



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:14 PM UTC

PDB ID : 8J5K / pdb\_00008j5k  
EMDB ID : EMD-35987  
Title : Structural insights into photosystem II supercomplex and trimeric FCP antennae of a centric diatom *Cyclotella meneghiniana*  
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.  
Deposited on : 2023-04-23  
Resolution : 2.93 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>.

---

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

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

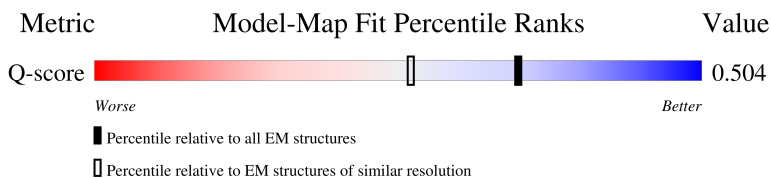
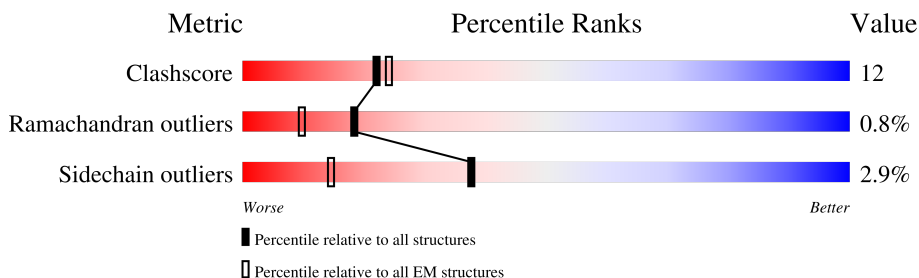
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 Å.

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



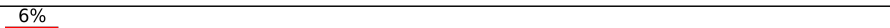
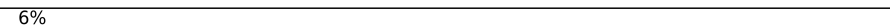
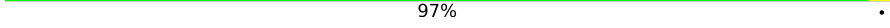
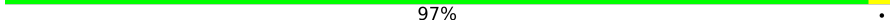
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13037 ( 2.43 - 3.43 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 333    |                  |
| 1   | a     | 333    |                  |
| 2   | B     | 481    |                  |
| 2   | b     | 481    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | C     | 450    |    |
| 3   | c     | 450    |    |
| 4   | D     | 340    |    |
| 4   | d     | 340    |    |
| 5   | E     | 75     |    |
| 5   | e     | 75     |    |
| 6   | F     | 31     |    |
| 6   | f     | 31     |    |
| 7   | H     | 65     |    |
| 7   | h     | 65     |    |
| 8   | I     | 34     |    |
| 8   | i     | 34     |    |
| 9   | J     | 34     |  |
| 9   | j     | 34     |  |
| 10  | K     | 37     |  |
| 10  | k     | 37     |  |
| 11  | L     | 37     |  |
| 11  | l     | 37     |  |
| 12  | M     | 41     |  |
| 12  | m     | 41     |  |
| 13  | N     | 30     |  |
| 13  | n     | 30     |  |
| 14  | O     | 248    |  |
| 14  | o     | 248    |  |
| 15  | Q     | 145    |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | q     | 145    |                  |
| 16  | T     | 29     |                  |
| 16  | t     | 29     |                  |
| 17  | U     | 92     |                  |
| 17  | u     | 92     |                  |
| 18  | V     | 136    |                  |
| 18  | v     | 136    |                  |
| 19  | W     | 50     |                  |
| 19  | w     | 50     |                  |
| 20  | X     | 34     |                  |
| 20  | x     | 34     |                  |
| 21  | Y     | 33     |                  |
| 21  | y     | 33     |                  |
| 22  | Z     | 59     |                  |
| 22  | z     | 59     |                  |
| 23  | 0     | 169    |                  |
| 23  | 5     | 169    |                  |
| 24  | 2     | 164    |                  |
| 24  | 7     | 164    |                  |
| 25  | 1     | 164    |                  |
| 25  | 6     | 164    |                  |
| 26  | P     | 214    |                  |
| 26  | p     | 214    |                  |
| 27  | 4     | 153    |                  |
| 27  | 9     | 153    |                  |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 28  | 3     | 163    | <div> <div>77%</div> <div>84%</div> <div>16%</div> </div> |
| 28  | 8     | 163    | <div> <div>77%</div> <div>85%</div> <div>15%</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 0     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 0     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 201 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 205 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 206 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 207 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 208 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 209 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 210 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 211 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 212 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 213 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 214 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 215 | X         | -        | -       | -                |
| 31  | CLA  | 1     | 216 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 313 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 2     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 204 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 205 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 206 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 207 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 208 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 209 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 210 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 211 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 212 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 213 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 201 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 205 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 206 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 207 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 208 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 209 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 210 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 6     | 211 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 212 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 213 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 214 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 215 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 216 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 304 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 204 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 205 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 206 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 207 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 208 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 209 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 210 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 211 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 212 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 213 | X         | -        | -       | -                |
| 31  | CLA  | A     | 403 | X         | -        | -       | -                |
| 31  | CLA  | A     | 404 | X         | -        | -       | -                |
| 31  | CLA  | A     | 407 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | B     | 501 | X         | -        | -       | -                |
| 31  | CLA  | B     | 502 | X         | -        | -       | -                |
| 31  | CLA  | B     | 503 | X         | -        | -       | -                |
| 31  | CLA  | B     | 504 | X         | -        | -       | -                |
| 31  | CLA  | B     | 505 | X         | -        | -       | -                |
| 31  | CLA  | B     | 506 | X         | -        | -       | -                |
| 31  | CLA  | B     | 507 | X         | -        | -       | -                |
| 31  | CLA  | B     | 508 | X         | -        | -       | -                |
| 31  | CLA  | B     | 509 | X         | -        | -       | -                |
| 31  | CLA  | B     | 510 | X         | -        | -       | -                |
| 31  | CLA  | B     | 511 | X         | -        | -       | -                |
| 31  | CLA  | B     | 512 | X         | -        | -       | -                |
| 31  | CLA  | B     | 513 | X         | -        | -       | -                |
| 31  | CLA  | B     | 514 | X         | -        | -       | -                |
| 31  | CLA  | B     | 515 | X         | -        | -       | -                |
| 31  | CLA  | B     | 516 | X         | -        | -       | -                |
| 31  | CLA  | C     | 502 | X         | -        | -       | -                |
| 31  | CLA  | C     | 503 | X         | -        | -       | -                |
| 31  | CLA  | C     | 504 | X         | -        | -       | -                |
| 31  | CLA  | C     | 505 | X         | -        | -       | -                |
| 31  | CLA  | C     | 506 | X         | -        | -       | -                |
| 31  | CLA  | C     | 507 | X         | -        | -       | -                |
| 31  | CLA  | C     | 508 | X         | -        | -       | -                |
| 31  | CLA  | C     | 509 | X         | -        | -       | -                |
| 31  | CLA  | C     | 510 | X         | -        | -       | -                |
| 31  | CLA  | C     | 511 | X         | -        | -       | -                |
| 31  | CLA  | C     | 512 | X         | -        | -       | -                |
| 31  | CLA  | C     | 513 | X         | -        | -       | -                |
| 31  | CLA  | C     | 514 | X         | -        | -       | -                |
| 31  | CLA  | D     | 401 | X         | -        | -       | -                |
| 31  | CLA  | D     | 403 | X         | -        | -       | -                |
| 31  | CLA  | D     | 404 | X         | -        | -       | -                |
| 31  | CLA  | P     | 601 | X         | -        | -       | -                |
| 31  | CLA  | P     | 602 | X         | -        | -       | -                |
| 31  | CLA  | P     | 603 | X         | -        | -       | -                |
| 31  | CLA  | P     | 604 | X         | -        | -       | -                |
| 31  | CLA  | P     | 605 | X         | -        | -       | -                |
| 31  | CLA  | P     | 606 | X         | -        | -       | -                |
| 31  | CLA  | P     | 607 | X         | -        | -       | -                |
| 31  | CLA  | P     | 608 | X         | -        | -       | -                |
| 31  | CLA  | P     | 609 | X         | -        | -       | -                |
| 31  | CLA  | W     | 202 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | Z     | 101 | X         | -        | -       | -                |
| 31  | CLA  | a     | 403 | X         | -        | -       | -                |
| 31  | CLA  | a     | 404 | X         | -        | -       | -                |
| 31  | CLA  | a     | 407 | X         | -        | -       | -                |
| 31  | CLA  | b     | 502 | X         | -        | -       | -                |
| 31  | CLA  | b     | 503 | X         | -        | -       | -                |
| 31  | CLA  | b     | 504 | X         | -        | -       | -                |
| 31  | CLA  | b     | 505 | X         | -        | -       | -                |
| 31  | CLA  | b     | 506 | X         | -        | -       | -                |
| 31  | CLA  | b     | 507 | X         | -        | -       | -                |
| 31  | CLA  | b     | 508 | X         | -        | -       | -                |
| 31  | CLA  | b     | 509 | X         | -        | -       | -                |
| 31  | CLA  | b     | 510 | X         | -        | -       | -                |
| 31  | CLA  | b     | 511 | X         | -        | -       | -                |
| 31  | CLA  | b     | 512 | X         | -        | -       | -                |
| 31  | CLA  | b     | 513 | X         | -        | -       | -                |
| 31  | CLA  | b     | 514 | X         | -        | -       | -                |
| 31  | CLA  | b     | 515 | X         | -        | -       | -                |
| 31  | CLA  | b     | 516 | X         | -        | -       | -                |
| 31  | CLA  | b     | 517 | X         | -        | -       | -                |
| 31  | CLA  | c     | 502 | X         | -        | -       | -                |
| 31  | CLA  | c     | 503 | X         | -        | -       | -                |
| 31  | CLA  | c     | 504 | X         | -        | -       | -                |
| 31  | CLA  | c     | 505 | X         | -        | -       | -                |
| 31  | CLA  | c     | 506 | X         | -        | -       | -                |
| 31  | CLA  | c     | 507 | X         | -        | -       | -                |
| 31  | CLA  | c     | 508 | X         | -        | -       | -                |
| 31  | CLA  | c     | 509 | X         | -        | -       | -                |
| 31  | CLA  | c     | 510 | X         | -        | -       | -                |
| 31  | CLA  | c     | 511 | X         | -        | -       | -                |
| 31  | CLA  | c     | 512 | X         | -        | -       | -                |
| 31  | CLA  | c     | 513 | X         | -        | -       | -                |
| 31  | CLA  | c     | 514 | X         | -        | -       | -                |
| 31  | CLA  | d     | 401 | X         | -        | -       | -                |
| 31  | CLA  | d     | 403 | X         | -        | -       | -                |
| 31  | CLA  | d     | 404 | X         | -        | -       | -                |
| 31  | CLA  | p     | 601 | X         | -        | -       | -                |
| 31  | CLA  | p     | 602 | X         | -        | -       | -                |
| 31  | CLA  | p     | 603 | X         | -        | -       | -                |
| 31  | CLA  | p     | 604 | X         | -        | -       | -                |
| 31  | CLA  | p     | 605 | X         | -        | -       | -                |
| 31  | CLA  | p     | 606 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | p     | 607 | X         | -        | -       | -                |
| 31  | CLA  | p     | 608 | X         | -        | -       | -                |
| 31  | CLA  | p     | 609 | X         | -        | -       | -                |
| 31  | CLA  | w     | 202 | X         | -        | -       | -                |
| 31  | CLA  | z     | 101 | X         | -        | -       | -                |

## 2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 71446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PsbA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 333      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2530  | 1656 | 421 | 439 | 14 |         |       |
| 1   | a     | 333      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2530  | 1656 | 421 | 439 | 14 |         |       |

- Molecule 2 is a protein called PsbB.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2456 | 635 | 646 | 11 |         |       |
| 2   | b     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2456 | 635 | 646 | 11 |         |       |

- Molecule 3 is a protein called PsbC.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3437  | 2252 | 579 | 595 | 11 |         |       |
| 3   | c     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3437  | 2252 | 579 | 595 | 11 |         |       |

- Molecule 4 is a protein called PsbD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2667  | 1765 | 437 | 455 | 10 |         |       |
| 4   | d     | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2667  | 1765 | 437 | 455 | 10 |         |       |

- Molecule 5 is a protein called PsbE.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5   | E     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 602   | 392 | 101 | 109 |         |       |
| 5   | e     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 602   | 392 | 101 | 109 |         |       |

- Molecule 6 is a protein called PsbF.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 6   | F     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 242   | 166 | 41 | 35 |         |       |
| 6   | f     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 242   | 166 | 41 | 35 |         |       |

- Molecule 7 is a protein called PsbH.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | H     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 499   | 331 | 82 | 85 | 1 |         |       |
| 7   | h     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 499   | 331 | 82 | 85 | 1 |         |       |

- Molecule 8 is a protein called PsbI.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 266   | 179 | 40 | 46 | 1 |         |       |
| 8   | i     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 266   | 179 | 40 | 46 | 1 |         |       |

- Molecule 9 is a protein called PsbJ.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | J     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 247   | 167 | 38 | 42 |         |       |
| 9   | j     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 247   | 167 | 38 | 42 |         |       |

- Molecule 10 is a protein called PsbK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | K     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 294   | 205 | 44 | 45 |         |       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 294   | 205 | 44 | 45 |         |       |

- Molecule 11 is a protein called PsbL.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 294   | 197 | 46 | 51 |         |       |
| 11  | l     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 294   | 197 | 46 | 51 |         |       |

- Molecule 12 is a protein called PsbM.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 12  | M     | 41       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 295   | 193 | 49 | 53 |         |       |
| 12  | m     | 41       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 295   | 193 | 49 | 53 |         |       |

- Molecule 13 is a protein called Psb34.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 13  | N     | 30       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 150   | 90 | 30 | 30 |         |       |
| 13  | n     | 30       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 150   | 90 | 30 | 30 |         |       |

- Molecule 14 is a protein called PsbO.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | O     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1151 | 304 | 362 | 7 |         |       |
| 14  | o     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1151 | 304 | 362 | 7 |         |       |

- Molecule 15 is a protein called PsbQ'.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | Q     | 145      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1050  | 654 | 182 | 214 |         |       |
| 15  | q     | 145      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1050  | 654 | 182 | 214 |         |       |

- Molecule 16 is a protein called PsbT.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | T     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 234   | 164 | 32 | 36 | 2 |         |       |
| 16  | t     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 234   | 164 | 32 | 36 | 2 |         |       |

- Molecule 17 is a protein called PsbU.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | U     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 678   | 436 | 111 | 130 | 1 |         |       |
| 17  | u     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 678   | 436 | 111 | 130 | 1 |         |       |

- Molecule 18 is a protein called PsbV.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | V     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 612 | 169 | 194 | 4 |         |       |
| 18  | v     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 612 | 169 | 194 | 4 |         |       |

- Molecule 19 is a protein called PsbW.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | W     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 338   | 211 | 56 | 68 | 3 |         |       |
| 19  | w     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 338   | 211 | 56 | 68 | 3 |         |       |

- Molecule 20 is a protein called PsbX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | X     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 233   | 150 | 39 | 43 | 1 |         |       |
| 20  | x     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 233   | 150 | 39 | 43 | 1 |         |       |

- Molecule 21 is a protein called PsbY.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 21  | Y     | 33       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 216   | 137 | 39 | 40 |         |       |
| 21  | y     | 33       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 216   | 137 | 39 | 40 |         |       |

- Molecule 22 is a protein called PsbZ.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | Z     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 413   | 270 | 65 | 77 | 1 |         |       |
| 22  | z     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 413   | 270 | 65 | 77 | 1 |         |       |

- Molecule 23 is a protein called FCPII-G, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | 5     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1280  | 827 | 211 | 239 | 3 |         |       |
| 23  | 0     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1280  | 827 | 211 | 239 | 3 |         |       |

- Molecule 24 is a protein called FCPII-H2, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 7     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1222  | 808 | 198 | 212 | 4 |         |       |
| 24  | 2     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1222  | 808 | 198 | 212 | 4 |         |       |

- Molecule 25 is a protein called FCPII-H1, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 6     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1209  | 796 | 210 | 201 | 2 |         |       |
| 25  | 1     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1209  | 796 | 210 | 201 | 2 |         |       |

- Molecule 26 is a protein called FCPII-I, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | p     | 214      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1265  | 789 | 230 | 245 | 1 |         |       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 214      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1265  | 789 | 230 | 245 | 1 |         |       |

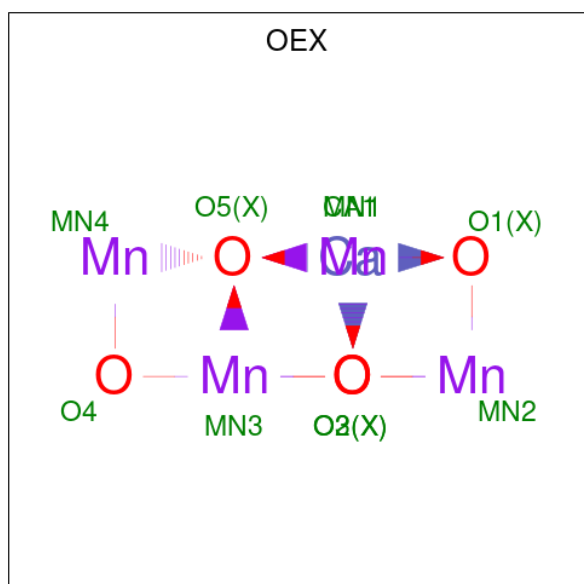
- Molecule 27 is a protein called FCPII-K, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 27  | 4     | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 27  | 9     | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |

- Molecule 28 is a protein called FCPII-J, fucoxanthin chlorophyll a/c binding protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28  | 3     | 163      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 992   | 616 | 192 | 184 |         |       |
| 28  | 8     | 163      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 992   | 616 | 192 | 184 |         |       |

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 29  | A     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |

Continued on next page...

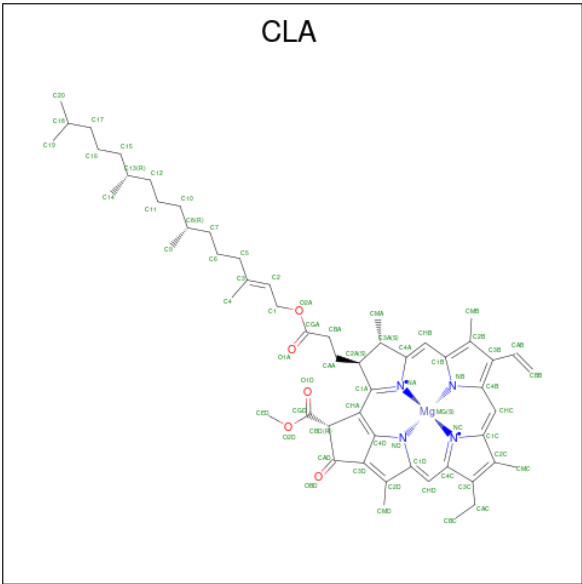
Continued from previous page...

| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 29  | a     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 30  | a     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | B     | 1        | Total<br>61 | C<br>52 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 31  | B     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | C     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | D     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | D     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | W     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | Z     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | b     | 1        | Total<br>61 | C<br>52 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 31  | b     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | c     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 31  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 31  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | w     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | p     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | p     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | p     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | p     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | p     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | p     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | p     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | p     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | p     | 1        | Total<br>39 | C<br>32 | Mg<br>1 | N<br>4 | O<br>2 | 0       |
| 31  | 4     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>35 | C<br>29 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 4     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 4     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>34 | C<br>28 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 4     | 1        | Total<br>35 | C<br>29 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 3     | 1        | Total<br>34 | C<br>28 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 3     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 3     | 1        | Total<br>33 | C<br>27 | Mg<br>1 | N<br>4 | O<br>1 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 35    | 29 | 1  | 4 | 1 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 39    | 33 | 1  | 4 | 1 |         |
| 31  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 35    | 29 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 31  | P     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 39    | 32 | 1  | 4 | 2 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 35    | 29 | 1  | 4 | 1 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 31  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | 9     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 9     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 9     | 1        | Total<br>34 | C<br>28 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 9     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 9     | 1        | Total<br>35 | C<br>29 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>34 | C<br>28 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 8     | 1        | Total<br>33 | C<br>27 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 8     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 8     | 1        | Total<br>35 | C<br>29 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 8     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 8     | 1        | Total<br>39 | C<br>33 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 8     | 1        | Total<br>35 | C<br>29 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 0     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 0     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 0     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 0     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

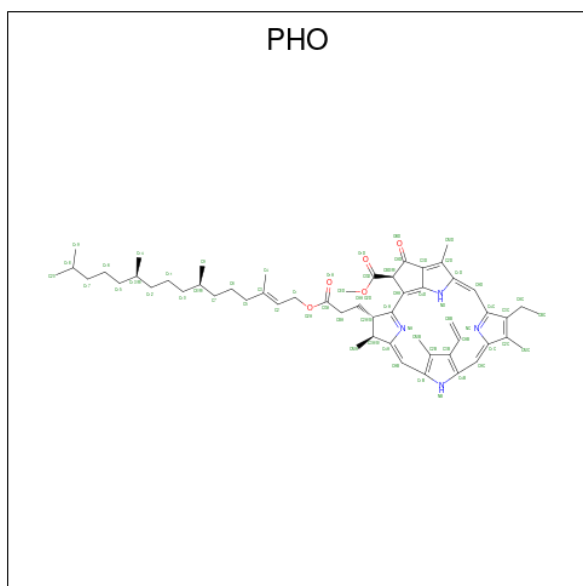
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | 0     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 0     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 0     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 0     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 0     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 0     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 0     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 2     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 2     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 2     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 2     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 2     | 1        | Total<br>38 | C<br>32 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 31  | 2     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | 1     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 1     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |

*Continued on next page...*

Continued from previous page...

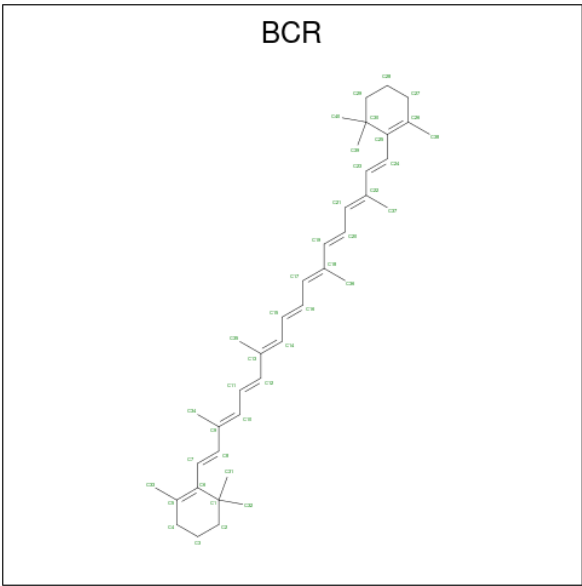
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 31  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 32  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 32  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 32  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 32  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 33  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 33  | D     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

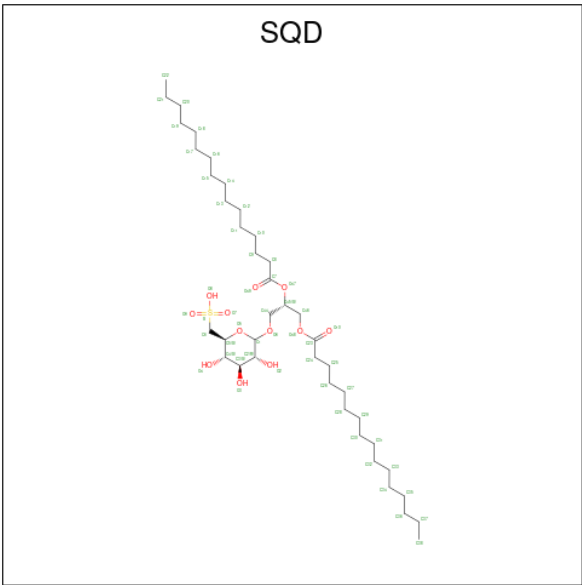
Continued on next page...



*Continued from previous page...*

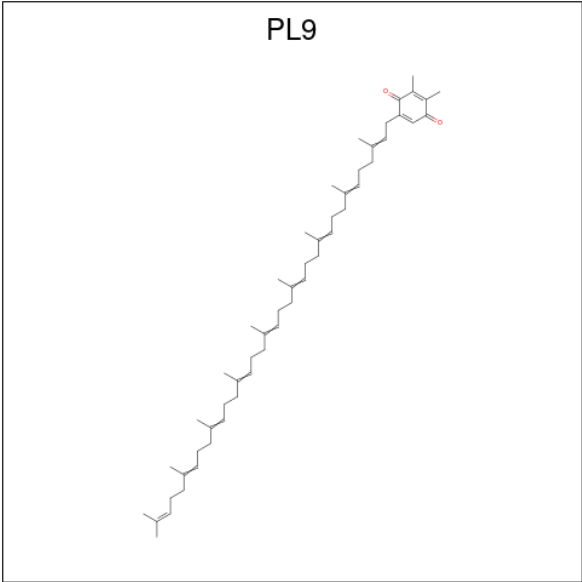
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 33  | H     | 1        | Total C<br>40 40 | 0       |
| 33  | K     | 1        | Total C<br>40 40 | 0       |
| 33  | a     | 1        | Total C<br>40 40 | 0       |
| 33  | b     | 1        | Total C<br>40 40 | 0       |
| 33  | b     | 1        | Total C<br>40 40 | 0       |
| 33  | b     | 1        | Total C<br>40 40 | 0       |
| 33  | c     | 1        | Total C<br>40 40 | 0       |
| 33  | c     | 1        | Total C<br>40 40 | 0       |
| 33  | c     | 1        | Total C<br>40 40 | 0       |
| 33  | d     | 1        | Total C<br>40 40 | 0       |
| 33  | h     | 1        | Total C<br>40 40 | 0       |
| 33  | k     | 1        | Total C<br>40 40 | 0       |

- Molecule 34 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) (labeled as "Ligand of Interest" by depositor).



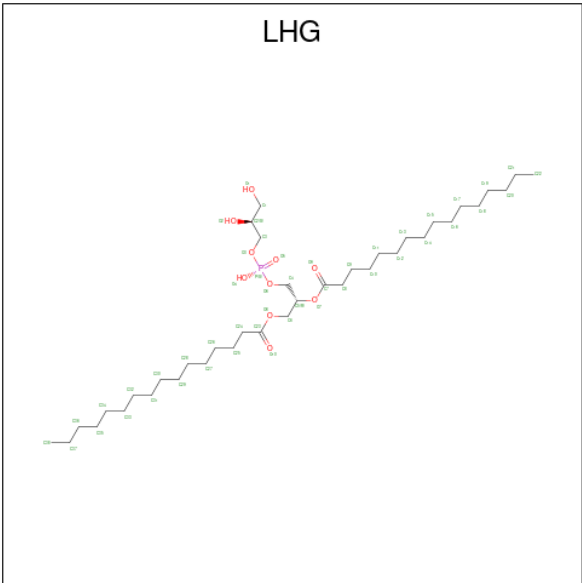
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 34  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 34  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 34  | B     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 34  | B     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 40    | 27 | 12 | 1 |         |
| 34  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 34  | b     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 40    | 27 | 12 | 1 |         |
| 34  | 5     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 48    | 35 | 12 | 1 |         |
| 34  | 0     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 48    | 35 | 12 | 1 |         |

- Molecule 35 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>) (labeled as "Ligand of Interest" by depositor).



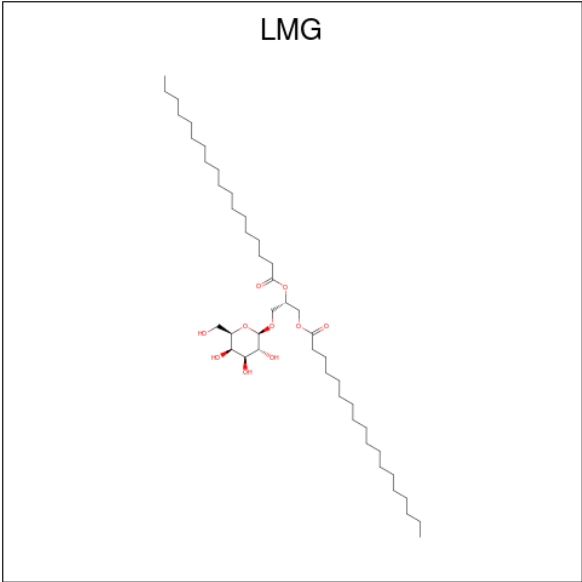
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 32    | 30 | 2 |         |
| 35  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 35  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 32    | 30 | 2 |         |
| 35  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 36  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 36  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 26    | 15 | 10 | 1 |         |
| 36  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 36  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 38 | 9  | 1 |         |
| 36  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 34    | 23 | 10 | 1 |         |
| 36  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 28    | 19 | 8  | 1 |         |
| 36  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 36  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 36  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 26    | 15 | 10 | 1 |         |
| 36  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 38 | 9  | 1 |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 34    | 23 | 10 | 1 |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 28    | 19 | 8  | 1 |         |
| 36  | h     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 37  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 28    | 18 | 10 |         |
| 37  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 37  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 37  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |
| 37  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 37  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 50    | 40 | 10 |         |
| 37  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 37  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 37  | W     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 37  | Y     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 37  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 28    | 18 | 10 |         |
| 37  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 37  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 37  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |

Continued on next page...

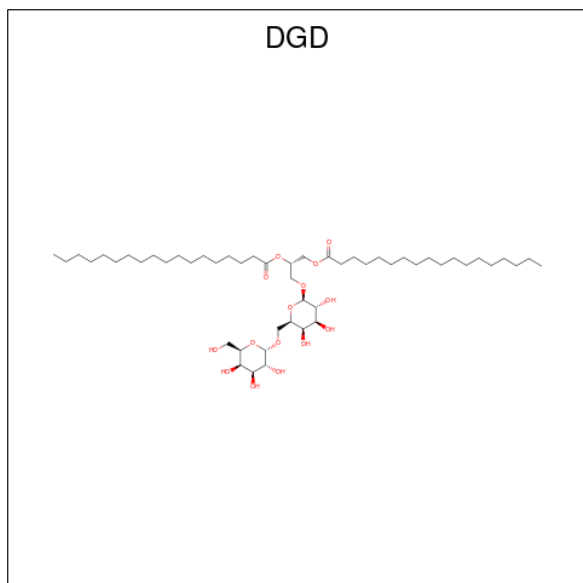
Continued from previous page...

| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 37  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 37  | j     | 1        | Total | C  | O  | 0       |
|     |       |          | 50    | 40 | 10 |         |
| 37  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 37  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 37  | w     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 37  | y     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 37  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 37  | 0     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |

- Molecule 38 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

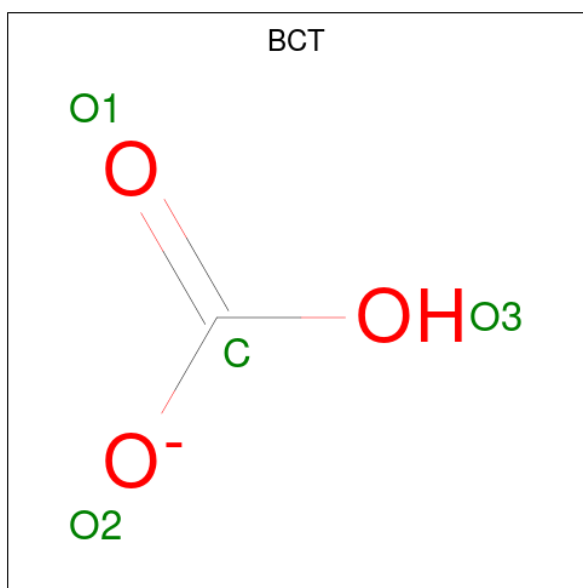
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 38  | C     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 38  | c     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



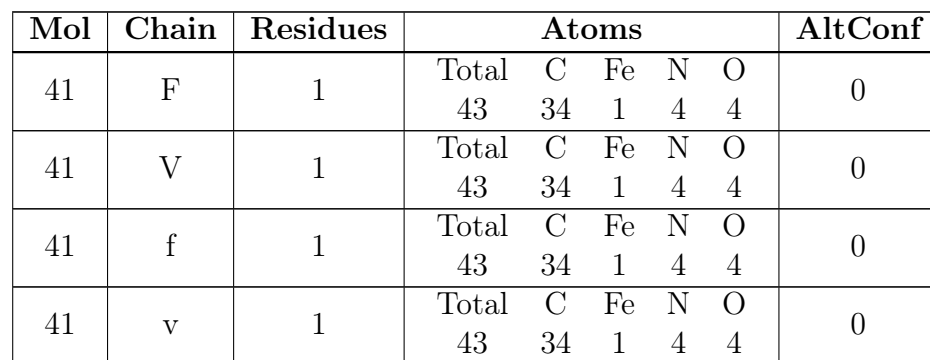
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 39  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 39  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 39  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 39  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 39  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 39  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 39  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 39  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).

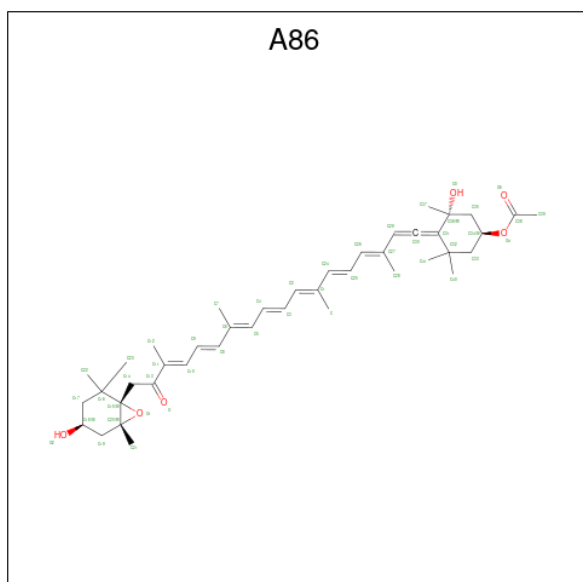


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 40  | D     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |
| 40  | d     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ) (labeled as "Ligand of Interest" by depositor).



- Molecule 42 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).





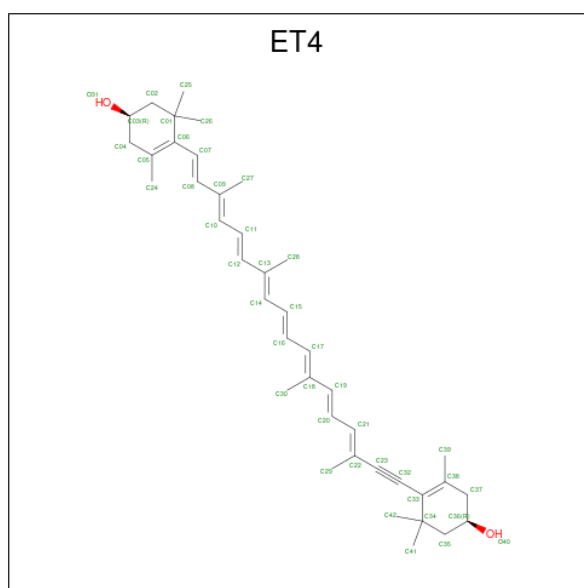
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 42  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | p     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

*Continued on next page...*

Continued from previous page...

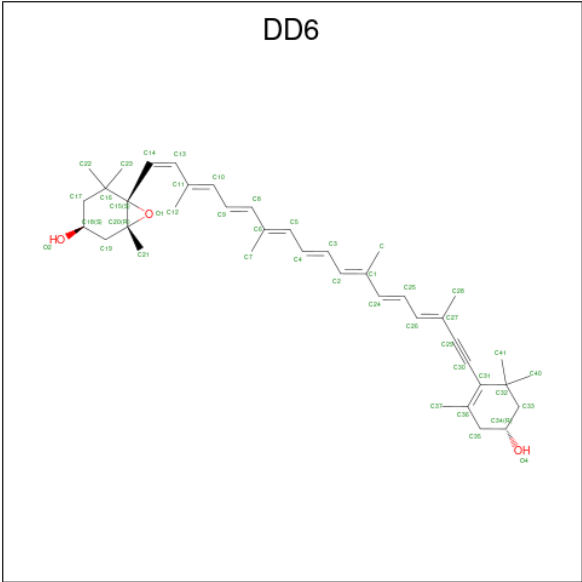
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 42  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 42  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

- Molecule 43 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 43  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 43  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 44 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

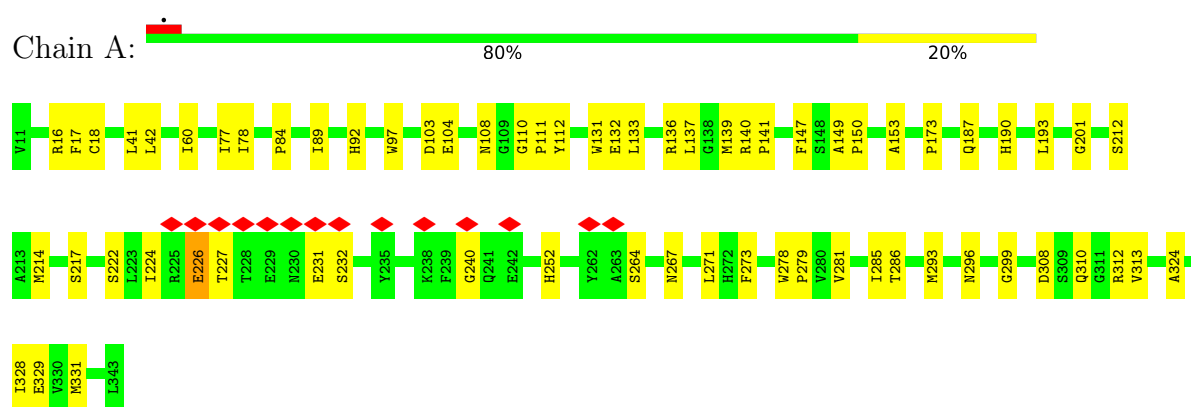


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 44  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | p     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 44  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |

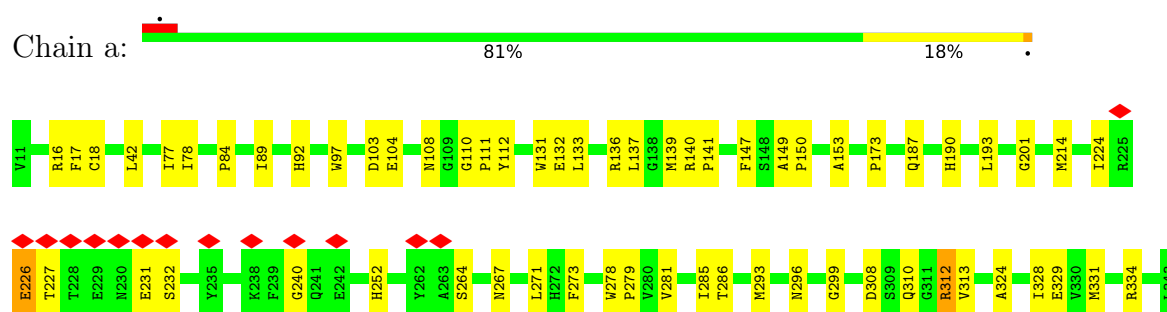
### 3 Residue-property plots [i](#)

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.

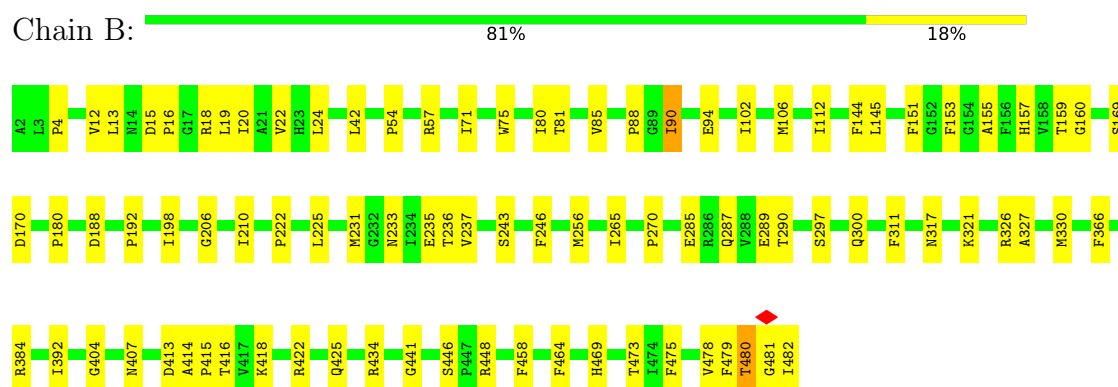
#### • Molecule 1: PsbA



#### • Molecule 1: PsbA

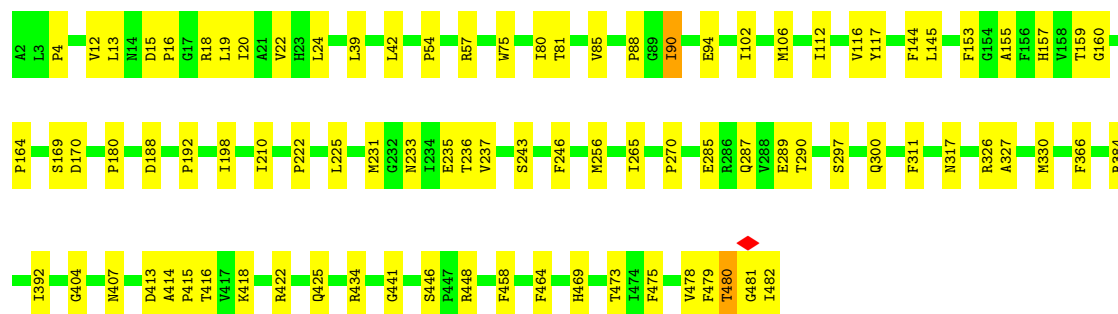


#### • Molecule 2: PsbB



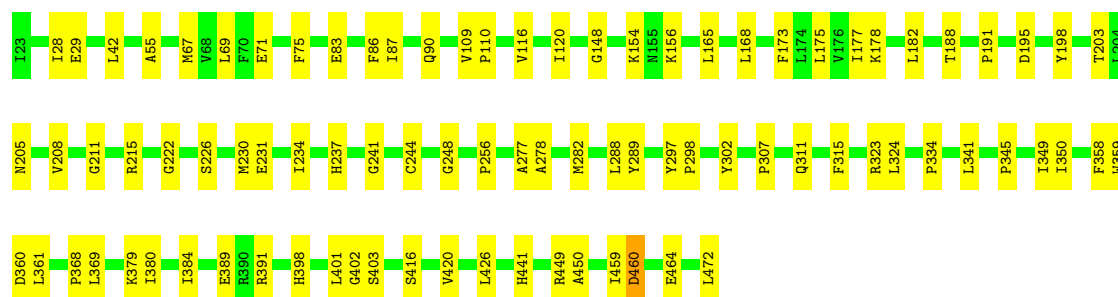
- Molecule 2: PsbB

Chain b:  81% 18%



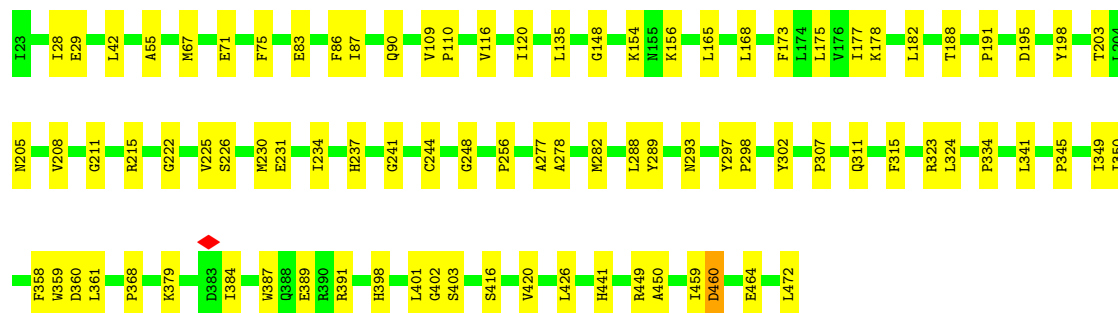
- Molecule 3: PsbC

Chain C:  80% 19%



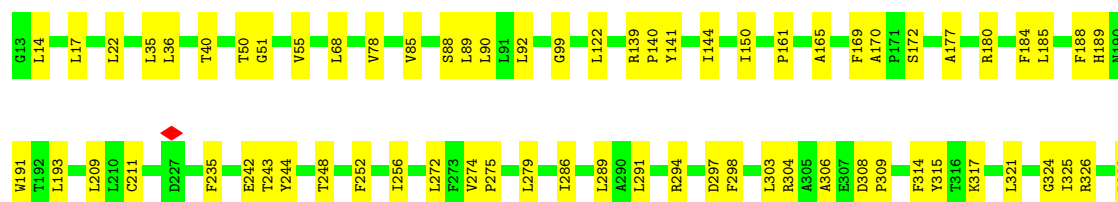
- Molecule 3: PsbC

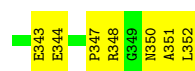
Chain c:  80% 20%



- Molecule 4: PsbD

Chain D:  78% 22%





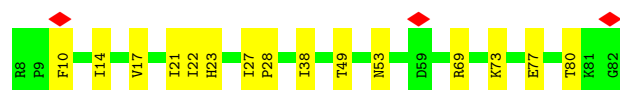
• Molecule 4: PsbD

Chain d: 79% 21%



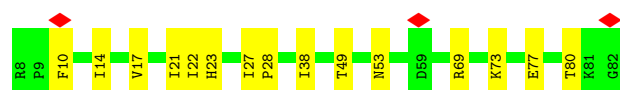
• Molecule 5: PsbE

Chain E: 80% 20%



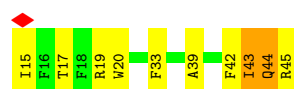
• Molecule 5: PsbE

Chain e: 80% 20%



• Molecule 6: PsbF

Chain F: 68% 26% 6%



• Molecule 6: PsbF

Chain f: 68% 26% 6%

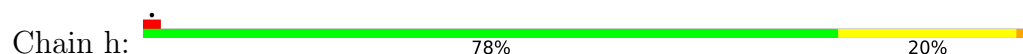


• Molecule 7: PsbH

Chain H: 78% 20%



• Molecule 7: PsbH



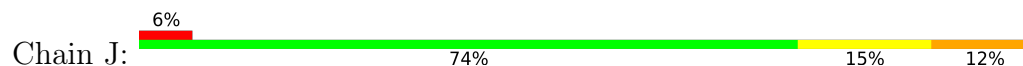
• Molecule 8: PsbI



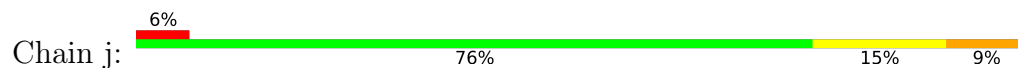
• Molecule 8: PsbI



• Molecule 9: PsbJ



• Molecule 9: PsbJ



• Molecule 10: PsbK



• Molecule 10: PsbK





• Molecule 11: PsbL

Chain L: 78% 22%



• Molecule 11: PsbL

Chain l: 78% 22%



• Molecule 12: PsbM

Chain M: 73% 24% .



• Molecule 12: PsbM

Chain m: 73% 24% .



• Molecule 13: Psb34

Chain N: 7% 97% .



• Molecule 13: Psb34

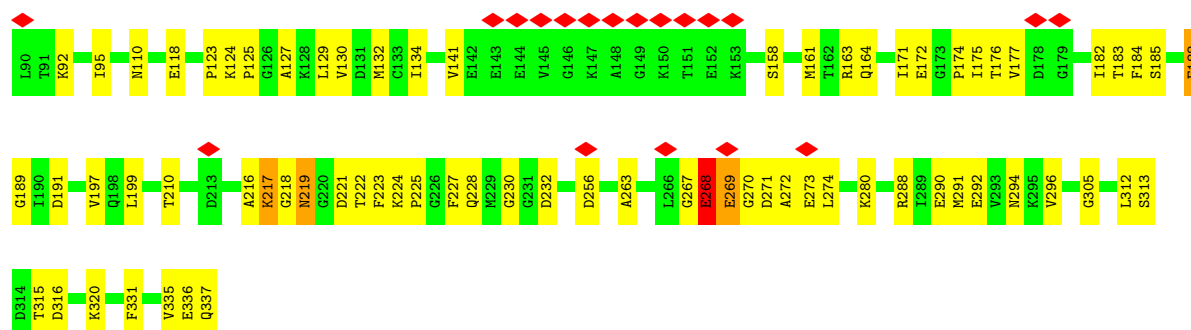
Chain n: 10% 97% .



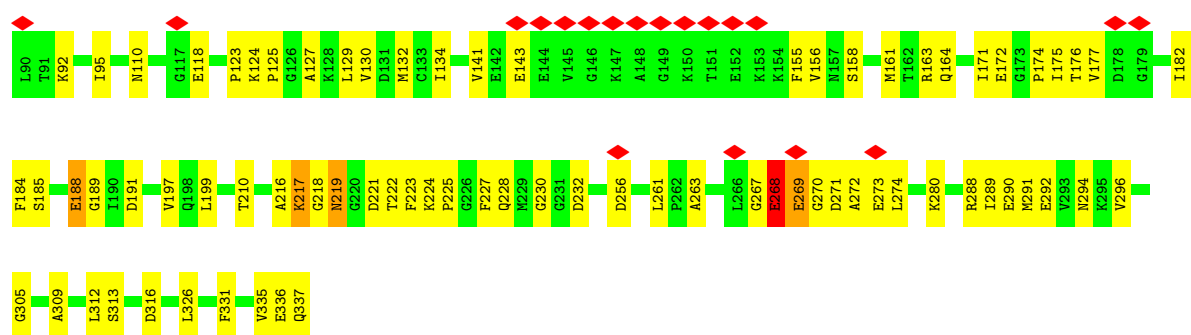
• Molecule 14: PsbO

Chain O: 8% 71% 27% .

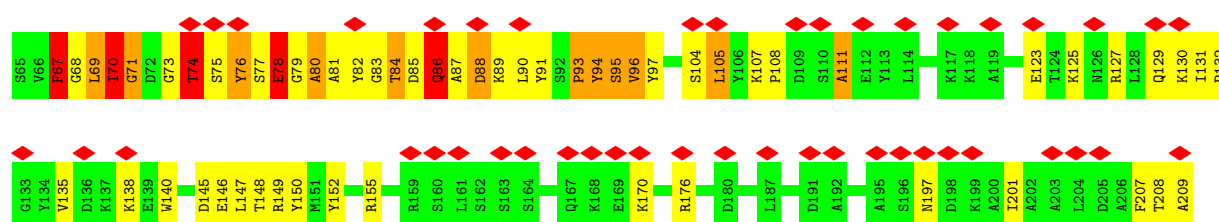




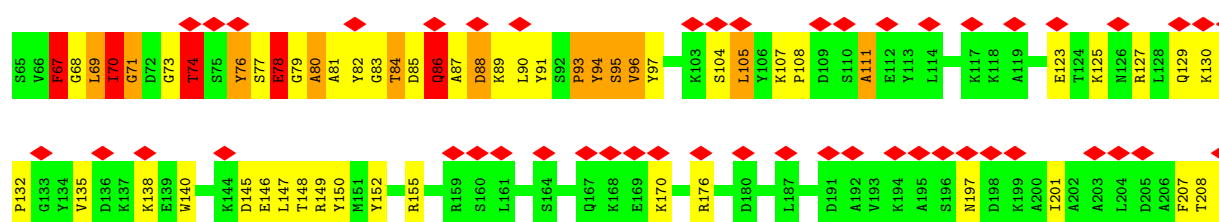
• Molecule 14: PsbO



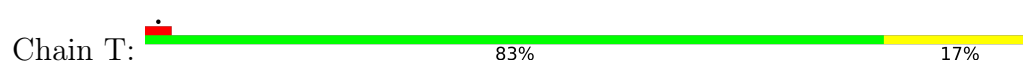
• Molecule 15: PsbQ'



• Molecule 15: PsbQ'

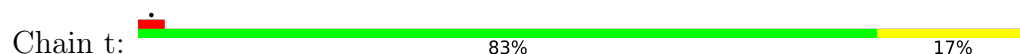


• Molecule 16: PsbT

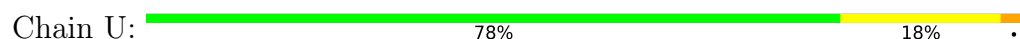




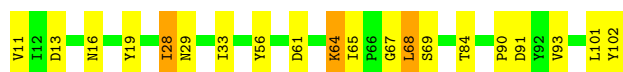
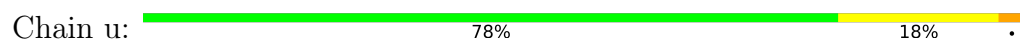
• Molecule 16: PsbT



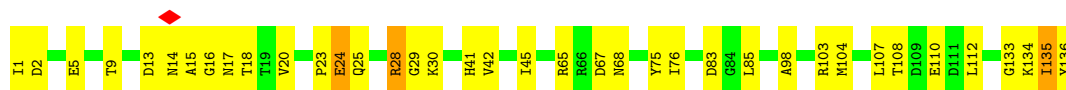
• Molecule 17: PsbU



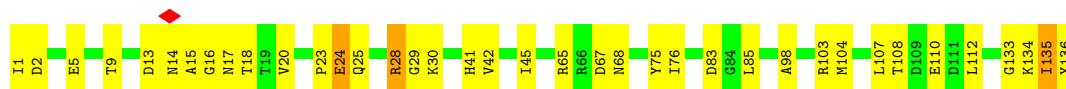
• Molecule 17: PsbU



• Molecule 18: PsbV



• Molecule 18: PsbV

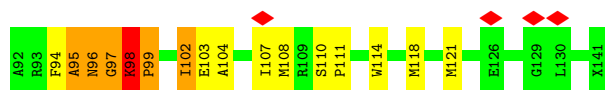


• Molecule 19: PsbW



• Molecule 19: PsbW





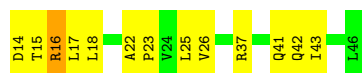
• Molecule 20: PsbX



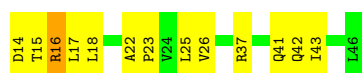
• Molecule 20: PsbX



• Molecule 21: PsbY



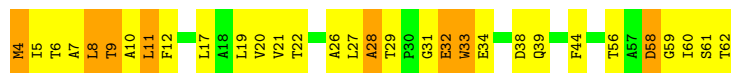
• Molecule 21: PsbY



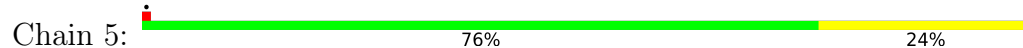
• Molecule 22: PsbZ

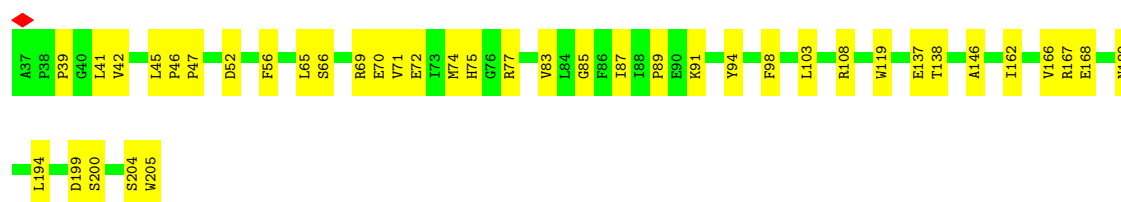


• Molecule 22: PsbZ

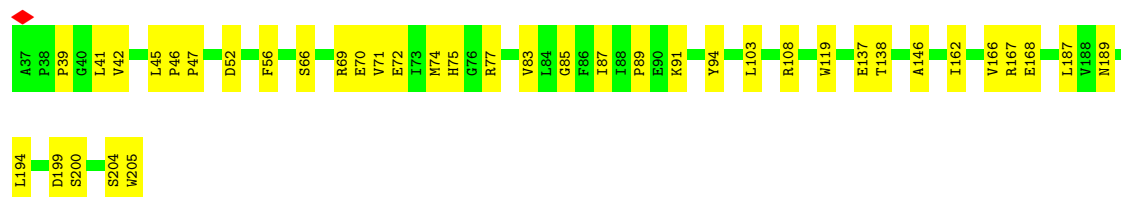
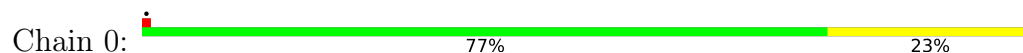


• Molecule 23: FCPH-G, fucoxanthin chlorophyll a/c binding protein

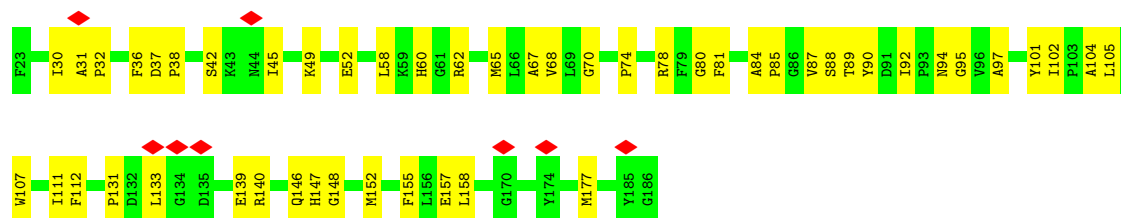




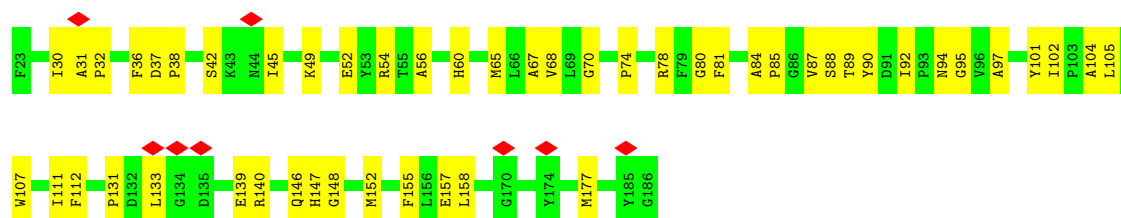
- Molecule 23: FCPH-G, fucoxanthin chlorophyll a/c binding protein



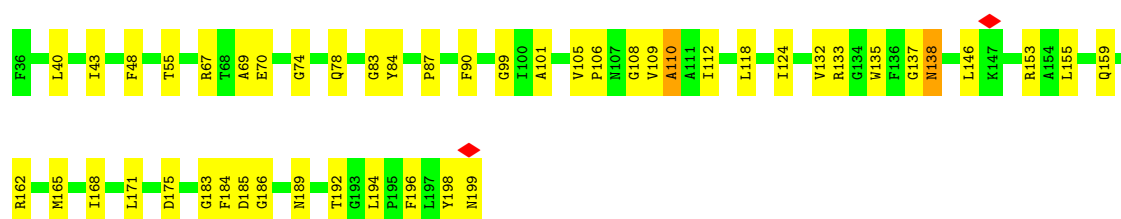
- Molecule 24: FCPH-H2, fucoxanthin chlorophyll a/c binding protein



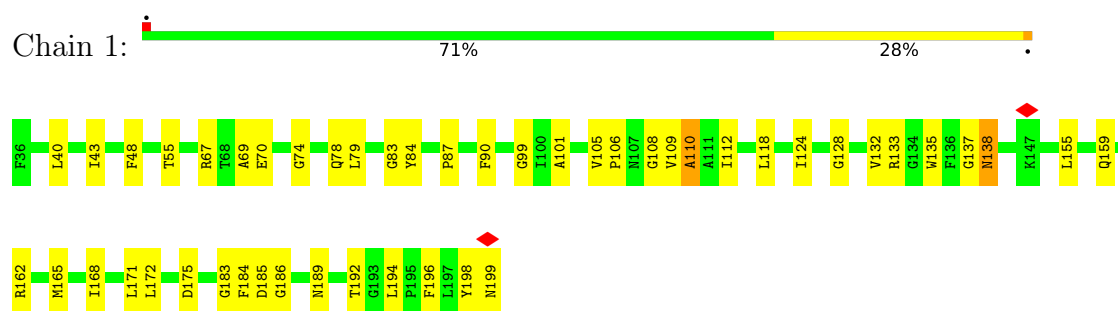
- Molecule 24: FCPH-H2, fucoxanthin chlorophyll a/c binding protein



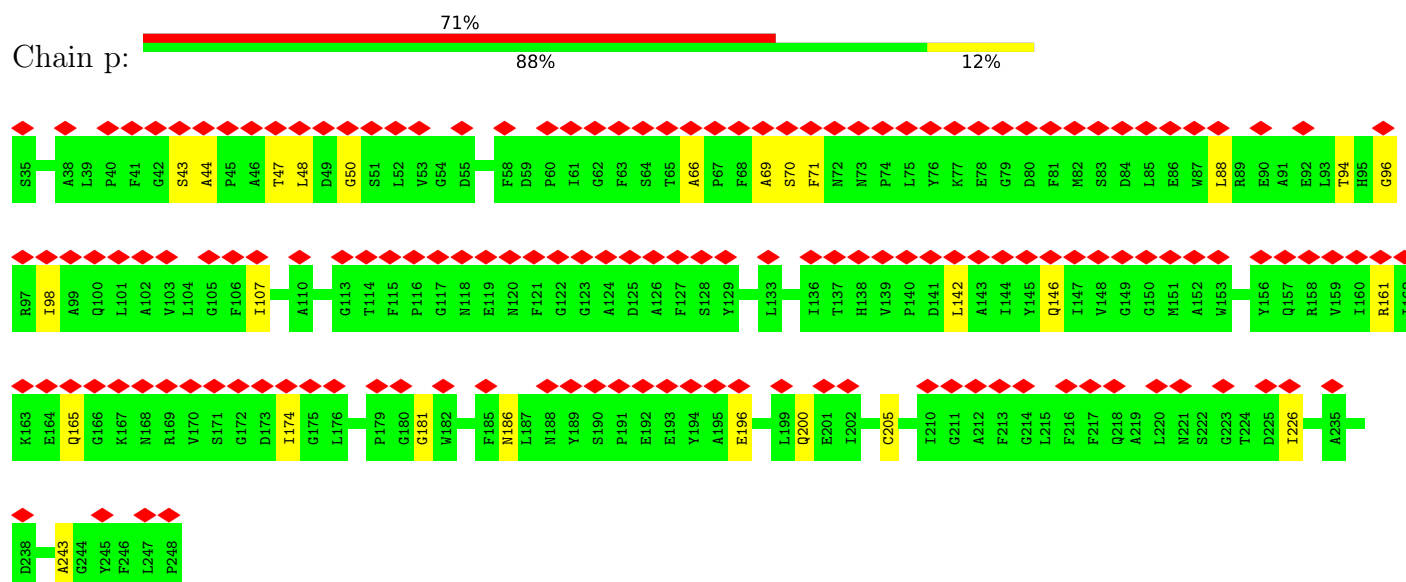
- Molecule 25: FCPH-H1, fucoxanthin chlorophyll a/c binding protein



