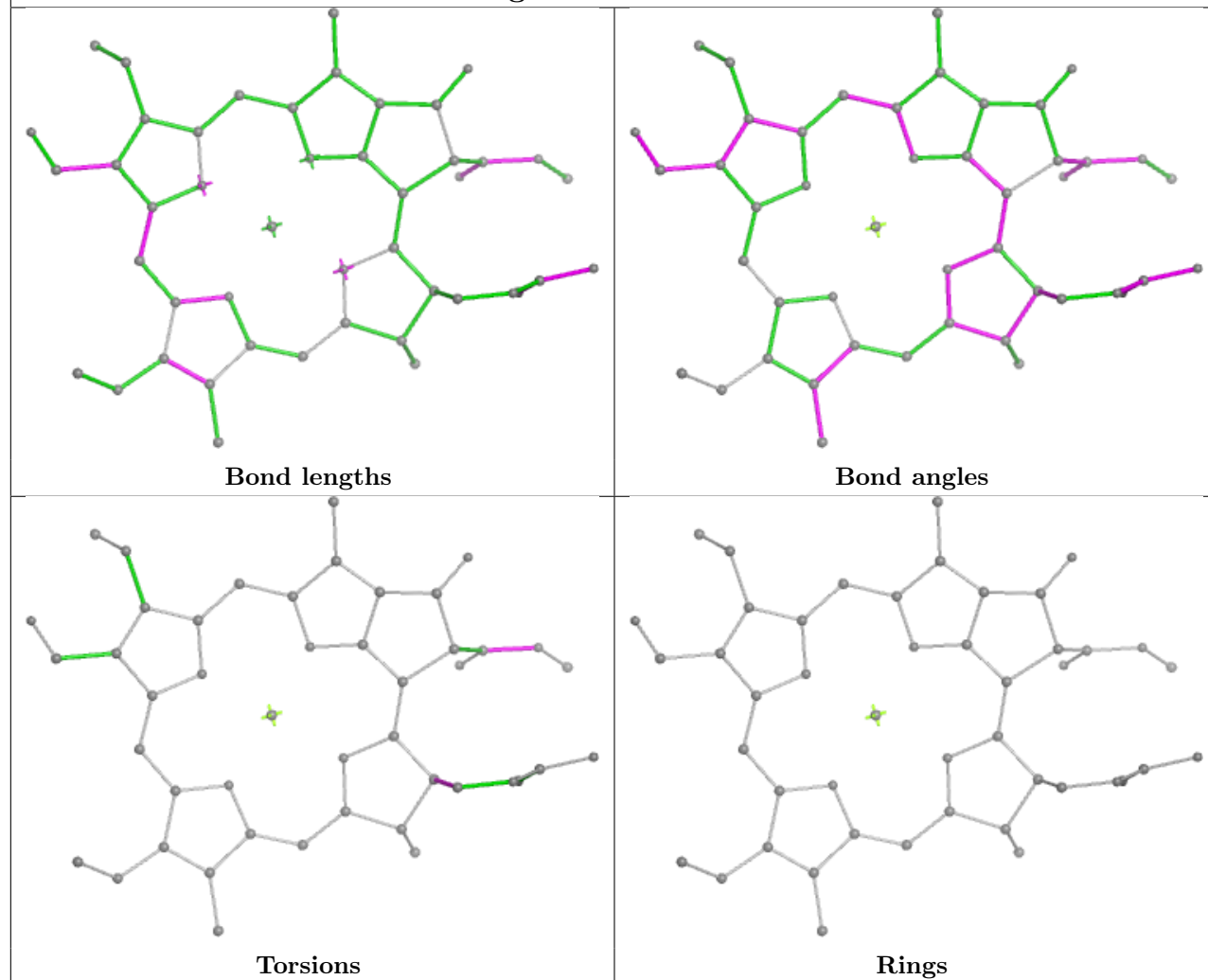
## Ligand CLA y 305



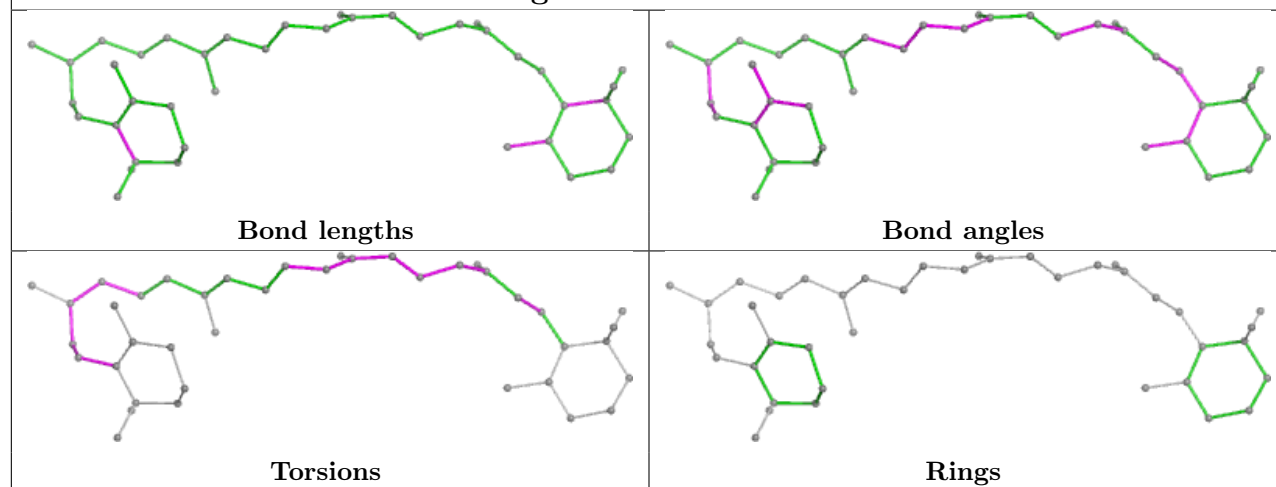
## Ligand CLA C 502

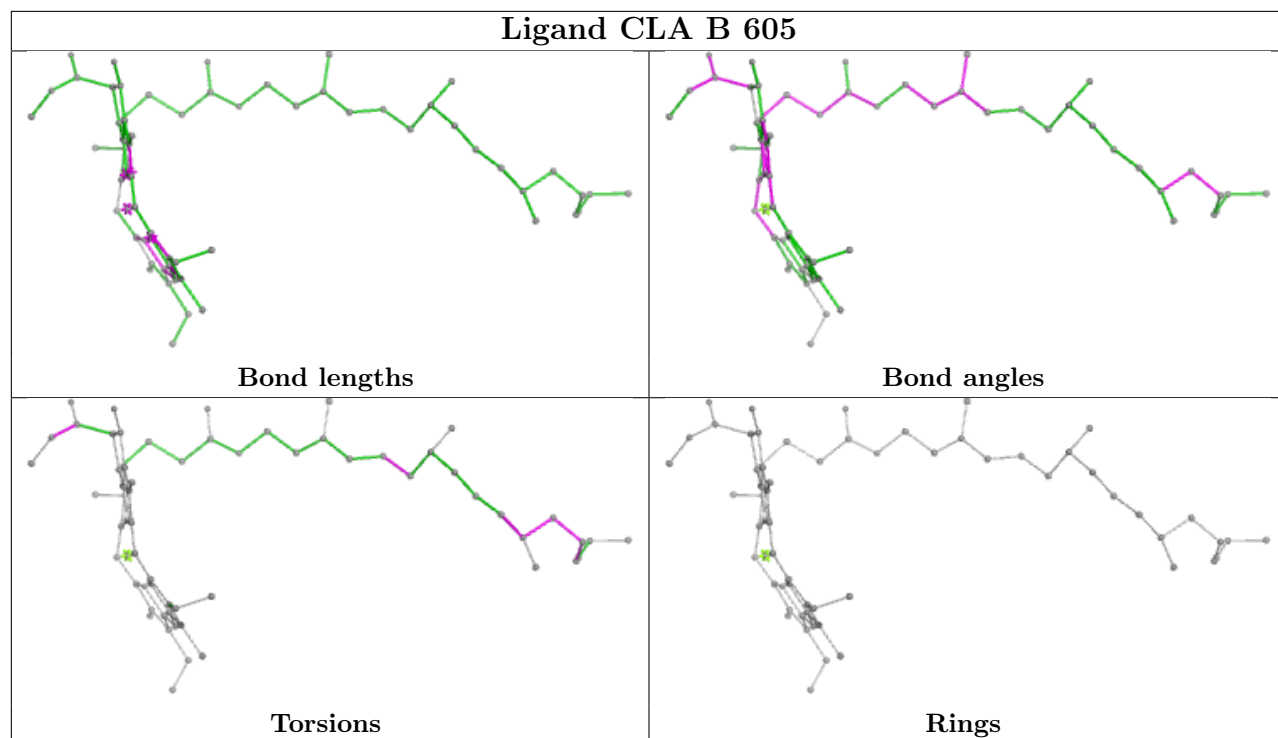
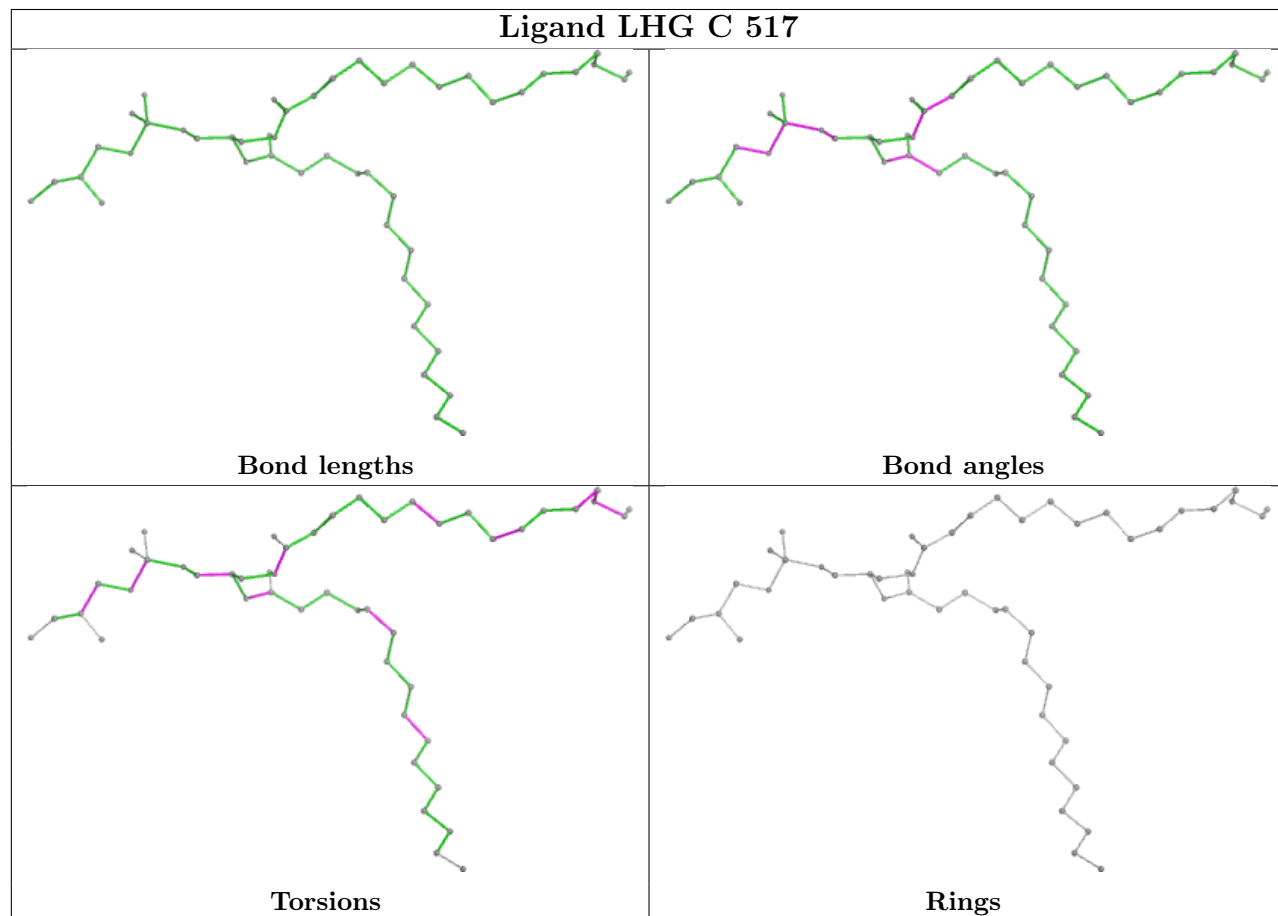