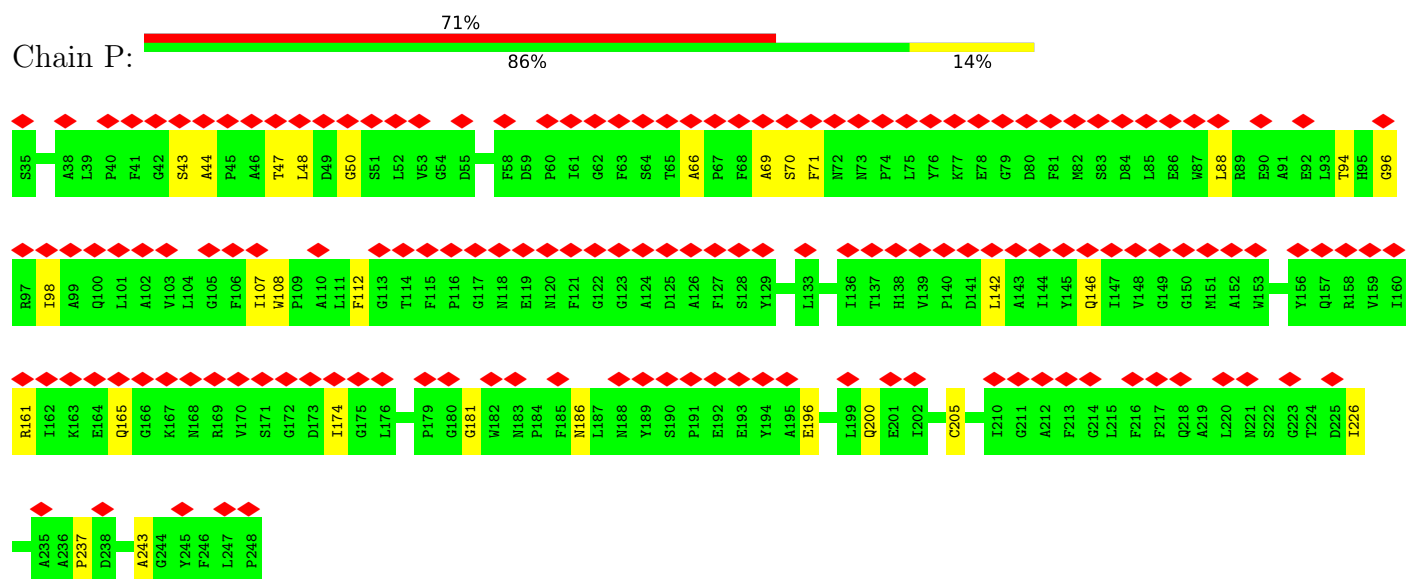
- Molecule 25: FCPH-H1, fucoxanthin chlorophyll a/c binding protein



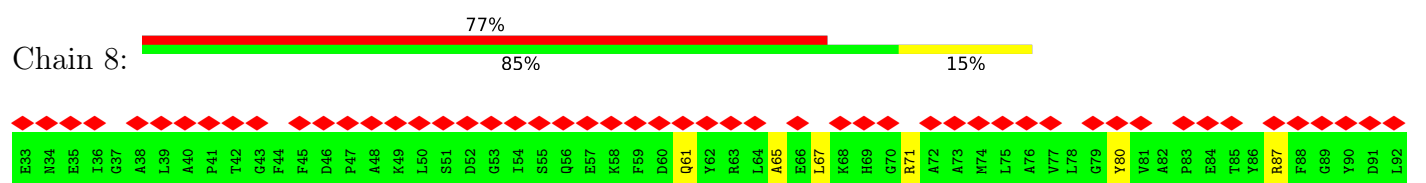
- Molecule 26: FCPH-I, fucoxanthin chlorophyll a/c binding protein

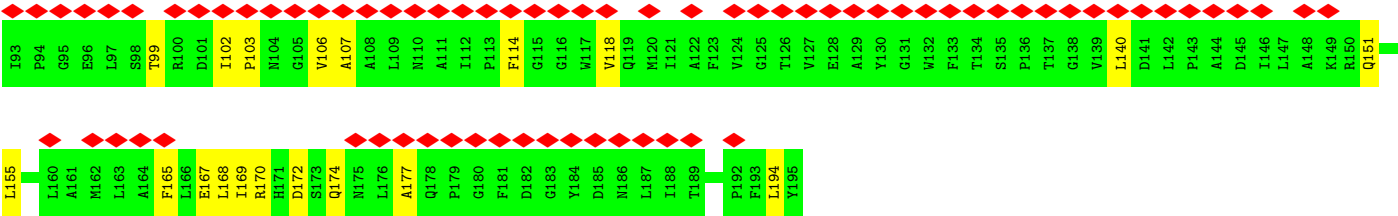


- Molecule 26: FCPH-I, fucoxanthin chlorophyll a/c binding protein



- Molecule 27: FCPH-K, fucoxanthin chlorophyll a/c binding protein





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 153326                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.709                                   | Depositor |
| Minimum map value                    | -0.314                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.018                                   | Depositor |
| Recommended contour level            | 0.158                                   | Depositor |
| Map size (Å)                         | 542.72, 542.72, 542.72                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | 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: A86, BCR, OEX, PL9, CLA, BCT, DD6, SQD, HEM, ET4, DGD, CL, PHO, FE2, LMG, 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   | A     | 0.28         | 0/2609       | 0.39        | 0/3563        |
| 1   | a     | 0.28         | 0/2609       | 0.40        | 0/3563        |
| 2   | B     | 0.24         | 0/3878       | 0.36        | 0/5282        |
| 2   | b     | 0.24         | 0/3878       | 0.36        | 0/5282        |
| 3   | C     | 0.21         | 0/3553       | 0.35        | 0/4850        |
| 3   | c     | 0.22         | 0/3553       | 0.35        | 0/4850        |
| 4   | D     | 0.20         | 0/2759       | 0.34        | 0/3766        |
| 4   | d     | 0.20         | 0/2759       | 0.34        | 0/3766        |
| 5   | E     | 0.20         | 0/620        | 0.33        | 0/847         |
| 5   | e     | 0.20         | 0/620        | 0.33        | 0/847         |
| 6   | F     | 0.56         | 0/250        | 0.64        | 0/340         |
| 6   | f     | 0.56         | 0/250        | 0.64        | 0/340         |
| 7   | H     | 0.34         | 0/509        | 0.50        | 0/696         |
| 7   | h     | 0.34         | 0/509        | 0.50        | 0/696         |
| 8   | I     | 0.40         | 0/273        | 0.51        | 0/371         |
| 8   | i     | 0.40         | 0/273        | 0.51        | 0/371         |
| 9   | J     | 0.80         | 2/253 (0.8%) | 0.96        | 4/344 (1.2%)  |
| 9   | j     | 0.79         | 2/253 (0.8%) | 0.96        | 4/344 (1.2%)  |
| 10  | K     | 0.51         | 0/305        | 0.59        | 0/420         |
| 10  | k     | 0.51         | 0/305        | 0.59        | 0/420         |
| 11  | L     | 0.31         | 0/303        | 0.43        | 0/415         |
| 11  | l     | 0.31         | 0/303        | 0.43        | 0/415         |
| 12  | M     | 0.33         | 0/299        | 0.39        | 0/404         |
| 12  | m     | 0.33         | 0/299        | 0.39        | 0/404         |
| 14  | O     | 0.24         | 0/1853       | 0.40        | 0/2505        |
| 14  | o     | 0.25         | 0/1853       | 0.40        | 0/2505        |
| 15  | Q     | 0.35         | 0/1065       | 0.63        | 1/1439 (0.1%) |
| 15  | q     | 0.35         | 0/1065       | 0.63        | 1/1439 (0.1%) |
| 16  | T     | 0.22         | 0/240        | 0.34        | 0/325         |
| 16  | t     | 0.23         | 0/240        | 0.34        | 0/325         |
| 17  | U     | 0.21         | 0/693        | 0.36        | 0/945         |
| 17  | u     | 0.21         | 0/693        | 0.36        | 0/945         |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 18  | V     | 0.33         | 0/996          | 0.46        | 0/1364          |
| 18  | v     | 0.33         | 0/996          | 0.46        | 0/1364          |
| 19  | W     | 0.46         | 0/310          | 0.85        | 3/421 (0.7%)    |
| 19  | w     | 0.42         | 0/310          | 0.85        | 3/421 (0.7%)    |
| 20  | X     | 0.35         | 0/233          | 0.45        | 0/315           |
| 20  | x     | 0.35         | 0/233          | 0.45        | 0/315           |
| 21  | Y     | 0.49         | 0/216          | 0.72        | 0/297           |
| 21  | y     | 0.50         | 0/216          | 0.72        | 0/297           |
| 22  | Z     | 0.40         | 0/419          | 0.45        | 0/578           |
| 22  | z     | 0.40         | 0/419          | 0.45        | 0/578           |
| 23  | 0     | 0.27         | 0/1312         | 0.48        | 0/1792          |
| 23  | 5     | 0.27         | 0/1312         | 0.49        | 0/1792          |
| 24  | 2     | 0.24         | 0/1258         | 0.44        | 0/1714          |
| 24  | 7     | 0.24         | 0/1258         | 0.44        | 0/1714          |
| 25  | 1     | 0.31         | 0/1242         | 0.47        | 0/1697          |
| 25  | 6     | 0.31         | 0/1242         | 0.47        | 0/1697          |
| 26  | P     | 0.33         | 0/1287         | 0.69        | 1/1778 (0.1%)   |
| 26  | p     | 0.33         | 0/1287         | 0.69        | 1/1778 (0.1%)   |
| 28  | 3     | 0.39         | 0/1003         | 0.65        | 0/1373          |
| 28  | 8     | 0.39         | 0/1003         | 0.65        | 0/1373          |
| All | All   | 0.29         | 4/55476 (0.0%) | 0.46        | 18/75682 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 9   | j     | 34  | SER  | N-CA  | 5.75 | 1.54        | 1.46     |
| 9   | J     | 34  | SER  | N-CA  | 5.72 | 1.54        | 1.46     |
| 9   | j     | 33  | TYR  | CA-C  | 5.59 | 1.60        | 1.52     |
| 9   | J     | 33  | TYR  | CA-C  | 5.57 | 1.60        | 1.52     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | J     | 33  | TYR  | N-CA-C | 6.89  | 122.03      | 112.45   |
| 9   | j     | 33  | TYR  | N-CA-C | 6.87  | 122.00      | 112.45   |
| 9   | J     | 34  | SER  | N-CA-C | 6.75  | 122.07      | 107.49   |
| 9   | j     | 34  | SER  | N-CA-C | 6.75  | 122.07      | 107.49   |
| 19  | w     | 97  | GLY  | N-CA-C | -6.11 | 102.47      | 111.03   |
| 9   | j     | 30  | TYR  | N-CA-C | -5.95 | 104.80      | 111.28   |
| 9   | J     | 30  | TYR  | N-CA-C | -5.92 | 104.82      | 111.28   |
| 19  | W     | 98  | LYS  | CA-C-N | -5.64 | 112.79      | 119.84   |
| 19  | W     | 98  | LYS  | C-N-CA | -5.64 | 112.79      | 119.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | j     | 32  | SER  | N-CA-C  | -5.46 | 104.77      | 111.75   |
| 9   | J     | 32  | SER  | N-CA-C  | -5.42 | 104.81      | 111.75   |
| 19  | W     | 97  | GLY  | N-CA-C  | -5.42 | 102.52      | 110.97   |
| 26  | p     | 243 | ALA  | CB-CA-C | -5.32 | 110.42      | 116.54   |
| 15  | Q     | 93  | PRO  | N-CA-C  | -5.32 | 101.91      | 110.74   |
| 15  | q     | 93  | PRO  | N-CA-C  | -5.31 | 101.93      | 110.74   |
| 26  | P     | 243 | ALA  | CB-CA-C | -5.30 | 110.44      | 116.54   |
| 19  | w     | 98  | LYS  | CA-C-N  | -5.25 | 113.28      | 119.84   |
| 19  | w     | 98  | LYS  | C-N-CA  | -5.25 | 113.28      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2530  | 0        | 2400     | 56      | 0            |
| 1   | a     | 2530  | 0        | 2400     | 53      | 0            |
| 2   | B     | 3748  | 0        | 3581     | 61      | 0            |
| 2   | b     | 3748  | 0        | 3581     | 64      | 0            |
| 3   | C     | 3437  | 0        | 3297     | 74      | 0            |
| 3   | c     | 3437  | 0        | 3297     | 74      | 0            |
| 4   | D     | 2667  | 0        | 2551     | 61      | 0            |
| 4   | d     | 2667  | 0        | 2551     | 57      | 0            |
| 5   | E     | 602   | 0        | 576      | 10      | 0            |
| 5   | e     | 602   | 0        | 576      | 10      | 0            |
| 6   | F     | 242   | 0        | 237      | 12      | 0            |
| 6   | f     | 242   | 0        | 237      | 12      | 0            |
| 7   | H     | 499   | 0        | 521      | 17      | 0            |
| 7   | h     | 499   | 0        | 521      | 16      | 0            |
| 8   | I     | 266   | 0        | 264      | 11      | 0            |
| 8   | i     | 266   | 0        | 264      | 11      | 0            |
| 9   | J     | 247   | 0        | 256      | 7       | 0            |
| 9   | j     | 247   | 0        | 256      | 5       | 0            |
| 10  | K     | 294   | 0        | 295      | 10      | 0            |
| 10  | k     | 294   | 0        | 295      | 10      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | L     | 294   | 0        | 281      | 7       | 0            |
| 11  | l     | 294   | 0        | 281      | 7       | 0            |
| 12  | M     | 295   | 0        | 292      | 6       | 0            |
| 12  | m     | 295   | 0        | 292      | 6       | 0            |
| 13  | N     | 150   | 0        | 33       | 1       | 0            |
| 13  | n     | 150   | 0        | 33       | 1       | 0            |
| 14  | O     | 1824  | 0        | 1775     | 54      | 0            |
| 14  | o     | 1824  | 0        | 1775     | 54      | 0            |
| 15  | Q     | 1050  | 0        | 988      | 67      | 0            |
| 15  | q     | 1050  | 0        | 988      | 65      | 0            |
| 16  | T     | 234   | 0        | 241      | 4       | 0            |
| 16  | t     | 234   | 0        | 241      | 4       | 0            |
| 17  | U     | 678   | 0        | 663      | 16      | 0            |
| 17  | u     | 678   | 0        | 663      | 17      | 0            |
| 18  | V     | 979   | 0        | 942      | 27      | 0            |
| 18  | v     | 979   | 0        | 942      | 28      | 0            |
| 19  | W     | 338   | 0        | 254      | 17      | 0            |
| 19  | w     | 338   | 0        | 254      | 18      | 0            |
| 20  | X     | 233   | 0        | 254      | 17      | 0            |
| 20  | x     | 233   | 0        | 254      | 19      | 0            |
| 21  | Y     | 216   | 0        | 210      | 12      | 0            |
| 21  | y     | 216   | 0        | 210      | 11      | 0            |
| 22  | Z     | 413   | 0        | 402      | 22      | 0            |
| 22  | z     | 413   | 0        | 402      | 24      | 0            |
| 23  | 0     | 1280  | 0        | 1242     | 42      | 0            |
| 23  | 5     | 1280  | 0        | 1242     | 43      | 0            |
| 24  | 2     | 1222  | 0        | 1142     | 64      | 0            |
| 24  | 7     | 1222  | 0        | 1142     | 63      | 0            |
| 25  | 1     | 1209  | 0        | 1150     | 43      | 0            |
| 25  | 6     | 1209  | 0        | 1150     | 40      | 0            |
| 26  | P     | 1265  | 0        | 946      | 18      | 0            |
| 26  | p     | 1265  | 0        | 946      | 16      | 0            |
| 27  | 4     | 765   | 0        | 161      | 3       | 0            |
| 27  | 9     | 765   | 0        | 161      | 2       | 0            |
| 28  | 3     | 992   | 0        | 778      | 20      | 0            |
| 28  | 8     | 992   | 0        | 778      | 19      | 0            |
| 29  | A     | 10    | 0        | 0        | 0       | 0            |
| 29  | a     | 10    | 0        | 0        | 0       | 0            |
| 30  | A     | 1     | 0        | 0        | 0       | 0            |
| 30  | a     | 1     | 0        | 0        | 0       | 0            |
| 31  | 0     | 528   | 0        | 439      | 21      | 0            |
| 31  | 1     | 580   | 0        | 441      | 14      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | 2     | 525   | 0        | 395      | 22      | 0            |
| 31  | 3     | 416   | 0        | 257      | 8       | 0            |
| 31  | 4     | 372   | 0        | 234      | 0       | 0            |
| 31  | 5     | 528   | 0        | 439      | 21      | 0            |
| 31  | 6     | 580   | 0        | 441      | 15      | 0            |
| 31  | 7     | 525   | 0        | 395      | 22      | 0            |
| 31  | 8     | 416   | 0        | 257      | 7       | 0            |
| 31  | 9     | 372   | 0        | 234      | 0       | 0            |
| 31  | A     | 174   | 0        | 170      | 4       | 0            |
| 31  | B     | 959   | 0        | 994      | 39      | 0            |
| 31  | C     | 792   | 0        | 822      | 19      | 0            |
| 31  | D     | 186   | 0        | 190      | 4       | 0            |
| 31  | P     | 341   | 0        | 213      | 10      | 0            |
| 31  | W     | 45    | 0        | 33       | 1       | 0            |
| 31  | Z     | 51    | 0        | 41       | 6       | 0            |
| 31  | a     | 174   | 0        | 170      | 3       | 0            |
| 31  | b     | 959   | 0        | 994      | 34      | 0            |
| 31  | c     | 792   | 0        | 822      | 20      | 0            |
| 31  | d     | 186   | 0        | 190      | 4       | 0            |
| 31  | p     | 341   | 0        | 213      | 10      | 0            |
| 31  | w     | 45    | 0        | 33       | 1       | 0            |
| 31  | z     | 51    | 0        | 41       | 6       | 0            |
| 32  | A     | 128   | 0        | 148      | 4       | 0            |
| 32  | a     | 128   | 0        | 148      | 3       | 0            |
| 33  | A     | 40    | 0        | 56       | 3       | 0            |
| 33  | B     | 120   | 0        | 168      | 13      | 0            |
| 33  | C     | 120   | 0        | 168      | 6       | 0            |
| 33  | D     | 40    | 0        | 56       | 2       | 0            |
| 33  | H     | 40    | 0        | 56       | 2       | 0            |
| 33  | K     | 40    | 0        | 56       | 2       | 0            |
| 33  | a     | 40    | 0        | 56       | 3       | 0            |
| 33  | b     | 120   | 0        | 168      | 12      | 0            |
| 33  | c     | 120   | 0        | 168      | 8       | 0            |
| 33  | d     | 40    | 0        | 56       | 1       | 0            |
| 33  | h     | 40    | 0        | 56       | 2       | 0            |
| 33  | k     | 40    | 0        | 56       | 2       | 0            |
| 34  | 0     | 48    | 0        | 63       | 5       | 0            |
| 34  | 5     | 48    | 0        | 63       | 5       | 0            |
| 34  | A     | 108   | 0        | 156      | 6       | 0            |
| 34  | B     | 94    | 0        | 122      | 3       | 0            |
| 34  | a     | 54    | 0        | 78       | 0       | 0            |
| 34  | b     | 40    | 0        | 44       | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | A     | 32    | 0        | 39       | 3       | 0            |
| 35  | D     | 55    | 0        | 80       | 3       | 0            |
| 35  | a     | 32    | 0        | 39       | 3       | 0            |
| 35  | d     | 55    | 0        | 80       | 4       | 0            |
| 36  | A     | 69    | 0        | 81       | 4       | 0            |
| 36  | B     | 49    | 0        | 74       | 4       | 0            |
| 36  | D     | 110   | 0        | 141      | 9       | 0            |
| 36  | H     | 42    | 0        | 54       | 6       | 0            |
| 36  | a     | 69    | 0        | 81       | 4       | 0            |
| 36  | b     | 49    | 0        | 74       | 4       | 0            |
| 36  | d     | 110   | 0        | 141      | 9       | 0            |
| 36  | h     | 42    | 0        | 54       | 5       | 0            |
| 37  | 0     | 48    | 0        | 69       | 1       | 0            |
| 37  | 5     | 48    | 0        | 69       | 1       | 0            |
| 37  | B     | 28    | 0        | 26       | 1       | 0            |
| 37  | C     | 51    | 0        | 72       | 4       | 0            |
| 37  | D     | 123   | 0        | 156      | 2       | 0            |
| 37  | J     | 50    | 0        | 73       | 3       | 0            |
| 37  | M     | 91    | 0        | 122      | 2       | 0            |
| 37  | W     | 48    | 0        | 66       | 2       | 0            |
| 37  | Y     | 46    | 0        | 62       | 3       | 0            |
| 37  | b     | 28    | 0        | 26       | 1       | 0            |
| 37  | c     | 51    | 0        | 72       | 4       | 0            |
| 37  | d     | 123   | 0        | 156      | 3       | 0            |
| 37  | j     | 50    | 0        | 73       | 2       | 0            |
| 37  | m     | 91    | 0        | 122      | 2       | 0            |
| 37  | w     | 48    | 0        | 66       | 2       | 0            |
| 37  | y     | 46    | 0        | 62       | 4       | 0            |
| 38  | C     | 1     | 0        | 0        | 0       | 0            |
| 38  | c     | 1     | 0        | 0        | 0       | 0            |
| 39  | C     | 179   | 0        | 232      | 10      | 0            |
| 39  | H     | 62    | 0        | 82       | 4       | 0            |
| 39  | c     | 179   | 0        | 232      | 10      | 0            |
| 39  | h     | 62    | 0        | 82       | 4       | 0            |
| 40  | D     | 4     | 0        | 1        | 0       | 0            |
| 40  | d     | 4     | 0        | 1        | 0       | 0            |
| 41  | F     | 43    | 0        | 30       | 3       | 0            |
| 41  | V     | 43    | 0        | 30       | 6       | 0            |
| 41  | f     | 43    | 0        | 30       | 3       | 0            |
| 41  | v     | 43    | 0        | 30       | 6       | 0            |
| 42  | 0     | 144   | 0        | 0        | 1       | 0            |
| 42  | 1     | 48    | 0        | 0        | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 42  | 2     | 96    | 0        | 0        | 0       | 0            |
| 42  | 3     | 96    | 0        | 0        | 0       | 0            |
| 42  | 4     | 144   | 0        | 0        | 0       | 0            |
| 42  | 5     | 144   | 0        | 0        | 1       | 0            |
| 42  | 6     | 48    | 0        | 0        | 1       | 0            |
| 42  | 7     | 96    | 0        | 0        | 0       | 0            |
| 42  | 8     | 96    | 0        | 0        | 0       | 0            |
| 42  | 9     | 144   | 0        | 0        | 0       | 0            |
| 42  | P     | 48    | 0        | 0        | 0       | 0            |
| 42  | p     | 48    | 0        | 0        | 0       | 0            |
| 43  | 0     | 42    | 0        | 0        | 0       | 0            |
| 43  | 5     | 42    | 0        | 0        | 0       | 0            |
| 44  | 1     | 86    | 0        | 0        | 3       | 0            |
| 44  | 2     | 86    | 0        | 0        | 24      | 0            |
| 44  | 3     | 43    | 0        | 0        | 1       | 0            |
| 44  | 6     | 86    | 0        | 0        | 3       | 0            |
| 44  | 7     | 86    | 0        | 0        | 25      | 0            |
| 44  | 8     | 43    | 0        | 0        | 1       | 0            |
| 44  | P     | 43    | 0        | 0        | 7       | 0            |
| 44  | p     | 43    | 0        | 0        | 7       | 0            |
| All | All   | 71446 | 0        | 64844    | 1569    | 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 12.

All (1569) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 24:7:65:MET:HG2  | 44:7:304:DD6:C3   | 1.71                     | 1.19              |
| 24:2:65:MET:HG2  | 44:2:304:DD6:C3   | 1.71                     | 1.19              |
| 31:B:514:CLA:H43 | 33:B:517:BCR:H383 | 1.19                     | 1.14              |
| 31:b:515:CLA:H43 | 33:b:518:BCR:H383 | 1.19                     | 1.13              |
| 31:p:604:CLA:C2B | 44:p:611:DD6:C37  | 2.31                     | 1.09              |
| 31:P:604:CLA:C2B | 44:P:611:DD6:C37  | 2.31                     | 1.09              |
| 15:Q:145:ASP:HB3 | 15:Q:149:ARG:HH21 | 1.17                     | 1.08              |
| 24:2:37:ASP:HA   | 44:2:303:DD6:O2   | 1.54                     | 1.06              |
| 24:7:37:ASP:HA   | 44:7:303:DD6:O2   | 1.54                     | 1.05              |
| 24:7:155:PHE:CE2 | 44:7:303:DD6:C24  | 2.39                     | 1.05              |
| 24:2:155:PHE:CE2 | 44:2:303:DD6:C24  | 2.39                     | 1.05              |
| 31:p:604:CLA:CMB | 44:p:611:DD6:C37  | 2.35                     | 1.04              |
| 31:P:604:CLA:CMB | 44:P:611:DD6:C37  | 2.35                     | 1.03              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:2:68:VAL:HG11  | 44:2:304:DD6:C26  | 1.89                     | 1.02              |
| 15:q:145:ASP:HB3  | 15:q:149:ARG:HH21 | 1.17                     | 1.02              |
| 24:7:68:VAL:HG11  | 44:7:304:DD6:C26  | 1.89                     | 1.01              |
| 44:7:304:DD6:C8   | 31:7:310:CLA:HHC  | 1.92                     | 1.00              |
| 44:2:304:DD6:C8   | 31:2:310:CLA:HHC  | 1.92                     | 1.00              |
| 15:q:67:PHE:C     | 15:q:74:THR:HG21  | 1.86                     | 1.00              |
| 24:7:36:PHE:CD2   | 44:7:303:DD6:C22  | 2.45                     | 0.99              |
| 15:Q:67:PHE:C     | 15:Q:74:THR:HG21  | 1.86                     | 0.99              |
| 24:2:36:PHE:CD2   | 44:2:303:DD6:C22  | 2.45                     | 0.99              |
| 31:b:515:CLA:C4   | 33:b:518:BCR:H383 | 2.02                     | 0.90              |
| 6:F:44:GLN:HG2    | 15:Q:68:GLY:HA3   | 1.54                     | 0.89              |
| 6:f:44:GLN:HG2    | 15:q:68:GLY:HA3   | 1.54                     | 0.89              |
| 15:Q:108:PRO:HG2  | 15:Q:111:ALA:HB2  | 1.54                     | 0.89              |
| 15:q:108:PRO:HG2  | 15:q:111:ALA:HB2  | 1.53                     | 0.88              |
| 31:B:514:CLA:C4   | 33:B:517:BCR:H383 | 2.02                     | 0.87              |
| 31:B:514:CLA:H43  | 33:B:517:BCR:C38  | 2.05                     | 0.85              |
| 15:q:170:LYS:NZ   | 15:q:207:PHE:HA   | 1.92                     | 0.84              |
| 15:Q:170:LYS:NZ   | 15:Q:207:PHE:HA   | 1.92                     | 0.84              |
| 19:W:99:PRO:HG3   | 37:W:201:LMG:HC71 | 1.59                     | 0.84              |
| 14:O:219:ASN:HD21 | 14:O:228:GLN:HB2  | 1.42                     | 0.84              |
| 31:b:515:CLA:H43  | 33:b:518:BCR:C38  | 2.05                     | 0.84              |
| 44:2:304:DD6:C8   | 31:2:310:CLA:CHC  | 2.56                     | 0.83              |
| 44:7:304:DD6:C8   | 31:7:310:CLA:CHC  | 2.56                     | 0.83              |
| 14:o:219:ASN:HD21 | 14:o:228:GLN:HB2  | 1.42                     | 0.82              |
| 24:7:38:PRO:HD2   | 44:7:303:DD6:C18  | 2.09                     | 0.82              |
| 24:2:38:PRO:HD2   | 44:2:303:DD6:C18  | 2.09                     | 0.82              |
| 15:Q:69:LEU:HD12  | 15:Q:73:GLY:HA3   | 1.61                     | 0.82              |
| 20:x:92:ILE:CD1   | 23:5:119:TRP:HE1  | 1.93                     | 0.81              |
| 15:q:69:LEU:HD12  | 15:q:73:GLY:HA3   | 1.61                     | 0.80              |
| 31:p:604:CLA:HMB1 | 44:p:611:DD6:C37  | 2.10                     | 0.80              |
| 3:c:334:PRO:HG2   | 4:d:350:ASN:HD21  | 1.45                     | 0.80              |
| 3:C:334:PRO:HG2   | 4:D:350:ASN:HD21  | 1.45                     | 0.80              |
| 15:Q:77:SER:C     | 15:Q:79:GLY:H     | 1.91                     | 0.78              |
| 15:q:77:SER:C     | 15:q:79:GLY:H     | 1.91                     | 0.78              |
| 31:P:604:CLA:HMB1 | 44:P:611:DD6:C37  | 2.10                     | 0.78              |
| 2:b:441:GLY:HA2   | 14:o:263:ALA:HB3  | 1.63                     | 0.78              |
| 2:B:441:GLY:HA2   | 14:O:263:ALA:HB3  | 1.64                     | 0.77              |
| 18:V:28:ARG:HH12  | 18:V:110:GLU:HG3  | 1.47                     | 0.77              |
| 25:6:189:ASN:HB3  | 25:6:199:ASN:C    | 2.09                     | 0.77              |
| 25:1:189:ASN:HB3  | 25:1:199:ASN:C    | 2.09                     | 0.77              |
| 18:v:28:ARG:HH12  | 18:v:110:GLU:HG3  | 1.47                     | 0.77              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:w:99:PRO:HG3   | 37:w:201:LMG:HC71 | 1.65                     | 0.77              |
| 19:W:102:ILE:HG13 | 19:W:104:ALA:H    | 1.50                     | 0.77              |
| 1:A:97:TRP:CZ3    | 8:I:8:VAL:HG11    | 2.20                     | 0.76              |
| 2:B:404:GLY:H     | 2:B:407:ASN:HB2   | 1.51                     | 0.76              |
| 14:o:174:PRO:HD2  | 14:o:185:SER:O    | 1.86                     | 0.76              |
| 23:5:71:VAL:HG13  | 23:5:75:HIS:CE1   | 2.20                     | 0.76              |
| 24:2:155:PHE:CD2  | 44:2:303:DD6:C24  | 2.69                     | 0.76              |
| 24:7:155:PHE:CD2  | 44:7:303:DD6:C24  | 2.69                     | 0.76              |
| 2:b:404:GLY:H     | 2:b:407:ASN:HB2   | 1.51                     | 0.75              |
| 20:X:92:ILE:CD1   | 23:0:119:TRP:HE1  | 1.99                     | 0.75              |
| 19:w:102:ILE:HG13 | 19:w:104:ALA:H    | 1.50                     | 0.75              |
| 23:0:71:VAL:HG13  | 23:0:75:HIS:CE1   | 2.20                     | 0.75              |
| 14:O:174:PRO:HD2  | 14:O:185:SER:O    | 1.85                     | 0.75              |
| 10:K:44:LEU:CB    | 33:K:101:BCR:H351 | 2.17                     | 0.75              |
| 10:k:44:LEU:CB    | 33:k:101:BCR:H351 | 2.17                     | 0.75              |
| 1:a:97:TRP:CZ3    | 8:i:8:VAL:HG11    | 2.20                     | 0.74              |
| 18:V:104:MET:HG3  | 18:V:107:LEU:HD12 | 1.69                     | 0.74              |
| 26:p:107:ILE:CD1  | 26:p:226:ILE:HG21 | 2.18                     | 0.74              |
| 18:v:104:MET:HG3  | 18:v:107:LEU:HD12 | 1.69                     | 0.73              |
| 2:b:160:GLY:HA3   | 2:b:180:PRO:HB3   | 1.70                     | 0.73              |
| 24:7:38:PRO:HD2   | 44:7:303:DD6:C19  | 2.19                     | 0.73              |
| 2:B:160:GLY:HA3   | 2:B:180:PRO:HB3   | 1.70                     | 0.73              |
| 26:P:107:ILE:CD1  | 26:P:226:ILE:HG21 | 2.18                     | 0.73              |
| 24:2:38:PRO:HD2   | 44:2:303:DD6:C19  | 2.19                     | 0.73              |
| 15:Q:93:PRO:O     | 15:Q:94:TYR:C     | 2.32                     | 0.72              |
| 15:Q:85:ASP:HB3   | 15:Q:96:VAL:HG12  | 1.70                     | 0.72              |
| 15:q:93:PRO:O     | 15:q:94:TYR:C     | 2.32                     | 0.72              |
| 31:D:404:CLA:H111 | 7:H:48:LEU:HD21   | 1.71                     | 0.72              |
| 1:A:131:TRP:HZ2   | 3:C:449:ARG:HD2   | 1.55                     | 0.72              |
| 2:b:24:LEU:HD21   | 31:b:517:CLA:HAB  | 1.70                     | 0.72              |
| 2:B:24:LEU:HD21   | 31:B:516:CLA:HAB  | 1.70                     | 0.72              |
| 15:q:85:ASP:HB3   | 15:q:96:VAL:HG12  | 1.70                     | 0.72              |
| 28:8:80:TYR:HD2   | 28:8:168:LEU:HD13 | 1.55                     | 0.72              |
| 3:C:178:LYS:HA    | 3:C:182:LEU:HB2   | 1.71                     | 0.71              |
| 2:B:384:ARG:HE    | 17:U:101:LEU:HD23 | 1.55                     | 0.71              |
| 23:5:41:LEU:HD12  | 23:5:69:ARG:HE    | 1.55                     | 0.71              |
| 3:c:178:LYS:HA    | 3:c:182:LEU:HB2   | 1.71                     | 0.71              |
| 1:a:190:HIS:HB3   | 1:a:293:MET:HE2   | 1.72                     | 0.71              |
| 15:q:145:ASP:CB   | 15:q:149:ARG:HH21 | 2.00                     | 0.71              |
| 1:a:140:ARG:NH2   | 36:a:412:LHG:O5   | 2.22                     | 0.71              |
| 23:0:41:LEU:HD12  | 23:0:69:ARG:HE    | 1.55                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:0:167:ARG:HD3  | 31:0:311:CLA:HBA1 | 1.72                     | 0.71              |
| 31:d:404:CLA:H111 | 7:h:48:LEU:HD21   | 1.71                     | 0.71              |
| 5:E:22:ILE:HG13   | 5:E:23:HIS:HD1    | 1.56                     | 0.71              |
| 2:b:384:ARG:HE    | 17:u:101:LEU:HD23 | 1.55                     | 0.70              |
| 5:e:22:ILE:HG13   | 5:e:23:HIS:HD1    | 1.56                     | 0.70              |
| 1:A:140:ARG:NH2   | 36:A:413:LHG:O5   | 2.22                     | 0.70              |
| 23:5:167:ARG:HD3  | 31:5:311:CLA:HBA1 | 1.72                     | 0.70              |
| 28:3:80:TYR:HD2   | 28:3:168:LEU:HD13 | 1.55                     | 0.70              |
| 1:A:190:HIS:HB3   | 1:A:293:MET:HE2   | 1.72                     | 0.70              |
| 1:a:131:TRP:HZ2   | 3:c:449:ARG:HD2   | 1.55                     | 0.70              |
| 33:A:408:BCR:H351 | 34:A:411:SQD:H371 | 1.74                     | 0.70              |
| 34:B:522:SQD:H371 | 33:a:408:BCR:H351 | 1.74                     | 0.70              |
| 10:K:48:LEU:HA    | 10:K:51:VAL:HG12  | 1.73                     | 0.70              |
| 36:D:412:LHG:HC81 | 36:H:103:LHG:H241 | 1.73                     | 0.69              |
| 36:d:412:LHG:HC81 | 36:h:103:LHG:H241 | 1.73                     | 0.69              |
| 10:k:48:LEU:HA    | 10:k:51:VAL:HG12  | 1.73                     | 0.69              |
| 15:q:77:SER:C     | 15:q:79:GLY:N     | 2.50                     | 0.69              |
| 15:Q:145:ASP:CB   | 15:Q:149:ARG:HH21 | 2.00                     | 0.69              |
| 28:3:67:LEU:HD11  | 28:3:71:ARG:CZ    | 2.23                     | 0.69              |
| 3:c:449:ARG:HH12  | 8:i:28:PRO:HG3    | 1.58                     | 0.69              |
| 7:h:41:PRO:HB2    | 31:5:314:CLA:HMD3 | 1.74                     | 0.69              |
| 24:7:107:TRP:O    | 24:7:111:ILE:HG13 | 1.93                     | 0.69              |
| 37:c:521:LMG:H121 | 37:c:521:LMG:H301 | 1.75                     | 0.69              |
| 24:2:107:TRP:O    | 24:2:111:ILE:HG13 | 1.93                     | 0.69              |
| 6:F:44:GLN:O      | 6:F:45:ARG:C      | 2.36                     | 0.68              |
| 24:7:37:ASP:CA    | 44:7:303:DD6:O2   | 2.38                     | 0.68              |
| 15:Q:125:LYS:C    | 15:Q:129:GLN:HE22 | 2.02                     | 0.68              |
| 6:f:44:GLN:O      | 6:f:45:ARG:C      | 2.36                     | 0.68              |
| 21:y:23:PRO:O     | 21:y:26:VAL:HB    | 1.94                     | 0.68              |
| 3:c:368:PRO:HB3   | 15:q:149:ARG:HB3  | 1.74                     | 0.68              |
| 4:d:314:PHE:HA    | 4:d:317:LYS:HD3   | 1.76                     | 0.68              |
| 25:1:165:MET:HE1  | 31:1:206:CLA:HHC  | 1.76                     | 0.68              |
| 37:C:521:LMG:H301 | 37:C:521:LMG:H121 | 1.75                     | 0.67              |
| 4:d:14:LEU:HD23   | 36:d:412:LHG:HC92 | 1.76                     | 0.67              |
| 28:8:67:LEU:HD11  | 28:8:71:ARG:CZ    | 2.23                     | 0.67              |
| 15:q:125:LYS:C    | 15:q:129:GLN:HE22 | 2.02                     | 0.67              |
| 3:C:368:PRO:HB3   | 15:Q:149:ARG:HB3  | 1.75                     | 0.67              |
| 41:v:201:HEM:HBC2 | 41:v:201:HEM:HHD  | 1.76                     | 0.67              |
| 20:x:92:ILE:HD12  | 23:5:119:TRP:HE1  | 1.60                     | 0.67              |
| 3:C:449:ARG:HH12  | 8:I:28:PRO:HG3    | 1.58                     | 0.67              |
| 4:D:139:ARG:HD2   | 4:D:141:TYR:CE2   | 2.30                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:M:102:LMG:H292 | 37:M:102:LMG:H112 | 1.77                     | 0.67              |
| 31:c:509:CLA:H72  | 10:k:46:PHE:HZ    | 1.60                     | 0.67              |
| 4:D:314:PHE:HA    | 4:D:317:LYS:HD3   | 1.77                     | 0.67              |
| 15:Q:170:LYS:HZ3  | 15:Q:207:PHE:HA   | 1.60                     | 0.67              |
| 41:V:201:HEM:HBC2 | 41:V:201:HEM:HHD  | 1.76                     | 0.66              |
| 37:m:102:LMG:H292 | 37:m:102:LMG:H112 | 1.77                     | 0.66              |
| 24:2:37:ASP:CA    | 44:2:303:DD6:O2   | 2.38                     | 0.66              |
| 20:x:92:ILE:HD12  | 23:5:119:TRP:NE1  | 2.10                     | 0.66              |
| 21:Y:23:PRO:O     | 21:Y:26:VAL:HB    | 1.94                     | 0.66              |
| 4:d:139:ARG:HD2   | 4:d:141:TYR:CE2   | 2.30                     | 0.66              |
| 14:o:132:MET:HB3  | 14:o:171:ILE:HB   | 1.77                     | 0.66              |
| 25:6:165:MET:HE1  | 31:6:206:CLA:HHC  | 1.76                     | 0.66              |
| 15:q:170:LYS:HZ3  | 15:q:207:PHE:HA   | 1.59                     | 0.66              |
| 26:p:96:GLY:HA3   | 26:p:205:CYS:HB3  | 1.77                     | 0.66              |
| 24:2:36:PHE:HD2   | 44:2:303:DD6:C22  | 2.08                     | 0.66              |
| 31:C:509:CLA:H72  | 10:K:46:PHE:HZ    | 1.60                     | 0.65              |
| 14:O:219:ASN:ND2  | 14:O:228:GLN:HB2  | 2.12                     | 0.65              |
| 24:2:133:LEU:HD21 | 31:2:310:CLA:HAA2 | 1.78                     | 0.65              |
| 20:x:92:ILE:HD11  | 23:5:119:TRP:HE1  | 1.61                     | 0.65              |
| 3:C:368:PRO:HG3   | 15:Q:148:THR:HG23 | 1.78                     | 0.65              |
| 3:c:368:PRO:HG3   | 15:q:148:THR:HG23 | 1.78                     | 0.65              |
| 26:P:96:GLY:HA3   | 26:P:205:CYS:HB3  | 1.77                     | 0.65              |
| 14:O:132:MET:HB3  | 14:O:171:ILE:HB   | 1.77                     | 0.65              |
| 26:P:88:LEU:HG    | 31:P:602:CLA:HHB  | 1.79                     | 0.65              |
| 18:v:65:ARG:NH2   | 18:v:67:ASP:OD2   | 2.30                     | 0.65              |
| 24:7:133:LEU:HD21 | 31:7:310:CLA:HAA2 | 1.78                     | 0.64              |
| 1:A:240:GLY:HA3   | 16:T:29:ILE:HG23  | 1.79                     | 0.64              |
| 2:b:265:ILE:HD12  | 2:b:270:PRO:HA    | 1.79                     | 0.64              |
| 36:D:411:LHG:HC81 | 20:X:89:ALA:HB3   | 1.79                     | 0.64              |
| 1:A:17:PHE:HE2    | 8:I:18:LEU:HD11   | 1.61                     | 0.64              |
| 36:d:411:LHG:HC81 | 20:x:89:ALA:HB3   | 1.79                     | 0.64              |
| 3:C:256:PRO:HA    | 31:C:507:CLA:HED3 | 1.79                     | 0.64              |
| 2:b:326:ARG:NH2   | 4:d:297:ASP:OD2   | 2.31                     | 0.64              |
| 26:P:107:ILE:HD13 | 26:P:226:ILE:HG21 | 1.80                     | 0.64              |
| 18:V:65:ARG:NH2   | 18:V:67:ASP:OD2   | 2.30                     | 0.64              |
| 1:a:17:PHE:HE2    | 8:i:18:LEU:HD11   | 1.62                     | 0.64              |
| 24:7:36:PHE:CE2   | 44:7:303:DD6:C22  | 2.81                     | 0.64              |
| 24:2:84:ALA:HB3   | 24:2:87:VAL:HG12  | 1.80                     | 0.64              |
| 14:O:175:ILE:HG23 | 14:O:182:ILE:HG23 | 1.80                     | 0.64              |
| 2:b:469:HIS:O     | 2:b:473:THR:HG23  | 1.98                     | 0.64              |
| 14:o:175:ILE:HG23 | 14:o:182:ILE:HG23 | 1.80                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:o:219:ASN:ND2  | 14:o:228:GLN:HB2  | 2.12                     | 0.63              |
| 22:Z:5:ILE:O      | 22:Z:9:THR:HG22   | 1.99                     | 0.63              |
| 23:5:41:LEU:HB3   | 23:5:69:ARG:HH21  | 1.62                     | 0.63              |
| 24:7:84:ALA:HB3   | 24:7:87:VAL:HG12  | 1.80                     | 0.63              |
| 26:p:88:LEU:HG    | 31:p:602:CLA:HBB  | 1.79                     | 0.63              |
| 22:z:5:ILE:O      | 22:z:9:THR:HG22   | 1.99                     | 0.63              |
| 2:B:469:HIS:O     | 2:B:473:THR:HG23  | 1.98                     | 0.63              |
| 15:q:145:ASP:HB3  | 15:q:149:ARG:NH2  | 2.02                     | 0.63              |
| 2:B:265:ILE:HD12  | 2:B:270:PRO:HA    | 1.79                     | 0.63              |
| 3:C:177:ILE:HG23  | 31:8:313:CLA:HMB3 | 1.81                     | 0.63              |
| 6:F:44:GLN:HB2    | 15:Q:80:ALA:HB1   | 1.81                     | 0.63              |
| 14:O:269:GLU:CD   | 14:O:269:GLU:H    | 2.06                     | 0.63              |
| 26:p:107:ILE:HD13 | 26:p:226:ILE:HG21 | 1.80                     | 0.63              |
| 1:a:240:GLY:HA3   | 16:t:29:ILE:HG23  | 1.79                     | 0.63              |
| 24:7:155:PHE:CZ   | 44:7:303:DD6:C24  | 2.82                     | 0.63              |
| 23:0:41:LEU:HB3   | 23:0:69:ARG:HH21  | 1.62                     | 0.63              |
| 24:2:65:MET:SD    | 31:2:310:CLA:HMC3 | 2.39                     | 0.63              |
| 2:B:326:ARG:NH2   | 4:D:297:ASP:OD2   | 2.31                     | 0.62              |
| 15:Q:77:SER:C     | 15:Q:79:GLY:N     | 2.50                     | 0.62              |
| 14:o:269:GLU:H    | 14:o:269:GLU:CD   | 2.06                     | 0.62              |
| 3:c:256:PRO:HA    | 31:c:507:CLA:HED3 | 1.79                     | 0.62              |
| 3:c:288:LEU:HD12  | 39:c:518:DGD:HB52 | 1.81                     | 0.62              |
| 6:f:44:GLN:HB2    | 15:q:80:ALA:HB1   | 1.81                     | 0.62              |
| 24:2:36:PHE:CE2   | 44:2:303:DD6:C22  | 2.81                     | 0.62              |
| 36:d:407:LHG:H182 | 16:t:17:ILE:HD11  | 1.81                     | 0.62              |
| 15:q:77:SER:O     | 15:q:79:GLY:N     | 2.33                     | 0.62              |
| 22:Z:26:ALA:HA    | 22:Z:32:GLU:HG2   | 1.82                     | 0.62              |
| 20:X:92:ILE:HD12  | 23:0:119:TRP:HE1  | 1.64                     | 0.62              |
| 3:c:311:GLN:HG3   | 3:c:361:LEU:HD13  | 1.82                     | 0.62              |
| 25:6:194:LEU:HB3  | 25:6:196:PHE:CZ   | 2.35                     | 0.62              |
| 31:0:313:CLA:HBB2 | 34:0:316:SQD:H251 | 1.82                     | 0.62              |
| 1:a:187:GLN:HE22  | 1:a:193:LEU:HG    | 1.64                     | 0.62              |
| 24:2:155:PHE:CZ   | 44:2:303:DD6:C26  | 2.83                     | 0.62              |
| 24:2:155:PHE:CZ   | 44:2:303:DD6:C24  | 2.82                     | 0.62              |
| 31:5:313:CLA:HBB2 | 34:5:316:SQD:H251 | 1.82                     | 0.61              |
| 1:A:187:GLN:HE22  | 1:A:193:LEU:HG    | 1.64                     | 0.61              |
| 24:7:155:PHE:CZ   | 44:7:303:DD6:C26  | 2.83                     | 0.61              |
| 12:M:4:GLN:HG3    | 12:M:6:GLY:H      | 1.66                     | 0.61              |
| 14:o:129:LEU:HG   | 14:o:175:ILE:HD11 | 1.82                     | 0.61              |
| 24:7:65:MET:SD    | 31:7:310:CLA:HMC3 | 2.39                     | 0.61              |
| 2:B:422:ARG:NH1   | 14:O:256:ASP:OD2  | 2.33                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:D:407:LHG:H182 | 16:T:17:ILE:HD11  | 1.81                     | 0.61              |
| 14:O:129:LEU:HG   | 14:O:175:ILE:HD11 | 1.82                     | 0.61              |
| 15:Q:125:LYS:O    | 15:Q:129:GLN:NE2  | 2.33                     | 0.61              |
| 14:o:158:SER:HB2  | 14:o:197:VAL:HG22 | 1.82                     | 0.61              |
| 23:5:138:THR:HG23 | 31:5:308:CLA:HAC2 | 1.81                     | 0.61              |
| 3:C:87:ILE:HD11   | 3:C:426:LEU:HG    | 1.82                     | 0.61              |
| 7:H:41:PRO:HB2    | 31:0:314:CLA:HMD3 | 1.82                     | 0.61              |
| 14:O:158:SER:HB2  | 14:O:197:VAL:HG22 | 1.83                     | 0.61              |
| 23:5:194:LEU:HD11 | 23:5:205:TRP:HZ3  | 1.66                     | 0.61              |
| 44:2:303:DD6:C9   | 31:2:306:CLA:HMC1 | 2.31                     | 0.61              |
| 3:C:311:GLN:HG3   | 3:C:361:LEU:HD13  | 1.82                     | 0.61              |
| 15:q:68:GLY:N     | 15:q:74:THR:HG21  | 2.16                     | 0.61              |
| 15:q:125:LYS:O    | 15:q:129:GLN:NE2  | 2.33                     | 0.61              |
| 20:x:92:ILE:HD11  | 31:5:307:CLA:O2A  | 2.00                     | 0.61              |
| 3:C:288:LEU:HD12  | 39:C:518:DGD:HB52 | 1.81                     | 0.61              |
| 15:Q:77:SER:O     | 15:Q:79:GLY:N     | 2.33                     | 0.61              |
| 22:z:26:ALA:HA    | 22:z:32:GLU:HG2   | 1.82                     | 0.61              |
| 2:b:422:ARG:NH1   | 14:o:256:ASP:OD2  | 2.33                     | 0.61              |
| 25:1:194:LEU:HB3  | 25:1:196:PHE:CZ   | 2.35                     | 0.61              |
| 14:o:267:GLY:O    | 14:o:268:GLU:C    | 2.43                     | 0.60              |
| 23:0:138:THR:HG23 | 31:0:308:CLA:HAC2 | 1.82                     | 0.60              |
| 23:0:194:LEU:HD11 | 23:0:205:TRP:HZ3  | 1.66                     | 0.60              |
| 15:Q:68:GLY:N     | 15:Q:74:THR:HG21  | 2.16                     | 0.60              |
| 10:k:57:SER:O     | 10:k:58:PHE:C     | 2.43                     | 0.60              |
| 44:7:303:DD6:C9   | 31:7:306:CLA:HMC1 | 2.31                     | 0.60              |
| 10:K:57:SER:O     | 10:K:58:PHE:C     | 2.43                     | 0.60              |
| 2:B:237:VAL:HG22  | 31:B:510:CLA:HBC2 | 1.83                     | 0.60              |
| 20:X:92:ILE:HD11  | 31:0:307:CLA:O2A  | 2.00                     | 0.60              |
| 12:m:4:GLN:HG3    | 12:m:6:GLY:H      | 1.65                     | 0.60              |
| 25:6:70:GLU:OE2   | 25:6:162:ARG:NE   | 2.27                     | 0.60              |
| 31:p:603:CLA:HMC1 | 44:p:611:DD6:C    | 2.31                     | 0.60              |
| 31:3:310:CLA:HHC  | 31:3:310:CLA:HBB1 | 1.84                     | 0.60              |
| 20:X:92:ILE:HD12  | 23:0:119:TRP:NE1  | 2.16                     | 0.60              |
| 31:c:502:CLA:H71  | 31:c:502:CLA:HBB1 | 1.84                     | 0.60              |
| 24:7:155:PHE:CE1  | 44:7:303:DD6:C26  | 2.85                     | 0.60              |
| 26:p:44:ALA:HB3   | 26:p:47:THR:HB    | 1.83                     | 0.60              |
| 31:P:603:CLA:HMC1 | 44:P:611:DD6:C    | 2.31                     | 0.60              |
| 5:e:38:ILE:HD11   | 6:f:39:ALA:HB3    | 1.83                     | 0.60              |
| 25:6:74:GLY:O     | 25:6:78:GLN:HG3   | 2.01                     | 0.60              |
| 14:O:267:GLY:O    | 14:O:268:GLU:C    | 2.43                     | 0.60              |
| 5:E:38:ILE:HD11   | 6:F:39:ALA:HB3    | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:148:GLY:O     | 3:c:156:LYS:NZ    | 2.35                     | 0.60              |
| 3:C:148:GLY:O     | 3:C:156:LYS:NZ    | 2.35                     | 0.59              |
| 31:C:502:CLA:HBB1 | 31:C:502:CLA:H71  | 1.84                     | 0.59              |
| 3:c:449:ARG:NH2   | 31:c:506:CLA:O1D  | 2.33                     | 0.59              |
| 24:2:155:PHE:CE1  | 44:2:303:DD6:C26  | 2.84                     | 0.59              |
| 25:1:74:GLY:O     | 25:1:78:GLN:HG3   | 2.01                     | 0.59              |
| 2:B:413:ASP:OD1   | 2:B:414:ALA:N     | 2.35                     | 0.59              |
| 3:C:289:TYR:HE2   | 31:C:502:CLA:HAA2 | 1.66                     | 0.59              |
| 2:b:237:VAL:HG22  | 31:b:511:CLA:HBC2 | 1.83                     | 0.59              |
| 3:c:87:ILE:HD11   | 3:c:426:LEU:HG    | 1.82                     | 0.59              |
| 15:Q:89:LYS:O     | 15:Q:90:LEU:C     | 2.45                     | 0.59              |
| 4:D:303:LEU:O     | 4:D:306:ALA:N     | 2.35                     | 0.59              |
| 4:d:172:SER:HB2   | 4:d:177:ALA:HB1   | 1.85                     | 0.59              |
| 31:p:604:CLA:C3B  | 44:p:611:DD6:C37  | 2.80                     | 0.59              |
| 31:8:310:CLA:HHC  | 31:8:310:CLA:HBB1 | 1.84                     | 0.59              |
| 15:Q:145:ASP:HB3  | 15:Q:149:ARG:NH2  | 2.02                     | 0.59              |
| 4:D:14:LEU:HD23   | 36:D:412:LHG:HC92 | 1.84                     | 0.59              |
| 21:Y:25:LEU:HD12  | 37:Y:101:LMG:H142 | 1.83                     | 0.59              |
| 3:c:289:TYR:HE2   | 31:c:502:CLA:HAA2 | 1.66                     | 0.59              |
| 24:2:38:PRO:CD    | 44:2:303:DD6:C18  | 2.81                     | 0.59              |
| 2:b:413:ASP:HB3   | 2:b:416:THR:HG22  | 1.85                     | 0.59              |
| 3:C:289:TYR:CE2   | 31:C:502:CLA:HAA2 | 2.38                     | 0.59              |
| 4:D:298:PHE:N     | 4:D:315:TYR:OH    | 2.36                     | 0.59              |
| 1:a:84:PRO:HA     | 1:a:112:TYR:CG    | 2.38                     | 0.59              |
| 3:c:289:TYR:CE2   | 31:c:502:CLA:HAA2 | 2.38                     | 0.59              |
| 26:P:44:ALA:HB3   | 26:P:47:THR:HB    | 1.83                     | 0.59              |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG    | 2.38                     | 0.58              |
| 4:D:172:SER:HB2   | 4:D:177:ALA:HB1   | 1.85                     | 0.58              |
| 4:d:303:LEU:O     | 4:d:306:ALA:N     | 2.35                     | 0.58              |
| 14:o:141:VAL:HB   | 14:o:199:LEU:HD21 | 1.85                     | 0.58              |
| 24:7:36:PHE:HD2   | 44:7:303:DD6:C22  | 2.08                     | 0.58              |
| 17:u:16:ASN:HB3   | 17:u:19:TYR:HD2   | 1.68                     | 0.58              |
| 26:p:200:GLN:NE2  | 31:p:607:CLA:OBD  | 2.37                     | 0.58              |
| 15:q:89:LYS:O     | 15:q:90:LEU:C     | 2.45                     | 0.58              |
| 21:y:25:LEU:HD12  | 37:y:101:LMG:H142 | 1.83                     | 0.58              |
| 26:P:200:GLN:NE2  | 31:P:607:CLA:OBD  | 2.37                     | 0.58              |
| 31:P:604:CLA:C3B  | 44:P:611:DD6:C37  | 2.80                     | 0.58              |
| 3:C:449:ARG:NH2   | 31:C:506:CLA:O1D  | 2.33                     | 0.58              |
| 2:b:413:ASP:OD1   | 2:b:414:ALA:N     | 2.35                     | 0.58              |
| 4:d:51:GLY:HA2    | 4:d:55:VAL:HG12   | 1.85                     | 0.58              |
| 24:7:84:ALA:HB1   | 24:7:85:PRO:HD2   | 1.85                     | 0.58              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:1:70:GLU:OE2   | 25:1:162:ARG:NE   | 2.27                     | 0.58              |
| 31:B:501:CLA:HAC1 | 33:H:101:BCR:H383 | 1.86                     | 0.58              |
| 24:7:38:PRO:CD    | 44:7:303:DD6:C18  | 2.81                     | 0.58              |
| 23:0:42:VAL:HG23  | 23:0:162:ILE:HG23 | 1.86                     | 0.58              |
| 4:D:351:ALA:HB1   | 17:U:102:TYR:HE2  | 1.68                     | 0.58              |
| 5:E:53:ASN:O      | 18:V:1:ILE:N      | 2.37                     | 0.58              |
| 5:e:53:ASN:O      | 18:v:1:ILE:N      | 2.37                     | 0.58              |
| 1:A:42:LEU:HB3    | 33:A:408:BCR:H353 | 1.86                     | 0.57              |
| 2:B:413:ASP:HB3   | 2:B:416:THR:HG22  | 1.85                     | 0.57              |
| 15:Q:69:LEU:O     | 15:Q:71:GLY:N     | 2.38                     | 0.57              |
| 1:a:42:LEU:HB3    | 33:a:408:BCR:H353 | 1.86                     | 0.57              |
| 4:d:351:ALA:HB1   | 17:u:102:TYR:HE2  | 1.68                     | 0.57              |
| 24:2:84:ALA:HB1   | 24:2:85:PRO:HD2   | 1.85                     | 0.57              |
| 17:U:16:ASN:HB3   | 17:U:19:TYR:HD2   | 1.68                     | 0.57              |
| 20:X:92:ILE:HD11  | 23:0:119:TRP:HE1  | 1.67                     | 0.57              |
| 4:d:298:PHE:N     | 4:d:315:TYR:OH    | 2.36                     | 0.57              |
| 15:q:132:PRO:HA   | 15:q:135:VAL:HG12 | 1.85                     | 0.57              |
| 24:7:38:PRO:HD2   | 44:7:303:DD6:O2   | 2.04                     | 0.57              |
| 4:D:50:THR:HG22   | 6:F:33:PHE:HZ     | 1.68                     | 0.57              |
| 17:U:61:ASP:HA    | 17:U:64:LYS:HD2   | 1.86                     | 0.57              |
| 4:d:50:THR:HG22   | 6:f:33:PHE:HZ     | 1.68                     | 0.57              |
| 25:1:165:MET:HE1  | 31:1:206:CLA:CHC  | 2.34                     | 0.57              |
| 31:b:502:CLA:HAC1 | 33:h:101:BCR:H383 | 1.86                     | 0.57              |
| 15:Q:132:PRO:HA   | 15:Q:135:VAL:HG12 | 1.85                     | 0.57              |
| 25:6:165:MET:HE1  | 31:6:206:CLA:CHC  | 2.34                     | 0.57              |
| 14:O:141:VAL:HB   | 14:O:199:LEU:HD21 | 1.85                     | 0.57              |
| 17:u:61:ASP:HA    | 17:u:64:LYS:HD2   | 1.86                     | 0.57              |
| 19:w:94:PHE:O     | 19:w:95:ALA:C     | 2.47                     | 0.57              |
| 23:5:42:VAL:HG23  | 23:5:162:ILE:HG23 | 1.86                     | 0.57              |
| 18:V:83:ASP:CG    | 18:V:85:LEU:HD13  | 2.30                     | 0.57              |
| 15:q:83:GLY:O     | 15:q:84:THR:C     | 2.46                     | 0.57              |
| 41:v:201:HEM:HMB1 | 41:v:201:HEM:HBB2 | 1.86                     | 0.57              |
| 28:8:80:TYR:CD2   | 28:8:168:LEU:HD13 | 2.39                     | 0.57              |
| 24:2:38:PRO:CD    | 44:2:303:DD6:O2   | 2.53                     | 0.57              |
| 25:1:132:VAL:HG13 | 25:1:133:ARG:H    | 1.68                     | 0.57              |
| 41:V:201:HEM:HMB1 | 41:V:201:HEM:HBB2 | 1.86                     | 0.57              |
| 20:X:104:ALA:O    | 20:X:108:ILE:HG22 | 2.04                     | 0.57              |
| 15:q:69:LEU:O     | 15:q:71:GLY:N     | 2.38                     | 0.57              |
| 18:v:83:ASP:CG    | 18:v:85:LEU:HD13  | 2.30                     | 0.57              |
| 1:A:331:MET:HE3   | 4:D:347:PRO:HB2   | 1.86                     | 0.56              |
| 3:C:350:ILE:HG21  | 3:C:359:TRP:HB2   | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:C:521:LMG:H292 | 31:Z:101:CLA:HBD  | 1.86                     | 0.56              |
| 4:D:193:LEU:O     | 11:L:35:TYR:OH    | 2.20                     | 0.56              |
| 35:D:406:PL9:H111 | 36:D:407:LHG:H102 | 1.87                     | 0.56              |
| 15:Q:83:GLY:O     | 15:Q:84:THR:C     | 2.46                     | 0.56              |
| 19:W:99:PRO:CG    | 37:W:201:LMG:HC71 | 2.32                     | 0.56              |
| 20:x:92:ILE:CD1   | 23:5:119:TRP:NE1  | 2.64                     | 0.56              |
| 25:6:159:GLN:OE1  | 25:6:162:ARG:NH1  | 2.38                     | 0.56              |
| 1:a:331:MET:HE3   | 4:d:347:PRO:HB2   | 1.87                     | 0.56              |
| 2:b:198:ILE:HD13  | 31:b:504:CLA:HED2 | 1.87                     | 0.56              |
| 4:d:297:ASP:HA    | 4:d:315:TYR:OH    | 2.05                     | 0.56              |
| 25:6:132:VAL:HG13 | 25:6:133:ARG:H    | 1.68                     | 0.56              |
| 25:1:159:GLN:OE1  | 25:1:162:ARG:NH1  | 2.38                     | 0.56              |
| 4:D:51:GLY:HA2    | 4:D:55:VAL:HG12   | 1.86                     | 0.56              |
| 4:D:297:ASP:HA    | 4:D:315:TYR:OH    | 2.05                     | 0.56              |
| 2:b:15:ASP:O      | 2:b:16:PRO:C      | 2.49                     | 0.56              |
| 37:c:521:LMG:H292 | 31:z:101:CLA:HBD  | 1.86                     | 0.56              |
| 14:o:336:GLU:HG3  | 14:o:336:GLU:O    | 2.05                     | 0.56              |
| 26:p:181:GLY:HA3  | 26:p:186:ASN:HA   | 1.87                     | 0.56              |
| 28:3:165:PHE:O    | 28:3:169:ILE:HG22 | 2.06                     | 0.56              |
| 41:F:101:HEM:HBB2 | 41:F:101:HEM:HMB1 | 1.88                     | 0.56              |
| 20:x:104:ALA:O    | 20:x:108:ILE:HG22 | 2.04                     | 0.56              |
| 24:7:38:PRO:CD    | 44:7:303:DD6:O2   | 2.53                     | 0.56              |
| 23:0:66:SER:O     | 23:0:70:GLU:HG2   | 2.05                     | 0.56              |
| 24:2:38:PRO:HD2   | 44:2:303:DD6:O2   | 2.04                     | 0.56              |
| 2:B:392:ILE:HG21  | 2:B:418:LYS:HG2   | 1.87                     | 0.56              |
| 7:H:42:ILE:HG12   | 31:0:314:CLA:C3D  | 2.35                     | 0.56              |
| 3:c:278:ALA:O     | 3:c:282:MET:HG3   | 2.05                     | 0.56              |
| 26:P:181:GLY:HA3  | 26:P:186:ASN:HA   | 1.87                     | 0.56              |
| 2:b:106:MET:HE2   | 31:b:517:CLA:H151 | 1.88                     | 0.56              |
| 21:y:22:ALA:HB3   | 21:y:23:PRO:HD3   | 1.88                     | 0.56              |
| 28:8:165:PHE:O    | 28:8:169:ILE:HG22 | 2.06                     | 0.56              |
| 32:A:406:PHO:HBC3 | 4:D:279:LEU:HD12  | 1.88                     | 0.56              |
| 21:Y:22:ALA:HB3   | 21:Y:23:PRO:HD3   | 1.87                     | 0.56              |
| 41:f:101:HEM:HMB1 | 41:f:101:HEM:HBB2 | 1.88                     | 0.56              |
| 18:v:24:GLU:HG3   | 18:v:25:GLN:N     | 2.20                     | 0.56              |
| 2:B:434:ARG:HH22  | 14:O:267:GLY:HA3  | 1.71                     | 0.56              |
| 22:Z:21:VAL:HG13  | 22:Z:22:THR:HG23  | 1.87                     | 0.56              |
| 4:d:36:LEU:O      | 4:d:40:THR:OG1    | 2.20                     | 0.56              |
| 23:5:47:PRO:HG3   | 31:5:304:CLA:NB   | 2.21                     | 0.56              |
| 14:O:336:GLU:HG3  | 14:O:336:GLU:O    | 2.05                     | 0.56              |
| 22:Z:28:ALA:O     | 22:Z:29:THR:C     | 2.49                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:6:40:LEU:O     | 25:6:67:ARG:NH2   | 2.39                     | 0.56              |
| 25:1:40:LEU:O     | 25:1:67:ARG:NH2   | 2.39                     | 0.56              |
| 3:c:350:ILE:HG21  | 3:c:359:TRP:HB2   | 1.87                     | 0.55              |
| 35:d:406:PL9:H111 | 36:d:407:LHG:H102 | 1.87                     | 0.55              |
| 4:D:139:ARG:HG2   | 4:D:140:PRO:HD2   | 1.88                     | 0.55              |
| 23:5:66:SER:O     | 23:5:70:GLU:HG2   | 2.05                     | 0.55              |
| 3:C:278:ALA:O     | 3:C:282:MET:HG3   | 2.05                     | 0.55              |
| 1:a:153:ALA:HB1   | 31:a:403:CLA:HED1 | 1.89                     | 0.55              |
| 2:b:434:ARG:HH22  | 14:o:267:GLY:HA3  | 1.70                     | 0.55              |
| 4:d:139:ARG:HG2   | 4:d:140:PRO:HD2   | 1.88                     | 0.55              |
| 9:j:23:THR:O      | 9:j:27:LEU:HD23   | 2.07                     | 0.55              |
| 23:0:47:PRO:HG3   | 31:0:304:CLA:NB   | 2.21                     | 0.55              |
| 3:C:323:ARG:NH2   | 3:C:389:GLU:OE2   | 2.36                     | 0.55              |
| 14:O:123:PRO:HA   | 14:O:337:GLN:HE22 | 1.72                     | 0.55              |
| 19:W:94:PHE:O     | 19:W:95:ALA:C     | 2.49                     | 0.55              |
| 2:b:392:ILE:HG21  | 2:b:418:LYS:HG2   | 1.87                     | 0.55              |
| 4:d:193:LEU:O     | 11:l:35:TYR:OH    | 2.20                     | 0.55              |
| 24:7:133:LEU:HD12 | 24:7:140:ARG:HG3  | 1.89                     | 0.55              |
| 28:3:103:PRO:HB2  | 28:3:107:ALA:HB3  | 1.89                     | 0.55              |
| 28:8:103:PRO:HB2  | 28:8:107:ALA:HB3  | 1.89                     | 0.55              |
| 23:0:39:PRO:HG2   | 23:0:41:LEU:HD23  | 1.89                     | 0.55              |
| 1:A:139:MET:HE1   | 4:D:252:PHE:HB2   | 1.89                     | 0.55              |
| 18:V:24:GLU:HG3   | 18:V:25:GLN:N     | 2.20                     | 0.55              |
| 23:5:71:VAL:HG13  | 23:5:75:HIS:HE1   | 1.70                     | 0.55              |
| 1:A:133:LEU:HD23  | 4:D:256:ILE:HG12  | 1.89                     | 0.55              |
| 35:A:410:PL9:HC2  | 35:A:410:PL9:H103 | 1.88                     | 0.55              |
| 2:B:15:ASP:O      | 2:B:16:PRO:C      | 2.49                     | 0.55              |
| 2:B:198:ILE:HD13  | 31:B:503:CLA:HED2 | 1.87                     | 0.55              |
| 2:B:458:PHE:HB3   | 31:B:504:CLA:HBC2 | 1.89                     | 0.55              |
| 3:C:379:LYS:CE    | 15:Q:149:ARG:HH22 | 2.20                     | 0.55              |
| 3:c:379:LYS:CE    | 15:q:149:ARG:HH22 | 2.20                     | 0.55              |
| 24:2:133:LEU:HD12 | 24:2:140:ARG:HG3  | 1.89                     | 0.55              |
| 2:B:106:MET:HE2   | 31:B:516:CLA:H151 | 1.88                     | 0.55              |
| 7:H:48:LEU:HD13   | 36:H:103:LHG:H161 | 1.89                     | 0.55              |
| 32:a:406:PHO:HBC3 | 4:d:279:LEU:HD12  | 1.88                     | 0.55              |
| 14:O:294:ASN:HB2  | 14:O:305:GLY:HA2  | 1.88                     | 0.55              |
| 8:i:9:TYR:OH      | 19:w:99:PRO:HB2   | 2.06                     | 0.55              |
| 27:4:70:UNK:O     | 27:4:73:UNK:N     | 2.40                     | 0.55              |
| 35:a:410:PL9:H103 | 35:a:410:PL9:HC2  | 1.88                     | 0.55              |
| 2:b:458:PHE:HB3   | 31:b:505:CLA:HBC2 | 1.89                     | 0.55              |
| 23:5:74:MET:HE1   | 31:5:308:CLA:OBD  | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:B:508:CLA:HBC3 | 31:B:509:CLA:H122 | 1.89                     | 0.55              |
| 9:J:23:THR:O      | 9:J:27:LEU:HD23   | 2.07                     | 0.55              |
| 14:O:182:ILE:HG21 | 14:O:223:PHE:CZ   | 2.42                     | 0.55              |
| 23:5:39:PRO:HG2   | 23:5:41:LEU:HD23  | 1.89                     | 0.55              |
| 24:2:30:ILE:HG22  | 24:2:31:ALA:H     | 1.72                     | 0.55              |
| 25:1:84:TYR:HD2   | 25:1:171:LEU:HD13 | 1.72                     | 0.55              |
| 17:U:90:PRO:HA    | 17:U:93:VAL:HG22  | 1.89                     | 0.54              |
| 22:z:21:VAL:HG13  | 22:z:22:THR:HG23  | 1.87                     | 0.54              |
| 24:7:81:PHE:O     | 24:7:89:THR:HG22  | 2.07                     | 0.54              |
| 27:9:70:UNK:O     | 27:9:73:UNK:N     | 2.40                     | 0.54              |
| 3:C:83:GLU:OE1    | 18:V:103:ARG:NH2  | 2.37                     | 0.54              |
| 4:D:68:LEU:HD23   | 5:E:49:THR:HG21   | 1.90                     | 0.54              |
| 14:o:182:ILE:HG21 | 14:o:223:PHE:CZ   | 2.42                     | 0.54              |
| 17:u:90:PRO:HA    | 17:u:93:VAL:HG22  | 1.89                     | 0.54              |
| 24:2:81:PHE:O     | 24:2:89:THR:HG22  | 2.07                     | 0.54              |
| 14:o:294:ASN:HB2  | 14:o:305:GLY:HA2  | 1.88                     | 0.54              |
| 16:t:7:THR:O      | 16:t:11:ILE:HG12  | 2.07                     | 0.54              |
| 22:z:28:ALA:O     | 22:z:29:THR:C     | 2.49                     | 0.54              |
| 24:7:30:ILE:HG22  | 24:7:31:ALA:H     | 1.72                     | 0.54              |
| 1:A:153:ALA:HB1   | 31:A:403:CLA:HED1 | 1.89                     | 0.54              |
| 1:a:139:MET:HE1   | 4:d:252:PHE:HB2   | 1.89                     | 0.54              |
| 37:d:409:LMG:O4   | 37:d:409:LMG:O5   | 2.23                     | 0.54              |
| 24:2:68:VAL:CG1   | 44:2:304:DD6:C26  | 2.76                     | 0.54              |
| 41:V:201:HEM:HBA2 | 41:V:201:HEM:HHA  | 1.90                     | 0.54              |
| 31:c:505:CLA:H51  | 39:c:520:DGD:HB72 | 1.90                     | 0.54              |
| 4:d:68:LEU:HD23   | 5:e:49:THR:HG21   | 1.89                     | 0.54              |
| 23:0:74:MET:HE1   | 31:0:308:CLA:OBD  | 2.07                     | 0.54              |
| 22:Z:9:THR:O      | 22:Z:10:ALA:C     | 2.48                     | 0.54              |
| 31:b:509:CLA:HBC3 | 31:b:510:CLA:H122 | 1.89                     | 0.54              |
| 19:w:110:SER:HG   | 19:w:114:TRP:CD1  | 2.26                     | 0.54              |
| 28:3:80:TYR:CD2   | 28:3:168:LEU:HD13 | 2.39                     | 0.54              |
| 1:A:77:ILE:HD13   | 11:L:30:VAL:HG13  | 1.90                     | 0.54              |
| 3:C:459:ILE:O     | 3:C:460:ASP:HB2   | 2.07                     | 0.54              |
| 21:Y:23:PRO:C     | 21:Y:26:VAL:HB    | 2.32                     | 0.54              |
| 1:a:187:GLN:NE2   | 1:a:193:LEU:HG    | 2.22                     | 0.54              |
| 31:b:516:CLA:H2   | 31:b:517:CLA:HBB2 | 1.90                     | 0.54              |
| 41:f:101:HEM:HBC2 | 41:f:101:HEM:HMC2 | 1.90                     | 0.54              |
| 24:2:60:HIS:CB    | 24:2:152:MET:HE2  | 2.38                     | 0.54              |
| 25:1:99:GLY:O     | 25:1:101:ALA:N    | 2.40                     | 0.54              |
| 3:c:109:VAL:HG11  | 31:z:101:CLA:H52  | 1.90                     | 0.54              |
| 22:z:58:ASP:O     | 22:z:59:GLY:C     | 2.50                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:2:30:ILE:HG22  | 24:2:32:PRO:HD2   | 1.90                     | 0.54              |
| 41:F:101:HEM:HBC2 | 41:F:101:HEM:HMC2 | 1.90                     | 0.54              |
| 8:I:9:TYR:OH      | 19:W:99:PRO:HB2   | 2.08                     | 0.54              |
| 14:O:221:ASP:O    | 14:O:222:THR:C    | 2.51                     | 0.54              |
| 1:a:224:ILE:O     | 1:a:226:GLU:HG3   | 2.08                     | 0.54              |
| 3:c:116:VAL:HG21  | 33:c:515:BCR:HC22 | 1.90                     | 0.54              |
| 22:z:56:THR:HG23  | 31:z:101:CLA:HBB1 | 1.90                     | 0.54              |
| 2:B:415:PRO:HG3   | 17:U:13:ASP:OD2   | 2.08                     | 0.53              |
| 3:C:109:VAL:HG11  | 31:Z:101:CLA:H52  | 1.90                     | 0.53              |
| 16:T:7:THR:O      | 16:T:11:ILE:HG12  | 2.07                     | 0.53              |
| 20:X:92:ILE:CD1   | 23:0:119:TRP:NE1  | 2.70                     | 0.53              |
| 22:Z:58:ASP:O     | 22:Z:59:GLY:C     | 2.50                     | 0.53              |
| 3:c:459:ILE:O     | 3:c:460:ASP:HB2   | 2.07                     | 0.53              |
| 19:w:99:PRO:CG    | 37:w:201:LMG:HC71 | 2.36                     | 0.53              |
| 22:z:9:THR:O      | 22:z:10:ALA:C     | 2.48                     | 0.53              |
| 23:0:199:ASP:O    | 23:0:200:SER:OG   | 2.24                     | 0.53              |
| 3:C:315:PHE:HZ    | 3:C:384:ILE:HD11  | 1.73                     | 0.53              |
| 3:c:83:GLU:OE1    | 18:v:103:ARG:NH2  | 2.37                     | 0.53              |
| 21:y:23:PRO:C     | 21:y:26:VAL:HB    | 2.32                     | 0.53              |
| 25:6:84:TYR:HD2   | 25:6:171:LEU:HD13 | 1.72                     | 0.53              |
| 1:A:187:GLN:HE21  | 31:A:403:CLA:HAC1 | 1.74                     | 0.53              |
| 1:A:187:GLN:NE2   | 1:A:193:LEU:HG    | 2.23                     | 0.53              |
| 3:C:416:SER:HB2   | 18:V:42:VAL:HG23  | 1.91                     | 0.53              |
| 22:Z:56:THR:HG23  | 31:Z:101:CLA:HBB1 | 1.90                     | 0.53              |
| 3:c:315:PHE:HZ    | 3:c:384:ILE:HD11  | 1.74                     | 0.53              |
| 18:v:76:ILE:HG21  | 18:v:112:LEU:HD22 | 1.90                     | 0.53              |
| 41:v:201:HEM:HHA  | 41:v:201:HEM:HBA2 | 1.90                     | 0.53              |
| 24:7:60:HIS:CB    | 24:7:152:MET:HE2  | 2.38                     | 0.53              |
| 1:A:224:ILE:O     | 1:A:226:GLU:HG3   | 2.08                     | 0.53              |
| 18:V:76:ILE:HG21  | 18:V:112:LEU:HD22 | 1.90                     | 0.53              |
| 4:d:161:PRO:HB3   | 4:d:170:ALA:HB2   | 1.90                     | 0.53              |
| 24:7:30:ILE:HG22  | 24:7:32:PRO:HD2   | 1.90                     | 0.53              |
| 25:1:83:GLY:O     | 25:1:87:PRO:HD2   | 2.09                     | 0.53              |
| 9:J:34:SER:HG     | 15:Q:81:ALA:HA    | 1.74                     | 0.53              |
| 1:a:133:LEU:HD23  | 4:d:256:ILE:HG12  | 1.89                     | 0.53              |
| 14:o:123:PRO:HA   | 14:o:337:GLN:HE22 | 1.72                     | 0.53              |
| 19:w:102:ILE:HG13 | 19:w:104:ALA:N    | 2.23                     | 0.53              |
| 24:7:68:VAL:CG1   | 44:7:304:DD6:C26  | 2.76                     | 0.53              |
| 31:C:505:CLA:H51  | 39:C:520:DGD:HB72 | 1.90                     | 0.53              |
| 1:a:77:ILE:HD13   | 11:l:30:VAL:HG13  | 1.90                     | 0.53              |
| 3:c:323:ARG:NH2   | 3:c:389:GLU:OE2   | 2.36                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:x:92:ILE:HD12  | 23:5:119:TRP:CD1  | 2.43                     | 0.53              |
| 25:6:83:GLY:O     | 25:6:87:PRO:HD2   | 2.09                     | 0.53              |
| 1:A:278:TRP:HB3   | 1:A:279:PRO:HD3   | 1.91                     | 0.53              |
| 2:B:153:PHE:CE1   | 2:B:157:HIS:HD2   | 2.27                     | 0.53              |
| 2:B:481:GLY:N     | 4:D:139:ARG:HH21  | 2.07                     | 0.53              |
| 28:3:99:THR:HA    | 28:3:102:ILE:HD13 | 1.91                     | 0.53              |
| 2:b:311:PHE:O     | 2:b:317:ASN:ND2   | 2.42                     | 0.53              |
| 22:z:38:ASP:OD1   | 22:z:39:GLN:N     | 2.42                     | 0.53              |
| 23:5:47:PRO:HG3   | 31:5:304:CLA:C4B  | 2.38                     | 0.53              |
| 1:A:328:ILE:HG23  | 4:D:321:LEU:HD22  | 1.91                     | 0.52              |
| 7:H:45:ILE:HD13   | 36:H:103:LHG:H141 | 1.91                     | 0.52              |
| 1:a:328:ILE:HG23  | 4:d:321:LEU:HD22  | 1.91                     | 0.52              |
| 2:b:153:PHE:CE1   | 2:b:157:HIS:HD2   | 2.27                     | 0.52              |
| 2:b:222:PRO:HB3   | 7:h:38:GLY:HA3    | 1.91                     | 0.52              |
| 2:b:415:PRO:HG3   | 17:u:13:ASP:OD2   | 2.08                     | 0.52              |
| 3:c:334:PRO:HG2   | 4:d:350:ASN:ND2   | 2.22                     | 0.52              |
| 39:c:520:DGD:HBW2 | 39:c:520:DGD:HAT2 | 1.91                     | 0.52              |
| 15:q:86:GLN:O     | 15:q:87:ALA:C     | 2.52                     | 0.52              |
| 1:a:278:TRP:HB3   | 1:a:279:PRO:HD3   | 1.91                     | 0.52              |
| 3:c:87:ILE:HD11   | 3:c:426:LEU:CG    | 2.39                     | 0.52              |
| 3:C:116:VAL:HG21  | 33:C:515:BCR:HC22 | 1.91                     | 0.52              |
| 21:Y:42:GLN:O     | 21:Y:43:ILE:C     | 2.52                     | 0.52              |
| 22:Z:38:ASP:OD1   | 22:Z:39:GLN:N     | 2.41                     | 0.52              |
| 3:c:203:THR:HG23  | 3:c:231:GLU:HB3   | 1.91                     | 0.52              |
| 14:o:188:GLU:HG2  | 14:o:189:GLY:N    | 2.24                     | 0.52              |
| 14:o:221:ASP:O    | 14:o:222:THR:C    | 2.51                     | 0.52              |
| 17:u:67:GLY:O     | 17:u:68:LEU:C     | 2.52                     | 0.52              |
| 23:0:47:PRO:HG3   | 31:0:304:CLA:C4B  | 2.38                     | 0.52              |
| 1:A:324:ALA:HB1   | 4:D:325:ILE:HD11  | 1.91                     | 0.52              |
| 4:D:161:PRO:HB3   | 4:D:170:ALA:HB2   | 1.90                     | 0.52              |
| 3:c:173:PHE:O     | 3:c:177:ILE:HG12  | 2.09                     | 0.52              |
| 3:c:416:SER:HB2   | 18:v:42:VAL:HG23  | 1.91                     | 0.52              |
| 31:B:515:CLA:H2   | 31:B:516:CLA:HBB2 | 1.90                     | 0.52              |
| 3:C:173:PHE:O     | 3:C:177:ILE:HG12  | 2.09                     | 0.52              |
| 39:C:520:DGD:HBW2 | 39:C:520:DGD:HAT2 | 1.91                     | 0.52              |
| 15:Q:197:ASN:O    | 15:Q:201:ILE:HG12 | 2.10                     | 0.52              |
| 2:b:22:VAL:HG13   | 31:b:515:CLA:HMB2 | 1.91                     | 0.52              |
| 37:y:101:LMG:H292 | 37:y:101:LMG:H152 | 1.92                     | 0.52              |
| 24:7:32:PRO:HG3   | 31:7:305:CLA:C4B  | 2.39                     | 0.52              |
| 31:B:514:CLA:C16  | 33:B:517:BCR:H351 | 2.40                     | 0.52              |
| 15:Q:86:GLN:O     | 15:Q:87:ALA:C     | 2.52                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:17:PHE:CE2    | 8:i:18:LEU:HD11   | 2.45                     | 0.52              |
| 2:b:235:GLU:HB3   | 2:b:473:THR:HG22  | 1.91                     | 0.52              |
| 18:v:76:ILE:HD11  | 41:v:201:HEM:HMB1 | 1.92                     | 0.52              |
| 25:6:165:MET:O    | 25:6:168:ILE:HG22 | 2.09                     | 0.52              |
| 24:2:32:PRO:HG3   | 31:2:305:CLA:C4B  | 2.39                     | 0.52              |
| 1:A:331:MET:HG3   | 4:D:324:GLY:HA3   | 1.92                     | 0.52              |
| 2:B:22:VAL:HG13   | 31:B:514:CLA:HMB2 | 1.91                     | 0.52              |
| 2:B:222:PRO:HB3   | 7:H:38:GLY:HA3    | 1.91                     | 0.52              |
| 2:B:311:PHE:O     | 2:B:317:ASN:ND2   | 2.42                     | 0.52              |
| 17:U:67:GLY:O     | 17:U:68:LEU:C     | 2.52                     | 0.52              |
| 4:d:35:LEU:HD21   | 20:x:105:LEU:HD11 | 1.91                     | 0.52              |
| 14:o:110:ASN:HD21 | 14:o:164:GLN:C    | 2.18                     | 0.52              |
| 25:1:165:MET:O    | 25:1:168:ILE:HG22 | 2.09                     | 0.52              |
| 3:C:87:ILE:HD11   | 3:C:426:LEU:CG    | 2.39                     | 0.52              |
| 19:W:102:ILE:HG13 | 19:W:104:ALA:N    | 2.23                     | 0.52              |