## Ligand CHL r 605

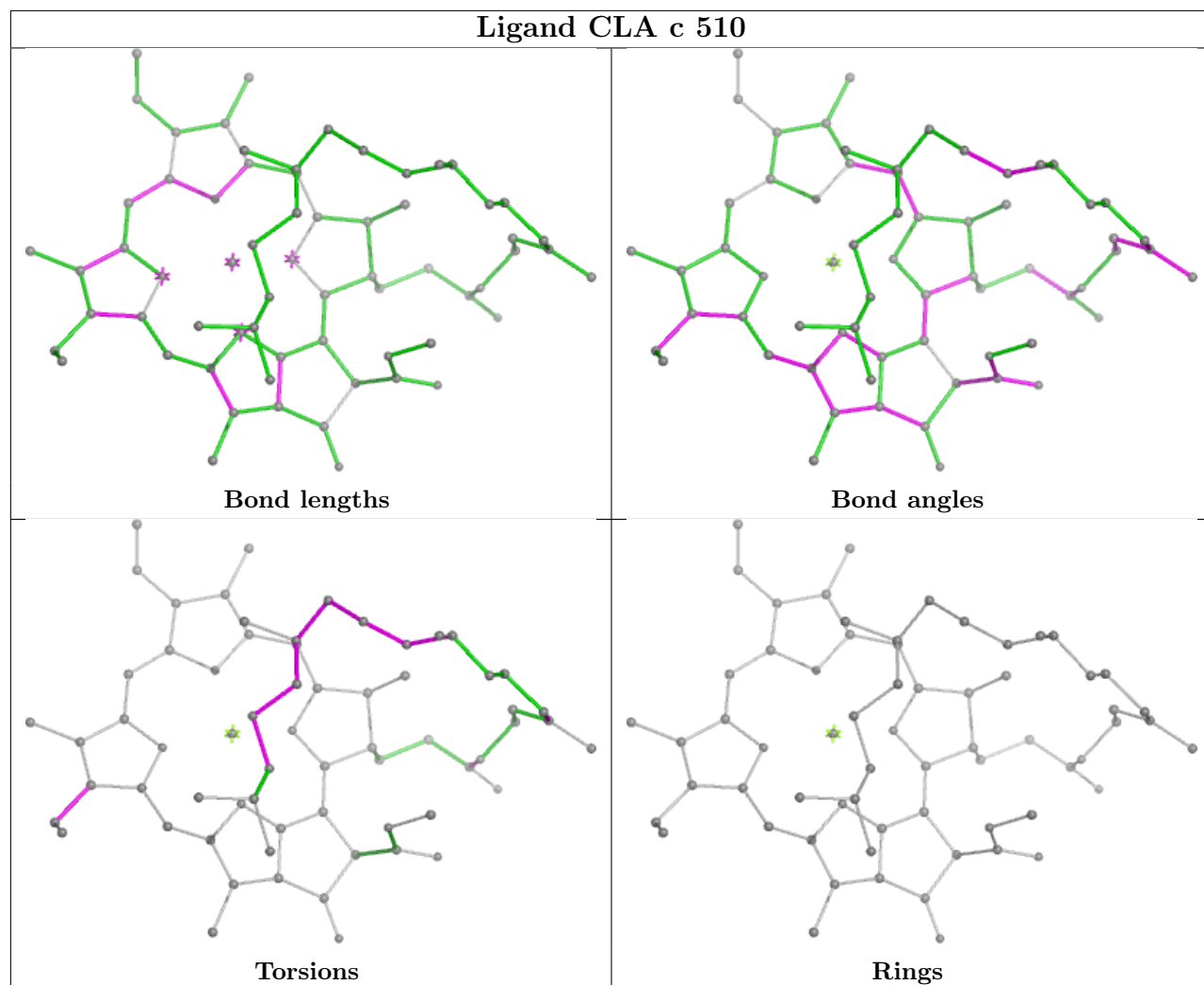


## Ligand BCR T 101

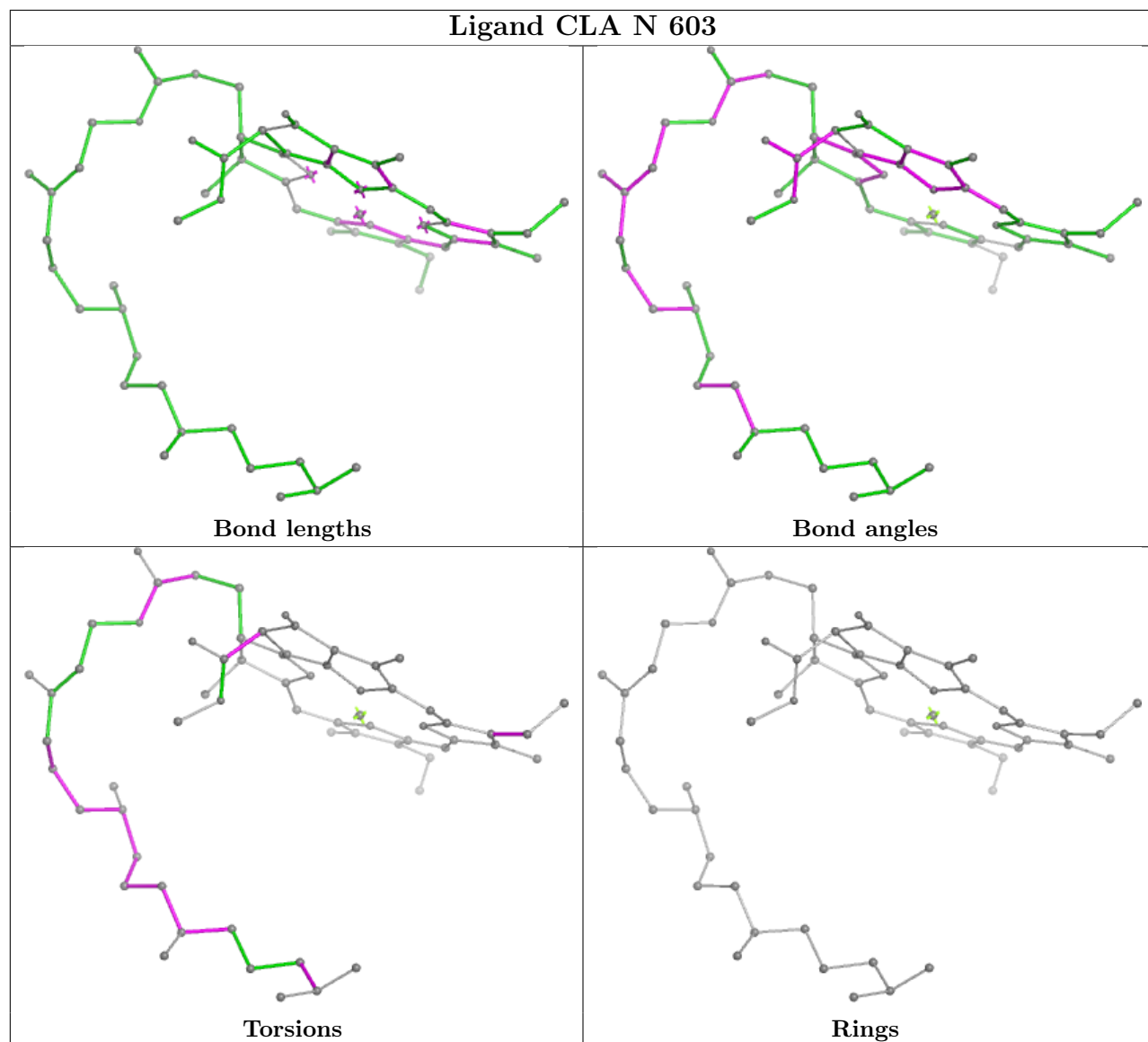


**Ligand CLA B 605****Ligand LHG C 517**

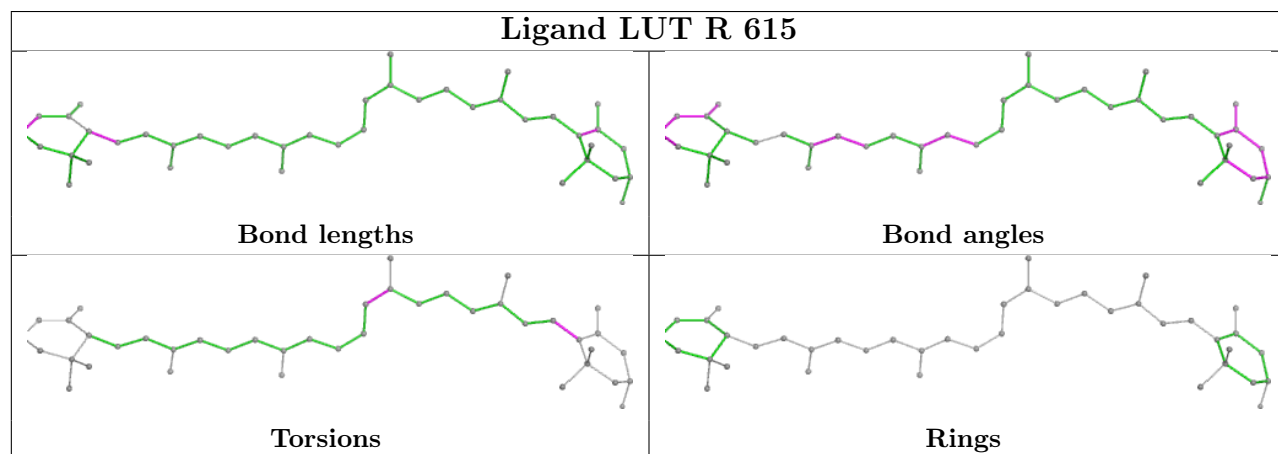
## Ligand CLA c 510

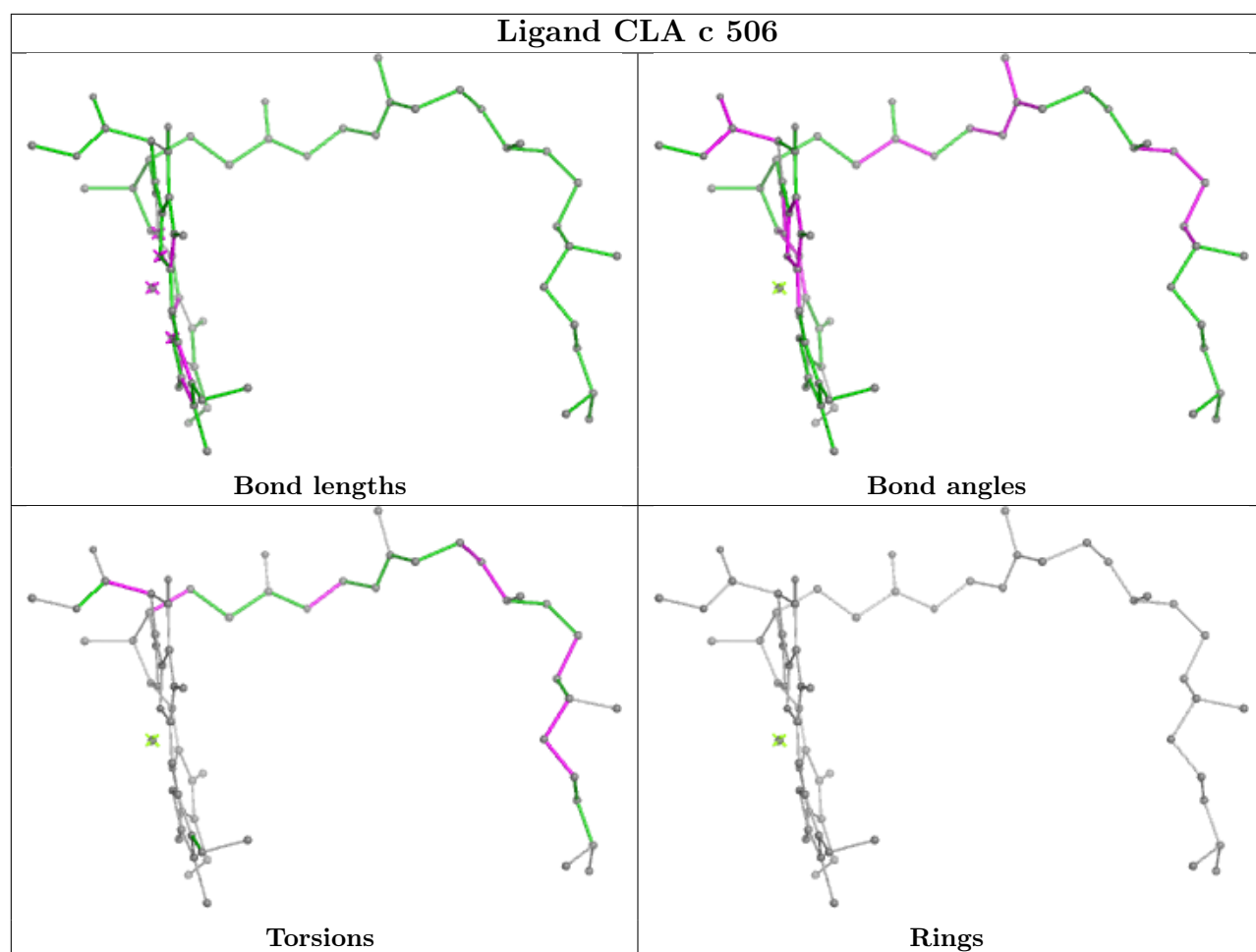


## Ligand CLA N 603

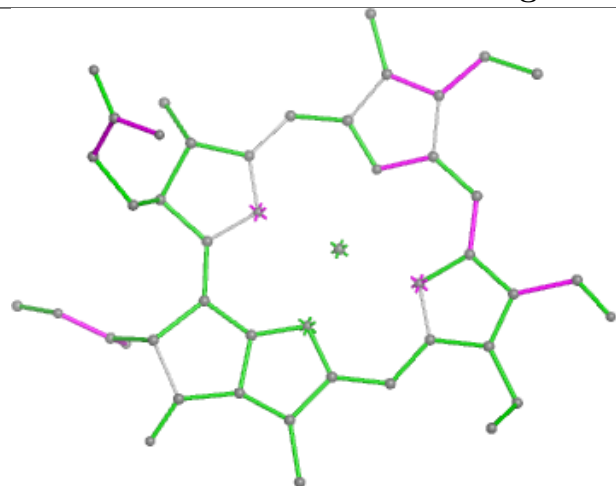


## Ligand LUT R 615

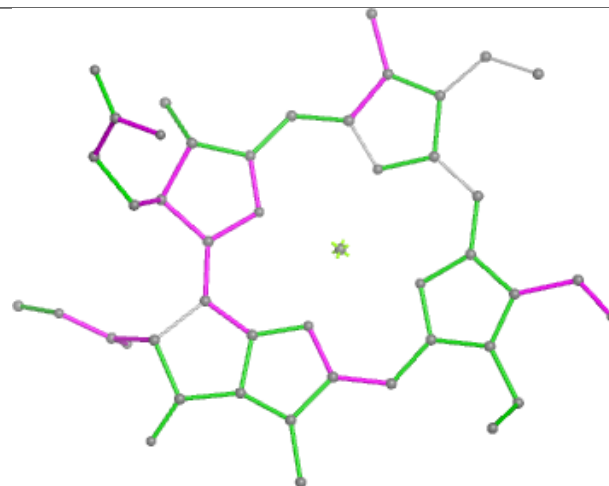




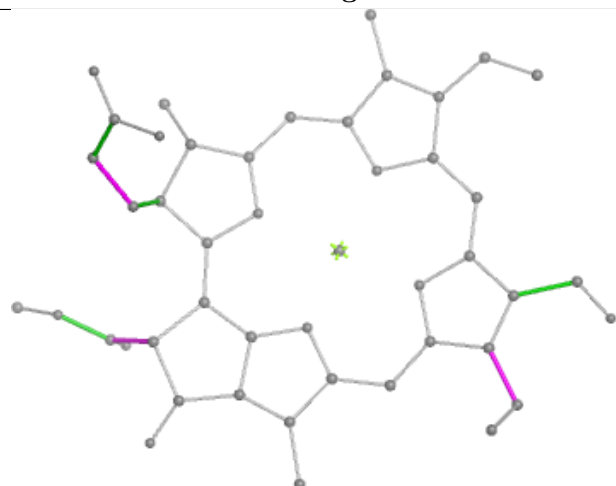
## Ligand CHL 1 301



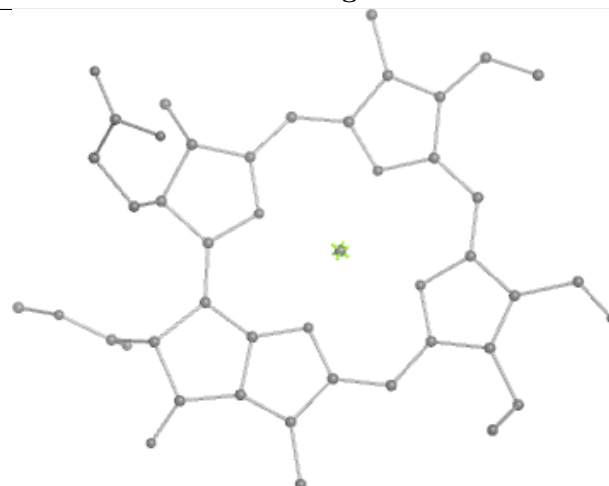
Bond lengths



Bond angles

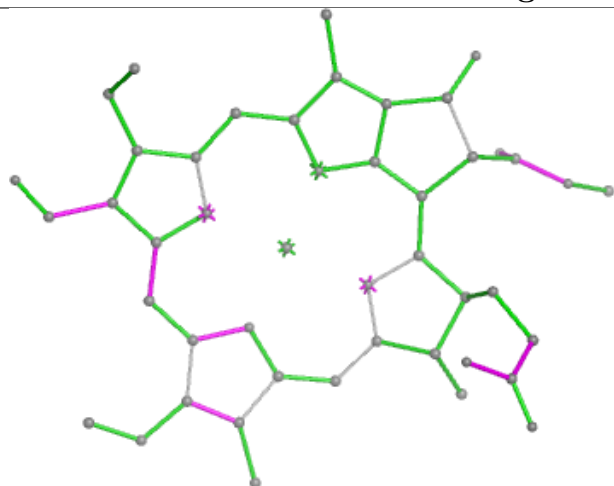


Torsions

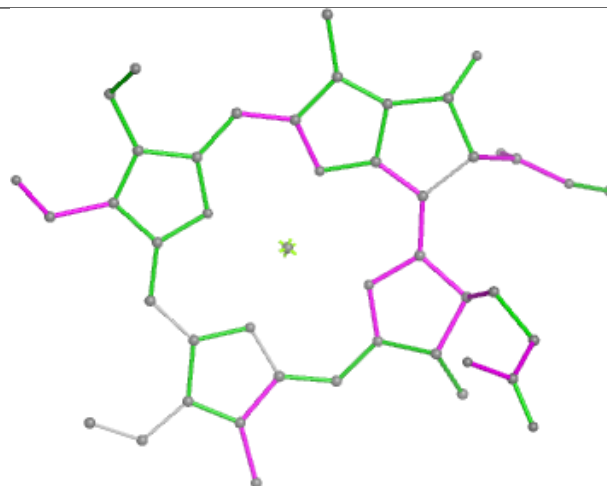


Rings

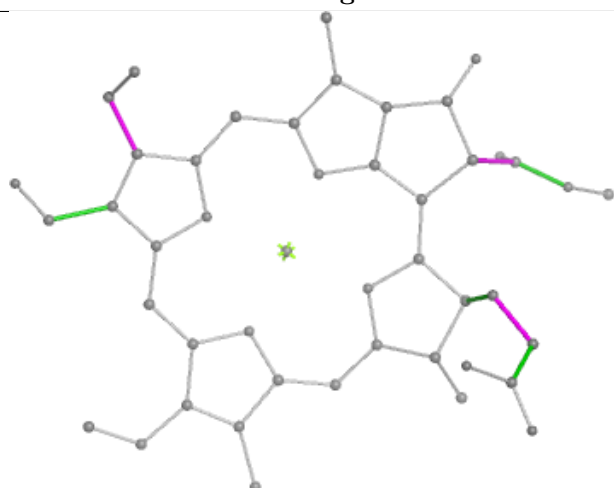
## Ligand CHL 5 301



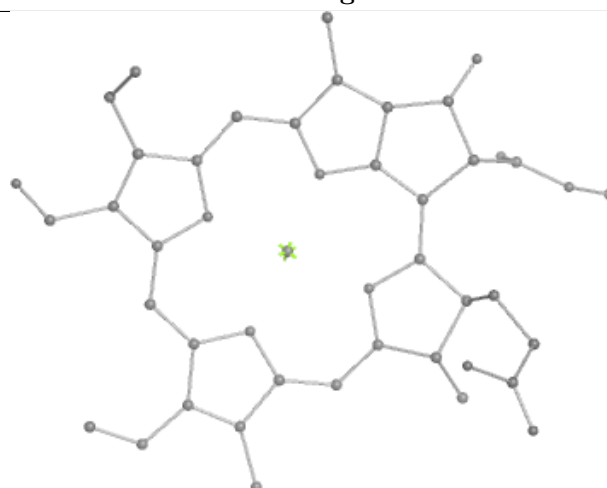
Bond lengths



Bond angles



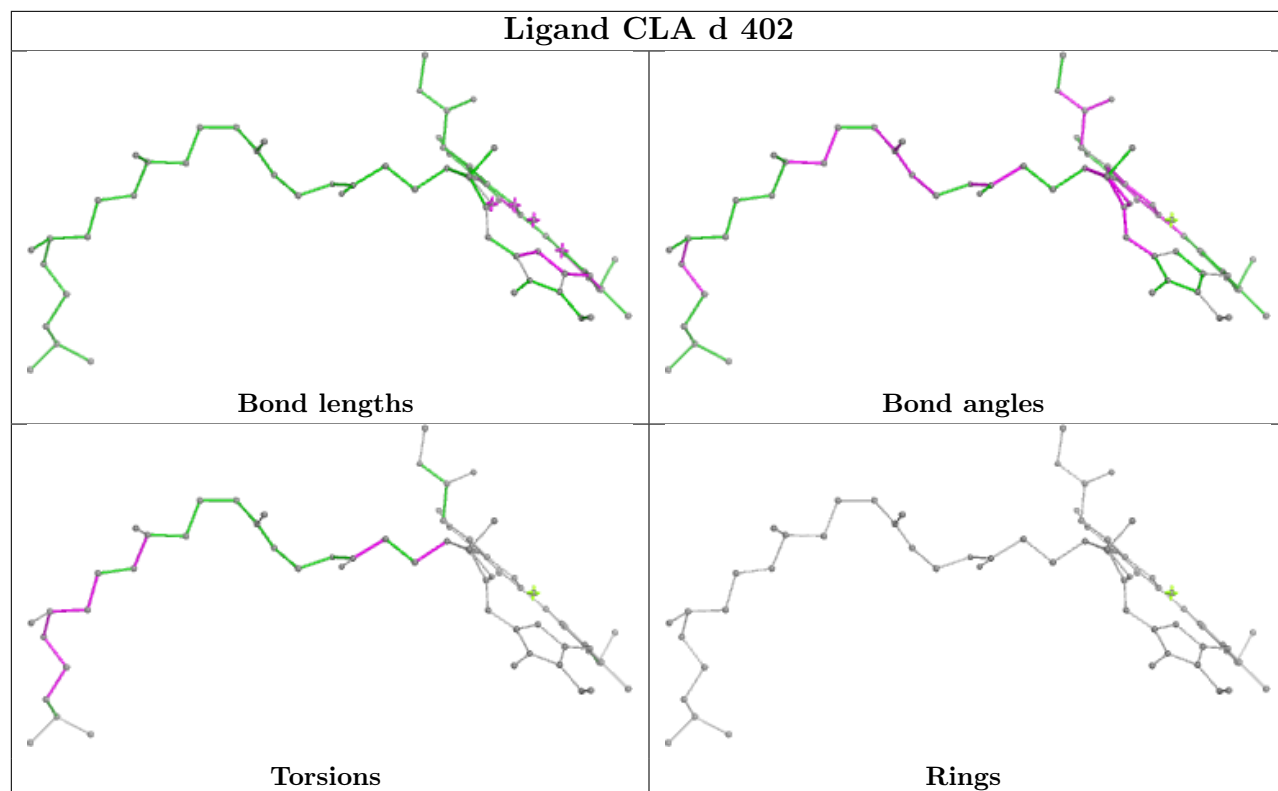
Torsions



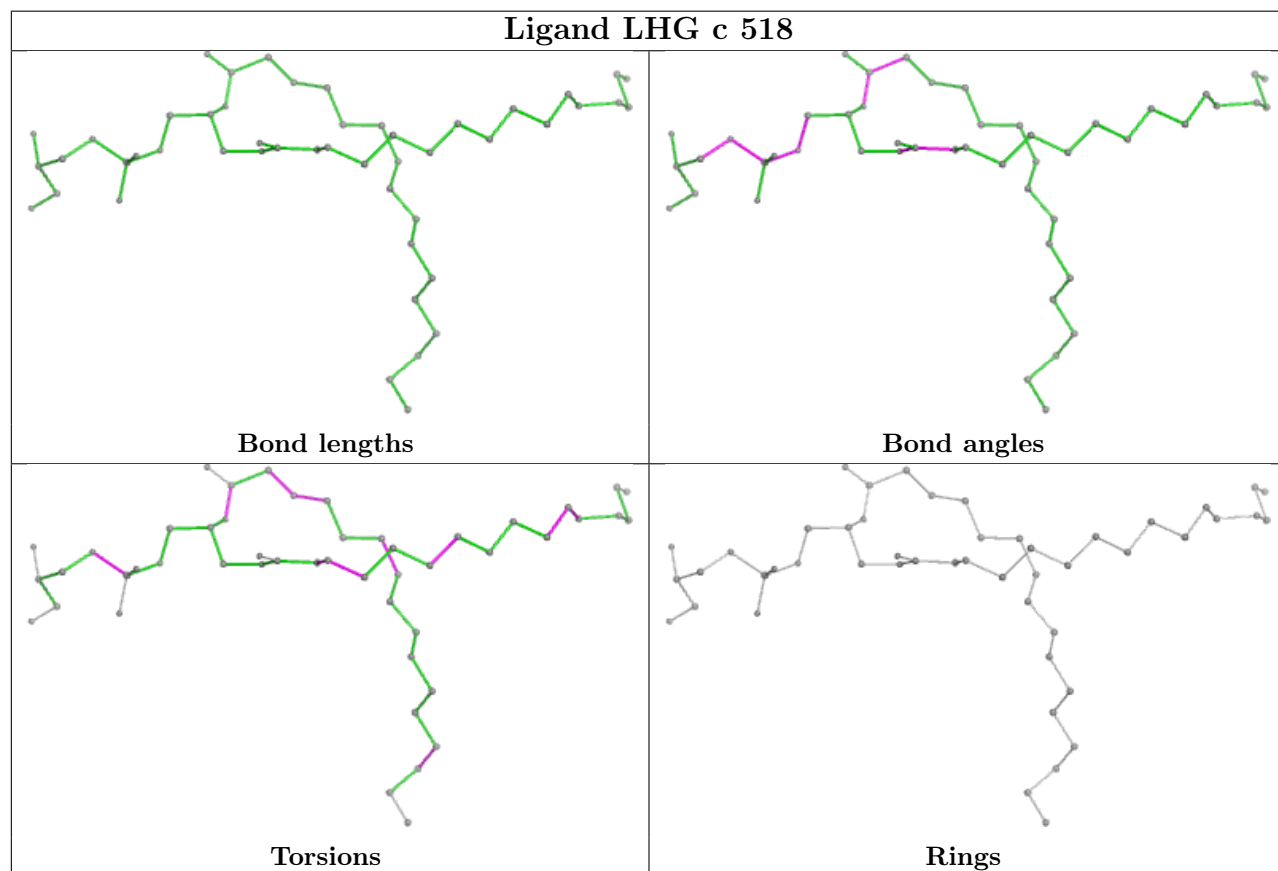
Rings



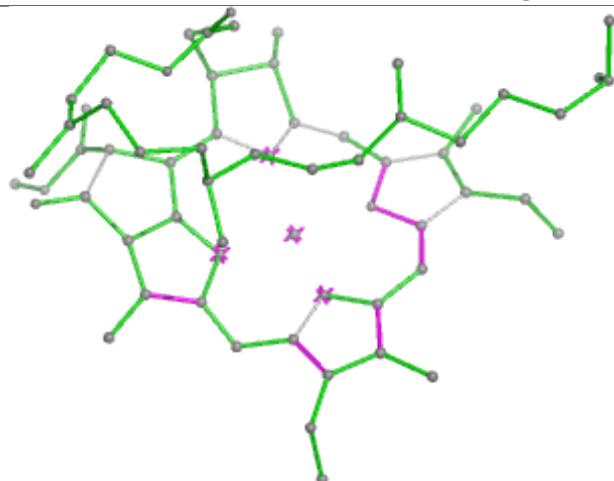
## Ligand CLA d 402



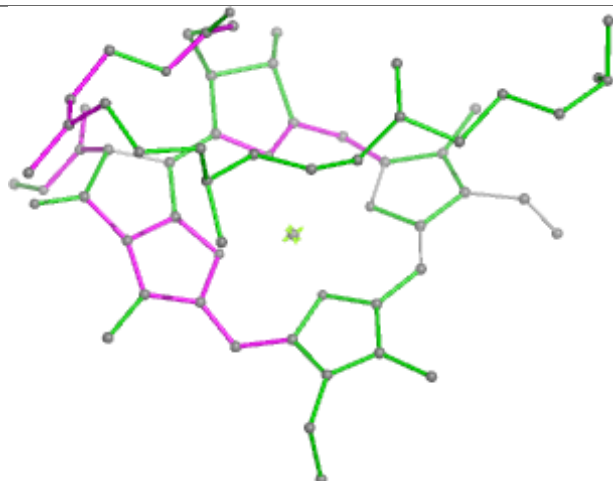
## Ligand LHG c 518



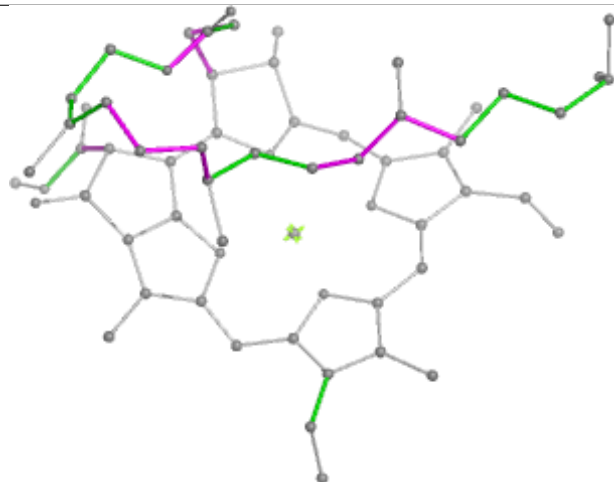
## Ligand CLA b 601



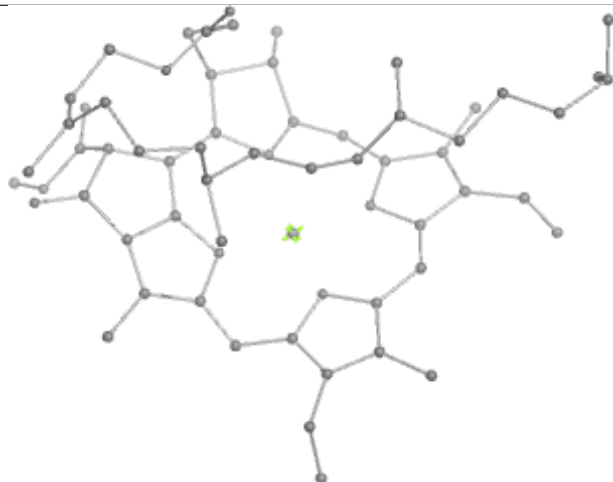
Bond lengths



Bond angles

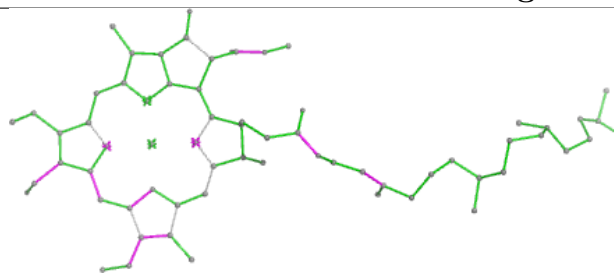


Torsions

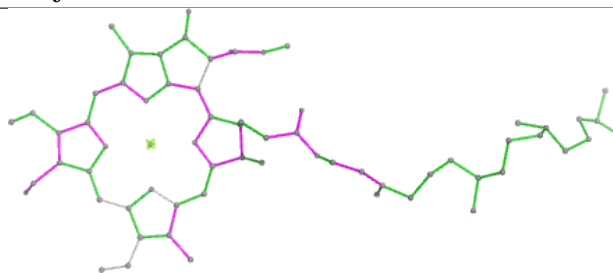


Rings

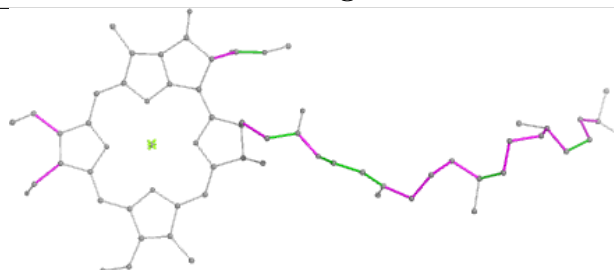
## Ligand CHL y 302



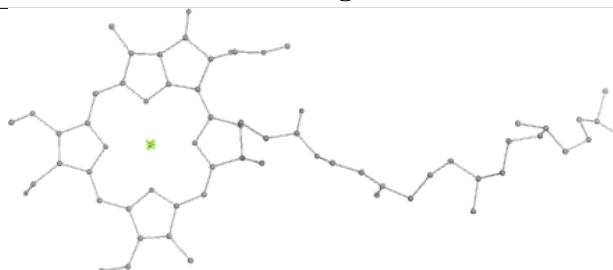
Bond lengths



Bond angles

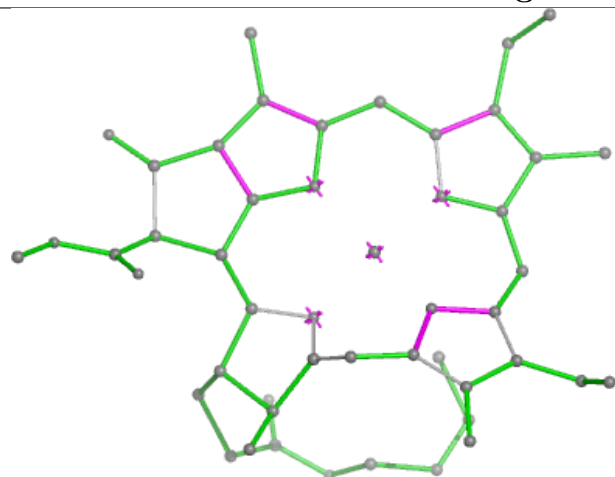


Torsions

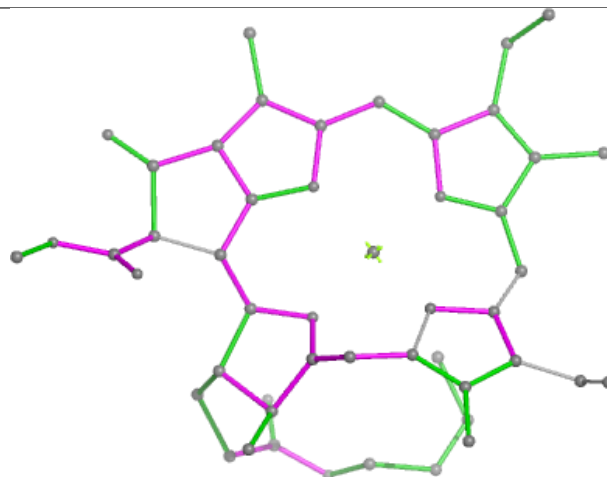


Rings

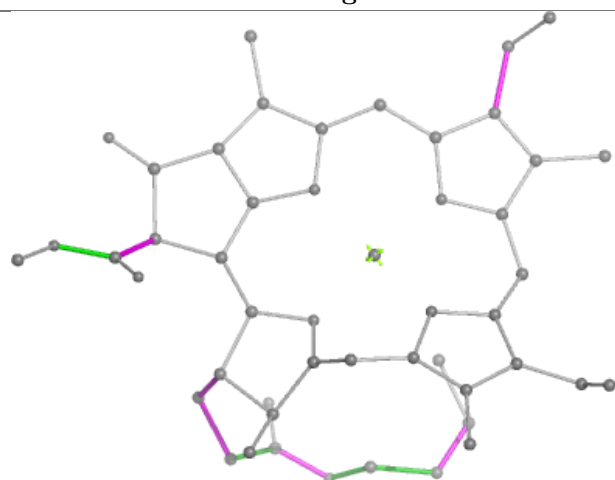
## Ligand CLA R 610



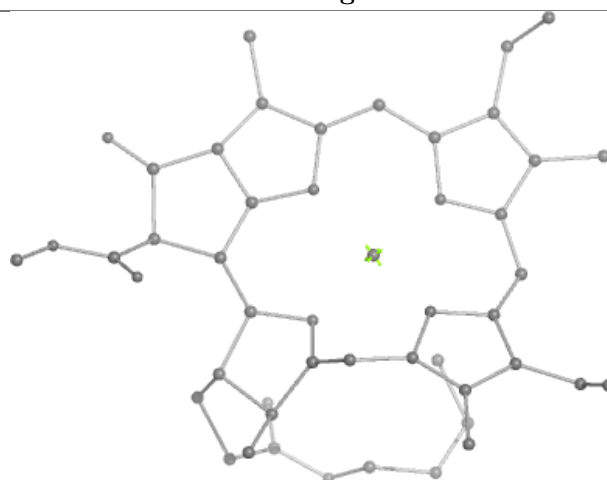
Bond lengths



Bond angles

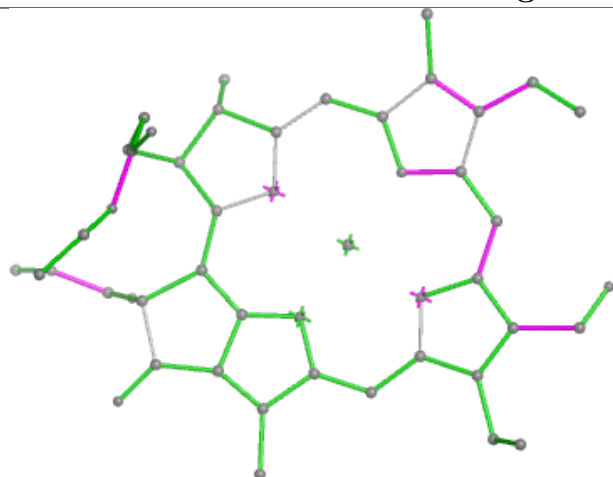


Torsions

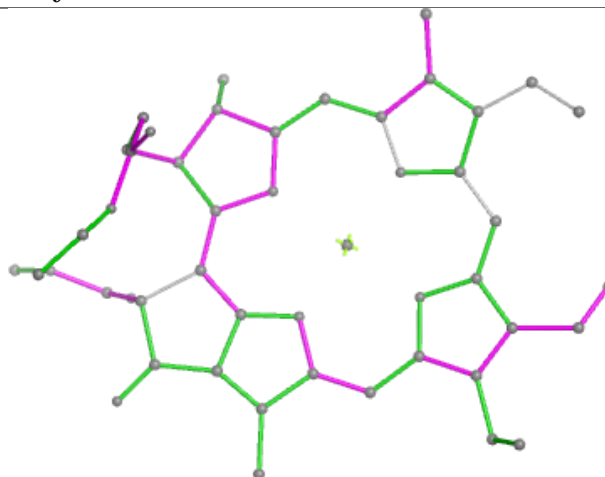


Rings

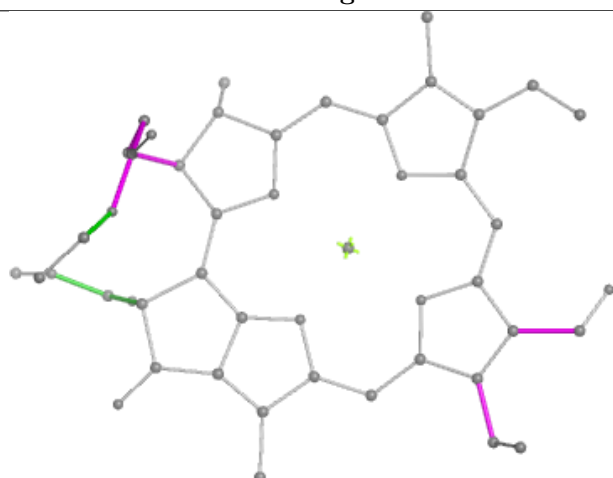
## Ligand CHL y 306



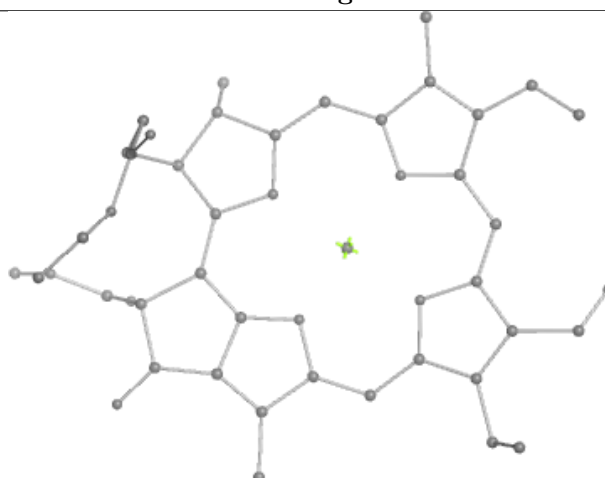
Bond lengths



Bond angles

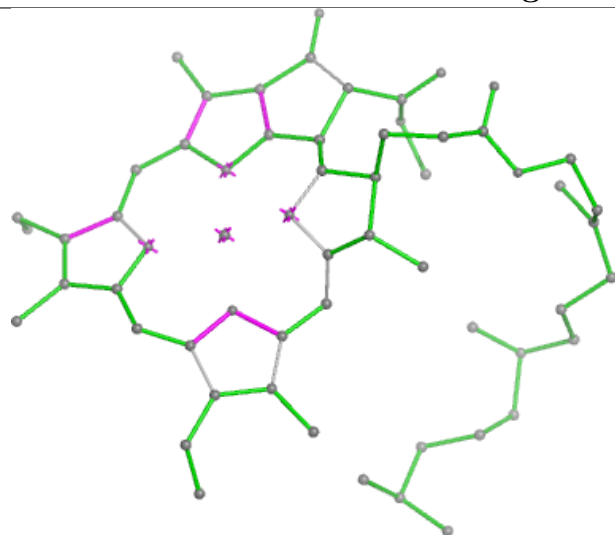


Torsions

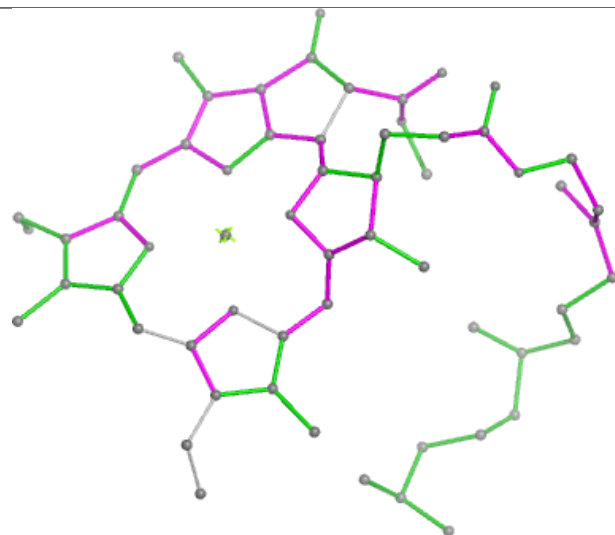


Rings

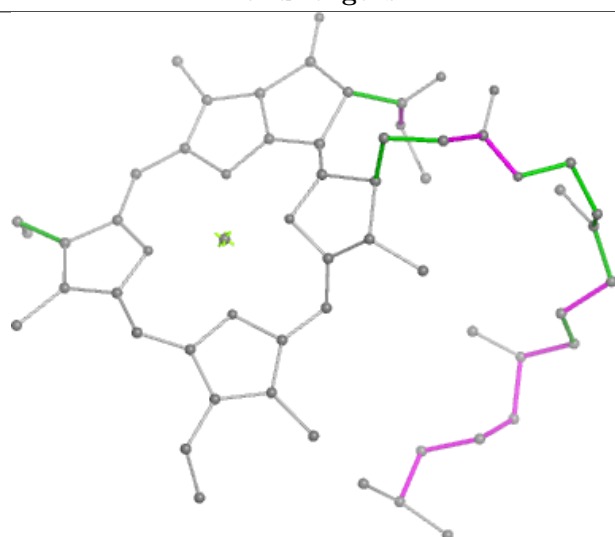
## Ligand CLA r 603



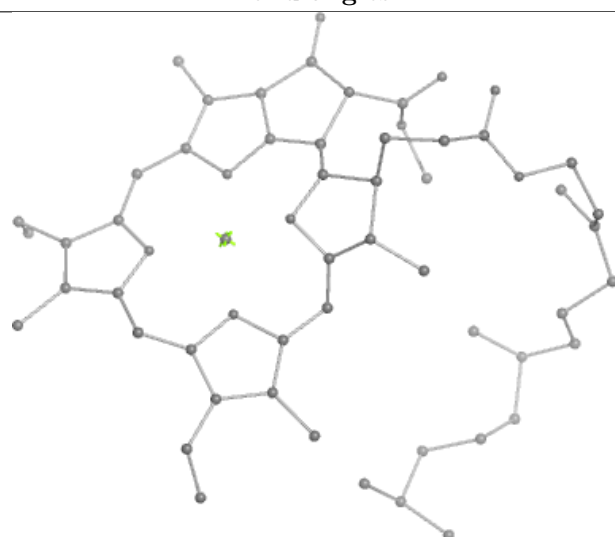
Bond lengths



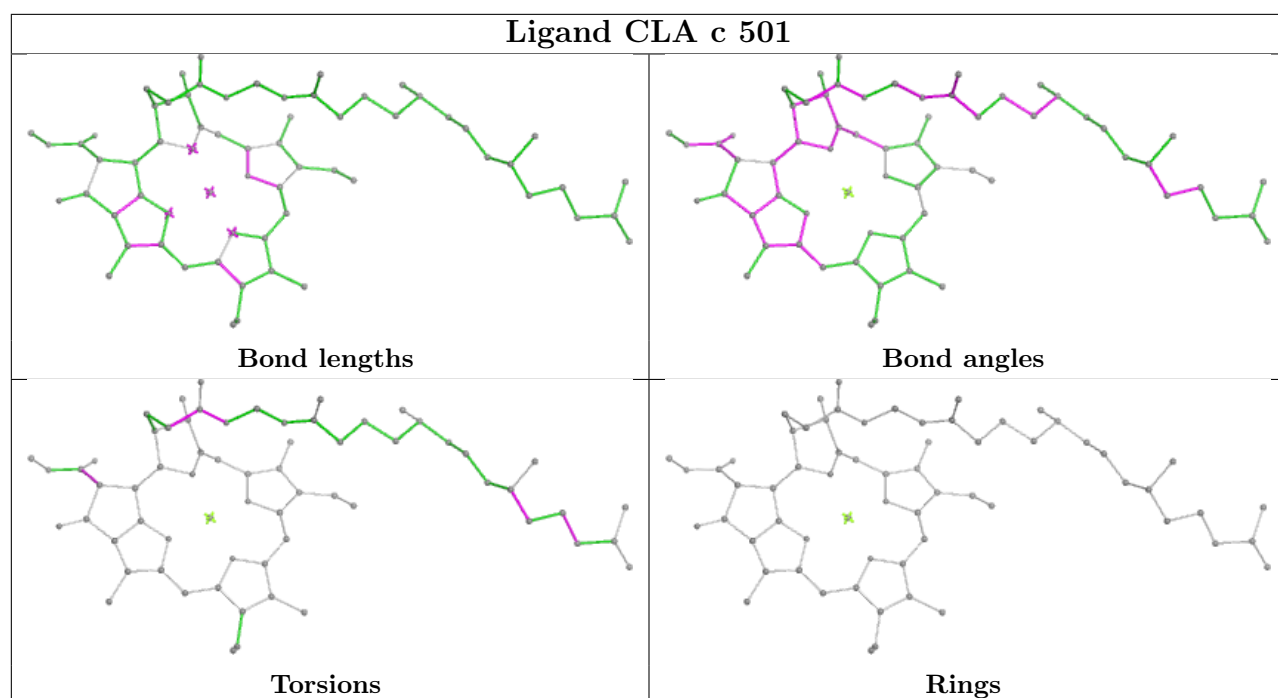
Bond angles



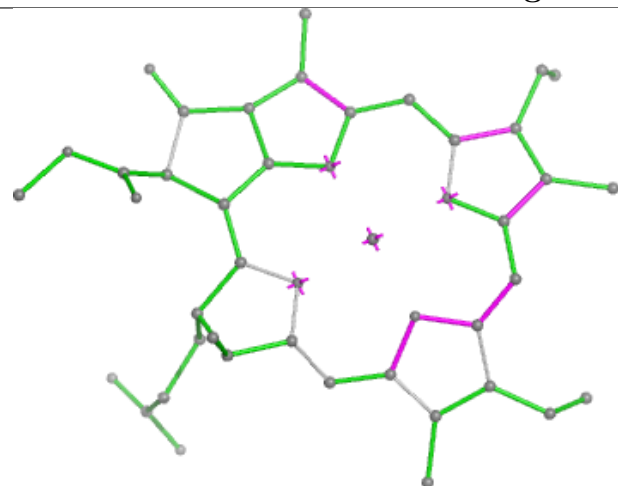
Torsions



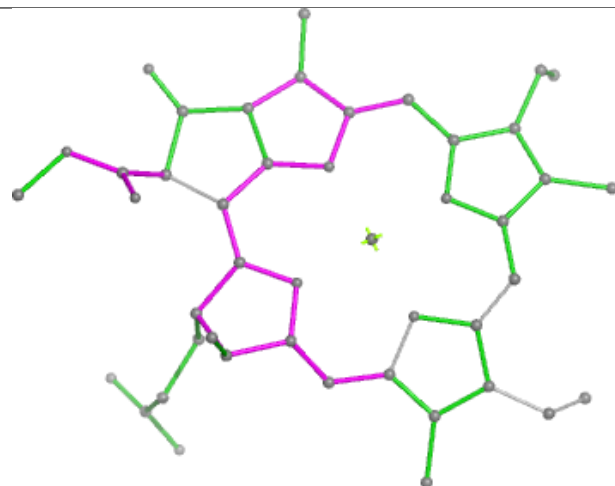
Rings



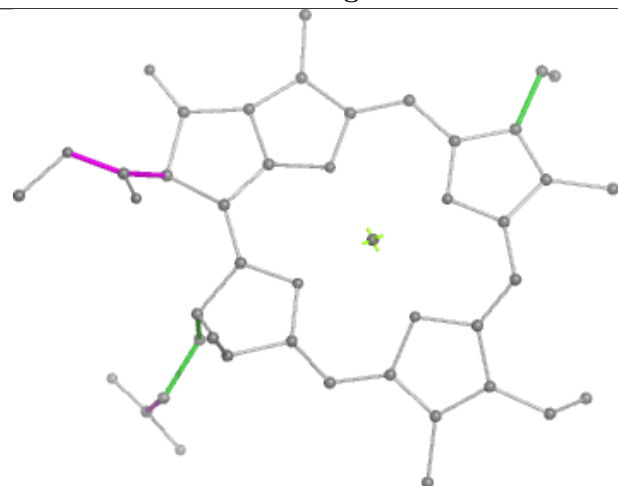
## Ligand CLA s 309



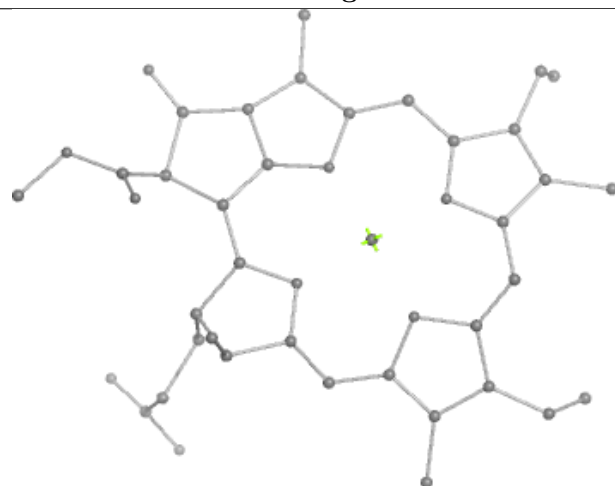
Bond lengths



Bond angles

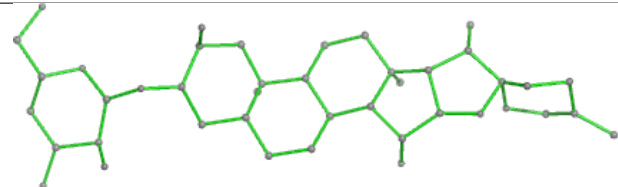


Torsions

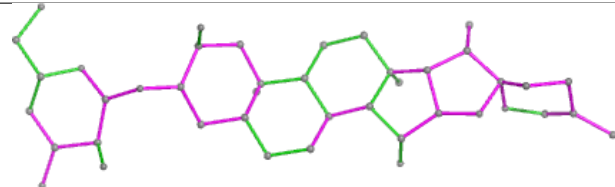


Rings

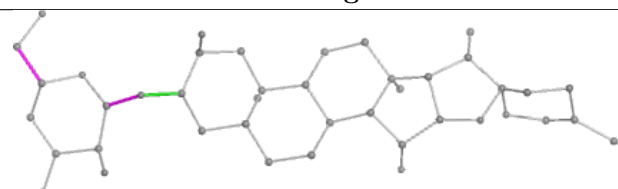
## Ligand AJP s 319



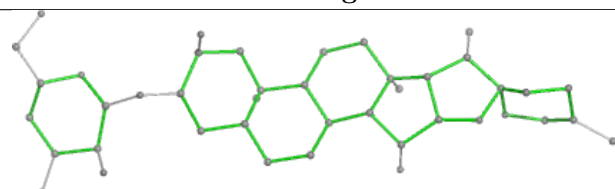
Bond lengths



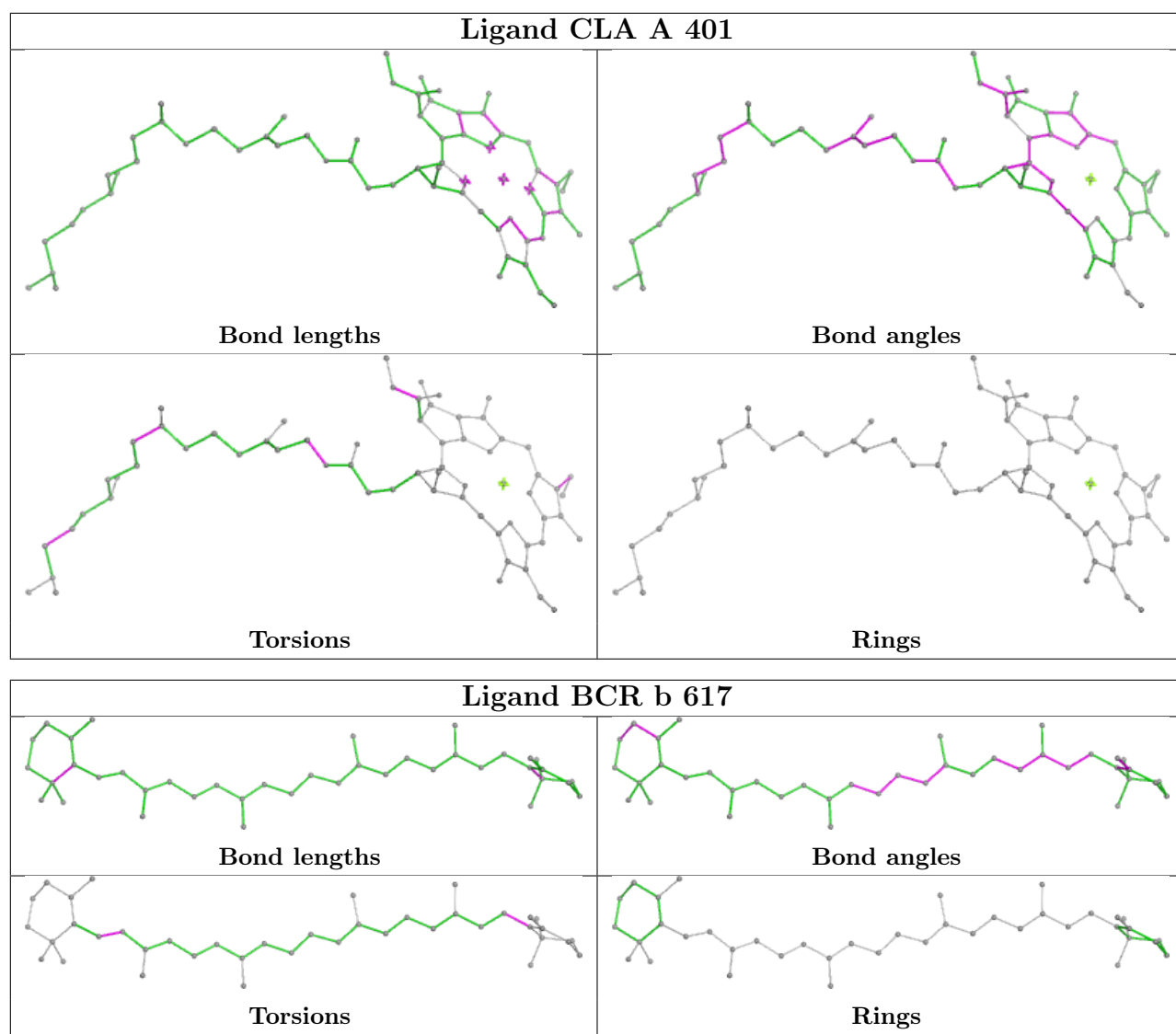
Bond angles



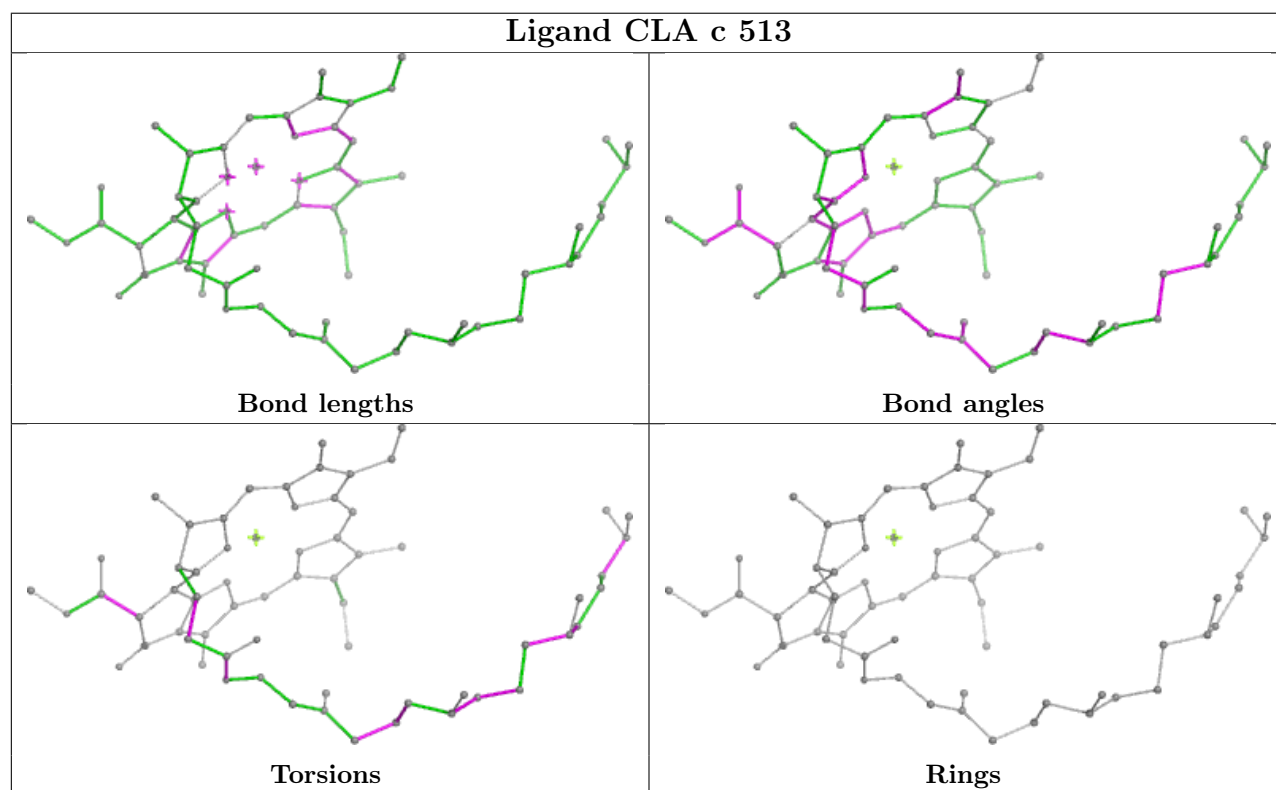
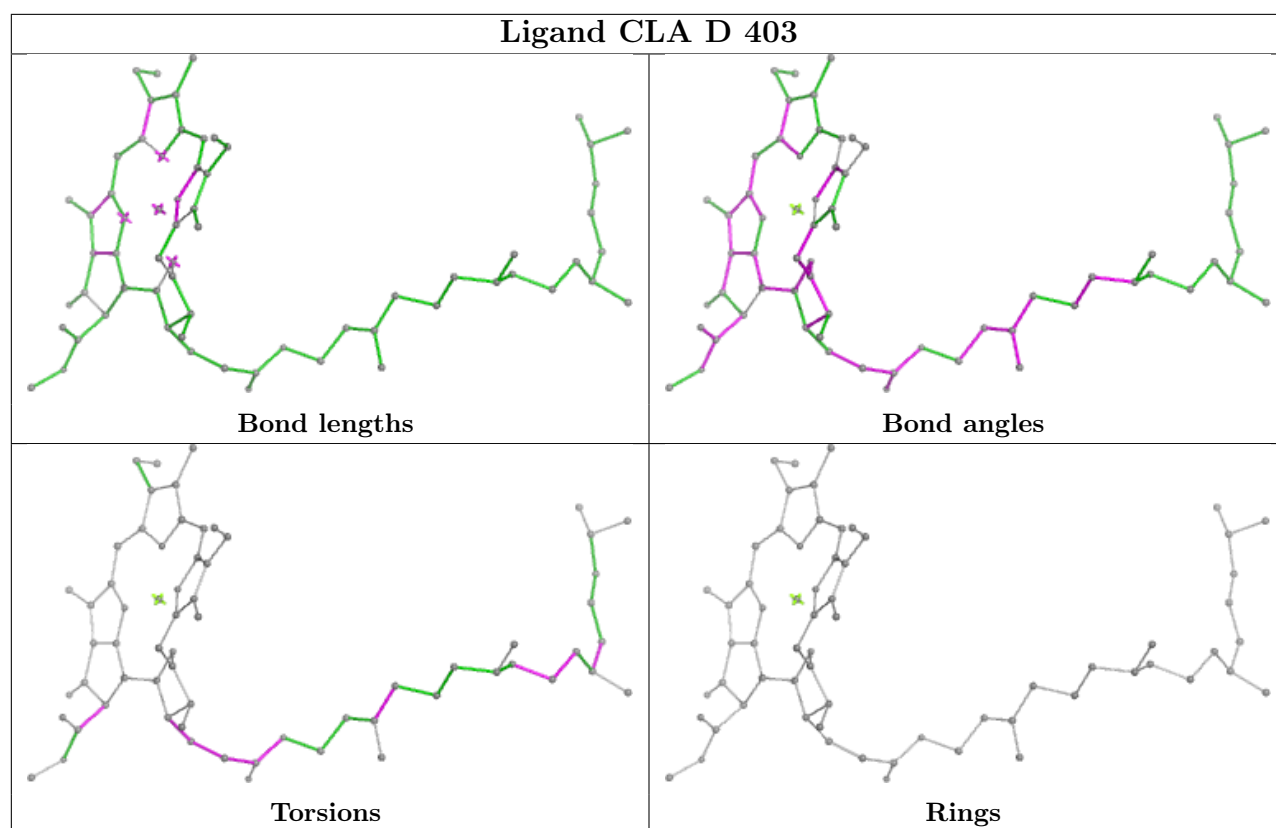
Torsions