| 1:a:187:GLN:HE21  | 31:a:403:CLA:HAC1 | 1.74                     | 0.52              |
| 18:v:9:THR:HG22   | 18:v:18:THR:HB    | 1.92                     | 0.52              |
| 21:y:42:GLN:O     | 21:y:43:ILE:C     | 2.52                     | 0.52              |
| 25:6:99:GLY:O     | 25:6:101:ALA:N    | 2.40                     | 0.52              |
| 23:0:71:VAL:HG13  | 23:0:75:HIS:HE1   | 1.71                     | 0.52              |
| 14:O:188:GLU:HG2  | 14:O:189:GLY:N    | 2.24                     | 0.51              |
| 19:W:110:SER:HG   | 19:W:114:TRP:CD1  | 2.28                     | 0.51              |
| 20:X:92:ILE:HD11  | 31:0:307:CLA:C1   | 2.40                     | 0.51              |
| 2:b:233:ASN:O     | 2:b:236:THR:HG22  | 2.10                     | 0.51              |
| 2:b:481:GLY:N     | 4:d:139:ARG:HH21  | 2.07                     | 0.51              |
| 15:Q:69:LEU:O     | 15:Q:70:ILE:C     | 2.53                     | 0.51              |
| 37:Y:101:LMG:H152 | 37:Y:101:LMG:H292 | 1.92                     | 0.51              |
| 1:a:267:ASN:HA    | 4:d:235:PHE:CD2   | 2.45                     | 0.51              |
| 3:C:402:GLY:HA3   | 3:C:420:VAL:HG22  | 1.91                     | 0.51              |
| 18:V:76:ILE:HD11  | 41:V:201:HEM:HMB1 | 1.92                     | 0.51              |
| 21:Y:23:PRO:HA    | 21:Y:26:VAL:HB    | 1.92                     | 0.51              |
| 1:a:331:MET:HG3   | 4:d:324:GLY:HA3   | 1.92                     | 0.51              |
| 28:3:170:ARG:O    | 28:3:174:GLN:HG2  | 2.10                     | 0.51              |
| 28:8:99:THR:HA    | 28:8:102:ILE:HD13 | 1.91                     | 0.51              |
| 2:B:233:ASN:O     | 2:B:236:THR:HG22  | 2.10                     | 0.51              |
| 2:B:235:GLU:HB3   | 2:B:473:THR:HG22  | 1.91                     | 0.51              |
| 31:C:509:CLA:C7   | 10:K:46:PHE:HZ    | 2.24                     | 0.51              |
| 18:V:9:THR:HG22   | 18:V:18:THR:HB    | 1.92                     | 0.51              |
| 1:a:324:ALA:HB1   | 4:d:325:ILE:HD11  | 1.91                     | 0.51              |
| 14:o:132:MET:HE2  | 14:o:134:ILE:HD11 | 1.92                     | 0.51              |
| 21:y:23:PRO:HA    | 21:y:26:VAL:HB    | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:5:204:SER:O    | 25:6:186:GLY:HA3  | 2.11                     | 0.51              |
| 28:8:170:ARG:O    | 28:8:174:GLN:HG2  | 2.10                     | 0.51              |
| 2:B:192:PRO:HG3   | 7:H:61:TYR:CD1    | 2.46                     | 0.51              |
| 3:C:203:THR:HG23  | 3:C:231:GLU:HB3   | 1.91                     | 0.51              |
| 7:h:42:ILE:HG12   | 31:5:314:CLA:C3D  | 2.41                     | 0.51              |
| 36:h:103:LHG:H261 | 36:h:103:LHG:H131 | 1.92                     | 0.51              |
| 19:w:97:GLY:O     | 19:w:98:LYS:C     | 2.52                     | 0.51              |
| 23:5:146:ALA:HA   | 31:5:308:CLA:HBC2 | 1.93                     | 0.51              |
| 25:6:133:ARG:HH21 | 31:6:201:CLA:HED1 | 1.76                     | 0.51              |
| 4:D:35:LEU:HD21   | 20:X:105:LEU:HD11 | 1.91                     | 0.51              |
| 14:O:280:LYS:O    | 17:U:11:VAL:N     | 2.44                     | 0.51              |
| 31:b:515:CLA:C16  | 33:b:518:BCR:H351 | 2.40                     | 0.51              |
| 36:d:411:LHG:HC81 | 20:x:89:ALA:CB    | 2.40                     | 0.51              |
| 15:q:197:ASN:O    | 15:q:201:ILE:HG12 | 2.10                     | 0.51              |
| 1:A:267:ASN:HA    | 4:D:235:PHE:CD2   | 2.45                     | 0.51              |
| 1:A:296:ASN:HB3   | 3:C:401:LEU:HD13  | 1.93                     | 0.51              |
| 3:C:464:GLU:OE2   | 4:D:248:THR:OG1   | 2.29                     | 0.51              |
| 14:O:110:ASN:HD21 | 14:O:164:GLN:C    | 2.18                     | 0.51              |
| 22:Z:6:THR:O      | 22:Z:9:THR:HG23   | 2.11                     | 0.51              |
| 26:p:161:ARG:O    | 26:p:165:GLN:N    | 2.34                     | 0.51              |
| 26:P:161:ARG:O    | 26:P:165:GLN:N    | 2.34                     | 0.51              |
| 33:B:519:BCR:H333 | 13:N:17:UNK:CB    | 2.41                     | 0.51              |
| 3:C:334:PRO:HG2   | 4:D:350:ASN:ND2   | 2.22                     | 0.51              |
| 15:Q:68:GLY:HA2   | 15:Q:74:THR:OG1   | 2.11                     | 0.51              |
| 7:h:41:PRO:HB2    | 31:5:314:CLA:CMD  | 2.40                     | 0.51              |
| 14:o:280:LYS:O    | 17:u:11:VAL:N     | 2.44                     | 0.51              |
| 22:z:6:THR:O      | 22:z:9:THR:HG23   | 2.11                     | 0.51              |
| 1:a:17:PHE:O      | 1:a:18:CYS:C      | 2.54                     | 0.51              |
| 19:w:121:MET:HA   | 19:w:121:MET:HE2  | 1.93                     | 0.51              |
| 25:6:108:GLY:HA3  | 25:6:175:ASP:OD2  | 2.11                     | 0.51              |
| 26:p:69:ALA:O     | 26:p:71:PHE:N     | 2.43                     | 0.51              |
| 31:B:503:CLA:HAB  | 31:B:505:CLA:H152 | 1.93                     | 0.51              |
| 3:C:67:MET:O      | 3:C:71:GLU:HG3    | 2.11                     | 0.51              |
| 4:D:36:LEU:O      | 4:D:40:THR:OG1    | 2.20                     | 0.51              |
| 10:K:58:PHE:O     | 10:K:59:ARG:C     | 2.54                     | 0.51              |
| 3:c:402:GLY:HA3   | 3:c:420:VAL:HG22  | 1.92                     | 0.51              |
| 4:d:191:TRP:CE3   | 4:d:289:LEU:HD11  | 2.46                     | 0.51              |
| 23:5:42:VAL:HG22  | 23:5:166:VAL:HG23 | 1.93                     | 0.51              |
| 26:p:48:LEU:HG    | 26:p:50:GLY:H     | 1.76                     | 0.51              |
| 23:0:204:SER:O    | 25:1:186:GLY:HA3  | 2.11                     | 0.51              |
| 44:2:303:DD6:C37  | 31:2:307:CLA:C2B  | 2.89                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:191:TRP:CE3   | 4:D:289:LEU:HD11  | 2.47                     | 0.50              |
| 36:H:103:LHG:H261 | 36:H:103:LHG:H131 | 1.92                     | 0.50              |
| 14:O:132:MET:HE2  | 14:O:134:ILE:HD11 | 1.92                     | 0.50              |
| 19:W:121:MET:HE2  | 19:W:121:MET:HA   | 1.93                     | 0.50              |
| 2:b:192:PRO:HG3   | 7:h:61:TYR:CD1    | 2.46                     | 0.50              |
| 18:v:134:LYS:O    | 18:v:135:ILE:C    | 2.54                     | 0.50              |
| 20:x:92:ILE:HD11  | 31:5:307:CLA:C1   | 2.41                     | 0.50              |
| 23:0:137:GLU:HG3  | 31:0:308:CLA:HMC2 | 1.93                     | 0.50              |
| 31:b:507:CLA:OBD  | 37:b:521:LMG:O5   | 2.30                     | 0.50              |
| 3:c:324:LEU:HD13  | 17:u:33:ILE:HD13  | 1.92                     | 0.50              |
| 31:P:604:CLA:HMB3 | 44:P:611:DD6:C37  | 2.37                     | 0.50              |
| 17:U:28:ILE:HG13  | 17:U:84:THR:O     | 2.11                     | 0.50              |
| 3:c:67:MET:O      | 3:c:71:GLU:HG3    | 2.11                     | 0.50              |
| 15:q:68:GLY:HA2   | 15:q:74:THR:OG1   | 2.11                     | 0.50              |
| 15:q:69:LEU:O     | 15:q:70:ILE:C     | 2.53                     | 0.50              |
| 17:u:28:ILE:HG13  | 17:u:84:THR:O     | 2.11                     | 0.50              |
| 25:1:132:VAL:HG13 | 25:1:133:ARG:N    | 2.26                     | 0.50              |
| 14:O:127:ALA:HB1  | 14:O:336:GLU:O    | 2.12                     | 0.50              |
| 33:b:520:BCR:H333 | 13:n:17:UNK:CB    | 2.41                     | 0.50              |
| 3:c:191:PRO:HB3   | 15:q:147:LEU:HG   | 1.94                     | 0.50              |
| 3:c:464:GLU:OE2   | 4:d:248:THR:OG1   | 2.29                     | 0.50              |
| 22:z:31:GLY:O     | 22:z:32:GLU:C     | 2.53                     | 0.50              |
| 25:6:132:VAL:HG13 | 25:6:133:ARG:N    | 2.26                     | 0.50              |
| 2:B:54:PRO:HD2    | 2:B:57:ARG:HB2    | 1.93                     | 0.50              |
| 18:V:134:LYS:O    | 18:V:135:ILE:C    | 2.54                     | 0.50              |
| 31:c:509:CLA:C7   | 10:k:46:PHE:HZ    | 2.24                     | 0.50              |
| 14:o:127:ALA:HB1  | 14:o:336:GLU:O    | 2.12                     | 0.50              |
| 21:y:22:ALA:O     | 21:y:26:VAL:HG23  | 2.12                     | 0.50              |
| 23:5:137:GLU:HG3  | 31:5:308:CLA:HMC2 | 1.93                     | 0.50              |
| 44:7:303:DD6:C37  | 31:7:307:CLA:C2B  | 2.90                     | 0.50              |
| 23:0:74:MET:HE2   | 23:0:77:ARG:HD2   | 1.94                     | 0.50              |
| 14:O:130:VAL:O    | 14:O:172:GLU:HG2  | 2.12                     | 0.50              |
| 21:Y:22:ALA:O     | 21:Y:26:VAL:HG23  | 2.12                     | 0.50              |
| 2:b:54:PRO:HD2    | 2:b:57:ARG:HB2    | 1.93                     | 0.50              |
| 3:c:83:GLU:OE2    | 3:c:398:HIS:NE2   | 2.45                     | 0.50              |
| 1:A:89:ILE:HD11   | 1:A:108:ASN:HB3   | 1.94                     | 0.50              |
| 28:3:65:ALA:HA    | 31:3:308:CLA:OBD  | 2.12                     | 0.50              |
| 25:1:133:ARG:HH21 | 31:1:201:CLA:HED1 | 1.76                     | 0.50              |
| 3:C:191:PRO:HB3   | 15:Q:147:LEU:HG   | 1.94                     | 0.50              |
| 4:d:189:HIS:HA    | 4:d:294:ARG:HD2   | 1.94                     | 0.50              |
| 3:C:324:LEU:HD13  | 17:U:33:ILE:HD13  | 1.93                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:1:MET:HE3     | 34:b:501:SQD:H3   | 1.94                     | 0.50              |
| 23:0:42:VAL:HG22  | 23:0:166:VAL:HG23 | 1.93                     | 0.50              |
| 14:O:294:ASN:O    | 14:O:296:VAL:HG23 | 2.12                     | 0.49              |
| 3:c:345:PRO:HB3   | 14:o:163:ARG:HD3  | 1.94                     | 0.49              |
| 15:q:127:ARG:O    | 15:q:130:LYS:HG2  | 2.12                     | 0.49              |
| 1:A:17:PHE:CE2    | 8:I:18:LEU:HD11   | 2.45                     | 0.49              |
| 11:L:5:ASN:OD1    | 11:L:6:PRO:HD2    | 2.11                     | 0.49              |
| 3:c:55:ALA:HB1    | 33:c:517:BCR:H373 | 1.94                     | 0.49              |
| 24:2:78:ARG:HB3   | 24:2:89:THR:O     | 2.12                     | 0.49              |
| 25:1:108:GLY:HA3  | 25:1:175:ASP:OD2  | 2.11                     | 0.49              |
| 4:D:189:HIS:HA    | 4:D:294:ARG:HD2   | 1.94                     | 0.49              |
| 11:l:5:ASN:OD1    | 11:l:6:PRO:HD2    | 2.11                     | 0.49              |
| 14:o:130:VAL:O    | 14:o:172:GLU:HG2  | 2.12                     | 0.49              |
| 14:o:294:ASN:O    | 14:o:296:VAL:HG23 | 2.12                     | 0.49              |
| 22:z:33:TRP:O     | 22:z:34:GLU:C     | 2.56                     | 0.49              |
| 31:0:308:CLA:H2A  | 31:0:308:CLA:O1A  | 2.12                     | 0.49              |
| 2:B:19:LEU:O      | 2:B:20:ILE:C      | 2.56                     | 0.49              |
| 31:B:506:CLA:OBD  | 37:B:520:LMG:O5   | 2.30                     | 0.49              |
| 26:P:88:LEU:HD23  | 31:P:602:CLA:H3A  | 1.95                     | 0.49              |
| 23:0:146:ALA:HA   | 31:0:308:CLA:HBC2 | 1.93                     | 0.49              |
| 1:A:214:MET:SD    | 35:A:410:PL9:H102 | 2.52                     | 0.49              |
| 2:B:153:PHE:HE1   | 2:B:157:HIS:HD2   | 1.61                     | 0.49              |
| 3:C:83:GLU:OE2    | 3:C:398:HIS:NE2   | 2.45                     | 0.49              |
| 36:D:411:LHG:HC81 | 20:X:89:ALA:CB    | 2.43                     | 0.49              |
| 6:F:42:PHE:O      | 6:F:44:GLN:N      | 2.46                     | 0.49              |
| 20:X:108:ILE:HG23 | 20:X:109:SER:H    | 1.78                     | 0.49              |
| 22:Z:31:GLY:O     | 22:Z:32:GLU:C     | 2.53                     | 0.49              |
| 10:k:58:PHE:O     | 10:k:59:ARG:C     | 2.54                     | 0.49              |
| 2:B:155:ALA:O     | 2:B:159:THR:OG1   | 2.30                     | 0.49              |
| 3:C:307:PRO:HB2   | 3:C:361:LEU:HD12  | 1.95                     | 0.49              |
| 6:F:19:ARG:O      | 6:F:20:TRP:C      | 2.54                     | 0.49              |
| 15:Q:127:ARG:O    | 15:Q:130:LYS:HG2  | 2.12                     | 0.49              |
| 1:a:214:MET:SD    | 35:a:410:PL9:H102 | 2.52                     | 0.49              |
| 31:b:504:CLA:HAB  | 31:b:506:CLA:H152 | 1.93                     | 0.49              |
| 1:A:190:HIS:HB3   | 1:A:293:MET:CE    | 2.41                     | 0.49              |
| 34:B:523:SQD:H3   | 8:i:1:MET:HE3     | 1.94                     | 0.49              |
| 3:C:345:PRO:HB3   | 14:O:163:ARG:HD3  | 1.94                     | 0.49              |
| 8:I:9:TYR:OH      | 19:W:99:PRO:HG2   | 2.12                     | 0.49              |
| 1:a:190:HIS:HB3   | 1:a:293:MET:CE    | 2.41                     | 0.49              |
| 2:b:42:LEU:HD13   | 2:b:94:GLU:HG3    | 1.94                     | 0.49              |
| 4:d:122:LEU:HG    | 4:d:150:ILE:HG12  | 1.95                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:f:19:ARG:O      | 6:f:20:TRP:C      | 2.54                     | 0.49              |
| 26:P:48:LEU:HG    | 26:P:50:GLY:H     | 1.76                     | 0.49              |
| 44:1:204:DD6:C10  | 31:1:211:CLA:H52  | 2.43                     | 0.49              |
| 20:X:92:ILE:HD12  | 23:0:119:TRP:CD1  | 2.47                     | 0.49              |
| 1:a:271:LEU:HD11  | 35:a:410:PL9:HC8  | 1.95                     | 0.49              |
| 1:a:296:ASN:HB3   | 3:c:401:LEU:HD13  | 1.93                     | 0.49              |
| 22:z:4:MET:O      | 22:z:5:ILE:C      | 2.56                     | 0.49              |
| 2:b:145:LEU:HD21  | 31:b:505:CLA:H143 | 1.95                     | 0.49              |
| 9:j:31:GLY:C      | 9:j:33:TYR:N      | 2.68                     | 0.49              |
| 26:p:88:LEU:HD23  | 31:p:602:CLA:H3A  | 1.95                     | 0.49              |
| 28:8:65:ALA:HA    | 31:8:308:CLA:OBD  | 2.12                     | 0.49              |
| 2:B:145:LEU:HD21  | 31:B:504:CLA:H143 | 1.95                     | 0.49              |
| 39:C:519:DGD:HA72 | 39:C:519:DGD:HA41 | 1.54                     | 0.49              |
| 31:b:509:CLA:H172 | 31:b:510:CLA:H192 | 1.95                     | 0.49              |
| 3:c:90:GLN:HB3    | 3:c:302:TYR:CZ    | 2.48                     | 0.49              |
| 6:f:42:PHE:O      | 6:f:44:GLN:N      | 2.46                     | 0.49              |
| 19:w:94:PHE:O     | 19:w:96:ASN:N     | 2.46                     | 0.49              |
| 20:x:108:ILE:HG23 | 20:x:109:SER:H    | 1.77                     | 0.49              |
| 24:7:30:ILE:HG22  | 24:7:31:ALA:N     | 2.27                     | 0.49              |
| 3:C:90:GLN:HB3    | 3:C:302:TYR:CZ    | 2.48                     | 0.48              |
| 31:C:509:CLA:H72  | 10:K:46:PHE:CZ    | 2.45                     | 0.48              |
| 36:a:411:LHG:O4   | 4:d:141:TYR:OH    | 2.24                     | 0.48              |
| 5:e:10:PHE:O      | 5:e:14:ILE:HG12   | 2.13                     | 0.48              |
| 7:h:48:LEU:HD13   | 36:h:103:LHG:H161 | 1.95                     | 0.48              |
| 23:5:74:MET:HE2   | 23:5:77:ARG:HD2   | 1.94                     | 0.48              |
| 26:P:69:ALA:O     | 26:P:71:PHE:N     | 2.43                     | 0.48              |
| 24:2:30:ILE:HG22  | 24:2:31:ALA:N     | 2.27                     | 0.48              |
| 1:A:131:TRP:CH2   | 31:C:506:CLA:HAA2 | 2.48                     | 0.48              |
| 2:B:102:ILE:HD13  | 33:B:518:BCR:H401 | 1.94                     | 0.48              |
| 2:B:112:ILE:HG21  | 33:B:519:BCR:H393 | 1.95                     | 0.48              |
| 4:D:122:LEU:HG    | 4:D:150:ILE:HG12  | 1.95                     | 0.48              |
| 5:E:10:PHE:O      | 5:E:14:ILE:HG12   | 2.14                     | 0.48              |
| 1:a:89:ILE:HD11   | 1:a:108:ASN:HB3   | 1.94                     | 0.48              |
| 2:b:243:SER:HA    | 2:b:246:PHE:CE1   | 2.48                     | 0.48              |
| 1:A:110:GLY:N     | 1:A:111:PRO:HD2   | 2.29                     | 0.48              |
| 2:B:243:SER:HA    | 2:B:246:PHE:CE1   | 2.49                     | 0.48              |
| 19:W:104:ALA:O    | 19:W:108:MET:HG3  | 2.14                     | 0.48              |
| 32:a:405:PHO:NC   | 4:d:209:LEU:HD13  | 2.29                     | 0.48              |
| 2:b:102:ILE:HD13  | 33:b:519:BCR:H401 | 1.94                     | 0.48              |
| 2:b:112:ILE:HG21  | 33:b:520:BCR:H393 | 1.95                     | 0.48              |
| 2:b:155:ALA:O     | 2:b:159:THR:OG1   | 2.30                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:q:104:SER:O    | 15:q:105:LEU:HD22 | 2.13                     | 0.48              |
| 23:5:45:LEU:HB3   | 23:5:47:PRO:HD2   | 1.96                     | 0.48              |
| 23:5:103:LEU:HD22 | 23:5:108:ARG:O    | 2.13                     | 0.48              |
| 31:5:308:CLA:H2A  | 31:5:308:CLA:O1A  | 2.12                     | 0.48              |
| 24:7:65:MET:HE2   | 24:7:147:HIS:HB3  | 1.95                     | 0.48              |
| 24:7:102:ILE:HB   | 24:7:107:TRP:NE1  | 2.28                     | 0.48              |
| 24:7:104:ALA:HB3  | 25:6:112:ILE:O    | 2.13                     | 0.48              |
| 23:0:194:LEU:HD11 | 23:0:205:TRP:CZ3  | 2.48                     | 0.48              |
| 2:B:42:LEU:HD13   | 2:B:94:GLU:HG3    | 1.94                     | 0.48              |
| 5:E:23:HIS:NE2    | 41:F:101:HEM:ND   | 2.62                     | 0.48              |
| 15:Q:76:TYR:CG    | 15:Q:77:SER:N     | 2.81                     | 0.48              |
| 1:a:131:TRP:CH2   | 31:c:506:CLA:HAA2 | 2.48                     | 0.48              |
| 31:7:309:CLA:H12  | 31:6:201:CLA:HMD2 | 1.94                     | 0.48              |
| 23:0:45:LEU:HB3   | 23:0:47:PRO:HD2   | 1.96                     | 0.48              |
| 23:0:85:GLY:O     | 23:0:89:PRO:HD2   | 2.14                     | 0.48              |
| 1:A:97:TRP:CH2    | 8:I:8:VAL:HG11    | 2.49                     | 0.48              |
| 1:A:310:GLN:HG3   | 18:V:2:ASP:O      | 2.14                     | 0.48              |
| 15:Q:104:SER:O    | 15:Q:105:LEU:HD22 | 2.13                     | 0.48              |
| 39:c:520:DGD:HAW2 | 39:c:520:DGD:HA82 | 1.94                     | 0.48              |
| 23:5:194:LEU:HD11 | 23:5:205:TRP:CZ3  | 2.48                     | 0.48              |
| 23:0:103:LEU:HD22 | 23:0:108:ARG:O    | 2.13                     | 0.48              |
| 25:1:78:GLN:HB3   | 44:1:204:DD6:C3   | 2.43                     | 0.48              |
| 3:C:154:LYS:HB3   | 3:C:256:PRO:HG2   | 1.95                     | 0.48              |
| 1:a:110:GLY:N     | 1:a:111:PRO:HD2   | 2.29                     | 0.48              |
| 2:b:153:PHE:HE1   | 2:b:157:HIS:HD2   | 1.61                     | 0.48              |
| 24:7:74:PRO:HB2   | 24:7:94:ASN:ND2   | 2.29                     | 0.48              |
| 24:2:65:MET:HE2   | 24:2:147:HIS:HB3  | 1.96                     | 0.48              |
| 24:2:74:PRO:HB2   | 24:2:94:ASN:ND2   | 2.29                     | 0.48              |
| 1:A:17:PHE:O      | 1:A:18:CYS:C      | 2.54                     | 0.48              |
| 2:b:4:PRO:HB3     | 36:b:522:LHG:HC31 | 1.95                     | 0.48              |
| 4:d:286:ILE:HD13  | 4:d:289:LEU:HD12  | 1.95                     | 0.48              |
| 6:f:42:PHE:O      | 6:f:43:ILE:C      | 2.57                     | 0.48              |
| 19:w:104:ALA:O    | 19:w:108:MET:HG3  | 2.14                     | 0.48              |
| 26:P:66:ALA:HA    | 28:8:140:LEU:HA   | 1.96                     | 0.48              |
| 44:8:303:DD6:C9   | 31:8:305:CLA:HMC2 | 2.44                     | 0.48              |
| 31:A:403:CLA:H203 | 36:D:407:LHG:H161 | 1.96                     | 0.48              |
| 3:C:55:ALA:HB1    | 33:C:517:BCR:H373 | 1.94                     | 0.48              |
| 22:Z:33:TRP:O     | 22:Z:34:GLU:C     | 2.56                     | 0.48              |
| 18:v:76:ILE:HD11  | 41:v:201:HEM:CMB  | 2.44                     | 0.48              |
| 23:5:85:GLY:O     | 23:5:89:PRO:HD2   | 2.13                     | 0.48              |
| 24:7:80:GLY:HA2   | 24:7:90:TYR:CE2   | 2.49                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:6:43:ILE:HD12  | 25:6:155:LEU:HD21 | 1.96                     | 0.48              |
| 24:2:104:ALA:HB3  | 25:1:112:ILE:O    | 2.13                     | 0.48              |
| 31:2:309:CLA:HMB3 | 31:2:309:CLA:HBB1 | 1.96                     | 0.48              |
| 18:V:76:ILE:HD11  | 41:V:201:HEM:CMB  | 2.44                     | 0.48              |
| 44:6:204:DD6:C10  | 31:6:211:CLA:H52  | 2.43                     | 0.48              |
| 24:2:102:ILE:HB   | 24:2:107:TRP:NE1  | 2.28                     | 0.48              |
| 32:A:405:PHO:NC   | 4:D:209:LEU:HD13  | 2.29                     | 0.48              |
| 1:a:84:PRO:HD3    | 1:a:173:PRO:HB3   | 1.96                     | 0.48              |
| 3:c:307:PRO:HB2   | 3:c:361:LEU:HD12  | 1.95                     | 0.48              |
| 14:o:230:GLY:HA2  | 14:o:290:GLU:HA   | 1.96                     | 0.48              |
| 26:p:66:ALA:HA    | 28:3:140:LEU:HA   | 1.95                     | 0.48              |
| 31:p:604:CLA:HMB3 | 44:p:611:DD6:C37  | 2.37                     | 0.48              |
| 37:D:409:LMG:HC3  | 37:D:410:LMG:HC2  | 1.96                     | 0.47              |
| 4:d:85:VAL:HG11   | 4:d:90:LEU:HD21   | 1.96                     | 0.47              |
| 15:q:76:TYR:CG    | 15:q:77:SER:N     | 2.81                     | 0.47              |
| 15:q:170:LYS:NZ   | 15:q:207:PHE:HD1  | 2.12                     | 0.47              |
| 19:w:108:MET:O    | 19:w:111:PRO:HD2  | 2.14                     | 0.47              |
| 24:7:78:ARG:HB3   | 24:7:89:THR:O     | 2.12                     | 0.47              |
| 25:6:78:GLN:HB3   | 44:6:204:DD6:C3   | 2.43                     | 0.47              |
| 24:2:80:GLY:HA2   | 24:2:90:TYR:CE2   | 2.49                     | 0.47              |
| 36:B:521:LHG:O4   | 36:D:407:LHG:O1   | 2.31                     | 0.47              |
| 3:C:205:ASN:HB3   | 3:C:208:VAL:HG12  | 1.96                     | 0.47              |
| 1:a:131:TRP:HZ2   | 3:c:449:ARG:CD    | 2.25                     | 0.47              |
| 3:c:205:ASN:HB3   | 3:c:208:VAL:HG12  | 1.96                     | 0.47              |
| 39:c:519:DGD:C5A  | 39:c:520:DGD:HB42 | 2.44                     | 0.47              |
| 5:e:73:LYS:O      | 5:e:77:GLU:HG3    | 2.15                     | 0.47              |
| 34:0:316:SQD:O4   | 25:1:184:PHE:O    | 2.30                     | 0.47              |
| 31:2:309:CLA:H12  | 31:1:201:CLA:HMD2 | 1.95                     | 0.47              |
| 1:A:78:ILE:HD13   | 11:L:34:SER:OG    | 2.15                     | 0.47              |
| 2:B:4:PRO:HB3     | 36:B:521:LHG:HC31 | 1.95                     | 0.47              |
| 2:B:327:ALA:HB1   | 37:M:101:LMG:HC8  | 1.96                     | 0.47              |
| 4:D:184:PHE:HD2   | 4:D:185:LEU:HD12  | 1.79                     | 0.47              |
| 4:D:286:ILE:HD13  | 4:D:289:LEU:HD12  | 1.95                     | 0.47              |
| 7:H:78:ILE:HD13   | 7:H:78:ILE:HA     | 1.72                     | 0.47              |
| 1:a:310:GLN:HG3   | 18:v:2:ASP:O      | 2.14                     | 0.47              |
| 2:b:327:ALA:HB1   | 37:m:101:LMG:HC8  | 1.96                     | 0.47              |
| 3:c:154:LYS:HB3   | 3:c:256:PRO:HG2   | 1.95                     | 0.47              |
| 14:o:224:LYS:O    | 14:o:225:PRO:C    | 2.57                     | 0.47              |
| 15:q:138:LYS:NZ   | 15:q:140:TRP:HZ2  | 2.12                     | 0.47              |
| 28:3:87:ARG:NH1   | 28:3:99:THR:O     | 2.47                     | 0.47              |
| 28:3:114:PHE:O    | 28:3:118:VAL:HG23 | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:131:TRP:HZ2   | 3:C:449:ARG:CD    | 2.25                     | 0.47              |
| 14:O:230:GLY:HA2  | 14:O:290:GLU:HA   | 1.96                     | 0.47              |
| 15:Q:170:LYS:NZ   | 15:Q:207:PHE:HD1  | 2.12                     | 0.47              |
| 3:c:195:ASP:HB2   | 15:q:155:ARG:HD3  | 1.96                     | 0.47              |
| 37:d:409:LMG:HC3  | 37:d:410:LMG:HC2  | 1.95                     | 0.47              |
| 5:e:23:HIS:NE2    | 41:f:101:HEM:ND   | 2.62                     | 0.47              |
| 24:7:92:ILE:HG13  | 31:7:307:CLA:HED3 | 1.96                     | 0.47              |
| 34:0:316:SQD:H45  | 34:0:316:SQD:H1   | 1.72                     | 0.47              |
| 14:O:224:LYS:O    | 14:O:225:PRO:C    | 2.57                     | 0.47              |
| 44:3:303:DD6:C9   | 31:3:305:CLA:HMC2 | 2.44                     | 0.47              |
| 25:1:165:MET:CE   | 31:1:206:CLA:HHC  | 2.44                     | 0.47              |
| 1:A:271:LEU:HD11  | 35:A:410:PL9:HC8  | 1.95                     | 0.47              |
| 2:B:366:PHE:O     | 2:B:425:GLN:NE2   | 2.45                     | 0.47              |
| 31:B:508:CLA:H172 | 31:B:509:CLA:H192 | 1.95                     | 0.47              |
| 3:C:175:LEU:HD23  | 3:C:237:HIS:CD2   | 2.50                     | 0.47              |
| 39:C:520:DGD:HAW2 | 39:C:520:DGD:HA82 | 1.94                     | 0.47              |
| 5:E:73:LYS:O      | 5:E:77:GLU:HG3    | 2.15                     | 0.47              |
| 15:Q:138:LYS:NZ   | 15:Q:140:TRP:HZ2  | 2.12                     | 0.47              |
| 31:5:304:CLA:HBC2 | 31:5:311:CLA:HBC1 | 1.96                     | 0.47              |
| 1:A:201:GLY:HA3   | 1:A:286:THR:OG1   | 2.15                     | 0.47              |
| 3:C:198:TYR:HB2   | 15:Q:176:ARG:HH12 | 1.79                     | 0.47              |
| 7:H:48:LEU:HD13   | 36:H:103:LHG:C16  | 2.44                     | 0.47              |
| 1:a:78:ILE:HD13   | 11:l:34:SER:OG    | 2.15                     | 0.47              |
| 1:a:97:TRP:CH2    | 8:i:8:VAL:HG11    | 2.49                     | 0.47              |
| 4:d:184:PHE:HD2   | 4:d:185:LEU:HD12  | 1.80                     | 0.47              |
| 8:i:9:TYR:OH      | 19:w:99:PRO:HG2   | 2.15                     | 0.47              |
| 14:o:92:LYS:HA    | 14:o:95:ILE:HG22  | 1.97                     | 0.47              |
| 14:o:312:LEU:HD23 | 14:o:313:SER:O    | 2.15                     | 0.47              |
| 18:v:14:ASN:O     | 18:v:15:ALA:C     | 2.58                     | 0.47              |
| 24:7:102:ILE:HD11 | 31:7:307:CLA:HAA2 | 1.96                     | 0.47              |
| 31:1:210:CLA:HBA1 | 31:1:210:CLA:CHA  | 2.45                     | 0.47              |
| 4:D:85:VAL:HG11   | 4:D:90:LEU:HD21   | 1.96                     | 0.47              |
| 18:V:14:ASN:O     | 18:V:15:ALA:C     | 2.58                     | 0.47              |
| 19:W:108:MET:O    | 19:W:111:PRO:HD2  | 2.14                     | 0.47              |
| 22:Z:4:MET:O      | 22:Z:5:ILE:C      | 2.56                     | 0.47              |
| 15:q:70:ILE:O     | 15:q:71:GLY:C     | 2.57                     | 0.47              |
| 31:0:304:CLA:HBC2 | 31:0:311:CLA:HBC1 | 1.96                     | 0.47              |
| 3:C:195:ASP:HB2   | 15:Q:155:ARG:HD3  | 1.96                     | 0.47              |
| 14:O:312:LEU:HD23 | 14:O:313:SER:O    | 2.15                     | 0.47              |
| 37:D:409:LMG:O2   | 37:D:410:LMG:O10  | 2.29                     | 0.47              |
| 15:Q:207:PHE:O    | 15:Q:209:ALA:N    | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:h:78:ILE:HD13   | 7:h:78:ILE:HA     | 1.72                     | 0.47              |
| 25:6:171:LEU:HD23 | 25:6:171:LEU:HA   | 1.77                     | 0.47              |
| 42:6:202:A86:C21  | 31:6:214:CLA:H3A  | 2.45                     | 0.47              |
| 28:8:87:ARG:NH1   | 28:8:99:THR:O     | 2.47                     | 0.47              |
| 25:1:43:ILE:HD12  | 25:1:155:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:141:PRO:HG3   | 3:C:450:ALA:HB2   | 1.96                     | 0.46              |
| 3:C:75:PHE:HD1    | 3:C:86:PHE:HE2    | 1.63                     | 0.46              |
| 17:U:64:LYS:O     | 17:U:65:ILE:C     | 2.58                     | 0.46              |
| 31:Z:101:CLA:H3A  | 31:Z:101:CLA:HBA1 | 1.52                     | 0.46              |
| 12:m:17:LEU:HB2   | 12:m:18:PRO:HD3   | 1.97                     | 0.46              |
| 15:q:207:PHE:O    | 15:q:209:ALA:N    | 2.48                     | 0.46              |
| 31:7:309:CLA:HMB3 | 31:7:309:CLA:HBB1 | 1.95                     | 0.46              |
| 28:8:114:PHE:O    | 28:8:118:VAL:HG23 | 2.14                     | 0.46              |
| 24:2:45:ILE:HG22  | 24:2:49:LYS:HB2   | 1.97                     | 0.46              |
| 24:2:80:GLY:H     | 24:2:89:THR:HG23  | 1.80                     | 0.46              |
| 4:D:92:LEU:HD23   | 4:D:99:GLY:HA2    | 1.97                     | 0.46              |
| 31:a:403:CLA:H203 | 36:d:407:LHG:H161 | 1.96                     | 0.46              |
| 2:b:19:LEU:O      | 2:b:20:ILE:C      | 2.56                     | 0.46              |
| 3:c:165:LEU:HD23  | 3:c:248:GLY:N     | 2.30                     | 0.46              |
| 3:c:198:TYR:HB2   | 15:q:176:ARG:HH12 | 1.80                     | 0.46              |
| 24:2:92:ILE:HG13  | 31:2:307:CLA:HED3 | 1.96                     | 0.46              |
| 1:A:84:PRO:HD3    | 1:A:173:PRO:HB3   | 1.96                     | 0.46              |
| 39:C:519:DGD:C5A  | 39:C:520:DGD:HB42 | 2.44                     | 0.46              |
| 14:O:218:GLY:HA3  | 14:O:227:PHE:CZ   | 2.50                     | 0.46              |
| 4:d:291:LEU:HD21  | 39:h:102:DGD:HBN2 | 1.97                     | 0.46              |
| 4:d:304:ARG:NH1   | 4:d:308:ASP:HB3   | 2.31                     | 0.46              |
| 14:o:232:ASP:OD1  | 14:o:288:ARG:NH1  | 2.48                     | 0.46              |
| 15:q:86:GLN:HB3   | 15:q:87:ALA:H     | 1.44                     | 0.46              |
| 22:z:26:ALA:O     | 22:z:27:LEU:C     | 2.59                     | 0.46              |
| 4:D:291:LEU:HD21  | 39:H:102:DGD:HBN2 | 1.97                     | 0.46              |
| 1:a:281:VAL:O     | 1:a:285:ILE:HG12  | 2.16                     | 0.46              |
| 33:b:520:BCR:H403 | 33:b:520:BCR:H371 | 1.97                     | 0.46              |
| 3:c:175:LEU:HD23  | 3:c:237:HIS:CD2   | 2.50                     | 0.46              |
| 31:6:210:CLA:CHA  | 31:6:210:CLA:HBA1 | 2.45                     | 0.46              |
| 25:1:48:PHE:CZ    | 25:1:55:THR:HG21  | 2.50                     | 0.46              |
| 2:B:75:TRP:HD1    | 2:B:88:PRO:HG2    | 1.81                     | 0.46              |
| 7:H:61:TYR:HD2    | 39:H:102:DGD:C1B  | 2.28                     | 0.46              |
| 17:U:28:ILE:HG13  | 17:U:28:ILE:H     | 1.58                     | 0.46              |
| 1:a:201:GLY:HA3   | 1:a:286:THR:OG1   | 2.15                     | 0.46              |
| 2:b:75:TRP:HD1    | 2:b:88:PRO:HG2    | 1.80                     | 0.46              |
| 31:b:505:CLA:H192 | 31:b:505:CLA:H161 | 1.70                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:75:PHE:HD1    | 3:c:86:PHE:HE2    | 1.63                     | 0.46              |
| 24:7:45:ILE:HG22  | 24:7:49:LYS:HB2   | 1.97                     | 0.46              |
| 25:6:48:PHE:CZ    | 25:6:55:THR:HG21  | 2.50                     | 0.46              |
| 6:F:42:PHE:O      | 6:F:43:ILE:C      | 2.57                     | 0.46              |
| 14:O:92:LYS:HA    | 14:O:95:ILE:HG22  | 1.97                     | 0.46              |
| 18:V:16:GLY:O     | 18:V:17:ASN:C     | 2.58                     | 0.46              |
| 22:Z:4:MET:HB3    | 22:Z:4:MET:HE3    | 1.63                     | 0.46              |
| 17:u:91:ASP:N     | 17:u:91:ASP:OD1   | 2.48                     | 0.46              |
| 24:7:80:GLY:H     | 24:7:89:THR:HG23  | 1.81                     | 0.46              |
| 44:7:303:DD6:C8   | 31:7:306:CLA:HMC1 | 2.45                     | 0.46              |
| 42:1:202:A86:C21  | 31:1:214:CLA:H3A  | 2.45                     | 0.46              |
| 1:A:281:VAL:O     | 1:A:285:ILE:HG12  | 2.16                     | 0.46              |
| 9:J:31:GLY:C      | 9:J:33:TYR:N      | 2.68                     | 0.46              |
| 14:O:315:THR:OG1  | 14:O:320:LYS:O    | 2.29                     | 0.46              |
| 25:6:109:VAL:N    | 25:6:175:ASP:OD2  | 2.44                     | 0.46              |
| 14:O:232:ASP:OD1  | 14:O:288:ARG:NH1  | 2.48                     | 0.46              |
| 22:Z:56:THR:HG23  | 31:Z:101:CLA:CBB  | 2.46                     | 0.46              |
| 5:e:17:VAL:O      | 5:e:21:ILE:HG23   | 2.16                     | 0.46              |
| 6:f:44:GLN:HB2    | 15:q:80:ALA:CB    | 2.45                     | 0.46              |
| 14:o:218:GLY:HA3  | 14:o:227:PHE:CZ   | 2.50                     | 0.46              |
| 21:y:16:ARG:H     | 21:y:16:ARG:HG2   | 1.51                     | 0.46              |
| 31:2:309:CLA:H41  | 31:2:309:CLA:H62  | 1.71                     | 0.46              |
| 25:1:87:PRO:HA    | 25:1:90:PHE:O     | 2.16                     | 0.46              |
| 4:D:304:ARG:NH1   | 4:D:308:ASP:HB3   | 2.31                     | 0.46              |
| 22:Z:26:ALA:O     | 22:Z:27:LEU:C     | 2.59                     | 0.46              |
| 4:d:343:GLU:HG2   | 4:d:344:GLU:N     | 2.31                     | 0.46              |
| 22:z:56:THR:HG23  | 31:z:101:CLA:CBB  | 2.46                     | 0.46              |
| 34:0:316:SQD:H252 | 34:0:316:SQD:H82  | 1.98                     | 0.46              |
| 44:2:303:DD6:C8   | 31:2:306:CLA:HMC1 | 2.45                     | 0.46              |
| 39:C:519:DGD:HA51 | 39:C:520:DGD:HB42 | 1.98                     | 0.46              |
| 1:a:141:PRO:HG3   | 3:c:450:ALA:HB2   | 1.96                     | 0.46              |
| 14:o:269:GLU:CD   | 14:o:269:GLU:N    | 2.72                     | 0.46              |
| 15:q:127:ARG:HB3  | 15:q:146:GLU:OE2  | 2.16                     | 0.46              |
| 22:z:7:ALA:O      | 22:z:8:LEU:C      | 2.58                     | 0.46              |
| 23:5:69:ARG:NH1   | 23:5:72:GLU:OE1   | 2.49                     | 0.46              |
| 34:5:316:SQD:H252 | 34:5:316:SQD:H82  | 1.98                     | 0.46              |
| 24:2:102:ILE:HD11 | 31:2:307:CLA:HAA2 | 1.96                     | 0.46              |
| 3:C:165:LEU:HD23  | 3:C:248:GLY:N     | 2.31                     | 0.45              |
| 31:C:512:CLA:H101 | 33:C:517:BCR:H402 | 1.98                     | 0.45              |
| 3:c:307:PRO:HB3   | 3:c:358:PHE:CD1   | 2.51                     | 0.45              |
| 4:d:92:LEU:HD23   | 4:d:99:GLY:HA2    | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:0:69:ARG:NH1   | 23:0:72:GLU:OE1   | 2.49                     | 0.45              |
| 32:A:405:PHO:H141 | 31:D:401:CLA:HBB1 | 1.98                     | 0.45              |
| 31:B:504:CLA:H93  | 31:B:504:CLA:H61  | 1.72                     | 0.45              |
| 5:E:17:VAL:O      | 5:E:21:ILE:HG23   | 2.16                     | 0.45              |
| 12:M:17:LEU:HB2   | 12:M:18:PRO:HD3   | 1.97                     | 0.45              |
| 15:Q:70:ILE:O     | 15:Q:71:GLY:C     | 2.57                     | 0.45              |
| 36:b:522:LHG:HC11 | 11:l:13:LEU:HA    | 1.98                     | 0.45              |
| 4:d:51:GLY:HA3    | 4:d:78:VAL:HG22   | 1.98                     | 0.45              |
| 4:d:88:SER:HB2    | 5:e:69:ARG:NH2    | 2.32                     | 0.45              |
| 7:h:41:PRO:O      | 7:h:45:ILE:HG12   | 2.17                     | 0.45              |
| 19:w:107:ILE:O    | 19:w:111:PRO:HD3  | 2.16                     | 0.45              |
| 25:6:105:VAL:HG12 | 25:6:106:PRO:O    | 2.16                     | 0.45              |
| 1:A:137:LEU:HB2   | 1:A:139:MET:HE3   | 1.98                     | 0.45              |
| 4:D:88:SER:HB2    | 5:E:69:ARG:NH2    | 2.31                     | 0.45              |
| 4:D:297:ASP:HA    | 4:D:315:TYR:HH    | 1.81                     | 0.45              |
| 7:H:41:PRO:O      | 7:H:45:ILE:HG12   | 2.17                     | 0.45              |
| 3:c:55:ALA:HB1    | 33:c:517:BCR:C37  | 2.47                     | 0.45              |
| 7:h:61:TYR:HD2    | 39:h:102:DGD:C1B  | 2.28                     | 0.45              |
| 15:q:78:GLU:OE2   | 18:v:23:PRO:HB3   | 2.16                     | 0.45              |
| 15:q:95:SER:C     | 15:q:97:TYR:N     | 2.74                     | 0.45              |
| 34:A:411:SQD:H271 | 34:A:411:SQD:H242 | 1.85                     | 0.45              |
| 33:B:519:BCR:H403 | 33:B:519:BCR:H371 | 1.97                     | 0.45              |
| 14:O:269:GLU:CD   | 14:O:269:GLU:N    | 2.72                     | 0.45              |
| 15:Q:123:GLU:OE1  | 15:Q:127:ARG:NE   | 2.49                     | 0.45              |
| 18:V:13:ASP:C     | 18:V:68:ASN:HD22  | 2.25                     | 0.45              |
| 19:W:107:ILE:O    | 19:W:111:PRO:HD3  | 2.16                     | 0.45              |
| 3:c:177:ILE:HG23  | 31:3:313:CLA:HMB3 | 1.98                     | 0.45              |
| 23:5:199:ASP:O    | 23:5:200:SER:OG   | 2.24                     | 0.45              |
| 25:6:48:PHE:HZ    | 25:6:55:THR:HG21  | 1.82                     | 0.45              |
| 25:6:135:TRP:C    | 25:6:137:GLY:H    | 2.25                     | 0.45              |
| 23:0:45:LEU:HD21  | 23:0:166:VAL:HG11 | 1.99                     | 0.45              |
| 25:1:135:TRP:C    | 25:1:137:GLY:H    | 2.25                     | 0.45              |
| 1:A:132:GLU:O     | 1:A:136:ARG:HG2   | 2.16                     | 0.45              |
| 3:C:222:GLY:O     | 3:C:226:SER:OG    | 2.34                     | 0.45              |
| 3:C:307:PRO:HB3   | 3:C:358:PHE:CD1   | 2.51                     | 0.45              |
| 39:C:519:DGD:HAH1 | 39:C:520:DGD:HBW1 | 1.99                     | 0.45              |
| 39:H:102:DGD:HBF2 | 39:H:102:DGD:HBE2 | 1.75                     | 0.45              |
| 12:M:25:LEU:O     | 12:M:28:GLN:HG3   | 2.17                     | 0.45              |
| 15:Q:78:GLU:OE2   | 18:V:23:PRO:HB3   | 2.16                     | 0.45              |
| 18:V:29:GLY:O     | 18:V:30:LYS:C     | 2.60                     | 0.45              |
| 19:W:97:GLY:O     | 19:W:98:LYS:C     | 2.57                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:391:ARG:NH2   | 15:q:152:TYR:OH   | 2.50                     | 0.45              |
| 31:c:509:CLA:H72  | 10:k:46:PHE:CZ    | 2.45                     | 0.45              |
| 39:c:519:DGD:HA51 | 39:c:520:DGD:HB42 | 1.98                     | 0.45              |
| 14:o:182:ILE:HG12 | 14:o:221:ASP:HA   | 1.99                     | 0.45              |
| 17:u:64:LYS:O     | 17:u:65:ILE:C     | 2.58                     | 0.45              |
| 24:7:65:MET:HE3   | 24:7:148:GLY:HA2  | 1.97                     | 0.45              |
| 28:8:61:GLN:OE1   | 28:8:61:GLN:N     | 2.42                     | 0.45              |
| 28:8:167:GLU:HB2  | 31:8:311:CLA:C4B  | 2.47                     | 0.45              |
| 25:1:48:PHE:HZ    | 25:1:55:THR:HG21  | 1.82                     | 0.45              |
| 8:I:31:ASN:O      | 8:I:32:PRO:C      | 2.60                     | 0.45              |
| 15:Q:95:SER:C     | 15:Q:97:TYR:N     | 2.74                     | 0.45              |
| 37:Y:101:LMG:H111 | 37:Y:101:LMG:H141 | 1.43                     | 0.45              |
| 32:a:405:PHO:H141 | 31:d:401:CLA:HBB1 | 1.98                     | 0.45              |
| 31:b:507:CLA:H72  | 33:b:520:BCR:H311 | 1.99                     | 0.45              |
| 14:o:132:MET:HE3  | 14:o:291:MET:HE1  | 1.98                     | 0.45              |
| 15:q:95:SER:C     | 15:q:97:TYR:H     | 2.25                     | 0.45              |
| 37:y:101:LMG:H141 | 37:y:101:LMG:H111 | 1.43                     | 0.45              |
| 24:7:65:MET:HE3   | 24:7:148:GLY:CA   | 2.47                     | 0.45              |
| 24:2:65:MET:HE3   | 24:2:148:GLY:CA   | 2.47                     | 0.45              |
| 31:B:512:CLA:HBB1 | 31:B:512:CLA:HMB1 | 1.99                     | 0.45              |
| 3:C:55:ALA:HB1    | 33:C:517:BCR:C37  | 2.47                     | 0.45              |
| 14:O:183:THR:HG22 | 14:O:217:LYS:HD2  | 1.99                     | 0.45              |
| 1:a:137:LEU:HB2   | 1:a:139:MET:HE3   | 1.98                     | 0.45              |
| 7:h:45:ILE:HD13   | 36:h:103:LHG:H141 | 1.98                     | 0.45              |
| 23:5:46:PRO:O     | 23:5:47:PRO:C     | 2.60                     | 0.45              |
| 28:3:167:GLU:HB2  | 31:3:311:CLA:C4B  | 2.47                     | 0.45              |
| 24:2:131:PRO:HD2  | 31:2:310:CLA:HED3 | 1.98                     | 0.45              |
| 36:B:521:LHG:HC11 | 11:L:13:LEU:HA    | 1.98                     | 0.45              |
| 3:C:391:ARG:NH2   | 15:Q:152:TYR:OH   | 2.50                     | 0.45              |
| 8:I:2:LEU:HD11    | 19:W:102:ILE:HG21 | 1.99                     | 0.45              |
| 3:c:289:TYR:CE2   | 3:c:297:TYR:HE2   | 2.35                     | 0.45              |
| 3:c:315:PHE:CZ    | 3:c:384:ILE:HD11  | 2.52                     | 0.45              |
| 31:c:512:CLA:H101 | 33:c:517:BCR:H402 | 1.99                     | 0.45              |
| 17:u:61:ASP:O     | 17:u:64:LYS:HG2   | 2.17                     | 0.45              |
| 18:v:29:GLY:O     | 18:v:30:LYS:C     | 2.60                     | 0.45              |
| 18:v:133:GLY:O    | 18:v:134:LYS:C    | 2.60                     | 0.45              |
| 21:y:15:THR:OG1   | 21:y:18:LEU:HD23  | 2.16                     | 0.45              |
| 24:7:37:ASP:OD2   | 24:7:42:SER:OG    | 2.28                     | 0.45              |
| 24:7:105:LEU:HD13 | 25:6:112:ILE:HG21 | 1.99                     | 0.45              |
| 26:P:196:GLU:O    | 26:P:200:GLN:HG2  | 2.17                     | 0.45              |
| 24:2:65:MET:HE3   | 24:2:148:GLY:HA2  | 1.97                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:149:ALA:HB3   | 1:A:150:PRO:HD3   | 1.98                     | 0.45              |
| 31:B:506:CLA:H72  | 33:B:519:BCR:H311 | 1.99                     | 0.45              |
| 6:F:44:GLN:HB2    | 15:Q:80:ALA:CB    | 2.45                     | 0.45              |
| 1:a:312:ARG:HE    | 1:a:312:ARG:HB3   | 1.54                     | 0.45              |
| 25:6:165:MET:CE   | 31:6:206:CLA:HHC  | 2.44                     | 0.45              |
| 25:1:105:VAL:HG12 | 25:1:106:PRO:O    | 2.16                     | 0.45              |
| 4:D:343:GLU:HG2   | 4:D:344:GLU:N     | 2.31                     | 0.45              |
| 15:Q:95:SER:C     | 15:Q:97:TYR:H     | 2.25                     | 0.45              |
| 21:Y:15:THR:OG1   | 21:Y:18:LEU:HD23  | 2.16                     | 0.45              |
| 22:Z:9:THR:O      | 22:Z:12:PHE:N     | 2.50                     | 0.45              |
| 1:a:147:PHE:O     | 1:a:150:PRO:HD2   | 2.17                     | 0.45              |
| 2:b:297:SER:HB3   | 2:b:300:GLN:HG2   | 1.99                     | 0.45              |
| 3:c:277:ALA:HB2   | 3:c:441:HIS:CG    | 2.52                     | 0.45              |
| 6:f:44:GLN:CG     | 15:q:68:GLY:HA3   | 2.37                     | 0.45              |
| 14:o:228:GLN:NE2  | 14:o:292:GLU:OE1  | 2.50                     | 0.45              |
| 15:q:67:PHE:HD1   | 15:q:67:PHE:HA    | 1.66                     | 0.45              |
| 18:v:16:GLY:O     | 18:v:17:ASN:C     | 2.58                     | 0.45              |
| 23:5:45:LEU:HD21  | 23:5:166:VAL:HG11 | 1.99                     | 0.45              |
| 25:1:110:ALA:C    | 25:1:112:ILE:H    | 2.25                     | 0.45              |
| 1:A:41:LEU:HD23   | 1:A:41:LEU:HA     | 1.82                     | 0.44              |
| 37:J:101:LMG:H231 | 37:J:101:LMG:H261 | 1.34                     | 0.44              |
| 14:O:132:MET:HE3  | 14:O:291:MET:HE1  | 1.98                     | 0.44              |
| 15:Q:127:ARG:HB3  | 15:Q:146:GLU:OE2  | 2.17                     | 0.44              |
| 1:a:132:GLU:O     | 1:a:136:ARG:HG2   | 2.16                     | 0.44              |
| 39:c:519:DGD:HA41 | 39:c:519:DGD:HA72 | 1.54                     | 0.44              |
| 39:c:519:DGD:HAH1 | 39:c:520:DGD:HBW1 | 1.99                     | 0.44              |
| 8:i:31:ASN:O      | 8:i:32:PRO:C      | 2.60                     | 0.44              |
| 9:j:12:LEU:HD23   | 9:j:12:LEU:HA     | 1.74                     | 0.44              |
| 15:q:107:LYS:HG3  | 18:v:98:ALA:HB3   | 1.99                     | 0.44              |
| 18:v:75:TYR:CZ    | 41:v:201:HEM:HAA2 | 2.52                     | 0.44              |
| 24:7:131:PRO:HD2  | 31:7:310:CLA:HED3 | 1.98                     | 0.44              |
| 3:C:277:ALA:HB2   | 3:C:441:HIS:CG    | 2.52                     | 0.44              |
| 4:D:51:GLY:HA3    | 4:D:78:VAL:HG22   | 1.98                     | 0.44              |
| 37:j:101:LMG:H261 | 37:j:101:LMG:H231 | 1.34                     | 0.44              |
| 28:3:151:GLN:O    | 28:3:155:LEU:HG   | 2.18                     | 0.44              |
| 14:O:228:GLN:NE2  | 14:O:292:GLU:OE1  | 2.50                     | 0.44              |
| 31:c:509:CLA:HBB1 | 31:c:509:CLA:HMB3 | 1.99                     | 0.44              |
| 25:6:87:PRO:HA    | 25:6:90:PHE:O     | 2.16                     | 0.44              |
| 31:3:307:CLA:HBA2 | 31:3:307:CLA:H3A  | 1.68                     | 0.44              |
| 28:8:151:GLN:O    | 28:8:155:LEU:HG   | 2.18                     | 0.44              |
| 23:0:52:ASP:OD1   | 31:0:305:CLA:HBA2 | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:147:PHE:O     | 1:A:150:PRO:HD2   | 2.17                     | 0.44              |
| 32:A:405:PHO:H141 | 32:A:405:PHO:H161 | 1.73                     | 0.44              |
| 3:C:315:PHE:CZ    | 3:C:384:ILE:HD11  | 2.52                     | 0.44              |
| 33:D:405:BCR:H15C | 33:D:405:BCR:H351 | 1.90                     | 0.44              |
| 37:J:101:LMG:H172 | 37:J:101:LMG:H201 | 1.21                     | 0.44              |
| 18:V:75:TYR:CZ    | 41:V:201:HEM:HAA2 | 2.52                     | 0.44              |
| 22:Z:7:ALA:O      | 22:Z:8:LEU:C      | 2.58                     | 0.44              |
| 3:c:116:VAL:O     | 3:c:120:ILE:HG12  | 2.18                     | 0.44              |
| 19:w:95:ALA:O     | 19:w:96:ASN:HB2   | 2.16                     | 0.44              |
| 31:7:309:CLA:H62  | 31:7:309:CLA:H41  | 1.71                     | 0.44              |
| 26:p:196:GLU:O    | 26:p:200:GLN:HG2  | 2.17                     | 0.44              |
| 24:2:49:LYS:O     | 24:2:52:GLU:N     | 2.51                     | 0.44              |
| 31:B:506:CLA:H72  | 31:B:506:CLA:H112 | 1.68                     | 0.44              |
| 14:O:182:ILE:HG12 | 14:O:221:ASP:HA   | 1.99                     | 0.44              |
| 15:Q:107:LYS:HG3  | 18:V:98:ALA:CB    | 2.48                     | 0.44              |
| 18:V:133:GLY:O    | 18:V:134:LYS:C    | 2.60                     | 0.44              |
| 33:c:515:BCR:H15C | 33:c:515:BCR:H351 | 1.86                     | 0.44              |
| 39:c:519:DGD:O5E  | 39:c:519:DGD:O4E  | 2.30                     | 0.44              |
| 28:3:61:GLN:OE1   | 28:3:61:GLN:N     | 2.42                     | 0.44              |
| 7:H:41:PRO:HB2    | 31:0:314:CLA:CMD  | 2.46                     | 0.44              |
| 10:K:37:VAL:O     | 10:K:40:VAL:HG12  | 2.18                     | 0.44              |
| 1:a:149:ALA:HB3   | 1:a:150:PRO:HD3   | 1.98                     | 0.44              |
| 33:b:518:BCR:H351 | 33:b:518:BCR:H15C | 1.86                     | 0.44              |
| 31:c:510:CLA:H141 | 31:c:510:CLA:H161 | 1.83                     | 0.44              |
| 18:v:13:ASP:C     | 18:v:68:ASN:HD22  | 2.25                     | 0.44              |
| 31:z:101:CLA:HBA1 | 31:z:101:CLA:H3A  | 1.52                     | 0.44              |
| 23:5:52:ASP:OD1   | 31:5:305:CLA:HBA2 | 2.17                     | 0.44              |
| 31:5:308:CLA:H51  | 31:5:308:CLA:H12  | 1.79                     | 0.44              |
| 25:6:196:PHE:C    | 25:6:198:TYR:H    | 2.25                     | 0.44              |
| 25:1:196:PHE:C    | 25:1:198:TYR:H    | 2.25                     | 0.44              |
| 2:B:330:MET:HE3   | 2:B:446:SER:HA    | 2.00                     | 0.44              |
| 33:B:517:BCR:H24C | 33:B:517:BCR:H371 | 1.80                     | 0.44              |
| 3:C:289:TYR:CE2   | 3:C:297:TYR:HE2   | 2.35                     | 0.44              |
| 15:Q:107:LYS:HG3  | 18:V:98:ALA:HB3   | 1.99                     | 0.44              |
| 31:b:515:CLA:H91  | 31:b:515:CLA:H111 | 1.63                     | 0.44              |
| 36:b:522:LHG:O2   | 11:l:14:ASN:OD1   | 2.34                     | 0.44              |
| 37:d:409:LMG:O2   | 37:d:410:LMG:O10  | 2.29                     | 0.44              |
| 14:o:183:THR:HG22 | 14:o:217:LYS:HD2  | 1.99                     | 0.44              |
| 15:q:76:TYR:O     | 15:q:77:SER:HB3   | 2.17                     | 0.44              |
| 22:z:9:THR:O      | 22:z:12:PHE:N     | 2.50                     | 0.44              |
| 31:0:305:CLA:CGA  | 31:0:305:CLA:H3A  | 2.48                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:2:37:ASP:OD2   | 31:2:306:CLA:HBA2 | 2.18                     | 0.44              |
| 24:2:105:LEU:HD13 | 25:1:112:ILE:HG21 | 1.99                     | 0.44              |
| 3:C:341:LEU:HD12  | 3:C:349:ILE:HG22  | 2.00                     | 0.44              |
| 12:M:20:LEU:HD12  | 12:m:20:LEU:HD12  | 1.99                     | 0.44              |