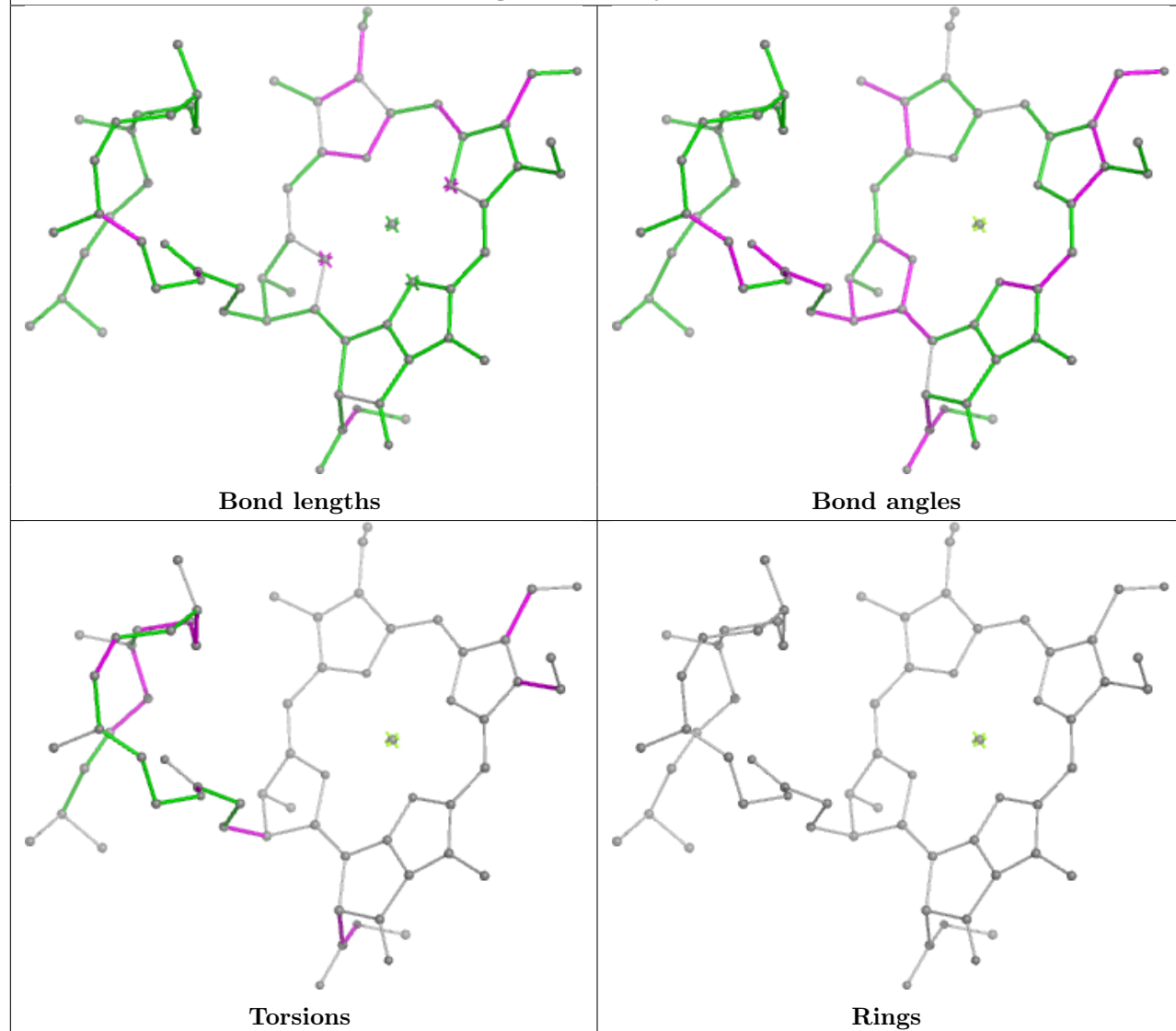
Rings



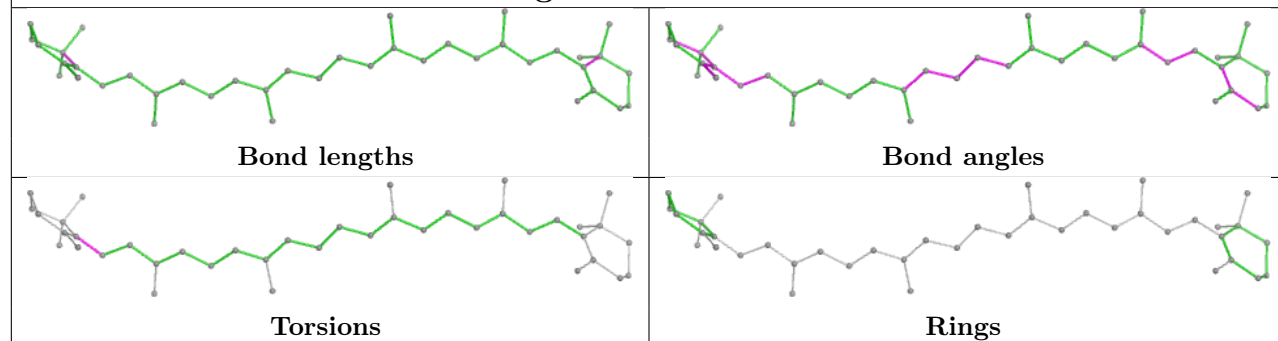




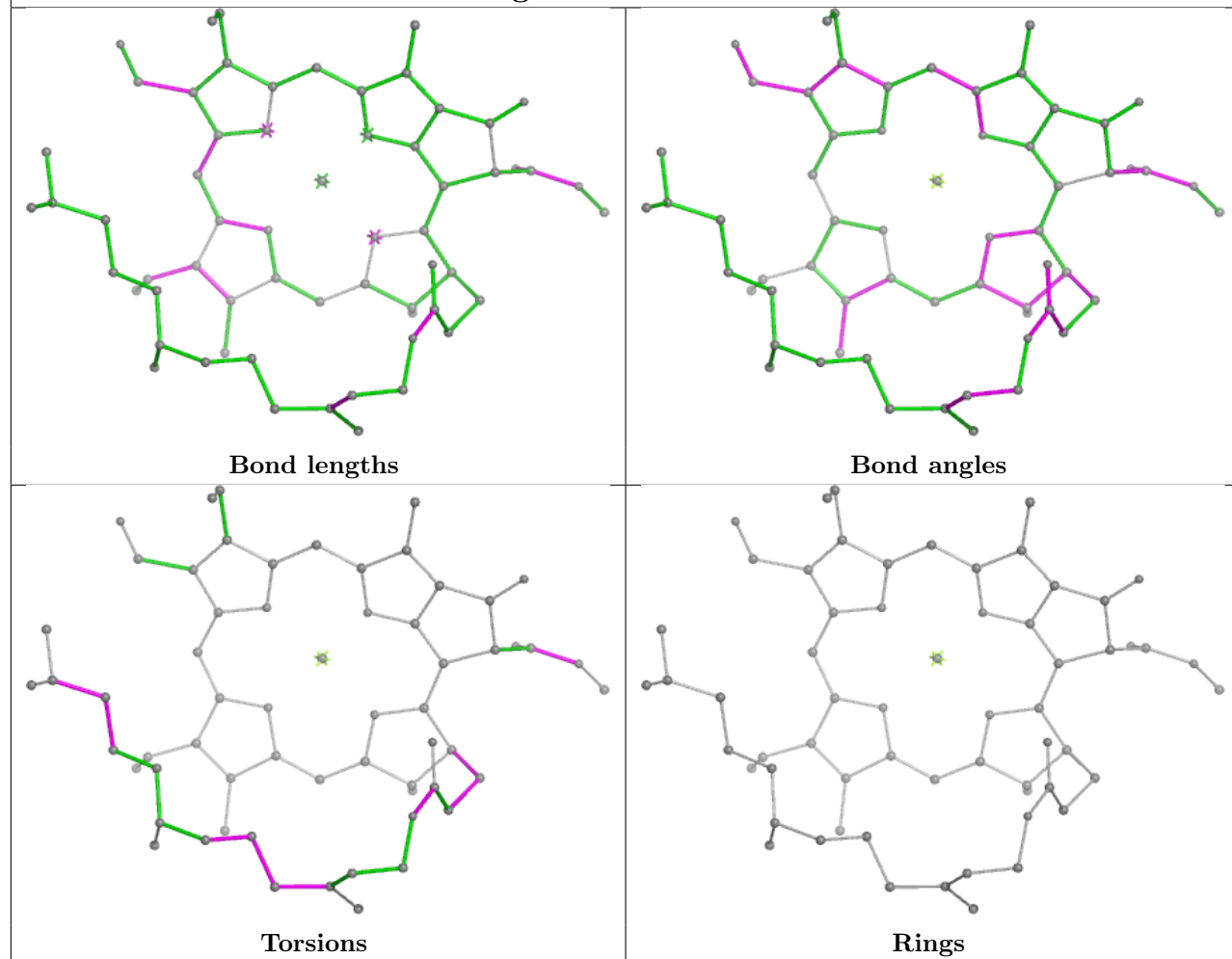
## Ligand CHL y 309



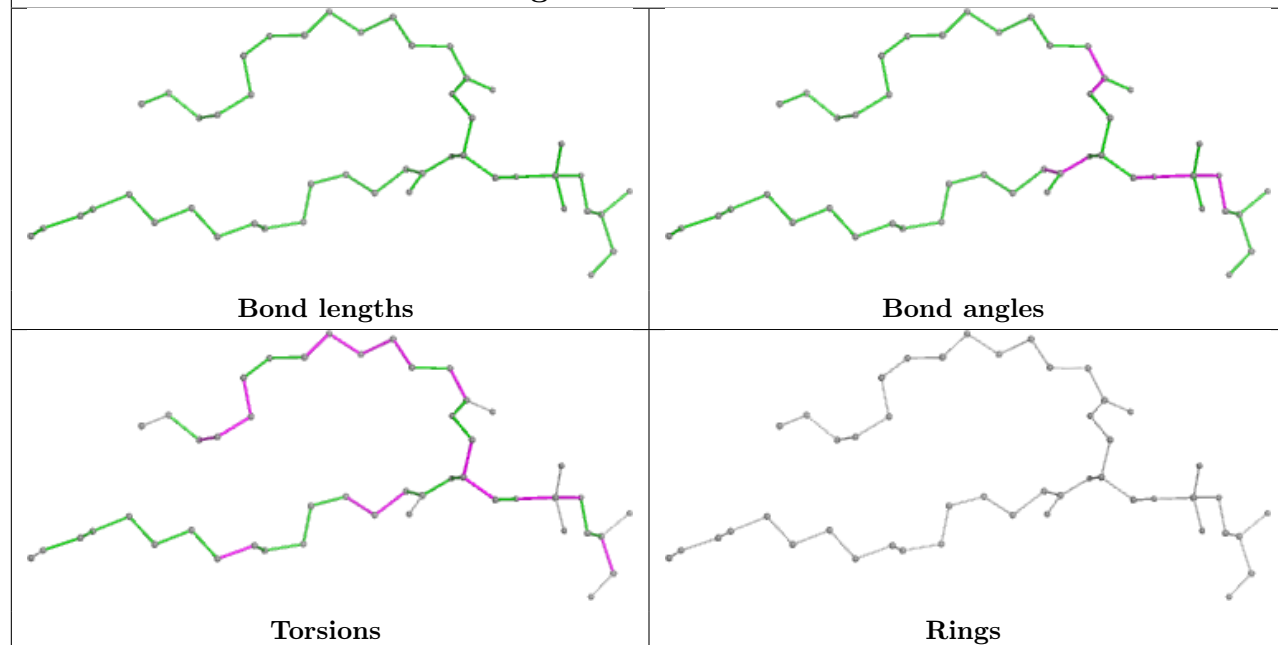
## Ligand BCR c 514



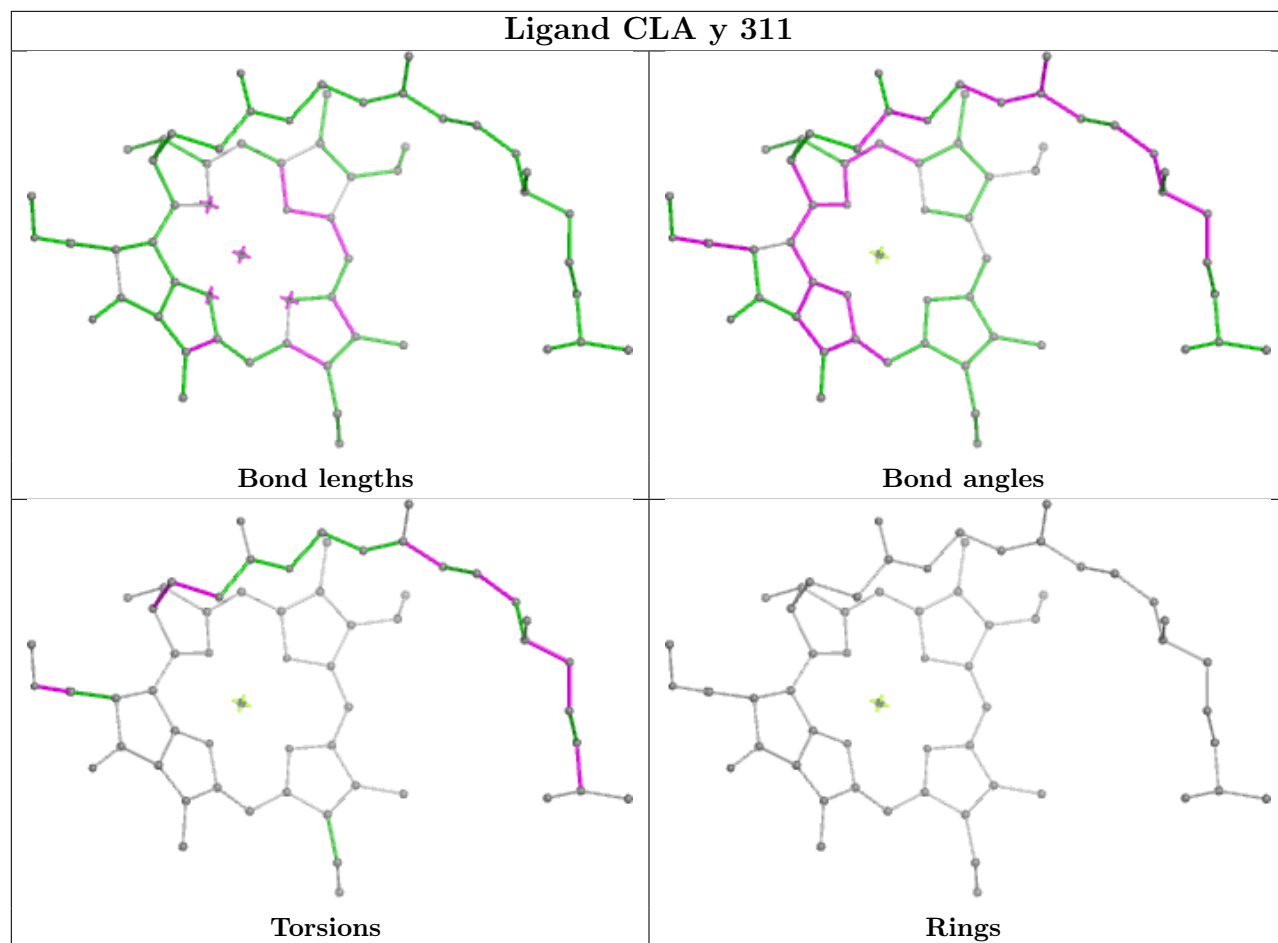
## Ligand CHL R 607



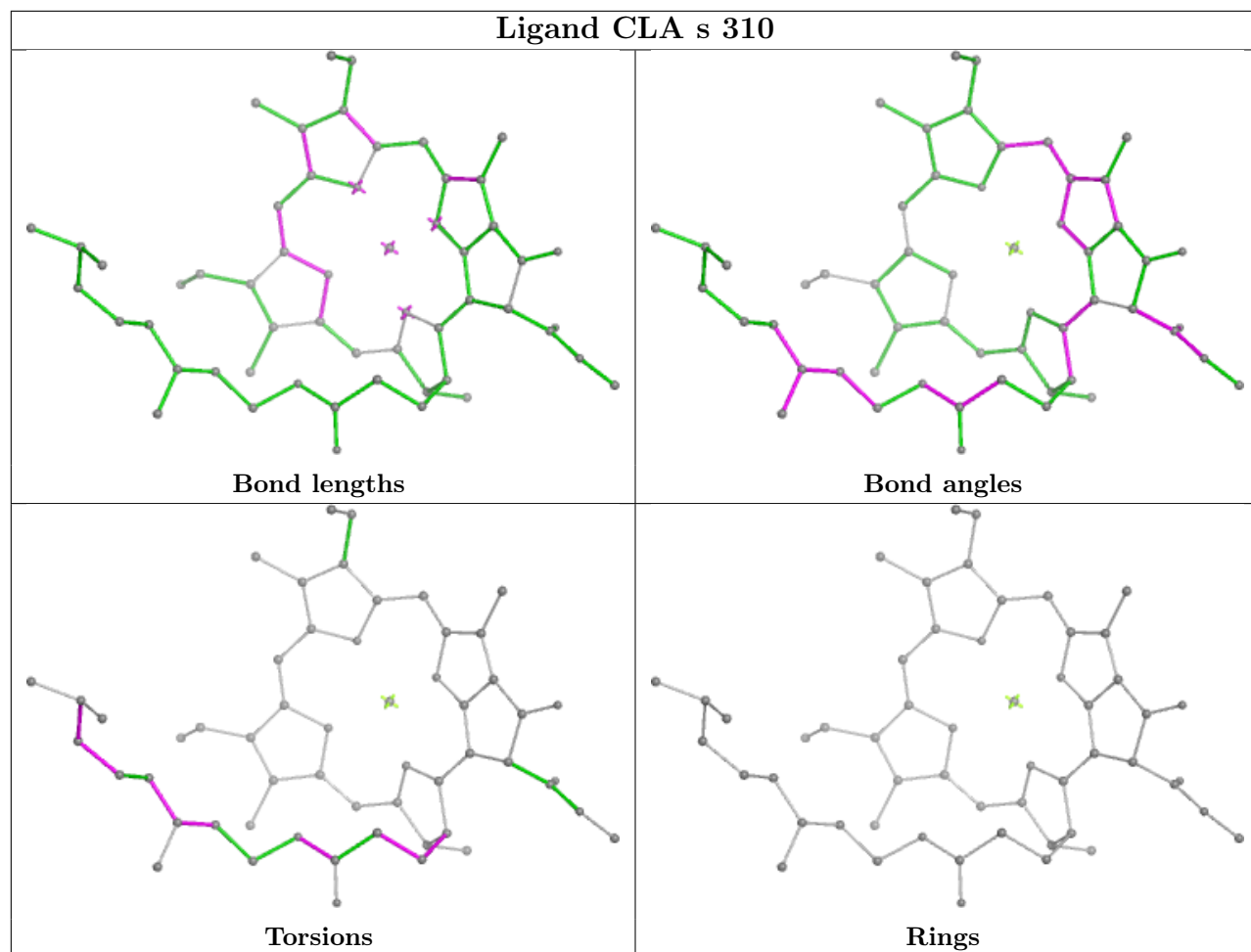
## Ligand LHG B 621



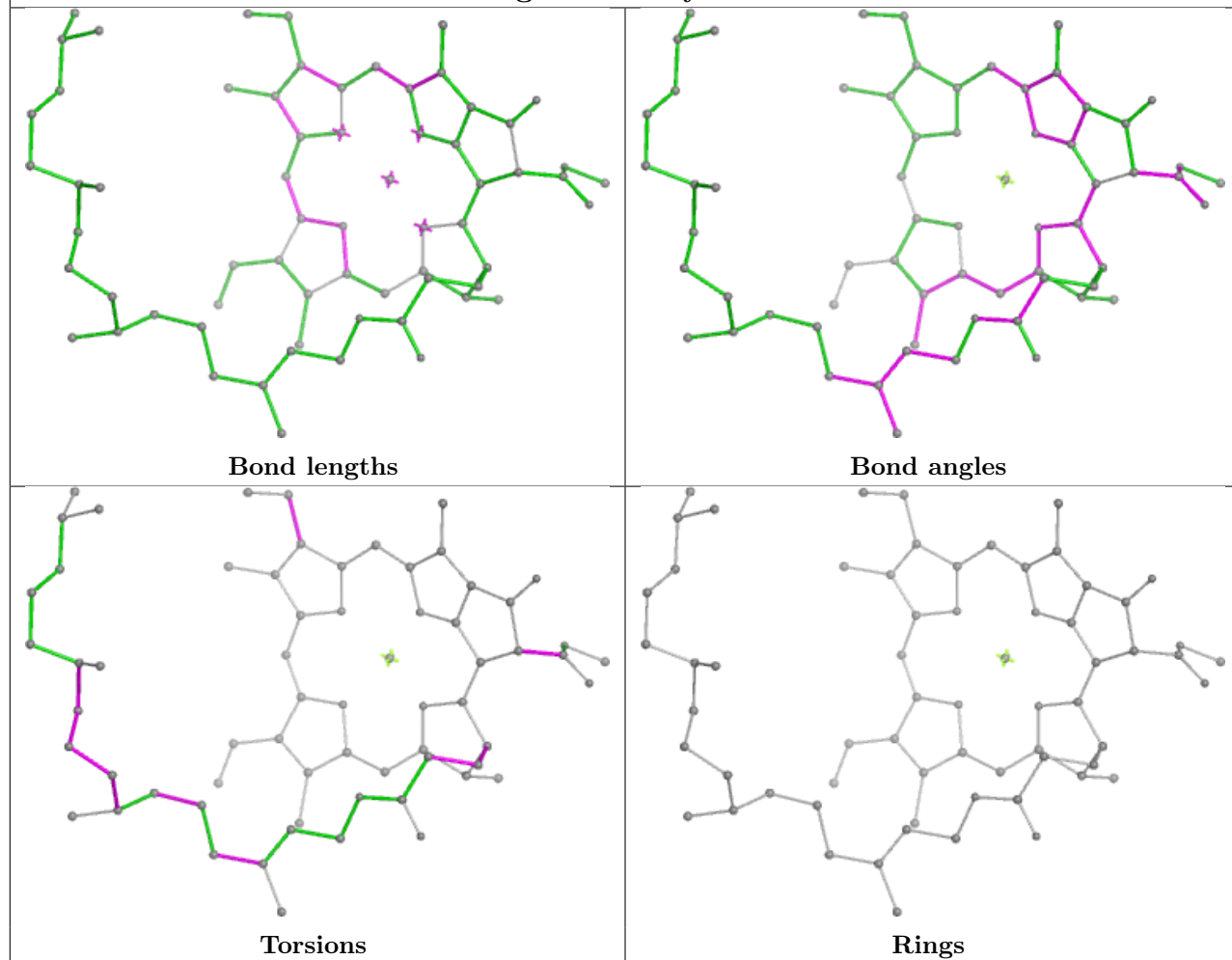
## Ligand CLA y 311



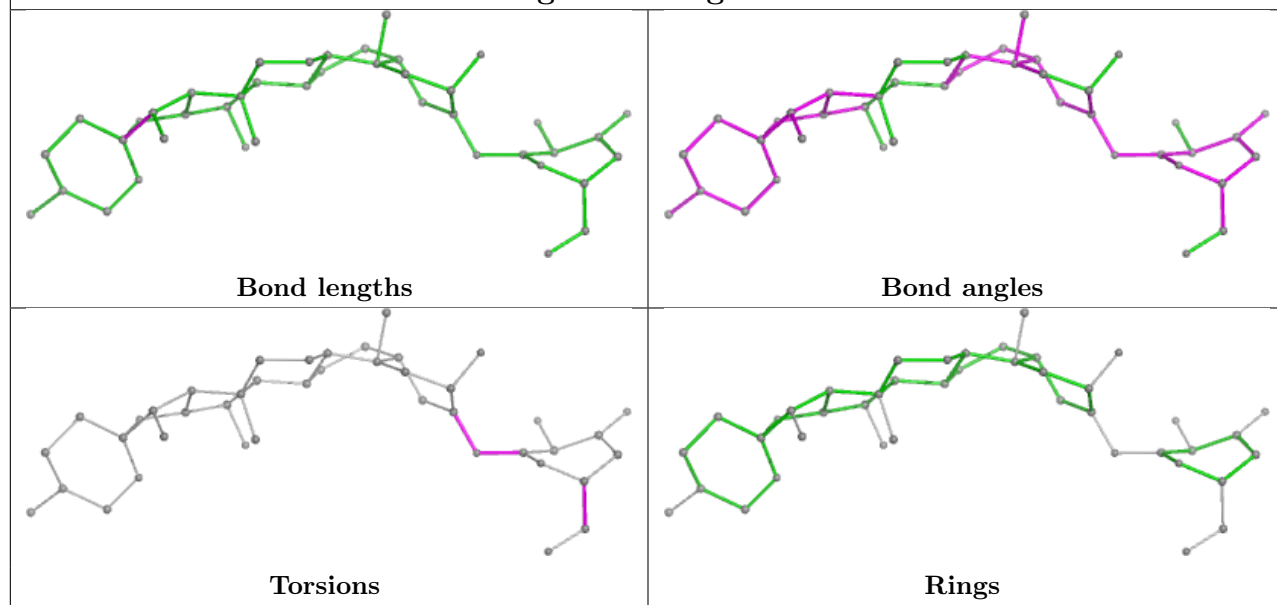
## Ligand CLA s 310

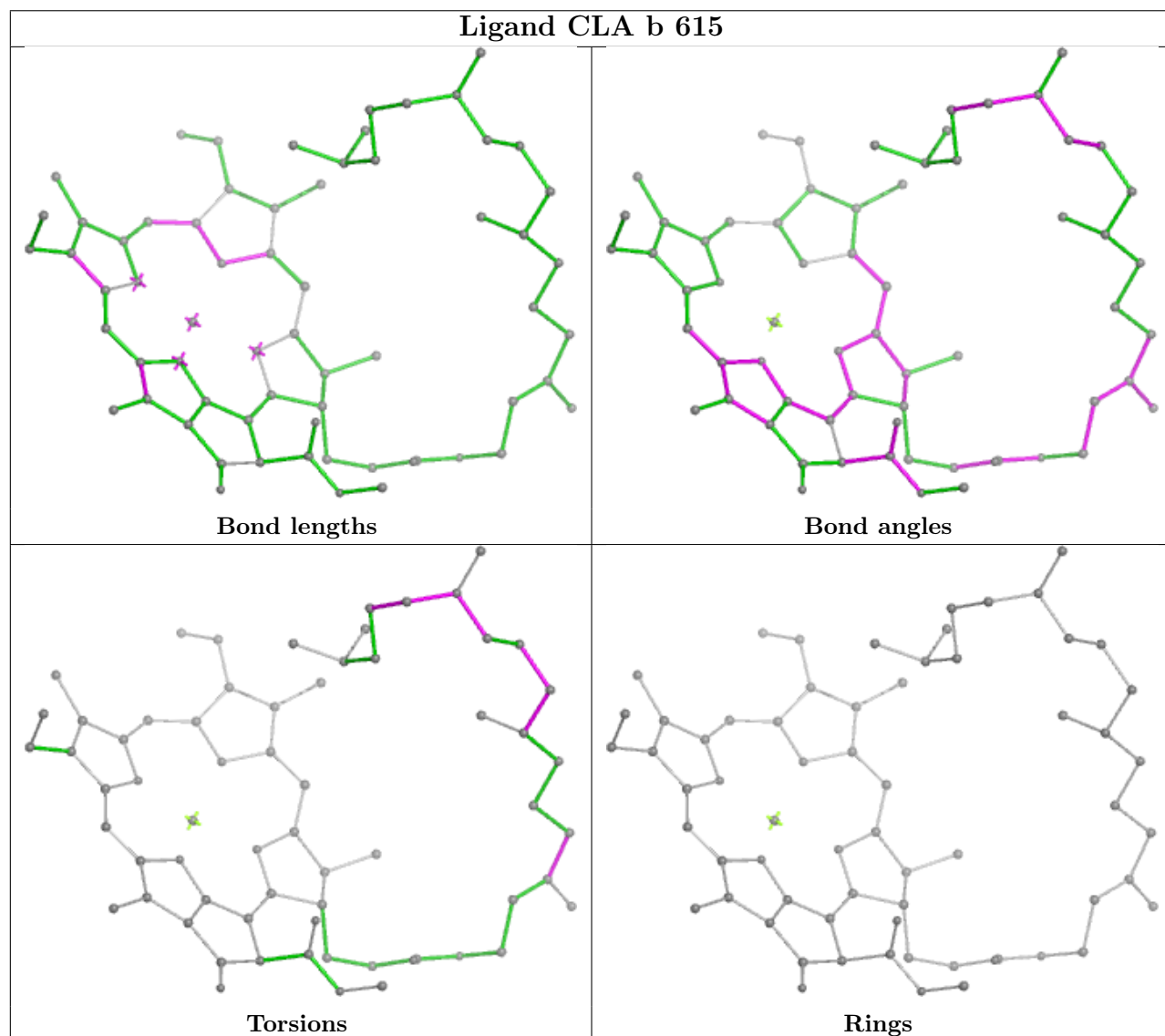
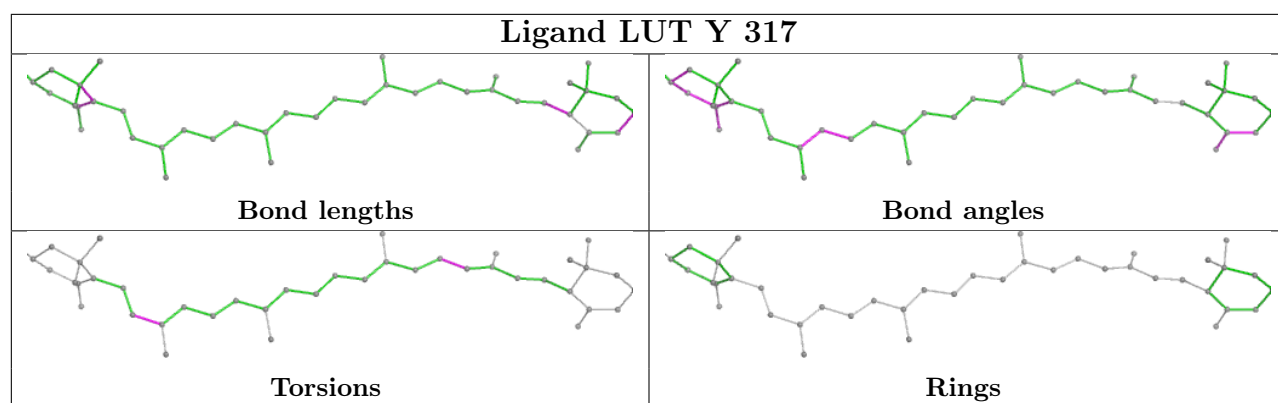


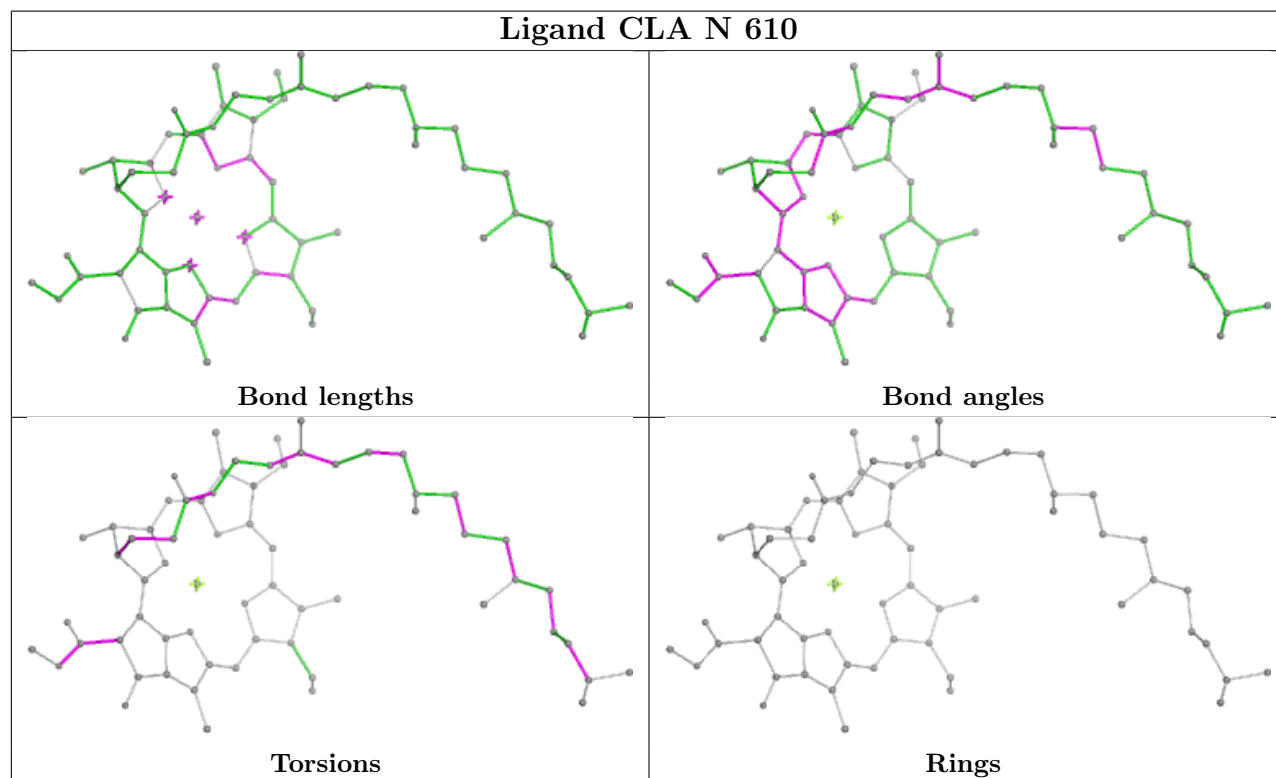
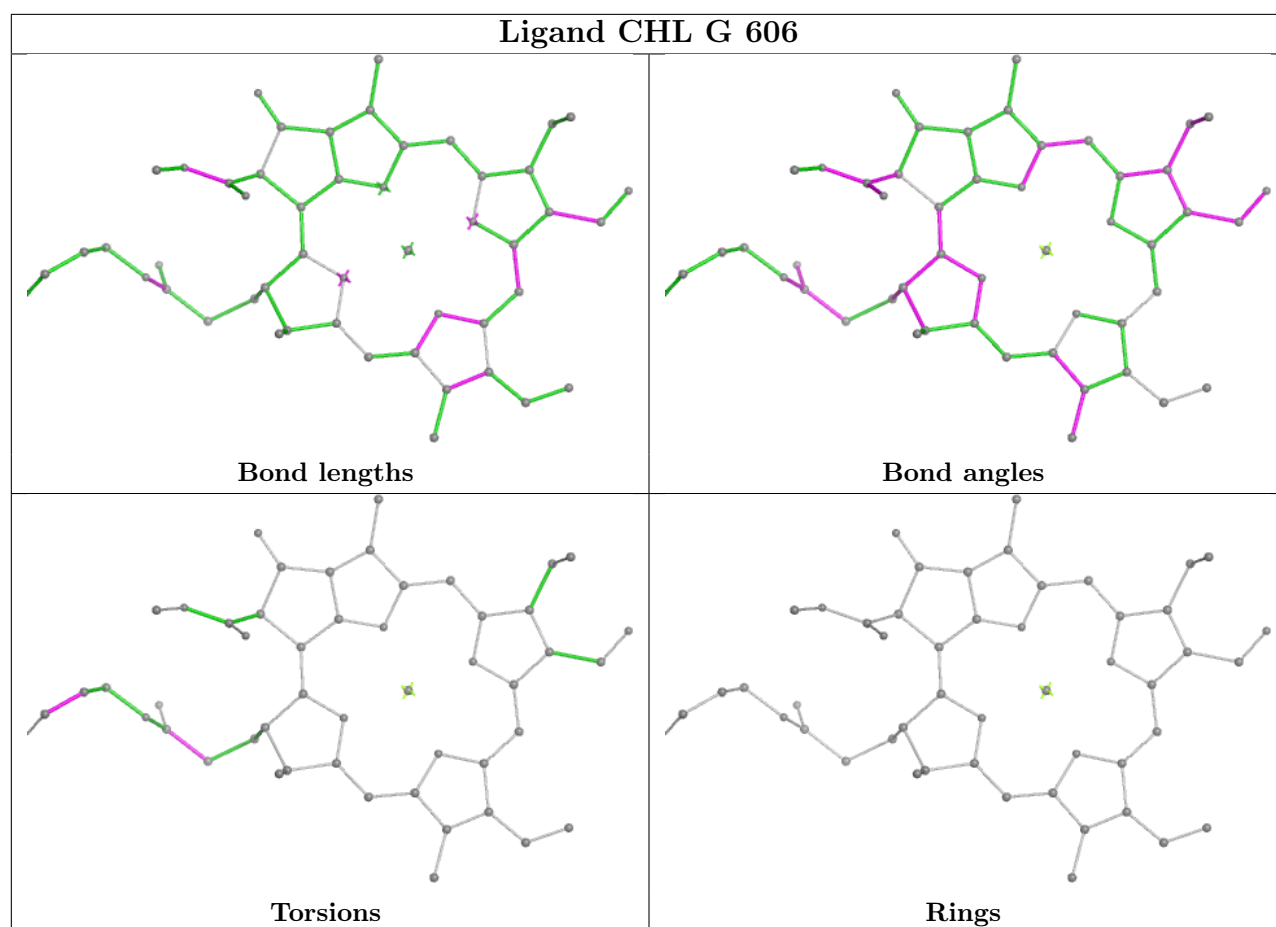
## Ligand CLA y 303