| 14:O:191:ASP:O    | 14:O:210:THR:HA   | 2.18                     | 0.44              |
| 12:m:25:LEU:O     | 12:m:28:GLN:HG3   | 2.17                     | 0.44              |
| 17:u:64:LYS:HE2   | 17:u:64:LYS:HB3   | 1.84                     | 0.44              |
| 27:9:74:UNK:O     | 27:9:76:UNK:N     | 2.51                     | 0.44              |
| 24:2:60:HIS:HB3   | 24:2:152:MET:HE2  | 1.99                     | 0.44              |
| 25:1:109:VAL:N    | 25:1:175:ASP:OD2  | 2.44                     | 0.44              |
| 2:B:297:SER:HB3   | 2:B:300:GLN:HG2   | 1.99                     | 0.44              |
| 31:C:511:CLA:HMA1 | 31:C:511:CLA:H2   | 2.00                     | 0.44              |
| 4:D:235:PHE:CD1   | 4:D:243:THR:HG21  | 2.52                     | 0.44              |
| 20:X:108:ILE:HG23 | 20:X:109:SER:N    | 2.33                     | 0.44              |
| 31:b:507:CLA:H72  | 31:b:507:CLA:H112 | 1.68                     | 0.44              |
| 33:c:517:BCR:H371 | 33:c:517:BCR:H24C | 1.81                     | 0.44              |
| 4:d:89:LEU:HG     | 7:h:62:ASN:ND2    | 2.33                     | 0.44              |
| 18:v:104:MET:HE2  | 18:v:104:MET:HB2  | 1.89                     | 0.44              |
| 22:z:5:ILE:HG23   | 22:z:6:THR:H      | 1.83                     | 0.44              |
| 31:5:305:CLA:H3A  | 31:5:305:CLA:CGA  | 2.48                     | 0.44              |
| 24:7:112:PHE:HA   | 31:7:309:CLA:HBB2 | 1.99                     | 0.44              |
| 31:2:309:CLA:CGA  | 25:1:132:VAL:HG11 | 2.48                     | 0.44              |
| 1:A:92:HIS:NE2    | 3:C:360:ASP:OD2   | 2.52                     | 0.43              |
| 3:C:205:ASN:HD22  | 26:P:237:PRO:HG3  | 1.83                     | 0.43              |
| 2:b:366:PHE:O     | 2:b:425:GLN:NE2   | 2.45                     | 0.43              |
| 3:c:341:LEU:HD12  | 3:c:349:ILE:HG22  | 2.00                     | 0.43              |
| 8:i:2:LEU:HD11    | 19:w:102:ILE:HG21 | 1.99                     | 0.43              |
| 14:o:271:ASP:OD1  | 14:o:271:ASP:N    | 2.50                     | 0.43              |
| 31:6:211:CLA:H92  | 31:6:211:CLA:H61  | 1.69                     | 0.43              |
| 31:B:511:CLA:H112 | 31:B:511:CLA:H72  | 1.75                     | 0.43              |
| 3:C:116:VAL:O     | 3:C:120:ILE:HG12  | 2.18                     | 0.43              |
| 31:D:404:CLA:H61  | 31:D:404:CLA:H41  | 1.79                     | 0.43              |
| 17:U:61:ASP:O     | 17:U:64:LYS:HG2   | 2.17                     | 0.43              |
| 22:Z:5:ILE:HG23   | 22:Z:6:THR:H      | 1.83                     | 0.43              |
| 2:b:330:MET:HE3   | 2:b:446:SER:HA    | 2.00                     | 0.43              |
| 15:q:170:LYS:HE3  | 15:q:170:LYS:HB3  | 1.69                     | 0.43              |
| 17:u:28:ILE:HG13  | 17:u:28:ILE:H     | 1.58                     | 0.43              |
| 24:7:37:ASP:OD2   | 31:7:306:CLA:HBA2 | 2.18                     | 0.43              |
| 25:6:138:ASN:O    | 25:6:138:ASN:ND2  | 2.51                     | 0.43              |
| 28:8:194:LEU:HD21 | 31:8:314:CLA:HMD2 | 2.00                     | 0.43              |
| 23:0:46:PRO:O     | 23:0:47:PRO:C     | 2.60                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:A:411:SQD:H322 | 34:A:411:SQD:H291 | 1.70                     | 0.43              |
| 31:B:513:CLA:HMB3 | 31:B:513:CLA:HBB1 | 1.99                     | 0.43              |
| 31:C:509:CLA:HBB1 | 31:C:509:CLA:HMB3 | 1.99                     | 0.43              |
| 4:D:36:LEU:HD23   | 4:D:36:LEU:H      | 1.83                     | 0.43              |
| 35:D:406:PL9:H401 | 36:D:407:LHG:H212 | 1.99                     | 0.43              |
| 31:b:515:CLA:O1D  | 31:b:515:CLA:H2A  | 2.19                     | 0.43              |
| 36:b:522:LHG:O4   | 36:d:407:LHG:O1   | 2.31                     | 0.43              |
| 24:7:157:GLU:HB2  | 31:7:312:CLA:C4B  | 2.49                     | 0.43              |
| 27:4:74:UNK:O     | 27:4:76:UNK:N     | 2.51                     | 0.43              |
| 24:2:112:PHE:HA   | 31:2:309:CLA:HBB2 | 1.99                     | 0.43              |
| 9:J:31:GLY:O      | 9:J:32:SER:C      | 2.61                     | 0.43              |
| 39:c:518:DGD:O5E  | 39:c:518:DGD:O4E  | 2.24                     | 0.43              |
| 4:d:235:PHE:CD1   | 4:d:243:THR:HG21  | 2.52                     | 0.43              |
| 9:j:31:GLY:O      | 9:j:32:SER:C      | 2.61                     | 0.43              |
| 37:5:315:LMG:O5   | 37:5:315:LMG:O4   | 2.35                     | 0.43              |
| 24:7:49:LYS:O     | 24:7:52:GLU:N     | 2.50                     | 0.43              |
| 31:0:307:CLA:H3A  | 31:0:307:CLA:HBA2 | 1.47                     | 0.43              |
| 37:0:315:LMG:O5   | 37:0:315:LMG:O4   | 2.35                     | 0.43              |
| 25:1:124:ILE:O    | 31:1:210:CLA:HAB  | 2.18                     | 0.43              |
| 9:J:34:SER:OG     | 15:Q:81:ALA:HA    | 2.18                     | 0.43              |
| 14:O:184:PHE:H    | 14:O:216:ALA:HB3  | 1.84                     | 0.43              |
| 17:U:91:ASP:N     | 17:U:91:ASP:OD1   | 2.48                     | 0.43              |
| 31:Z:101:CLA:HMA2 | 31:Z:101:CLA:H2   | 2.01                     | 0.43              |
| 3:c:211:GLY:O     | 3:c:215:ARG:HB3   | 2.18                     | 0.43              |
| 10:k:37:VAL:O     | 10:k:40:VAL:HG12  | 2.18                     | 0.43              |
| 10:k:47:LEU:HB2   | 33:k:101:BCR:H19C | 2.00                     | 0.43              |
| 15:q:123:GLU:OE1  | 15:q:127:ARG:NE   | 2.49                     | 0.43              |
| 23:5:91:LYS:HE2   | 34:5:316:SQD:H442 | 2.00                     | 0.43              |
| 24:7:60:HIS:HB3   | 24:7:152:MET:HE2  | 1.99                     | 0.43              |
| 25:6:110:ALA:C    | 25:6:112:ILE:H    | 2.26                     | 0.43              |
| 28:3:167:GLU:CD   | 28:3:170:ARG:HH21 | 2.27                     | 0.43              |
| 31:1:210:CLA:H62  | 31:1:210:CLA:H41  | 1.70                     | 0.43              |
| 34:B:522:SQD:H271 | 34:B:522:SQD:H242 | 1.85                     | 0.43              |
| 35:D:406:PL9:H502 | 16:T:10:LEU:HD13  | 2.01                     | 0.43              |
| 10:K:47:LEU:HB2   | 33:K:101:BCR:H19C | 2.00                     | 0.43              |
| 14:O:92:LYS:HD3   | 14:O:95:ILE:CG2   | 2.48                     | 0.43              |
| 14:O:272:ALA:C    | 14:O:274:LEU:N    | 2.76                     | 0.43              |
| 3:c:225:VAL:O     | 3:c:293:ASN:ND2   | 2.49                     | 0.43              |
| 4:d:165:ALA:HB3   | 4:d:169:PHE:HE2   | 1.84                     | 0.43              |
| 31:7:309:CLA:CGA  | 25:6:132:VAL:HG11 | 2.48                     | 0.43              |
| 26:p:43:SER:HB3   | 26:p:47:THR:HG21  | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:8:167:GLU:CD   | 28:8:170:ARG:HH21 | 2.27                     | 0.43              |
| 24:2:60:HIS:HB2   | 24:2:152:MET:HE2  | 2.01                     | 0.43              |
| 31:B:504:CLA:H192 | 31:B:504:CLA:H161 | 1.70                     | 0.43              |
| 3:C:211:GLY:O     | 3:C:215:ARG:HB3   | 2.18                     | 0.43              |
| 19:W:108:MET:HE2  | 19:W:108:MET:HB2  | 1.91                     | 0.43              |
| 21:Y:16:ARG:H     | 21:Y:16:ARG:HG2   | 1.51                     | 0.43              |
| 33:a:408:BCR:H20C | 33:a:408:BCR:H361 | 1.79                     | 0.43              |
| 31:b:514:CLA:H72  | 31:b:514:CLA:H112 | 1.90                     | 0.43              |
| 33:b:520:BCR:H11C | 33:b:520:BCR:H341 | 1.87                     | 0.43              |
| 31:c:511:CLA:HMA1 | 31:c:511:CLA:H2   | 2.00                     | 0.43              |
| 24:7:158:LEU:HG   | 44:7:304:DD6:C37  | 2.49                     | 0.43              |
| 25:6:124:ILE:O    | 31:6:210:CLA:HAB  | 2.18                     | 0.43              |
| 2:B:413:ASP:CG    | 2:B:415:PRO:HD2   | 2.44                     | 0.43              |
| 3:C:459:ILE:HG21  | 3:C:464:GLU:HG3   | 2.01                     | 0.43              |
| 31:5:307:CLA:HBA2 | 31:5:307:CLA:H3A  | 1.47                     | 0.43              |
| 25:6:109:VAL:C    | 25:6:110:ALA:O    | 2.62                     | 0.43              |
| 26:P:142:LEU:O    | 26:P:146:GLN:HG2  | 2.19                     | 0.43              |
| 24:2:177:MET:HE2  | 24:2:177:MET:HB2  | 1.93                     | 0.43              |
| 4:D:165:ALA:HB3   | 4:D:169:PHE:HE2   | 1.84                     | 0.43              |
| 4:D:242:GLU:HG3   | 4:D:244:TYR:H     | 1.84                     | 0.43              |
| 37:J:101:LMG:H221 | 37:J:101:LMG:H192 | 1.51                     | 0.43              |
| 15:Q:76:TYR:O     | 15:Q:77:SER:HB3   | 2.17                     | 0.43              |
| 1:a:92:HIS:NE2    | 3:c:360:ASP:OD2   | 2.51                     | 0.43              |
| 35:d:406:PL9:H401 | 36:d:407:LHG:H212 | 1.99                     | 0.43              |
| 31:z:101:CLA:HMA2 | 31:z:101:CLA:H2   | 2.01                     | 0.43              |
| 23:5:94:TYR:CD2   | 23:5:194:LEU:HD23 | 2.53                     | 0.43              |
| 28:3:194:LEU:HD21 | 31:3:314:CLA:HMD2 | 2.00                     | 0.43              |
| 36:B:521:LHG:O2   | 11:L:14:ASN:OD1   | 2.34                     | 0.43              |
| 1:a:329:GLU:HG2   | 4:d:352:LEU:HD21  | 2.00                     | 0.43              |
| 3:c:230:MET:O     | 3:c:234:ILE:HG12  | 2.19                     | 0.43              |
| 4:d:36:LEU:HD23   | 4:d:36:LEU:H      | 1.83                     | 0.43              |
| 18:v:41:HIS:HA    | 18:v:45:ILE:O     | 2.19                     | 0.43              |
| 24:7:88:SER:C     | 24:7:90:TYR:H     | 2.27                     | 0.43              |
| 26:P:43:SER:HB3   | 26:P:47:THR:HG21  | 2.01                     | 0.43              |
| 31:B:510:CLA:H161 | 31:B:510:CLA:H202 | 1.69                     | 0.42              |
| 31:B:514:CLA:O1D  | 31:B:514:CLA:H2A  | 2.19                     | 0.42              |
| 31:B:516:CLA:H12  | 31:B:516:CLA:H51  | 1.77                     | 0.42              |
| 6:F:44:GLN:CG     | 15:Q:68:GLY:HA3   | 2.37                     | 0.42              |
| 2:b:231:MET:HG2   | 31:b:511:CLA:HAC1 | 2.01                     | 0.42              |
| 8:i:10:THR:O      | 8:i:11:THR:C      | 2.61                     | 0.42              |
| 9:j:34:SER:OG     | 15:q:81:ALA:HA    | 2.18                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:o:191:ASP:O    | 14:o:210:THR:HA   | 2.18                     | 0.42              |
| 2:B:256:MET:HG2   | 2:B:448:ARG:HG3   | 2.02                     | 0.42              |
| 7:H:52:ILE:HD12   | 20:X:91:LEU:HD13  | 2.01                     | 0.42              |
| 14:O:124:LYS:HB3  | 14:O:124:LYS:HE3  | 1.86                     | 0.42              |
| 14:O:256:ASP:OD1  | 14:O:256:ASP:N    | 2.51                     | 0.42              |
| 3:c:188:THR:CG2   | 3:c:298:PRO:HB3   | 2.49                     | 0.42              |
| 7:h:52:ILE:HD12   | 20:x:91:LEU:HD13  | 2.01                     | 0.42              |
| 24:2:158:LEU:HG   | 44:2:304:DD6:C37  | 2.49                     | 0.42              |
| 25:1:109:VAL:C    | 25:1:110:ALA:O    | 2.62                     | 0.42              |
| 25:1:138:ASN:O    | 25:1:138:ASN:ND2  | 2.51                     | 0.42              |
| 2:B:90:ILE:HG12   | 2:B:90:ILE:O      | 2.18                     | 0.42              |
| 31:C:510:CLA:H141 | 31:C:510:CLA:H161 | 1.83                     | 0.42              |
| 37:C:521:LMG:H241 | 37:C:521:LMG:H211 | 1.71                     | 0.42              |
| 37:C:521:LMG:H381 | 37:C:521:LMG:H412 | 1.41                     | 0.42              |
| 5:E:27:ILE:HB     | 5:E:28:PRO:HD3    | 2.02                     | 0.42              |
| 9:J:12:LEU:HD23   | 9:J:12:LEU:HA     | 1.74                     | 0.42              |
| 22:Z:5:ILE:O      | 22:Z:6:THR:C      | 2.61                     | 0.42              |
| 7:h:73:ASP:OD1    | 39:h:102:DGD:O4E  | 2.36                     | 0.42              |
| 39:h:102:DGD:HBF2 | 39:h:102:DGD:HBE2 | 1.75                     | 0.42              |
| 14:o:92:LYS:HD3   | 14:o:95:ILE:CG2   | 2.48                     | 0.42              |
| 20:x:108:ILE:HG23 | 20:x:109:SER:N    | 2.33                     | 0.42              |
| 24:7:92:ILE:HG22  | 24:7:101:TYR:CD2  | 2.54                     | 0.42              |
| 28:3:106:VAL:HG13 | 28:3:172:ASP:OD2  | 2.18                     | 0.42              |
| 24:2:88:SER:C     | 24:2:90:TYR:H     | 2.28                     | 0.42              |
| 24:2:92:ILE:HG22  | 24:2:101:TYR:CD2  | 2.54                     | 0.42              |
| 25:1:69:ALA:HB2   | 31:1:210:CLA:HED3 | 2.02                     | 0.42              |
| 44:1:203:DD6:C9   | 31:1:206:CLA:HMC1 | 2.49                     | 0.42              |
| 1:A:103:ASP:C     | 14:O:161:MET:HE1  | 2.45                     | 0.42              |
| 1:A:104:GLU:OE2   | 14:O:163:ARG:HG2  | 2.19                     | 0.42              |
| 2:B:231:MET:HG2   | 31:B:510:CLA:HAC1 | 2.01                     | 0.42              |
| 15:Q:82:TYR:O     | 15:Q:83:GLY:C     | 2.61                     | 0.42              |
| 31:d:404:CLA:H61  | 31:d:404:CLA:H41  | 1.79                     | 0.42              |
| 15:q:107:LYS:HG3  | 18:v:98:ALA:CB    | 2.48                     | 0.42              |
| 23:5:65:LEU:HA    | 23:5:65:LEU:HD12  | 1.79                     | 0.42              |
| 44:6:203:DD6:C9   | 31:6:206:CLA:HMC1 | 2.49                     | 0.42              |
| 28:3:169:ILE:HG13 | 31:3:312:CLA:HAC1 | 2.00                     | 0.42              |
| 23:0:94:TYR:CD2   | 23:0:194:LEU:HD23 | 2.53                     | 0.42              |
| 3:C:168:LEU:HD23  | 3:C:168:LEU:HA    | 1.90                     | 0.42              |
| 4:D:89:LEU:HG     | 7:H:62:ASN:ND2    | 2.33                     | 0.42              |
| 33:H:101:BCR:H24C | 33:H:101:BCR:H371 | 1.87                     | 0.42              |
| 15:Q:69:LEU:N     | 15:Q:74:THR:OG1   | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:Z:11:LEU:O     | 22:Z:12:PHE:C     | 2.62                     | 0.42              |
| 2:b:169:SER:OG    | 2:b:170:ASP:N     | 2.52                     | 0.42              |
| 31:c:512:CLA:H171 | 22:z:20:VAL:HG23  | 2.01                     | 0.42              |
| 35:d:406:PL9:H502 | 16:t:10:LEU:HD13  | 2.01                     | 0.42              |
| 14:o:184:PHE:H    | 14:o:216:ALA:HB3  | 1.84                     | 0.42              |
| 24:7:60:HIS:HB2   | 24:7:152:MET:HE2  | 2.01                     | 0.42              |
| 25:1:171:LEU:HA   | 25:1:171:LEU:HD23 | 1.77                     | 0.42              |
| 2:B:321:LYS:HA    | 2:B:321:LYS:HD3   | 1.90                     | 0.42              |
| 4:D:351:ALA:HB1   | 17:U:102:TYR:CE2  | 2.53                     | 0.42              |
| 14:O:124:LYS:HD2  | 14:O:125:PRO:O    | 2.20                     | 0.42              |
| 2:b:256:MET:HG2   | 2:b:448:ARG:HG3   | 2.02                     | 0.42              |
| 3:c:135:LEU:HD23  | 3:c:135:LEU:HA    | 1.85                     | 0.42              |
| 3:c:387:TRP:NE1   | 15:q:149:ARG:O    | 2.49                     | 0.42              |
| 26:p:142:LEU:O    | 26:p:146:GLN:HG2  | 2.19                     | 0.42              |
| 23:0:187:LEU:HD23 | 23:0:187:LEU:HA   | 1.88                     | 0.42              |
| 3:C:67:MET:HE1    | 31:C:505:CLA:CHD  | 2.49                     | 0.42              |
| 31:C:510:CLA:O1A  | 31:C:510:CLA:H2A  | 2.19                     | 0.42              |
| 21:Y:15:THR:C     | 21:Y:17:LEU:N     | 2.76                     | 0.42              |
| 1:a:103:ASP:C     | 14:o:161:MET:HE1  | 2.45                     | 0.42              |
| 36:a:411:LHG:H272 | 2:b:464:PHE:CE2   | 2.55                     | 0.42              |
| 3:c:165:LEU:HG    | 3:c:244:CYS:O     | 2.20                     | 0.42              |
| 14:o:124:LYS:HD2  | 14:o:125:PRO:O    | 2.19                     | 0.42              |
| 28:8:169:ILE:HG13 | 31:8:312:CLA:HAC1 | 2.01                     | 0.42              |
| 24:2:157:GLU:HB2  | 31:2:312:CLA:C4B  | 2.49                     | 0.42              |
| 34:A:409:SQD:H351 | 34:A:409:SQD:H322 | 1.84                     | 0.42              |
| 8:I:10:THR:O      | 8:I:11:THR:C      | 2.61                     | 0.42              |
| 31:b:505:CLA:H93  | 31:b:505:CLA:H61  | 1.72                     | 0.42              |
| 31:c:510:CLA:H2A  | 31:c:510:CLA:O1A  | 2.19                     | 0.42              |
| 37:c:521:LMG:H371 | 37:c:521:LMG:H341 | 1.61                     | 0.42              |
| 15:q:69:LEU:N     | 15:q:74:THR:OG1   | 2.53                     | 0.42              |
| 31:6:210:CLA:H41  | 31:6:210:CLA:H62  | 1.70                     | 0.42              |
| 28:8:106:VAL:O    | 28:8:107:ALA:C    | 2.63                     | 0.42              |
| 23:0:56:PHE:CD2   | 31:0:305:CLA:H42  | 2.55                     | 0.42              |
| 31:0:308:CLA:H51  | 31:0:308:CLA:H12  | 1.79                     | 0.42              |
| 3:C:165:LEU:HG    | 3:C:244:CYS:O     | 2.20                     | 0.42              |
| 3:C:188:THR:CG2   | 3:C:298:PRO:HB3   | 2.49                     | 0.42              |
| 3:C:230:MET:O     | 3:C:234:ILE:HG12  | 2.19                     | 0.42              |
| 33:D:405:BCR:H20C | 33:D:405:BCR:H361 | 1.87                     | 0.42              |
| 14:O:175:ILE:CG2  | 14:O:182:ILE:HG23 | 2.48                     | 0.42              |
| 18:V:41:HIS:HA    | 18:V:45:ILE:O     | 2.19                     | 0.42              |
| 1:a:104:GLU:OE2   | 14:o:163:ARG:HG2  | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:308:ASP:O     | 6:f:45:ARG:HD2    | 2.20                     | 0.42              |
| 31:b:511:CLA:H202 | 31:b:511:CLA:H161 | 1.69                     | 0.42              |
| 3:c:42:LEU:HD21   | 31:c:512:CLA:H2A  | 2.02                     | 0.42              |
| 31:c:508:CLA:H62  | 31:c:508:CLA:H41  | 1.84                     | 0.42              |
| 5:e:27:ILE:HB     | 5:e:28:PRO:HD3    | 2.02                     | 0.42              |
| 15:q:82:TYR:O     | 15:q:83:GLY:C     | 2.61                     | 0.42              |
| 37:y:101:LMG:H382 | 37:y:101:LMG:H412 | 1.77                     | 0.42              |
| 23:5:56:PHE:CD2   | 31:5:305:CLA:H42  | 2.55                     | 0.42              |
| 24:7:147:HIS:CD2  | 31:7:310:CLA:HBB2 | 2.55                     | 0.42              |
| 25:6:118:LEU:HB3  | 31:6:209:CLA:O1D  | 2.20                     | 0.42              |
| 28:8:106:VAL:HG13 | 28:8:172:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:308:ASP:O     | 6:F:45:ARG:HD2    | 2.20                     | 0.42              |
| 1:A:329:GLU:HG2   | 4:D:352:LEU:HD21  | 2.00                     | 0.42              |
| 3:C:42:LEU:HD21   | 31:C:512:CLA:H2A  | 2.02                     | 0.42              |
| 15:Q:123:GLU:HG3  | 15:Q:150:TYR:CE2  | 2.55                     | 0.42              |
| 15:Q:170:LYS:HE3  | 15:Q:170:LYS:HB3  | 1.69                     | 0.42              |
| 2:b:413:ASP:CG    | 2:b:415:PRO:HD2   | 2.44                     | 0.42              |
| 2:b:464:PHE:HE1   | 4:d:144:ILE:HG23  | 1.85                     | 0.42              |
| 3:c:459:ILE:HG21  | 3:c:464:GLU:HG3   | 2.01                     | 0.42              |
| 31:c:509:CLA:H142 | 31:c:511:CLA:H102 | 2.02                     | 0.42              |
| 15:q:123:GLU:HG3  | 15:q:150:TYR:CE2  | 2.55                     | 0.42              |
| 22:z:5:ILE:O      | 22:z:6:THR:C      | 2.61                     | 0.42              |
| 23:0:189:ASN:O    | 23:0:189:ASN:OD1  | 2.38                     | 0.42              |
| 25:1:118:LEU:HB3  | 31:1:209:CLA:O1D  | 2.20                     | 0.42              |
| 31:1:210:CLA:HED2 | 31:1:210:CLA:HBD  | 1.86                     | 0.42              |
| 1:A:217:SER:HA    | 4:D:272:LEU:HD12  | 2.02                     | 0.41              |
| 1:A:299:GLY:O     | 3:C:403:SER:HB2   | 2.20                     | 0.41              |
| 36:A:412:LHG:H272 | 2:B:464:PHE:CE2   | 2.55                     | 0.41              |
| 31:B:504:CLA:H12  | 31:B:505:CLA:ND   | 2.35                     | 0.41              |
| 31:B:513:CLA:H72  | 31:B:513:CLA:H112 | 1.90                     | 0.41              |
| 3:C:379:LYS:HD3   | 15:Q:149:ARG:HH22 | 1.85                     | 0.41              |
| 31:C:512:CLA:H171 | 22:Z:20:VAL:HG23  | 2.01                     | 0.41              |
| 33:C:516:BCR:H323 | 31:W:202:CLA:HBB2 | 2.02                     | 0.41              |
| 15:Q:67:PHE:O     | 15:Q:74:THR:HG21  | 2.18                     | 0.41              |
| 31:b:505:CLA:H12  | 31:b:506:CLA:ND   | 2.35                     | 0.41              |
| 33:c:516:BCR:H323 | 31:w:202:CLA:HBB2 | 2.02                     | 0.41              |
| 20:x:108:ILE:O    | 20:x:109:SER:C    | 2.63                     | 0.41              |
| 23:5:83:VAL:HG11  | 42:5:303:A86:C8   | 2.50                     | 0.41              |
| 28:3:106:VAL:O    | 28:3:107:ALA:C    | 2.63                     | 0.41              |
| 23:0:168:GLU:HB2  | 31:0:310:CLA:C1B  | 2.50                     | 0.41              |
| 25:1:79:LEU:HD23  | 25:1:79:LEU:HA    | 1.87                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:212:SER:HB2   | 4:D:211:CYS:HB2   | 2.02                     | 0.41              |
| 39:C:520:DGD:HB91 | 39:C:520:DGD:HB61 | 1.87                     | 0.41              |
| 4:D:17:LEU:HD11   | 20:X:110:LYS:HG3  | 2.02                     | 0.41              |
| 14:O:130:VAL:HG13 | 14:O:336:GLU:HG2  | 2.02                     | 0.41              |
| 2:b:188:ASP:OD1   | 2:b:188:ASP:N     | 2.53                     | 0.41              |
| 2:b:287:GLN:O     | 2:b:290:THR:HG22  | 2.21                     | 0.41              |
| 2:b:392:ILE:HG21  | 2:b:418:LYS:CG    | 2.50                     | 0.41              |
| 3:c:173:PHE:CE1   | 3:c:241:GLY:HA3   | 2.56                     | 0.41              |
| 25:6:69:ALA:HB2   | 31:6:210:CLA:HED3 | 2.02                     | 0.41              |
| 31:6:210:CLA:HED2 | 31:6:210:CLA:HBD  | 1.86                     | 0.41              |
| 24:2:36:PHE:HB3   | 31:2:306:CLA:C3D  | 2.50                     | 0.41              |
| 25:1:183:GLY:C    | 25:1:185:ASP:H    | 2.28                     | 0.41              |
| 2:B:464:PHE:HE1   | 4:D:144:ILE:HG23  | 1.85                     | 0.41              |
| 2:b:222:PRO:HG2   | 2:b:225:LEU:HB2   | 2.02                     | 0.41              |
| 31:b:503:CLA:HBB1 | 31:b:503:CLA:HMB3 | 2.01                     | 0.41              |
| 3:c:67:MET:HE1    | 31:c:505:CLA:CHD  | 2.50                     | 0.41              |
| 33:c:516:BCR:H20C | 33:c:516:BCR:H361 | 1.85                     | 0.41              |
| 4:d:17:LEU:HD11   | 20:x:110:LYS:HG3  | 2.03                     | 0.41              |
| 15:q:131:ILE:N    | 15:q:132:PRO:HD2  | 2.35                     | 0.41              |
| 18:v:5:GLU:OE2    | 18:v:20:VAL:HG21  | 2.21                     | 0.41              |
| 20:x:80:MET:HB3   | 23:5:98:PHE:O     | 2.20                     | 0.41              |
| 24:7:36:PHE:HB3   | 31:7:306:CLA:C3D  | 2.50                     | 0.41              |
| 24:7:84:ALA:HB1   | 24:7:85:PRO:CD    | 2.49                     | 0.41              |
| 28:3:107:ALA:O    | 28:3:108:ALA:C    | 2.63                     | 0.41              |
| 23:0:91:LYS:HE2   | 34:0:316:SQD:H442 | 2.00                     | 0.41              |
| 24:2:37:ASP:OD2   | 24:2:42:SER:OG    | 2.28                     | 0.41              |
| 1:A:222:SER:O     | 1:A:222:SER:OG    | 2.37                     | 0.41              |
| 1:A:273:PHE:HZ    | 36:A:413:LHG:H112 | 1.86                     | 0.41              |
| 2:B:287:GLN:O     | 2:B:290:THR:HG22  | 2.21                     | 0.41              |
| 31:B:502:CLA:HBB1 | 31:B:502:CLA:HMB3 | 2.01                     | 0.41              |
| 33:B:517:BCR:H351 | 33:B:517:BCR:H15C | 1.86                     | 0.41              |
| 31:C:509:CLA:H142 | 31:C:511:CLA:H102 | 2.02                     | 0.41              |
| 19:W:102:ILE:O    | 19:W:103:GLU:C    | 2.63                     | 0.41              |
| 1:a:299:GLY:O     | 3:c:403:SER:HB2   | 2.20                     | 0.41              |
| 2:b:90:ILE:O      | 2:b:90:ILE:HG12   | 2.18                     | 0.41              |
| 7:h:48:LEU:HD13   | 36:h:103:LHG:C16  | 2.50                     | 0.41              |
| 12:m:7:ALA:O      | 12:m:8:TYR:C      | 2.61                     | 0.41              |
| 14:o:289:ILE:HG13 | 14:o:309:ALA:HB2  | 2.03                     | 0.41              |
| 21:y:37:ARG:O     | 21:y:41:GLN:HG2   | 2.21                     | 0.41              |
| 25:6:183:GLY:C    | 25:6:185:ASP:H    | 2.28                     | 0.41              |
| 24:2:67:ALA:O     | 24:2:70:GLY:N     | 2.52                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:2:148:GLY:O    | 24:2:152:MET:HG3  | 2.21                     | 0.41              |
| 2:B:418:LYS:O     | 2:B:422:ARG:HG3   | 2.21                     | 0.41              |
| 6:F:45:ARG:NH2    | 15:Q:79:GLY:HA3   | 2.36                     | 0.41              |
| 15:Q:86:GLN:HB3   | 15:Q:87:ALA:H     | 1.44                     | 0.41              |
| 15:Q:88:ASP:C     | 15:Q:90:LEU:H     | 2.28                     | 0.41              |
| 1:a:273:PHE:HZ    | 36:a:412:LHG:H112 | 1.86                     | 0.41              |
| 31:b:512:CLA:H112 | 31:b:512:CLA:H72  | 1.75                     | 0.41              |
| 4:d:242:GLU:HG3   | 4:d:244:TYR:H     | 1.84                     | 0.41              |
| 15:q:88:ASP:C     | 15:q:90:LEU:H     | 2.28                     | 0.41              |
| 15:q:93:PRO:O     | 15:q:95:SER:N     | 2.53                     | 0.41              |
| 15:q:105:LEU:HB2  | 18:v:108:THR:HG22 | 2.02                     | 0.41              |
| 23:5:168:GLU:HB2  | 31:5:310:CLA:C1B  | 2.51                     | 0.41              |
| 24:7:30:ILE:HD12  | 24:7:146:GLN:CD   | 2.45                     | 0.41              |
| 24:7:95:GLY:O     | 24:7:97:ALA:N     | 2.46                     | 0.41              |
| 25:6:146:LEU:HD13 | 25:6:153:ARG:HG3  | 2.03                     | 0.41              |
| 31:p:603:CLA:CMC  | 44:p:611:DD6:C    | 2.97                     | 0.41              |
| 23:0:83:VAL:O     | 23:0:87:ILE:HG12  | 2.20                     | 0.41              |
| 1:A:193:LEU:HD11  | 31:A:403:CLA:HMC2 | 2.03                     | 0.41              |
| 2:B:188:ASP:OD1   | 2:B:188:ASP:N     | 2.53                     | 0.41              |
| 2:B:475:PHE:HB3   | 2:B:478:VAL:HG12  | 2.02                     | 0.41              |
| 31:B:516:CLA:O1D  | 31:B:516:CLA:HBA2 | 2.20                     | 0.41              |
| 3:C:173:PHE:CE1   | 3:C:241:GLY:HA3   | 2.55                     | 0.41              |
| 4:D:188:PHE:CZ    | 4:D:326:ARG:HG3   | 2.56                     | 0.41              |
| 31:D:404:CLA:H61  | 31:D:404:CLA:H92  | 1.83                     | 0.41              |
| 12:M:7:ALA:O      | 12:M:8:TYR:C      | 2.61                     | 0.41              |
| 21:Y:37:ARG:O     | 21:Y:41:GLN:HG2   | 2.21                     | 0.41              |
| 2:b:144:PHE:HE1   | 2:b:210:ILE:HG23  | 1.85                     | 0.41              |
| 19:w:114:TRP:O    | 19:w:118:MET:HG2  | 2.20                     | 0.41              |
| 23:5:83:VAL:O     | 23:5:87:ILE:HG12  | 2.20                     | 0.41              |
| 31:2:309:CLA:H111 | 31:2:309:CLA:H71  | 1.69                     | 0.41              |
| 33:A:408:BCR:H351 | 33:A:408:BCR:H15C | 1.92                     | 0.41              |
| 34:A:409:SQD:H222 | 34:A:409:SQD:H191 | 1.86                     | 0.41              |
| 36:A:412:LHG:O4   | 4:D:141:TYR:OH    | 2.24                     | 0.41              |
| 2:B:151:PHE:HB2   | 2:B:206:GLY:HA3   | 2.03                     | 0.41              |
| 2:B:256:MET:O     | 2:B:448:ARG:NH1   | 2.47                     | 0.41              |
| 31:B:504:CLA:H111 | 31:B:515:CLA:H42  | 2.03                     | 0.41              |
| 33:B:518:BCR:H24C | 33:B:518:BCR:H371 | 1.87                     | 0.41              |
| 7:H:73:ASP:OD1    | 39:H:102:DGD:O4E  | 2.36                     | 0.41              |
| 12:M:3:VAL:HG23   | 12:M:4:GLN:N      | 2.35                     | 0.41              |
| 14:O:118:GLU:HA   | 14:O:296:VAL:H    | 1.85                     | 0.41              |
| 15:Q:105:LEU:HB2  | 18:V:108:THR:HG22 | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:252:HIS:CD2   | 1:a:264:SER:HB2   | 2.56                     | 0.41              |
| 2:b:22:VAL:HG11   | 31:b:513:CLA:CAB  | 2.51                     | 0.41              |
| 31:b:505:CLA:H111 | 31:b:516:CLA:H42  | 2.03                     | 0.41              |
| 31:b:517:CLA:O1D  | 31:b:517:CLA:HBA2 | 2.20                     | 0.41              |
| 3:c:222:GLY:O     | 3:c:226:SER:OG    | 2.34                     | 0.41              |
| 4:d:188:PHE:CZ    | 4:d:326:ARG:HG3   | 2.56                     | 0.41              |
| 6:f:45:ARG:NH2    | 15:q:79:GLY:HA3   | 2.36                     | 0.41              |
| 14:o:272:ALA:C    | 14:o:274:LEU:N    | 2.76                     | 0.41              |
| 22:z:11:LEU:O     | 22:z:12:PHE:C     | 2.62                     | 0.41              |
| 24:2:56:ALA:O     | 24:2:60:HIS:ND1   | 2.51                     | 0.41              |
| 2:B:169:SER:OG    | 2:B:170:ASP:N     | 2.52                     | 0.41              |
| 2:B:285:GLU:O     | 2:B:289:GLU:HG2   | 2.21                     | 0.41              |
| 31:B:504:CLA:HBD  | 31:B:505:CLA:H42  | 2.03                     | 0.41              |
| 31:B:508:CLA:H141 | 31:B:508:CLA:H161 | 1.95                     | 0.41              |
| 3:C:369:LEU:HD23  | 3:C:380:ILE:HG12  | 2.03                     | 0.41              |
| 4:D:235:PHE:HD1   | 4:D:243:THR:HG21  | 1.86                     | 0.41              |
| 4:D:274:VAL:HB    | 4:D:275:PRO:HD3   | 2.03                     | 0.41              |
| 10:K:42:PRO:O     | 10:K:43:VAL:C     | 2.63                     | 0.41              |
| 14:O:271:ASP:OD1  | 14:O:271:ASP:N    | 2.50                     | 0.41              |
| 18:V:5:GLU:OE2    | 18:V:20:VAL:HG21  | 2.21                     | 0.41              |
| 22:Z:17:LEU:HA    | 22:Z:20:VAL:HG12  | 2.03                     | 0.41              |
| 2:b:157:HIS:ND1   | 2:b:164:PRO:HD2   | 2.36                     | 0.41              |
| 2:b:418:LYS:O     | 2:b:422:ARG:HG3   | 2.21                     | 0.41              |
| 3:c:168:LEU:HD23  | 3:c:168:LEU:HA    | 1.90                     | 0.41              |
| 4:d:274:VAL:HB    | 4:d:275:PRO:HD3   | 2.03                     | 0.41              |
| 37:j:101:LMG:H192 | 37:j:101:LMG:H221 | 1.51                     | 0.41              |
| 14:o:130:VAL:HG13 | 14:o:336:GLU:HG2  | 2.02                     | 0.41              |
| 23:5:189:ASN:OD1  | 23:5:189:ASN:O    | 2.38                     | 0.41              |
| 24:7:148:GLY:O    | 24:7:152:MET:HG3  | 2.21                     | 0.41              |
| 23:0:83:VAL:HG11  | 42:0:303:A86:C8   | 2.50                     | 0.41              |
| 24:2:30:ILE:HD12  | 24:2:146:GLN:CD   | 2.45                     | 0.41              |
| 33:B:517:BCR:H20C | 33:B:517:BCR:H361 | 1.84                     | 0.41              |
| 33:C:517:BCR:H361 | 33:C:517:BCR:H20C | 1.84                     | 0.41              |
| 4:D:22:LEU:HD23   | 4:D:22:LEU:HA     | 1.91                     | 0.41              |
| 4:D:180:ARG:HH21  | 4:D:333:ASP:CG    | 2.29                     | 0.41              |
| 9:J:29:ILE:O      | 9:J:30:TYR:C      | 2.62                     | 0.41              |
| 14:O:134:ILE:HD13 | 14:O:331:PHE:HB2  | 2.03                     | 0.41              |
| 15:Q:74:THR:HB    | 15:Q:75:SER:H     | 1.64                     | 0.41              |
| 15:Q:93:PRO:O     | 15:Q:95:SER:N     | 2.53                     | 0.41              |
| 15:Q:105:LEU:HD13 | 15:Q:105:LEU:HA   | 1.84                     | 0.41              |
| 15:Q:131:ILE:N    | 15:Q:132:PRO:HD2  | 2.35                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:U:28:ILE:HD13  | 17:U:56:TYR:HD2   | 1.86                     | 0.41              |
| 18:V:134:LYS:O    | 18:V:136:TYR:N    | 2.54                     | 0.41              |
| 2:b:285:GLU:O     | 2:b:289:GLU:HG2   | 2.21                     | 0.41              |
| 31:b:505:CLA:HBD  | 31:b:506:CLA:H42  | 2.03                     | 0.41              |
| 37:c:521:LMG:H202 | 37:c:521:LMG:H172 | 1.81                     | 0.41              |
| 33:h:101:BCR:H24C | 33:h:101:BCR:H371 | 1.87                     | 0.41              |
| 17:u:28:ILE:HD13  | 17:u:56:TYR:HD2   | 1.86                     | 0.41              |
| 18:v:134:LYS:O    | 18:v:136:TYR:N    | 2.54                     | 0.41              |
| 22:z:4:MET:HB3    | 22:z:4:MET:HE3    | 1.63                     | 0.41              |
| 23:5:71:VAL:O     | 23:5:75:HIS:ND1   | 2.31                     | 0.41              |
| 27:4:80:UNK:C     | 27:4:82:UNK:N     | 2.84                     | 0.41              |
| 26:P:94:THR:O     | 26:P:98:ILE:HG12  | 2.21                     | 0.41              |
| 24:2:95:GLY:O     | 24:2:97:ALA:N     | 2.46                     | 0.41              |
| 24:2:147:HIS:CD2  | 31:2:310:CLA:HBB2 | 2.55                     | 0.41              |
| 21:Y:16:ARG:HE    | 21:Y:16:ARG:HB3   | 1.77                     | 0.41              |
| 3:c:379:LYS:HD3   | 15:q:149:ARG:HH22 | 1.85                     | 0.41              |
| 35:d:406:PL9:H38  | 35:d:406:PL9:H421 | 1.84                     | 0.41              |
| 14:o:143:GLU:HG3  | 14:o:156:VAL:HG11 | 2.03                     | 0.41              |
| 22:z:60:ILE:C     | 22:z:62:THR:H     | 2.29                     | 0.41              |
| 31:7:309:CLA:H111 | 31:7:309:CLA:H71  | 1.69                     | 0.41              |
| 26:p:94:THR:O     | 26:p:98:ILE:HG12  | 2.21                     | 0.41              |
| 31:P:603:CLA:CMC  | 44:P:611:DD6:C    | 2.97                     | 0.41              |
| 24:2:84:ALA:HB1   | 24:2:85:PRO:CD    | 2.49                     | 0.41              |
| 31:B:505:CLA:H162 | 31:B:505:CLA:H193 | 1.86                     | 0.40              |
| 7:H:45:ILE:HD13   | 36:H:103:LHG:C14  | 2.49                     | 0.40              |
| 15:Q:170:LYS:HZ1  | 15:Q:207:PHE:HD1  | 1.69                     | 0.40              |
| 2:b:441:GLY:O     | 14:o:261:LEU:HA   | 2.21                     | 0.40              |
| 33:b:519:BCR:H361 | 33:b:519:BCR:H20C | 1.85                     | 0.40              |
| 3:c:109:VAL:N     | 3:c:110:PRO:HD2   | 2.36                     | 0.40              |
| 4:d:309:PRO:HG2   | 14:o:316:ASP:OD2  | 2.21                     | 0.40              |
| 4:d:351:ALA:HB1   | 17:u:102:TYR:CE2  | 2.53                     | 0.40              |
| 7:h:53:PHE:O      | 7:h:57:ILE:HG12   | 2.21                     | 0.40              |
| 14:o:155:PHE:CE1  | 14:o:326:LEU:HB2  | 2.56                     | 0.40              |
| 22:z:17:LEU:HA    | 22:z:20:VAL:HG12  | 2.03                     | 0.40              |
| 22:z:19:LEU:HD21  | 22:z:44:PHE:HE1   | 1.87                     | 0.40              |
| 24:2:54:ARG:NH2   | 31:2:306:CLA:O1D  | 2.55                     | 0.40              |
| 25:1:128:GLY:O    | 25:1:132:VAL:HG12 | 2.21                     | 0.40              |
| 2:B:222:PRO:HG2   | 2:B:225:LEU:HB2   | 2.02                     | 0.40              |
| 31:B:514:CLA:OBD  | 11:L:11:VAL:HG21  | 2.21                     | 0.40              |
| 19:W:114:TRP:O    | 19:W:118:MET:HG2  | 2.20                     | 0.40              |
| 2:b:39:LEU:HD23   | 2:b:39:LEU:HA     | 1.92                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:d:405:BCR:H11C | 33:d:405:BCR:H341 | 1.94                     | 0.40              |
| 10:k:42:PRO:O     | 10:k:43:VAL:C     | 2.63                     | 0.40              |
| 12:m:3:VAL:HG23   | 12:m:4:GLN:N      | 2.35                     | 0.40              |
| 15:q:68:GLY:CA    | 15:q:74:THR:OG1   | 2.69                     | 0.40              |
| 24:7:58:LEU:O     | 24:7:62:ARG:HG3   | 2.21                     | 0.40              |
| 44:7:304:DD6:C5   | 31:7:310:CLA:HAB  | 2.52                     | 0.40              |
| 26:P:108:TRP:HA   | 26:P:112:PHE:H    | 1.86                     | 0.40              |
| 23:0:71:VAL:O     | 23:0:75:HIS:ND1   | 2.31                     | 0.40              |
| 2:B:71:ILE:HD13   | 31:B:506:CLA:HED3 | 2.04                     | 0.40              |
| 3:C:109:VAL:N     | 3:C:110:PRO:HD2   | 2.36                     | 0.40              |
| 7:H:53:PHE:O      | 7:H:57:ILE:HG12   | 2.21                     | 0.40              |
| 14:O:172:GLU:HB2  | 14:O:188:GLU:OE1  | 2.22                     | 0.40              |
| 2:b:475:PHE:HB3   | 2:b:478:VAL:HG12  | 2.02                     | 0.40              |
| 31:d:404:CLA:H61  | 31:d:404:CLA:H92  | 1.83                     | 0.40              |
| 21:y:15:THR:C     | 21:y:17:LEU:N     | 2.76                     | 0.40              |
| 24:7:177:MET:HE2  | 24:7:177:MET:HB2  | 1.93                     | 0.40              |
| 25:1:67:ARG:NH1   | 25:1:70:GLU:OE1   | 2.55                     | 0.40              |
| 25:1:172:LEU:HD23 | 25:1:172:LEU:HA   | 1.84                     | 0.40              |
| 2:B:144:PHE:HE1   | 2:B:210:ILE:HG23  | 1.85                     | 0.40              |
| 3:C:69:LEU:HD23   | 3:C:69:LEU:HA     | 1.91                     | 0.40              |
| 2:b:414:ALA:HB3   | 2:b:415:PRO:HD3   | 2.04                     | 0.40              |
| 4:d:159:LEU:HD23  | 4:d:159:LEU:HA    | 1.88                     | 0.40              |
| 20:x:93:ALA:O     | 20:x:96:VAL:HG12  | 2.21                     | 0.40              |
| 34:5:316:SQD:H1   | 34:5:316:SQD:H45  | 1.71                     | 0.40              |
| 24:7:67:ALA:O     | 24:7:70:GLY:N     | 2.52                     | 0.40              |
| 1:A:252:HIS:CD2   | 1:A:264:SER:HB2   | 2.56                     | 0.40              |
| 34:A:409:SQD:H381 | 39:C:519:DGD:HAT1 | 2.03                     | 0.40              |
| 2:B:22:VAL:HG11   | 31:B:512:CLA:CAB  | 2.51                     | 0.40              |
| 4:D:309:PRO:HG2   | 14:O:316:ASP:OD2  | 2.21                     | 0.40              |
| 20:X:108:ILE:O    | 20:X:109:SER:C    | 2.63                     | 0.40              |
| 1:a:334:ARG:O     | 4:d:350:ASN:HB2   | 2.22                     | 0.40              |
| 2:b:116:VAL:HG12  | 2:b:117:TYR:CD1   | 2.57                     | 0.40              |
| 2:b:256:MET:O     | 2:b:448:ARG:NH1   | 2.47                     | 0.40              |
| 31:b:515:CLA:OBD  | 11:l:11:VAL:HG21  | 2.21                     | 0.40              |
| 14:o:118:GLU:HA   | 14:o:296:VAL:H    | 1.85                     | 0.40              |
| 14:o:134:ILE:HD13 | 14:o:331:PHE:HB2  | 2.03                     | 0.40              |
| 14:o:172:GLU:HB2  | 14:o:188:GLU:OE1  | 2.22                     | 0.40              |
| 19:w:102:ILE:O    | 19:w:103:GLU:C    | 2.63                     | 0.40              |
| 34:5:316:SQD:O4   | 25:6:184:PHE:O    | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 331/333 (99%)  | 316 (96%) | 15 (4%) | 0        | 100         | 100 |
| 1   | a     | 331/333 (99%)  | 316 (96%) | 15 (4%) | 0        | 100         | 100 |
| 2   | B     | 479/481 (100%) | 456 (95%) | 22 (5%) | 1 (0%)   | 43          | 65  |
| 2   | b     | 479/481 (100%) | 456 (95%) | 22 (5%) | 1 (0%)   | 43          | 65  |
| 3   | C     | 448/450 (100%) | 435 (97%) | 12 (3%) | 1 (0%)   | 43          | 65  |
| 3   | c     | 448/450 (100%) | 435 (97%) | 12 (3%) | 1 (0%)   | 43          | 65  |
| 4   | D     | 338/340 (99%)  | 325 (96%) | 13 (4%) | 0        | 100         | 100 |
| 4   | d     | 338/340 (99%)  | 325 (96%) | 13 (4%) | 0        | 100         | 100 |
| 5   | E     | 73/75 (97%)    | 70 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 5   | e     | 73/75 (97%)    | 70 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | F     | 29/31 (94%)    | 26 (90%)  | 2 (7%)  | 1 (3%)   | 3           | 7   |
| 6   | f     | 29/31 (94%)    | 26 (90%)  | 2 (7%)  | 1 (3%)   | 3           | 7   |
| 7   | H     | 63/65 (97%)    | 58 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 7   | h     | 63/65 (97%)    | 58 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 8   | I     | 32/34 (94%)    | 31 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | i     | 32/34 (94%)    | 31 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | J     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 9   | j     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 10  | K     | 35/37 (95%)    | 33 (94%)  | 2 (6%)  | 0        | 100         | 100 |
| 10  | k     | 35/37 (95%)    | 33 (94%)  | 2 (6%)  | 0        | 100         | 100 |
| 11  | L     | 35/37 (95%)    | 35 (100%) | 0       | 0        | 100         | 100 |
| 11  | l     | 35/37 (95%)    | 35 (100%) | 0       | 0        | 100         | 100 |
| 12  | M     | 39/41 (95%)    | 39 (100%) | 0       | 0        | 100         | 100 |
| 12  | m     | 39/41 (95%)    | 39 (100%) | 0       | 0        | 100         | 100 |
| 14  | O     | 246/248 (99%)  | 223 (91%) | 21 (8%) | 2 (1%)   | 16          | 36  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 14  | o     | 246/248 (99%)   | 223 (91%)  | 21 (8%)  | 2 (1%)   | 16          | 36  |
| 15  | Q     | 143/145 (99%)   | 113 (79%)  | 17 (12%) | 13 (9%)  | 0           | 1   |
| 15  | q     | 143/145 (99%)   | 113 (79%)  | 17 (12%) | 13 (9%)  | 0           | 1   |
| 16  | T     | 27/29 (93%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 16  | t     | 27/29 (93%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 17  | U     | 90/92 (98%)     | 82 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 17  | u     | 90/92 (98%)     | 82 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 18  | V     | 134/136 (98%)   | 125 (93%)  | 8 (6%)   | 1 (1%)   | 18          | 40  |
| 18  | v     | 134/136 (98%)   | 125 (93%)  | 8 (6%)   | 1 (1%)   | 18          | 40  |
| 19  | W     | 42/50 (84%)     | 36 (86%)   | 2 (5%)   | 4 (10%)  | 0           | 1   |
| 19  | w     | 42/50 (84%)     | 36 (86%)   | 2 (5%)   | 4 (10%)  | 0           | 1   |
| 20  | X     | 32/34 (94%)     | 29 (91%)   | 2 (6%)   | 1 (3%)   | 3           | 8   |
| 20  | x     | 32/34 (94%)     | 29 (91%)   | 2 (6%)   | 1 (3%)   | 3           | 8   |
| 21  | Y     | 31/33 (94%)     | 26 (84%)   | 5 (16%)  | 0        | 100         | 100 |
| 21  | y     | 31/33 (94%)     | 26 (84%)   | 5 (16%)  | 0        | 100         | 100 |
| 22  | Z     | 57/59 (97%)     | 44 (77%)   | 11 (19%) | 2 (4%)   | 3           | 7   |
| 22  | z     | 57/59 (97%)     | 44 (77%)   | 11 (19%) | 2 (4%)   | 3           | 7   |
| 23  | 0     | 167/169 (99%)   | 143 (86%)  | 24 (14%) | 0        | 100         | 100 |
| 23  | 5     | 167/169 (99%)   | 143 (86%)  | 24 (14%) | 0        | 100         | 100 |
| 24  | 2     | 162/164 (99%)   | 143 (88%)  | 19 (12%) | 0        | 100         | 100 |
| 24  | 7     | 162/164 (99%)   | 143 (88%)  | 19 (12%) | 0        | 100         | 100 |
| 25  | 1     | 162/164 (99%)   | 135 (83%)  | 26 (16%) | 1 (1%)   | 21          | 45  |
| 25  | 6     | 162/164 (99%)   | 135 (83%)  | 26 (16%) | 1 (1%)   | 21          | 45  |
| 26  | P     | 212/214 (99%)   | 172 (81%)  | 38 (18%) | 2 (1%)   | 14          | 34  |
| 26  | p     | 212/214 (99%)   | 173 (82%)  | 37 (18%) | 2 (1%)   | 14          | 34  |
| 28  | 3     | 161/163 (99%)   | 140 (87%)  | 20 (12%) | 1 (1%)   | 21          | 45  |
| 28  | 8     | 161/163 (99%)   | 140 (87%)  | 20 (12%) | 1 (1%)   | 21          | 45  |
| All | All   | 7200/7316 (98%) | 6589 (92%) | 551 (8%) | 60 (1%)  | 18          | 36  |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 460 | ASP  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 43  | ILE  |
| 14  | O     | 268 | GLU  |
| 15  | Q     | 70  | ILE  |
| 15  | Q     | 84  | THR  |
| 15  | Q     | 86  | GLN  |
| 22  | Z     | 33  | TRP  |
| 3   | c     | 460 | ASP  |
| 6   | f     | 43  | ILE  |
| 14  | o     | 268 | GLU  |
| 15  | q     | 70  | ILE  |
| 15  | q     | 84  | THR  |
| 15  | q     | 86  | GLN  |
| 22  | z     | 33  | TRP  |
| 28  | 3     | 177 | ALA  |
| 28  | 8     | 177 | ALA  |
| 2   | B     | 480 | THR  |
| 15  | Q     | 78  | GLU  |
| 15  | Q     | 80  | ALA  |
| 15  | Q     | 91  | TYR  |
| 15  | Q     | 94  | TYR  |
| 15  | Q     | 111 | ALA  |
| 15  | Q     | 208 | THR  |
| 19  | W     | 98  | LYS  |
| 19  | W     | 99  | PRO  |
| 2   | b     | 480 | THR  |
| 15  | q     | 78  | GLU  |
| 15  | q     | 80  | ALA  |
| 15  | q     | 91  | TYR  |
| 15  | q     | 94  | TYR  |
| 15  | q     | 111 | ALA  |
| 15  | q     | 208 | THR  |
| 19  | w     | 98  | LYS  |
| 19  | w     | 99  | PRO  |
| 25  | 6     | 110 | ALA  |
| 25  | 1     | 110 | ALA  |
| 15  | Q     | 71  | GLY  |
| 15  | Q     | 76  | TYR  |
| 19  | W     | 96  | ASN  |
| 20  | X     | 112 | ASP  |
| 15  | q     | 71  | GLY  |
| 15  | q     | 76  | TYR  |
| 19  | w     | 95  | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | x     | 112 | ASP  |
| 14  | O     | 270 | GLY  |
| 15  | Q     | 67  | PHE  |
| 14  | o     | 270 | GLY  |
| 15  | q     | 67  | PHE  |
| 26  | p     | 174 | ILE  |
| 26  | P     | 174 | ILE  |
| 15  | Q     | 74  | THR  |
| 22  | Z     | 28  | ALA  |
| 15  | q     | 74  | THR  |
| 19  | w     | 96  | ASN  |
| 22  | z     | 28  | ALA  |
| 26  | p     | 70  | SER  |
| 26  | P     | 70  | SER  |
| 19  | W     | 95  | ALA  |
| 18  | V     | 135 | ILE  |
| 18  | v     | 135 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | A     | 250/272 (92%) | 242 (97%)  | 8 (3%)   | 34          | 59 |
| 1   | a     | 250/272 (92%) | 243 (97%)  | 7 (3%)   | 38          | 63 |
| 2   | B     | 370/384 (96%) | 360 (97%)  | 10 (3%)  | 39          | 64 |
| 2   | b     | 370/384 (96%) | 360 (97%)  | 10 (3%)  | 39          | 64 |
| 3   | C     | 337/355 (95%) | 334 (99%)  | 3 (1%)   | 70          | 82 |
| 3   | c     | 337/355 (95%) | 334 (99%)  | 3 (1%)   | 70          | 82 |
| 4   | D     | 265/272 (97%) | 264 (100%) | 1 (0%)   | 84          | 92 |
| 4   | d     | 265/272 (97%) | 264 (100%) | 1 (0%)   | 84          | 92 |
| 5   | E     | 65/69 (94%)   | 64 (98%)   | 1 (2%)   | 57          | 75 |
| 5   | e     | 65/69 (94%)   | 64 (98%)   | 1 (2%)   | 57          | 75 |
| 6   | F     | 22/25 (88%)   | 19 (86%)   | 3 (14%)  | 3           | 10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 6   | f     | 22/25 (88%)   | 19 (86%)  | 3 (14%)  | 3           | 10  |
| 7   | H     | 52/54 (96%)   | 49 (94%)  | 3 (6%)   | 18          | 40  |
| 7   | h     | 52/54 (96%)   | 49 (94%)  | 3 (6%)   | 18          | 40  |
| 8   | I     | 30/33 (91%)   | 27 (90%)  | 3 (10%)  | 7           | 19  |
| 8   | i     | 30/33 (91%)   | 27 (90%)  | 3 (10%)  | 7           | 19  |
| 9   | J     | 26/26 (100%)  | 26 (100%) | 0        | 100         | 100 |
| 9   | j     | 26/26 (100%)  | 26 (100%) | 0        | 100         | 100 |
| 10  | K     | 30/32 (94%)   | 29 (97%)  | 1 (3%)   | 33          | 58  |
| 10  | k     | 30/32 (94%)   | 29 (97%)  | 1 (3%)   | 33          | 58  |
| 11  | L     | 31/33 (94%)   | 31 (100%) | 0        | 100         | 100 |
| 11  | l     | 31/33 (94%)   | 31 (100%) | 0        | 100         | 100 |
| 12  | M     | 26/30 (87%)   | 24 (92%)  | 2 (8%)   | 12          | 28  |
| 12  | m     | 26/30 (87%)   | 24 (92%)  | 2 (8%)   | 12          | 28  |
| 14  | O     | 185/201 (92%) | 176 (95%) | 9 (5%)   | 22          | 47  |
| 14  | o     | 185/201 (92%) | 176 (95%) | 9 (5%)   | 22          | 47  |
| 15  | Q     | 99/116 (85%)  | 89 (90%)  | 10 (10%) | 7           | 19  |
| 15  | q     | 99/116 (85%)  | 89 (90%)  | 10 (10%) | 7           | 19  |
| 16  | T     | 24/26 (92%)   | 24 (100%) | 0        | 100         | 100 |
| 16  | t     | 24/26 (92%)   | 24 (100%) | 0        | 100         | 100 |
| 17  | U     | 70/77 (91%)   | 65 (93%)  | 5 (7%)   | 13          | 31  |
| 17  | u     | 70/77 (91%)   | 65 (93%)  | 5 (7%)   | 13          | 31  |
| 18  | V     | 101/114 (89%) | 99 (98%)  | 2 (2%)   | 48          | 70  |
| 18  | v     | 101/114 (89%) | 99 (98%)  | 2 (2%)   | 48          | 70  |
| 19  | W     | 25/34 (74%)   | 24 (96%)  | 1 (4%)   | 28          | 53  |
| 19  | w     | 25/34 (74%)   | 24 (96%)  | 1 (4%)   | 28          | 53  |
| 20  | X     | 25/26 (96%)   | 24 (96%)  | 1 (4%)   | 28          | 53  |
| 20  | x     | 25/26 (96%)   | 24 (96%)  | 1 (4%)   | 28          | 53  |
| 21  | Y     | 18/26 (69%)   | 16 (89%)  | 2 (11%)  | 6           | 16  |
| 21  | y     | 18/26 (69%)   | 16 (89%)  | 2 (11%)  | 6           | 16  |
| 22  | Z     | 39/48 (81%)   | 32 (82%)  | 7 (18%)  | 2           | 4   |
| 22  | z     | 39/48 (81%)   | 32 (82%)  | 7 (18%)  | 2           | 4   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 23  | 0     | 129/136 (95%)   | 129 (100%) | 0        | 100         | 100 |
| 23  | 5     | 129/136 (95%)   | 129 (100%) | 0        | 100         | 100 |
| 24  | 2     | 110/131 (84%)   | 109 (99%)  | 1 (1%)   | 70          | 82  |
| 24  | 7     | 110/131 (84%)   | 109 (99%)  | 1 (1%)   | 70          | 82  |
| 25  | 1     | 107/129 (83%)   | 105 (98%)  | 2 (2%)   | 50          | 71  |
| 25  | 6     | 107/129 (83%)   | 105 (98%)  | 2 (2%)   | 50          | 71  |
| 26  | P     | 70/166 (42%)    | 70 (100%)  | 0        | 100         | 100 |
| 26  | p     | 70/166 (42%)    | 70 (100%)  | 0        | 100         | 100 |
| 28  | 3     | 54/128 (42%)    | 54 (100%)  | 0        | 100         | 100 |
| 28  | 8     | 54/128 (42%)    | 54 (100%)  | 0        | 100         | 100 |
| All | All   | 5120/5886 (87%) | 4971 (97%) | 149 (3%) | 38          | 62  |