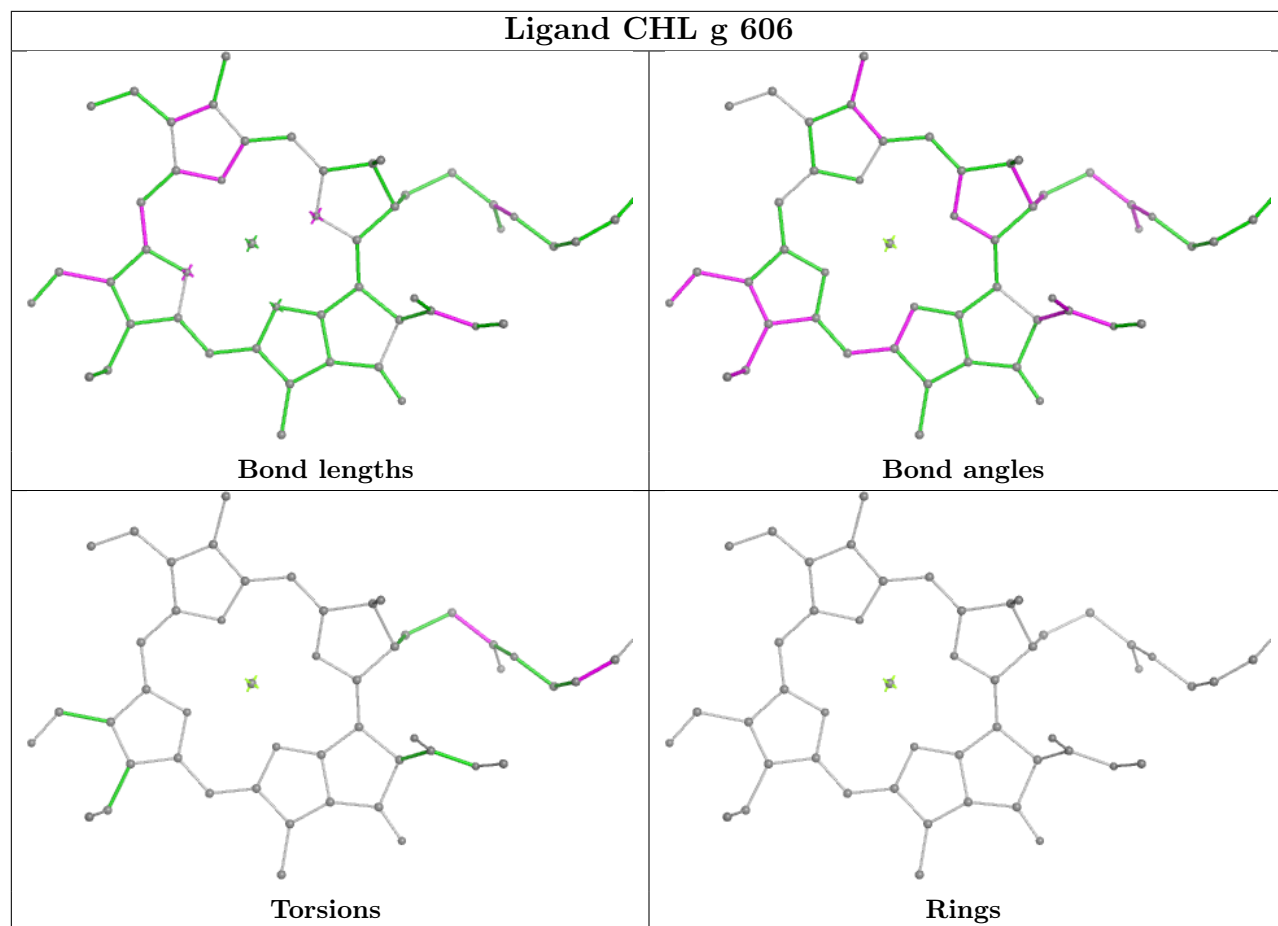
## Ligand AJP g 618



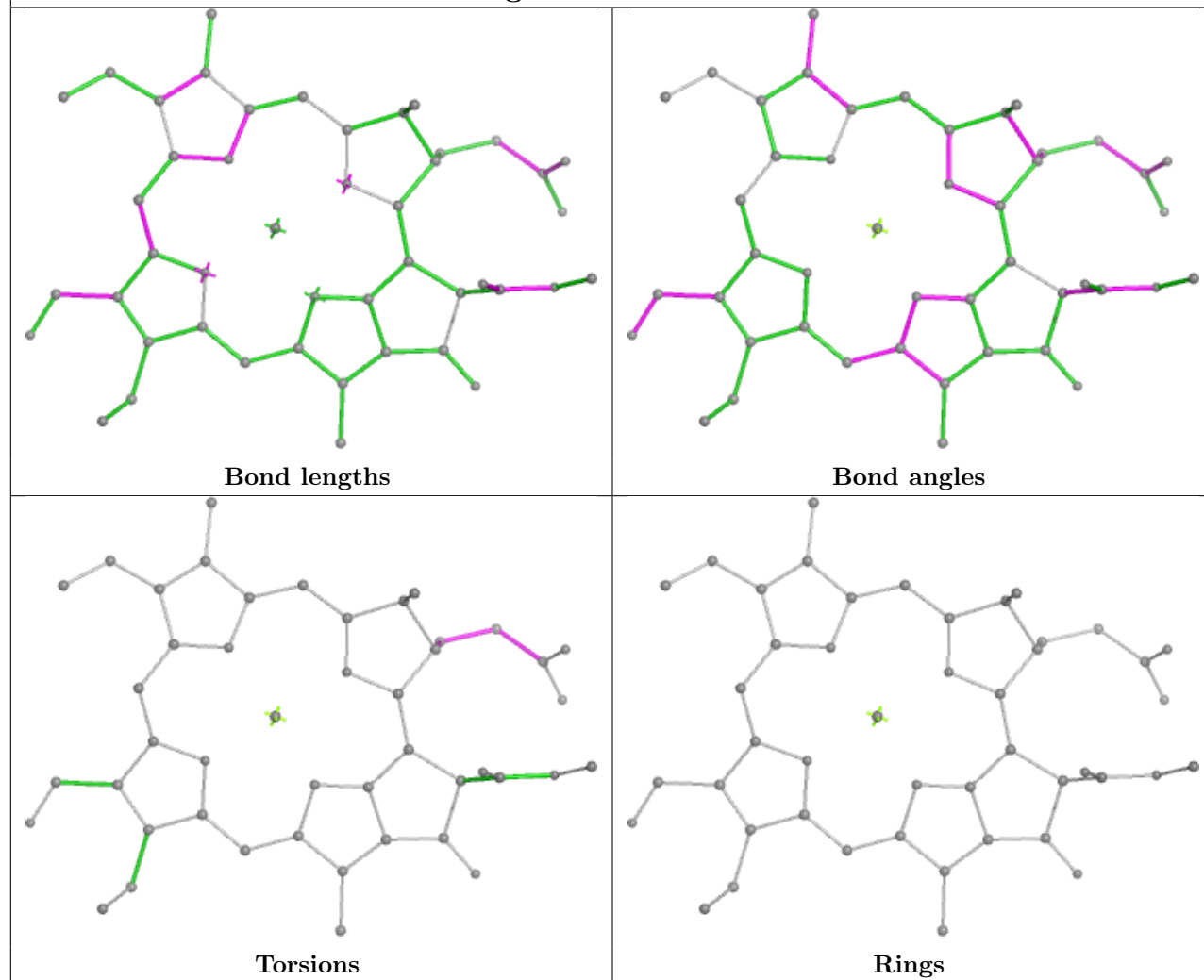




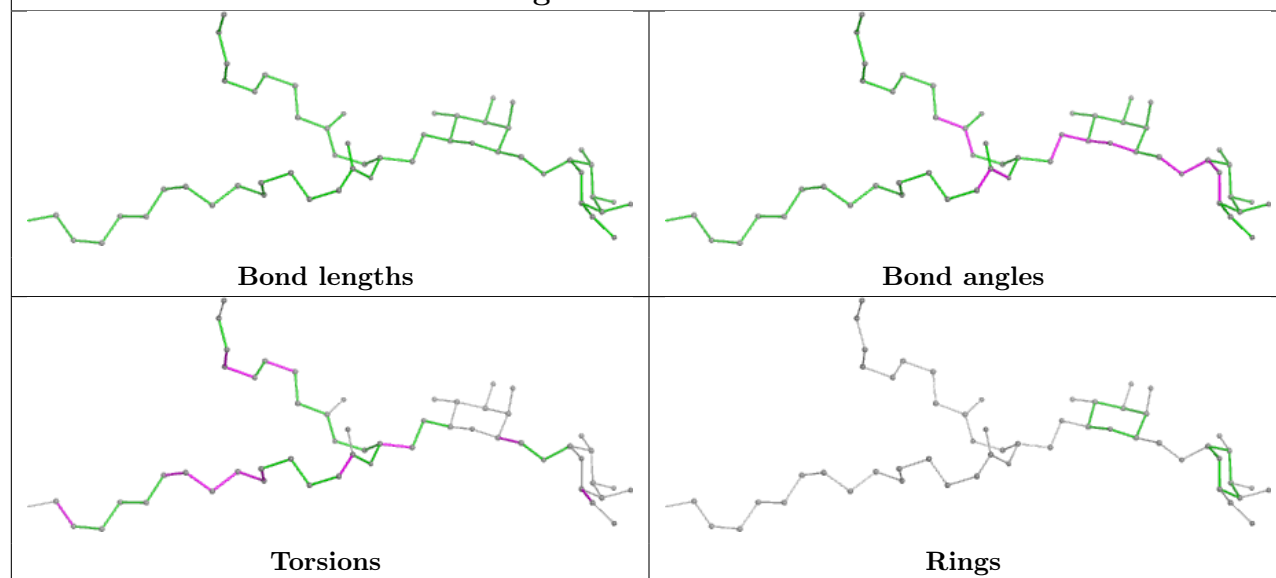


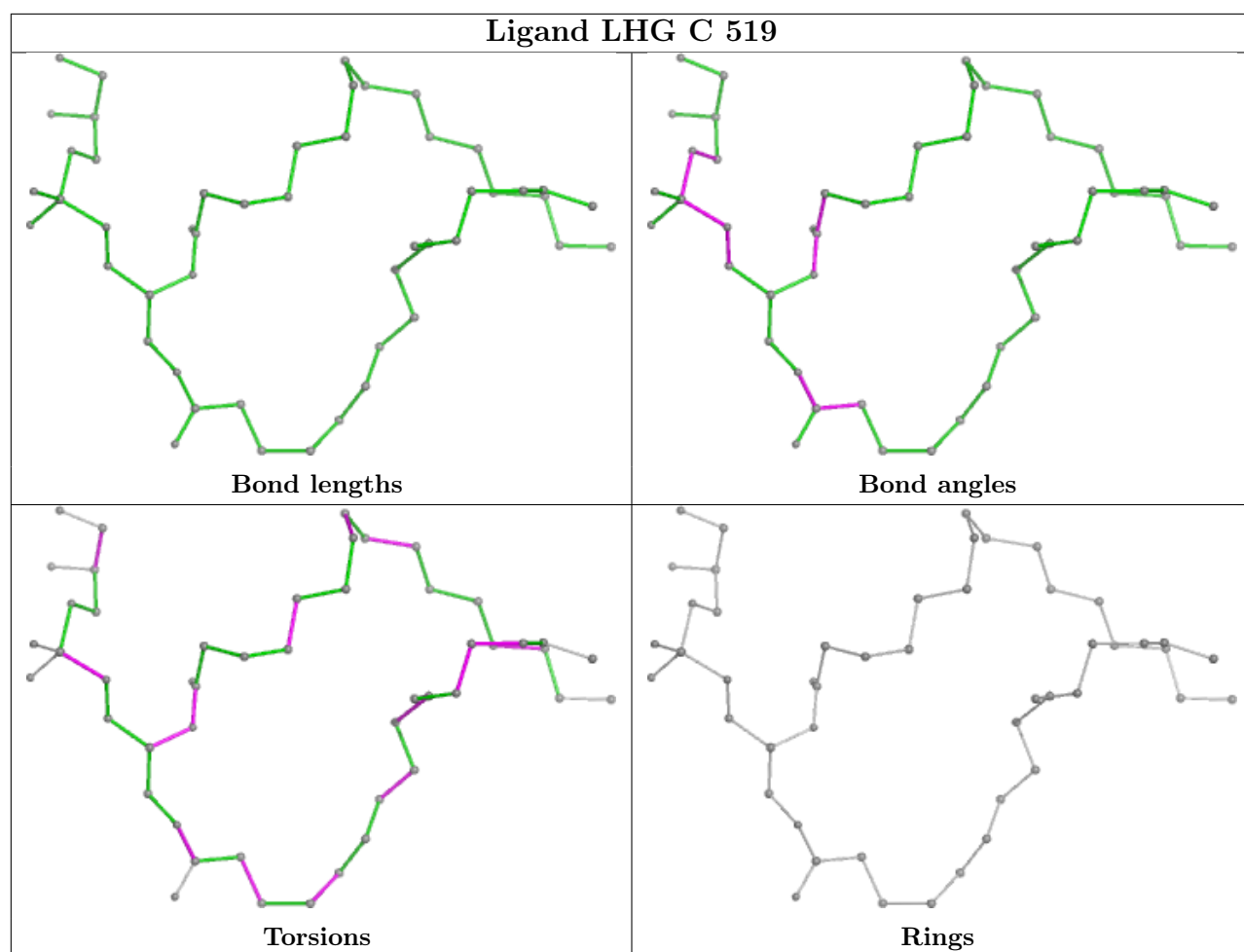


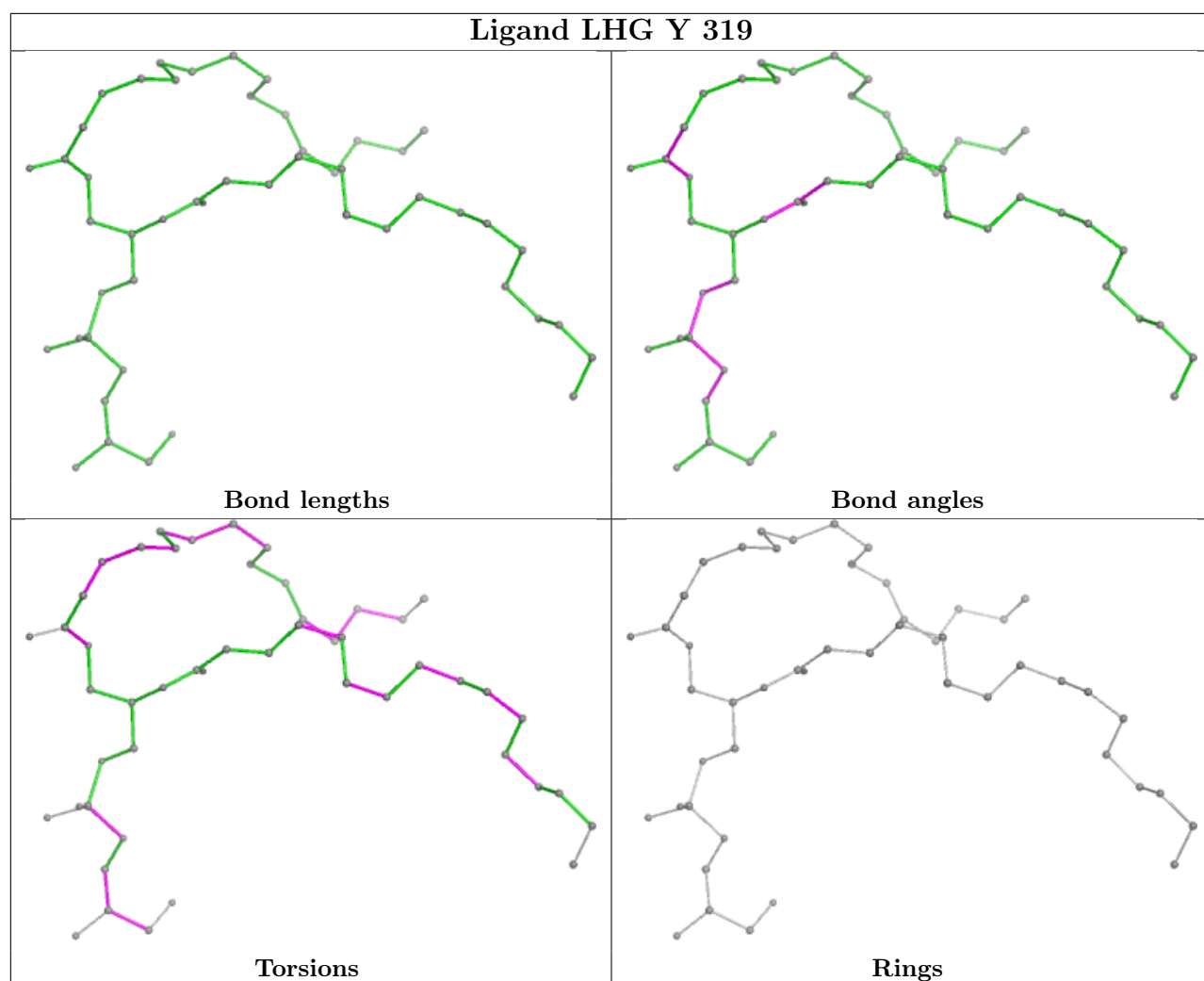
## Ligand CHL 5 302

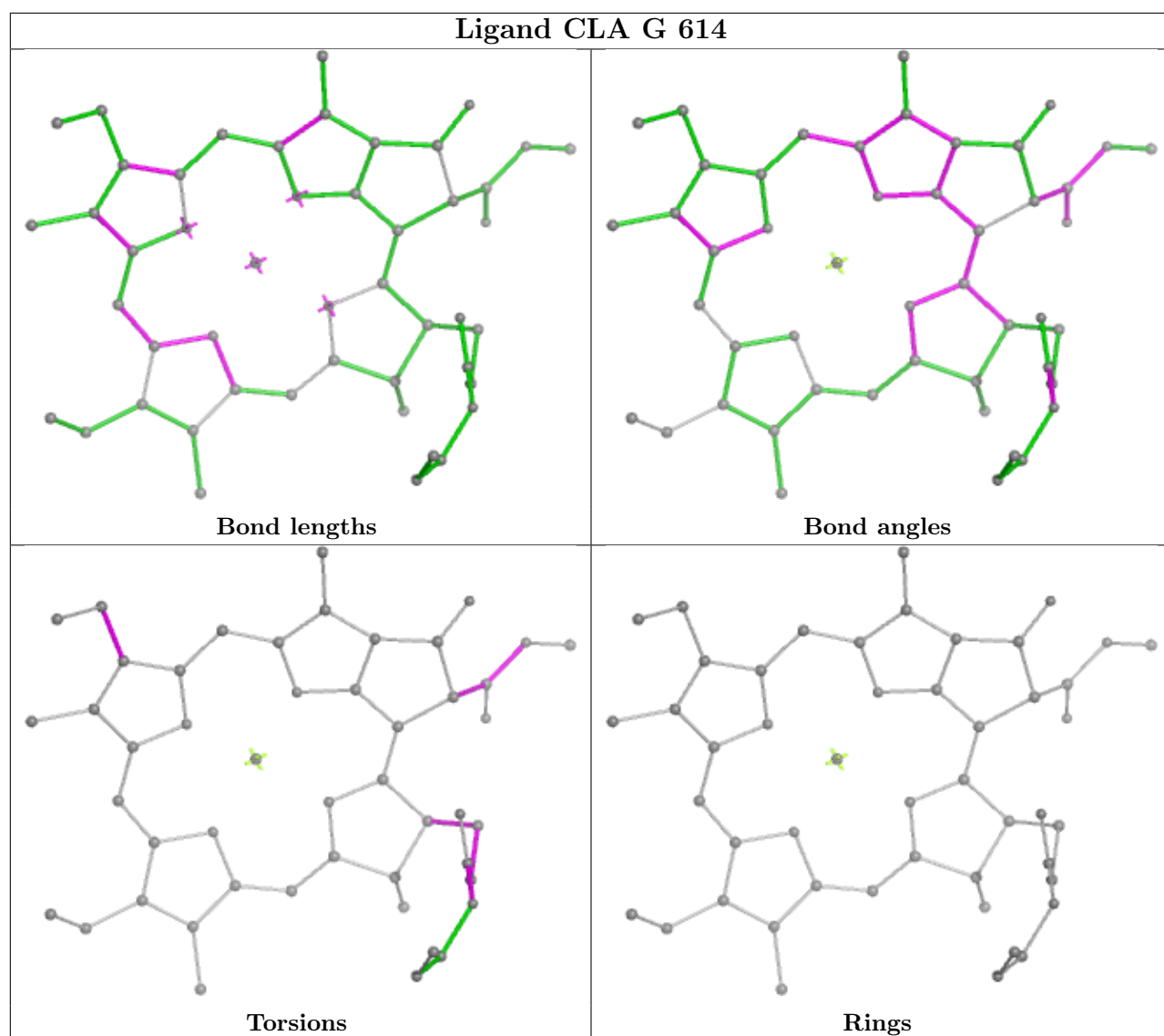


## Ligand DGD c 515

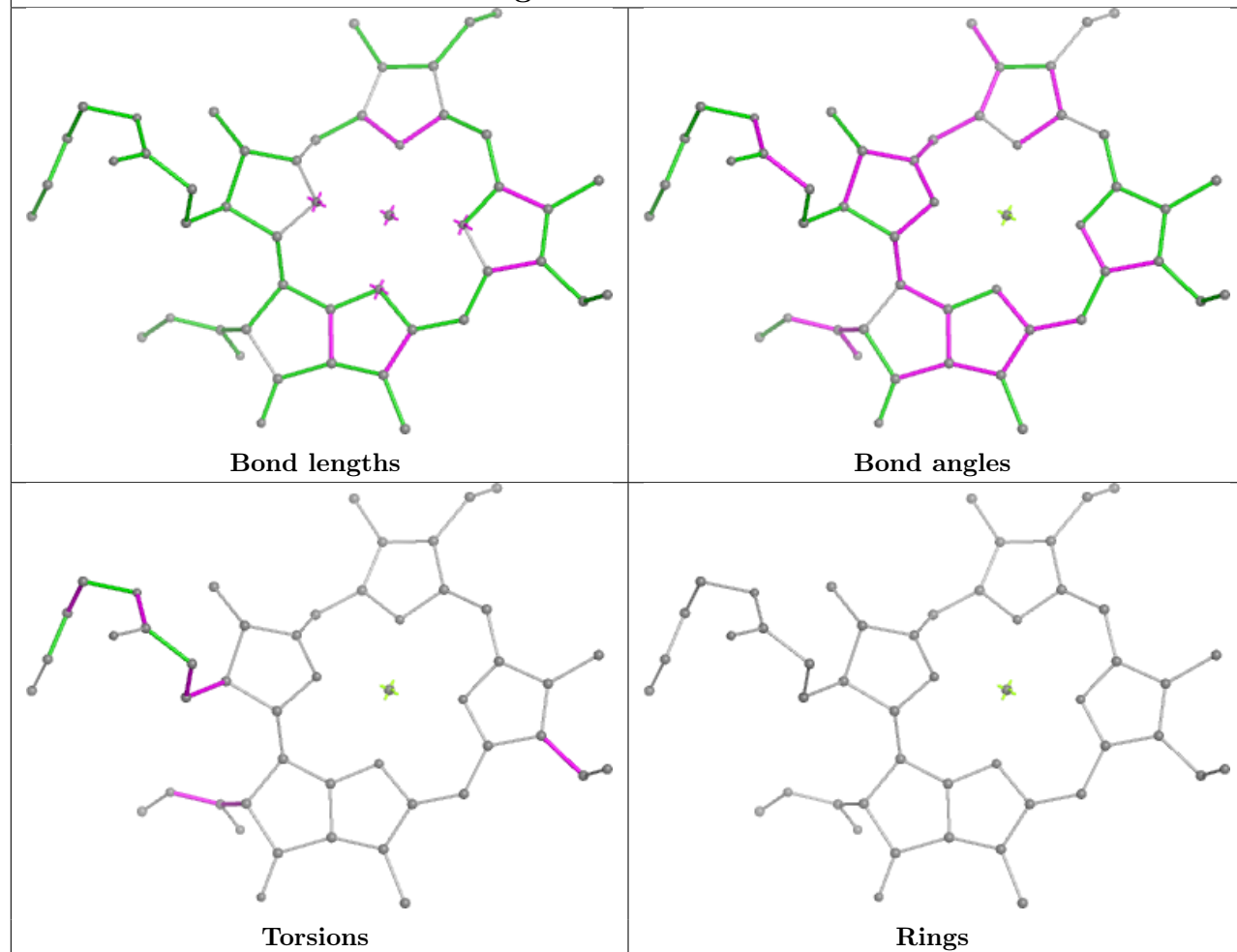




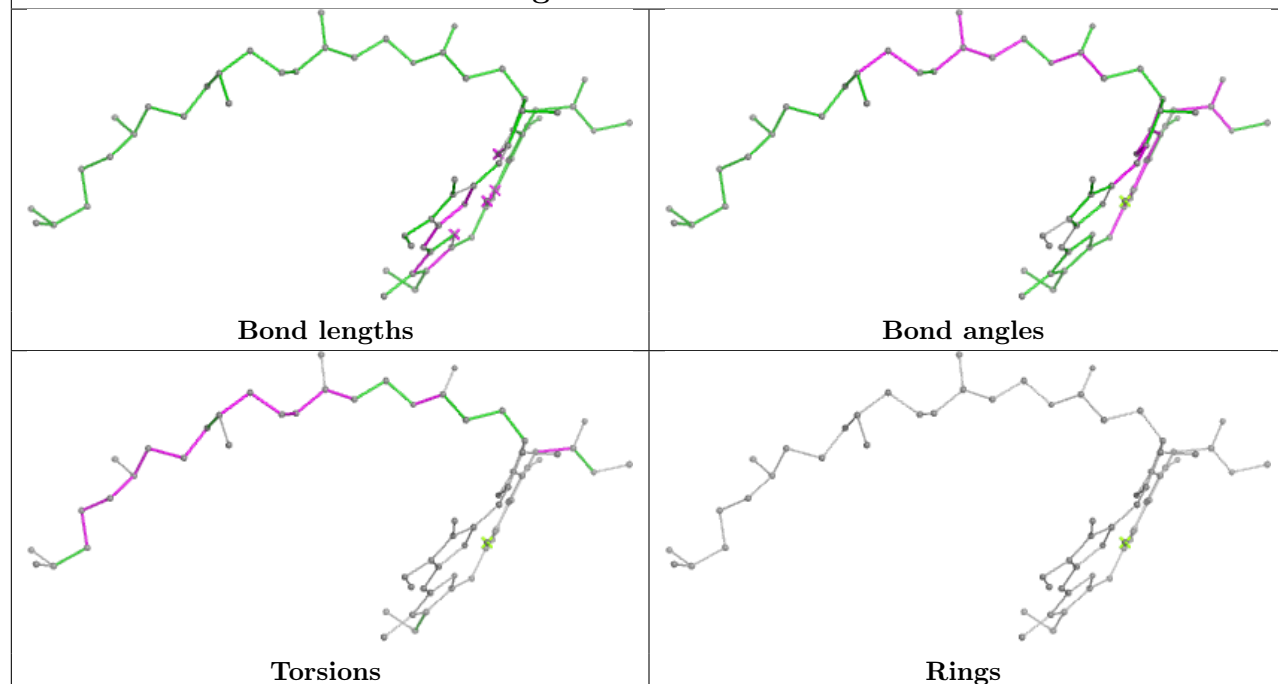




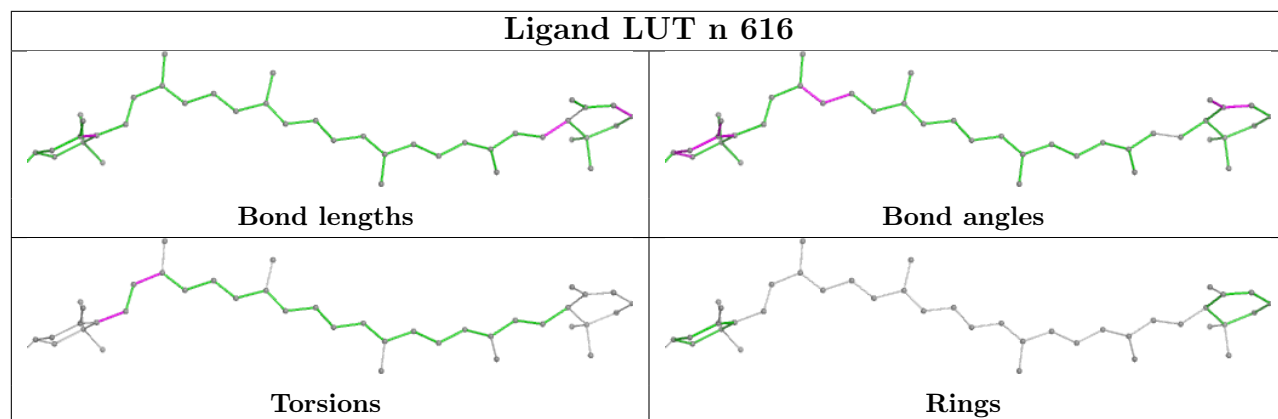
## Ligand CLA R 601



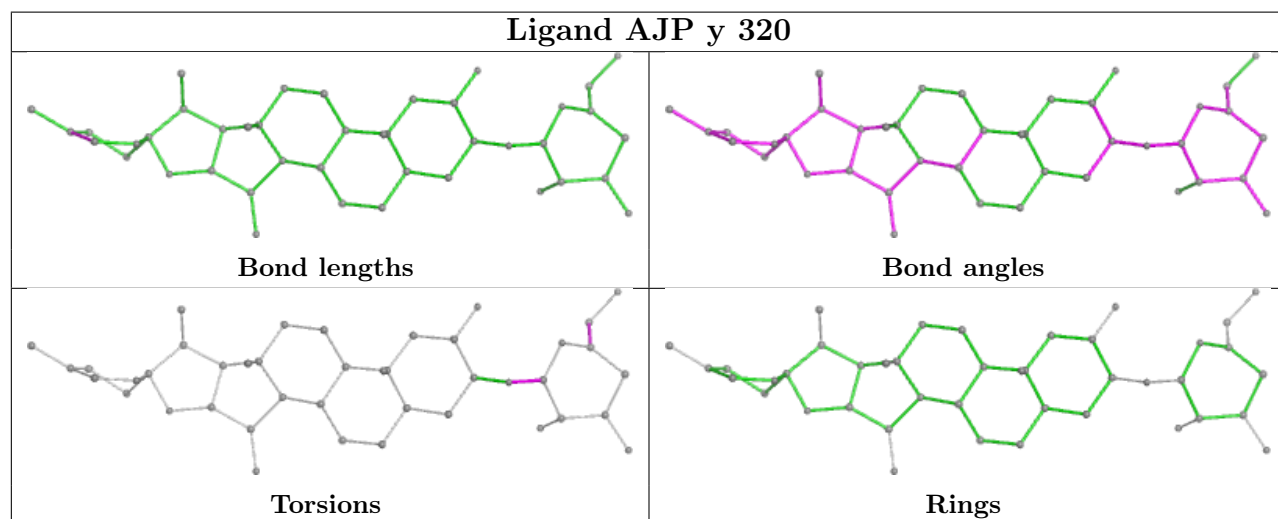
## Ligand CLA B 607



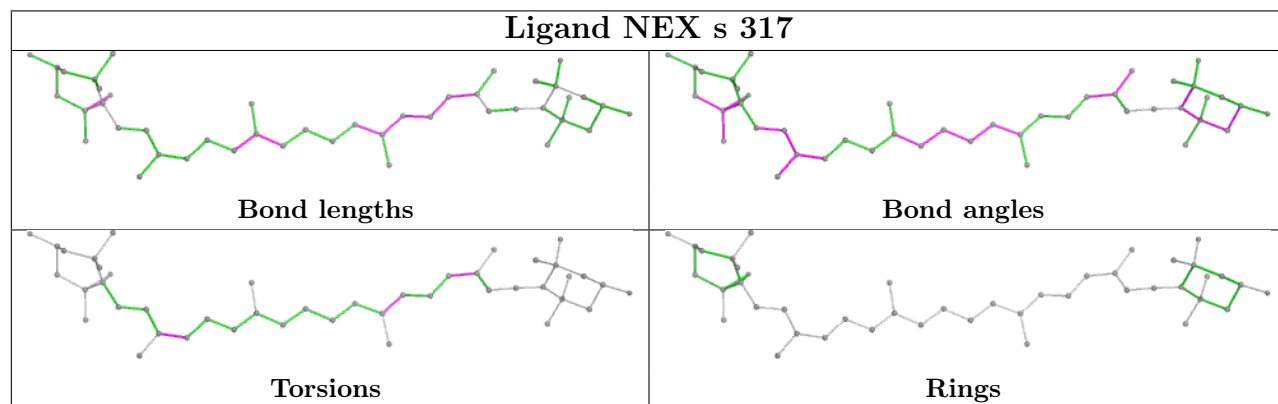
## Ligand LUT n 616



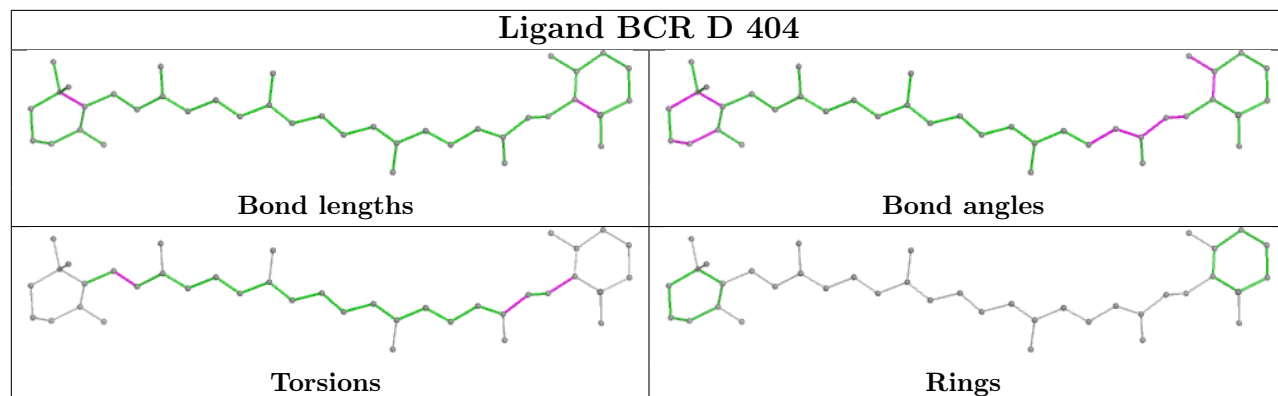
## Ligand AJP y 320

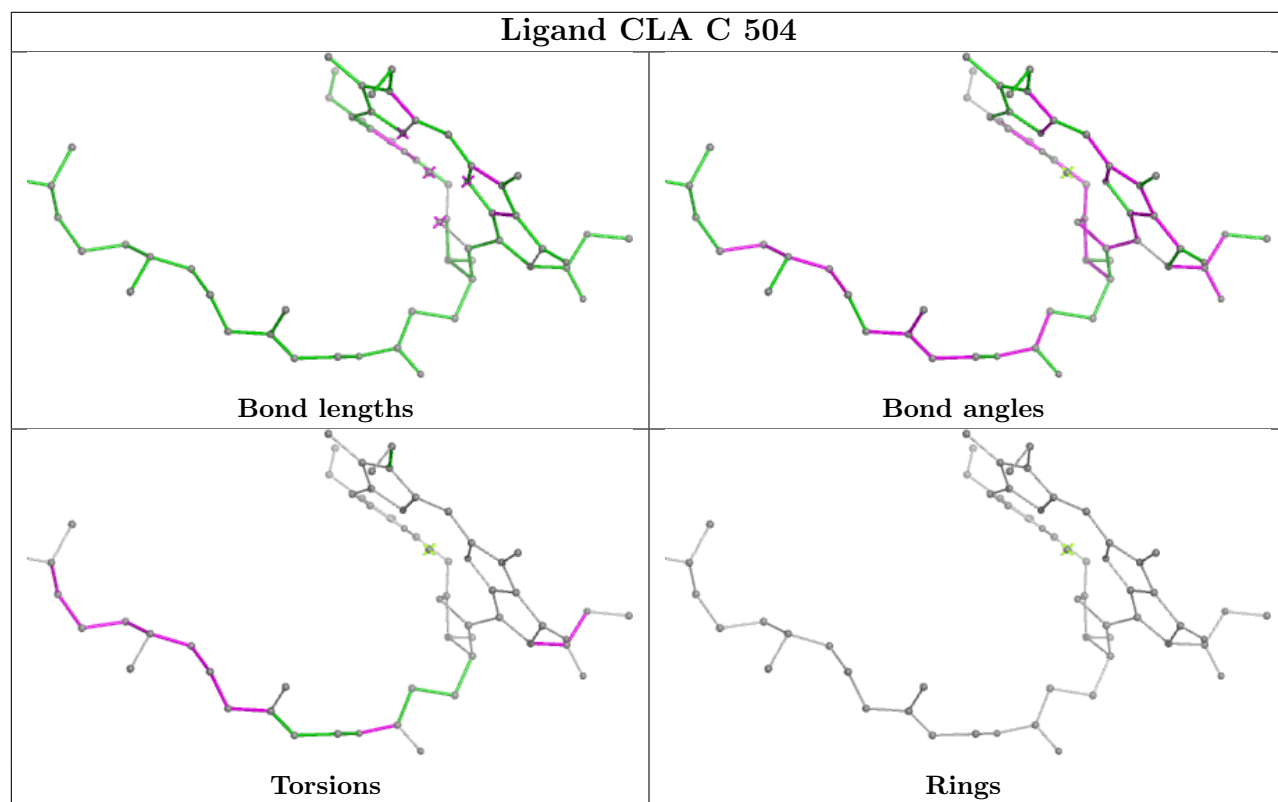
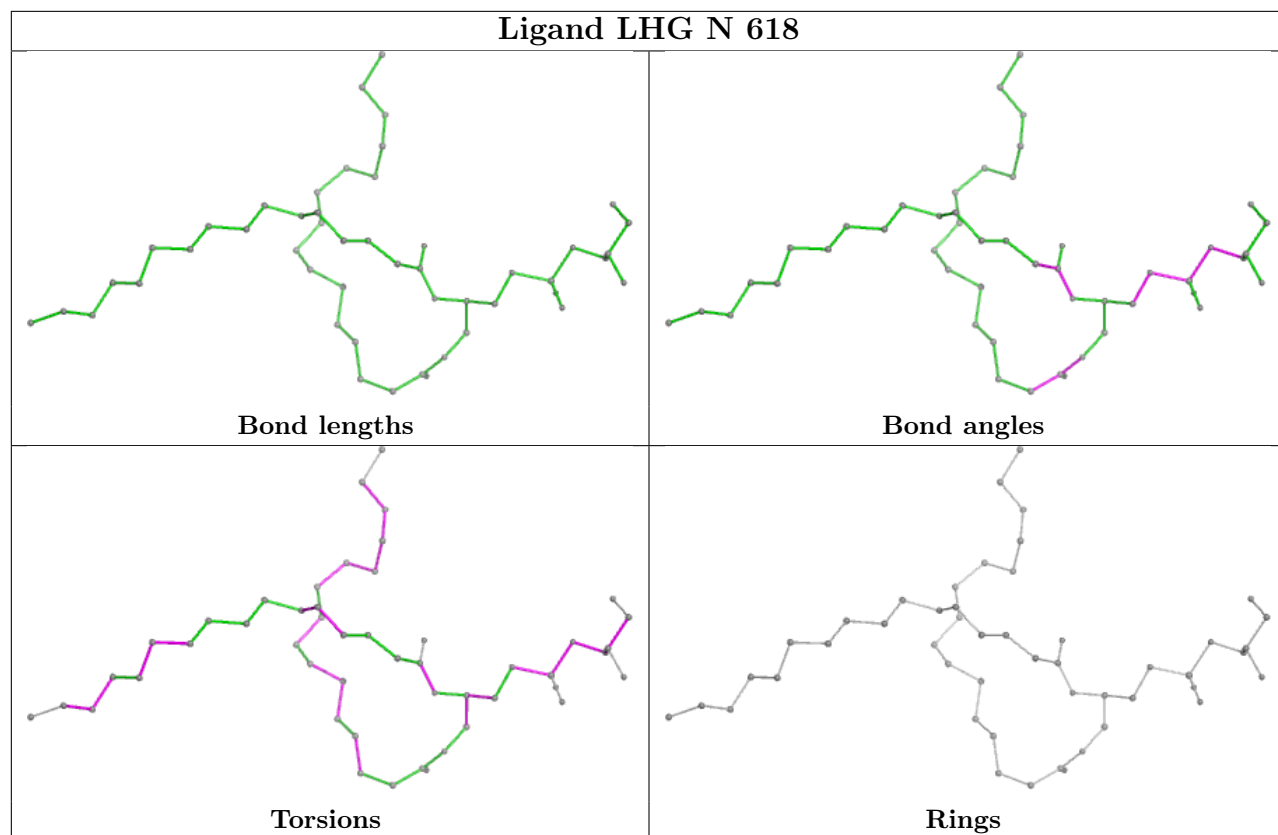