All (149) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ARG  |
| 1   | A     | 60  | ILE  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 227 | THR  |
| 1   | A     | 231 | GLU  |
| 1   | A     | 232 | SER  |
| 1   | A     | 312 | ARG  |
| 1   | A     | 313 | VAL  |
| 2   | B     | 12  | VAL  |
| 2   | B     | 13  | LEU  |
| 2   | B     | 18  | ARG  |
| 2   | B     | 80  | ILE  |
| 2   | B     | 81  | THR  |
| 2   | B     | 85  | VAL  |
| 2   | B     | 90  | ILE  |
| 2   | B     | 479 | PHE  |
| 2   | B     | 480 | THR  |
| 2   | B     | 482 | ILE  |
| 3   | C     | 28  | ILE  |
| 3   | C     | 29  | GLU  |
| 3   | C     | 472 | LEU  |
| 4   | D     | 348 | ARG  |
| 5   | E     | 80  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 15  | ILE  |
| 6   | F     | 17  | THR  |
| 6   | F     | 44  | GLN  |
| 7   | H     | 16  | ARG  |
| 7   | H     | 18  | ARG  |
| 7   | H     | 78  | ILE  |
| 8   | I     | 10  | THR  |
| 8   | I     | 31  | ASN  |
| 8   | I     | 33  | ASN  |
| 10  | K     | 59  | ARG  |
| 12  | M     | 2   | GLU  |
| 12  | M     | 3   | VAL  |
| 14  | O     | 176 | THR  |
| 14  | O     | 177 | VAL  |
| 14  | O     | 188 | GLU  |
| 14  | O     | 217 | LYS  |
| 14  | O     | 219 | ASN  |
| 14  | O     | 268 | GLU  |
| 14  | O     | 269 | GLU  |
| 14  | O     | 273 | GLU  |
| 14  | O     | 335 | VAL  |
| 15  | Q     | 67  | PHE  |
| 15  | Q     | 69  | LEU  |
| 15  | Q     | 70  | ILE  |
| 15  | Q     | 74  | THR  |
| 15  | Q     | 78  | GLU  |
| 15  | Q     | 86  | GLN  |
| 15  | Q     | 88  | ASP  |
| 15  | Q     | 95  | SER  |
| 15  | Q     | 96  | VAL  |
| 15  | Q     | 105 | LEU  |
| 17  | U     | 28  | ILE  |
| 17  | U     | 29  | ASN  |
| 17  | U     | 64  | LYS  |
| 17  | U     | 68  | LEU  |
| 17  | U     | 69  | SER  |
| 18  | V     | 24  | GLU  |
| 18  | V     | 28  | ARG  |
| 19  | W     | 102 | ILE  |
| 20  | X     | 110 | LYS  |
| 21  | Y     | 14  | ASP  |
| 21  | Y     | 16  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | Z     | 4   | MET  |
| 22  | Z     | 8   | LEU  |
| 22  | Z     | 9   | THR  |
| 22  | Z     | 11  | LEU  |
| 22  | Z     | 32  | GLU  |
| 22  | Z     | 58  | ASP  |
| 22  | Z     | 61  | SER  |
| 1   | a     | 16  | ARG  |
| 1   | a     | 226 | GLU  |
| 1   | a     | 227 | THR  |
| 1   | a     | 231 | GLU  |
| 1   | a     | 232 | SER  |
| 1   | a     | 312 | ARG  |
| 1   | a     | 313 | VAL  |
| 2   | b     | 12  | VAL  |
| 2   | b     | 13  | LEU  |
| 2   | b     | 18  | ARG  |
| 2   | b     | 80  | ILE  |
| 2   | b     | 81  | THR  |
| 2   | b     | 85  | VAL  |
| 2   | b     | 90  | ILE  |
| 2   | b     | 479 | PHE  |
| 2   | b     | 480 | THR  |
| 2   | b     | 482 | ILE  |
| 3   | c     | 28  | ILE  |
| 3   | c     | 29  | GLU  |
| 3   | c     | 472 | LEU  |
| 4   | d     | 348 | ARG  |
| 5   | e     | 80  | THR  |
| 6   | f     | 15  | ILE  |
| 6   | f     | 17  | THR  |
| 6   | f     | 44  | GLN  |
| 7   | h     | 16  | ARG  |
| 7   | h     | 18  | ARG  |
| 7   | h     | 78  | ILE  |
| 8   | i     | 10  | THR  |
| 8   | i     | 31  | ASN  |
| 8   | i     | 33  | ASN  |
| 10  | k     | 59  | ARG  |
| 12  | m     | 2   | GLU  |
| 12  | m     | 3   | VAL  |
| 14  | o     | 176 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | o     | 177 | VAL  |
| 14  | o     | 188 | GLU  |
| 14  | o     | 217 | LYS  |
| 14  | o     | 219 | ASN  |
| 14  | o     | 268 | GLU  |
| 14  | o     | 269 | GLU  |
| 14  | o     | 273 | GLU  |
| 14  | o     | 335 | VAL  |
| 15  | q     | 67  | PHE  |
| 15  | q     | 69  | LEU  |
| 15  | q     | 70  | ILE  |
| 15  | q     | 74  | THR  |
| 15  | q     | 78  | GLU  |
| 15  | q     | 86  | GLN  |
| 15  | q     | 88  | ASP  |
| 15  | q     | 95  | SER  |
| 15  | q     | 96  | VAL  |
| 15  | q     | 105 | LEU  |
| 17  | u     | 28  | ILE  |
| 17  | u     | 29  | ASN  |
| 17  | u     | 64  | LYS  |
| 17  | u     | 68  | LEU  |
| 17  | u     | 69  | SER  |
| 18  | v     | 24  | GLU  |
| 18  | v     | 28  | ARG  |
| 19  | w     | 102 | ILE  |
| 20  | x     | 110 | LYS  |
| 21  | y     | 14  | ASP  |
| 21  | y     | 16  | ARG  |
| 22  | z     | 4   | MET  |
| 22  | z     | 8   | LEU  |
| 22  | z     | 9   | THR  |
| 22  | z     | 11  | LEU  |
| 22  | z     | 32  | GLU  |
| 22  | z     | 58  | ASP  |
| 22  | z     | 61  | SER  |
| 24  | 7     | 139 | GLU  |
| 25  | 6     | 138 | ASN  |
| 25  | 6     | 192 | THR  |
| 24  | 2     | 139 | GLU  |
| 25  | 1     | 138 | ASN  |
| 25  | 1     | 192 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 165 | GLN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 187 | GLN  |
| 2   | B     | 26  | HIS  |
| 2   | B     | 114 | HIS  |
| 2   | B     | 157 | HIS  |
| 2   | B     | 179 | GLN  |
| 3   | C     | 228 | ASN  |
| 4   | D     | 117 | HIS  |
| 4   | D     | 197 | HIS  |
| 4   | D     | 350 | ASN  |
| 5   | E     | 61  | GLN  |
| 7   | H     | 69  | ASN  |
| 10  | K     | 53  | GLN  |
| 14  | O     | 265 | GLN  |
| 15  | Q     | 129 | GLN  |
| 17  | U     | 16  | ASN  |
| 1   | a     | 165 | GLN  |
| 1   | a     | 181 | ASN  |
| 1   | a     | 187 | GLN  |
| 2   | b     | 26  | HIS  |
| 2   | b     | 114 | HIS  |
| 2   | b     | 157 | HIS  |
| 3   | c     | 228 | ASN  |
| 4   | d     | 117 | HIS  |
| 4   | d     | 197 | HIS  |
| 4   | d     | 350 | ASN  |
| 5   | e     | 61  | GLN  |
| 7   | h     | 69  | ASN  |
| 10  | k     | 53  | GLN  |
| 14  | o     | 265 | GLN  |
| 15  | q     | 129 | GLN  |
| 17  | u     | 16  | ASN  |
| 21  | y     | 42  | GLN  |
| 23  | 5     | 171 | GLN  |
| 23  | 5     | 185 | GLN  |
| 23  | 5     | 189 | ASN  |
| 23  | 5     | 196 | ASN  |
| 26  | p     | 200 | GLN  |
| 26  | P     | 200 | GLN  |
| 23  | 0     | 171 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | 0     | 185 | GLN  |
| 23  | 0     | 189 | ASN  |
| 23  | 0     | 196 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 336 ligands modelled in this entry, 4 are monoatomic - leaving 332 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 | $\# Z  > 2$ |
| 31  | CLA  | 7     | 309 | 24   | 63,67,73     | 1.21 | 9 (14%)     | 74,105,113  | 1.32 | 7 (9%)      |
| 37  | LMG  | y     | 101 | -    | 46,46,55     | 0.75 | 1 (2%)      | 54,54,63    | 1.39 | 11 (20%)    |
| 39  | DGD  | C     | 518 | -    | 56,56,67     | 0.95 | 3 (5%)      | 70,70,81    | 1.45 | 11 (15%)    |
| 31  | CLA  | 8     | 309 | -    | 43,48,73     | 1.40 | 9 (20%)     | 51,83,113   | 1.70 | 6 (11%)     |
| 31  | CLA  | 9     | 213 | -    | 37,43,73     | 1.67 | 10 (27%)    | 49,76,113   | 1.69 | 11 (22%)    |
| 32  | PHO  | a     | 406 | -    | 58,69,69     | 2.09 | 10 (17%)    | 55,99,99    | 1.46 | 7 (12%)     |
| 31  | CLA  | B     | 505 | -    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.28 | 5 (6%)      |
| 31  | CLA  | 4     | 205 | -    | 38,43,73     | 1.61 | 11 (28%)    | 48,75,113   | 1.47 | 5 (10%)     |
| 31  | CLA  | B     | 516 | -    | 69,73,73     | 1.17 | 9 (13%)     | 82,113,113  | 1.30 | 6 (7%)      |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 42  | A86  | 1     | 202 | -    | 47,50,50     | 1.48 | 6 (12%)  | 51,76,76    | 2.40 | 15 (29%) |
| 31  | CLA  | 6     | 212 | -    | 45,49,73     | 1.40 | 7 (15%)  | 54,84,113   | 1.49 | 6 (11%)  |
| 36  | LHG  | d     | 407 | -    | 44,47,48     | 0.56 | 1 (2%)   | 44,51,54    | 1.23 | 6 (13%)  |
| 34  | SQD  | B     | 522 | -    | 52,54,54     | 0.94 | 2 (3%)   | 62,65,65    | 1.60 | 12 (19%) |
| 42  | A86  | 6     | 202 | -    | 47,50,50     | 1.49 | 6 (12%)  | 51,76,76    | 2.40 | 15 (29%) |
| 42  | A86  | 4     | 203 | -    | 47,50,50     | 1.82 | 6 (12%)  | 51,76,76    | 3.65 | 22 (43%) |
| 44  | DD6  | 2     | 303 | -    | 40,45,45     | 1.57 | 2 (5%)   | 51,67,67    | 2.17 | 17 (33%) |
| 31  | CLA  | 2     | 305 | -    | 45,49,73     | 1.40 | 8 (17%)  | 54,84,113   | 1.51 | 6 (11%)  |
| 35  | PL9  | D     | 406 | -    | 55,55,55     | 1.32 | 5 (9%)   | 68,69,69    | 1.53 | 12 (17%) |
| 31  | CLA  | C     | 502 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 31  | CLA  | c     | 504 | -    | 55,59,73     | 1.29 | 9 (16%)  | 64,96,113   | 1.46 | 7 (10%)  |
| 31  | CLA  | 0     | 312 | -    | 46,50,73     | 1.39 | 8 (17%)  | 53,85,113   | 1.44 | 4 (7%)   |
| 31  | CLA  | 1     | 210 | 25   | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 31  | CLA  | 8     | 314 | -    | 39,43,73     | 1.61 | 10 (25%) | 50,76,113   | 1.52 | 7 (14%)  |
| 37  | LMG  | D     | 409 | -    | 37,37,55     | 0.78 | 1 (2%)   | 45,45,63    | 1.33 | 7 (15%)  |
| 31  | CLA  | 6     | 214 | 25   | 40,46,73     | 1.45 | 8 (20%)  | 52,80,113   | 1.52 | 7 (13%)  |
| 31  | CLA  | 3     | 306 | -    | 35,41,73     | 1.74 | 10 (28%) | 47,72,113   | 1.66 | 8 (17%)  |
| 42  | A86  | 9     | 203 | -    | 47,50,50     | 1.82 | 6 (12%)  | 51,76,76    | 3.64 | 22 (43%) |
| 37  | LMG  | 5     | 315 | -    | 48,48,55     | 0.77 | 1 (2%)   | 56,56,63    | 1.29 | 6 (10%)  |
| 44  | DD6  | 6     | 203 | -    | 40,45,45     | 1.57 | 2 (5%)   | 51,67,67    | 2.16 | 17 (33%) |
| 31  | CLA  | B     | 514 | -    | 64,68,73     | 1.20 | 9 (14%)  | 75,106,113  | 1.31 | 5 (6%)   |
| 31  | CLA  | 6     | 216 | 25   | 40,46,73     | 1.45 | 7 (17%)  | 52,80,113   | 1.46 | 5 (9%)   |
| 31  | CLA  | 4     | 207 | -    | 40,46,73     | 1.44 | 8 (20%)  | 52,80,113   | 1.59 | 6 (11%)  |
| 31  | CLA  | c     | 509 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 8 (9%)   |
| 31  | CLA  | a     | 404 | -    | 53,57,73     | 1.29 | 9 (16%)  | 61,93,113   | 1.45 | 6 (9%)   |
| 31  | CLA  | 1     | 206 | 25   | 49,53,73     | 1.35 | 7 (14%)  | 58,89,113   | 1.50 | 5 (8%)   |
| 42  | A86  | 7     | 301 | -    | 47,50,50     | 1.54 | 5 (10%)  | 51,76,76    | 2.59 | 18 (35%) |
| 42  | A86  | P     | 610 | -    | 47,50,50     | 1.60 | 7 (14%)  | 51,76,76    | 3.91 | 25 (49%) |
| 31  | CLA  | 3     | 311 | 28   | 43,48,73     | 1.44 | 8 (18%)  | 51,83,113   | 1.57 | 6 (11%)  |
| 31  | CLA  | W     | 202 | 19   | 49,53,73     | 1.35 | 10 (20%) | 58,89,113   | 1.47 | 7 (12%)  |
| 33  | BCR  | k     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 36  | LHG  | B     | 521 | -    | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31 | 6 (11%)  |
| 31  | CLA  | 7     | 316 | -    | 45,49,73     | 1.41 | 8 (17%)  | 54,84,113   | 1.48 | 6 (11%)  |
| 31  | CLA  | 8     | 308 | -    | 40,43,73     | 1.57 | 11 (27%) | 46,73,113   | 2.00 | 6 (13%)  |
| 37  | LMG  | J     | 101 | -    | 50,50,55     | 0.79 | 1 (2%)   | 58,58,63    | 1.35 | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 3     | 314 | -    | 39,43,73     | 1.61 | 11 (28%) | 50,76,113   | 1.53 | 7 (14%)  |
| 31  | CLA  | C     | 510 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 31  | CLA  | 9     | 212 | -    | 40,44,73     | 1.59 | 10 (25%) | 51,77,113   | 1.54 | 6 (11%)  |
| 31  | CLA  | B     | 511 | -    | 68,72,73     | 1.18 | 9 (13%)  | 80,111,113  | 1.34 | 7 (8%)   |
| 31  | CLA  | 1     | 208 | -    | 51,55,73     | 1.34 | 9 (17%)  | 60,91,113   | 1.41 | 5 (8%)   |
| 31  | CLA  | 9     | 211 | -    | 37,42,73     | 1.65 | 10 (27%) | 47,74,113   | 1.50 | 5 (10%)  |
| 31  | CLA  | 5     | 313 | 23   | 40,46,73     | 1.46 | 7 (17%)  | 52,80,113   | 1.51 | 5 (9%)   |
| 31  | CLA  | 9     | 207 | -    | 40,46,73     | 1.44 | 8 (20%)  | 52,80,113   | 1.60 | 6 (11%)  |
| 31  | CLA  | z     | 101 | -    | 55,59,73     | 1.32 | 8 (14%)  | 64,96,113   | 1.35 | 5 (7%)   |
| 31  | CLA  | b     | 517 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 31  | CLA  | 4     | 206 | -    | 39,45,73     | 1.50 | 9 (23%)  | 49,78,113   | 1.49 | 6 (12%)  |
| 31  | CLA  | 9     | 205 | -    | 38,43,73     | 1.62 | 12 (31%) | 48,75,113   | 1.48 | 5 (10%)  |
| 36  | LHG  | a     | 412 | -    | 25,25,48     | 0.82 | 1 (4%)   | 28,31,54    | 1.30 | 2 (7%)   |
| 43  | ET4  | 0     | 302 | -    | 41,43,43     | 1.72 | 10 (24%) | 52,60,60    | 2.18 | 14 (26%) |
| 37  | LMG  | w     | 201 | -    | 48,48,55     | 0.77 | 1 (2%)   | 56,56,63    | 1.34 | 7 (12%)  |
| 33  | BCR  | b     | 518 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 42  | A86  | 7     | 302 | -    | 47,50,50     | 1.79 | 7 (14%)  | 51,76,76    | 2.85 | 17 (33%) |
| 31  | CLA  | 2     | 306 | 24   | 49,53,73     | 1.36 | 8 (16%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 31  | CLA  | A     | 404 | -    | 53,57,73     | 1.29 | 9 (16%)  | 61,93,113   | 1.45 | 6 (9%)   |
| 33  | BCR  | K     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 37  | LMG  | c     | 521 | -    | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 1.05 | 4 (6%)   |
| 31  | CLA  | A     | 407 | -    | 64,68,73     | 1.19 | 8 (12%)  | 76,107,113  | 1.34 | 9 (11%)  |
| 31  | CLA  | c     | 507 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 42  | A86  | 3     | 301 | -    | 47,50,50     | 1.77 | 9 (19%)  | 51,76,76    | 4.95 | 22 (43%) |
| 31  | CLA  | p     | 604 | -    | 43,48,73     | 1.40 | 9 (20%)  | 51,83,113   | 1.57 | 7 (13%)  |
| 31  | CLA  | C     | 512 | 3    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 5 (6%)   |
| 44  | DD6  | 1     | 203 | -    | 40,45,45     | 1.58 | 2 (5%)   | 51,67,67    | 2.16 | 17 (33%) |
| 43  | ET4  | 5     | 302 | -    | 41,43,43     | 1.72 | 10 (24%) | 52,60,60    | 2.18 | 14 (26%) |
| 31  | CLA  | c     | 511 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 31  | CLA  | 8     | 305 | -    | 44,49,73     | 1.40 | 10 (22%) | 50,84,113   | 1.55 | 5 (10%)  |
| 31  | CLA  | 1     | 211 | 25   | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.33 | 6 (8%)   |
| 31  | CLA  | b     | 510 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 31  | CLA  | 2     | 315 | 24   | 40,46,73     | 1.47 | 9 (22%)  | 52,80,113   | 1.51 | 6 (11%)  |
| 37  | LMG  | D     | 408 | -    | 46,46,55     | 0.77 | 1 (2%)   | 54,54,63    | 1.34 | 6 (11%)  |
| 31  | CLA  | 5     | 306 | -    | 49,53,73     | 1.37 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | c     | 514 | -    | 53,57,73     | 1.30 | 8 (15%)  | 61,93,113   | 1.44 | 6 (9%)   |
| 39  | DGD  | c     | 518 | -    | 56,56,67     | 0.95 | 3 (5%)   | 70,70,81    | 1.44 | 11 (15%) |
| 32  | PHO  | A     | 406 | -    | 58,69,69     | 2.10 | 10 (17%) | 55,99,99    | 1.46 | 7 (12%)  |
| 42  | A86  | 0     | 303 | -    | 47,50,50     | 1.53 | 7 (14%)  | 51,76,76    | 2.73 | 22 (43%) |
| 31  | CLA  | p     | 607 | -    | 38,44,73     | 1.61 | 10 (26%) | 50,77,113   | 1.50 | 6 (12%)  |
| 31  | CLA  | 0     | 314 | 23   | 40,46,73     | 1.46 | 8 (20%)  | 52,80,113   | 1.50 | 6 (11%)  |
| 36  | LHG  | D     | 411 | -    | 33,33,48     | 0.74 | 2 (6%)   | 36,39,54    | 1.34 | 4 (11%)  |
| 31  | CLA  | 7     | 311 | -    | 47,51,73     | 1.38 | 8 (17%)  | 55,86,113   | 1.38 | 6 (10%)  |
| 33  | BCR  | C     | 515 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 34  | SQD  | A     | 409 | -    | 52,54,54     | 0.96 | 4 (7%)   | 62,65,65    | 1.43 | 8 (12%)  |
| 31  | CLA  | p     | 603 | -    | 39,45,73     | 1.47 | 9 (23%)  | 51,79,113   | 1.66 | 7 (13%)  |
| 31  | CLA  | B     | 515 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.31 | 7 (8%)   |
| 31  | CLA  | 7     | 313 | 24   | 40,46,73     | 1.46 | 7 (17%)  | 52,80,113   | 1.49 | 6 (11%)  |
| 31  | CLA  | 6     | 205 | -    | 45,49,73     | 1.40 | 8 (17%)  | 54,84,113   | 1.47 | 5 (9%)   |
| 31  | CLA  | 8     | 307 | -    | 46,50,73     | 1.37 | 10 (21%) | 55,84,113   | 1.44 | 5 (9%)   |
| 31  | CLA  | p     | 606 | -    | 39,45,73     | 1.50 | 10 (25%) | 49,78,113   | 1.51 | 6 (12%)  |
| 31  | CLA  | 0     | 304 | -    | 45,49,73     | 1.41 | 8 (17%)  | 54,84,113   | 1.53 | 6 (11%)  |
| 31  | CLA  | b     | 515 | -    | 64,68,73     | 1.20 | 9 (14%)  | 75,106,113  | 1.31 | 5 (6%)   |
| 41  | HEM  | v     | 201 | 18   | 50,50,50     | 1.29 | 5 (10%)  | 67,82,82    | 1.27 | 5 (7%)   |
| 39  | DGD  | c     | 520 | -    | 63,63,67     | 0.85 | 2 (3%)   | 77,77,81    | 0.94 | 3 (3%)   |
| 31  | CLA  | 2     | 307 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.44 | 5 (8%)   |
| 31  | CLA  | A     | 403 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 31  | CLA  | C     | 509 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 8 (9%)   |
| 36  | LHG  | b     | 522 | -    | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31 | 6 (11%)  |
| 31  | CLA  | 7     | 310 | 24   | 59,63,73     | 1.25 | 8 (13%)  | 70,101,113  | 1.36 | 6 (8%)   |
| 42  | A86  | 4     | 201 | -    | 47,50,50     | 1.69 | 6 (12%)  | 51,76,76    | 3.96 | 23 (45%) |
| 31  | CLA  | 2     | 314 | -    | 40,46,73     | 1.47 | 8 (20%)  | 52,80,113   | 1.50 | 6 (11%)  |
| 44  | DD6  | 2     | 304 | -    | 40,45,45     | 1.58 | 2 (5%)   | 51,67,67    | 2.45 | 15 (29%) |
| 31  | CLA  | c     | 505 | -    | 68,72,73     | 1.16 | 8 (11%)  | 80,111,113  | 1.29 | 4 (5%)   |
| 31  | CLA  | 6     | 213 | 25   | 43,48,73     | 1.43 | 8 (18%)  | 51,83,113   | 1.45 | 5 (9%)   |
| 31  | CLA  | B     | 503 | -    | 68,72,73     | 1.16 | 9 (13%)  | 80,111,113  | 1.28 | 5 (6%)   |
| 33  | BCR  | b     | 519 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 31  | CLA  | 2     | 308 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.44 | 6 (10%)  |
| 33  | BCR  | c     | 515 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 31  | CLA  | 4     | 209 | -    | 45,49,73     | 1.38 | 9 (20%)  | 54,84,113   | 1.56 | 5 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | DGD  | C     | 519 | -    | 63,63,67     | 0.92 | 3 (4%)   | 77,77,81    | 1.45 | 12 (15%) |
| 31  | CLA  | 3     | 305 | -    | 44,49,73     | 1.41 | 10 (22%) | 50,84,113   | 1.54 | 5 (10%)  |
| 31  | CLA  | 6     | 206 | 25   | 49,53,73     | 1.35 | 8 (16%)  | 58,89,113   | 1.51 | 5 (8%)   |
| 44  | DD6  | 7     | 303 | -    | 40,45,45     | 1.58 | 2 (5%)   | 51,67,67    | 2.16 | 17 (33%) |
| 39  | DGD  | C     | 520 | -    | 63,63,67     | 0.85 | 2 (3%)   | 77,77,81    | 0.93 | 3 (3%)   |
| 31  | CLA  | P     | 605 | -    | 39,45,73     | 1.46 | 10 (25%) | 51,79,113   | 1.64 | 5 (9%)   |
| 31  | CLA  | c     | 508 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.32 | 4 (4%)   |
| 31  | CLA  | 2     | 310 | 24   | 59,63,73     | 1.25 | 8 (13%)  | 70,101,113  | 1.37 | 6 (8%)   |
| 34  | SQD  | 5     | 316 | -    | 46,48,54     | 1.03 | 6 (13%)  | 56,59,65    | 1.39 | 8 (14%)  |
| 31  | CLA  | 1     | 205 | -    | 45,49,73     | 1.41 | 9 (20%)  | 54,84,113   | 1.46 | 5 (9%)   |
| 34  | SQD  | B     | 523 | -    | 38,40,54     | 1.11 | 3 (7%)   | 48,51,65    | 1.70 | 11 (22%) |
| 31  | CLA  | 0     | 309 | 23   | 45,49,73     | 1.41 | 9 (20%)  | 54,84,113   | 1.50 | 6 (11%)  |
| 34  | SQD  | b     | 501 | -    | 38,40,54     | 1.11 | 3 (7%)   | 48,51,65    | 1.70 | 11 (22%) |
| 37  | LMG  | B     | 520 | -    | 28,28,55     | 0.94 | 1 (3%)   | 36,36,63    | 1.35 | 7 (19%)  |
| 31  | CLA  | P     | 606 | -    | 39,45,73     | 1.50 | 10 (25%) | 49,78,113   | 1.51 | 6 (12%)  |
| 37  | LMG  | m     | 101 | -    | 51,51,55     | 0.77 | 1 (1%)   | 59,59,63    | 1.41 | 9 (15%)  |
| 31  | CLA  | B     | 513 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 31  | CLA  | 6     | 201 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.48 | 7 (11%)  |
| 34  | SQD  | a     | 409 | -    | 52,54,54     | 0.96 | 4 (7%)   | 62,65,65    | 1.43 | 8 (12%)  |
| 42  | A86  | p     | 610 | -    | 47,50,50     | 1.60 | 7 (14%)  | 51,76,76    | 3.91 | 24 (47%) |
| 39  | DGD  | c     | 519 | -    | 63,63,67     | 0.92 | 3 (4%)   | 77,77,81    | 1.45 | 12 (15%) |
| 31  | CLA  | p     | 602 | -    | 45,49,73     | 1.39 | 9 (20%)  | 54,84,113   | 1.60 | 9 (16%)  |
| 31  | CLA  | C     | 503 | -    | 68,72,73     | 1.18 | 9 (13%)  | 80,111,113  | 1.31 | 6 (7%)   |
| 31  | CLA  | d     | 401 | -    | 63,67,73     | 1.20 | 8 (12%)  | 74,105,113  | 1.37 | 7 (9%)   |
| 36  | LHG  | h     | 103 | -    | 41,41,48     | 0.65 | 1 (2%)   | 44,47,54    | 1.16 | 3 (6%)   |
| 31  | CLA  | 6     | 210 | 25   | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 31  | CLA  | B     | 510 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 4 (4%)   |
| 44  | DD6  | P     | 611 | -    | 40,45,45     | 1.55 | 2 (5%)   | 51,67,67    | 1.87 | 14 (27%) |
| 31  | CLA  | 4     | 208 | -    | 43,48,73     | 1.45 | 10 (23%) | 51,83,113   | 1.61 | 8 (15%)  |
| 42  | A86  | 4     | 202 | -    | 47,50,50     | 1.85 | 7 (14%)  | 51,76,76    | 3.72 | 28 (54%) |
| 31  | CLA  | C     | 514 | -    | 53,57,73     | 1.30 | 8 (15%)  | 61,93,113   | 1.44 | 6 (9%)   |
| 31  | CLA  | B     | 504 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.38 | 7 (8%)   |
| 31  | CLA  | 6     | 208 | -    | 51,55,73     | 1.33 | 8 (15%)  | 60,91,113   | 1.41 | 5 (8%)   |
| 31  | CLA  | 8     | 313 | -    | 41,47,73     | 1.43 | 10 (24%) | 51,81,113   | 1.46 | 4 (7%)   |
| 31  | CLA  | Z     | 101 | -    | 55,59,73     | 1.31 | 8 (14%)  | 64,96,113   | 1.35 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 44  | DD6  | 8     | 303 | -    | 40,45,45     | 1.61 | 3 (7%)   | 51,67,67    | 2.83 | 16 (31%) |
| 31  | CLA  | C     | 511 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 31  | CLA  | B     | 506 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.33 | 6 (7%)   |
| 31  | CLA  | a     | 407 | -    | 64,68,73     | 1.19 | 8 (12%)  | 76,107,113  | 1.35 | 9 (11%)  |
| 41  | HEM  | f     | 101 | 5,6  | 50,50,50     | 1.36 | 9 (18%)  | 67,82,82    | 1.03 | 1 (1%)   |
| 31  | CLA  | C     | 504 | -    | 55,59,73     | 1.30 | 9 (16%)  | 64,96,113   | 1.46 | 7 (10%)  |
| 37  | LMG  | M     | 101 | -    | 51,51,55     | 0.76 | 1 (1%)   | 59,59,63    | 1.41 | 9 (15%)  |
| 31  | CLA  | 2     | 312 | 24   | 39,44,73     | 1.55 | 9 (23%)  | 50,77,113   | 1.59 | 9 (18%)  |
| 31  | CLA  | P     | 607 | -    | 38,44,73     | 1.61 | 10 (26%) | 50,77,113   | 1.48 | 6 (12%)  |
| 40  | BCT  | d     | 402 | 30   | 3,3,3        | 1.12 | 0        | 2,3,3       | 4.14 | 2 (100%) |
| 31  | CLA  | 5     | 314 | 23   | 40,46,73     | 1.47 | 8 (20%)  | 52,80,113   | 1.49 | 6 (11%)  |
| 37  | LMG  | j     | 101 | -    | 50,50,55     | 0.80 | 1 (2%)   | 58,58,63    | 1.34 | 6 (10%)  |
| 31  | CLA  | b     | 508 | -    | 45,49,73     | 1.39 | 9 (20%)  | 54,84,113   | 1.51 | 7 (12%)  |
| 31  | CLA  | c     | 503 | -    | 68,72,73     | 1.17 | 9 (13%)  | 80,111,113  | 1.31 | 6 (7%)   |
| 42  | A86  | 5     | 317 | -    | 47,50,50     | 1.54 | 5 (10%)  | 51,76,76    | 2.60 | 17 (33%) |
| 31  | CLA  | D     | 404 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.32 | 5 (6%)   |
| 36  | LHG  | D     | 407 | -    | 44,47,48     | 0.56 | 1 (2%)   | 44,51,54    | 1.23 | 6 (13%)  |
| 33  | BCR  | b     | 520 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 31  | CLA  | b     | 509 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 31  | CLA  | p     | 605 | -    | 39,45,73     | 1.46 | 10 (25%) | 51,79,113   | 1.65 | 5 (9%)   |
| 31  | CLA  | 4     | 210 | -    | 40,46,73     | 1.44 | 9 (22%)  | 52,80,113   | 1.58 | 7 (13%)  |
| 37  | LMG  | m     | 102 | -    | 40,40,55     | 0.86 | 1 (2%)   | 48,48,63    | 1.30 | 5 (10%)  |
| 31  | CLA  | P     | 609 | -    | 42,47,73     | 1.44 | 9 (21%)  | 53,81,113   | 1.56 | 5 (9%)   |
| 31  | CLA  | c     | 510 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 31  | CLA  | 5     | 307 | -    | 65,69,73     | 1.20 | 7 (10%)  | 77,108,113  | 1.32 | 6 (7%)   |
| 41  | HEM  | F     | 101 | 5,6  | 50,50,50     | 1.35 | 8 (16%)  | 67,82,82    | 1.02 | 1 (1%)   |
| 31  | CLA  | 1     | 215 | -    | 40,46,73     | 1.45 | 8 (20%)  | 52,80,113   | 1.51 | 5 (9%)   |
| 31  | CLA  | 9     | 206 | -    | 39,45,73     | 1.48 | 9 (23%)  | 49,78,113   | 1.50 | 5 (10%)  |
| 31  | CLA  | 3     | 308 | -    | 40,43,73     | 1.57 | 11 (27%) | 46,73,113   | 2.00 | 5 (10%)  |
| 31  | CLA  | 0     | 310 | 23   | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.34 | 6 (8%)   |
| 31  | CLA  | C     | 513 | -    | 68,72,73     | 1.16 | 9 (13%)  | 80,111,113  | 1.27 | 6 (7%)   |
| 31  | CLA  | 0     | 311 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.47 | 4 (6%)   |
| 33  | BCR  | c     | 517 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 36  | LHG  | d     | 411 | -    | 33,33,48     | 0.73 | 2 (6%)   | 36,39,54    | 1.34 | 4 (11%)  |
| 32  | PHO  | a     | 405 | -    | 58,69,69     | 2.14 | 10 (17%) | 55,99,99    | 1.52 | 8 (14%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | BCR  | a     | 408 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.17 | 6 (10%)  |
| 31  | CLA  | 6     | 209 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.45 | 6 (10%)  |
| 31  | CLA  | 8     | 306 | -    | 35,41,73     | 1.74 | 10 (28%) | 47,72,113   | 1.65 | 8 (17%)  |
| 31  | CLA  | 4     | 211 | -    | 37,42,73     | 1.64 | 10 (27%) | 47,74,113   | 1.50 | 5 (10%)  |
| 31  | CLA  | w     | 202 | 19   | 49,53,73     | 1.36 | 10 (20%) | 58,89,113   | 1.46 | 7 (12%)  |
| 37  | LMG  | C     | 521 | -    | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 1.05 | 4 (6%)   |
| 31  | CLA  | B     | 512 | -    | 45,49,73     | 1.37 | 7 (15%)  | 54,84,113   | 1.57 | 8 (14%)  |
| 31  | CLA  | 2     | 309 | 24   | 63,67,73     | 1.21 | 9 (14%)  | 74,105,113  | 1.33 | 7 (9%)   |
| 31  | CLA  | 5     | 304 | -    | 45,49,73     | 1.40 | 8 (17%)  | 54,84,113   | 1.51 | 6 (11%)  |
| 39  | DGD  | H     | 102 | -    | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 1.42 | 10 (12%) |
| 42  | A86  | 5     | 301 | -    | 47,50,50     | 1.61 | 5 (10%)  | 51,76,76    | 3.00 | 18 (35%) |
| 31  | CLA  | p     | 601 | 26   | 39,44,73     | 1.51 | 8 (20%)  | 50,77,113   | 1.69 | 7 (14%)  |
| 39  | DGD  | h     | 102 | -    | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 1.42 | 10 (12%) |
| 31  | CLA  | 8     | 312 | -    | 44,49,73     | 1.40 | 7 (15%)  | 50,84,113   | 1.42 | 4 (8%)   |
| 44  | DD6  | 7     | 304 | -    | 40,45,45     | 1.58 | 2 (5%)   | 51,67,67    | 2.45 | 15 (29%) |
| 31  | CLA  | d     | 404 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 5 (6%)   |
| 31  | CLA  | P     | 602 | -    | 45,49,73     | 1.39 | 9 (20%)  | 54,84,113   | 1.60 | 9 (16%)  |
| 31  | CLA  | 3     | 309 | -    | 43,48,73     | 1.40 | 8 (18%)  | 51,83,113   | 1.69 | 6 (11%)  |
| 31  | CLA  | 0     | 307 | -    | 65,69,73     | 1.21 | 8 (12%)  | 77,108,113  | 1.33 | 6 (7%)   |
| 42  | A86  | 9     | 201 | -    | 47,50,50     | 1.68 | 6 (12%)  | 51,76,76    | 3.94 | 22 (43%) |
| 31  | CLA  | 1     | 212 | -    | 45,49,73     | 1.41 | 7 (15%)  | 54,84,113   | 1.48 | 6 (11%)  |
| 31  | CLA  | 7     | 308 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.45 | 6 (10%)  |
| 35  | PL9  | a     | 410 | -    | 32,32,55     | 1.09 | 4 (12%)  | 39,40,69    | 1.57 | 9 (23%)  |
| 31  | CLA  | 2     | 313 | 24   | 40,46,73     | 1.47 | 7 (17%)  | 52,80,113   | 1.49 | 6 (11%)  |
| 31  | CLA  | 0     | 313 | 23   | 40,46,73     | 1.46 | 8 (20%)  | 52,80,113   | 1.52 | 5 (9%)   |
| 31  | CLA  | B     | 509 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 31  | CLA  | 6     | 215 | -    | 40,46,73     | 1.45 | 8 (20%)  | 52,80,113   | 1.51 | 5 (9%)   |
| 37  | LMG  | M     | 102 | -    | 40,40,55     | 0.86 | 1 (2%)   | 48,48,63    | 1.30 | 4 (8%)   |
| 31  | CLA  | P     | 608 | -    | 41,46,73     | 1.55 | 10 (24%) | 49,80,113   | 1.52 | 8 (16%)  |
| 44  | DD6  | 3     | 303 | -    | 40,45,45     | 1.61 | 3 (7%)   | 51,67,67    | 2.83 | 16 (31%) |
| 42  | A86  | 5     | 303 | -    | 47,50,50     | 1.53 | 7 (14%)  | 51,76,76    | 2.74 | 22 (43%) |
| 31  | CLA  | 6     | 207 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.41 | 6 (10%)  |
| 33  | BCR  | A     | 408 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.17 | 6 (10%)  |
| 31  | CLA  | 9     | 204 | -    | 40,46,73     | 1.46 | 9 (22%)  | 52,80,113   | 1.52 | 5 (9%)   |
| 36  | LHG  | a     | 411 | -    | 42,42,48     | 0.70 | 1 (2%)   | 45,48,54    | 1.29 | 5 (11%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 7     | 305 | -    | 45,49,73     | 1.41 | 8 (17%)  | 54,84,113   | 1.51 | 6 (11%)  |
| 31  | CLA  | 1     | 214 | 25   | 40,46,73     | 1.45 | 8 (20%)  | 52,80,113   | 1.53 | 7 (13%)  |
| 31  | CLA  | C     | 507 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 36  | LHG  | d     | 412 | -    | 27,27,48     | 0.89 | 2 (7%)   | 30,32,54    | 1.77 | 4 (13%)  |
| 31  | CLA  | P     | 604 | -    | 43,48,73     | 1.40 | 9 (20%)  | 51,83,113   | 1.58 | 7 (13%)  |
| 31  | CLA  | c     | 513 | -    | 68,72,73     | 1.16 | 8 (11%)  | 80,111,113  | 1.26 | 6 (7%)   |
| 42  | A86  | 0     | 301 | -    | 47,50,50     | 1.61 | 5 (10%)  | 51,76,76    | 3.00 | 18 (35%) |
| 31  | CLA  | 2     | 316 | -    | 45,49,73     | 1.41 | 8 (17%)  | 54,84,113   | 1.48 | 6 (11%)  |
| 37  | LMG  | d     | 410 | -    | 40,40,55     | 0.94 | 3 (7%)   | 48,48,63    | 1.36 | 6 (12%)  |
| 31  | CLA  | 5     | 311 | -    | 49,53,73     | 1.37 | 9 (18%)  | 58,89,113   | 1.47 | 4 (6%)   |
| 31  | CLA  | 5     | 305 | 23   | 65,69,73     | 1.21 | 9 (13%)  | 77,108,113  | 1.33 | 6 (7%)   |
| 31  | CLA  | 5     | 308 | -    | 65,69,73     | 1.21 | 8 (12%)  | 77,108,113  | 1.33 | 6 (7%)   |
| 31  | CLA  | p     | 608 | -    | 41,46,73     | 1.56 | 10 (24%) | 49,80,113   | 1.54 | 8 (16%)  |
| 31  | CLA  | 2     | 311 | -    | 47,51,73     | 1.38 | 8 (17%)  | 55,86,113   | 1.38 | 6 (10%)  |
| 29  | OEX  | A     | 401 | 3,1  | 0,15,15      | -    | -        | -           | -    | -        |
| 31  | CLA  | b     | 505 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.37 | 6 (7%)   |
| 31  | CLA  | d     | 403 | -    | 66,70,73     | 1.27 | 10 (15%) | 80,109,113  | 1.34 | 8 (10%)  |
| 33  | BCR  | d     | 405 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 31  | CLA  | b     | 502 | -    | 47,51,73     | 1.37 | 8 (17%)  | 55,86,113   | 1.46 | 4 (7%)   |
| 31  | CLA  | 9     | 209 | -    | 45,49,73     | 1.37 | 9 (20%)  | 54,84,113   | 1.56 | 5 (9%)   |
| 35  | PL9  | A     | 410 | -    | 32,32,55     | 1.09 | 4 (12%)  | 39,40,69    | 1.57 | 9 (23%)  |
| 33  | BCR  | H     | 101 | -    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 31  | CLA  | 3     | 310 | -    | 40,43,73     | 1.58 | 10 (25%) | 48,75,113   | 1.61 | 5 (10%)  |
| 33  | BCR  | B     | 517 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 31  | CLA  | b     | 503 | -    | 64,69,73     | 1.18 | 8 (12%)  | 73,106,113  | 1.26 | 5 (6%)   |
| 31  | CLA  | b     | 513 | -    | 45,49,73     | 1.36 | 7 (15%)  | 54,84,113   | 1.57 | 8 (14%)  |
| 37  | LMG  | D     | 410 | -    | 40,40,55     | 0.94 | 3 (7%)   | 48,48,63    | 1.36 | 6 (12%)  |
| 31  | CLA  | B     | 508 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 31  | CLA  | 5     | 309 | 23   | 45,49,73     | 1.40 | 8 (17%)  | 54,84,113   | 1.50 | 6 (11%)  |
| 31  | CLA  | c     | 512 | 3    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 37  | LMG  | 0     | 315 | -    | 48,48,55     | 0.77 | 0        | 56,56,63    | 1.29 | 6 (10%)  |
| 36  | LHG  | H     | 103 | -    | 41,41,48     | 0.66 | 1 (2%)   | 44,47,54    | 1.17 | 3 (6%)   |
| 42  | A86  | 3     | 302 | -    | 47,50,50     | 1.81 | 7 (14%)  | 51,76,76    | 3.04 | 24 (47%) |
| 34  | SQD  | 0     | 316 | -    | 46,48,54     | 1.04 | 6 (13%)  | 56,59,65    | 1.39 | 8 (14%)  |
| 31  | CLA  | C     | 505 | -    | 68,72,73     | 1.16 | 8 (11%)  | 80,111,113  | 1.30 | 4 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 1     | 213 | 25   | 43,48,73     | 1.43 | 8 (18%)  | 51,83,113   | 1.44 | 5 (9%)   |
| 36  | LHG  | A     | 412 | -    | 42,42,48     | 0.70 | 1 (2%)   | 45,48,54    | 1.29 | 5 (11%)  |
| 31  | CLA  | 6     | 211 | 25   | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.33 | 6 (8%)   |
| 33  | BCR  | B     | 518 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 33  | BCR  | C     | 516 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.30 | 8 (14%)  |
| 31  | CLA  | 8     | 304 | -    | 39,42,73     | 1.66 | 12 (30%) | 49,74,113   | 1.62 | 7 (14%)  |
| 31  | CLA  | p     | 609 | -    | 42,47,73     | 1.44 | 9 (21%)  | 53,81,113   | 1.56 | 7 (13%)  |
| 31  | CLA  | 4     | 213 | -    | 37,43,73     | 1.66 | 10 (27%) | 49,76,113   | 1.69 | 10 (20%) |
| 31  | CLA  | D     | 403 | -    | 66,70,73     | 1.28 | 10 (15%) | 80,109,113  | 1.34 | 8 (10%)  |
| 31  | CLA  | b     | 507 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.33 | 6 (7%)   |
| 31  | CLA  | 3     | 313 | -    | 41,47,73     | 1.43 | 10 (24%) | 51,81,113   | 1.47 | 4 (7%)   |
| 31  | CLA  | b     | 516 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 31  | CLA  | b     | 511 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 4 (4%)   |
| 37  | LMG  | d     | 409 | -    | 37,37,55     | 0.78 | 0        | 45,45,63    | 1.33 | 7 (15%)  |
| 31  | CLA  | 1     | 209 | -    | 48,52,73     | 1.49 | 9 (18%)  | 59,88,113   | 1.45 | 6 (10%)  |
| 31  | CLA  | c     | 502 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 42  | A86  | 8     | 301 | -    | 47,50,50     | 1.77 | 9 (19%)  | 51,76,76    | 4.95 | 22 (43%) |
| 31  | CLA  | b     | 504 | -    | 68,72,73     | 1.17 | 9 (13%)  | 80,111,113  | 1.28 | 6 (7%)   |
| 31  | CLA  | 7     | 306 | 24   | 49,53,73     | 1.36 | 8 (16%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 34  | SQD  | A     | 411 | -    | 52,54,54     | 0.94 | 2 (3%)   | 62,65,65    | 1.60 | 12 (19%) |
| 31  | CLA  | 1     | 216 | 25   | 40,46,73     | 1.45 | 6 (15%)  | 52,80,113   | 1.47 | 5 (9%)   |
| 29  | OEX  | a     | 401 | 3,1  | 0,15,15      | -    | -        | -           | -    | -        |
| 31  | CLA  | 3     | 312 | -    | 44,49,73     | 1.40 | 8 (18%)  | 50,84,113   | 1.43 | 4 (8%)   |
| 31  | CLA  | 1     | 207 | -    | 48,52,73     | 1.49 | 9 (18%)  | 59,88,113   | 1.41 | 6 (10%)  |
| 36  | LHG  | D     | 412 | -    | 27,27,48     | 0.89 | 2 (7%)   | 30,32,54    | 1.76 | 4 (13%)  |
| 42  | A86  | 8     | 302 | -    | 47,50,50     | 1.81 | 7 (14%)  | 51,76,76    | 3.03 | 24 (47%) |
| 36  | LHG  | A     | 413 | -    | 25,25,48     | 0.83 | 1 (4%)   | 28,31,54    | 1.31 | 2 (7%)   |
| 31  | CLA  | 3     | 307 | -    | 46,50,73     | 1.37 | 10 (21%) | 55,84,113   | 1.42 | 5 (9%)   |
| 33  | BCR  | c     | 516 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.31 | 8 (14%)  |
| 31  | CLA  | 3     | 304 | -    | 39,42,73     | 1.66 | 12 (30%) | 49,74,113   | 1.63 | 7 (14%)  |
| 31  | CLA  | a     | 403 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 31  | CLA  | 9     | 210 | -    | 40,46,73     | 1.44 | 9 (22%)  | 52,80,113   | 1.57 | 7 (13%)  |
| 31  | CLA  | 1     | 201 | -    | 48,52,73     | 1.48 | 9 (18%)  | 59,88,113   | 1.48 | 7 (11%)  |
| 44  | DD6  | 6     | 204 | -    | 40,45,45     | 1.72 | 3 (7%)   | 51,67,67    | 2.31 | 14 (27%) |
| 31  | CLA  | 8     | 310 | -    | 40,43,73     | 1.58 | 10 (25%) | 48,75,113   | 1.61 | 5 (10%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | BCR  | C     | 517 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 35  | PL9  | d     | 406 | -    | 55,55,55     | 1.32 | 5 (9%)   | 68,69,69    | 1.53 | 12 (17%) |
| 31  | CLA  | 8     | 311 | 28   | 43,48,73     | 1.43 | 8 (18%)  | 51,83,113   | 1.57 | 6 (11%)  |
| 41  | HEM  | V     | 201 | 18   | 50,50,50     | 1.29 | 5 (10%)  | 67,82,82    | 1.27 | 5 (7%)   |
| 33  | BCR  | D     | 405 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 31  | CLA  | c     | 506 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 31  | CLA  | 4     | 204 | -    | 40,46,73     | 1.46 | 9 (22%)  | 52,80,113   | 1.53 | 5 (9%)   |
| 37  | LMG  | b     | 521 | -    | 28,28,55     | 0.95 | 1 (3%)   | 36,36,63    | 1.35 | 7 (19%)  |
| 31  | CLA  | 7     | 307 | -    | 51,55,73     | 1.33 | 9 (17%)  | 60,91,113   | 1.44 | 5 (8%)   |
| 31  | CLA  | 7     | 312 | 24   | 39,44,73     | 1.56 | 10 (25%) | 50,77,113   | 1.60 | 10 (20%) |
| 31  | CLA  | 0     | 305 | 23   | 65,69,73     | 1.21 | 9 (13%)  | 77,108,113  | 1.34 | 6 (7%)   |
| 44  | DD6  | p     | 611 | -    | 40,45,45     | 1.54 | 2 (5%)   | 51,67,67    | 1.87 | 14 (27%) |
| 31  | CLA  | D     | 401 | -    | 63,67,73     | 1.20 | 8 (12%)  | 74,105,113  | 1.37 | 7 (9%)   |
| 42  | A86  | 0     | 317 | -    | 47,50,50     | 1.54 | 5 (10%)  | 51,76,76    | 2.60 | 17 (33%) |
| 31  | CLA  | 0     | 306 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 31  | CLA  | 5     | 310 | 23   | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.33 | 6 (8%)   |
| 33  | BCR  | B     | 519 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 40  | BCT  | D     | 402 | 30   | 3,3,3        | 1.11 | 0        | 2,3,3       | 4.14 | 2 (100%) |
| 42  | A86  | 2     | 302 | -    | 47,50,50     | 1.79 | 7 (14%)  | 51,76,76    | 2.85 | 17 (33%) |
| 42  | A86  | 9     | 202 | -    | 47,50,50     | 1.85 | 7 (14%)  | 51,76,76    | 3.72 | 28 (54%) |
| 31  | CLA  | B     | 507 | -    | 45,49,73     | 1.40 | 9 (20%)  | 54,84,113   | 1.51 | 6 (11%)  |
| 33  | BCR  | h     | 101 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 31  | CLA  | 0     | 308 | -    | 65,69,73     | 1.21 | 9 (13%)  | 77,108,113  | 1.32 | 6 (7%)   |
| 31  | CLA  | B     | 501 | -    | 47,51,73     | 1.37 | 8 (17%)  | 55,86,113   | 1.45 | 4 (7%)   |
| 32  | PHO  | A     | 405 | -    | 58,69,69     | 2.14 | 10 (17%) | 55,99,99    | 1.53 | 8 (14%)  |
| 31  | CLA  | 5     | 312 | -    | 46,50,73     | 1.40 | 8 (17%)  | 53,85,113   | 1.44 | 4 (7%)   |
| 37  | LMG  | d     | 408 | -    | 46,46,55     | 0.76 | 1 (2%)   | 54,54,63    | 1.34 | 7 (12%)  |
| 31  | CLA  | C     | 508 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.31 | 4 (4%)   |
| 31  | CLA  | B     | 502 | -    | 64,69,73     | 1.18 | 9 (14%)  | 73,106,113  | 1.25 | 5 (6%)   |
| 31  | CLA  | 7     | 314 | -    | 40,46,73     | 1.47 | 8 (20%)  | 52,80,113   | 1.51 | 6 (11%)  |
| 31  | CLA  | P     | 603 | -    | 39,45,73     | 1.48 | 9 (23%)  | 51,79,113   | 1.65 | 7 (13%)  |
| 31  | CLA  | b     | 512 | -    | 68,72,73     | 1.18 | 9 (13%)  | 80,111,113  | 1.33 | 7 (8%)   |
| 31  | CLA  | P     | 601 | 26   | 39,44,73     | 1.51 | 8 (20%)  | 50,77,113   | 1.67 | 7 (14%)  |
| 31  | CLA  | 9     | 208 | -    | 43,48,73     | 1.45 | 10 (23%) | 51,83,113   | 1.61 | 8 (15%)  |
| 31  | CLA  | b     | 506 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 7     | 315 | 24   | 40,46,73     | 1.47 | 8 (20%)  | 52,80,113   | 1.51 | 6 (11%)  |
| 37  | LMG  | Y     | 101 | -    | 46,46,55     | 0.75 | 1 (2%)   | 54,54,63    | 1.39 | 11 (20%) |
| 37  | LMG  | W     | 201 | -    | 48,48,55     | 0.76 | 1 (2%)   | 56,56,63    | 1.34 | 7 (12%)  |
| 31  | CLA  | C     | 506 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 31  | CLA  | 4     | 212 | -    | 40,44,73     | 1.60 | 10 (25%) | 51,77,113   | 1.53 | 6 (11%)  |
| 31  | CLA  | b     | 514 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 44  | DD6  | 1     | 204 | -    | 40,45,45     | 1.71 | 3 (7%)   | 51,67,67    | 2.30 | 14 (27%) |
| 42  | A86  | 2     | 301 | -    | 47,50,50     | 1.54 | 5 (10%)  | 51,76,76    | 2.59 | 18 (35%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 7     | 309 | 24   | 1/1/13/20 | 10/32/108/115 | -       |
| 37  | LMG  | y     | 101 | -    | -         | 18/41/61/70   | 0/1/1/1 |
| 39  | DGD  | C     | 518 | -    | -         | 19/44/84/95   | 0/2/2/2 |
| 31  | CLA  | 8     | 309 | -    | 1/1/10/20 | 3/8/84/115    | -       |
| 31  | CLA  | 9     | 213 | -    | 1/1/8/20  | -             | -       |
| 32  | PHO  | a     | 406 | -    | -         | 11/37/103/103 | 0/5/6/6 |
| 31  | CLA  | B     | 505 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 4     | 205 | -    | 1/1/7/20  | 0/2/70/115    | -       |
| 31  | CLA  | B     | 516 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 42  | A86  | 1     | 202 | -    | -         | 7/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 6     | 212 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 36  | LHG  | d     | 407 | -    | -         | 22/47/51/53   | -       |
| 34  | SQD  | B     | 522 | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 42  | A86  | 6     | 202 | -    | -         | 7/34/90/90    | 0/3/3/3 |
| 42  | A86  | 4     | 203 | -    | -         | 6/34/90/90    | 0/3/3/3 |
| 44  | DD6  | 2     | 303 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 31  | CLA  | 2     | 305 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 35  | PL9  | D     | 406 | -    | -         | 8/53/73/73    | 0/1/1/1 |
| 31  | CLA  | C     | 502 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | c     | 504 | -    | 1/1/12/20 | 4/23/99/115   | -       |
| 31  | CLA  | 0     | 312 | -    | 1/1/10/20 | 6/12/88/115   | -       |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 1     | 210 | 25   | 1/1/15/20 | 16/39/115/115 | -       |
| 31  | CLA  | 8     | 314 | -    | 1/1/8/20  | -             | -       |
| 37  | LMG  | D     | 409 | -    | -         | 13/32/52/70   | 0/1/1/1 |
| 31  | CLA  | 6     | 214 | 25   | 1/1/9/20  | 0/4/80/115    | -       |
| 31  | CLA  | 3     | 306 | -    | 1/1/7/20  | -             | -       |
| 42  | A86  | 9     | 203 | -    | -         | 6/34/90/90    | 0/3/3/3 |
| 37  | LMG  | 5     | 315 | -    | -         | 26/43/63/70   | 0/1/1/1 |
| 44  | DD6  | 6     | 203 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 31  | CLA  | B     | 514 | -    | 1/1/13/20 | 12/33/109/115 | -       |
| 31  | CLA  | 6     | 216 | 25   | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | 4     | 207 | -    | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | c     | 509 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 31  | CLA  | a     | 404 | -    | 1/1/11/20 | 1/20/96/115   | -       |
| 31  | CLA  | 1     | 206 | 25   | 1/1/11/20 | 6/15/91/115   | -       |
| 42  | A86  | 7     | 301 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 42  | A86  | P     | 610 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 3     | 311 | 28   | 1/1/10/20 | 2/8/84/115    | -       |
| 31  | CLA  | W     | 202 | 19   | 1/1/11/20 | 3/15/91/115   | -       |
| 33  | BCR  | k     | 101 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 36  | LHG  | B     | 521 | -    | -         | 18/53/53/53   | -       |
| 31  | CLA  | 7     | 316 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | 8     | 308 | -    | 1/1/6/20  | 4/6/66/115    | -       |
| 37  | LMG  | J     | 101 | -    | -         | 29/45/65/70   | 0/1/1/1 |
| 31  | CLA  | 3     | 314 | -    | 1/1/8/20  | -             | -       |
| 31  | CLA  | C     | 510 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 31  | CLA  | 9     | 212 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 31  | CLA  | B     | 511 | -    | 1/1/14/20 | 12/37/113/115 | -       |
| 31  | CLA  | 1     | 208 | -    | 1/1/11/20 | 6/18/94/115   | -       |
| 31  | CLA  | 9     | 211 | -    | 1/1/7/20  | -             | -       |
| 31  | CLA  | 5     | 313 | 23   | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | 9     | 207 | -    | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | z     | 101 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 31  | CLA  | b     | 517 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 31  | CLA  | 4     | 206 | -    | 1/1/8/20  | 2/4/76/115    | -       |
| 31  | CLA  | 9     | 205 | -    | 1/1/7/20  | 0/2/70/115    | -       |
| 36  | LHG  | a     | 412 | -    | -         | 11/29/29/53   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 43  | ET4  | 0     | 302 | -    | -         | 9/25/67/67    | 0/2/2/2 |
| 37  | LMG  | w     | 201 | -    | -         | 26/43/63/70   | 0/1/1/1 |
| 33  | BCR  | b     | 518 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 42  | A86  | 7     | 302 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 2     | 306 | 24   | 1/1/11/20 | 3/15/91/115   | -       |
| 31  | CLA  | A     | 404 | -    | 1/1/11/20 | 1/20/96/115   | -       |
| 33  | BCR  | K     | 101 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 37  | LMG  | c     | 521 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 31  | CLA  | A     | 407 | -    | 1/1/14/20 | 4/33/109/115  | -       |
| 31  | CLA  | c     | 507 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 42  | A86  | 3     | 301 | -    | -         | 12/34/90/90   | 0/3/3/3 |
| 31  | CLA  | p     | 604 | -    | 1/1/10/20 | 2/8/84/115    | -       |
| 31  | CLA  | C     | 512 | 3    | 1/1/15/20 | 8/39/115/115  | -       |
| 44  | DD6  | 1     | 203 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 43  | ET4  | 5     | 302 | -    | -         | 9/25/67/67    | 0/2/2/2 |
| 31  | CLA  | c     | 511 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | 8     | 305 | -    | 1/1/10/20 | 3/10/86/115   | -       |
| 31  | CLA  | 1     | 211 | 25   | 1/1/13/20 | 5/27/103/115  | -       |
| 31  | CLA  | b     | 510 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 2     | 315 | 24   | 1/1/9/20  | 2/4/80/115    | -       |
| 37  | LMG  | D     | 408 | -    | -         | 16/41/61/70   | 0/1/1/1 |
| 31  | CLA  | 5     | 306 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 31  | CLA  | c     | 514 | -    | 1/1/11/20 | 5/20/96/115   | -       |
| 39  | DGD  | c     | 518 | -    | -         | 19/44/84/95   | 0/2/2/2 |
| 32  | PHO  | A     | 406 | -    | -         | 11/37/103/103 | 0/5/6/6 |
| 42  | A86  | 0     | 303 | -    | -         | 5/34/90/90    | 0/3/3/3 |
| 31  | CLA  | p     | 607 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 31  | CLA  | 0     | 314 | 23   | 1/1/9/20  | 0/4/80/115    | -       |
| 36  | LHG  | D     | 411 | -    | -         | 26/38/38/53   | -       |
| 31  | CLA  | 7     | 311 | -    | 1/1/10/20 | 5/13/89/115   | -       |
| 33  | BCR  | C     | 515 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 34  | SQD  | A     | 409 | -    | -         | 14/49/69/69   | 0/1/1/1 |
| 31  | CLA  | p     | 603 | -    | 1/1/9/20  | 0/2/78/115    | -       |
| 31  | CLA  | B     | 515 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 31  | CLA  | 7     | 313 | 24   | 1/1/9/20  | 2/4/80/115    | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 6     | 205 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | 8     | 307 | -    | 1/1/9/20  | 2/11/83/115   | -       |
| 31  | CLA  | p     | 606 | -    | 1/1/8/20  | 2/4/76/115    | -       |
| 31  | CLA  | 0     | 304 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 31  | CLA  | b     | 515 | -    | 1/1/13/20 | 12/33/109/115 | -       |
| 41  | HEM  | v     | 201 | 18   | -         | 6/14/54/54    | -       |
| 39  | DGD  | c     | 520 | -    | -         | 8/51/91/95    | 0/2/2/2 |
| 31  | CLA  | 2     | 307 | -    | 1/1/11/20 | 3/18/94/115   | -       |
| 31  | CLA  | A     | 403 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | C     | 509 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 36  | LHG  | b     | 522 | -    | -         | 18/53/53/53   | -       |
| 31  | CLA  | 7     | 310 | 24   | 1/1/13/20 | 10/27/103/115 | -       |
| 42  | A86  | 4     | 201 | -    | -         | 7/34/90/90    | 1/3/3/3 |
| 31  | CLA  | 2     | 314 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 44  | DD6  | 2     | 304 | -    | -         | 10/26/80/80   | 0/3/3/3 |
| 31  | CLA  | c     | 505 | -    | 1/1/14/20 | 9/37/113/115  | -       |
| 31  | CLA  | 6     | 213 | 25   | 1/1/10/20 | 5/8/84/115    | -       |
| 31  | CLA  | B     | 503 | -    | 1/1/14/20 | 11/37/113/115 | -       |
| 33  | BCR  | b     | 519 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 2     | 308 | -    | 1/1/11/20 | 7/13/89/115   | -       |
| 33  | BCR  | c     | 515 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 4     | 209 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 39  | DGD  | C     | 519 | -    | -         | 22/51/91/95   | 0/2/2/2 |
| 31  | CLA  | 3     | 305 | -    | 1/1/10/20 | 3/10/86/115   | -       |
| 31  | CLA  | 6     | 206 | 25   | 1/1/11/20 | 6/15/91/115   | -       |
| 44  | DD6  | 7     | 303 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 39  | DGD  | C     | 520 | -    | -         | 8/51/91/95    | 0/2/2/2 |
| 31  | CLA  | P     | 605 | -    | 1/1/9/20  | 2/2/78/115    | -       |
| 31  | CLA  | c     | 508 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 31  | CLA  | 2     | 310 | 24   | 1/1/13/20 | 10/27/103/115 | -       |
| 34  | SQD  | 5     | 316 | -    | -         | 18/43/63/69   | 0/1/1/1 |
| 31  | CLA  | 1     | 205 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 34  | SQD  | B     | 523 | -    | -         | 14/35/55/69   | 0/1/1/1 |
| 31  | CLA  | 0     | 309 | 23   | 1/1/10/20 | 4/10/86/115   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 34  | SQD  | b     | 501 | -    | -         | 14/35/55/69   | 0/1/1/1 |
| 37  | LMG  | B     | 520 | -    | -         | 5/23/43/70    | 0/1/1/1 |
| 31  | CLA  | P     | 606 | -    | 1/1/8/20  | 2/4/76/115    | -       |
| 37  | LMG  | m     | 101 | -    | -         | 18/46/66/70   | 0/1/1/1 |
| 31  | CLA  | B     | 513 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 31  | CLA  | 6     | 201 | -    | 1/1/11/20 | 4/13/89/115   | -       |
| 34  | SQD  | a     | 409 | -    | -         | 14/49/69/69   | 0/1/1/1 |
| 42  | A86  | p     | 610 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 39  | DGD  | c     | 519 | -    | -         | 22/51/91/95   | 0/2/2/2 |
| 31  | CLA  | p     | 602 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | C     | 503 | -    | 1/1/14/20 | 14/37/113/115 | -       |
| 31  | CLA  | d     | 401 | -    | 1/1/13/20 | 2/32/108/115  | -       |
| 36  | LHG  | h     | 103 | -    | -         | 10/46/46/53   | -       |
| 31  | CLA  | 6     | 210 | 25   | 1/1/15/20 | 16/39/115/115 | -       |
| 31  | CLA  | B     | 510 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 44  | DD6  | P     | 611 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 31  | CLA  | 4     | 208 | -    | 1/1/10/20 | 2/8/84/115    | -       |
| 42  | A86  | 4     | 202 | -    | -         | 7/34/90/90    | 0/3/3/3 |
| 31  | CLA  | C     | 514 | -    | 1/1/11/20 | 5/20/96/115   | -       |
| 31  | CLA  | B     | 504 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | 6     | 208 | -    | 1/1/11/20 | 6/18/94/115   | -       |
| 31  | CLA  | 8     | 313 | -    | 1/1/9/20  | 3/6/82/115    | -       |
| 31  | CLA  | Z     | 101 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 44  | DD6  | 8     | 303 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 31  | CLA  | C     | 511 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | B     | 506 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 31  | CLA  | a     | 407 | -    | 1/1/14/20 | 4/33/109/115  | -       |
| 41  | HEM  | f     | 101 | 5,6  | -         | 4/14/54/54    | -       |
| 31  | CLA  | C     | 504 | -    | 1/1/12/20 | 4/23/99/115   | -       |
| 37  | LMG  | M     | 101 | -    | -         | 18/46/66/70   | 0/1/1/1 |
| 31  | CLA  | 2     | 312 | 24   | 1/1/9/20  | 0/2/78/115    | -       |
| 31  | CLA  | P     | 607 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 31  | CLA  | 5     | 314 | 23   | 1/1/9/20  | 0/4/80/115    | -       |
| 37  | LMG  | j     | 101 | -    | -         | 29/45/65/70   | 0/1/1/1 |
| 31  | CLA  | b     | 508 | -    | 1/1/10/20 | 2/10/86/115   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | c     | 503 | -    | 1/1/14/20 | 14/37/113/115 | -       |
| 42  | A86  | 5     | 317 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 31  | CLA  | D     | 404 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 36  | LHG  | D     | 407 | -    | -         | 22/47/51/53   | -       |
| 33  | BCR  | b     | 520 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | b     | 509 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 31  | CLA  | p     | 605 | -    | 1/1/9/20  | 2/2/78/115    | -       |
| 31  | CLA  | 4     | 210 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 37  | LMG  | m     | 102 | -    | -         | 12/35/55/70   | 0/1/1/1 |
| 31  | CLA  | P     | 609 | -    | 1/1/9/20  | 2/6/82/115    | -       |
| 31  | CLA  | c     | 510 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 31  | CLA  | 5     | 307 | -    | 1/1/14/20 | 20/35/111/115 | -       |
| 41  | HEM  | F     | 101 | 5,6  | -         | 4/14/54/54    | -       |
| 31  | CLA  | 1     | 215 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 31  | CLA  | 9     | 206 | -    | 1/1/8/20  | 2/4/76/115    | -       |
| 31  | CLA  | 3     | 308 | -    | 1/1/6/20  | 4/6/66/115    | -       |
| 31  | CLA  | 0     | 310 | 23   | 1/1/13/20 | 5/27/103/115  | -       |
| 31  | CLA  | C     | 513 | -    | 1/1/14/20 | 17/37/113/115 | -       |
| 31  | CLA  | 0     | 311 | -    | 1/1/11/20 | 9/15/91/115   | -       |
| 33  | BCR  | c     | 517 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 36  | LHG  | d     | 411 | -    | -         | 26/38/38/53   | -       |
| 32  | PHO  | a     | 405 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 33  | BCR  | a     | 408 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 6     | 209 | -    | 1/1/11/20 | 6/13/89/115   | -       |
| 31  | CLA  | 8     | 306 | -    | 1/1/7/20  | -             | -       |
| 31  | CLA  | 4     | 211 | -    | 1/1/7/20  | -             | -       |
| 31  | CLA  | w     | 202 | 19   | 1/1/11/20 | 3/15/91/115   | -       |
| 37  | LMG  | C     | 521 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 31  | CLA  | B     | 512 | -    | 1/1/10/20 | 0/10/86/115   | -       |
| 31  | CLA  | 2     | 309 | 24   | 1/1/13/20 | 10/32/108/115 | -       |
| 31  | CLA  | 5     | 304 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 39  | DGD  | H     | 102 | -    | -         | 16/51/91/95   | 0/2/2/2 |
| 42  | A86  | 5     | 301 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 31  | CLA  | p     | 601 | 26   | 1/1/9/20  | 2/2/78/115    | -       |
| 39  | DGD  | h     | 102 | -    | -         | 16/51/91/95   | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 8     | 312 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 44  | DD6  | 7     | 304 | -    | -         | 10/26/80/80   | 0/3/3/3 |
| 31  | CLA  | d     | 404 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 31  | CLA  | P     | 602 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | 3     | 309 | -    | 1/1/10/20 | 3/8/84/115    | -       |
| 31  | CLA  | 0     | 307 | -    | 1/1/14/20 | 20/35/111/115 | -       |
| 42  | A86  | 9     | 201 | -    | -         | 7/34/90/90    | 1/3/3/3 |
| 31  | CLA  | 1     | 212 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 31  | CLA  | 7     | 308 | -    | 1/1/11/20 | 7/13/89/115   | -       |
| 35  | PL9  | a     | 410 | -    | -         | 13/25/45/73   | 0/1/1/1 |
| 31  | CLA  | 2     | 313 | 24   | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | 0     | 313 | 23   | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | B     | 509 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 6     | 215 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 37  | LMG  | M     | 102 | -    | -         | 12/35/55/70   | 0/1/1/1 |
| 31  | CLA  | P     | 608 | -    | 1/1/9/20  | 3/6/78/115    | -       |
| 44  | DD6  | 3     | 303 | -    | -         | 3/26/80/80    | 0/3/3/3 |
| 42  | A86  | 5     | 303 | -    | -         | 5/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 6     | 207 | -    | 1/1/11/20 | 5/13/89/115   | -       |
| 33  | BCR  | A     | 408 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 9     | 204 | -    | 1/1/9/20  | 2/4/80/115    | -       |
| 36  | LHG  | a     | 411 | -    | -         | 13/47/47/53   | -       |
| 31  | CLA  | 7     | 305 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 31  | CLA  | 1     | 214 | 25   | 1/1/9/20  | 0/4/80/115    | -       |
| 31  | CLA  | C     | 507 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 36  | LHG  | d     | 412 | -    | -         | 17/29/29/53   | -       |
| 31  | CLA  | P     | 604 | -    | 1/1/10/20 | 2/8/84/115    | -       |
| 31  | CLA  | c     | 513 | -    | 1/1/14/20 | 17/37/113/115 | -       |
| 42  | A86  | 0     | 301 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 2     | 316 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 37  | LMG  | d     | 410 | -    | -         | 16/35/55/70   | 0/1/1/1 |
| 31  | CLA  | 5     | 311 | -    | 1/1/11/20 | 9/15/91/115   | -       |
| 31  | CLA  | 5     | 305 | 23   | 1/1/14/20 | 13/35/111/115 | -       |
| 31  | CLA  | 5     | 308 | -    | 1/1/14/20 | 9/35/111/115  | -       |
| 31  | CLA  | p     | 608 | -    | 1/1/9/20  | 2/6/78/115    | -       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 2     | 311 | -    | 1/1/10/20 | 5/13/89/115   | -       |
| 31  | CLA  | b     | 505 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 31  | CLA  | d     | 403 | -    | 1/1/14/20 | 5/33/109/115  | -       |
| 33  | BCR  | d     | 405 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 31  | CLA  | b     | 502 | -    | 1/1/10/20 | 3/13/89/115   | -       |
| 31  | CLA  | 9     | 209 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 35  | PL9  | A     | 410 | -    | -         | 13/25/45/73   | 0/1/1/1 |
| 33  | BCR  | H     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 3     | 310 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 33  | BCR  | B     | 517 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | b     | 503 | -    | 1/1/12/20 | 14/29/107/115 | -       |
| 31  | CLA  | b     | 513 | -    | 1/1/10/20 | 0/10/86/115   | -       |
| 37  | LMG  | D     | 410 | -    | -         | 16/35/55/70   | 0/1/1/1 |
| 31  | CLA  | B     | 508 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 31  | CLA  | 5     | 309 | 23   | 1/1/10/20 | 4/10/86/115   | -       |
| 31  | CLA  | c     | 512 | 3    | 1/1/15/20 | 8/39/115/115  | -       |
| 37  | LMG  | 0     | 315 | -    | -         | 26/43/63/70   | 0/1/1/1 |
| 36  | LHG  | H     | 103 | -    | -         | 10/46/46/53   | -       |
| 42  | A86  | 3     | 302 | -    | -         | 6/34/90/90    | 0/3/3/3 |
| 34  | SQD  | 0     | 316 | -    | -         | 18/43/63/69   | 0/1/1/1 |
| 31  | CLA  | C     | 505 | -    | 1/1/14/20 | 9/37/113/115  | -       |
| 31  | CLA  | 1     | 213 | 25   | 1/1/10/20 | 5/8/84/115    | -       |
| 36  | LHG  | A     | 412 | -    | -         | 13/47/47/53   | -       |
| 31  | CLA  | 6     | 211 | 25   | 1/1/13/20 | 5/27/103/115  | -       |
| 33  | BCR  | B     | 518 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 33  | BCR  | C     | 516 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 8     | 304 | -    | 1/1/8/20  | -             | -       |
| 31  | CLA  | p     | 609 | -    | 1/1/9/20  | 2/6/82/115    | -       |
| 31  | CLA  | 4     | 213 | -    | 1/1/8/20  | -             | -       |
| 31  | CLA  | D     | 403 | -    | 1/1/14/20 | 5/33/109/115  | -       |
| 31  | CLA  | b     | 507 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 31  | CLA  | 3     | 313 | -    | 1/1/9/20  | 3/6/82/115    | -       |
| 31  | CLA  | b     | 516 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 31  | CLA  | b     | 511 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 37  | LMG  | d     | 409 | -    | -         | 13/32/52/70   | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 1     | 209 | -    | 1/1/11/20 | 6/13/89/115   | -       |
| 31  | CLA  | c     | 502 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 42  | A86  | 8     | 301 | -    | -         | 12/34/90/90   | 0/3/3/3 |
| 31  | CLA  | b     | 504 | -    | 1/1/14/20 | 11/37/113/115 | -       |
| 31  | CLA  | 7     | 306 | 24   | 1/1/11/20 | 3/15/91/115   | -       |
| 34  | SQD  | A     | 411 | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 31  | CLA  | 1     | 216 | 25   | 1/1/9/20  | 2/4/80/115    | -       |
| 31  | CLA  | 3     | 312 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 31  | CLA  | 1     | 207 | -    | 1/1/11/20 | 5/13/89/115   | -       |
| 36  | LHG  | D     | 412 | -    | -         | 17/29/29/53   | -       |
| 42  | A86  | 8     | 302 | -    | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | LHG  | A     | 413 | -    | -         | 11/29/29/53   | -       |
| 31  | CLA  | 3     | 307 | -    | 1/1/9/20  | 2/11/83/115   | -       |
| 33  | BCR  | c     | 516 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 3     | 304 | -    | 1/1/8/20  | -             | -       |
| 31  | CLA  | a     | 403 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 9     | 210 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 31  | CLA  | 1     | 201 | -    | 1/1/11/20 | 4/13/89/115   | -       |
| 44  | DD6  | 6     | 204 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 31  | CLA  | 8     | 310 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 33  | BCR  | C     | 517 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 35  | PL9  | d     | 406 | -    | -         | 8/53/73/73    | 0/1/1/1 |
| 31  | CLA  | 8     | 311 | 28   | 1/1/10/20 | 2/8/84/115    | -       |
| 41  | HEM  | V     | 201 | 18   | -         | 6/14/54/54    | -       |
| 33  | BCR  | D     | 405 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 31  | CLA  | c     | 506 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 31  | CLA  | 4     | 204 | -    | 1/1/9/20  | 2/4/80/115    | -       |
| 37  | LMG  | b     | 521 | -    | -         | 5/23/43/70    | 0/1/1/1 |
| 31  | CLA  | 7     | 307 | -    | 1/1/11/20 | 3/18/94/115   | -       |
| 31  | CLA  | 7     | 312 | 24   | 1/1/9/20  | 0/2/78/115    | -       |
| 31  | CLA  | 0     | 305 | 23   | 1/1/14/20 | 13/35/111/115 | -       |
| 44  | DD6  | p     | 611 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 31  | CLA  | D     | 401 | -    | 1/1/13/20 | 2/32/108/115  | -       |
| 42  | A86  | 0     | 317 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 31  | CLA  | 0     | 306 | -    | 1/1/11/20 | 3/15/91/115   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 5     | 310 | 23   | 1/1/13/20 | 5/27/103/115  | -       |
| 33  | BCR  | B     | 519 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 42  | A86  | 2     | 302 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 42  | A86  | 9     | 202 | -    | -         | 7/34/90/90    | 0/3/3/3 |
| 31  | CLA  | B     | 507 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 33  | BCR  | h     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 0     | 308 | -    | 1/1/14/20 | 9/35/111/115  | -       |
| 31  | CLA  | B     | 501 | -    | 1/1/10/20 | 3/13/89/115   | -       |
| 32  | PHO  | A     | 405 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 31  | CLA  | 5     | 312 | -    | 1/1/10/20 | 6/12/88/115   | -       |
| 37  | LMG  | d     | 408 | -    | -         | 16/41/61/70   | 0/1/1/1 |
| 31  | CLA  | C     | 508 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 31  | CLA  | B     | 502 | -    | 1/1/12/20 | 14/29/107/115 | -       |
| 31  | CLA  | 7     | 314 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 31  | CLA  | P     | 603 | -    | 1/1/9/20  | 0/2/78/115    | -       |
| 31  | CLA  | b     | 512 | -    | 1/1/14/20 | 12/37/113/115 | -       |
| 31  | CLA  | P     | 601 | 26   | 1/1/9/20  | 2/2/78/115    | -       |
| 31  | CLA  | 9     | 208 | -    | 1/1/10/20 | 2/8/84/115    | -       |
| 31  | CLA  | b     | 506 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 31  | CLA  | 7     | 315 | 24   | 1/1/9/20  | 2/4/80/115    | -       |
| 37  | LMG  | Y     | 101 | -    | -         | 18/41/61/70   | 0/1/1/1 |
| 37  | LMG  | W     | 201 | -    | -         | 26/43/63/70   | 0/1/1/1 |
| 31  | CLA  | C     | 506 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 31  | CLA  | 4     | 212 | -    | 1/1/8/20  | 0/2/74/115    | -       |
| 31  | CLA  | b     | 514 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 44  | DD6  | 1     | 204 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 42  | A86  | 2     | 301 | -    | -         | 8/34/90/90    | 0/3/3/3 |