## Ligand NEX s 317

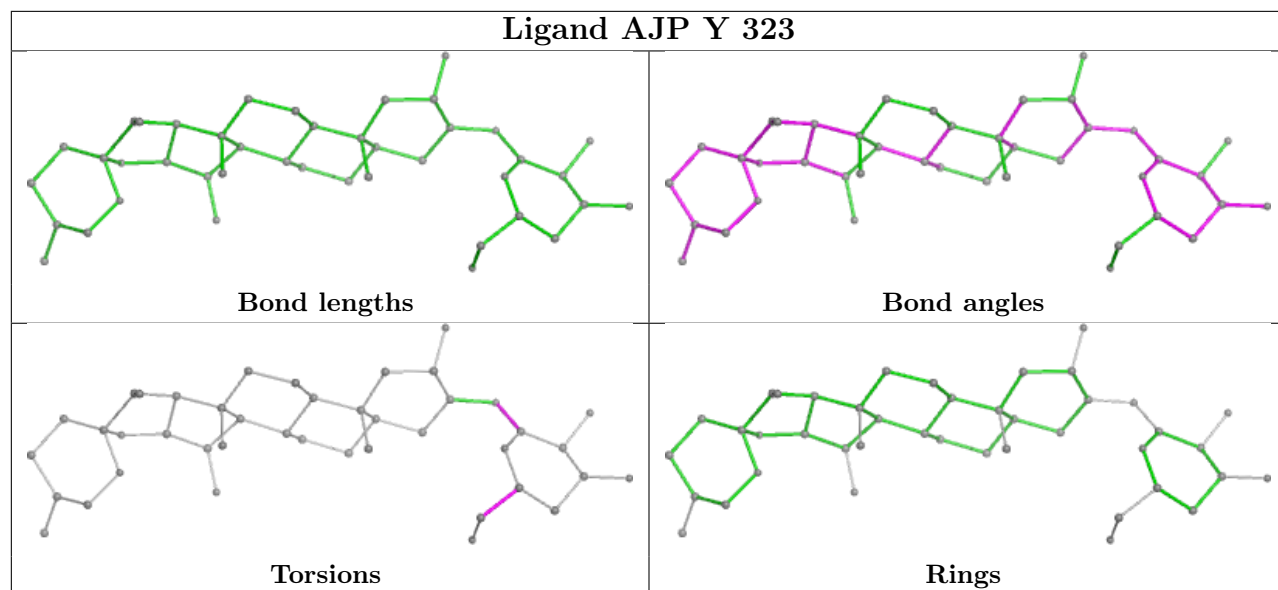


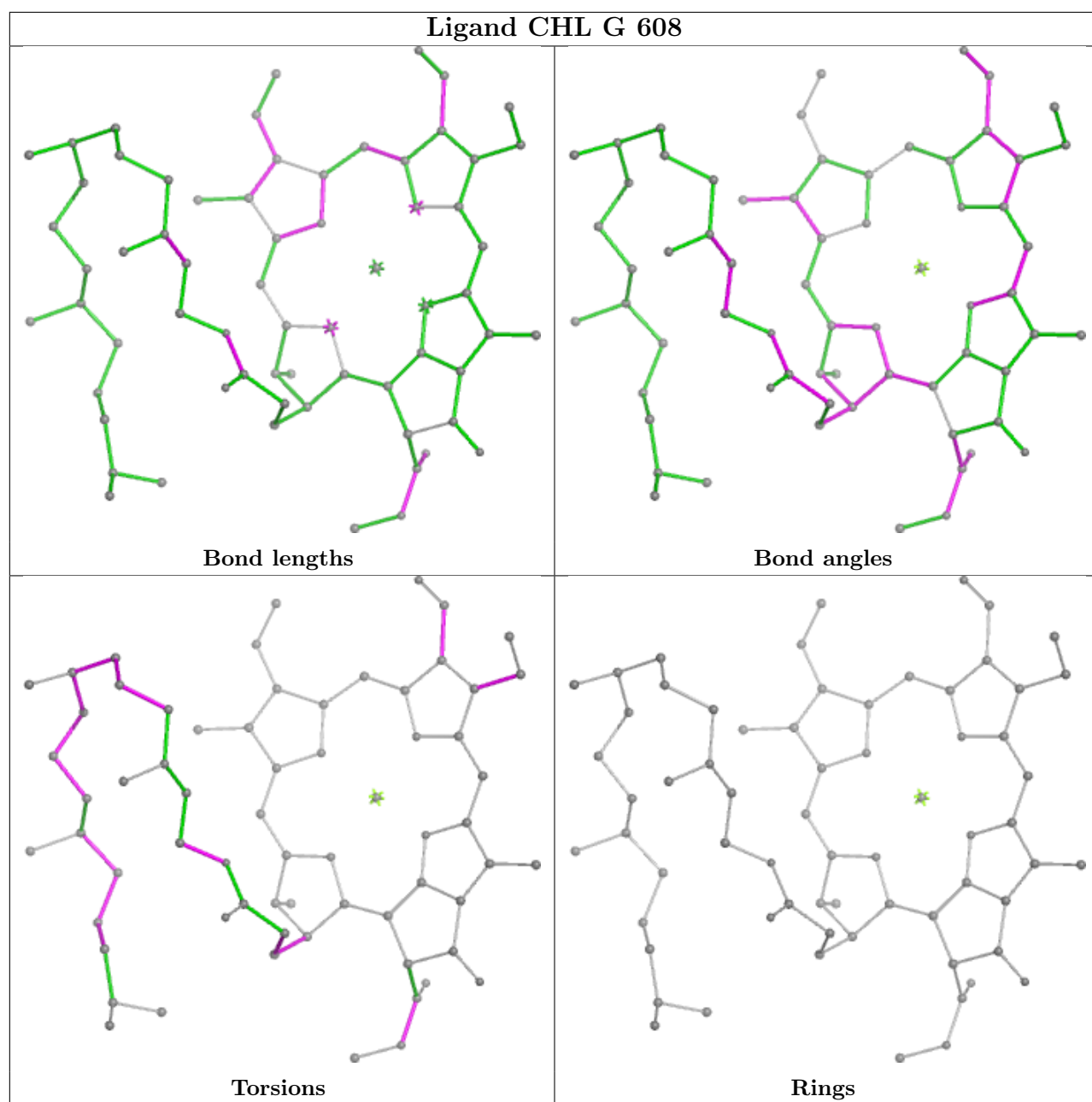
## Ligand BCR D 404

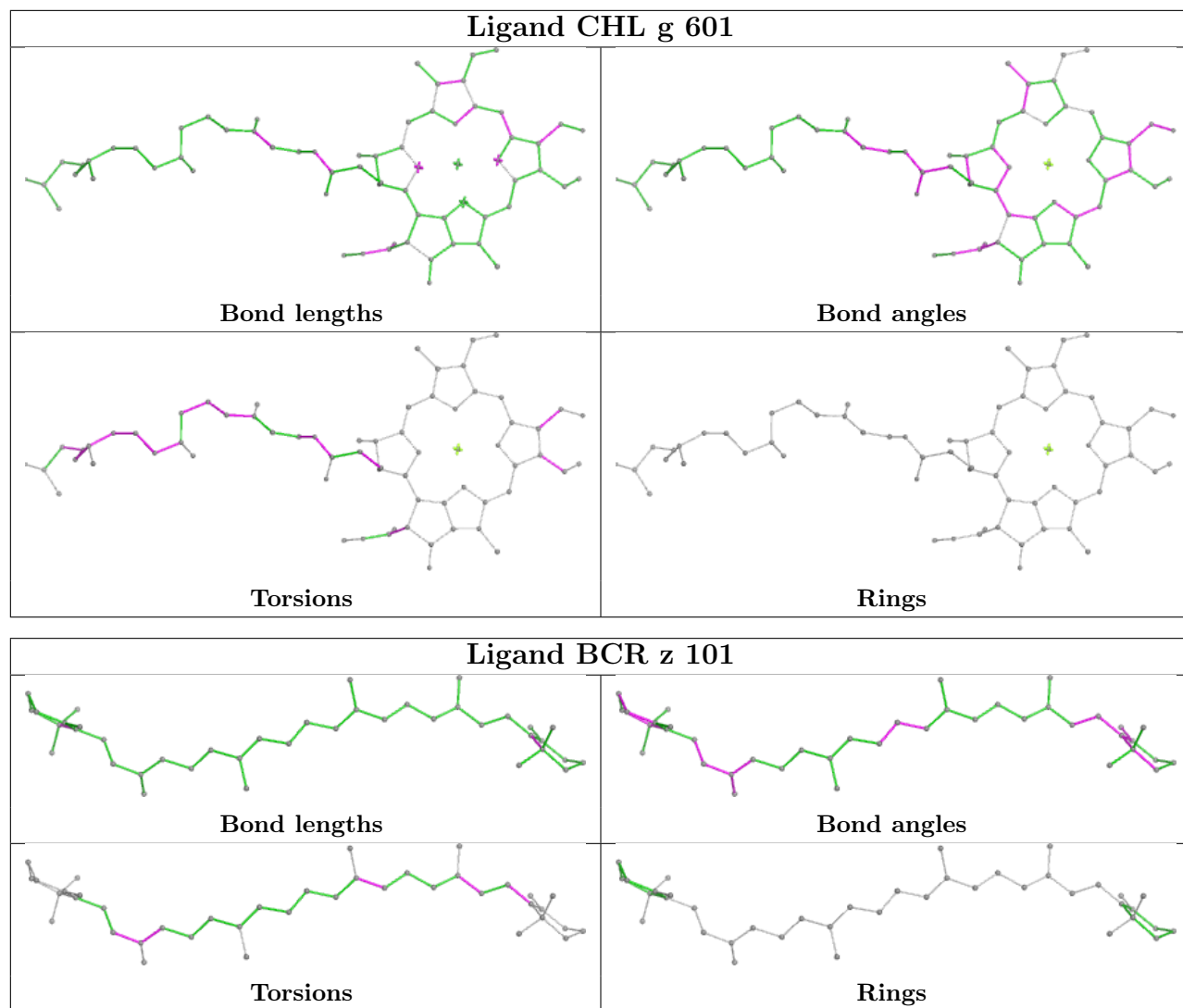




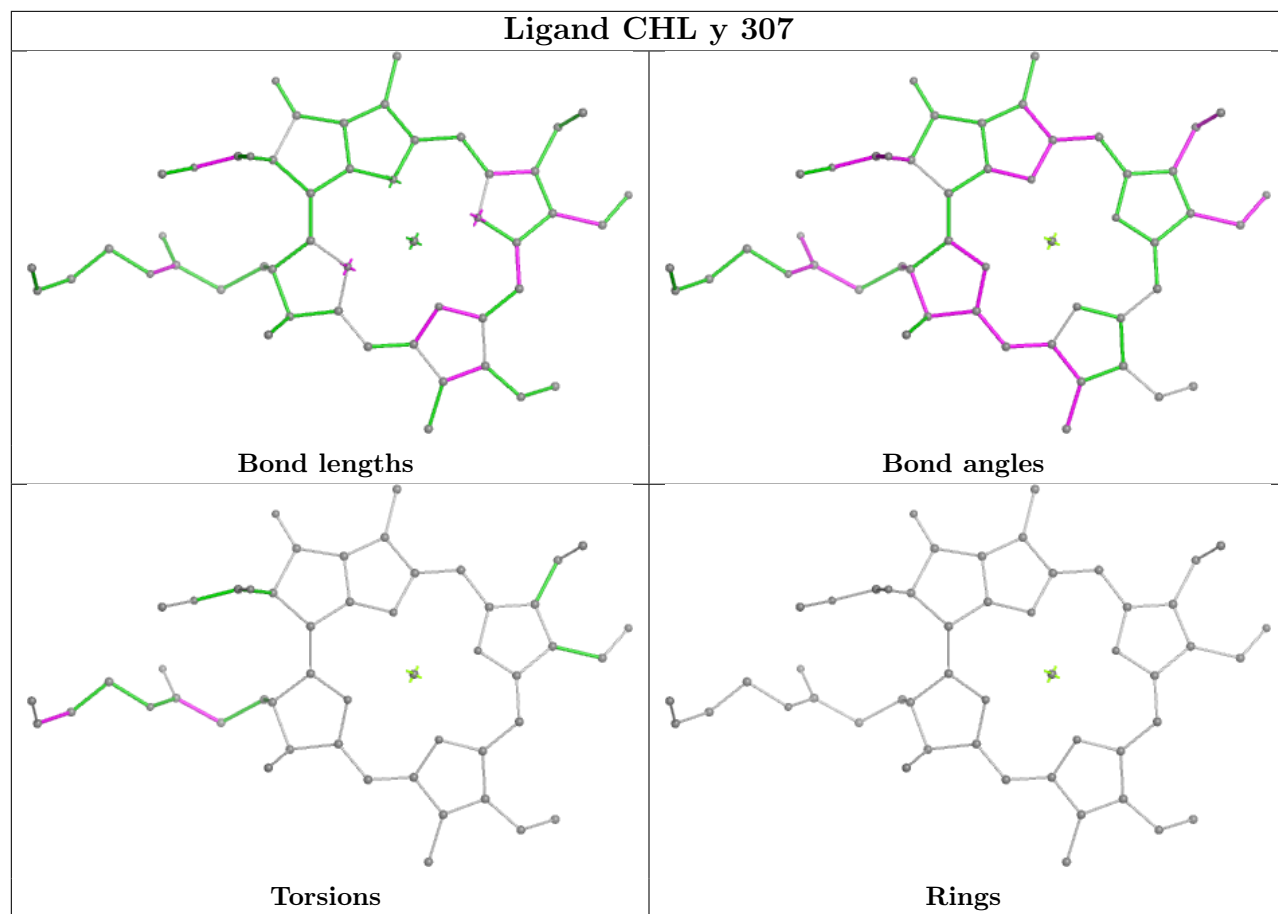




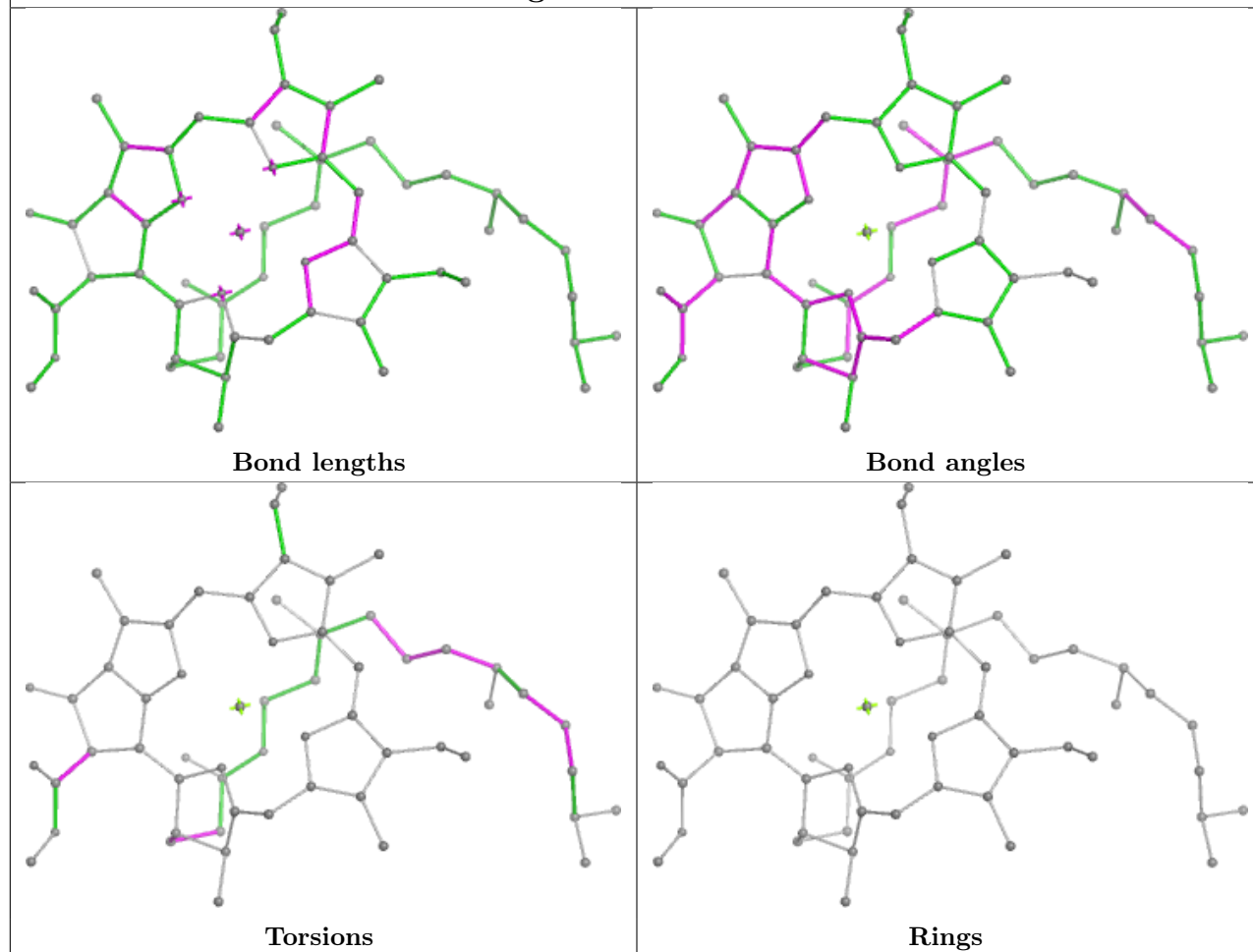




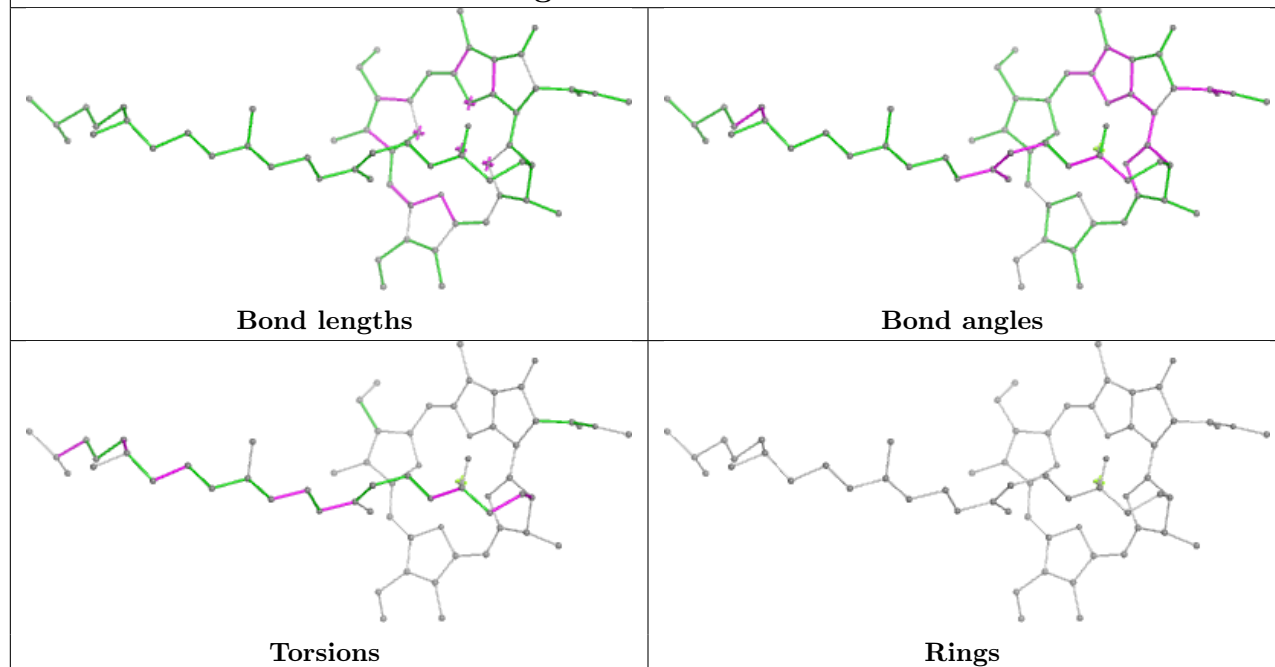
## Ligand CHL y 307

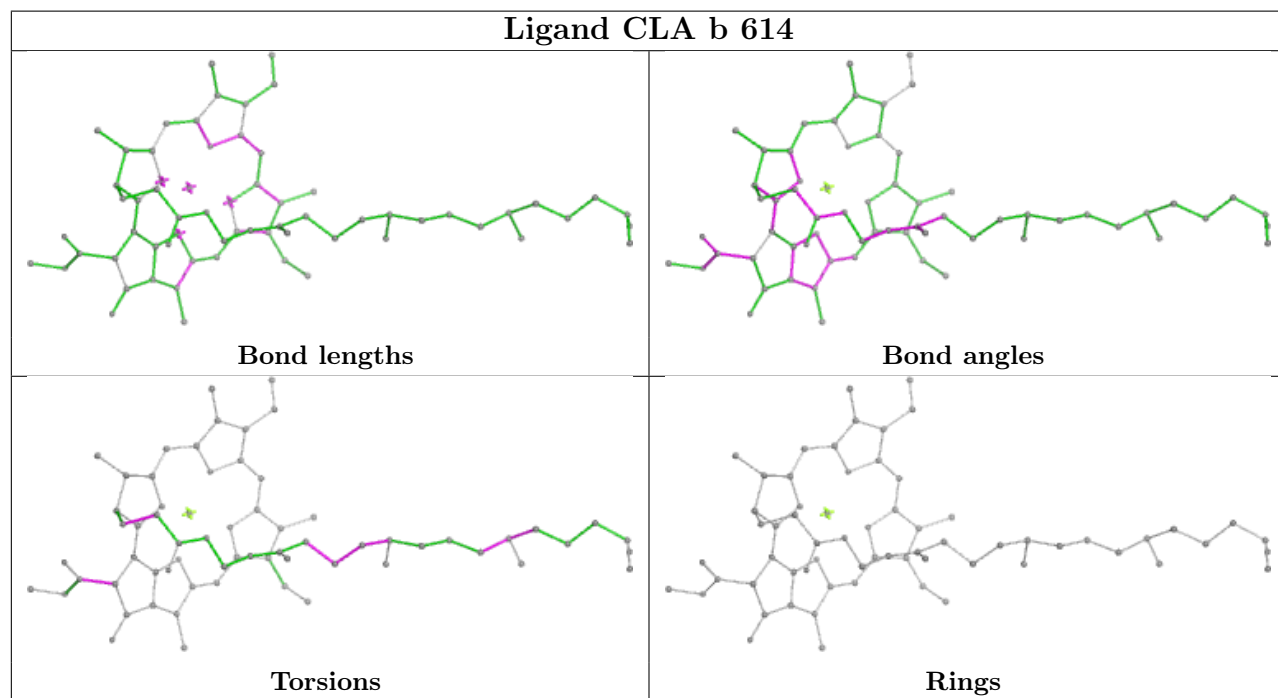
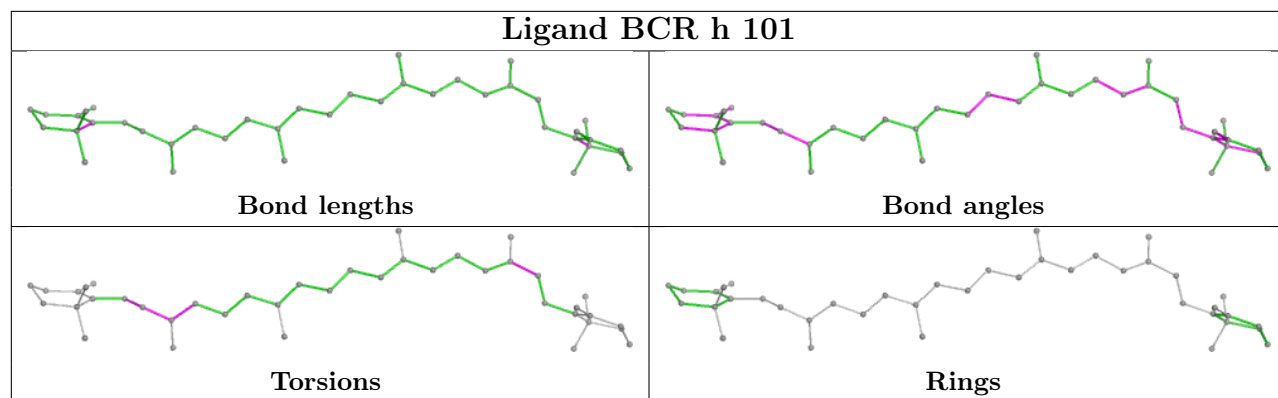


## Ligand CLA r 612

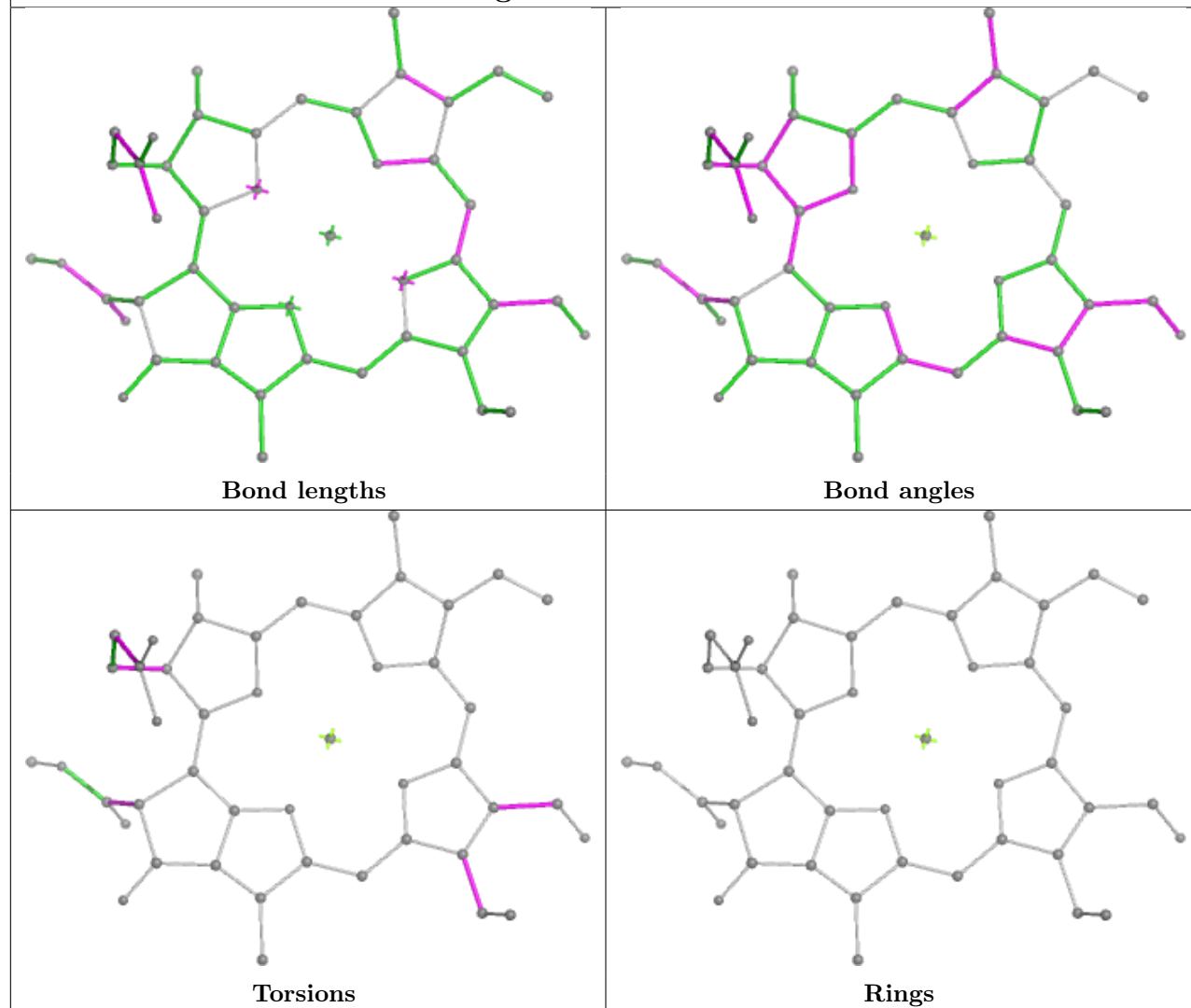


## Ligand CLA b 608

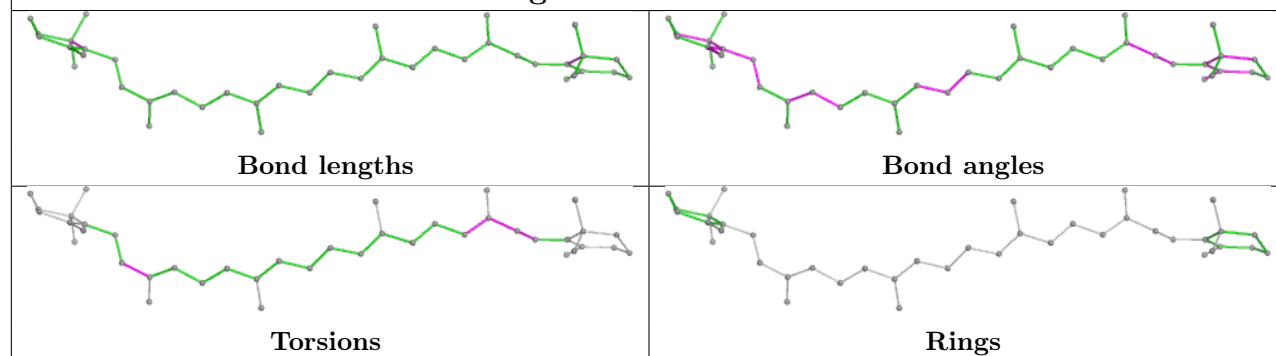


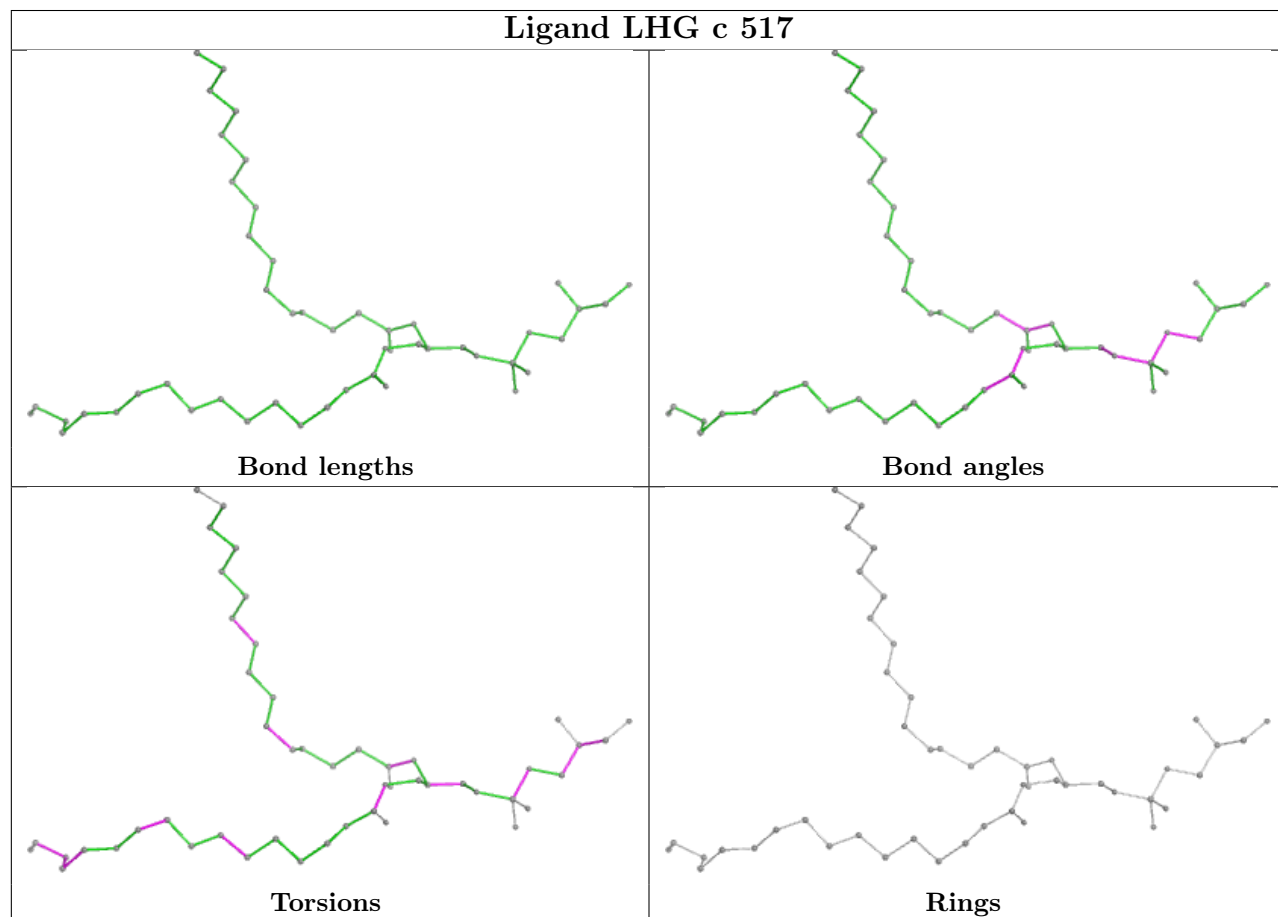
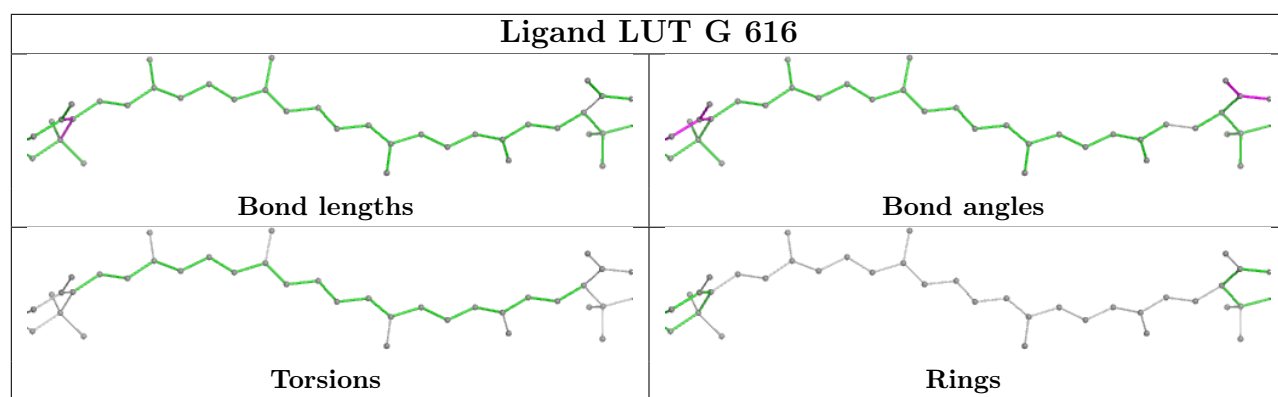


## Ligand CHL G 605

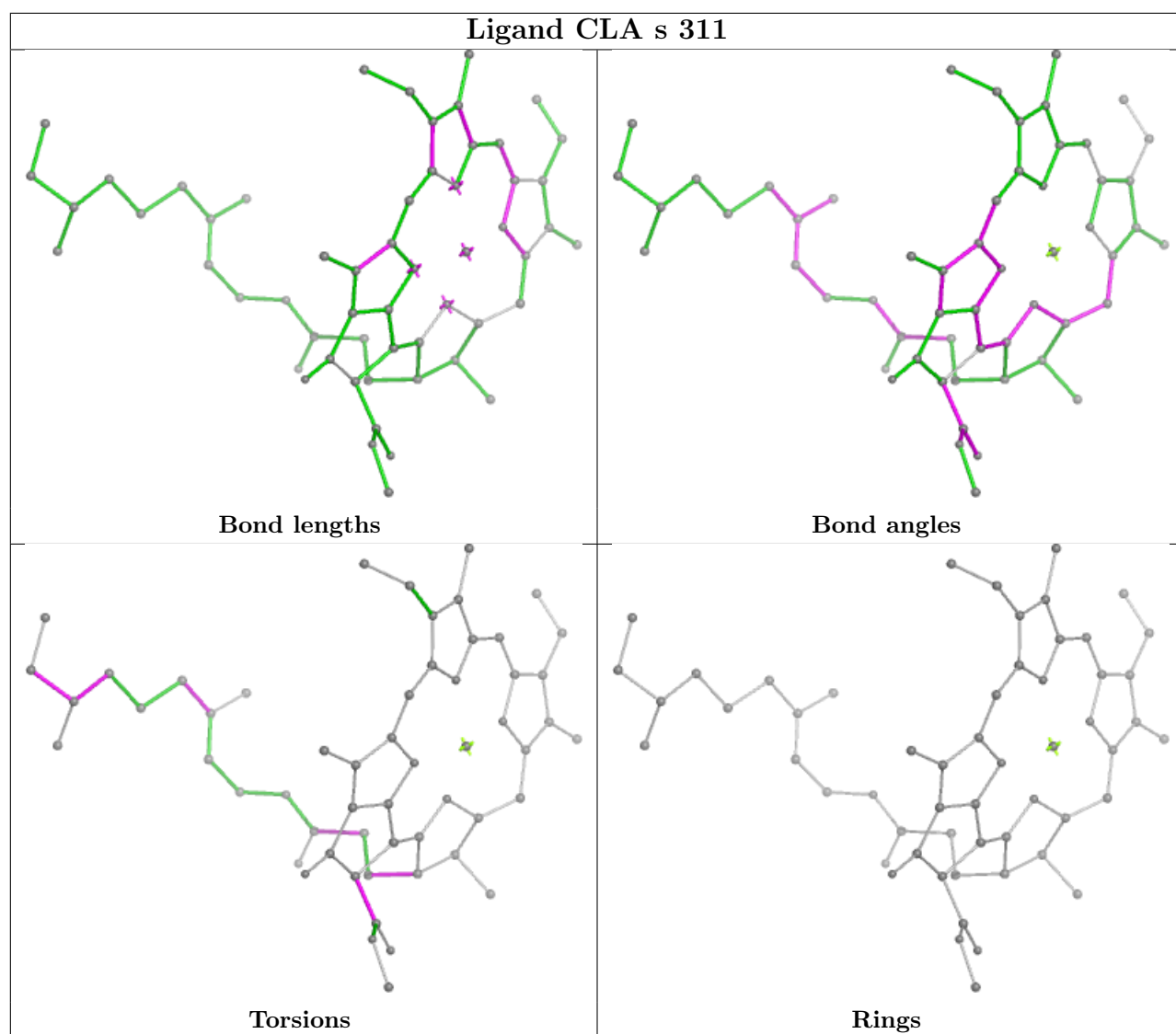


## Ligand BCR H 101

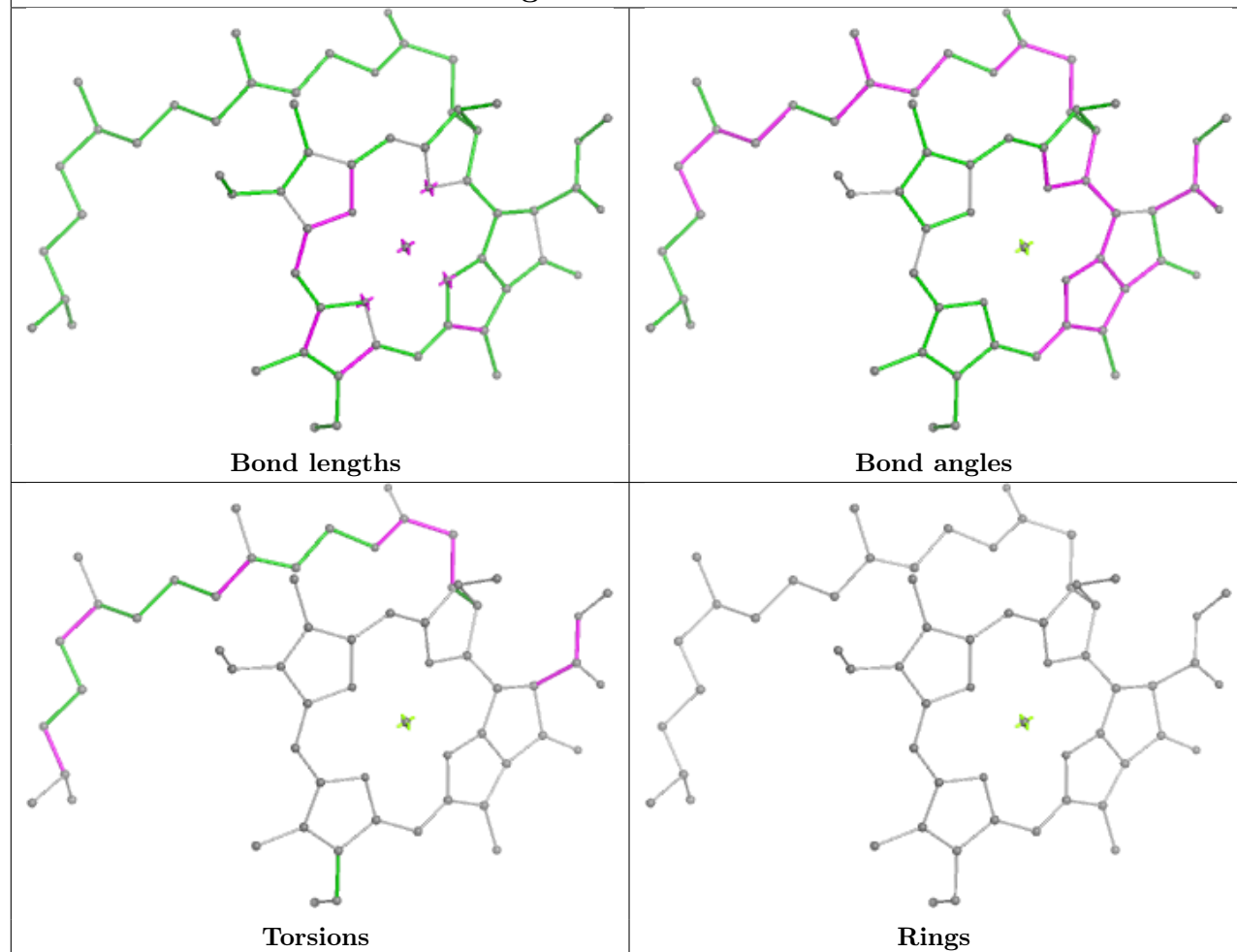




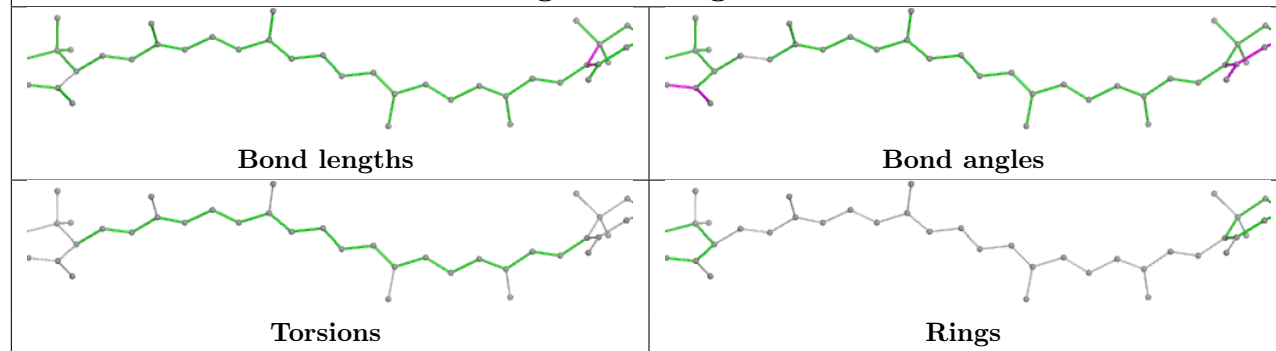




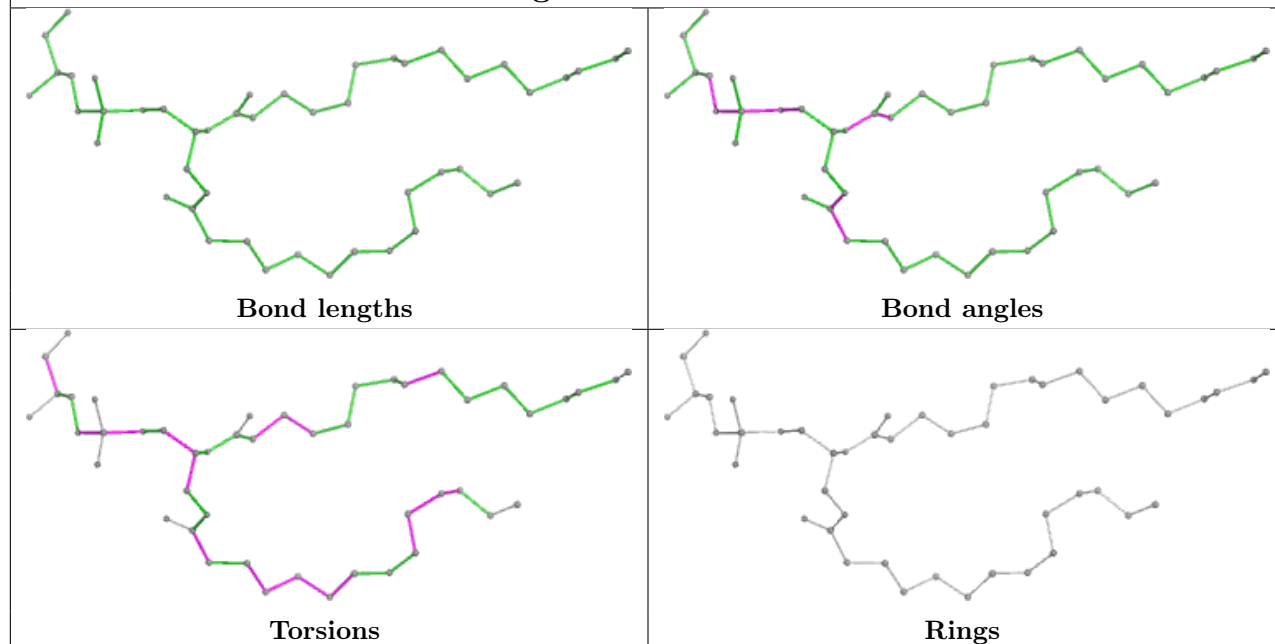
## Ligand CLA r 602



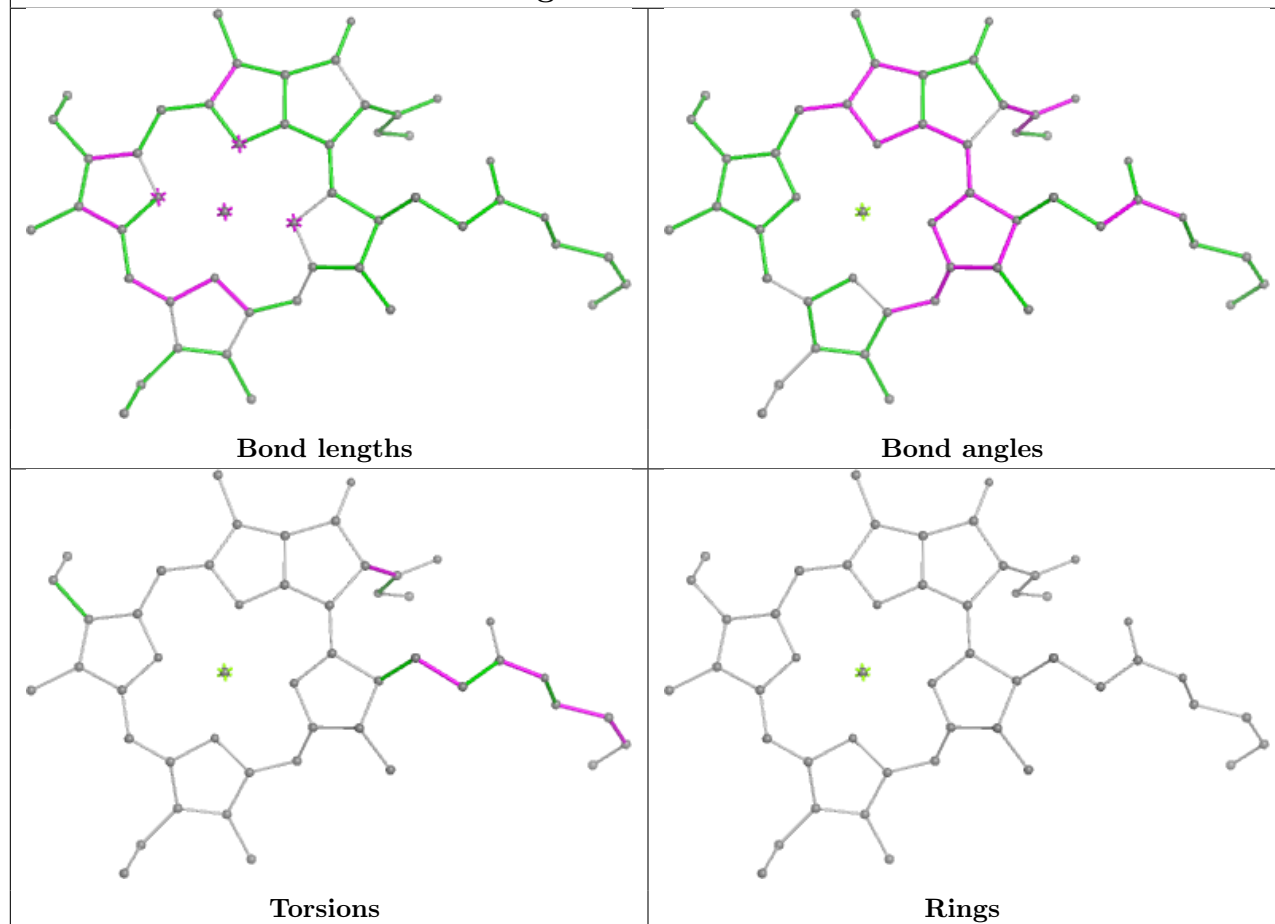
## Ligand LUT g 616



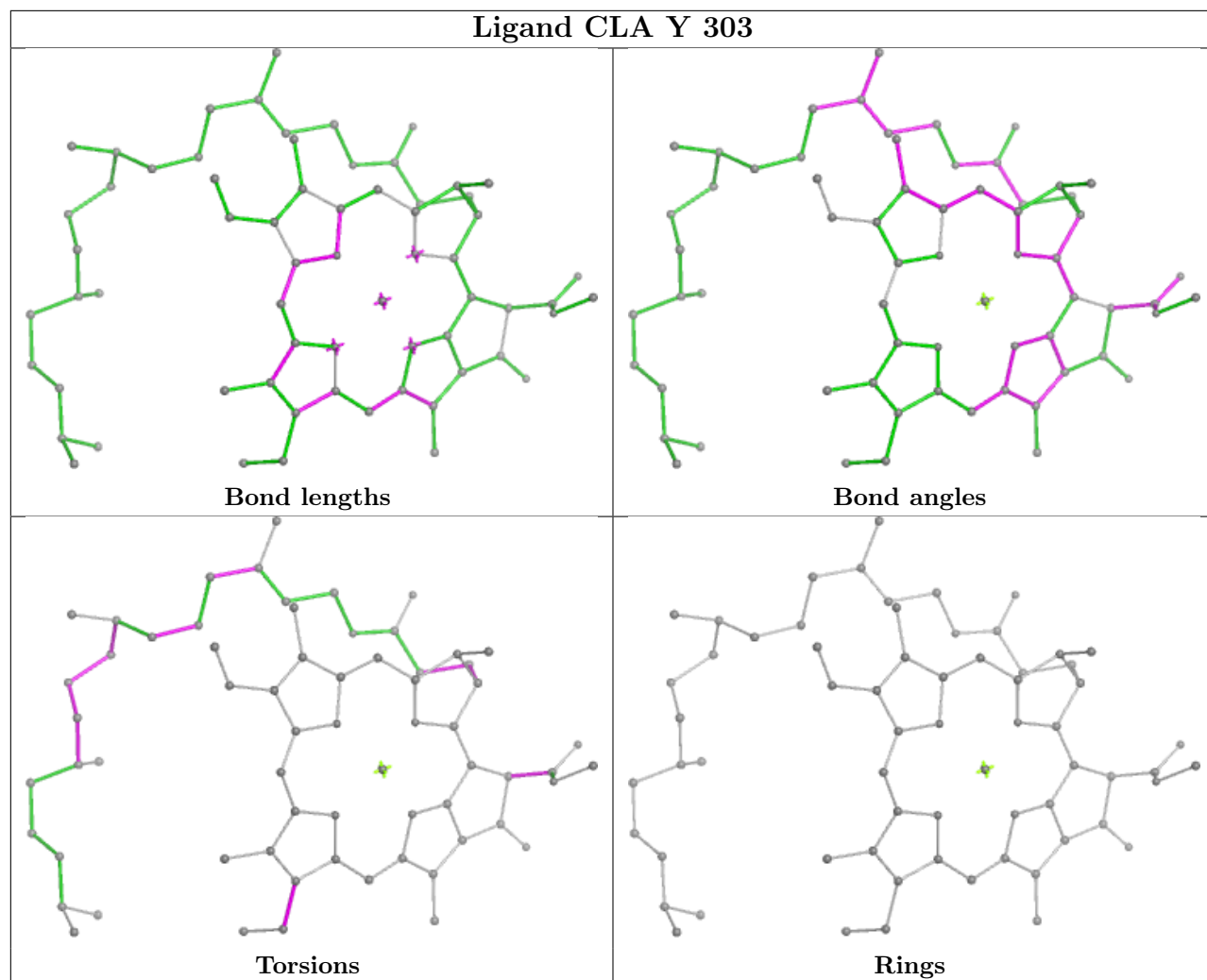
## Ligand LHG b 621



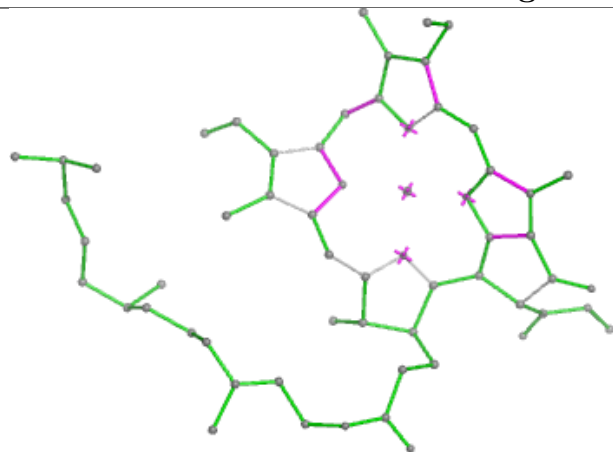
## Ligand CLA s 312



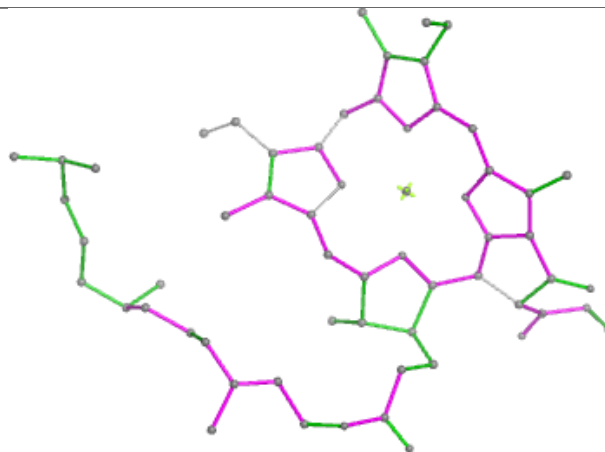
## Ligand CLA Y 303



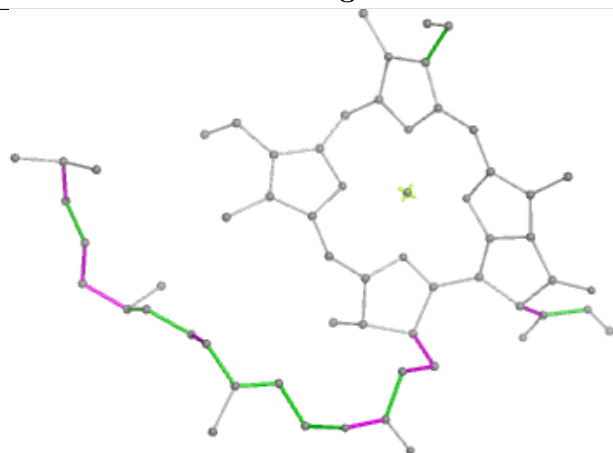
## Ligand CLA 6 602



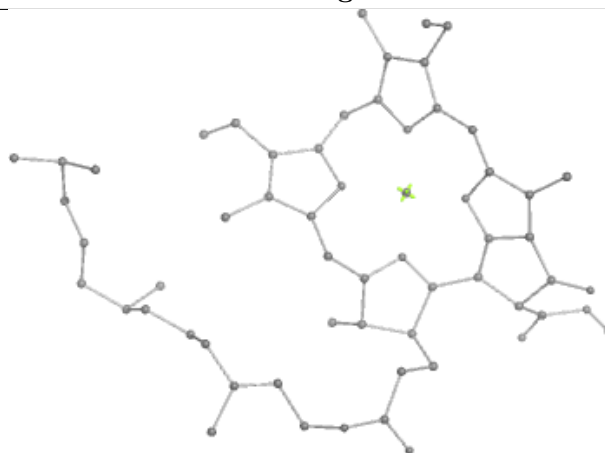
Bond lengths



Bond angles

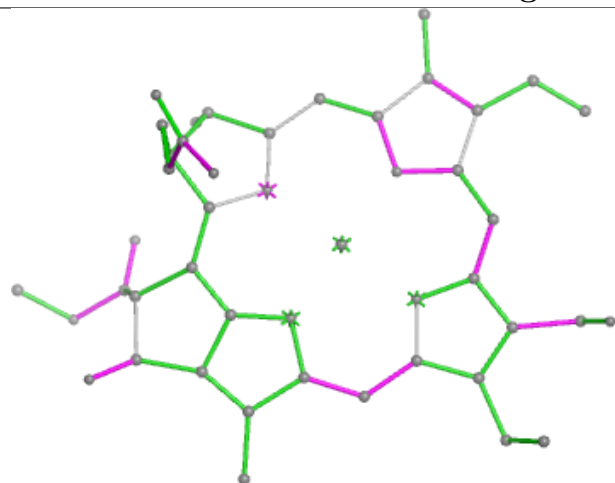


Torsions

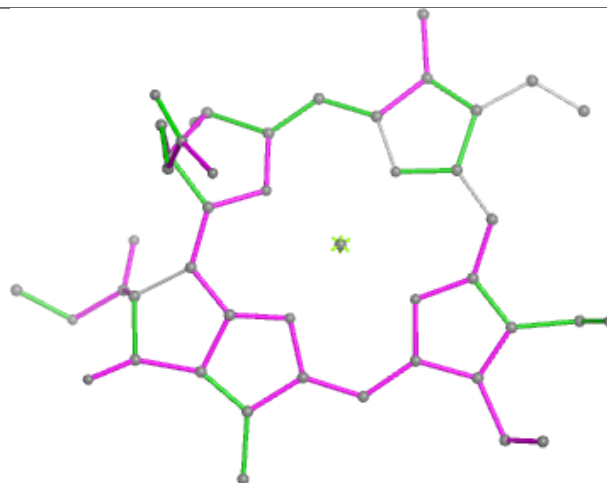


Rings

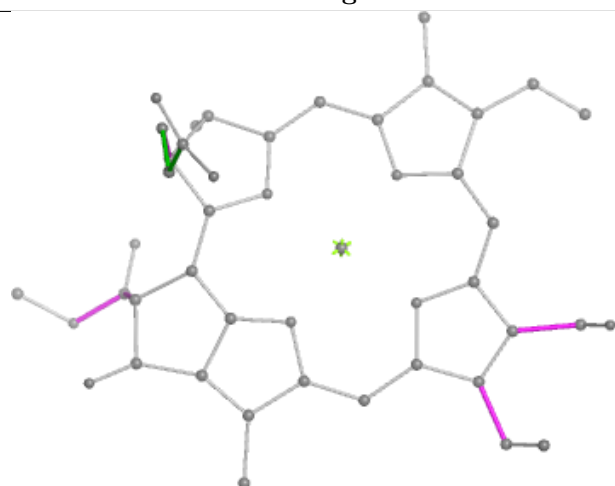
## Ligand CHL 2 603



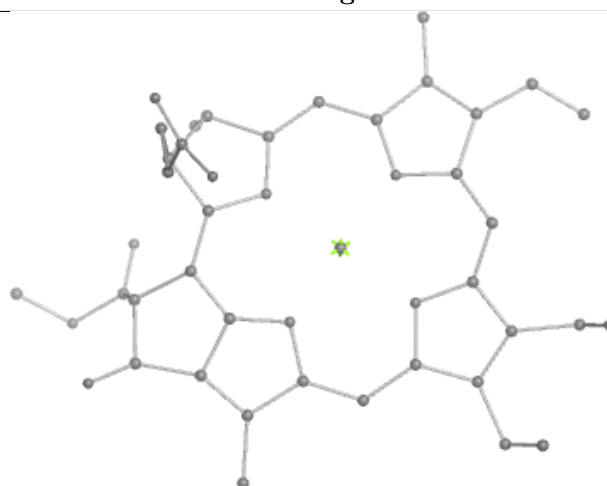
Bond lengths



Bond angles

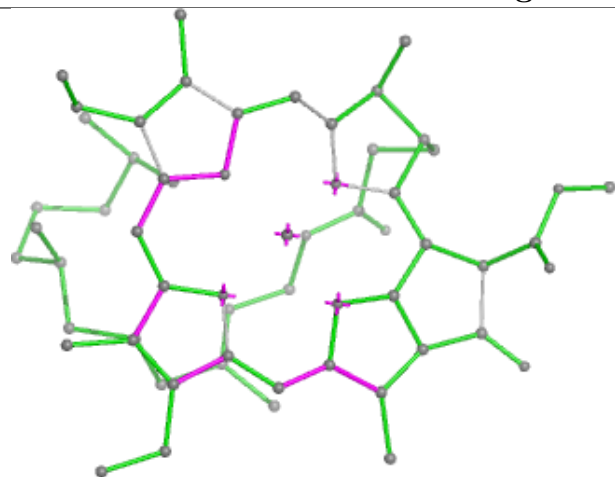


Torsions

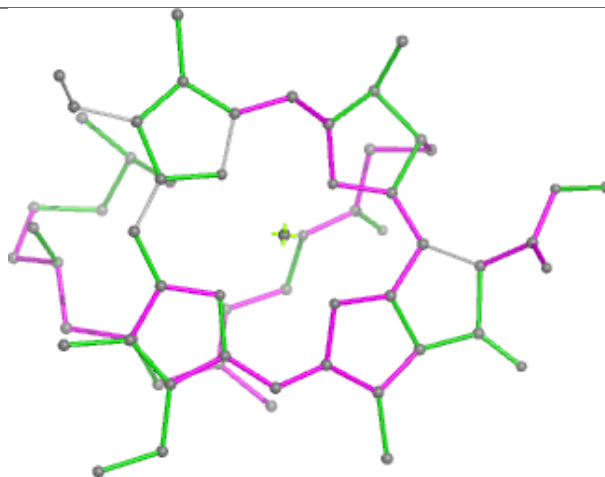


Rings

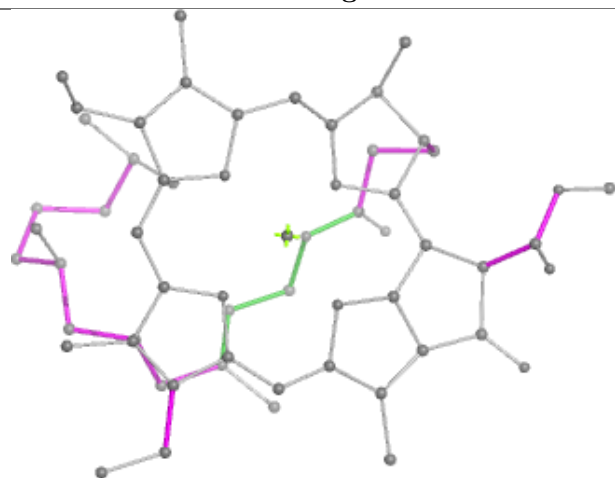
## Ligand CLA N 613



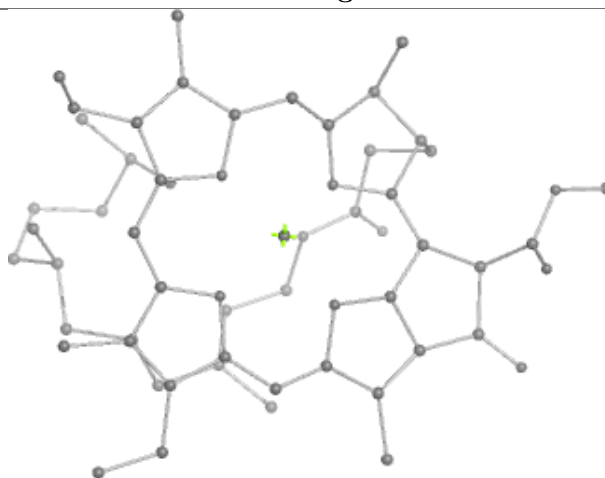
Bond lengths



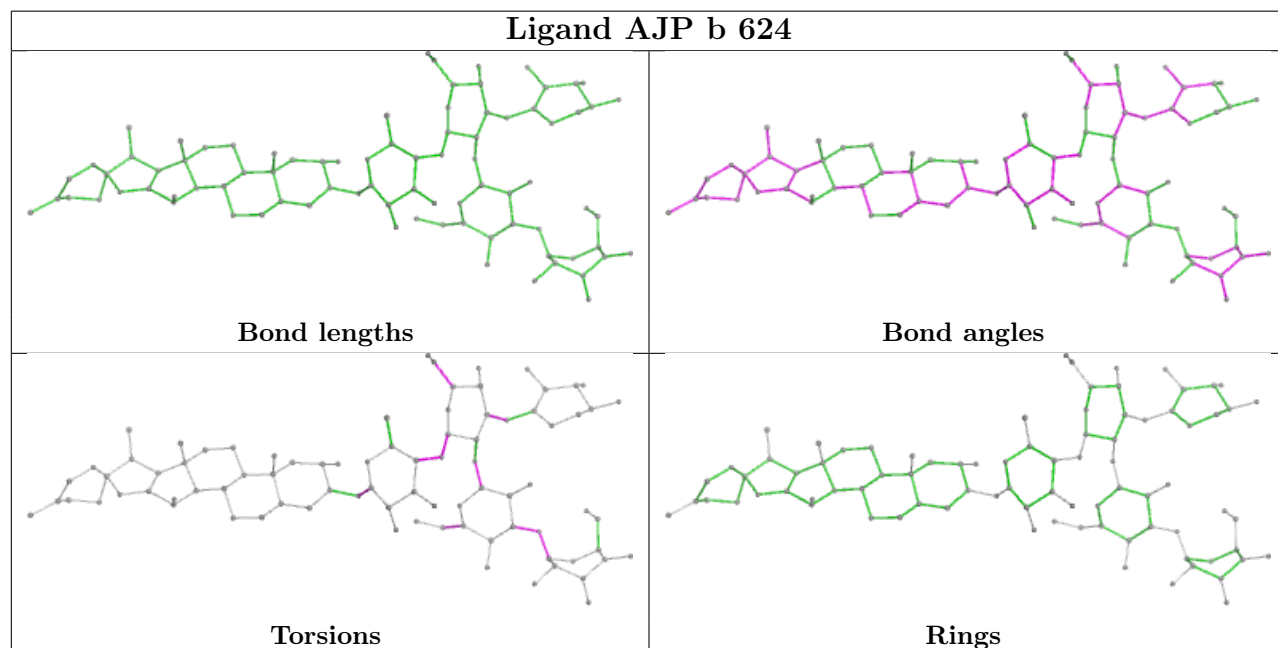
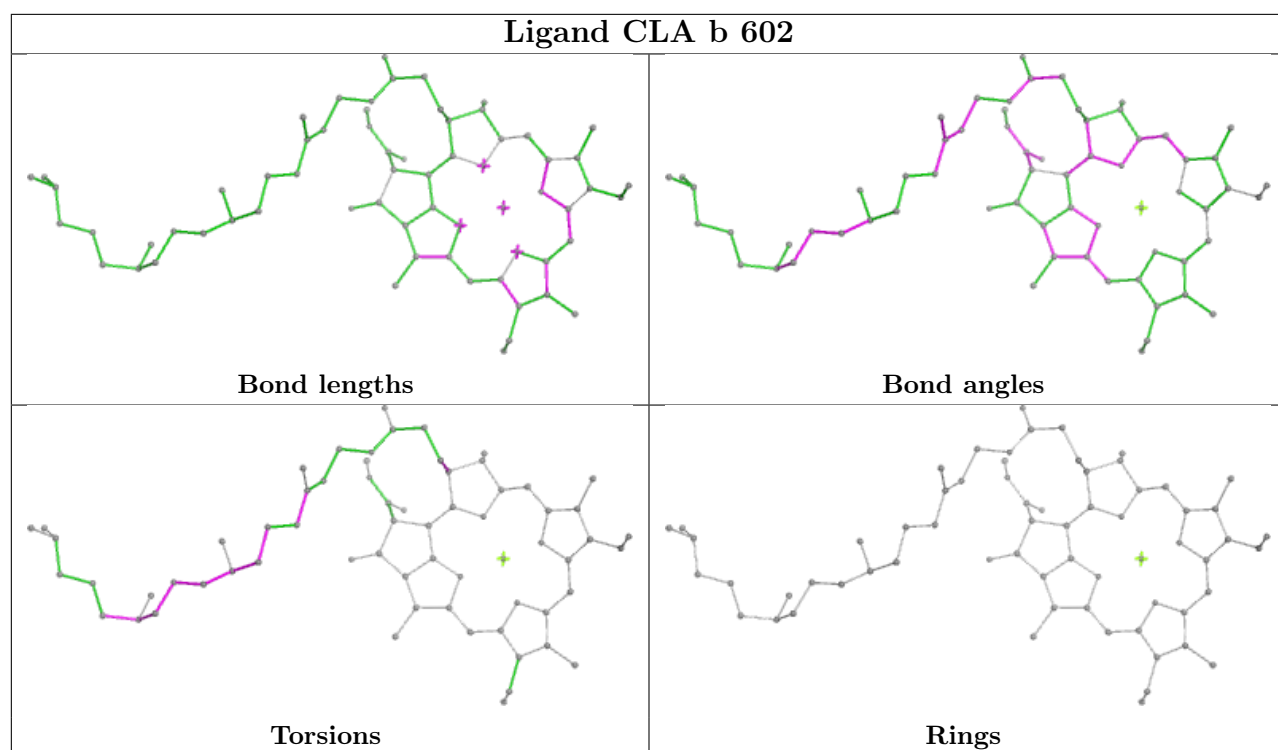
Bond angles



Torsions

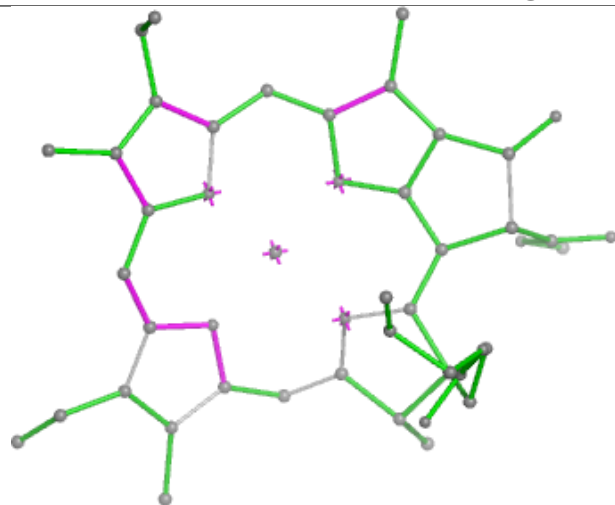


Rings

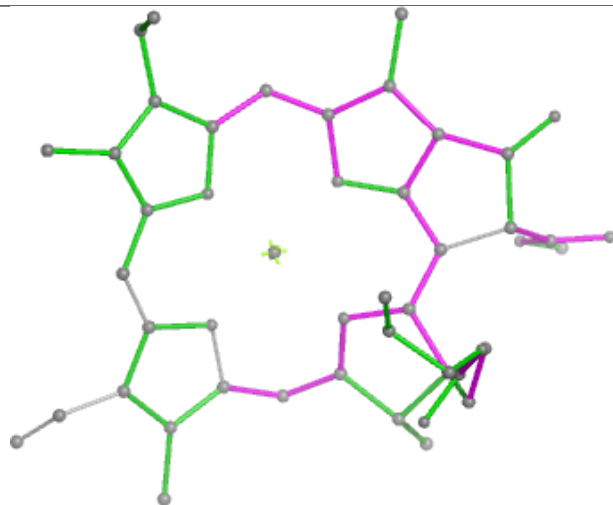




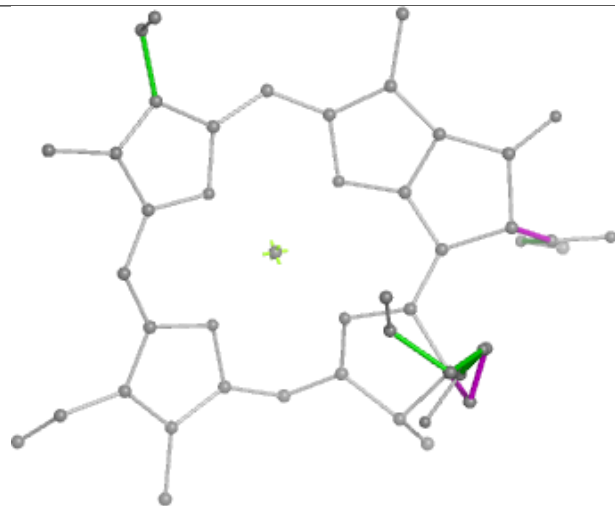
## Ligand CLA r 604



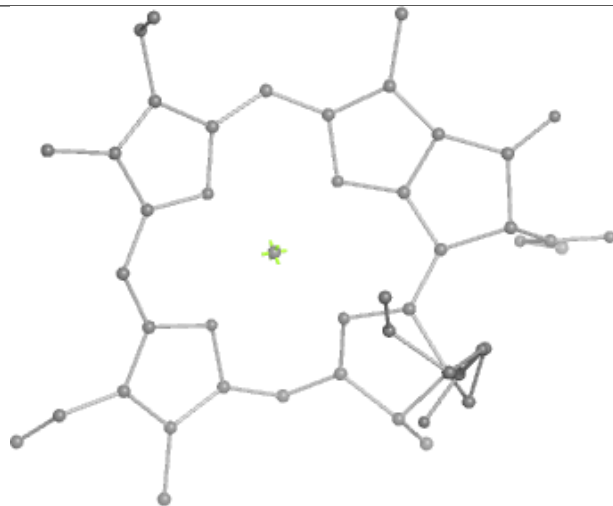
Bond lengths



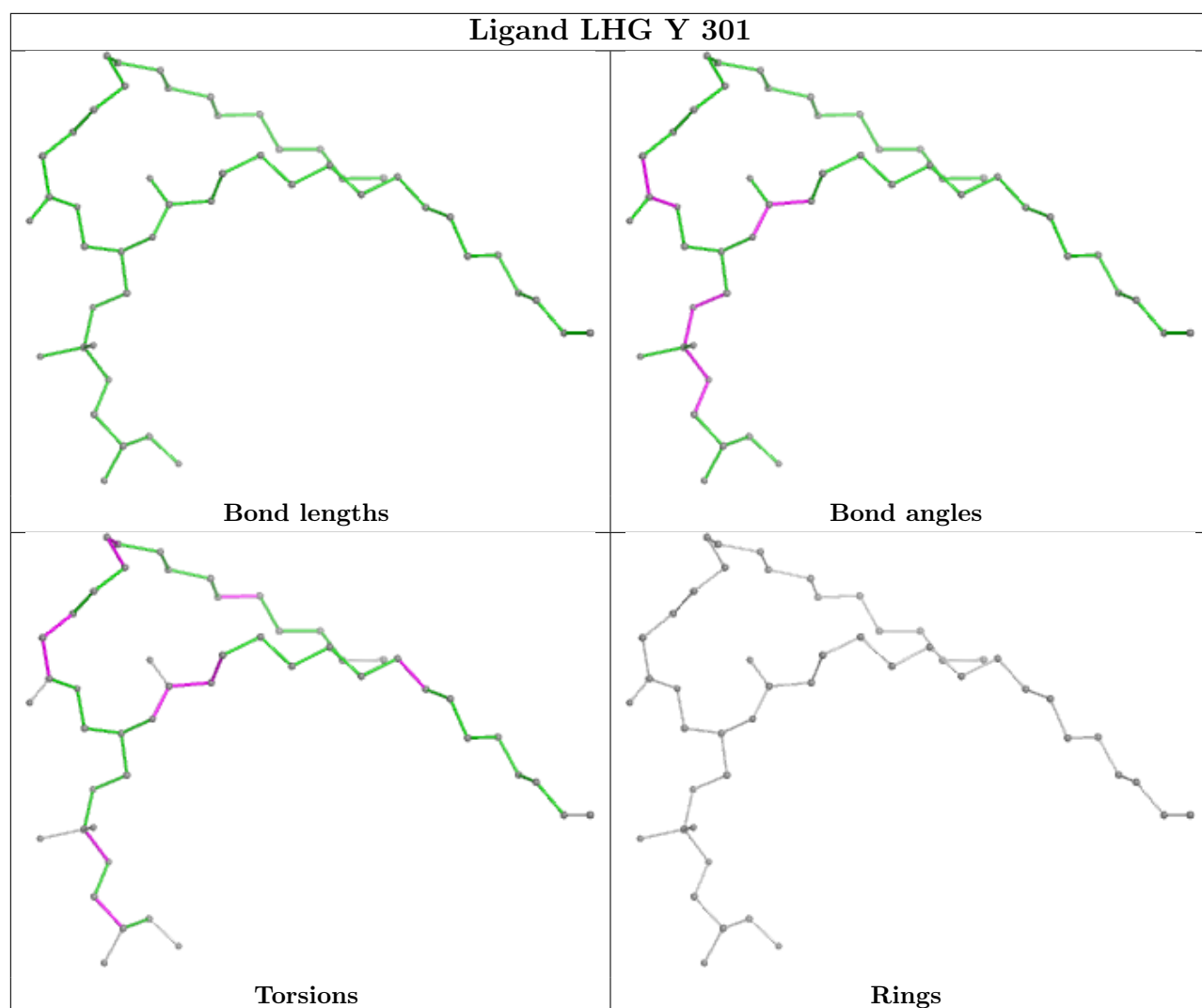
Bond angles



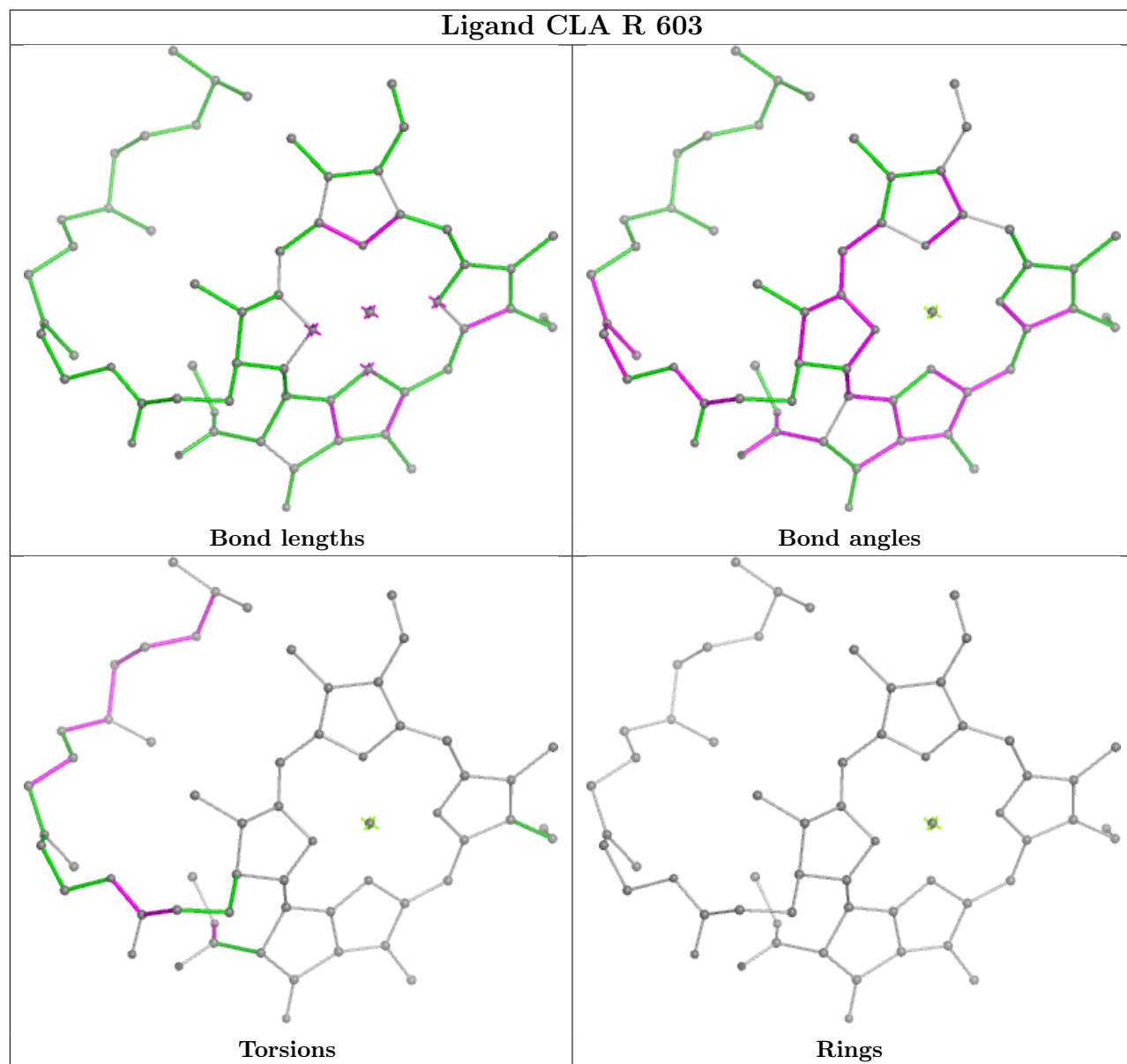
Torsions

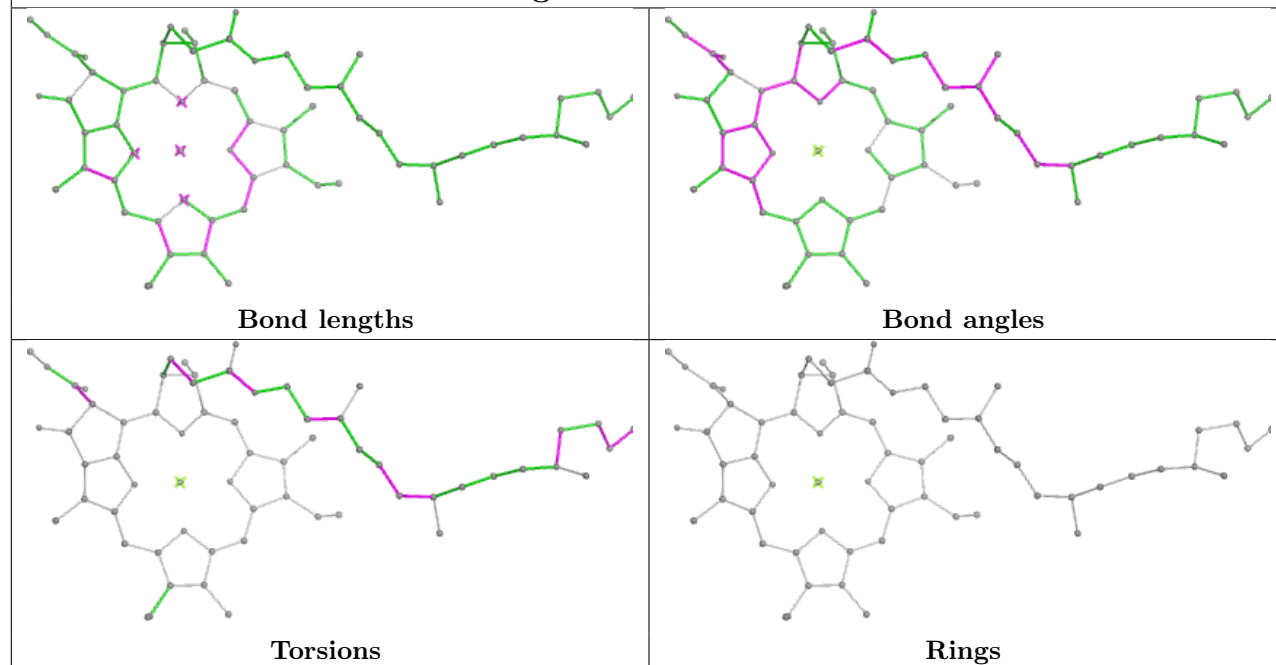
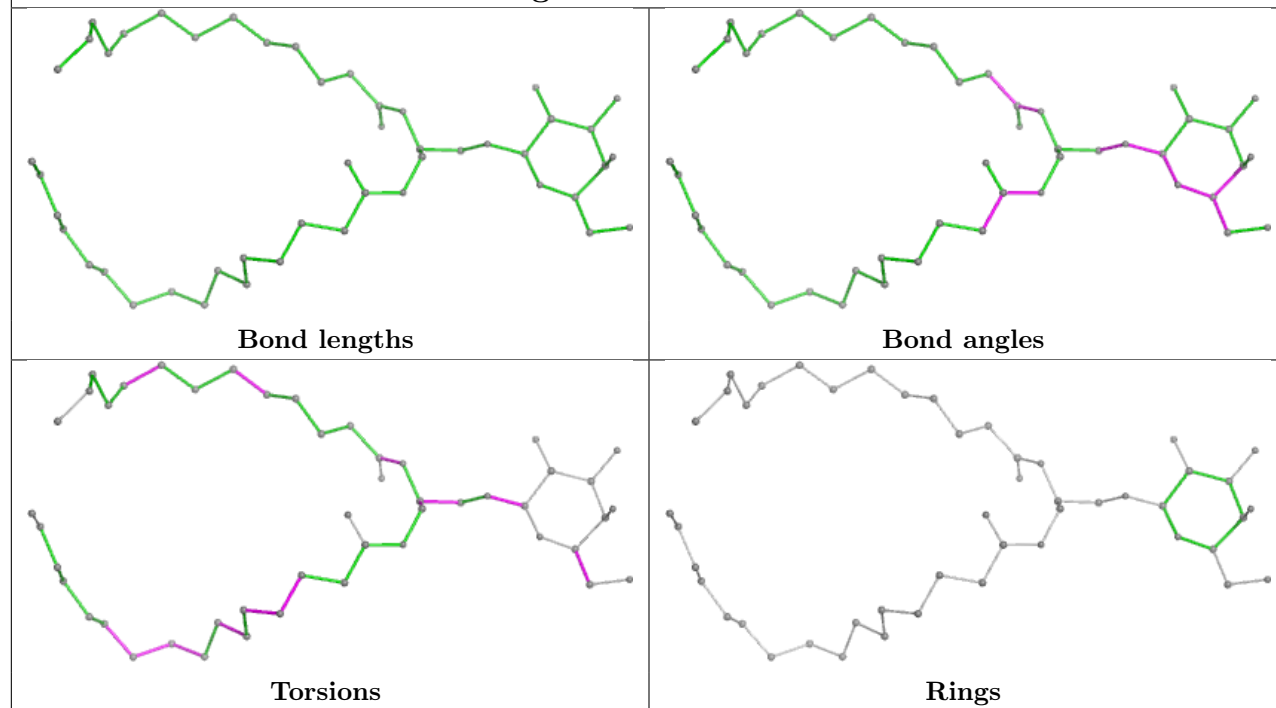


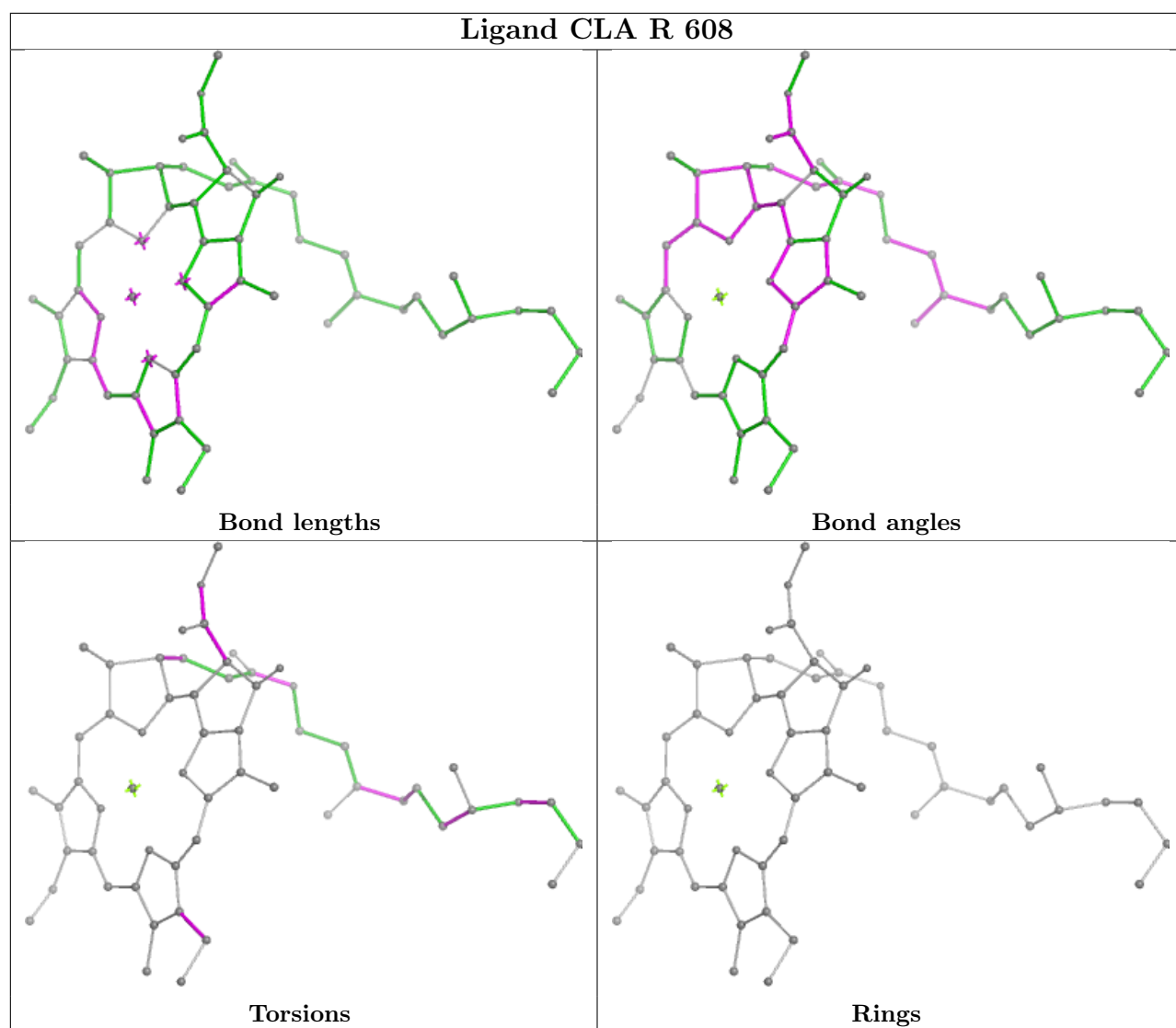
Rings



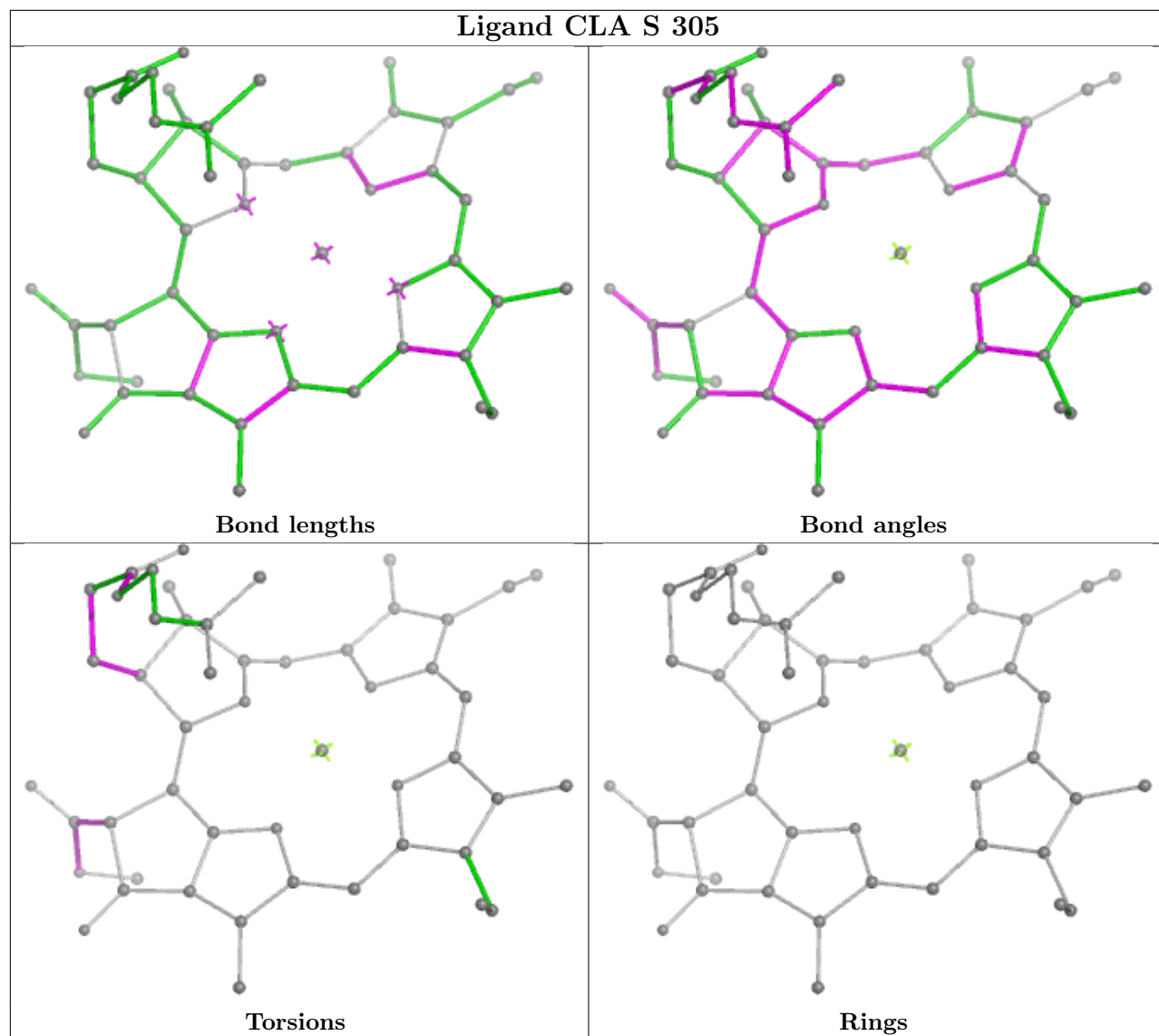
## Ligand CLA R 603

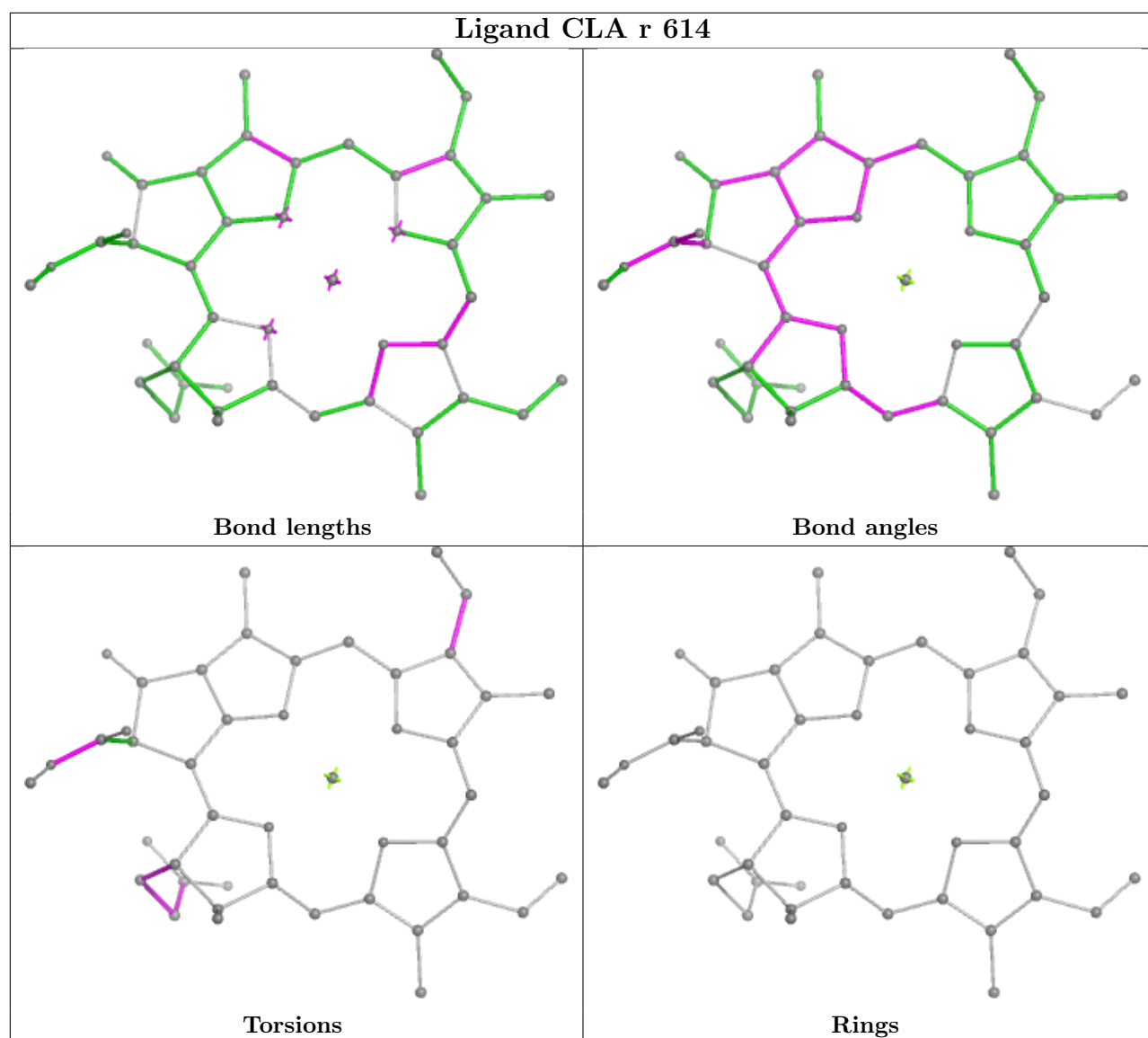


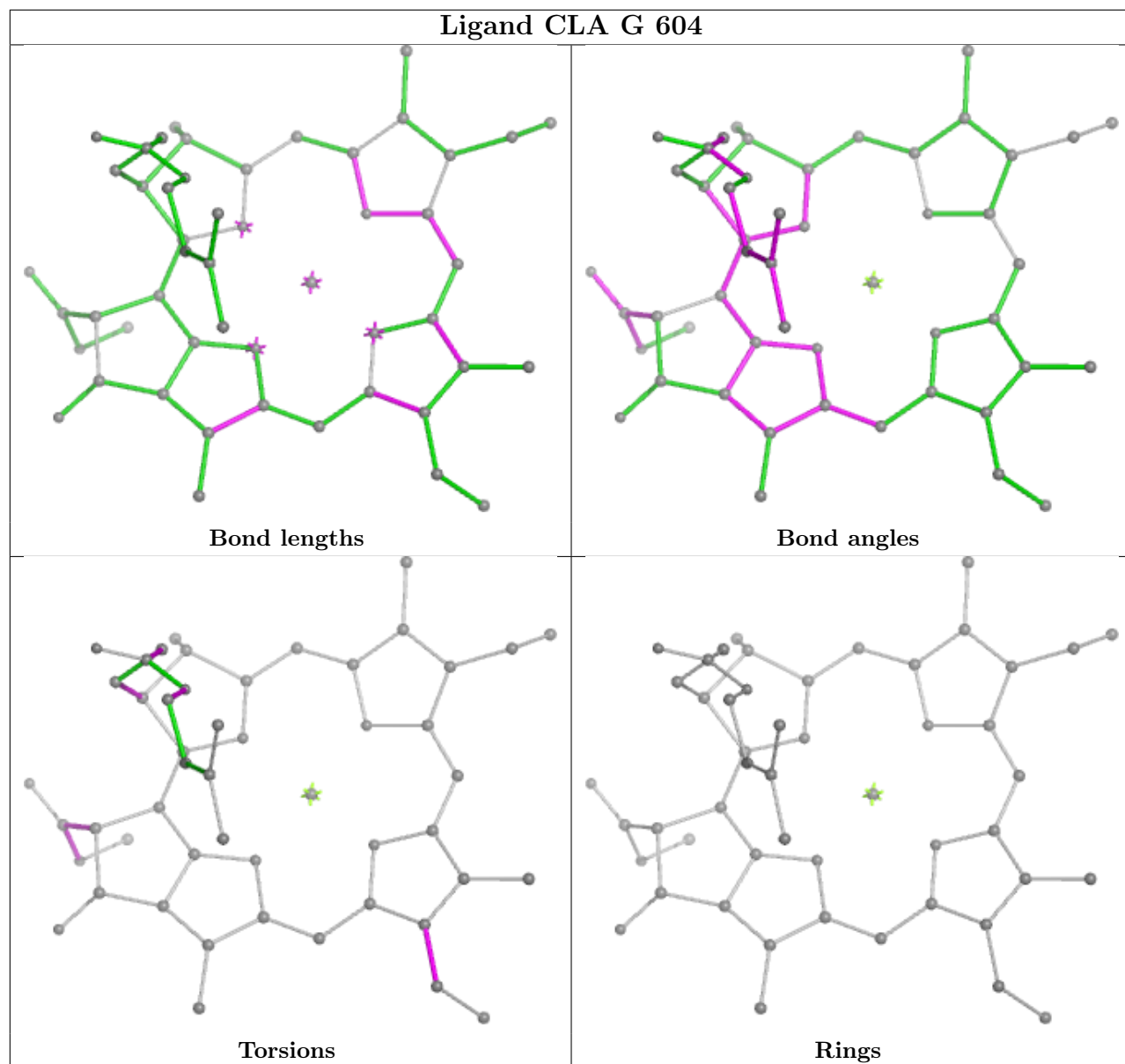
**Ligand CLA B 603****Ligand LMG a 409**



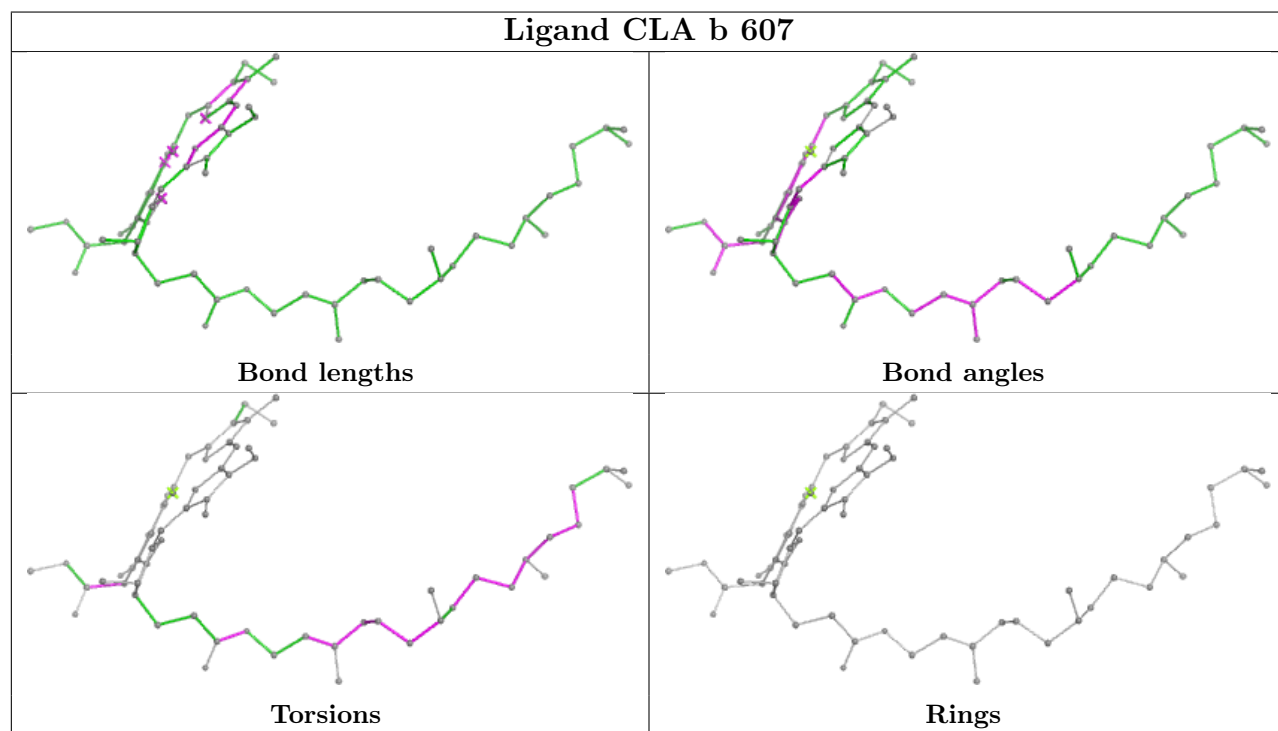
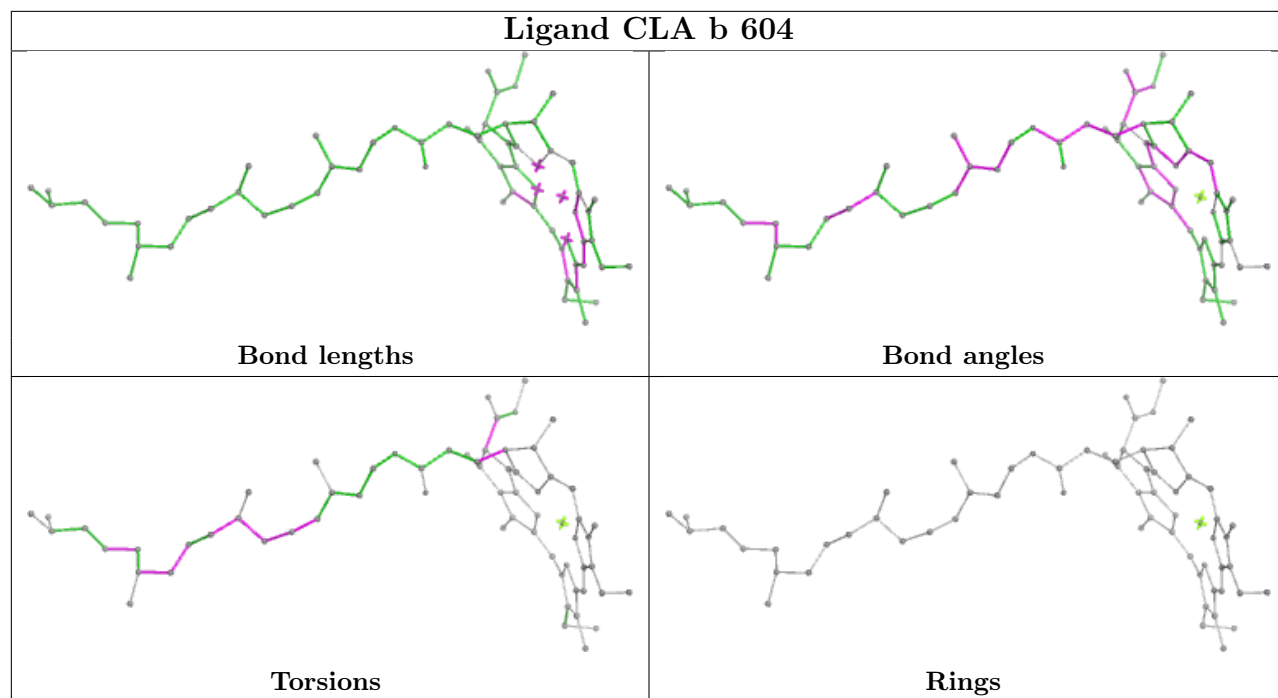
## Ligand CLA S 305



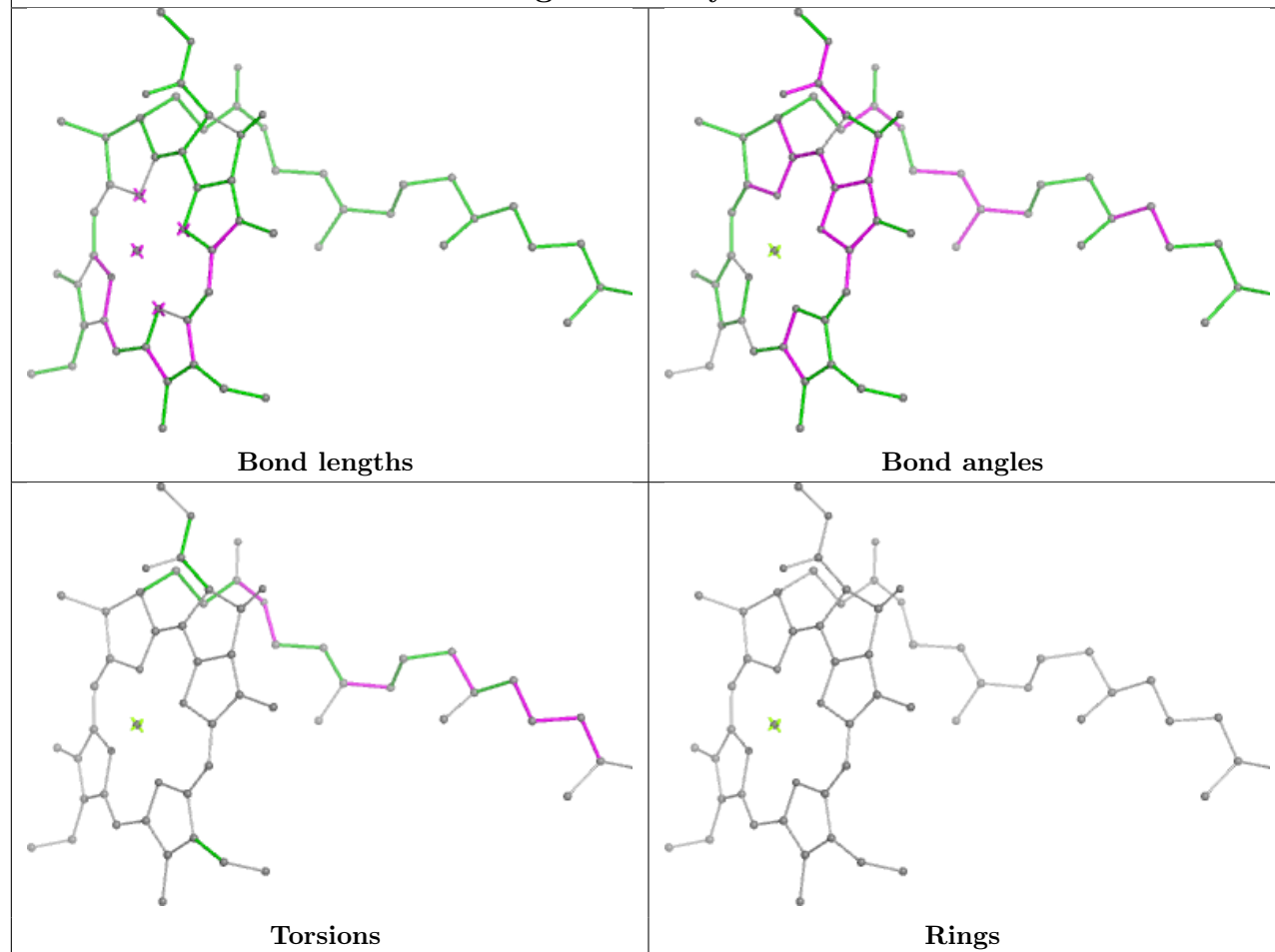




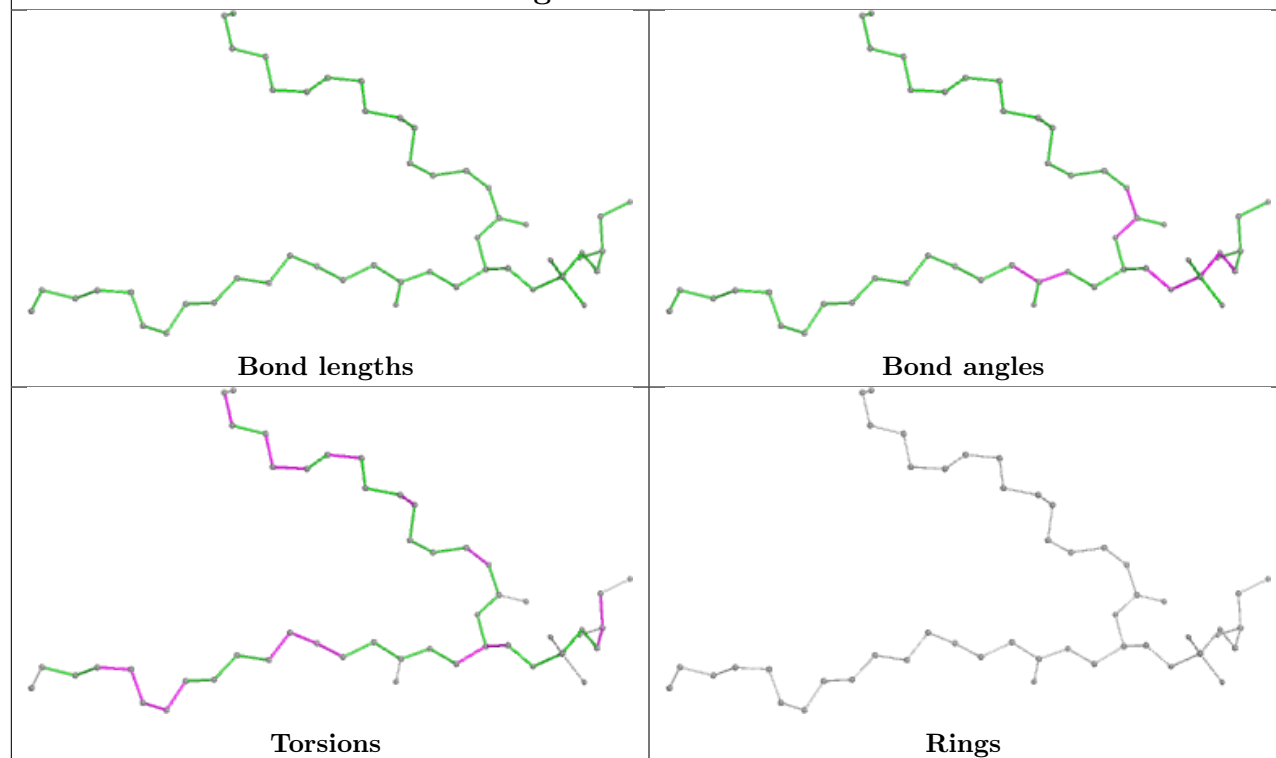


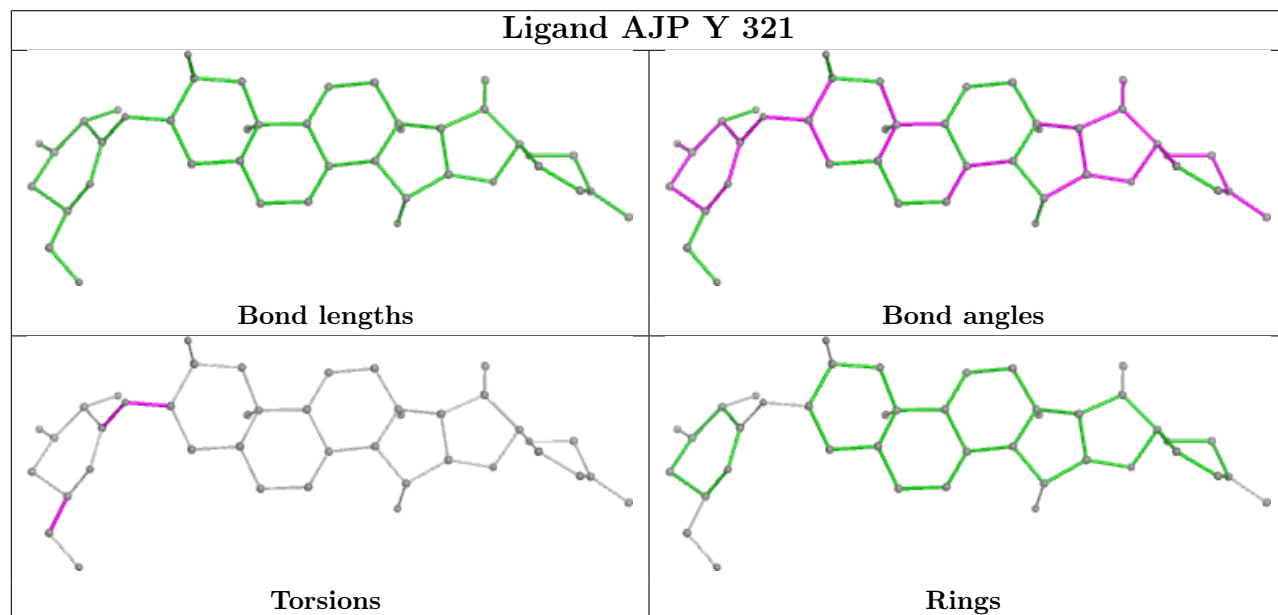
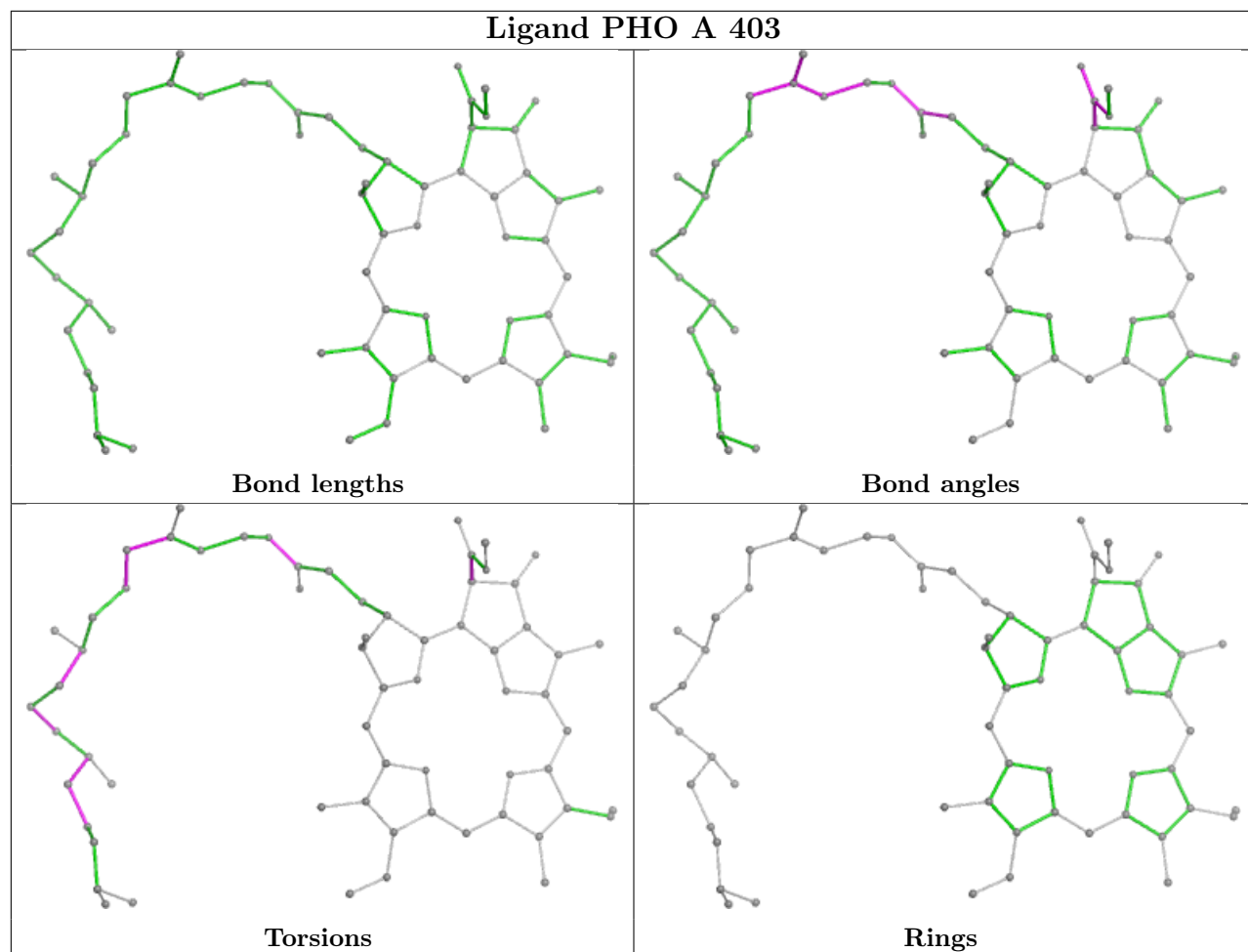


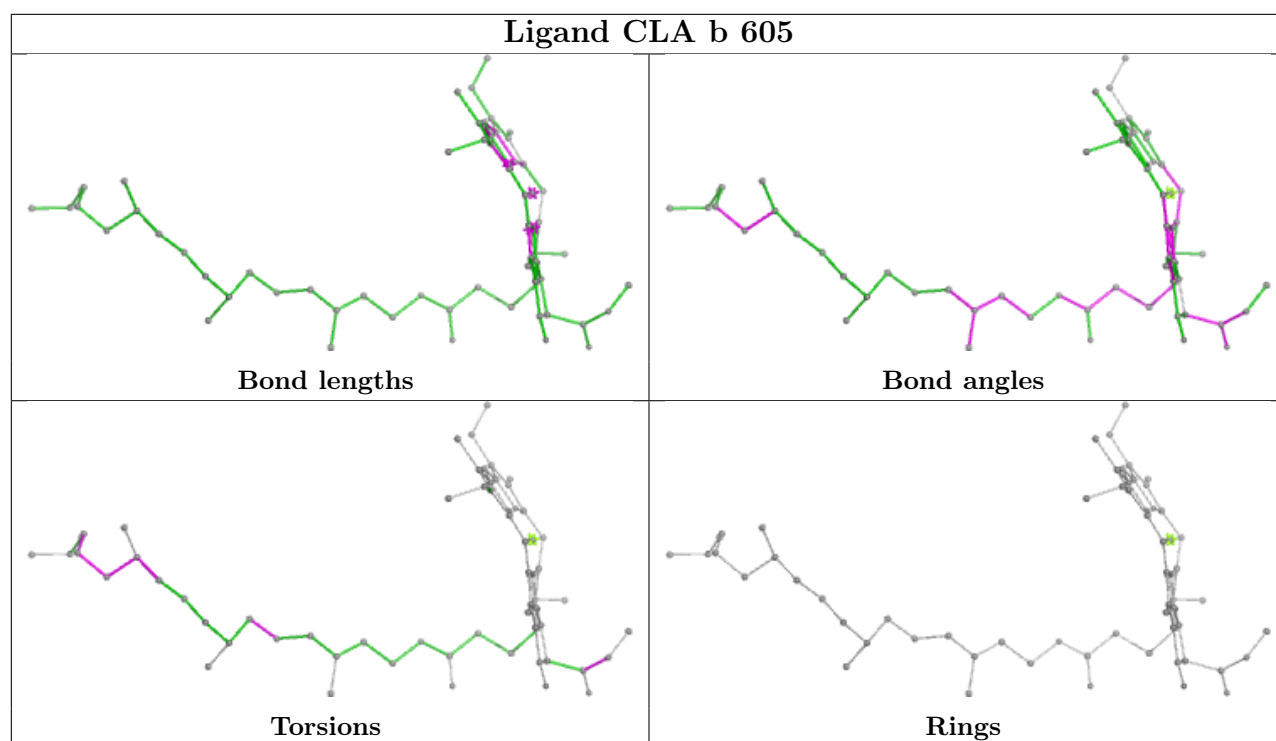
## Ligand CLA y 312



## Ligand LHG S 301







## 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.

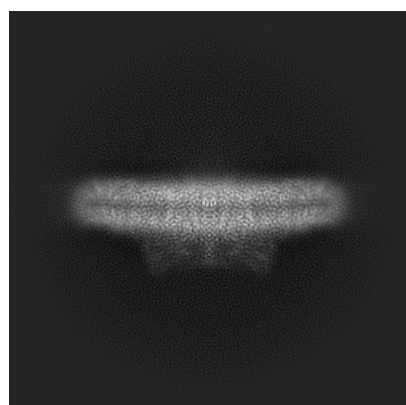
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13078. These allow visual inspection of the internal detail of the map and identification of artifacts.

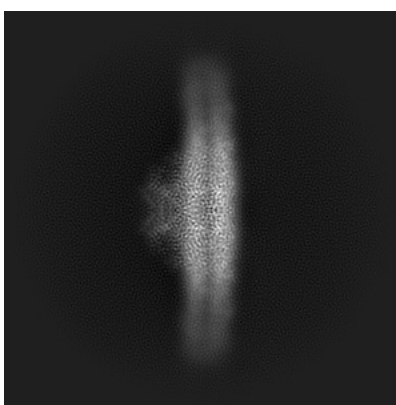
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

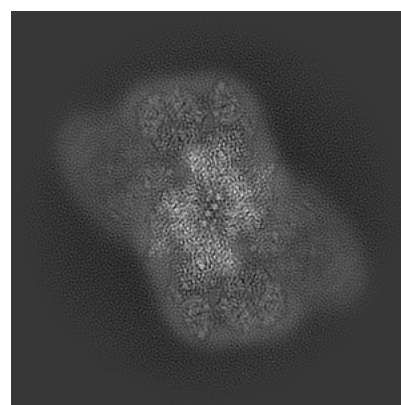
#### 6.1.1 Primary map



X



Y

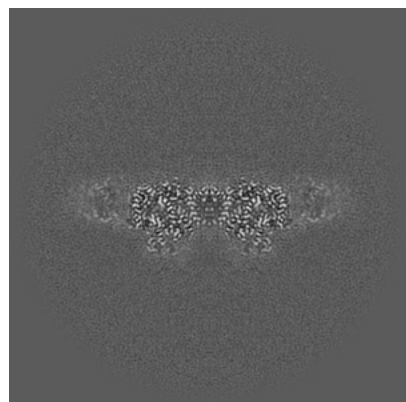


Z

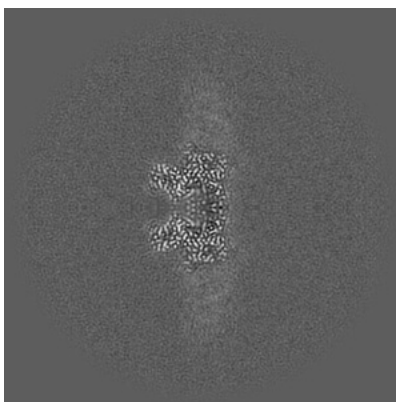
The images above show the map projected in three orthogonal directions.

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

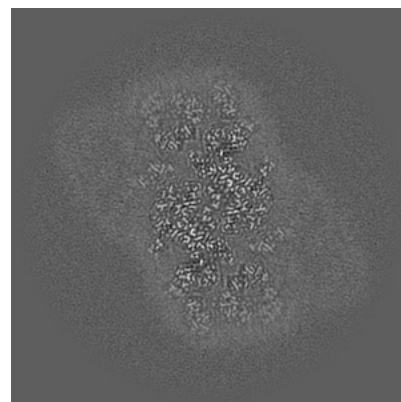
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

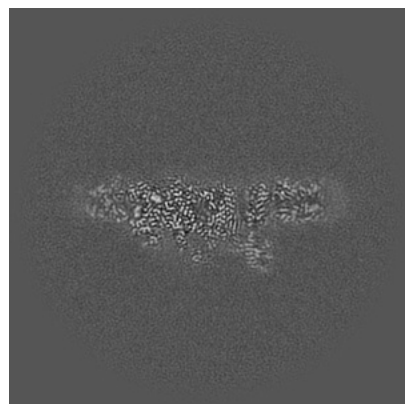


Z Index: 250

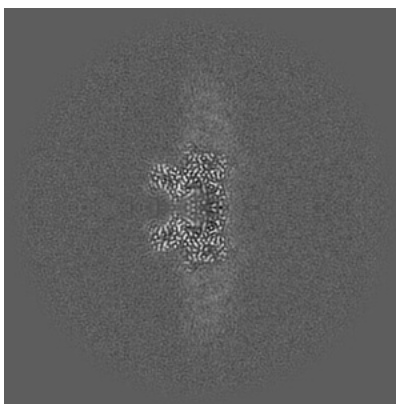
The images above show central slices of the map in three orthogonal directions.

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

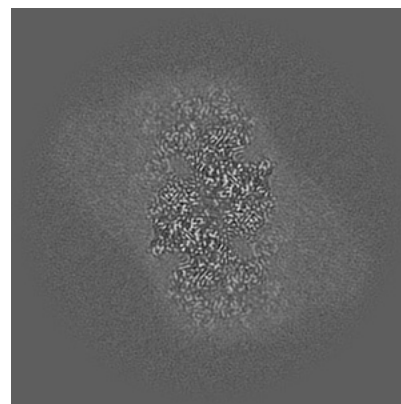
### 6.3.1 Primary map



X Index: 228



Y Index: 250

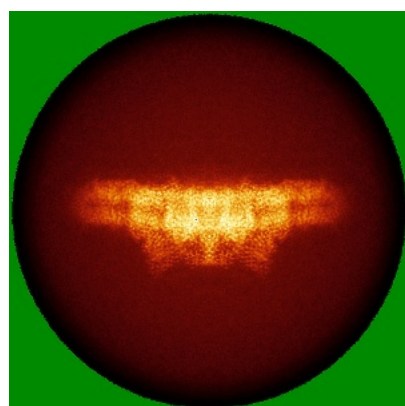


Z Index: 239

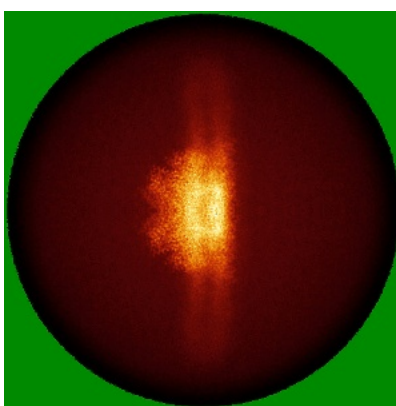
The images above show the largest variance slices of the map in three orthogonal directions.

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

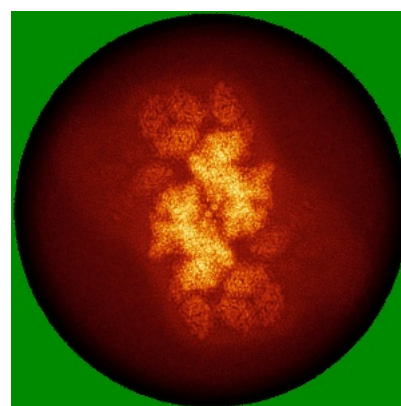
### 6.4.1 Primary map



X



Y

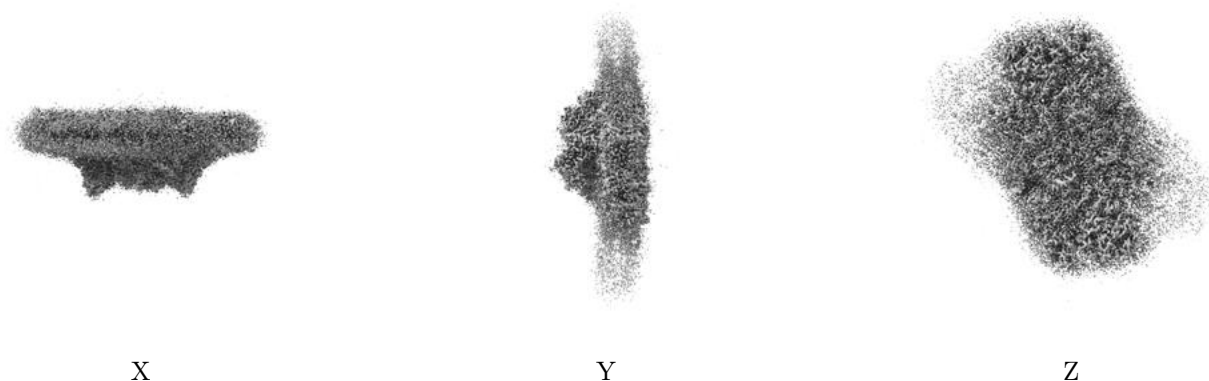


Z

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 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

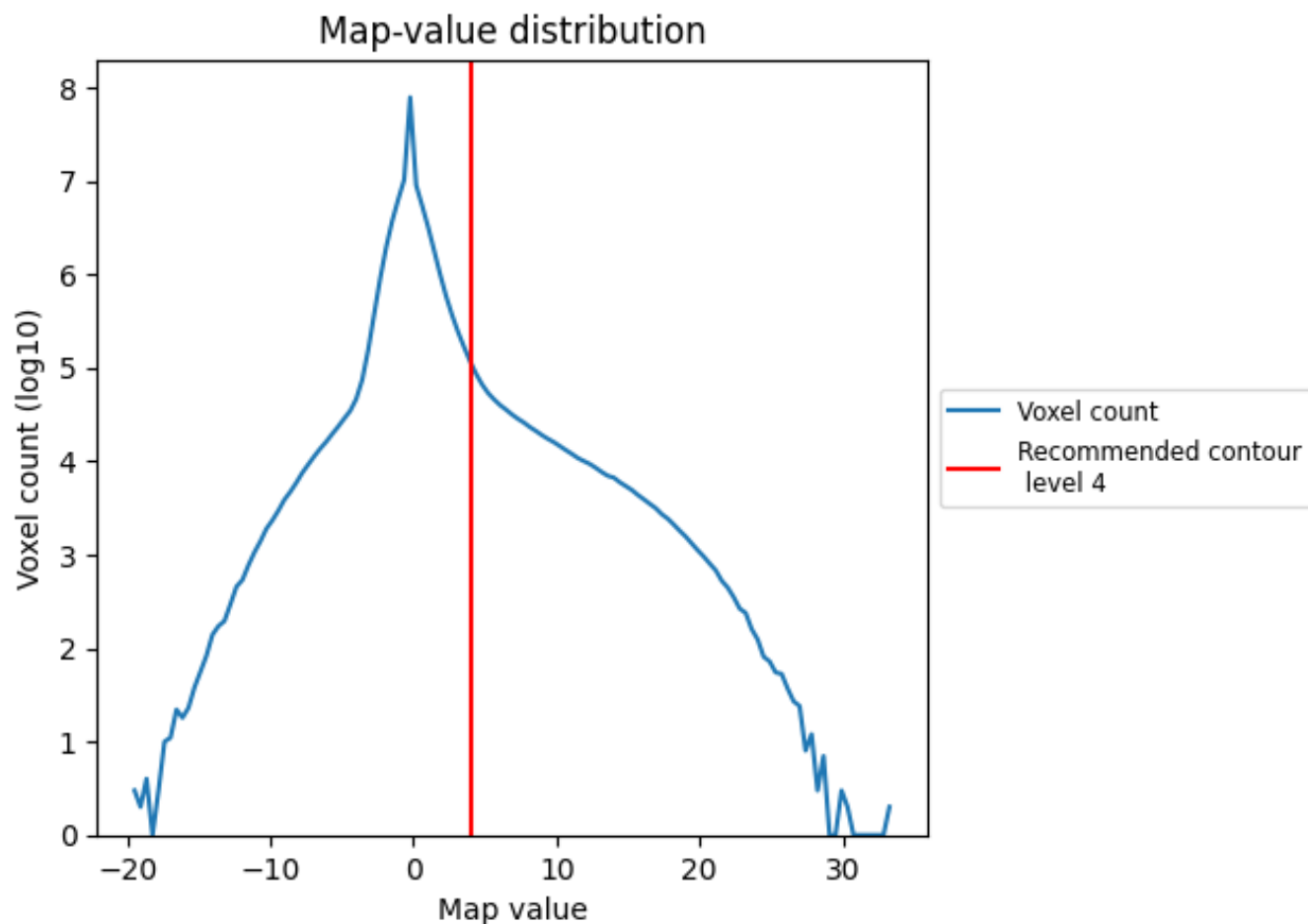
## 6.6 Mask visualisation [i](#)

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.

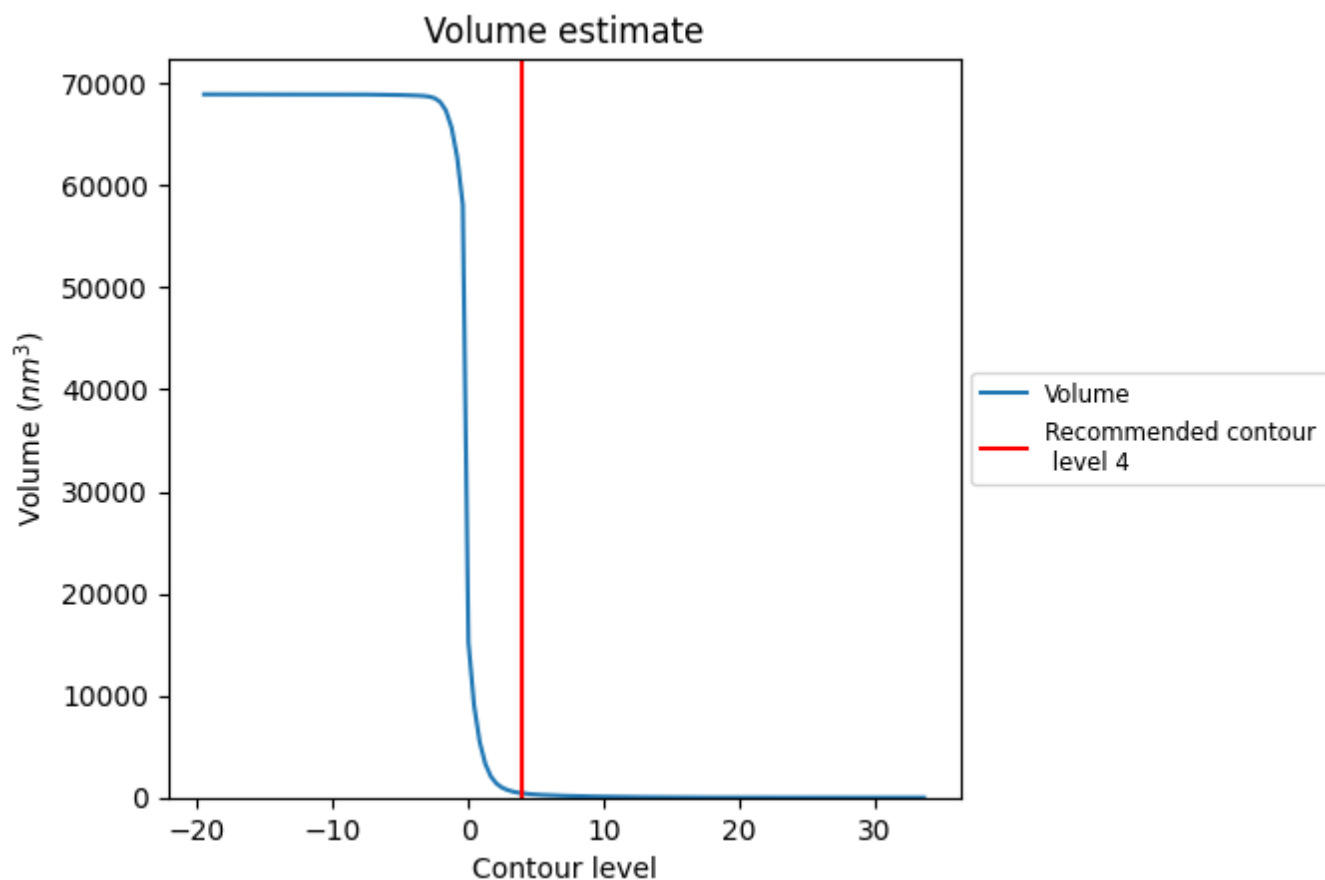
### 7.1 Map-value distribution [i](#)



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.



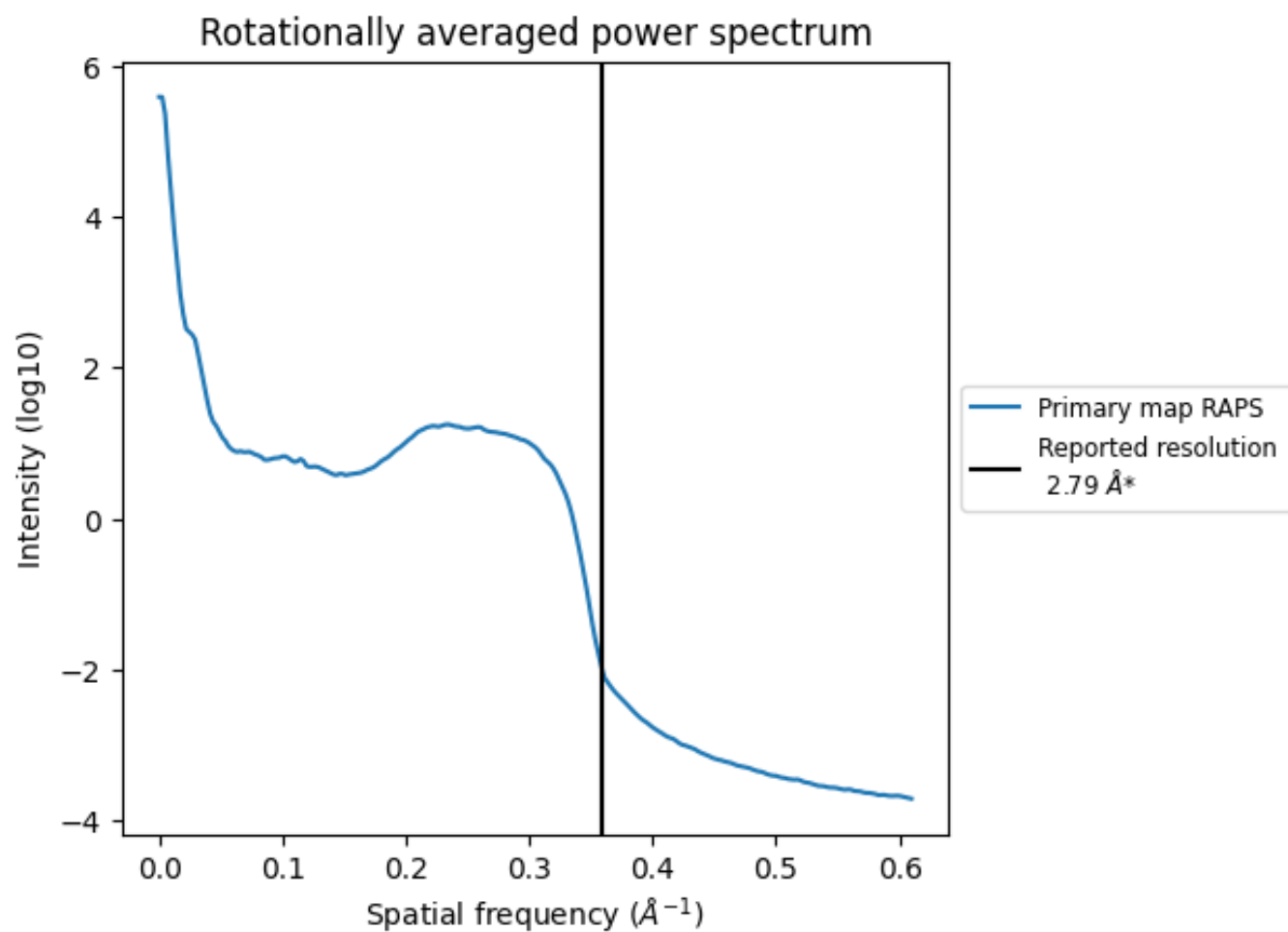
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 423 nm<sup>3</sup>; this corresponds to an approximate mass of 382 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 0.358 Å<sup>-1</sup>

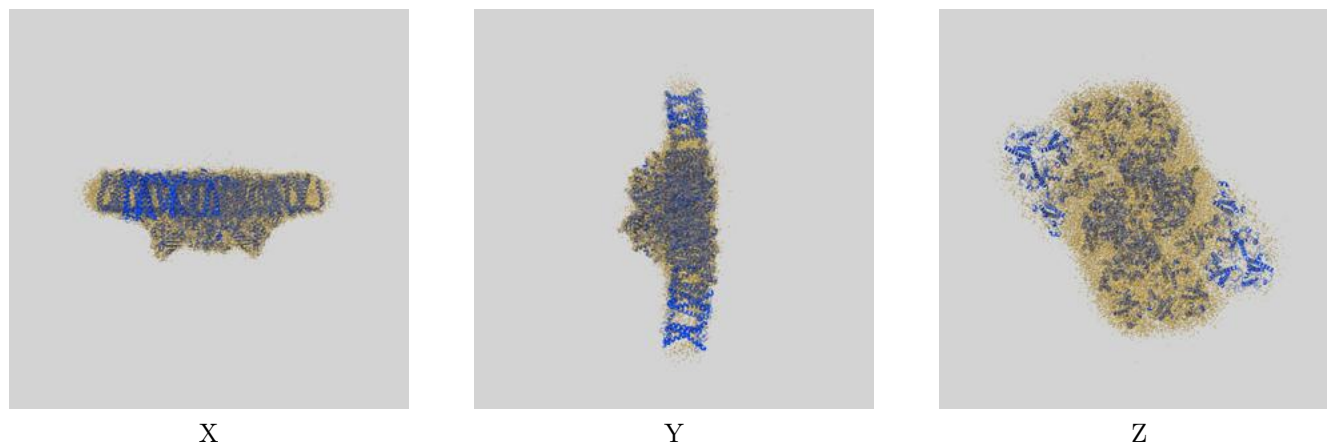
## 8 Fourier-Shell correlation ⓘ

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

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

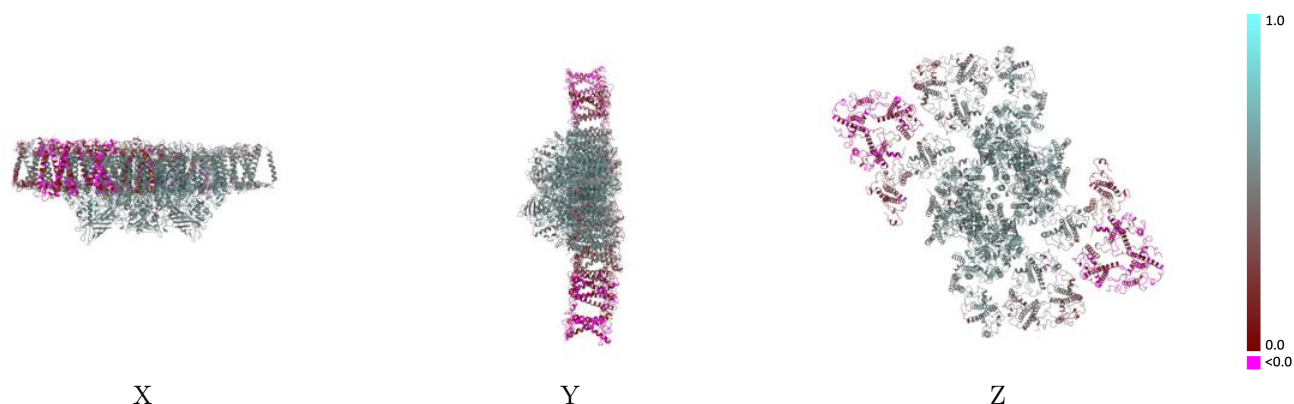
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section [3](#) on page [43](#).

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



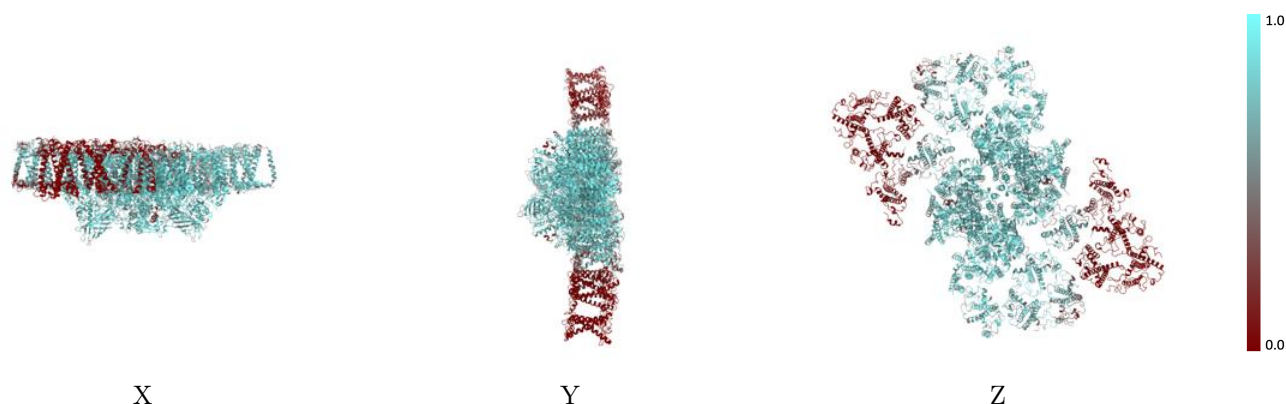
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



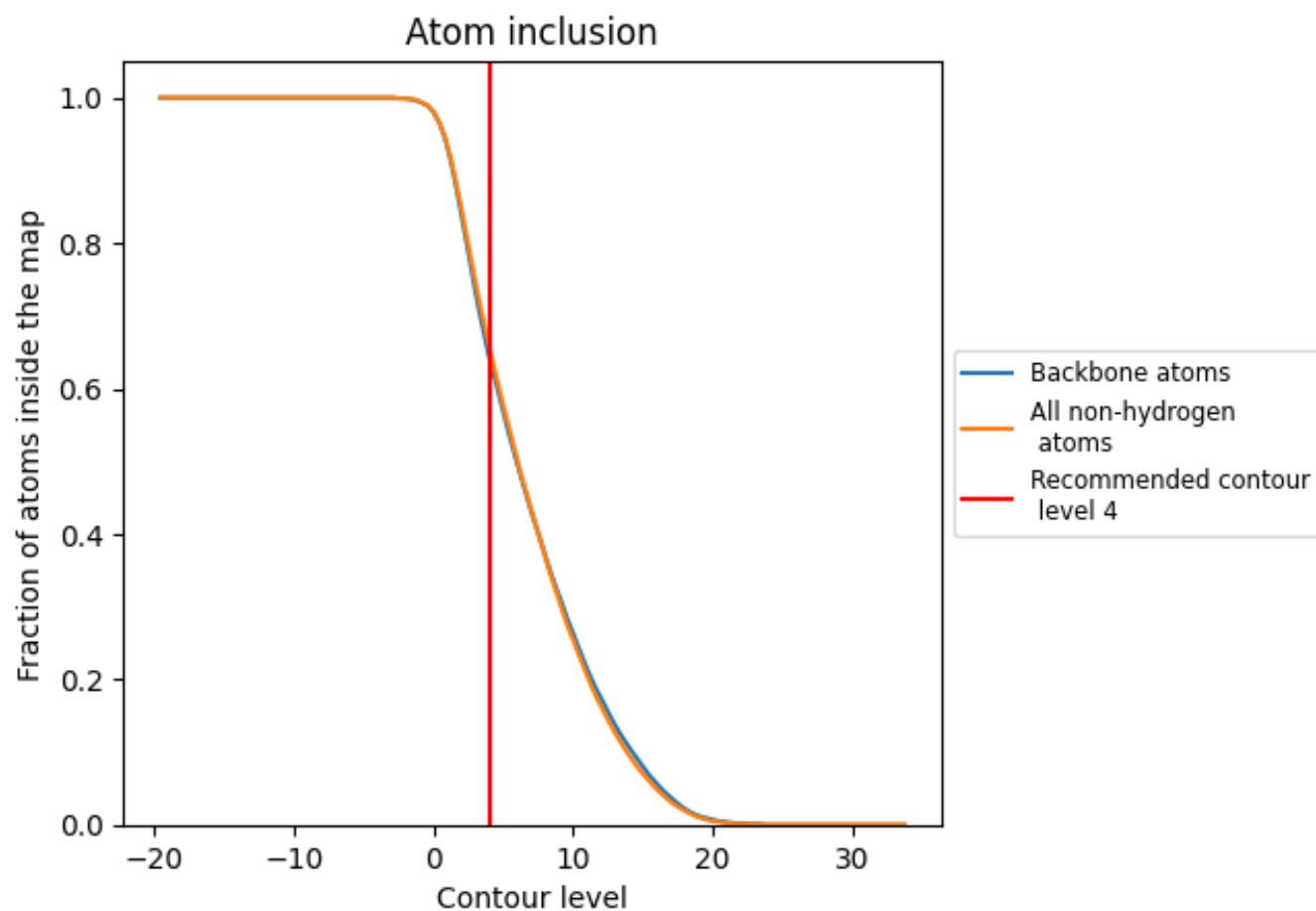
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 66% 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 (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.6570   |  0.4650   |
| 1     |  0.0340   |  0.0670   |
| 2     |  0.0320   |  0.1050   |
| 3     |  0.0060   |  0.0400   |
| 4     |  0.0870   |  0.2440   |
| 5     |  0.0340   |  0.0680   |
| 6     |  0.0320   |  0.1040   |
| 7     |  0.0060   |  0.0410   |
| 8     |  0.0870   |  0.2450   |
| A     |  0.8540   |  0.5740   |
| B     |  0.8690   |  0.5810   |
| C     |  0.8730   |  0.5820   |
| D     |  0.8800   |  0.5890   |
| E     |  0.7940   |  0.5260   |
| F     |  0.7710  |  0.5100  |
| G     |  0.5250 |  0.3940 |
| H     |  0.7940 |  0.5510 |
| I     |  0.8820 |  0.6010 |
| K     |  0.8250 |  0.5570 |
| L     |  0.8350 |  0.5430 |
| M     |  0.8310 |  0.5620 |
| N     |  0.6500 |  0.4540 |
| O     |  0.7370 |  0.5090 |
| R     |  0.6280 |  0.4770 |
| S     |  0.7300 |  0.5110 |
| T     |  0.8010 |  0.5660 |
| U     |  0.2770 |  0.4110 |
| W     |  0.8340 |  0.5810 |
| X     |  0.6210 |  0.4490 |
| Y     |  0.7790 |  0.5100 |
| Z     |  0.7270 |  0.5140 |
| a     |  0.8550 |  0.5750 |
| b     |  0.8680 |  0.5800 |
| c     |  0.8700 |  0.5820 |
| d     |  0.8760 |  0.5900 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| e     |  0.7920 |  0.5240 |
| f     |  0.7750 |  0.5080 |
| g     |  0.5270 |  0.3930 |
| h     |  0.7920 |  0.5510 |
| i     |  0.8940 |  0.5980 |
| k     |  0.8400 |  0.5590 |
| l     |  0.8350 |  0.5420 |
| m     |  0.8230 |  0.5660 |
| n     |  0.6500 |  0.4530 |
| o     |  0.7360 |  0.5130 |
| r     |  0.6250 |  0.4760 |
| s     |  0.7260 |  0.5110 |
| t     |  0.8080 |  0.5700 |
| u     |  0.2820 |  0.4040 |
| w     |  0.8340 |  0.5760 |
| x     |  0.6250 |  0.4400 |
| y     |  0.7770 |  0.5080 |
| z     |  0.7150 |  0.5110 |