All (2228) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | A     | 406 | PHO  | C1B-C2B | 9.26  | 1.49        | 1.39     |
| 32  | a     | 406 | PHO  | C1B-C2B | 9.25  | 1.49        | 1.39     |
| 32  | A     | 405 | PHO  | C1B-C2B | 9.23  | 1.49        | 1.39     |
| 32  | a     | 405 | PHO  | C1B-C2B | 9.23  | 1.49        | 1.39     |
| 44  | 6     | 204 | DD6  | C30-C31 | -9.20 | 1.24        | 1.42     |
| 44  | 1     | 204 | DD6  | C30-C31 | -9.15 | 1.24        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 44  | 7     | 304 | DD6  | C30-C31 | -8.69 | 1.25        | 1.42     |
| 44  | 2     | 304 | DD6  | C30-C31 | -8.69 | 1.25        | 1.42     |
| 32  | A     | 405 | PHO  | C3B-C4B | 8.49  | 1.50        | 1.41     |
| 32  | a     | 405 | PHO  | C3B-C4B | 8.49  | 1.50        | 1.41     |
| 44  | P     | 611 | DD6  | C30-C31 | -8.37 | 1.26        | 1.42     |
| 32  | a     | 406 | PHO  | C3B-C4B | 8.36  | 1.49        | 1.41     |
| 32  | A     | 406 | PHO  | C3B-C4B | 8.35  | 1.49        | 1.41     |
| 44  | 1     | 203 | DD6  | C30-C31 | -8.33 | 1.26        | 1.42     |
| 44  | p     | 611 | DD6  | C30-C31 | -8.32 | 1.26        | 1.42     |
| 44  | 7     | 303 | DD6  | C30-C31 | -8.28 | 1.26        | 1.42     |
| 44  | 2     | 303 | DD6  | C30-C31 | -8.28 | 1.26        | 1.42     |
| 44  | 6     | 203 | DD6  | C30-C31 | -8.27 | 1.26        | 1.42     |
| 44  | 8     | 303 | DD6  | C30-C31 | -8.21 | 1.26        | 1.42     |
| 44  | 3     | 303 | DD6  | C30-C31 | -8.19 | 1.26        | 1.42     |
| 42  | 4     | 202 | A86  | C20-C15 | 7.05  | 1.57        | 1.48     |
| 42  | 9     | 202 | A86  | C20-C15 | 7.03  | 1.57        | 1.48     |
| 42  | 4     | 203 | A86  | C20-C15 | 6.84  | 1.57        | 1.48     |
| 42  | 9     | 203 | A86  | C20-C15 | 6.80  | 1.56        | 1.48     |
| 42  | 3     | 302 | A86  | C20-C15 | 5.75  | 1.55        | 1.48     |
| 42  | 7     | 302 | A86  | C30-C31 | -5.74 | 1.23        | 1.30     |
| 42  | 2     | 302 | A86  | C30-C31 | -5.72 | 1.23        | 1.30     |
| 42  | 4     | 201 | A86  | C20-C15 | 5.69  | 1.55        | 1.48     |
| 42  | 8     | 302 | A86  | C20-C15 | 5.67  | 1.55        | 1.48     |
| 42  | 9     | 201 | A86  | C20-C15 | 5.62  | 1.55        | 1.48     |
| 42  | 4     | 202 | A86  | O4-C38  | 5.32  | 1.47        | 1.35     |
| 42  | 9     | 202 | A86  | O4-C38  | 5.30  | 1.46        | 1.35     |
| 42  | 6     | 202 | A86  | O4-C38  | 5.24  | 1.46        | 1.35     |
| 42  | 1     | 202 | A86  | O4-C38  | 5.24  | 1.46        | 1.35     |
| 42  | 0     | 301 | A86  | O4-C38  | 5.24  | 1.46        | 1.35     |
| 42  | 9     | 203 | A86  | O4-C38  | 5.22  | 1.46        | 1.35     |
| 42  | 4     | 203 | A86  | O4-C38  | 5.22  | 1.46        | 1.35     |
| 42  | 5     | 301 | A86  | O4-C38  | 5.21  | 1.46        | 1.35     |
| 42  | 2     | 302 | A86  | O4-C38  | 5.13  | 1.46        | 1.35     |
| 42  | 7     | 302 | A86  | O4-C38  | 5.11  | 1.46        | 1.35     |
| 42  | 0     | 301 | A86  | C20-C15 | 5.03  | 1.54        | 1.48     |
| 42  | 2     | 301 | A86  | O4-C38  | 5.03  | 1.46        | 1.35     |
| 42  | 5     | 301 | A86  | C20-C15 | 5.02  | 1.54        | 1.48     |
| 42  | 7     | 301 | A86  | O4-C38  | 5.02  | 1.46        | 1.35     |
| 42  | 5     | 317 | A86  | O4-C38  | 5.00  | 1.46        | 1.35     |
| 42  | 8     | 302 | A86  | C30-C31 | -5.00 | 1.24        | 1.30     |
| 42  | 0     | 317 | A86  | O4-C38  | 4.97  | 1.46        | 1.35     |
| 42  | 3     | 302 | A86  | C30-C31 | -4.96 | 1.24        | 1.30     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | p     | 610 | A86  | C20-C15 | 4.93  | 1.54        | 1.48     |
| 42  | 3     | 302 | A86  | O4-C38  | 4.92  | 1.46        | 1.35     |
| 42  | 8     | 302 | A86  | O4-C38  | 4.91  | 1.46        | 1.35     |
| 42  | P     | 610 | A86  | C20-C15 | 4.88  | 1.54        | 1.48     |
| 42  | 8     | 301 | A86  | O4-C38  | 4.74  | 1.45        | 1.35     |
| 42  | 8     | 301 | A86  | C20-C15 | 4.72  | 1.54        | 1.48     |
| 42  | 3     | 301 | A86  | C20-C15 | 4.71  | 1.54        | 1.48     |
| 42  | 3     | 301 | A86  | O4-C38  | 4.69  | 1.45        | 1.35     |
| 42  | 0     | 303 | A86  | O4-C38  | 4.60  | 1.45        | 1.35     |
| 42  | 5     | 303 | A86  | O4-C38  | 4.60  | 1.45        | 1.35     |
| 42  | 9     | 201 | A86  | O4-C38  | 4.56  | 1.45        | 1.35     |
| 42  | 4     | 201 | A86  | O4-C38  | 4.56  | 1.45        | 1.35     |
| 42  | P     | 610 | A86  | O4-C38  | 4.47  | 1.45        | 1.35     |
| 43  | 5     | 302 | ET4  | C08-C07 | 4.45  | 1.46        | 1.33     |
| 42  | p     | 610 | A86  | O4-C38  | 4.42  | 1.45        | 1.35     |
| 43  | 0     | 302 | ET4  | C08-C07 | 4.41  | 1.46        | 1.33     |
| 42  | 7     | 301 | A86  | C30-C31 | -4.30 | 1.25        | 1.30     |
| 42  | 2     | 301 | A86  | C30-C31 | -4.30 | 1.25        | 1.30     |
| 42  | 0     | 317 | A86  | C30-C31 | -4.26 | 1.25        | 1.30     |
| 42  | 0     | 317 | A86  | C20-C15 | 4.26  | 1.53        | 1.48     |
| 42  | 2     | 302 | A86  | C30-C29 | -4.25 | 1.25        | 1.31     |
| 42  | 8     | 302 | A86  | C30-C29 | -4.25 | 1.25        | 1.31     |
| 42  | 7     | 302 | A86  | O1-C20  | -4.24 | 1.40        | 1.46     |
| 42  | 2     | 302 | A86  | O1-C20  | -4.24 | 1.40        | 1.46     |
| 42  | 7     | 302 | A86  | C30-C29 | -4.23 | 1.25        | 1.31     |
| 42  | 4     | 203 | A86  | O1-C20  | -4.22 | 1.40        | 1.46     |
| 42  | 3     | 302 | A86  | C30-C29 | -4.22 | 1.25        | 1.31     |
| 42  | 5     | 317 | A86  | C30-C31 | -4.22 | 1.25        | 1.30     |
| 42  | 5     | 303 | A86  | C30-C31 | -4.22 | 1.25        | 1.30     |
| 42  | 0     | 303 | A86  | C30-C31 | -4.20 | 1.25        | 1.30     |
| 42  | 3     | 301 | A86  | C30-C31 | -4.20 | 1.25        | 1.30     |
| 37  | c     | 521 | LMG  | O8-C28  | 4.20  | 1.45        | 1.33     |
| 39  | c     | 520 | DGD  | O1G-C1A | 4.20  | 1.45        | 1.33     |
| 39  | C     | 520 | DGD  | O1G-C1A | 4.20  | 1.45        | 1.33     |
| 42  | 5     | 317 | A86  | C20-C15 | 4.20  | 1.53        | 1.48     |
| 37  | C     | 521 | LMG  | O8-C28  | 4.19  | 1.45        | 1.33     |
| 42  | 9     | 203 | A86  | O1-C20  | -4.19 | 1.40        | 1.46     |
| 32  | a     | 405 | PHO  | C1D-C2D | 4.17  | 1.44        | 1.39     |
| 42  | 4     | 201 | A86  | O1-C20  | -4.16 | 1.40        | 1.46     |
| 42  | 8     | 301 | A86  | C30-C31 | -4.15 | 1.25        | 1.30     |
| 32  | A     | 405 | PHO  | C1D-C2D | 4.12  | 1.44        | 1.39     |
| 42  | 5     | 301 | A86  | C30-C31 | -4.12 | 1.25        | 1.30     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | 6     | 202 | A86  | C30-C31 | -4.10 | 1.25        | 1.30     |
| 42  | 2     | 301 | A86  | C20-C15 | 4.10  | 1.53        | 1.48     |
| 42  | 9     | 201 | A86  | O1-C20  | -4.10 | 1.40        | 1.46     |
| 42  | 9     | 202 | A86  | O1-C20  | -4.09 | 1.40        | 1.46     |
| 42  | 0     | 301 | A86  | C30-C31 | -4.08 | 1.25        | 1.30     |
| 39  | C     | 520 | DGD  | O2G-C1B | 4.07  | 1.45        | 1.34     |
| 39  | c     | 520 | DGD  | O2G-C1B | 4.07  | 1.45        | 1.34     |
| 35  | D     | 406 | PL9  | C3-C4   | -4.06 | 1.43        | 1.49     |
| 35  | d     | 406 | PL9  | C3-C4   | -4.04 | 1.43        | 1.49     |
| 42  | 4     | 202 | A86  | O1-C20  | -4.04 | 1.41        | 1.46     |
| 42  | 7     | 301 | A86  | C20-C15 | 4.04  | 1.53        | 1.48     |
| 42  | 7     | 302 | A86  | C20-C15 | 4.03  | 1.53        | 1.48     |
| 42  | 2     | 302 | A86  | C20-C15 | 4.03  | 1.53        | 1.48     |
| 42  | 3     | 301 | A86  | C21-C20 | 4.02  | 1.57        | 1.51     |
| 43  | 5     | 302 | ET4  | C19-C18 | 4.02  | 1.54        | 1.46     |
| 42  | 1     | 202 | A86  | C30-C31 | -4.02 | 1.25        | 1.30     |
| 42  | 5     | 303 | A86  | C20-C15 | 4.01  | 1.53        | 1.48     |
| 33  | b     | 518 | BCR  | C1-C6   | -4.01 | 1.48        | 1.53     |
| 42  | p     | 610 | A86  | O1-C20  | -3.99 | 1.41        | 1.46     |
| 33  | B     | 517 | BCR  | C1-C6   | -3.99 | 1.48        | 1.53     |
| 42  | P     | 610 | A86  | O1-C20  | -3.99 | 1.41        | 1.46     |
| 43  | 0     | 302 | ET4  | C19-C18 | 3.99  | 1.54        | 1.46     |
| 42  | 8     | 301 | A86  | C21-C20 | 3.98  | 1.57        | 1.51     |
| 37  | c     | 521 | LMG  | O7-C10  | 3.97  | 1.45        | 1.34     |
| 42  | 0     | 303 | A86  | C20-C15 | 3.95  | 1.53        | 1.48     |
| 37  | C     | 521 | LMG  | O7-C10  | 3.95  | 1.45        | 1.34     |
| 42  | 9     | 203 | A86  | C30-C31 | -3.95 | 1.26        | 1.30     |
| 42  | 7     | 301 | A86  | O1-C20  | -3.94 | 1.41        | 1.46     |
| 42  | 2     | 301 | A86  | O1-C20  | -3.94 | 1.41        | 1.46     |
| 42  | 3     | 301 | A86  | O1-C20  | -3.94 | 1.41        | 1.46     |
| 42  | 4     | 203 | A86  | C30-C31 | -3.93 | 1.26        | 1.30     |
| 42  | 8     | 301 | A86  | O1-C20  | -3.92 | 1.41        | 1.46     |
| 33  | a     | 408 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 42  | 5     | 317 | A86  | O1-C20  | -3.86 | 1.41        | 1.46     |
| 33  | A     | 408 | BCR  | C1-C6   | -3.85 | 1.48        | 1.53     |
| 42  | 0     | 317 | A86  | O1-C20  | -3.84 | 1.41        | 1.46     |
| 42  | 7     | 302 | A86  | C32-C31 | -3.82 | 1.48        | 1.54     |
| 42  | 5     | 303 | A86  | C30-C29 | -3.81 | 1.25        | 1.31     |
| 42  | 0     | 303 | A86  | C30-C29 | -3.81 | 1.25        | 1.31     |
| 35  | D     | 406 | PL9  | C7-C3   | -3.80 | 1.46        | 1.51     |
| 33  | C     | 516 | BCR  | C1-C6   | -3.80 | 1.48        | 1.53     |
| 33  | c     | 516 | BCR  | C1-C6   | -3.80 | 1.48        | 1.53     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 43  | 5     | 302 | ET4  | C08-C09 | 3.79  | 1.54        | 1.46     |
| 43  | 0     | 302 | ET4  | C08-C09 | 3.79  | 1.54        | 1.46     |
| 35  | d     | 406 | PL9  | C7-C3   | -3.79 | 1.46        | 1.51     |
| 33  | b     | 520 | BCR  | C1-C6   | -3.78 | 1.48        | 1.53     |
| 42  | 2     | 302 | A86  | C32-C31 | -3.77 | 1.48        | 1.54     |
| 33  | B     | 519 | BCR  | C1-C6   | -3.75 | 1.49        | 1.53     |
| 33  | B     | 517 | BCR  | C30-C25 | -3.75 | 1.49        | 1.53     |
| 33  | b     | 518 | BCR  | C30-C25 | -3.75 | 1.49        | 1.53     |
| 42  | 8     | 302 | A86  | O1-C20  | -3.73 | 1.41        | 1.46     |
| 32  | A     | 405 | PHO  | C4D-CHA | 3.73  | 1.45        | 1.39     |
| 32  | a     | 405 | PHO  | C4D-CHA | 3.73  | 1.45        | 1.39     |
| 42  | 3     | 302 | A86  | O1-C20  | -3.72 | 1.41        | 1.46     |
| 33  | c     | 517 | BCR  | C1-C6   | -3.71 | 1.49        | 1.53     |
| 42  | 8     | 301 | A86  | C30-C29 | -3.70 | 1.25        | 1.31     |
| 42  | 7     | 301 | A86  | C30-C29 | -3.70 | 1.25        | 1.31     |
| 33  | C     | 517 | BCR  | C1-C6   | -3.70 | 1.49        | 1.53     |
| 31  | 8     | 308 | CLA  | C4D-ND  | -3.69 | 1.33        | 1.37     |
| 42  | 4     | 201 | A86  | C30-C31 | -3.68 | 1.26        | 1.30     |
| 33  | B     | 518 | BCR  | C1-C6   | -3.67 | 1.49        | 1.53     |
| 33  | b     | 519 | BCR  | C1-C6   | -3.67 | 1.49        | 1.53     |
| 42  | 2     | 301 | A86  | C30-C29 | -3.67 | 1.25        | 1.31     |
| 42  | 3     | 301 | A86  | C30-C29 | -3.67 | 1.25        | 1.31     |
| 42  | 6     | 202 | A86  | C30-C29 | -3.66 | 1.25        | 1.31     |
| 42  | 1     | 202 | A86  | C30-C29 | -3.66 | 1.25        | 1.31     |
| 31  | 3     | 308 | CLA  | C4D-ND  | -3.66 | 1.33        | 1.37     |
| 32  | A     | 406 | PHO  | C1D-C2D | 3.65  | 1.43        | 1.39     |
| 42  | 9     | 202 | A86  | C30-C31 | -3.64 | 1.26        | 1.30     |
| 33  | K     | 101 | BCR  | C1-C6   | -3.64 | 1.49        | 1.53     |
| 33  | k     | 101 | BCR  | C1-C6   | -3.64 | 1.49        | 1.53     |
| 31  | 4     | 212 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 42  | 4     | 202 | A86  | C30-C31 | -3.62 | 1.26        | 1.30     |
| 31  | 9     | 212 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 42  | 0     | 301 | A86  | O1-C20  | -3.61 | 1.41        | 1.46     |
| 42  | 5     | 301 | A86  | O1-C20  | -3.60 | 1.41        | 1.46     |
| 42  | 9     | 201 | A86  | C30-C31 | -3.60 | 1.26        | 1.30     |
| 33  | D     | 405 | BCR  | C30-C25 | -3.58 | 1.49        | 1.53     |
| 31  | 1     | 205 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 33  | c     | 515 | BCR  | C30-C25 | -3.56 | 1.49        | 1.53     |
| 32  | a     | 406 | PHO  | C1D-C2D | 3.55  | 1.43        | 1.39     |
| 33  | C     | 515 | BCR  | C30-C25 | -3.54 | 1.49        | 1.53     |
| 31  | 7     | 308 | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 31  | 8     | 310 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | 0     | 301 | A86  | C30-C29 | -3.53 | 1.26        | 1.31     |
| 43  | 5     | 302 | ET4  | C12-C13 | 3.52  | 1.53        | 1.46     |
| 43  | 0     | 302 | ET4  | C12-C13 | 3.52  | 1.53        | 1.46     |
| 42  | 6     | 202 | A86  | O1-C20  | -3.52 | 1.41        | 1.46     |
| 33  | K     | 101 | BCR  | C30-C25 | -3.52 | 1.49        | 1.53     |
| 31  | 7     | 305 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 42  | 5     | 317 | A86  | C30-C29 | -3.52 | 1.26        | 1.31     |
| 33  | d     | 405 | BCR  | C30-C25 | -3.52 | 1.49        | 1.53     |
| 31  | 2     | 308 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 31  | 7     | 316 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 31  | 3     | 310 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 31  | 2     | 315 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 31  | 1     | 208 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 31  | 7     | 313 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 33  | k     | 101 | BCR  | C30-C25 | -3.49 | 1.49        | 1.53     |
| 31  | 2     | 305 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 31  | 1     | 209 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 31  | 6     | 208 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 31  | 0     | 307 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 32  | A     | 406 | PHO  | C4D-CHA | 3.48  | 1.44        | 1.39     |
| 32  | a     | 406 | PHO  | C4D-CHA | 3.48  | 1.44        | 1.39     |
| 42  | 0     | 317 | A86  | C30-C29 | -3.48 | 1.26        | 1.31     |
| 42  | 5     | 301 | A86  | C30-C29 | -3.48 | 1.26        | 1.31     |
| 31  | 6     | 213 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 42  | 4     | 202 | A86  | C30-C29 | -3.48 | 1.26        | 1.31     |
| 31  | 2     | 316 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | 6     | 205 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | 1     | 214 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 31  | c     | 504 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 31  | 0     | 309 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 42  | 4     | 203 | A86  | C30-C29 | -3.45 | 1.26        | 1.31     |
| 31  | 7     | 315 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 31  | 1     | 207 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | 6     | 209 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | 6     | 211 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | 1     | 211 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | Z     | 101 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 42  | 9     | 203 | A86  | C30-C29 | -3.44 | 1.26        | 1.31     |
| 31  | 0     | 304 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | B     | 510 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | B     | 515 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 31  | 5     | 314 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 314 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 33  | C     | 515 | BCR  | C1-C6   | -3.44 | 1.49        | 1.53     |
| 31  | C     | 503 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | C     | 504 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | 6     | 214 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | 2     | 313 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | 6     | 212 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | 1     | 212 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | 7     | 310 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 31  | b     | 505 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | 0     | 308 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | 5     | 307 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | b     | 516 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | 1     | 213 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 42  | 9     | 202 | A86  | C30-C29 | -3.42 | 1.26        | 1.31     |
| 31  | 5     | 312 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | 0     | 312 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 31  | B     | 504 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | z     | 101 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 33  | c     | 515 | BCR  | C1-C6   | -3.41 | 1.49        | 1.53     |
| 31  | C     | 510 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | b     | 511 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | p     | 607 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | c     | 503 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | 5     | 309 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | C     | 513 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 31  | b     | 504 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | 1     | 215 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | 6     | 215 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | P     | 607 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | c     | 513 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | D     | 401 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | B     | 501 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | c     | 510 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 31  | 5     | 304 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 33  | d     | 405 | BCR  | C1-C6   | -3.39 | 1.49        | 1.53     |
| 31  | d     | 401 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | 5     | 308 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | 2     | 311 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | 2     | 310 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | C     | 508 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | a     | 403 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 5     | 310 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 31  | C     | 505 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 0     | 306 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | B     | 516 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | C     | 512 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 7     | 311 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 2     | 314 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 42  | 1     | 202 | A86  | O1-C20  | -3.38 | 1.41        | 1.46     |
| 31  | c     | 508 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 6     | 216 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 6     | 207 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 42  | 9     | 201 | A86  | C30-C29 | -3.38 | 1.26        | 1.31     |
| 31  | 7     | 312 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | 2     | 312 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 31  | A     | 407 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 31  | b     | 502 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 31  | c     | 505 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 31  | 7     | 314 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 31  | 5     | 306 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 31  | c     | 511 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 33  | D     | 405 | BCR  | C1-C6   | -3.37 | 1.49        | 1.53     |
| 31  | 8     | 314 | CLA  | CAB-C3B | -3.37 | 1.43        | 1.50     |
| 31  | B     | 503 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 31  | 2     | 307 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 31  | 5     | 313 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 31  | 0     | 313 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 7     | 307 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 42  | 4     | 201 | A86  | C30-C29 | -3.35 | 1.26        | 1.31     |
| 31  | C     | 514 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 0     | 310 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | B     | 505 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | B     | 507 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | B     | 513 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | c     | 512 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | b     | 506 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | C     | 507 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | a     | 407 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 31  | 1     | 216 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | 0     | 305 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 33  | h     | 101 | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 31  | 6     | 201 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | 1     | 201 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 512 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | C     | 511 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | b     | 510 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | a     | 404 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 33  | H     | 101 | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 31  | B     | 511 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 31  | B     | 509 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 33  | H     | 101 | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 31  | A     | 403 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 31  | A     | 404 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 33  | h     | 101 | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 31  | b     | 517 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 31  | 6     | 206 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | c     | 502 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 31  | 1     | 210 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | c     | 514 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 41  | F     | 101 | HEM  | FE-ND   | 3.31  | 2.05        | 1.94     |
| 31  | C     | 502 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | P     | 607 | CLA  | CAB-C3B | -3.31 | 1.44        | 1.50     |
| 31  | b     | 514 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 31  | c     | 507 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 41  | f     | 101 | HEM  | FE-ND   | 3.31  | 2.05        | 1.94     |
| 31  | 4     | 211 | CLA  | CAB-C3B | -3.31 | 1.44        | 1.50     |
| 31  | D     | 403 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 31  | 3     | 314 | CLA  | CAB-C3B | -3.30 | 1.44        | 1.50     |
| 31  | 3     | 307 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 31  | P     | 609 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 31  | 7     | 309 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 31  | 8     | 310 | CLA  | C4B-NB  | 3.29  | 1.42        | 1.37     |
| 31  | 5     | 305 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 33  | b     | 519 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 31  | 8     | 306 | CLA  | CAB-C3B | -3.29 | 1.44        | 1.50     |
| 33  | A     | 408 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 31  | D     | 404 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 31  | 9     | 211 | CLA  | CAB-C3B | -3.28 | 1.44        | 1.50     |
| 31  | P     | 604 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 31  | b     | 503 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 31  | 3     | 306 | CLA  | CAB-C3B | -3.27 | 1.44        | 1.50     |
| 31  | B     | 506 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | d     | 403 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 33  | B     | 518 | BCR  | C30-C25 | -3.27 | 1.49        | 1.53     |
| 31  | p     | 607 | CLA  | CAB-C3B | -3.27 | 1.44        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 310 | CLA  | C4B-NB  | 3.27  | 1.42        | 1.37     |
| 31  | 3     | 304 | CLA  | CAB-C3B | -3.27 | 1.44        | 1.50     |
| 31  | d     | 404 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 31  | C     | 509 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | 9     | 204 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | 8     | 307 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | 0     | 311 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | c     | 509 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | b     | 507 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | p     | 604 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | b     | 508 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | 9     | 211 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | 8     | 308 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 31  | p     | 603 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 9     | 205 | CLA  | CAB-C3B | -3.25 | 1.44        | 1.50     |
| 31  | 8     | 304 | CLA  | CAB-C3B | -3.25 | 1.44        | 1.50     |
| 31  | 2     | 309 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 1     | 206 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 31  | 4     | 205 | CLA  | CAB-C3B | -3.25 | 1.44        | 1.50     |
| 31  | B     | 512 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | B     | 502 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | d     | 403 | CLA  | CAB-C3B | -3.24 | 1.44        | 1.50     |
| 31  | b     | 513 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 33  | a     | 408 | BCR  | C30-C25 | -3.24 | 1.49        | 1.53     |
| 31  | P     | 603 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | b     | 509 | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 31  | 3     | 308 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | p     | 609 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | B     | 508 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | 4     | 210 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | 6     | 210 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 31  | D     | 403 | CLA  | CAB-C3B | -3.22 | 1.44        | 1.50     |
| 31  | 2     | 306 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 31  | 4     | 204 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 31  | 4     | 211 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 31  | C     | 506 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | b     | 515 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | 3     | 311 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | 9     | 213 | CLA  | CAB-C3B | -3.21 | 1.44        | 1.50     |
| 31  | 4     | 208 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | 1     | 201 | CLA  | CAB-C3B | -3.21 | 1.44        | 1.50     |
| 31  | p     | 608 | CLA  | CAB-C3B | -3.20 | 1.44        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 514 | CLA  | C1D-ND  | 3.20  | 1.42        | 1.37     |
| 31  | 9     | 208 | CLA  | C1D-ND  | 3.20  | 1.42        | 1.37     |
| 31  | 9     | 207 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | 8     | 304 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | c     | 506 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | 6     | 201 | CLA  | CAB-C3B | -3.19 | 1.44        | 1.50     |
| 31  | 4     | 207 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | 1     | 209 | CLA  | CAB-C3B | -3.19 | 1.44        | 1.50     |
| 31  | 7     | 306 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 31  | 9     | 210 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 31  | 9     | 212 | CLA  | CAB-C3B | -3.18 | 1.44        | 1.50     |
| 31  | 6     | 209 | CLA  | CAB-C3B | -3.18 | 1.44        | 1.50     |
| 31  | 3     | 314 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 42  | 1     | 202 | A86  | C20-C15 | 3.17  | 1.52        | 1.48     |
| 33  | c     | 516 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 31  | P     | 608 | CLA  | CAB-C3B | -3.17 | 1.44        | 1.50     |
| 31  | 3     | 304 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 31  | 4     | 213 | CLA  | CAB-C3B | -3.17 | 1.44        | 1.50     |
| 31  | 5     | 311 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 31  | 3     | 306 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 34  | B     | 523 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 31  | 6     | 207 | CLA  | CAB-C3B | -3.16 | 1.44        | 1.50     |
| 31  | 1     | 207 | CLA  | CAB-C3B | -3.16 | 1.44        | 1.50     |
| 34  | b     | 501 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 31  | 9     | 211 | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 31  | 8     | 314 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 31  | 4     | 212 | CLA  | CAB-C3B | -3.15 | 1.44        | 1.50     |
| 31  | 7     | 308 | CLA  | CAB-C3B | -3.14 | 1.44        | 1.50     |
| 31  | 9     | 205 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 31  | 8     | 311 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 31  | 2     | 308 | CLA  | CAB-C3B | -3.13 | 1.44        | 1.50     |
| 33  | B     | 519 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 31  | 4     | 211 | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 31  | 8     | 306 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 31  | P     | 602 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 33  | b     | 520 | BCR  | C30-C25 | -3.12 | 1.49        | 1.53     |
| 31  | p     | 602 | CLA  | C1D-ND  | 3.11  | 1.42        | 1.37     |
| 35  | D     | 406 | PL9  | C6-C1   | -3.11 | 1.43        | 1.48     |
| 34  | 5     | 316 | SQD  | O48-C23 | 3.10  | 1.42        | 1.33     |
| 34  | 0     | 316 | SQD  | O48-C23 | 3.10  | 1.42        | 1.33     |
| 31  | 5     | 304 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 35  | d     | 406 | PL9  | C6-C1   | -3.09 | 1.43        | 1.48     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 205 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 33  | C     | 516 | BCR  | C30-C25 | -3.09 | 1.49        | 1.53     |
| 42  | 6     | 202 | A86  | C20-C15 | 3.09  | 1.52        | 1.48     |
| 31  | 7     | 308 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 31  | p     | 606 | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 31  | 3     | 305 | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 34  | A     | 411 | SQD  | O48-C23 | 3.08  | 1.42        | 1.33     |
| 31  | 7     | 305 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |
| 31  | P     | 606 | CLA  | C1D-ND  | 3.07  | 1.41        | 1.37     |
| 31  | 4     | 206 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 31  | z     | 101 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 31  | 8     | 313 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 31  | 9     | 206 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | Z     | 101 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | b     | 502 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 31  | 4     | 213 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 34  | B     | 522 | SQD  | O48-C23 | 3.04  | 1.42        | 1.33     |
| 31  | 2     | 313 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 31  | B     | 501 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 31  | 4     | 206 | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 31  | 2     | 316 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 31  | 9     | 213 | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |
| 31  | 2     | 305 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 41  | f     | 101 | HEM  | CAB-C3B | 3.03  | 1.55        | 1.47     |
| 31  | 8     | 305 | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |
| 31  | 4     | 209 | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |
| 31  | 9     | 213 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 33  | c     | 517 | BCR  | C30-C25 | -3.02 | 1.49        | 1.53     |
| 41  | V     | 201 | HEM  | CAB-C3B | 3.02  | 1.55        | 1.47     |
| 31  | 3     | 312 | CLA  | C1D-ND  | 3.02  | 1.41        | 1.37     |
| 31  | p     | 601 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 31  | 4     | 212 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 31  | 3     | 313 | CLA  | C1D-ND  | 3.02  | 1.41        | 1.37     |
| 31  | 0     | 304 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 31  | 8     | 312 | CLA  | C1D-ND  | 3.02  | 1.41        | 1.37     |
| 41  | F     | 101 | HEM  | CAB-C3B | 3.01  | 1.55        | 1.47     |
| 34  | a     | 409 | SQD  | O48-C23 | 3.01  | 1.42        | 1.33     |
| 31  | 6     | 213 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 31  | 1     | 213 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 31  | 7     | 306 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 33  | C     | 517 | BCR  | C30-C25 | -3.01 | 1.49        | 1.53     |
| 31  | B     | 515 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 511 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 41  | v     | 201 | HEM  | CAB-C3B | 3.00  | 1.55        | 1.47     |
| 34  | A     | 409 | SQD  | O48-C23 | 3.00  | 1.42        | 1.33     |
| 31  | P     | 601 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 31  | 2     | 314 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 31  | 3     | 309 | CLA  | C1B-C2B | 3.00  | 1.50        | 1.43     |
| 31  | 9     | 212 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 42  | p     | 610 | A86  | C19-C18 | -3.00 | 1.48        | 1.52     |
| 31  | 5     | 314 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 31  | 1     | 216 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 31  | 2     | 308 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 31  | 7     | 313 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 41  | F     | 101 | HEM  | CAC-C3C | 2.99  | 1.55        | 1.47     |
| 31  | 8     | 309 | CLA  | C1B-C2B | 2.99  | 1.50        | 1.43     |
| 31  | b     | 516 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 41  | f     | 101 | HEM  | CAC-C3C | 2.98  | 1.55        | 1.47     |
| 31  | 4     | 213 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 31  | 3     | 304 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | 7     | 314 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | B     | 510 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | 8     | 304 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | 0     | 313 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 31  | 9     | 209 | CLA  | C1D-ND  | 2.96  | 1.41        | 1.37     |
| 31  | 7     | 315 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 31  | 1     | 208 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | 7     | 312 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | p     | 608 | CLA  | C1D-ND  | 2.95  | 1.41        | 1.37     |
| 31  | P     | 608 | CLA  | C1D-ND  | 2.95  | 1.41        | 1.37     |
| 31  | 1     | 214 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | 0     | 314 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 31  | 6     | 216 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 31  | 6     | 205 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 31  | 5     | 313 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 31  | P     | 606 | CLA  | MG-NB   | -2.94 | 2.00        | 2.05     |
| 31  | 7     | 316 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 1     | 211 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | p     | 606 | CLA  | MG-NB   | -2.93 | 2.00        | 2.05     |
| 31  | 6     | 201 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 6     | 208 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 1     | 201 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 9     | 206 | CLA  | C1D-ND  | 2.93  | 1.41        | 1.37     |
| 31  | 1     | 205 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 307 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | 2     | 315 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 31  | D     | 403 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 31  | 6     | 207 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 31  | 2     | 306 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 42  | P     | 610 | A86  | C19-C18 | -2.92 | 1.48        | 1.52     |
| 31  | 2     | 311 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 31  | 0     | 311 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | c     | 513 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 0     | 310 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | w     | 202 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 0     | 309 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 7     | 311 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | 1     | 207 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 31  | d     | 403 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | p     | 605 | CLA  | C1D-ND  | 2.90  | 1.41        | 1.37     |
| 31  | C     | 513 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | 3     | 308 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | 1     | 210 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 31  | W     | 202 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 31  | 9     | 204 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 31  | 5     | 307 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 44  | 8     | 303 | DD6  | O1-C20  | -2.89 | 1.42        | 1.46     |
| 31  | P     | 605 | CLA  | C1D-ND  | 2.89  | 1.41        | 1.37     |
| 31  | 5     | 306 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 31  | 4     | 204 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 31  | b     | 517 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 34  | b     | 501 | SQD  | O47-C7  | 2.88  | 1.42        | 1.34     |
| 31  | 8     | 310 | CLA  | C3C-C4C | 2.88  | 1.46        | 1.40     |
| 34  | B     | 523 | SQD  | O47-C7  | 2.88  | 1.42        | 1.34     |
| 41  | V     | 201 | HEM  | CAC-C3C | 2.88  | 1.55        | 1.47     |
| 31  | 3     | 306 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 44  | 3     | 303 | DD6  | O1-C20  | -2.88 | 1.42        | 1.46     |
| 31  | 2     | 312 | CLA  | C3C-C4C | 2.88  | 1.46        | 1.40     |
| 31  | 6     | 209 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | 1     | 209 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | 5     | 308 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | 0     | 308 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 31  | 1     | 212 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 41  | v     | 201 | HEM  | CAC-C3C | 2.88  | 1.55        | 1.47     |
| 31  | b     | 512 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 34  | B     | 522 | SQD  | O47-C7  | 2.87  | 1.42        | 1.34     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 214 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 3     | 310 | CLA  | C3C-C4C | 2.87  | 1.46        | 1.40     |
| 31  | B     | 508 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 6     | 211 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 5     | 312 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 0     | 312 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 31  | 6     | 210 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | 8     | 306 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 34  | A     | 411 | SQD  | O47-C7  | 2.86  | 1.42        | 1.34     |
| 31  | 3     | 314 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | B     | 511 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | 2     | 307 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | 7     | 312 | CLA  | C3C-C4C | 2.86  | 1.46        | 1.40     |
| 31  | 8     | 308 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | p     | 605 | CLA  | MG-NB   | -2.86 | 2.00        | 2.05     |
| 31  | B     | 516 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | b     | 509 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 31  | 0     | 306 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | 2     | 312 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | P     | 603 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | P     | 605 | CLA  | MG-NB   | -2.85 | 2.00        | 2.05     |
| 31  | p     | 608 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | 8     | 314 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | 3     | 304 | CLA  | C3C-C4C | 2.85  | 1.46        | 1.40     |
| 31  | 7     | 307 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 31  | 9     | 205 | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 31  | 8     | 306 | CLA  | C3C-C4C | 2.84  | 1.46        | 1.40     |
| 31  | P     | 606 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | C     | 507 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 5     | 305 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 0     | 305 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 5     | 310 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 7     | 310 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | 3     | 304 | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 31  | b     | 508 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | P     | 601 | CLA  | C3C-C4C | 2.83  | 1.46        | 1.40     |
| 34  | a     | 409 | SQD  | O47-C7  | 2.83  | 1.42        | 1.34     |
| 31  | 5     | 311 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | p     | 609 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | C     | 504 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | 6     | 215 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 31  | 1     | 215 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 304 | CLA  | C3C-C4C | 2.82  | 1.46        | 1.40     |
| 31  | 3     | 306 | CLA  | C3C-C4C | 2.82  | 1.46        | 1.40     |
| 31  | b     | 514 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | p     | 601 | CLA  | C3C-C4C | 2.82  | 1.46        | 1.40     |
| 42  | 5     | 303 | A86  | O1-C20  | -2.82 | 1.42        | 1.46     |
| 31  | B     | 507 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | c     | 504 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | b     | 510 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 31  | C     | 506 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 34  | A     | 409 | SQD  | O47-C7  | 2.81  | 1.42        | 1.34     |
| 31  | 6     | 212 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 31  | 9     | 210 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 42  | 0     | 303 | A86  | O1-C20  | -2.81 | 1.42        | 1.46     |
| 44  | 3     | 303 | DD6  | C28-C27 | -2.81 | 1.49        | 1.50     |
| 31  | 5     | 309 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 35  | A     | 410 | PL9  | C3-C4   | -2.80 | 1.45        | 1.49     |
| 31  | B     | 509 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | 4     | 205 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 31  | p     | 603 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | P     | 609 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | c     | 505 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 31  | 8     | 304 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 31  | c     | 511 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | B     | 505 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | c     | 506 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 31  | 1     | 210 | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 35  | a     | 410 | PL9  | C3-C4   | -2.79 | 1.45        | 1.49     |
| 44  | 8     | 303 | DD6  | C28-C27 | -2.79 | 1.49        | 1.50     |
| 31  | b     | 506 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 31  | 8     | 309 | CLA  | C1D-ND  | 2.78  | 1.41        | 1.37     |
| 34  | 0     | 316 | SQD  | O47-C7  | 2.78  | 1.42        | 1.34     |
| 31  | P     | 601 | CLA  | C1D-ND  | 2.78  | 1.41        | 1.37     |
| 31  | a     | 407 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 31  | c     | 507 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 31  | 3     | 309 | CLA  | C1D-ND  | 2.77  | 1.41        | 1.37     |
| 31  | 6     | 210 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 31  | P     | 608 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 31  | B     | 503 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 9     | 213 | CLA  | MG-NB   | -2.76 | 2.00        | 2.05     |
| 31  | 4     | 210 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 2     | 310 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 6     | 214 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 1     | 214 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 31  | B     | 504 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 7     | 309 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 31  | 2     | 309 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 34  | 5     | 316 | SQD  | O47-C7  | 2.76  | 1.42        | 1.34     |
| 31  | a     | 404 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | c     | 504 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 31  | C     | 511 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | C     | 505 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | p     | 606 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | p     | 601 | CLA  | C1D-ND  | 2.75  | 1.41        | 1.37     |
| 31  | b     | 505 | CLA  | C4B-NB  | 2.75  | 1.41        | 1.37     |
| 31  | 3     | 310 | CLA  | C3B-C4B | 2.75  | 1.50        | 1.42     |
| 31  | 8     | 310 | CLA  | C3B-C4B | 2.74  | 1.50        | 1.42     |
| 31  | d     | 403 | CLA  | C4B-C3B | 2.74  | 1.49        | 1.43     |
| 31  | A     | 404 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | c     | 508 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 39  | C     | 518 | DGD  | O2G-C2G | -2.74 | 1.40        | 1.46     |
| 31  | 4     | 213 | CLA  | MG-NB   | -2.74 | 2.00        | 2.05     |
| 31  | B     | 513 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 31  | C     | 504 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 41  | f     | 101 | HEM  | FE-NB   | 2.73  | 2.03        | 1.94     |
| 31  | 5     | 307 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 31  | 4     | 207 | CLA  | C4B-NB  | 2.73  | 1.41        | 1.37     |
| 39  | c     | 518 | DGD  | O2G-C2G | -2.73 | 1.40        | 1.46     |
| 31  | B     | 506 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | C     | 512 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | C     | 503 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 41  | V     | 201 | HEM  | FE-NC   | 2.72  | 2.04        | 1.95     |
| 31  | A     | 407 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | 6     | 212 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | 1     | 212 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | b     | 504 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | b     | 507 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 31  | b     | 513 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 31  | C     | 514 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 41  | F     | 101 | HEM  | FE-NB   | 2.72  | 2.03        | 1.94     |
| 31  | 0     | 311 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 42  | p     | 610 | A86  | C32-C31 | -2.71 | 1.50        | 1.54     |
| 31  | B     | 512 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 31  | C     | 509 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 31  | d     | 404 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 42  | P     | 610 | A86  | C32-C31 | -2.71 | 1.50        | 1.54     |
| 31  | 6     | 215 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 32  | a     | 406 | PHO  | CMC-C2C | -2.71 | 1.46        | 1.50     |
| 31  | 6     | 209 | CLA  | C4B-C3B | 2.70  | 1.49        | 1.43     |
| 31  | 0     | 314 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | 1     | 209 | CLA  | C4B-C3B | 2.70  | 1.49        | 1.43     |
| 41  | v     | 201 | HEM  | FE-NC   | 2.70  | 2.04        | 1.95     |
| 31  | 5     | 311 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | D     | 403 | CLA  | C4B-C3B | 2.70  | 1.49        | 1.43     |
| 31  | c     | 512 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | 9     | 207 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | 9     | 212 | CLA  | C4B-C3B | 2.70  | 1.49        | 1.43     |
| 31  | C     | 508 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | c     | 509 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | 1     | 206 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | P     | 601 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | a     | 403 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | P     | 602 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | 7     | 315 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | 8     | 313 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | 4     | 205 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 31  | 6     | 205 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 31  | 8     | 311 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | 9     | 204 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | 0     | 307 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | 3     | 313 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | W     | 202 | CLA  | C1D-ND  | 2.69  | 1.41        | 1.37     |
| 31  | 6     | 206 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 43  | 5     | 302 | ET4  | C20-C21 | 2.69  | 1.51        | 1.43     |
| 31  | 6     | 216 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | b     | 515 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | 1     | 215 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 31  | D     | 404 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 31  | 4     | 204 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 32  | a     | 405 | PHO  | CMC-C2C | -2.68 | 1.46        | 1.50     |
| 31  | 9     | 205 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | p     | 601 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | 2     | 315 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | B     | 502 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | 5     | 314 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | p     | 602 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | 0     | 313 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 43  | 0     | 302 | ET4  | C20-C21 | 2.68  | 1.51        | 1.43     |
| 31  | B     | 514 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | b     | 503 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 31  | C     | 512 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 31  | 1     | 207 | CLA  | C4B-C3B | 2.67  | 1.49        | 1.43     |
| 31  | 6     | 209 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 1     | 201 | CLA  | C4B-C3B | 2.67  | 1.49        | 1.43     |
| 31  | 4     | 209 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | 3     | 312 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | 4     | 212 | CLA  | C4B-C3B | 2.67  | 1.49        | 1.43     |
| 31  | A     | 403 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 31  | 3     | 311 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 32  | A     | 405 | PHO  | CMC-C2C | -2.67 | 1.46        | 1.50     |
| 31  | 1     | 216 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 32  | A     | 406 | PHO  | CMC-C2C | -2.67 | 1.46        | 1.50     |
| 31  | C     | 510 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 7     | 308 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 6     | 206 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 2     | 308 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | 1     | 206 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 31  | c     | 503 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | 6     | 207 | CLA  | C4B-C3B | 2.66  | 1.49        | 1.43     |
| 31  | P     | 608 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 36  | B     | 521 | LHG  | O7-C5   | -2.66 | 1.40        | 1.46     |
| 31  | 0     | 304 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 31  | c     | 514 | CLA  | C4B-NB  | 2.66  | 1.41        | 1.37     |
| 31  | w     | 202 | CLA  | C1D-ND  | 2.66  | 1.41        | 1.37     |
| 31  | D     | 401 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | 1     | 205 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | C     | 502 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | 5     | 310 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | P     | 609 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | 5     | 304 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | c     | 510 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | d     | 401 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 31  | 5     | 312 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | 6     | 211 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | 0     | 312 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | 1     | 211 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | d     | 404 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | 7     | 306 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 31  | D     | 404 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 314 | CLA  | C4B-C3B | 2.65  | 1.49        | 1.43     |
| 31  | 8     | 314 | CLA  | C4B-C3B | 2.65  | 1.49        | 1.43     |
| 31  | B     | 507 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | b     | 508 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 5     | 313 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 4     | 208 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 36  | b     | 522 | LHG  | O7-C5   | -2.64 | 1.40        | 1.46     |
| 31  | c     | 513 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 8     | 312 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 31  | p     | 608 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 1     | 209 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 6     | 207 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 7     | 312 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | B     | 515 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 7     | 314 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | 2     | 310 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 31  | b     | 510 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 7     | 311 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 7     | 316 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 9     | 209 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 31  | 8     | 314 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 3     | 311 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | c     | 512 | CLA  | C4B-NB  | 2.63  | 1.41        | 1.37     |
| 31  | c     | 506 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | c     | 505 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | b     | 516 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 0     | 310 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 6     | 208 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 31  | 2     | 306 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 1     | 207 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | c     | 508 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | z     | 101 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 6     | 201 | CLA  | C4B-C3B | 2.62  | 1.49        | 1.43     |
| 31  | B     | 509 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | C     | 505 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 3     | 314 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 9     | 211 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | C     | 513 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 1     | 201 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 44  | 7     | 303 | DD6  | O1-C20  | -2.62 | 1.42        | 1.46     |
| 31  | B     | 504 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | 2     | 307 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 41  | v     | 201 | HEM  | FE-NA   | 2.62  | 2.03        | 1.95     |
| 31  | 7     | 305 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 2     | 314 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 7     | 310 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | p     | 609 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 8     | 311 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 2     | 305 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 32  | A     | 405 | PHO  | CAC-C3C | -2.61 | 1.47        | 1.51     |
| 31  | c     | 510 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | 2     | 316 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 1     | 208 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | 9     | 208 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | 6     | 213 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | B     | 512 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 44  | 2     | 303 | DD6  | O1-C20  | -2.61 | 1.42        | 1.46     |
| 31  | 1     | 213 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | C     | 506 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | C     | 510 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | b     | 506 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 31  | c     | 502 | CLA  | C4B-NB  | 2.61  | 1.41        | 1.37     |
| 31  | 6     | 201 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | B     | 506 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | b     | 507 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 8     | 309 | CLA  | C4B-NB  | 2.60  | 1.41        | 1.37     |
| 31  | 2     | 311 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 4     | 211 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 7     | 313 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 2     | 313 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | B     | 505 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 41  | V     | 201 | HEM  | FE-NA   | 2.60  | 2.03        | 1.95     |
| 31  | 0     | 306 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | Z     | 101 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | c     | 502 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | p     | 602 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | C     | 514 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 7     | 307 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 31  | 3     | 309 | CLA  | C4B-NB  | 2.59  | 1.41        | 1.37     |
| 31  | C     | 511 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | C     | 508 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | b     | 513 | CLA  | C4B-NB  | 2.59  | 1.41        | 1.37     |
| 31  | c     | 503 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | 2     | 312 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 504 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | 7     | 308 | CLA  | C4B-C3B | 2.59  | 1.49        | 1.43     |
| 31  | 4     | 212 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | c     | 514 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 31  | 4     | 208 | CLA  | MG-NB   | -2.59 | 2.00        | 2.05     |
| 31  | 0     | 308 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 5     | 308 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | c     | 511 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 36  | a     | 411 | LHG  | O7-C5   | -2.58 | 1.40        | 1.46     |
| 31  | B     | 509 | CLA  | CMC-C2C | -2.58 | 1.45        | 1.50     |
| 31  | P     | 604 | CLA  | C4B-NB  | 2.58  | 1.41        | 1.37     |
| 31  | P     | 602 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 32  | a     | 405 | PHO  | CAC-C3C | -2.58 | 1.47        | 1.51     |
| 31  | b     | 505 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 8     | 306 | CLA  | C4B-C3B | 2.58  | 1.49        | 1.43     |
| 31  | P     | 607 | CLA  | C4B-NB  | 2.58  | 1.41        | 1.37     |
| 31  | b     | 510 | CLA  | CMC-C2C | -2.58 | 1.45        | 1.50     |
| 31  | C     | 502 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | 8     | 307 | CLA  | C4B-NB  | 2.58  | 1.41        | 1.37     |
| 31  | B     | 516 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | b     | 517 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 3     | 305 | CLA  | C4B-NB  | 2.57  | 1.41        | 1.37     |
| 31  | C     | 503 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 9     | 212 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | b     | 515 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | p     | 604 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 31  | 3     | 306 | CLA  | C4B-C3B | 2.56  | 1.49        | 1.43     |
| 31  | p     | 608 | CLA  | C4B-C3B | 2.56  | 1.49        | 1.43     |
| 36  | A     | 412 | LHG  | O7-C5   | -2.56 | 1.40        | 1.46     |
| 31  | 9     | 205 | CLA  | C4B-C3B | 2.56  | 1.49        | 1.43     |
| 31  | B     | 503 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | A     | 404 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 44  | 6     | 203 | DD6  | O1-C20  | -2.56 | 1.42        | 1.46     |
| 31  | P     | 608 | CLA  | C4B-C3B | 2.56  | 1.49        | 1.43     |
| 31  | 5     | 306 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | P     | 604 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 31  | 3     | 308 | CLA  | MG-NB   | -2.55 | 2.00        | 2.05     |
| 31  | 3     | 306 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | b     | 514 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | 2     | 308 | CLA  | C4B-C3B | 2.55  | 1.49        | 1.43     |
| 31  | 4     | 205 | CLA  | C4B-C3B | 2.55  | 1.49        | 1.43     |
| 44  | 1     | 203 | DD6  | O1-C20  | -2.55 | 1.42        | 1.46     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 209 | CLA  | MG-NB   | -2.55 | 2.00        | 2.05     |
| 32  | a     | 406 | PHO  | CMD-C2D | -2.55 | 1.46        | 1.51     |
| 36  | d     | 407 | LHG  | O7-C5   | -2.54 | 1.40        | 1.46     |
| 31  | b     | 503 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 9     | 213 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 3     | 307 | CLA  | C4B-NB  | 2.54  | 1.41        | 1.37     |
| 31  | p     | 607 | CLA  | C4B-NB  | 2.54  | 1.41        | 1.37     |
| 32  | a     | 405 | PHO  | CMD-C2D | -2.54 | 1.46        | 1.51     |
| 31  | b     | 509 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 9     | 208 | CLA  | MG-NB   | -2.54 | 2.00        | 2.05     |
| 31  | a     | 403 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | B     | 513 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | d     | 403 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | p     | 604 | CLA  | C4B-NB  | 2.54  | 1.41        | 1.37     |
| 31  | 8     | 308 | CLA  | MG-NB   | -2.54 | 2.00        | 2.05     |
| 31  | B     | 501 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 5     | 309 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 0     | 309 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | 4     | 209 | CLA  | MG-NB   | -2.54 | 2.00        | 2.05     |
| 31  | B     | 514 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | c     | 507 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | B     | 502 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | a     | 404 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | 4     | 207 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 36  | D     | 407 | LHG  | O7-C5   | -2.53 | 1.40        | 1.46     |
| 31  | 8     | 305 | CLA  | C4B-NB  | 2.53  | 1.41        | 1.37     |
| 31  | b     | 502 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | 3     | 305 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | B     | 510 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | 8     | 311 | CLA  | MG-NB   | -2.53 | 2.00        | 2.05     |
| 31  | 8     | 306 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | A     | 407 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | A     | 403 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | d     | 401 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | b     | 511 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | 7     | 309 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | 2     | 309 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 31  | P     | 607 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 31  | P     | 607 | CLA  | MG-NB   | -2.52 | 2.00        | 2.05     |
| 32  | A     | 406 | PHO  | CMD-C2D | -2.52 | 1.46        | 1.51     |
| 31  | 3     | 311 | CLA  | MG-NB   | -2.52 | 2.00        | 2.05     |
| 31  | D     | 401 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | C     | 507 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 37  | m     | 101 | LMG  | O7-C8   | -2.51 | 1.40        | 1.46     |
| 31  | D     | 403 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 35  | D     | 406 | PL9  | C53-C6  | -2.51 | 1.45        | 1.50     |
| 32  | A     | 405 | PHO  | CMD-C2D | -2.51 | 1.46        | 1.51     |
| 31  | a     | 407 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | p     | 607 | CLA  | C4B-C3B | 2.51  | 1.49        | 1.43     |
| 31  | 9     | 205 | CLA  | MG-NB   | -2.51 | 2.00        | 2.05     |
| 31  | 8     | 305 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | B     | 508 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | 9     | 207 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 31  | w     | 202 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 35  | d     | 406 | PL9  | C53-C6  | -2.50 | 1.45        | 1.50     |
| 31  | p     | 607 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | 3     | 313 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | P     | 607 | CLA  | C4B-C3B | 2.50  | 1.49        | 1.43     |
| 31  | w     | 202 | CLA  | MG-NB   | -2.50 | 2.00        | 2.05     |
| 31  | 4     | 213 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 31  | 4     | 205 | CLA  | MG-NB   | -2.49 | 2.00        | 2.05     |
| 37  | M     | 101 | LMG  | O7-C8   | -2.49 | 1.40        | 1.46     |
| 31  | 9     | 208 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | W     | 202 | CLA  | MG-NB   | -2.49 | 2.00        | 2.05     |
| 31  | 4     | 209 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 32  | A     | 405 | PHO  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 31  | 4     | 208 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | w     | 202 | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 31  | 8     | 313 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 32  | a     | 406 | PHO  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 31  | 3     | 312 | CLA  | MG-NB   | -2.48 | 2.00        | 2.05     |
| 31  | W     | 202 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 31  | p     | 607 | CLA  | MG-NB   | -2.48 | 2.00        | 2.05     |
| 31  | 3     | 307 | CLA  | MG-NB   | -2.48 | 2.00        | 2.05     |
| 31  | 4     | 211 | CLA  | C4B-C3B | 2.48  | 1.48        | 1.43     |
| 42  | 3     | 301 | A86  | C19-C18 | 2.47  | 1.55        | 1.52     |
| 31  | 9     | 211 | CLA  | C4B-C3B | 2.47  | 1.48        | 1.43     |
| 31  | W     | 202 | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 31  | 8     | 307 | CLA  | MG-NB   | -2.47 | 2.00        | 2.05     |
| 31  | P     | 603 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 31  | B     | 501 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 31  | p     | 605 | CLA  | C4B-NB  | 2.47  | 1.41        | 1.37     |
| 31  | 9     | 209 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 31  | 3     | 305 | CLA  | MG-NB   | -2.46 | 2.00        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | A     | 406 | PHO  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 32  | a     | 405 | PHO  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 31  | 4     | 207 | CLA  | MG-NB   | -2.46 | 2.00        | 2.05     |
| 31  | 4     | 206 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 31  | 8     | 312 | CLA  | MG-NB   | -2.45 | 2.00        | 2.05     |
| 39  | c     | 519 | DGD  | O1G-C1G | -2.45 | 1.39        | 1.45     |
| 42  | P     | 610 | A86  | C19-C20 | -2.45 | 1.48        | 1.52     |
| 31  | 4     | 206 | CLA  | MG-NB   | -2.44 | 2.00        | 2.05     |
| 39  | C     | 519 | DGD  | O1G-C1G | -2.44 | 1.39        | 1.45     |
| 31  | 9     | 207 | CLA  | MG-NB   | -2.44 | 2.00        | 2.05     |
| 31  | p     | 603 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 31  | B     | 511 | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 31  | b     | 502 | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 31  | 9     | 206 | CLA  | MG-NB   | -2.44 | 2.01        | 2.05     |
| 31  | p     | 605 | CLA  | MG-ND   | -2.44 | 2.01        | 2.05     |
| 31  | 8     | 305 | CLA  | MG-NB   | -2.43 | 2.01        | 2.05     |
| 31  | 3     | 307 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | 4     | 210 | CLA  | MG-NB   | -2.43 | 2.01        | 2.05     |
| 31  | 9     | 206 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 31  | b     | 512 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 42  | 8     | 301 | A86  | C13-C11 | -2.42 | 1.45        | 1.49     |
| 31  | 9     | 213 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 44  | 6     | 204 | DD6  | O1-C20  | -2.42 | 1.43        | 1.46     |
| 31  | 6     | 206 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 42  | p     | 610 | A86  | C19-C20 | -2.42 | 1.48        | 1.52     |
| 42  | 8     | 301 | A86  | C19-C18 | 2.42  | 1.55        | 1.52     |
| 31  | b     | 512 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | B     | 511 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | z     | 101 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 31  | 4     | 205 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 31  | c     | 509 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | 8     | 307 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 31  | Z     | 101 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 42  | P     | 610 | A86  | C13-C11 | -2.40 | 1.45        | 1.49     |
| 42  | p     | 610 | A86  | C13-C11 | -2.40 | 1.45        | 1.49     |
| 31  | 4     | 210 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 31  | 9     | 205 | CLA  | CHC-C1C | 2.40  | 1.43        | 1.38     |
| 31  | P     | 605 | CLA  | MG-ND   | -2.40 | 2.01        | 2.05     |
| 31  | c     | 503 | CLA  | MG-NB   | -2.40 | 2.01        | 2.05     |
| 31  | 2     | 306 | CLA  | CHC-C1C | 2.40  | 1.43        | 1.38     |
| 31  | 8     | 306 | CLA  | MG-NB   | -2.40 | 2.01        | 2.05     |
| 31  | 9     | 210 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 206 | CLA  | CHC-C1C | 2.40  | 1.43        | 1.38     |
| 31  | 1     | 206 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 31  | 3     | 308 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 31  | 3     | 309 | CLA  | MG-NB   | -2.39 | 2.01        | 2.05     |
| 31  | 5     | 305 | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 31  | 5     | 305 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 31  | 2     | 310 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.38     |
| 39  | h     | 102 | DGD  | O2G-C2G | -2.39 | 1.41        | 1.46     |
| 42  | 4     | 201 | A86  | C19-C18 | -2.39 | 1.48        | 1.52     |
| 31  | C     | 503 | CLA  | MG-NB   | -2.39 | 2.01        | 2.05     |
| 31  | C     | 509 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 31  | 2     | 310 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 37  | m     | 102 | LMG  | O7-C8   | -2.39 | 1.41        | 1.46     |
| 31  | P     | 606 | CLA  | MG-ND   | -2.39 | 2.01        | 2.05     |
| 41  | f     | 101 | HEM  | FE-NA   | 2.39  | 2.03        | 1.95     |
| 31  | P     | 606 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 31  | 8     | 308 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 31  | 3     | 306 | CLA  | MG-NB   | -2.39 | 2.01        | 2.05     |
| 37  | M     | 102 | LMG  | O7-C8   | -2.39 | 1.41        | 1.46     |
| 42  | 8     | 301 | A86  | C32-C31 | -2.38 | 1.50        | 1.54     |
| 31  | 8     | 309 | CLA  | MG-NB   | -2.38 | 2.01        | 2.05     |
| 31  | 7     | 306 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 31  | P     | 605 | CLA  | C4B-NB  | 2.38  | 1.41        | 1.37     |
| 31  | p     | 606 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 41  | F     | 101 | HEM  | FE-NA   | 2.38  | 2.03        | 1.95     |
| 44  | 1     | 204 | DD6  | O1-C20  | -2.38 | 1.43        | 1.46     |
| 31  | 8     | 313 | CLA  | MG-NB   | -2.38 | 2.01        | 2.05     |
| 42  | 3     | 301 | A86  | C13-C11 | -2.38 | 1.45        | 1.49     |
| 31  | 3     | 304 | CLA  | C4B-C3B | 2.38  | 1.48        | 1.43     |
| 31  | 4     | 213 | CLA  | CMB-C2B | -2.38 | 1.45        | 1.50     |
| 31  | P     | 603 | CLA  | MG-NB   | -2.37 | 2.01        | 2.05     |
| 31  | 8     | 304 | CLA  | C4B-C3B | 2.37  | 1.48        | 1.43     |
| 39  | H     | 102 | DGD  | O2G-C2G | -2.37 | 1.41        | 1.46     |
| 31  | z     | 101 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 31  | p     | 606 | CLA  | MG-ND   | -2.37 | 2.01        | 2.05     |
| 31  | c     | 514 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 31  | 1     | 206 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 31  | 0     | 305 | CLA  | CMC-C2C | -2.37 | 1.45        | 1.50     |
| 31  | 2     | 312 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | 3     | 308 | CLA  | CHA-C4D | 2.36  | 1.43        | 1.38     |
| 31  | 3     | 313 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 31  | 7     | 310 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | c     | 509 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 31  | 9     | 210 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 31  | 9     | 210 | CLA  | MG-NB   | -2.36 | 2.01        | 2.05     |
| 43  | 0     | 302 | ET4  | C16-C17 | 2.36  | 1.50        | 1.43     |
| 31  | 7     | 305 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | 2     | 305 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 42  | 9     | 201 | A86  | C19-C18 | -2.35 | 1.49        | 1.52     |
| 31  | c     | 509 | CLA  | CMB-C2B | -2.35 | 1.45        | 1.50     |
| 31  | 3     | 308 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | 7     | 316 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | 2     | 316 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | 4     | 210 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 32  | A     | 406 | PHO  | C3D-C4D | 2.35  | 1.44        | 1.41     |
| 31  | D     | 401 | CLA  | MG-NB   | -2.35 | 2.01        | 2.05     |
| 31  | 8     | 312 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 31  | C     | 509 | CLA  | MG-NB   | -2.35 | 2.01        | 2.05     |
| 32  | a     | 405 | PHO  | C3D-C4D | 2.35  | 1.44        | 1.41     |
| 31  | P     | 605 | CLA  | CMD-C2D | -2.35 | 1.46        | 1.50     |
| 31  | 1     | 216 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.38     |
| 31  | 3     | 314 | CLA  | MG-NB   | -2.35 | 2.01        | 2.05     |
| 31  | 9     | 206 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | 8     | 310 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 31  | p     | 603 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 31  | P     | 601 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 31  | 8     | 308 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | 0     | 305 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 31  | B     | 510 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | b     | 511 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | 6     | 211 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 31  | 6     | 211 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | 5     | 305 | CLA  | CMB-C2B | -2.34 | 1.46        | 1.50     |
| 31  | C     | 514 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 31  | p     | 601 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 43  | 5     | 302 | ET4  | C16-C17 | 2.34  | 1.50        | 1.43     |
| 31  | 8     | 310 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 31  | 7     | 312 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | 2     | 311 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | 4     | 206 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | C     | 511 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | C     | 509 | CLA  | CMB-C2B | -2.33 | 1.46        | 1.50     |
| 31  | 7     | 306 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | Z     | 101 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | c     | 518 | DGD  | O1G-C1G | -2.33 | 1.40        | 1.45     |
| 31  | 0     | 305 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | B     | 512 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | a     | 404 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | 7     | 309 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | 3     | 310 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 31  | 9     | 213 | CLA  | C4B-C3B | 2.33  | 1.48        | 1.43     |
| 31  | 0     | 308 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 31  | 7     | 311 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 39  | h     | 102 | DGD  | O1G-C1G | -2.32 | 1.40        | 1.45     |
| 31  | 7     | 313 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | 0     | 309 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 31  | A     | 403 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | p     | 608 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 31  | 7     | 310 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 31  | P     | 601 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | 0     | 304 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 31  | B     | 511 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 42  | 3     | 302 | A86  | C19-C18 | -2.32 | 1.49        | 1.52     |
| 37  | D     | 410 | LMG  | O1-C7   | -2.32 | 1.39        | 1.43     |
| 32  | a     | 406 | PHO  | C3D-C4D | 2.32  | 1.44        | 1.41     |
| 37  | d     | 410 | LMG  | O1-C7   | -2.32 | 1.39        | 1.43     |
| 35  | D     | 406 | PL9  | C52-C5  | -2.32 | 1.46        | 1.50     |
| 42  | 8     | 302 | A86  | C13-C11 | -2.32 | 1.45        | 1.49     |
| 31  | B     | 506 | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 35  | A     | 410 | PL9  | C6-C1   | -2.32 | 1.44        | 1.48     |
| 31  | 3     | 310 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 43  | 0     | 302 | ET4  | C01-C06 | 2.31  | 1.56        | 1.53     |
| 31  | d     | 404 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | a     | 403 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 39  | C     | 518 | DGD  | O1G-C1G | -2.31 | 1.40        | 1.45     |
| 31  | 8     | 308 | CLA  | CHA-C4D | 2.31  | 1.42        | 1.38     |
| 31  | 0     | 305 | CLA  | CMB-C2B | -2.31 | 1.46        | 1.50     |
| 31  | 3     | 312 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 31  | 1     | 211 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 39  | H     | 102 | DGD  | O1G-C1G | -2.31 | 1.40        | 1.45     |
| 31  | b     | 505 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | p     | 605 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 31  | P     | 604 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 4     | 213 | CLA  | C4B-C3B | 2.31  | 1.48        | 1.43     |
| 31  | P     | 603 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | B     | 504 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 503 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | d     | 401 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 8     | 314 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 2     | 313 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 31  | 8     | 304 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | c     | 511 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | p     | 602 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | b     | 512 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 1     | 211 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 31  | c     | 506 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 31  | 0     | 306 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 32  | A     | 405 | PHO  | C3D-C4D | 2.31  | 1.44        | 1.41     |
| 31  | 2     | 306 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 31  | P     | 602 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | 2     | 309 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 31  | A     | 404 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | 8     | 312 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 43  | 5     | 302 | ET4  | C15-C14 | 2.30  | 1.50        | 1.43     |
| 43  | 0     | 302 | ET4  | C15-C14 | 2.30  | 1.50        | 1.43     |
| 31  | 5     | 309 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | D     | 403 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | 7     | 306 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | 5     | 305 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 31  | a     | 407 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | p     | 601 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 42  | 3     | 301 | A86  | C32-C31 | -2.30 | 1.50        | 1.54     |
| 31  | 6     | 212 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | 2     | 312 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | p     | 606 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 31  | 2     | 313 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 31  | D     | 404 | CLA  | MG-NB   | -2.30 | 2.01        | 2.05     |
| 42  | 9     | 202 | A86  | C19-C18 | -2.30 | 1.49        | 1.52     |
| 31  | 7     | 316 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 31  | 6     | 216 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 6     | 208 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 1     | 208 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 5     | 306 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 3     | 304 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | B     | 513 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | b     | 513 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | b     | 514 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | P     | 608 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 515 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | P     | 608 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | C     | 502 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 37  | y     | 101 | LMG  | O7-C8   | -2.29 | 1.41        | 1.46     |
| 42  | 3     | 302 | A86  | C13-C11 | -2.29 | 1.45        | 1.49     |
| 31  | 0     | 307 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | 7     | 307 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | 2     | 307 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | b     | 503 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | b     | 504 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | 9     | 204 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | P     | 605 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 31  | 6     | 201 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | A     | 407 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 31  | B     | 505 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | 5     | 314 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | 0     | 314 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | 1     | 207 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 31  | c     | 510 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 31  | p     | 602 | CLA  | CMC-C2C | -2.28 | 1.46        | 1.50     |
| 31  | C     | 506 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | 3     | 311 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 31  | b     | 507 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | B     | 509 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 31  | 0     | 309 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 44  | p     | 611 | DD6  | O1-C20  | -2.28 | 1.43        | 1.46     |
| 31  | C     | 510 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | b     | 516 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | 5     | 308 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 42  | 4     | 202 | A86  | C19-C18 | -2.28 | 1.49        | 1.52     |
| 35  | d     | 406 | PL9  | C52-C5  | -2.28 | 1.46        | 1.50     |
| 31  | 5     | 304 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | p     | 603 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | b     | 506 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | 7     | 309 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | 2     | 309 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | 1     | 212 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 31  | 1     | 208 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 31  | 2     | 306 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 31  | p     | 605 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 42  | 8     | 302 | A86  | C19-C18 | -2.28 | 1.49        | 1.52     |
| 31  | 0     | 308 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 216 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | 7     | 312 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | B     | 516 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 6     | 207 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | 1     | 214 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 8     | 311 | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 31  | 4     | 208 | CLA  | MG-ND   | -2.27 | 2.01        | 2.05     |
| 31  | a     | 403 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | c     | 502 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 5     | 309 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | 0     | 306 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | c     | 514 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | B     | 502 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | d     | 403 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | 9     | 211 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 1     | 201 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 31  | 5     | 305 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 31  | a     | 407 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 37  | Y     | 101 | LMG  | O7-C8   | -2.27 | 1.41        | 1.46     |
| 35  | a     | 410 | PL9  | C6-C1   | -2.27 | 1.44        | 1.48     |
| 31  | 7     | 315 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | p     | 608 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | 2     | 315 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 31  | 6     | 214 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 8     | 306 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 31  | 5     | 307 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | C     | 514 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 42  | 1     | 202 | A86  | C13-C11 | -2.26 | 1.45        | 1.49     |
| 31  | P     | 602 | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 31  | 5     | 308 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | A     | 403 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | C     | 514 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 7     | 314 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 4     | 204 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 2     | 314 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 4     | 212 | CLA  | CBD-CAD | 2.26  | 1.56        | 1.51     |
| 37  | D     | 410 | LMG  | C3-C2   | 2.26  | 1.58        | 1.52     |
| 31  | B     | 502 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 7     | 314 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 2     | 314 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | 3     | 304 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 31  | b     | 509 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 43  | 0     | 302 | ET4  | C11-C10 | 2.26  | 1.50        | 1.43     |
| 31  | 0     | 310 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | p     | 604 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | b     | 508 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | c     | 514 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 7     | 311 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 2     | 311 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 31  | 1     | 205 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 37  | d     | 410 | LMG  | C3-C2   | 2.26  | 1.58        | 1.52     |
| 31  | 5     | 307 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 31  | B     | 508 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 31  | c     | 507 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | 8     | 305 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 9     | 208 | CLA  | MG-ND   | -2.25 | 2.01        | 2.05     |
| 31  | C     | 506 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 1     | 212 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 43  | 5     | 302 | ET4  | C01-C06 | 2.25  | 1.56        | 1.53     |
| 42  | 6     | 202 | A86  | C13-C11 | -2.25 | 1.45        | 1.49     |
| 31  | 6     | 212 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | 2     | 311 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | b     | 515 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 3     | 307 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | C     | 504 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 1     | 209 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | b     | 517 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 9     | 212 | CLA  | CBD-CAD | 2.25  | 1.56        | 1.51     |
| 31  | P     | 606 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 31  | B     | 513 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | a     | 403 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | b     | 514 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | c     | 506 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | c     | 508 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 31  | 3     | 305 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 2     | 316 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | b     | 512 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | p     | 609 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 31  | 6     | 205 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 7     | 313 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 31  | 1     | 216 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 31  | 9     | 204 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 2     | 307 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 3     | 313 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 312 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | 5     | 313 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 42  | 7     | 302 | A86  | C13-C11 | -2.24 | 1.45        | 1.49     |
| 31  | C     | 513 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | B     | 511 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | C     | 507 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | b     | 510 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | A     | 407 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 1     | 207 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | c     | 508 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | b     | 503 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | P     | 601 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 43  | 5     | 302 | ET4  | C11-C10 | 2.24  | 1.50        | 1.43     |
| 31  | 0     | 312 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | C     | 508 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | b     | 515 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 31  | 5     | 313 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 7     | 309 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | C     | 511 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | c     | 511 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 31  | B     | 507 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | 8     | 304 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 31  | 6     | 215 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 1     | 215 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 31  | 4     | 211 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 31  | p     | 602 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 35  | a     | 410 | PL9  | C7-C3   | -2.23 | 1.48        | 1.51     |
| 31  | 0     | 305 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 0     | 312 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | A     | 403 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | b     | 509 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 8     | 313 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 2     | 315 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 6     | 205 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | b     | 510 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 6     | 207 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 5     | 314 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 0     | 314 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | C     | 509 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 6     | 212 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 39  | C     | 519 | DGD  | O5D-C6D | -2.23 | 1.39        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | P     | 609 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | 6     | 201 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 31  | 5     | 310 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 9     | 206 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | c     | 504 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | 8     | 313 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | p     | 604 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 1     | 212 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 36  | D     | 412 | LHG  | O7-C5   | -2.23 | 1.41        | 1.46     |
| 36  | d     | 412 | LHG  | O7-C5   | -2.23 | 1.41        | 1.46     |
| 31  | C     | 511 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 6     | 213 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 1     | 213 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 32  | A     | 406 | PHO  | CAC-C3C | -2.23 | 1.47        | 1.51     |
| 35  | A     | 410 | PL9  | C7-C3   | -2.23 | 1.48        | 1.51     |
| 31  | 0     | 313 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | c     | 511 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 8     | 313 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 31  | b     | 515 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 6     | 209 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | 0     | 313 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | 4     | 204 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 39  | c     | 519 | DGD  | O5D-C6D | -2.23 | 1.39        | 1.43     |
| 44  | 7     | 304 | DD6  | O1-C20  | -2.23 | 1.43        | 1.46     |
| 44  | 2     | 304 | DD6  | O1-C20  | -2.23 | 1.43        | 1.46     |
| 31  | 5     | 306 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | c     | 509 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | 0     | 307 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 31  | P     | 602 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 31  | B     | 508 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 31  | p     | 601 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 31  | P     | 604 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 8     | 307 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 31  | 5     | 312 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | B     | 507 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | B     | 514 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 7     | 307 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 7     | 311 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | B     | 505 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 31  | 3     | 313 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | 6     | 208 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | 1     | 201 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 315 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | 5     | 306 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 31  | 0     | 306 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 37  | D     | 408 | LMG  | O7-C8   | -2.22 | 1.41        | 1.46     |
| 31  | p     | 609 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 31  | B     | 509 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 37  | d     | 408 | LMG  | O7-C8   | -2.22 | 1.41        | 1.46     |
| 31  | D     | 401 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | 4     | 207 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 31  | 0     | 312 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 32  | a     | 406 | PHO  | CAC-C3C | -2.22 | 1.47        | 1.51     |
| 31  | 8     | 305 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 31  | 3     | 305 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 31  | 4     | 206 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | 5     | 310 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 9     | 208 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 5     | 311 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 6     | 210 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 0     | 311 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | P     | 609 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | c     | 513 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | C     | 509 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | C     | 508 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | B     | 516 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 31  | C     | 507 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | 4     | 206 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 31  | C     | 512 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | 5     | 312 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 7     | 315 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 2     | 314 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 31  | b     | 511 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | b     | 508 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | B     | 516 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | p     | 603 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | 8     | 307 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 36  | D     | 412 | LHG  | P-O6    | 2.21  | 1.67        | 1.60     |
| 36  | d     | 412 | LHG  | P-O6    | 2.21  | 1.67        | 1.60     |
| 31  | W     | 202 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 32  | a     | 405 | PHO  | C4D-ND  | -2.21 | 1.35        | 1.38     |
| 31  | c     | 505 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | 5     | 313 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | B     | 514 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 212 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 31  | B     | 514 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 44  | P     | 611 | DD6  | O1-C20  | -2.21 | 1.43        | 1.46     |
| 31  | c     | 506 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 5     | 310 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 31  | b     | 506 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 4     | 208 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 31  | 3     | 313 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | c     | 503 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | B     | 511 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 37  | w     | 201 | LMG  | O7-C8   | -2.20 | 1.41        | 1.46     |
| 31  | 5     | 308 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | d     | 401 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | C     | 507 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 9     | 208 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | c     | 507 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 9     | 204 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 7     | 307 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | c     | 509 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | 0     | 308 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | A     | 407 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | b     | 505 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 6     | 206 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | 3     | 307 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 3     | 309 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 31  | 3     | 310 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 31  | B     | 502 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | B     | 505 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | b     | 512 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | b     | 504 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | 5     | 312 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | 3     | 314 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 31  | B     | 510 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 31  | 1     | 205 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 31  | 2     | 307 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 31  | p     | 606 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | P     | 603 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | 2     | 309 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | p     | 609 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | c     | 507 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | p     | 602 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 2     | 305 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | b     | 517 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | 9     | 208 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 37  | d     | 410 | LMG  | C1-C2   | 2.19  | 1.58        | 1.52     |
| 31  | c     | 512 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 35  | a     | 410 | PL9  | C53-C6  | -2.19 | 1.46        | 1.50     |
| 31  | w     | 202 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | b     | 517 | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 31  | P     | 602 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | z     | 101 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 39  | C     | 518 | DGD  | O5D-C6D | -2.19 | 1.40        | 1.43     |
| 31  | 0     | 310 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | D     | 403 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 3     | 304 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 44  | 1     | 204 | DD6  | C36-C31 | -2.19 | 1.32        | 1.35     |
| 31  | C     | 505 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | p     | 602 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | d     | 403 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 2     | 309 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | C     | 506 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | 5     | 308 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 0     | 308 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 1     | 210 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 39  | c     | 518 | DGD  | O5D-C6D | -2.19 | 1.40        | 1.43     |
| 31  | 6     | 215 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | 6     | 213 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | 1     | 213 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 31  | W     | 202 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 42  | 2     | 302 | A86  | C13-C11 | -2.19 | 1.45        | 1.49     |
| 31  | P     | 606 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 31  | 4     | 212 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | B     | 515 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 35  | A     | 410 | PL9  | C53-C6  | -2.19 | 1.46        | 1.50     |
| 31  | b     | 509 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 31  | P     | 609 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | B     | 513 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | p     | 603 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | b     | 516 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | 7     | 308 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | 2     | 308 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | c     | 512 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 0     | 310 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 207 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 37  | W     | 201 | LMG  | O7-C8   | -2.18 | 1.41        | 1.46     |
| 31  | 1     | 208 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 42  | 5     | 303 | A86  | C32-C31 | -2.18 | 1.50        | 1.54     |
| 42  | 0     | 303 | A86  | C32-C31 | -2.18 | 1.50        | 1.54     |
| 31  | C     | 512 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | b     | 503 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 5     | 304 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 0     | 304 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 5     | 314 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | B     | 508 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | d     | 403 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | a     | 403 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 4     | 204 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | B     | 503 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | B     | 504 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | c     | 505 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | b     | 507 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 37  | D     | 410 | LMG  | C1-C2   | 2.18  | 1.58        | 1.52     |
| 31  | 5     | 310 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 0     | 310 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | C     | 505 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 31  | 9     | 213 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | w     | 202 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 4     | 206 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | c     | 513 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 31  | 3     | 312 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 31  | a     | 407 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 36  | A     | 413 | LHG  | O7-C5   | -2.18 | 1.41        | 1.46     |
| 31  | 5     | 311 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | 0     | 311 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 31  | b     | 517 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 1     | 205 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 31  | 3     | 314 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | b     | 506 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 7     | 312 | CLA  | C1C-C2C | 2.17  | 1.46        | 1.42     |
| 31  | 7     | 309 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | 4     | 208 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 2     | 309 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 210 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 1     | 210 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | P     | 602 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 36  | a     | 412 | LHG  | O7-C5   | -2.17 | 1.41        | 1.46     |
| 31  | P     | 604 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | 7     | 305 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | b     | 504 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | C     | 503 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | 3     | 310 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | b     | 508 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 1     | 211 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 31  | 1     | 215 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | c     | 509 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 2     | 315 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 31  | b     | 514 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 31  | D     | 404 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | A     | 403 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | B     | 503 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | 8     | 312 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | C     | 503 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | c     | 503 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 31  | C     | 513 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 31  | 7     | 314 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 31  | C     | 506 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 6     | 214 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 3     | 307 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 3     | 311 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | D     | 403 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | B     | 506 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | P     | 603 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 4     | 213 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 9     | 205 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | d     | 404 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 31  | Z     | 101 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 41  | F     | 101 | HEM  | FE-NC   | 2.16  | 2.02        | 1.95     |
| 31  | 1     | 213 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | C     | 508 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 7     | 310 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 31  | 3     | 306 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | B     | 507 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 2     | 307 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | b     | 511 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 506 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 31  | 9     | 206 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 5     | 307 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | 8     | 308 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | p     | 606 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 41  | f     | 101 | HEM  | FE-NC   | 2.16  | 2.02        | 1.95     |
| 31  | 7     | 309 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | b     | 508 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 8     | 308 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | B     | 505 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 31  | P     | 609 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 31  | 9     | 210 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | 7     | 314 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 9     | 210 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 2     | 314 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 32  | A     | 405 | PHO  | C4D-ND  | -2.15 | 1.35        | 1.38     |
| 31  | 0     | 305 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | B     | 511 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 515 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | a     | 404 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 31  | b     | 511 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | B     | 507 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 4     | 209 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 516 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 3     | 305 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 8     | 307 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 5     | 309 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | 7     | 310 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | C     | 511 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 0     | 309 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | A     | 404 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 8     | 306 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 31  | 2     | 306 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 31  | B     | 514 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | P     | 608 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 9     | 209 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | c     | 508 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 4     | 208 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | a     | 404 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | b     | 515 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 307 | CLA  | MG-ND   | -2.15 | 2.01        | 2.05     |
| 31  | 0     | 314 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 31  | B     | 512 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 31  | 2     | 312 | CLA  | C1C-C2C | 2.15  | 1.46        | 1.42     |
| 31  | 2     | 311 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 31  | B     | 514 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | p     | 604 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | B     | 516 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 4     | 210 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | P     | 602 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 4     | 209 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 9     | 211 | CLA  | CBD-CAD | 2.14  | 1.56        | 1.51     |
| 31  | 9     | 205 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 7     | 314 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 3     | 314 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 9     | 209 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | p     | 606 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | 2     | 310 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 31  | c     | 504 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | b     | 503 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | b     | 515 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | 3     | 308 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | z     | 101 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 0     | 313 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | c     | 506 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | b     | 504 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | b     | 514 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 4     | 205 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 6     | 205 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | 3     | 307 | CLA  | MG-ND   | -2.14 | 2.01        | 2.05     |
| 31  | A     | 404 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 31  | p     | 601 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 8     | 305 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 31  | 6     | 213 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 31  | c     | 502 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 1     | 206 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 31  | b     | 513 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 509 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | b     | 517 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | P     | 606 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | B     | 513 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | b     | 512 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 6     | 214 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | c     | 511 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | B     | 510 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 1     | 201 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | B     | 503 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 0     | 311 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | P     | 607 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 306 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 2     | 310 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | c     | 510 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 31  | 9     | 212 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | 2     | 313 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | C     | 509 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 9     | 206 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | b     | 505 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 31  | B     | 502 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 307 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 1     | 209 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 4     | 212 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | 3     | 306 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | P     | 604 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | c     | 510 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 6     | 211 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | c     | 513 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 4     | 204 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 6     | 214 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | 6     | 208 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 31  | B     | 516 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 5     | 309 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 8     | 305 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | A     | 404 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | 4     | 210 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | B     | 515 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 31  | 4     | 205 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | 2     | 314 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 503 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 31  | B     | 514 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | b     | 515 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 31  | 0     | 304 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | C     | 510 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | c     | 507 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | 6     | 201 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | B     | 509 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | B     | 508 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | 4     | 211 | CLA  | CBD-CAD | 2.12  | 1.56        | 1.51     |
| 31  | 0     | 307 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | 2     | 316 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | C     | 504 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | p     | 604 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | C     | 513 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | c     | 508 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | p     | 602 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | p     | 609 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 7     | 313 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | 3     | 304 | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 31  | B     | 505 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | D     | 404 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | b     | 516 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | B     | 510 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | p     | 607 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | W     | 202 | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 31  | P     | 601 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | C     | 502 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | C     | 510 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 31  | 3     | 307 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 8     | 308 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | c     | 502 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | C     | 502 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | C     | 510 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | a     | 404 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | 5     | 305 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 31  | B     | 504 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 31  | b     | 506 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 4     | 213 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 31  | 1     | 216 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 37  | j     | 101 | LMG  | O8-C9   | -2.12 | 1.40        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 309 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 31  | p     | 604 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 31  | 9     | 204 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | 1     | 214 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | C     | 503 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | p     | 609 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | 8     | 308 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 36  | d     | 411 | LHG  | O7-C5   | -2.11 | 1.41        | 1.46     |
| 31  | p     | 608 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 34  | A     | 409 | SQD  | O2-C2   | -2.11 | 1.37        | 1.43     |
| 31  | 0     | 307 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 31  | C     | 505 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 5     | 305 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | b     | 510 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | P     | 606 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | D     | 401 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 9     | 204 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | p     | 604 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | B     | 506 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 31  | d     | 404 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 3     | 305 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 1     | 214 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | Z     | 101 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | b     | 502 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | 7     | 305 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 4     | 206 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 31  | P     | 608 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | 5     | 306 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | C     | 507 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 5     | 312 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 6     | 211 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 1     | 211 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | C     | 507 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | 7     | 308 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | 2     | 308 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 31  | B     | 510 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | c     | 510 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | 6     | 207 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 36  | D     | 411 | LHG  | O7-C5   | -2.11 | 1.41        | 1.46     |
| 34  | a     | 409 | SQD  | O2-C2   | -2.11 | 1.37        | 1.43     |
| 31  | C     | 513 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 307 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | C     | 514 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | c     | 514 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | B     | 515 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 3     | 304 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 1     | 201 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 8     | 314 | CLA  | CBD-CAD | 2.10  | 1.56        | 1.51     |
| 31  | b     | 504 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 5     | 309 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 6     | 216 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | w     | 202 | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 31  | A     | 407 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | w     | 202 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | b     | 507 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | 7     | 306 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | p     | 607 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | b     | 508 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | 9     | 209 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | 3     | 305 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | B     | 501 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | D     | 404 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | b     | 502 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | c     | 507 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | b     | 516 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 32  | a     | 406 | PHO  | C4D-ND  | -2.10 | 1.35        | 1.38     |
| 31  | P     | 609 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 31  | 8     | 312 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | 3     | 310 | CLA  | CBD-CAD | 2.10  | 1.56        | 1.51     |
| 31  | 7     | 310 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | P     | 604 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 2     | 305 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | 2     | 310 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 8     | 313 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | 7     | 311 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 8     | 304 | CLA  | CBD-CAD | 2.10  | 1.56        | 1.51     |
| 31  | D     | 401 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 31  | 0     | 306 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 32  | A     | 406 | PHO  | C4D-ND  | -2.10 | 1.35        | 1.38     |
| 34  | 5     | 316 | SQD  | O2-C2   | -2.10 | 1.37        | 1.43     |
| 31  | C     | 508 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 31  | c     | 508 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 34  | 0     | 316 | SQD  | O2-C2   | -2.10 | 1.37        | 1.43     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 215 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | 3     | 311 | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 31  | 1     | 215 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | c     | 505 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | d     | 401 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | B     | 501 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | 6     | 201 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | P     | 603 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 31  | 1     | 210 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 31  | 5     | 304 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 6     | 210 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 6     | 212 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 1     | 210 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | 1     | 212 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 31  | B     | 504 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | D     | 403 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 0     | 309 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | b     | 516 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | b     | 511 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | c     | 505 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 36  | H     | 103 | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 31  | a     | 407 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | b     | 517 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 5     | 307 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 8     | 307 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 1     | 209 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | 8     | 310 | CLA  | CBD-CAD | 2.09  | 1.56        | 1.51     |
| 31  | c     | 512 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | B     | 509 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 7     | 312 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | b     | 510 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 4     | 209 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 9     | 207 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 4     | 211 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 7     | 305 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | 2     | 305 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | C     | 504 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 1     | 214 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 3     | 304 | CLA  | CBD-CAD | 2.09  | 1.56        | 1.51     |
| 31  | 3     | 312 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 31  | B     | 507 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 6     | 209 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 211 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 9     | 207 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 1     | 211 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | P     | 607 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 2     | 308 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | C     | 503 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | c     | 503 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | C     | 512 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | P     | 605 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 2     | 305 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 2     | 312 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 31  | c     | 504 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | d     | 403 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | P     | 607 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 9     | 208 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | C     | 512 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 31  | 5     | 304 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 42  | 9     | 202 | A86  | C13-C11 | -2.09 | 1.45        | 1.49     |
| 31  | P     | 605 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 1     | 213 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | B     | 501 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 4     | 205 | CLA  | CBD-CAD | 2.09  | 1.56        | 1.51     |
| 31  | c     | 512 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 31  | 5     | 304 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | C     | 509 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | 9     | 213 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | d     | 404 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 31  | d     | 404 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 31  | 3     | 308 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 3     | 309 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 4     | 209 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 31  | 6     | 210 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 31  | b     | 502 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | d     | 403 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | 0     | 304 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | c     | 503 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | c     | 513 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | 7     | 316 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | p     | 605 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | 0     | 308 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | 4     | 204 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | d     | 401 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 44  | 6     | 204 | DD6  | C36-C31 | -2.08 | 1.32        | 1.35     |
| 31  | p     | 607 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | B     | 506 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | b     | 505 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 37  | J     | 101 | LMG  | O8-C9   | -2.08 | 1.40        | 1.45     |
| 31  | 4     | 207 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 4     | 205 | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 31  | b     | 513 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 43  | 5     | 302 | ET4  | C38-C33 | 2.08  | 1.37        | 1.35     |
| 43  | 0     | 302 | ET4  | C38-C33 | 2.08  | 1.37        | 1.35     |
| 31  | P     | 604 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | B     | 508 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | C     | 505 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | P     | 607 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | p     | 608 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 31  | 9     | 205 | CLA  | CBD-CAD | 2.08  | 1.56        | 1.51     |
| 31  | b     | 507 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | 5     | 313 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | 9     | 209 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | b     | 516 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | c     | 504 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 31  | C     | 508 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | P     | 608 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 31  | 8     | 313 | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 31  | 5     | 311 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | p     | 603 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 1     | 206 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | b     | 506 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | c     | 513 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | 7     | 305 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 6     | 215 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | W     | 202 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | p     | 606 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 2     | 313 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | c     | 510 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | C     | 502 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 9     | 205 | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 31  | 1     | 205 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | 3     | 307 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 4     | 208 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 9     | 211 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | b     | 502 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | c     | 502 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | B     | 502 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 6     | 209 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | 9     | 211 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | 0     | 313 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | C     | 504 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | p     | 607 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | p     | 608 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | B     | 511 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | D     | 403 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | B     | 509 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 7     | 316 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 31  | B     | 501 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | 0     | 309 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | b     | 510 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 31  | p     | 603 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | 4     | 207 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 31  | 9     | 206 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | p     | 605 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 31  | 1     | 215 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 31  | c     | 508 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 9     | 211 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 31  | C     | 511 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | c     | 511 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | b     | 512 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 4     | 213 | CLA  | CAC-C3C | -2.06 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 31  | b     | 509 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | w     | 202 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 41  | F     | 101 | HEM  | CMB-C2B | 2.06  | 1.55        | 1.50     |
| 31  | p     | 605 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 31  | C     | 512 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | B     | 503 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | B     | 512 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | D     | 404 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | c     | 511 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 5     | 314 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | 0     | 314 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 36  | h     | 103 | LHG  | P-O6    | 2.06  | 1.67        | 1.59     |
| 42  | 9     | 203 | A86  | C13-C11 | -2.06 | 1.45        | 1.49     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 313 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 34  | 0     | 316 | SQD  | O47-C45 | -2.06 | 1.41        | 1.46     |
| 31  | C     | 513 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 41  | f     | 101 | HEM  | CMB-C2B | 2.06  | 1.55        | 1.50     |
| 31  | 0     | 305 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | 4     | 212 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 0     | 308 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 34  | 0     | 316 | SQD  | O4-C4   | -2.06 | 1.37        | 1.43     |
| 31  | 0     | 314 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | P     | 605 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 31  | 7     | 312 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 3     | 314 | CLA  | CBD-CAD | 2.06  | 1.56        | 1.51     |
| 31  | C     | 508 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | C     | 510 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | c     | 506 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | 1     | 207 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 31  | 4     | 211 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 42  | 4     | 202 | A86  | C13-C11 | -2.06 | 1.45        | 1.49     |
| 31  | 4     | 207 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 31  | B     | 505 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 31  | c     | 504 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 31  | 5     | 310 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 0     | 310 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 9     | 210 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 4     | 212 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 2     | 308 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | C     | 514 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 1     | 208 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | C     | 504 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 41  | f     | 101 | HEM  | CMC-C2C | 2.05  | 1.55        | 1.50     |
| 31  | C     | 503 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 2     | 309 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | c     | 512 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | a     | 404 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | c     | 509 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 6     | 213 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | 1     | 213 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | 5     | 312 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | 0     | 312 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | c     | 514 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 0     | 312 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 5     | 310 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 0     | 310 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | z     | 101 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | D     | 404 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | 7     | 308 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 9     | 208 | CLA  | C1B-NB  | -2.05 | 1.35        | 1.37     |
| 31  | 7     | 306 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | 8     | 313 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 0     | 311 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | C     | 505 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | c     | 505 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | p     | 605 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | B     | 513 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | 7     | 307 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 2     | 307 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | 4     | 210 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | P     | 605 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 31  | 5     | 308 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 31  | p     | 609 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 31  | W     | 202 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | 7     | 313 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 31  | b     | 514 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 7     | 312 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | 6     | 206 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | A     | 403 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | b     | 504 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | 2     | 316 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 4     | 209 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 31  | 0     | 304 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 31  | B     | 515 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | 6     | 213 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | 4     | 204 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | 8     | 305 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | B     | 512 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 31  | C     | 502 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 41  | F     | 101 | HEM  | CMC-C2C | 2.04  | 1.55        | 1.50     |
| 31  | P     | 603 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | 7     | 315 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 42  | 5     | 303 | A86  | O1-C15  | -2.04 | 1.42        | 1.45     |
| 42  | 0     | 303 | A86  | O1-C15  | -2.04 | 1.42        | 1.45     |
| 31  | P     | 609 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 31  | Z     | 101 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | C     | 504 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | B     | 507 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | B     | 510 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | c     | 503 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 31  | 6     | 205 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 1     | 205 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 31  | 3     | 313 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 31  | 2     | 315 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | C     | 511 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 31  | 9     | 207 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 31  | 3     | 305 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 31  | 9     | 209 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 31  | 0     | 306 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 8     | 310 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 31  | b     | 505 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 42  | 4     | 203 | A86  | C13-C11 | -2.03 | 1.45        | 1.49     |
| 31  | c     | 504 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 31  | b     | 513 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 31  | 6     | 211 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 9     | 212 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 1     | 211 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 36  | D     | 411 | LHG  | P-O6    | 2.03  | 1.67        | 1.59     |
| 31  | 6     | 215 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 31  | C     | 506 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 7     | 316 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 0     | 307 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | a     | 403 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 209 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 1     | 209 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 208 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | A     | 404 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 31  | B     | 504 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | a     | 403 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 7     | 311 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 4     | 210 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 39  | C     | 519 | DGD  | O6D-C5D | -2.03 | 1.39        | 1.44     |
| 31  | B     | 506 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | a     | 407 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | P     | 606 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 31  | 9     | 213 | CLA  | CAC-C3C | -2.03 | 1.46        | 1.50     |
| 31  | 2     | 311 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 39  | c     | 519 | DGD  | O6D-C5D | -2.03 | 1.39        | 1.44     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 308 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 214 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 34  | 5     | 316 | SQD  | O4-C4   | -2.03 | 1.37        | 1.43     |
| 31  | b     | 508 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 0     | 311 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 34  | 5     | 316 | SQD  | O3-C3   | -2.03 | 1.37        | 1.43     |
| 34  | 0     | 316 | SQD  | O3-C3   | -2.03 | 1.37        | 1.43     |
| 31  | c     | 507 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 208 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 8     | 305 | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 31  | C     | 512 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | b     | 511 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 31  | 6     | 207 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | 1     | 207 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 36  | d     | 411 | LHG  | P-O6    | 2.03  | 1.67        | 1.59     |
| 31  | 3     | 310 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 31  | 9     | 210 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 33  | H     | 101 | BCR  | C33-C5  | -2.03 | 1.47        | 1.50     |
| 31  | B     | 506 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 31  | c     | 512 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 31  | b     | 507 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 37  | b     | 521 | LMG  | O7-C8   | -2.02 | 1.41        | 1.46     |
| 31  | A     | 407 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | c     | 502 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 1     | 210 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 37  | 5     | 315 | LMG  | O7-C8   | -2.02 | 1.41        | 1.46     |
| 31  | 7     | 309 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 2     | 306 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 2     | 312 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | d     | 401 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 31  | A     | 403 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | b     | 503 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 2     | 316 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | a     | 404 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 34  | B     | 523 | SQD  | O2-C2   | -2.02 | 1.38        | 1.43     |
| 34  | 5     | 316 | SQD  | O47-C45 | -2.02 | 1.41        | 1.46     |
| 31  | 7     | 307 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 1     | 215 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 34  | b     | 501 | SQD  | O2-C2   | -2.02 | 1.38        | 1.43     |
| 31  | 2     | 315 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | c     | 506 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 8     | 311 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 212 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 31  | 1     | 208 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 5     | 311 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 1     | 208 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 5     | 314 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 31  | 9     | 205 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | 6     | 206 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 37  | B     | 520 | LMG  | O7-C8   | -2.01 | 1.41        | 1.46     |
| 31  | d     | 404 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 31  | 3     | 312 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 0     | 311 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 0     | 309 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 41  | V     | 201 | HEM  | FE-ND   | 2.01  | 2.01        | 1.94     |
| 31  | 7     | 315 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 31  | 2     | 315 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 31  | 6     | 205 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 34  | A     | 409 | SQD  | O47-C45 | -2.01 | 1.41        | 1.46     |
| 31  | 4     | 211 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 41  | v     | 201 | HEM  | FE-ND   | 2.01  | 2.01        | 1.94     |
| 31  | B     | 502 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 31  | A     | 404 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 3     | 311 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 31  | C     | 507 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 34  | a     | 409 | SQD  | O47-C45 | -2.01 | 1.41        | 1.46     |
| 31  | C     | 513 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 3     | 314 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 1     | 214 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 31  | 4     | 208 | CLA  | C1B-NB  | -2.00 | 1.35        | 1.37     |
| 31  | D     | 401 | CLA  | CHC-C1C | 2.00  | 1.42        | 1.38     |
| 31  | 6     | 216 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 31  | C     | 510 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 31  | 9     | 204 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | 1     | 205 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 31  | 8     | 309 | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |
| 37  | D     | 409 | LMG  | O7-C8   | -2.00 | 1.41        | 1.46     |
| 41  | f     | 101 | HEM  | CMA-C3A | 2.00  | 1.54        | 1.50     |
| 31  | 3     | 309 | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |

All (2549) bond angle outliers are listed below:

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 42  | 3     | 301 | A86  | C40-C32-C31 | -17.41 | 94.89       | 110.47   |
| 42  | 8     | 301 | A86  | C40-C32-C31 | -17.36 | 94.94       | 110.47   |
| 42  | 8     | 301 | A86  | O1-C20-C19  | -16.74 | 97.80       | 113.49   |
| 42  | 3     | 301 | A86  | O1-C20-C19  | -16.71 | 97.83       | 113.49   |
| 42  | 9     | 202 | A86  | C20-O1-C15  | 14.55  | 67.28       | 61.03    |
| 42  | 4     | 202 | A86  | C20-O1-C15  | 14.54  | 67.28       | 61.03    |
| 42  | 4     | 203 | A86  | C20-O1-C15  | 13.97  | 67.03       | 61.03    |
| 42  | 9     | 203 | A86  | C20-O1-C15  | 13.84  | 66.98       | 61.03    |
| 42  | 4     | 201 | A86  | C41-C32-C31 | 12.99  | 122.10      | 110.47   |
| 42  | 9     | 201 | A86  | C41-C32-C31 | 12.99  | 122.10      | 110.47   |
| 42  | 4     | 201 | A86  | C20-O1-C15  | 12.72  | 66.50       | 61.03    |
| 42  | 9     | 201 | A86  | C20-O1-C15  | 12.54  | 66.42       | 61.03    |
| 42  | 3     | 302 | A86  | C20-O1-C15  | 12.07  | 66.22       | 61.03    |
| 42  | 8     | 302 | A86  | C20-O1-C15  | 11.99  | 66.18       | 61.03    |
| 42  | p     | 610 | A86  | C20-O1-C15  | 11.28  | 65.88       | 61.03    |
| 42  | P     | 610 | A86  | C20-O1-C15  | 11.24  | 65.86       | 61.03    |
| 42  | P     | 610 | A86  | C29-C30-C31 | -10.95 | 164.74      | 177.66   |
| 42  | p     | 610 | A86  | C29-C30-C31 | -10.92 | 164.77      | 177.66   |
| 42  | 8     | 301 | A86  | C35-C34-C33 | -10.17 | 91.62       | 109.89   |
| 42  | 3     | 301 | A86  | C35-C34-C33 | -10.16 | 91.64       | 109.89   |
| 44  | 8     | 303 | DD6  | C10-C9-C8   | 9.94   | 152.01      | 123.20   |
| 44  | 3     | 303 | DD6  | C10-C9-C8   | 9.92   | 151.93      | 123.20   |
| 42  | 9     | 203 | A86  | O1-C20-C21  | -9.80  | 104.10      | 115.05   |
| 42  | 0     | 301 | A86  | C20-O1-C15  | 9.78   | 65.23       | 61.03    |
| 42  | 3     | 301 | A86  | C23-C16-C22 | -9.75  | 93.20       | 107.37   |
| 42  | 5     | 301 | A86  | C20-O1-C15  | 9.74   | 65.21       | 61.03    |
| 42  | 4     | 203 | A86  | O1-C20-C21  | -9.73  | 104.17      | 115.05   |
| 42  | 8     | 301 | A86  | C23-C16-C22 | -9.73  | 93.23       | 107.37   |
| 42  | 5     | 303 | A86  | C20-O1-C15  | 9.50   | 65.11       | 61.03    |
| 42  | 0     | 303 | A86  | C20-O1-C15  | 9.41   | 65.07       | 61.03    |
| 42  | p     | 610 | A86  | C41-C32-C31 | -9.09  | 102.34      | 110.47   |
| 42  | P     | 610 | A86  | C41-C32-C31 | -9.06  | 102.36      | 110.47   |
| 42  | 8     | 301 | A86  | C20-O1-C15  | 9.05   | 64.92       | 61.03    |
| 42  | 3     | 301 | A86  | C20-O1-C15  | 9.03   | 64.91       | 61.03    |
| 42  | 4     | 202 | A86  | O4-C38-C39  | 8.72   | 126.64      | 111.09   |
| 42  | 9     | 202 | A86  | O4-C38-C39  | 8.72   | 126.64      | 111.09   |
| 42  | 7     | 302 | A86  | C20-O1-C15  | 8.63   | 64.74       | 61.03    |
| 42  | 2     | 302 | A86  | C20-O1-C15  | 8.63   | 64.74       | 61.03    |
| 44  | 8     | 303 | DD6  | C9-C10-C11  | 8.59   | 139.33      | 127.28   |
| 42  | 0     | 317 | A86  | C20-O1-C15  | 8.57   | 64.71       | 61.03    |
| 44  | 3     | 303 | DD6  | C9-C10-C11  | 8.55   | 139.26      | 127.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 5     | 317 | A86  | C20-O1-C15  | 8.49  | 64.68       | 61.03    |
| 42  | 8     | 301 | A86  | O1-C20-C21  | -8.46 | 105.59      | 115.05   |
| 42  | 2     | 301 | A86  | C20-O1-C15  | 8.46  | 64.67       | 61.03    |
| 42  | 3     | 301 | A86  | O1-C20-C21  | -8.44 | 105.61      | 115.05   |
| 42  | 7     | 301 | A86  | C20-O1-C15  | 8.41  | 64.64       | 61.03    |
| 42  | 9     | 201 | A86  | C33-C32-C31 | -8.27 | 101.17      | 109.21   |
| 42  | 4     | 201 | A86  | C33-C32-C31 | -8.26 | 101.19      | 109.21   |
| 31  | 8     | 309 | CLA  | C4A-NA-C1A  | 8.23  | 110.44      | 106.68   |
| 31  | 3     | 309 | CLA  | C4A-NA-C1A  | 8.15  | 110.40      | 106.68   |
| 44  | 7     | 304 | DD6  | C4-C5-C6    | -8.14 | 115.86      | 127.28   |
| 44  | 2     | 304 | DD6  | C4-C5-C6    | -8.14 | 115.86      | 127.28   |
| 42  | 5     | 301 | A86  | C25-C26-C27 | -7.94 | 116.14      | 127.28   |
| 42  | 0     | 301 | A86  | C25-C26-C27 | -7.91 | 116.19      | 127.28   |
| 44  | 8     | 303 | DD6  | C9-C8-C6    | 7.89  | 147.99      | 126.36   |
| 44  | 3     | 303 | DD6  | C9-C8-C6    | 7.87  | 147.93      | 126.36   |
| 42  | 4     | 201 | A86  | O4-C34-C35  | -7.83 | 87.58       | 107.64   |
| 42  | 9     | 201 | A86  | O4-C34-C35  | -7.83 | 87.59       | 107.64   |
| 44  | 7     | 304 | DD6  | C14-C13-C11 | -7.56 | 113.80      | 125.53   |
| 44  | 2     | 304 | DD6  | C14-C13-C11 | -7.56 | 113.80      | 125.53   |
| 42  | 7     | 302 | A86  | C3-C2-C1    | -7.49 | 116.77      | 127.28   |
| 42  | 3     | 301 | A86  | C21-C20-C19 | -7.49 | 105.83      | 114.24   |
| 42  | 2     | 302 | A86  | C3-C2-C1    | -7.47 | 116.81      | 127.28   |
| 42  | 8     | 301 | A86  | C21-C20-C19 | -7.46 | 105.86      | 114.24   |
| 42  | 4     | 202 | A86  | C34-O4-C38  | 7.37  | 130.86      | 117.85   |
| 42  | 9     | 202 | A86  | C34-O4-C38  | 7.37  | 130.86      | 117.85   |
| 31  | 3     | 308 | CLA  | CHA-C4D-ND  | 7.31  | 135.09      | 124.80   |
| 31  | 8     | 308 | CLA  | CHA-C4D-ND  | 7.30  | 135.07      | 124.80   |
| 42  | P     | 610 | A86  | C33-C32-C31 | 7.25  | 116.26      | 109.21   |
| 31  | 3     | 308 | CLA  | CHA-C4D-C3D | -7.24 | 113.01      | 125.21   |
| 42  | 4     | 203 | A86  | O4-C38-C39  | 7.23  | 123.99      | 111.09   |
| 42  | p     | 610 | A86  | C33-C32-C31 | 7.22  | 116.23      | 109.21   |
| 31  | 8     | 308 | CLA  | CHA-C4D-C3D | -7.21 | 113.05      | 125.21   |
| 42  | 9     | 203 | A86  | O4-C38-C39  | 7.21  | 123.95      | 111.09   |
| 31  | 3     | 304 | CLA  | C4A-NA-C1A  | 7.17  | 109.95      | 106.68   |
| 31  | c     | 508 | CLA  | C4A-NA-C1A  | 7.11  | 109.92      | 106.68   |
| 42  | 9     | 203 | A86  | O1-C20-C19  | 7.09  | 120.14      | 113.49   |
| 42  | 4     | 203 | A86  | O1-C20-C19  | 7.08  | 120.13      | 113.49   |
| 31  | 6     | 206 | CLA  | C4A-NA-C1A  | 7.07  | 109.91      | 106.68   |
| 31  | 8     | 304 | CLA  | C4A-NA-C1A  | 7.07  | 109.90      | 106.68   |
| 42  | 2     | 302 | A86  | O1-C20-C21  | -7.05 | 107.17      | 115.05   |
| 31  | b     | 507 | CLA  | C4A-NA-C1A  | 7.05  | 109.89      | 106.68   |
| 31  | C     | 512 | CLA  | C4A-NA-C1A  | 7.04  | 109.89      | 106.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | c     | 512 | CLA  | C4A-NA-C1A  | 7.04  | 109.89      | 106.68   |
| 42  | 7     | 302 | A86  | O1-C20-C21  | -7.03 | 107.19      | 115.05   |
| 31  | C     | 508 | CLA  | C4A-NA-C1A  | 7.00  | 109.87      | 106.68   |
| 31  | B     | 506 | CLA  | C4A-NA-C1A  | 6.99  | 109.87      | 106.68   |
| 42  | 0     | 301 | A86  | C29-C30-C31 | -6.99 | 169.41      | 177.66   |
| 44  | 7     | 303 | DD6  | C9-C10-C11  | -6.98 | 117.48      | 127.28   |
| 31  | b     | 510 | CLA  | C4A-NA-C1A  | 6.98  | 109.86      | 106.68   |
| 44  | 1     | 203 | DD6  | C9-C10-C11  | -6.98 | 117.49      | 127.28   |
| 31  | 6     | 210 | CLA  | C4A-NA-C1A  | 6.97  | 109.86      | 106.68   |
| 44  | 2     | 303 | DD6  | C9-C10-C11  | -6.97 | 117.51      | 127.28   |
| 44  | 6     | 203 | DD6  | C9-C10-C11  | -6.96 | 117.51      | 127.28   |
| 31  | B     | 509 | CLA  | C4A-NA-C1A  | 6.96  | 109.85      | 106.68   |
| 31  | b     | 516 | CLA  | C4A-NA-C1A  | 6.95  | 109.85      | 106.68   |
| 31  | 0     | 307 | CLA  | C4A-NA-C1A  | 6.94  | 109.84      | 106.68   |
| 42  | 5     | 301 | A86  | C29-C30-C31 | -6.93 | 169.49      | 177.66   |
| 44  | 7     | 304 | DD6  | C9-C10-C11  | -6.93 | 117.56      | 127.28   |
| 44  | 2     | 304 | DD6  | C9-C10-C11  | -6.93 | 117.56      | 127.28   |
| 31  | 1     | 206 | CLA  | C4A-NA-C1A  | 6.93  | 109.84      | 106.68   |
| 31  | c     | 504 | CLA  | C4A-NA-C1A  | 6.91  | 109.83      | 106.68   |
| 31  | C     | 504 | CLA  | C4A-NA-C1A  | 6.91  | 109.83      | 106.68   |
| 31  | B     | 512 | CLA  | C4A-NA-C1A  | 6.90  | 109.83      | 106.68   |
| 31  | b     | 513 | CLA  | C4A-NA-C1A  | 6.89  | 109.82      | 106.68   |
| 31  | 1     | 210 | CLA  | C4A-NA-C1A  | 6.89  | 109.82      | 106.68   |
| 42  | P     | 610 | A86  | O1-C20-C19  | 6.89  | 119.95      | 113.49   |
| 31  | 5     | 307 | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 31  | B     | 515 | CLA  | C4A-NA-C1A  | 6.85  | 109.80      | 106.68   |
| 31  | p     | 603 | CLA  | C4A-NA-C1A  | 6.85  | 109.80      | 106.68   |
| 42  | p     | 610 | A86  | O1-C20-C19  | 6.84  | 119.90      | 113.49   |
| 31  | 9     | 207 | CLA  | C4A-NA-C1A  | 6.83  | 109.80      | 106.68   |
| 31  | B     | 504 | CLA  | C4A-NA-C1A  | 6.76  | 109.76      | 106.68   |
| 31  | P     | 603 | CLA  | C4A-NA-C1A  | 6.76  | 109.76      | 106.68   |
| 42  | 1     | 202 | A86  | C20-O1-C15  | 6.76  | 63.93       | 61.03    |
| 42  | 6     | 202 | A86  | C20-O1-C15  | 6.76  | 63.93       | 61.03    |
| 31  | b     | 505 | CLA  | C4A-NA-C1A  | 6.76  | 109.76      | 106.68   |
| 31  | C     | 505 | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 31  | c     | 505 | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 31  | 4     | 207 | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 31  | 5     | 311 | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 31  | 0     | 311 | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 31  | 8     | 305 | CLA  | C4A-NA-C1A  | 6.72  | 109.74      | 106.68   |
| 31  | 2     | 310 | CLA  | C4A-NA-C1A  | 6.72  | 109.74      | 106.68   |
| 31  | p     | 601 | CLA  | C4A-NA-C1A  | 6.72  | 109.74      | 106.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | c     | 502 | CLA  | C4A-NA-C1A  | 6.70  | 109.74      | 106.68   |
| 31  | 8     | 311 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 31  | b     | 502 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 31  | a     | 403 | CLA  | C4A-NA-C1A  | 6.69  | 109.73      | 106.68   |
| 31  | 3     | 305 | CLA  | C4A-NA-C1A  | 6.69  | 109.73      | 106.68   |
| 31  | C     | 510 | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 31  | b     | 506 | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 31  | 1     | 214 | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 44  | 6     | 204 | DD6  | C14-C13-C11 | -6.67 | 115.17      | 125.53   |
| 31  | 2     | 306 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 31  | A     | 403 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 31  | 3     | 311 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 31  | p     | 609 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 31  | P     | 609 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 44  | 1     | 204 | DD6  | C14-C13-C11 | -6.66 | 115.20      | 125.53   |
| 42  | P     | 610 | A86  | C4-C5-C6    | -6.65 | 117.94      | 127.28   |
| 32  | A     | 405 | PHO  | C4D-CHA-CBD | -6.65 | 105.27      | 108.45   |
| 42  | p     | 610 | A86  | C4-C5-C6    | -6.64 | 117.96      | 127.28   |
| 32  | a     | 405 | PHO  | C4D-CHA-CBD | -6.64 | 105.27      | 108.45   |
| 31  | c     | 510 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 31  | B     | 505 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 31  | 7     | 306 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 31  | C     | 502 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 31  | b     | 517 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | 7     | 315 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | 9     | 209 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | 6     | 214 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 31  | 7     | 310 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 42  | 2     | 302 | A86  | O4-C38-C39  | 6.60  | 122.87      | 111.09   |
| 31  | B     | 501 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 43  | 0     | 302 | ET4  | C29-C22-C21 | -6.59 | 111.37      | 124.18   |
| 31  | B     | 507 | CLA  | C4A-NA-C1A  | 6.59  | 109.69      | 106.68   |
| 31  | 8     | 313 | CLA  | C4A-NA-C1A  | 6.59  | 109.69      | 106.68   |
| 43  | 5     | 302 | ET4  | C29-C22-C21 | -6.59 | 111.38      | 124.18   |
| 42  | 3     | 301 | A86  | C29-C30-C31 | -6.58 | 169.89      | 177.66   |
| 42  | 7     | 302 | A86  | O4-C38-C39  | 6.58  | 122.82      | 111.09   |
| 31  | 4     | 209 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 31  | P     | 604 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 31  | 3     | 313 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 31  | b     | 508 | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 31  | 0     | 304 | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 42  | 8     | 301 | A86  | C29-C30-C31 | -6.56 | 169.92      | 177.66   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | D     | 404 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 31  | B     | 516 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 42  | 4     | 201 | A86  | C21-C20-C19 | 6.55  | 121.59      | 114.24   |
| 31  | 2     | 315 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 42  | 4     | 203 | A86  | C29-C30-C31 | -6.52 | 169.96      | 177.66   |
| 42  | 9     | 203 | A86  | C29-C30-C31 | -6.52 | 169.96      | 177.66   |
| 31  | P     | 601 | CLA  | C4A-NA-C1A  | 6.52  | 109.66      | 106.68   |
| 31  | d     | 404 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 31  | B     | 510 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 31  | 4     | 204 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 42  | 9     | 201 | A86  | C21-C20-C19 | 6.49  | 121.54      | 114.24   |
| 31  | b     | 511 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 31  | a     | 407 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 31  | 6     | 215 | CLA  | C4A-NA-C1A  | 6.48  | 109.63      | 106.68   |
| 31  | 1     | 215 | CLA  | C4A-NA-C1A  | 6.48  | 109.63      | 106.68   |
| 31  | p     | 604 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 31  | 0     | 313 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 31  | 1     | 208 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 31  | 8     | 307 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 31  | b     | 514 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 31  | 5     | 304 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 31  | c     | 514 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 31  | 9     | 204 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 31  | A     | 407 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 31  | d     | 401 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 31  | D     | 401 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 31  | 5     | 313 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 31  | A     | 404 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 44  | 1     | 204 | DD6  | C3-C2-C1    | -6.42 | 118.28      | 127.28   |
| 31  | C     | 513 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 31  | 0     | 314 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 42  | 1     | 202 | A86  | C3-C2-C1    | -6.41 | 118.29      | 127.28   |
| 44  | 6     | 204 | DD6  | C3-C2-C1    | -6.41 | 118.29      | 127.28   |
| 31  | 6     | 205 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 42  | 6     | 202 | A86  | C3-C2-C1    | -6.40 | 118.30      | 127.28   |
| 31  | C     | 514 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | 5     | 305 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | 0     | 305 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | 2     | 305 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | a     | 404 | CLA  | C4A-NA-C1A  | 6.40  | 109.60      | 106.68   |
| 31  | C     | 506 | CLA  | C4A-NA-C1A  | 6.39  | 109.60      | 106.68   |
| 31  | 5     | 306 | CLA  | C4A-NA-C1A  | 6.39  | 109.60      | 106.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 31  | 1     | 211 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | B     | 513 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | c     | 506 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | 3     | 314 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | 1     | 209 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | 6     | 212 | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 31  | 3     | 310 | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 31  | 8     | 310 | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 31  | c     | 509 | CLA  | C4A-NA-C1A | 6.37 | 109.58      | 106.68   |
| 31  | 5     | 309 | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 42  | 4     | 201 | A86  | O4-C34-C33 | 6.36 | 123.91      | 107.64   |
| 31  | c     | 507 | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 31  | c     | 513 | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 31  | 6     | 213 | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 31  | 2     | 313 | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 31  | 7     | 316 | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 31  | 9     | 205 | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 31  | 2     | 309 | CLA  | C4A-NA-C1A | 6.34 | 109.57      | 106.68   |
| 31  | C     | 509 | CLA  | C4A-NA-C1A | 6.34 | 109.57      | 106.68   |
| 31  | 6     | 208 | CLA  | C4A-NA-C1A | 6.34 | 109.57      | 106.68   |
| 31  | 2     | 307 | CLA  | C4A-NA-C1A | 6.33 | 109.57      | 106.68   |
| 31  | 5     | 314 | CLA  | C4A-NA-C1A | 6.33 | 109.57      | 106.68   |
| 31  | 1     | 205 | CLA  | C4A-NA-C1A | 6.33 | 109.57      | 106.68   |
| 42  | 9     | 201 | A86  | O4-C34-C33 | 6.33 | 123.84      | 107.64   |
| 31  | 0     | 312 | CLA  | C4A-NA-C1A | 6.33 | 109.57      | 106.68   |
| 31  | C     | 507 | CLA  | C4A-NA-C1A | 6.33 | 109.56      | 106.68   |
| 31  | 7     | 305 | CLA  | C4A-NA-C1A | 6.32 | 109.56      | 106.68   |
| 42  | 5     | 301 | A86  | O4-C38-C39 | 6.32 | 122.36      | 111.09   |
| 31  | 5     | 312 | CLA  | C4A-NA-C1A | 6.32 | 109.56      | 106.68   |
| 31  | b     | 504 | CLA  | C4A-NA-C1A | 6.31 | 109.56      | 106.68   |
| 31  | 4     | 205 | CLA  | C4A-NA-C1A | 6.31 | 109.56      | 106.68   |
| 42  | 0     | 301 | A86  | O4-C38-C39 | 6.31 | 122.34      | 111.09   |
| 31  | 0     | 306 | CLA  | C4A-NA-C1A | 6.31 | 109.56      | 106.68   |
| 31  | d     | 403 | CLA  | C4A-NA-C1A | 6.30 | 109.56      | 106.68   |
| 31  | 1     | 212 | CLA  | C4A-NA-C1A | 6.30 | 109.56      | 106.68   |
| 31  | 7     | 307 | CLA  | C4A-NA-C1A | 6.30 | 109.55      | 106.68   |
| 31  | 6     | 209 | CLA  | C4A-NA-C1A | 6.30 | 109.55      | 106.68   |
| 31  | 3     | 307 | CLA  | C4A-NA-C1A | 6.30 | 109.55      | 106.68   |
| 31  | 6     | 211 | CLA  | C4A-NA-C1A | 6.30 | 109.55      | 106.68   |
| 31  | B     | 503 | CLA  | C4A-NA-C1A | 6.29 | 109.55      | 106.68   |
| 31  | 0     | 310 | CLA  | C4A-NA-C1A | 6.29 | 109.55      | 106.68   |
| 31  | D     | 403 | CLA  | C4A-NA-C1A | 6.29 | 109.55      | 106.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 310 | CLA  | C4A-NA-C1A  | 6.28  | 109.55      | 106.68   |
| 31  | 2     | 316 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 31  | 1     | 213 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 31  | 8     | 314 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 31  | 7     | 313 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 31  | 0     | 309 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 42  | p     | 610 | A86  | C21-C20-C19 | 6.26  | 121.27      | 114.24   |
| 31  | p     | 605 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 31  | b     | 503 | CLA  | C4A-NA-C1A  | 6.24  | 109.52      | 106.68   |
| 31  | 7     | 314 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 31  | 2     | 314 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 31  | 5     | 308 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 31  | 7     | 312 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 31  | 1     | 216 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 42  | 8     | 302 | A86  | O1-C20-C19  | 6.21  | 119.31      | 113.49   |
| 42  | P     | 610 | A86  | C21-C20-C19 | 6.21  | 121.22      | 114.24   |
| 31  | 7     | 309 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 42  | P     | 610 | A86  | O4-C38-C39  | 6.21  | 122.16      | 111.09   |
| 31  | B     | 511 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 42  | p     | 610 | A86  | O4-C38-C39  | 6.21  | 122.16      | 111.09   |
| 31  | B     | 502 | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 31  | p     | 608 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 42  | 3     | 302 | A86  | O1-C20-C19  | 6.17  | 119.28      | 113.49   |
| 31  | b     | 512 | CLA  | C4A-NA-C1A  | 6.17  | 109.49      | 106.68   |
| 31  | 7     | 308 | CLA  | C4A-NA-C1A  | 6.17  | 109.49      | 106.68   |
| 31  | c     | 503 | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 31  | 9     | 212 | CLA  | C4A-NA-C1A  | 6.15  | 109.49      | 106.68   |
| 31  | C     | 503 | CLA  | C4A-NA-C1A  | 6.15  | 109.49      | 106.68   |
| 31  | 4     | 213 | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 44  | 6     | 204 | DD6  | C9-C10-C11  | -6.13 | 118.69      | 127.28   |
| 31  | B     | 514 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 31  | 6     | 216 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 31  | P     | 605 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 31  | b     | 509 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 44  | 1     | 204 | DD6  | C9-C10-C11  | -6.12 | 118.70      | 127.28   |
| 31  | B     | 508 | CLA  | C4A-NA-C1A  | 6.11  | 109.47      | 106.68   |
| 31  | b     | 515 | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 31  | 2     | 308 | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 31  | 2     | 312 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 31  | Z     | 101 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 31  | 4     | 212 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 42  | 3     | 301 | A86  | O4-C38-C39  | 6.05  | 121.89      | 111.09   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 8     | 301 | A86  | O4-C38-C39  | 6.05  | 121.88      | 111.09   |
| 31  | 6     | 201 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 31  | 9     | 213 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 42  | 0     | 317 | A86  | C29-C30-C31 | -6.04 | 170.53      | 177.66   |
| 31  | 3     | 312 | CLA  | C4A-NA-C1A  | 6.04  | 109.44      | 106.68   |
| 31  | 0     | 308 | CLA  | C4A-NA-C1A  | 6.04  | 109.44      | 106.68   |
| 31  | 4     | 210 | CLA  | C4A-NA-C1A  | 6.04  | 109.43      | 106.68   |
| 31  | 3     | 306 | CLA  | C4A-NA-C1A  | 6.02  | 109.43      | 106.68   |
| 31  | z     | 101 | CLA  | C4A-NA-C1A  | 6.02  | 109.43      | 106.68   |
| 42  | 5     | 317 | A86  | C29-C30-C31 | -6.02 | 170.56      | 177.66   |
| 31  | 9     | 206 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 31  | 8     | 312 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 31  | 9     | 210 | CLA  | C4A-NA-C1A  | 6.00  | 109.42      | 106.68   |
| 31  | 8     | 306 | CLA  | C4A-NA-C1A  | 6.00  | 109.42      | 106.68   |
| 31  | 4     | 211 | CLA  | C4A-NA-C1A  | 5.96  | 109.40      | 106.68   |
| 42  | 4     | 202 | A86  | C29-C30-C31 | -5.96 | 170.63      | 177.66   |
| 31  | P     | 608 | CLA  | C4A-NA-C1A  | 5.95  | 109.39      | 106.68   |
| 42  | 9     | 202 | A86  | C29-C30-C31 | -5.93 | 170.67      | 177.66   |
| 31  | 4     | 206 | CLA  | C4A-NA-C1A  | 5.91  | 109.37      | 106.68   |
| 31  | 1     | 201 | CLA  | C4A-NA-C1A  | 5.88  | 109.36      | 106.68   |
| 31  | 9     | 211 | CLA  | C4A-NA-C1A  | 5.86  | 109.35      | 106.68   |
| 42  | 8     | 302 | A86  | O4-C38-C39  | 5.85  | 121.53      | 111.09   |
| 31  | 4     | 208 | CLA  | C4A-NA-C1A  | 5.85  | 109.35      | 106.68   |
| 42  | 8     | 301 | A86  | C41-C32-C31 | 5.84  | 115.70      | 110.47   |
| 32  | a     | 406 | PHO  | C4D-CHA-CBD | -5.84 | 105.65      | 108.45   |
| 31  | C     | 511 | CLA  | C4A-NA-C1A  | 5.84  | 109.34      | 106.68   |
| 42  | 3     | 302 | A86  | O4-C38-C39  | 5.84  | 121.50      | 111.09   |
| 31  | W     | 202 | CLA  | C4A-NA-C1A  | 5.83  | 109.34      | 106.68   |
| 32  | A     | 406 | PHO  | C4D-CHA-CBD | -5.83 | 105.66      | 108.45   |
| 31  | c     | 511 | CLA  | C4A-NA-C1A  | 5.79  | 109.32      | 106.68   |
| 42  | 3     | 301 | A86  | C41-C32-C31 | 5.78  | 115.65      | 110.47   |
| 31  | p     | 602 | CLA  | C4A-NA-C1A  | 5.78  | 109.31      | 106.68   |
| 31  | P     | 602 | CLA  | C4A-NA-C1A  | 5.78  | 109.31      | 106.68   |
| 42  | 7     | 302 | A86  | C35-C34-C33 | -5.78 | 99.51       | 109.89   |
| 42  | 2     | 302 | A86  | C35-C34-C33 | -5.78 | 99.51       | 109.89   |
| 31  | 2     | 311 | CLA  | C4A-NA-C1A  | 5.77  | 109.31      | 106.68   |
| 31  | 9     | 208 | CLA  | C4A-NA-C1A  | 5.76  | 109.31      | 106.68   |
| 31  | 7     | 311 | CLA  | C4A-NA-C1A  | 5.74  | 109.30      | 106.68   |
| 31  | w     | 202 | CLA  | C4A-NA-C1A  | 5.74  | 109.30      | 106.68   |
| 42  | 0     | 303 | A86  | O1-C20-C19  | -5.72 | 108.13      | 113.49   |
| 42  | 5     | 303 | A86  | O1-C20-C19  | -5.72 | 108.13      | 113.49   |
| 36  | D     | 412 | LHG  | O4-P-O5     | 5.69  | 133.02      | 110.83   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | d     | 412 | LHG  | O4-P-O5     | 5.69  | 133.01      | 110.83   |
| 42  | 0     | 317 | A86  | C35-C34-C33 | -5.69 | 99.67       | 109.89   |
| 42  | 5     | 317 | A86  | C35-C34-C33 | -5.68 | 99.69       | 109.89   |
| 42  | 0     | 303 | A86  | O1-C20-C21  | -5.65 | 108.73      | 115.05   |
| 42  | 4     | 202 | A86  | O1-C20-C15  | -5.64 | 56.96       | 59.23    |
| 42  | 6     | 202 | A86  | C25-C26-C27 | -5.62 | 119.40      | 127.28   |
| 42  | 8     | 302 | A86  | O1-C20-C21  | -5.61 | 108.78      | 115.05   |
| 42  | 9     | 202 | A86  | O1-C20-C15  | -5.61 | 56.97       | 59.23    |
| 42  | 5     | 303 | A86  | O1-C20-C21  | -5.61 | 108.78      | 115.05   |
| 42  | 3     | 302 | A86  | O1-C20-C21  | -5.60 | 108.79      | 115.05   |
| 42  | 7     | 301 | A86  | C35-C34-C33 | -5.59 | 99.84       | 109.89   |
| 42  | 2     | 301 | A86  | C35-C34-C33 | -5.59 | 99.84       | 109.89   |
| 31  | 6     | 207 | CLA  | C4A-NA-C1A  | 5.58  | 109.23      | 106.68   |
| 42  | 7     | 301 | A86  | C29-C30-C31 | -5.58 | 171.08      | 177.66   |
| 42  | 1     | 202 | A86  | C25-C26-C27 | -5.57 | 119.47      | 127.28   |
| 42  | 2     | 301 | A86  | C29-C30-C31 | -5.54 | 171.12      | 177.66   |
| 42  | 0     | 303 | A86  | C3-C2-C1    | -5.51 | 119.55      | 127.28   |
| 42  | 5     | 303 | A86  | C3-C2-C1    | -5.51 | 119.55      | 127.28   |
| 31  | 1     | 207 | CLA  | C4A-NA-C1A  | 5.49  | 109.18      | 106.68   |
| 44  | 2     | 303 | DD6  | C4-C5-C6    | -5.47 | 119.61      | 127.28   |
| 42  | 4     | 202 | A86  | C3-C2-C1    | -5.44 | 119.64      | 127.28   |
| 44  | 1     | 203 | DD6  | C4-C5-C6    | -5.43 | 119.66      | 127.28   |
| 44  | 6     | 203 | DD6  | C4-C5-C6    | -5.42 | 119.67      | 127.28   |
| 44  | 7     | 303 | DD6  | C4-C5-C6    | -5.41 | 119.68      | 127.28   |
| 42  | 9     | 202 | A86  | C3-C2-C1    | -5.41 | 119.69      | 127.28   |
| 40  | d     | 402 | BCT  | O2-C-O1     | 5.35  | 133.36      | 119.68   |
| 40  | D     | 402 | BCT  | O2-C-O1     | 5.35  | 133.35      | 119.68   |
| 44  | 6     | 204 | DD6  | C4-C5-C6    | -5.21 | 119.98      | 127.28   |
| 42  | 7     | 301 | A86  | C3-C2-C1    | -5.20 | 119.98      | 127.28   |
| 44  | 1     | 204 | DD6  | C4-C5-C6    | -5.19 | 120.00      | 127.28   |
| 42  | 2     | 301 | A86  | C3-C2-C1    | -5.16 | 120.04      | 127.28   |
| 44  | p     | 611 | DD6  | C4-C5-C6    | -5.11 | 120.11      | 127.28   |
| 44  | P     | 611 | DD6  | C4-C5-C6    | -5.11 | 120.12      | 127.28   |
| 42  | 5     | 301 | A86  | C35-C34-C33 | -5.09 | 100.74      | 109.89   |
| 42  | 0     | 301 | A86  | C35-C34-C33 | -5.08 | 100.76      | 109.89   |
| 42  | 3     | 302 | A86  | C25-C26-C27 | -5.05 | 120.19      | 127.28   |
| 35  | a     | 410 | PL9  | C7-C3-C4    | 5.04  | 121.06      | 116.91   |
| 35  | A     | 410 | PL9  | C7-C3-C4    | 5.04  | 121.06      | 116.91   |
| 42  | 8     | 302 | A86  | C25-C26-C27 | -5.04 | 120.22      | 127.28   |
| 42  | 6     | 202 | A86  | C4-C5-C6    | -5.03 | 120.22      | 127.28   |
| 42  | 1     | 202 | A86  | C4-C5-C6    | -5.03 | 120.22      | 127.28   |
| 31  | P     | 606 | CLA  | C4A-NA-C1A  | 5.01  | 108.96      | 106.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 43  | 5     | 302 | ET4  | C24-C05-C06 | -5.00 | 119.02      | 124.48   |
| 43  | 0     | 302 | ET4  | C24-C05-C06 | -5.00 | 119.03      | 124.48   |
| 42  | 2     | 301 | A86  | C4-C5-C6    | -4.97 | 120.30      | 127.28   |
| 31  | p     | 606 | CLA  | C4A-NA-C1A  | 4.97  | 108.95      | 106.68   |
| 42  | 7     | 301 | A86  | C4-C5-C6    | -4.97 | 120.31      | 127.28   |
| 44  | P     | 611 | DD6  | C21-C20-C19 | 4.96  | 119.81      | 114.24   |
| 44  | p     | 611 | DD6  | C21-C20-C19 | 4.95  | 119.80      | 114.24   |
| 31  | p     | 607 | CLA  | C4A-NA-C1A  | 4.94  | 108.93      | 106.68   |
| 44  | 8     | 303 | DD6  | C4-C5-C6    | -4.94 | 120.35      | 127.28   |
| 42  | 9     | 202 | A86  | O4-C38-O5   | -4.93 | 113.47      | 122.99   |
| 44  | 6     | 203 | DD6  | C3-C2-C1    | -4.93 | 120.36      | 127.28   |
| 42  | 4     | 202 | A86  | O4-C38-O5   | -4.93 | 113.48      | 122.99   |
| 35  | d     | 406 | PL9  | C7-C3-C4    | 4.91  | 120.95      | 116.91   |
| 42  | 4     | 201 | A86  | C4-C5-C6    | -4.91 | 120.39      | 127.28   |
| 42  | 9     | 201 | A86  | C4-C5-C6    | -4.91 | 120.40      | 127.28   |
| 42  | 5     | 301 | A86  | O1-C20-C19  | 4.90  | 118.09      | 113.49   |
| 42  | 0     | 301 | A86  | O1-C20-C19  | 4.90  | 118.08      | 113.49   |
| 35  | D     | 406 | PL9  | C7-C3-C4    | 4.90  | 120.94      | 116.91   |
| 44  | 2     | 303 | DD6  | C3-C2-C1    | -4.88 | 120.43      | 127.28   |
| 44  | 1     | 203 | DD6  | C3-C2-C1    | -4.88 | 120.43      | 127.28   |
| 44  | 3     | 303 | DD6  | C4-C5-C6    | -4.88 | 120.44      | 127.28   |
| 44  | 7     | 303 | DD6  | C3-C2-C1    | -4.87 | 120.45      | 127.28   |
| 42  | 5     | 317 | A86  | C3-C2-C1    | -4.78 | 120.58      | 127.28   |
| 31  | P     | 607 | CLA  | C4A-NA-C1A  | 4.75  | 108.85      | 106.68   |
| 42  | 0     | 317 | A86  | C3-C2-C1    | -4.73 | 120.64      | 127.28   |
| 42  | 5     | 317 | A86  | C4-C5-C6    | -4.72 | 120.66      | 127.28   |
| 42  | 0     | 317 | A86  | C4-C5-C6    | -4.71 | 120.67      | 127.28   |
| 44  | 3     | 303 | DD6  | C21-C20-C19 | 4.71  | 119.53      | 114.24   |
| 31  | 8     | 308 | CLA  | C4A-NA-C1A  | 4.71  | 108.83      | 106.68   |
| 44  | p     | 611 | DD6  | C3-C2-C1    | -4.70 | 120.69      | 127.28   |
| 44  | P     | 611 | DD6  | C3-C2-C1    | -4.68 | 120.72      | 127.28   |
| 42  | 4     | 203 | A86  | O1-C20-C15  | -4.67 | 57.35       | 59.23    |
| 44  | 8     | 303 | DD6  | C21-C20-C19 | 4.66  | 119.47      | 114.24   |
| 31  | 3     | 308 | CLA  | C4A-NA-C1A  | 4.66  | 108.80      | 106.68   |
| 42  | 9     | 203 | A86  | C4-C5-C6    | -4.62 | 120.79      | 127.28   |
| 42  | 4     | 201 | A86  | O1-C20-C15  | -4.62 | 57.37       | 59.23    |
| 42  | 4     | 203 | A86  | C4-C5-C6    | -4.61 | 120.81      | 127.28   |
| 42  | 0     | 301 | A86  | C4-C5-C6    | -4.60 | 120.83      | 127.28   |
| 42  | 4     | 203 | A86  | C3-C2-C1    | -4.59 | 120.83      | 127.28   |
| 42  | 9     | 203 | A86  | O1-C20-C15  | -4.59 | 57.38       | 59.23    |
| 36  | D     | 412 | LHG  | O3-P-O6     | -4.58 | 94.72       | 106.67   |
| 36  | d     | 412 | LHG  | O3-P-O6     | -4.58 | 94.72       | 106.67   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 5     | 301 | A86  | C4-C5-C6    | -4.57 | 120.86      | 127.28   |
| 42  | 4     | 201 | A86  | C29-C30-C31 | -4.57 | 172.27      | 177.66   |
| 42  | 9     | 201 | A86  | C29-C30-C31 | -4.57 | 172.27      | 177.66   |
| 42  | 5     | 303 | A86  | O1-C20-C15  | -4.57 | 57.39       | 59.23    |
| 42  | 9     | 203 | A86  | C3-C2-C1    | -4.57 | 120.88      | 127.28   |
| 42  | 9     | 201 | A86  | O1-C20-C15  | -4.54 | 57.40       | 59.23    |
| 42  | 5     | 303 | A86  | C36-C31-C32 | 4.54  | 124.20      | 119.70   |
| 42  | 0     | 303 | A86  | O1-C20-C15  | -4.53 | 57.41       | 59.23    |
| 42  | 4     | 203 | A86  | O1-C15-C20  | -4.52 | 55.62       | 59.45    |
| 42  | 9     | 203 | A86  | O1-C15-C20  | -4.50 | 55.64       | 59.45    |
| 42  | 9     | 202 | A86  | C41-C32-C31 | 4.50  | 114.50      | 110.47   |
| 42  | 0     | 303 | A86  | C36-C31-C32 | 4.49  | 124.15      | 119.70   |
| 42  | 7     | 302 | A86  | C4-C5-C6    | -4.49 | 120.99      | 127.28   |
| 42  | 2     | 302 | A86  | C4-C5-C6    | -4.48 | 121.00      | 127.28   |
| 36  | A     | 412 | LHG  | O4-P-O5     | 4.47  | 133.24      | 112.44   |
| 36  | A     | 413 | LHG  | O4-P-O5     | 4.47  | 133.23      | 112.44   |
| 36  | a     | 412 | LHG  | O4-P-O5     | 4.47  | 133.23      | 112.44   |
| 36  | a     | 411 | LHG  | O4-P-O5     | 4.47  | 133.22      | 112.44   |
| 42  | 0     | 303 | A86  | C4-C5-C6    | -4.43 | 121.06      | 127.28   |
| 36  | b     | 522 | LHG  | O4-P-O5     | 4.43  | 133.04      | 112.44   |
| 36  | B     | 521 | LHG  | O4-P-O5     | 4.43  | 133.03      | 112.44   |
| 42  | 4     | 203 | A86  | C35-C34-C33 | -4.42 | 101.94      | 109.89   |
| 42  | 9     | 203 | A86  | C35-C34-C33 | -4.41 | 101.97      | 109.89   |
| 36  | D     | 411 | LHG  | O4-P-O5     | 4.41  | 132.94      | 112.44   |
| 36  | d     | 411 | LHG  | O4-P-O5     | 4.40  | 132.93      | 112.44   |
| 42  | 4     | 202 | A86  | C41-C32-C31 | 4.39  | 114.40      | 110.47   |
| 42  | 9     | 202 | A86  | O1-C15-C20  | -4.37 | 55.74       | 59.45    |
| 42  | p     | 610 | A86  | C36-C31-C32 | -4.37 | 115.36      | 119.70   |
| 43  | 0     | 302 | ET4  | C19-C18-C17 | 4.36  | 125.87      | 119.01   |
| 42  | 5     | 303 | A86  | C4-C5-C6    | -4.36 | 121.16      | 127.28   |
| 43  | 5     | 302 | ET4  | C19-C18-C17 | 4.35  | 125.85      | 119.01   |
| 42  | P     | 610 | A86  | C36-C31-C32 | -4.35 | 115.38      | 119.70   |
| 42  | 4     | 202 | A86  | O1-C15-C20  | -4.35 | 55.76       | 59.45    |
| 42  | p     | 610 | A86  | C35-C34-C33 | -4.35 | 102.08      | 109.89   |
| 36  | H     | 103 | LHG  | O4-P-O5     | 4.34  | 132.64      | 112.44   |
| 42  | p     | 610 | A86  | C34-O4-C38  | -4.34 | 110.18      | 117.85   |
| 42  | 9     | 201 | A86  | O1-C20-C21  | -4.34 | 110.20      | 115.05   |
| 42  | P     | 610 | A86  | C35-C34-C33 | -4.33 | 102.10      | 109.89   |
| 36  | h     | 103 | LHG  | O4-P-O5     | 4.32  | 132.53      | 112.44   |
| 42  | 8     | 302 | A86  | C4-C5-C6    | -4.32 | 121.22      | 127.28   |
| 42  | P     | 610 | A86  | C34-O4-C38  | -4.31 | 110.22      | 117.85   |
| 42  | 5     | 303 | A86  | O4-C38-C39  | 4.30  | 118.77      | 111.09   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 0     | 303 | A86  | O4-C38-C39  | 4.29  | 118.74      | 111.09   |
| 42  | 3     | 302 | A86  | C4-C5-C6    | -4.29 | 121.26      | 127.28   |
| 42  | 5     | 317 | A86  | O1-C20-C21  | -4.29 | 110.26      | 115.05   |
| 42  | 2     | 301 | A86  | O1-C20-C21  | -4.27 | 110.27      | 115.05   |
| 42  | 4     | 201 | A86  | O1-C20-C21  | -4.27 | 110.28      | 115.05   |
| 42  | 7     | 301 | A86  | O1-C20-C21  | -4.26 | 110.29      | 115.05   |
| 42  | P     | 610 | A86  | O4-C38-O5   | -4.25 | 114.79      | 122.99   |
| 39  | c     | 519 | DGD  | O3G-C3G-C2G | -4.25 | 100.49      | 110.82   |
| 42  | 0     | 317 | A86  | O1-C20-C21  | -4.24 | 110.31      | 115.05   |
| 42  | 3     | 302 | A86  | O1-C20-C15  | -4.24 | 57.52       | 59.23    |
| 39  | C     | 519 | DGD  | O3G-C3G-C2G | -4.24 | 100.51      | 110.82   |
| 42  | 4     | 202 | A86  | C25-C26-C27 | -4.24 | 121.34      | 127.28   |
| 42  | p     | 610 | A86  | O4-C38-O5   | -4.23 | 114.83      | 122.99   |
| 42  | 9     | 202 | A86  | C25-C26-C27 | -4.22 | 121.36      | 127.28   |
| 39  | c     | 520 | DGD  | O2G-C1B-C2B | 4.21  | 120.60      | 111.48   |
| 42  | 0     | 301 | A86  | C12-C11-C13 | 4.21  | 122.83      | 116.00   |
| 42  | 5     | 301 | A86  | C12-C11-C13 | 4.20  | 122.81      | 116.00   |
| 44  | 6     | 204 | DD6  | C21-C20-C19 | 4.20  | 118.96      | 114.24   |
| 39  | C     | 520 | DGD  | O2G-C1B-C2B | 4.20  | 120.56      | 111.48   |
| 42  | 8     | 302 | A86  | O1-C20-C15  | -4.19 | 57.54       | 59.23    |
| 31  | P     | 602 | CLA  | CMA-C3A-C2A | -4.17 | 106.67      | 116.23   |
| 44  | 1     | 204 | DD6  | C21-C20-C19 | 4.17  | 118.92      | 114.24   |
| 31  | p     | 602 | CLA  | CMA-C3A-C2A | -4.17 | 106.68      | 116.23   |
| 44  | 2     | 303 | DD6  | C21-C20-C19 | 4.15  | 118.91      | 114.24   |
| 43  | 0     | 302 | ET4  | C16-C15-C14 | 4.15  | 132.01      | 123.52   |
| 31  | p     | 605 | CLA  | C3B-C4B-NB  | -4.14 | 106.83      | 110.53   |
| 42  | 3     | 301 | A86  | O1-C15-C20  | -4.14 | 55.94       | 59.45    |
| 43  | 5     | 302 | ET4  | C16-C15-C14 | 4.13  | 131.98      | 123.52   |
| 42  | 8     | 301 | A86  | O1-C15-C20  | -4.12 | 55.95       | 59.45    |
| 42  | 1     | 202 | A86  | C9-C10-C11  | -4.11 | 115.01      | 126.64   |
| 44  | 6     | 203 | DD6  | C21-C20-C19 | 4.11  | 118.86      | 114.24   |
| 44  | 7     | 303 | DD6  | C21-C20-C19 | 4.11  | 118.86      | 114.24   |
| 42  | 6     | 202 | A86  | C9-C10-C11  | -4.10 | 115.05      | 126.64   |
| 31  | P     | 605 | CLA  | C3B-C4B-NB  | -4.10 | 106.87      | 110.53   |
| 42  | 9     | 203 | A86  | C23-C16-C17 | -4.10 | 101.77      | 108.97   |
| 44  | 1     | 203 | DD6  | C21-C20-C19 | 4.10  | 118.84      | 114.24   |
| 42  | 9     | 201 | A86  | O1-C20-C19  | 4.09  | 117.33      | 113.49   |
| 42  | 4     | 203 | A86  | C23-C16-C17 | -4.08 | 101.80      | 108.97   |
| 43  | 0     | 302 | ET4  | C30-C18-C17 | -4.06 | 116.23      | 122.82   |
| 42  | 8     | 302 | A86  | C3-C2-C1    | -4.06 | 121.59      | 127.28   |
| 34  | B     | 523 | SQD  | O5-C5-C4    | 4.05  | 117.01      | 109.70   |
| 34  | b     | 501 | SQD  | O5-C5-C4    | 4.05  | 117.00      | 109.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 4     | 201 | A86  | O1-C20-C19  | 4.05  | 117.29      | 113.49   |
| 42  | 4     | 201 | A86  | C3-C2-C1    | -4.05 | 121.60      | 127.28   |
| 37  | C     | 521 | LMG  | O7-C10-C11  | 4.04  | 120.22      | 111.48   |
| 43  | 5     | 302 | ET4  | C30-C18-C17 | -4.03 | 116.28      | 122.82   |
| 44  | 7     | 304 | DD6  | C21-C20-C15 | -4.03 | 115.66      | 122.30   |
| 37  | c     | 521 | LMG  | O7-C10-C11  | 4.03  | 120.20      | 111.48   |
| 44  | 2     | 304 | DD6  | C21-C20-C15 | -4.03 | 115.67      | 122.30   |
| 42  | 3     | 302 | A86  | C3-C2-C1    | -4.02 | 121.64      | 127.28   |
| 42  | 0     | 317 | A86  | O4-C38-C39  | 4.00  | 118.23      | 111.09   |
| 42  | 5     | 301 | A86  | C3-C2-C1    | -4.00 | 121.67      | 127.28   |
| 42  | 9     | 201 | A86  | C3-C2-C1    | -4.00 | 121.67      | 127.28   |
| 42  | 9     | 202 | A86  | O1-C20-C19  | 3.99  | 117.23      | 113.49   |
| 42  | 8     | 301 | A86  | C34-O4-C38  | -3.99 | 110.81      | 117.85   |
| 42  | 7     | 302 | A86  | O1-C15-C20  | -3.98 | 56.07       | 59.45    |
| 42  | 2     | 302 | A86  | O1-C15-C20  | -3.98 | 56.07       | 59.45    |
| 31  | 4     | 209 | CLA  | CAA-C2A-C3A | -3.98 | 107.10      | 116.23   |
| 42  | 0     | 301 | A86  | C3-C2-C1    | -3.98 | 121.69      | 127.28   |
| 43  | 5     | 302 | ET4  | C27-C09-C10 | -3.98 | 116.37      | 122.82   |
| 39  | C     | 518 | DGD  | O3G-C3G-C2G | -3.98 | 101.15      | 110.82   |
| 42  | 3     | 301 | A86  | C34-O4-C38  | -3.98 | 110.83      | 117.85   |
| 42  | 5     | 317 | A86  | O4-C38-C39  | 3.97  | 118.17      | 111.09   |
| 39  | c     | 518 | DGD  | O3G-C3G-C2G | -3.97 | 101.17      | 110.82   |
| 43  | 0     | 302 | ET4  | C27-C09-C10 | -3.96 | 116.39      | 122.82   |
| 31  | 9     | 209 | CLA  | CAA-C2A-C3A | -3.96 | 107.14      | 116.23   |
| 35  | D     | 406 | PL9  | C7-C3-C2    | -3.96 | 118.72      | 123.39   |
| 42  | 4     | 202 | A86  | O1-C20-C19  | 3.96  | 117.20      | 113.49   |
| 35  | d     | 406 | PL9  | C7-C3-C2    | -3.96 | 118.73      | 123.39   |
| 34  | a     | 409 | SQD  | O9-S-O7     | -3.95 | 100.99      | 113.82   |
| 42  | 4     | 201 | A86  | C40-C32-C31 | -3.93 | 106.95      | 110.47   |
| 34  | A     | 409 | SQD  | O9-S-O7     | -3.93 | 101.04      | 113.82   |
| 31  | p     | 601 | CLA  | CAA-C2A-C3A | -3.93 | 107.23      | 116.23   |
| 42  | 4     | 201 | A86  | O1-C15-C20  | -3.91 | 56.13       | 59.45    |
| 31  | p     | 605 | CLA  | CAA-C2A-C3A | -3.91 | 107.27      | 116.23   |
| 31  | P     | 601 | CLA  | CAA-C2A-C3A | -3.90 | 107.28      | 116.23   |
| 31  | P     | 605 | CLA  | CAA-C2A-C3A | -3.90 | 107.28      | 116.23   |
| 42  | 9     | 201 | A86  | C40-C32-C31 | -3.90 | 106.98      | 110.47   |
| 42  | 9     | 202 | A86  | C28-C27-C26 | -3.90 | 116.50      | 122.82   |
| 42  | 4     | 202 | A86  | C28-C27-C26 | -3.88 | 116.53      | 122.82   |
| 42  | 2     | 301 | A86  | C41-C32-C31 | -3.88 | 107.00      | 110.47   |
| 42  | 5     | 317 | A86  | O4-C34-C33  | 3.88  | 117.56      | 107.64   |
| 34  | 5     | 316 | SQD  | O9-S-O7     | -3.88 | 101.21      | 113.82   |
| 34  | 0     | 316 | SQD  | O9-S-O7     | -3.88 | 101.22      | 113.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 7     | 301 | A86  | C41-C32-C31 | -3.87 | 107.01      | 110.47   |
| 42  | 9     | 201 | A86  | O4-C38-C39  | 3.87  | 117.99      | 111.09   |
| 42  | 4     | 201 | A86  | O4-C38-C39  | 3.87  | 117.99      | 111.09   |
| 42  | 9     | 201 | A86  | O1-C15-C20  | -3.86 | 56.18       | 59.45    |
| 42  | 0     | 317 | A86  | O4-C34-C33  | 3.85  | 117.50      | 107.64   |
| 34  | A     | 411 | SQD  | O9-S-O7     | -3.85 | 101.29      | 113.82   |
| 34  | B     | 522 | SQD  | O9-S-O7     | -3.85 | 101.30      | 113.82   |
| 42  | 5     | 301 | A86  | O1-C15-C20  | -3.84 | 56.19       | 59.45    |
| 42  | 0     | 301 | A86  | O1-C15-C20  | -3.84 | 56.19       | 59.45    |
| 44  | 3     | 303 | DD6  | C14-C13-C11 | -3.84 | 119.58      | 125.53   |
| 42  | 0     | 317 | A86  | O1-C15-C20  | -3.84 | 56.20       | 59.45    |
| 42  | 3     | 301 | A86  | C25-C26-C27 | -3.83 | 121.91      | 127.28   |
| 42  | 2     | 301 | A86  | O1-C15-C20  | -3.83 | 56.20       | 59.45    |
| 35  | A     | 410 | PL9  | C7-C3-C2    | -3.83 | 118.88      | 123.39   |
| 42  | 5     | 317 | A86  | O1-C15-C20  | -3.83 | 56.21       | 59.45    |
| 42  | 6     | 202 | A86  | C40-C32-C31 | -3.82 | 107.05      | 110.47   |
| 31  | 9     | 208 | CLA  | CAA-C2A-C1A | 3.82  | 121.24      | 111.81   |
| 44  | 8     | 303 | DD6  | C14-C13-C11 | -3.81 | 119.61      | 125.53   |
| 42  | 1     | 202 | A86  | C40-C32-C31 | -3.81 | 107.06      | 110.47   |
| 31  | 4     | 208 | CLA  | CAA-C2A-C1A | 3.81  | 121.22      | 111.81   |
| 42  | p     | 610 | A86  | C9-C8-C6    | -3.81 | 115.91      | 126.36   |
| 42  | 8     | 301 | A86  | C25-C26-C27 | -3.81 | 121.94      | 127.28   |
| 35  | a     | 410 | PL9  | C7-C3-C2    | -3.81 | 118.90      | 123.39   |
| 34  | B     | 522 | SQD  | C1-O5-C5    | 3.81  | 121.15      | 113.72   |
| 44  | P     | 611 | DD6  | C9-C10-C11  | -3.80 | 121.94      | 127.28   |
| 42  | P     | 610 | A86  | C9-C8-C6    | -3.80 | 115.94      | 126.36   |
| 42  | 4     | 203 | A86  | O4-C38-O5   | -3.80 | 115.65      | 122.99   |
| 34  | A     | 411 | SQD  | C1-O5-C5    | 3.80  | 121.14      | 113.72   |
| 42  | 7     | 301 | A86  | O1-C15-C20  | -3.79 | 56.23       | 59.45    |
| 42  | 4     | 203 | A86  | C23-C16-C22 | -3.79 | 101.86      | 107.37   |
| 42  | 9     | 203 | A86  | C23-C16-C22 | -3.78 | 101.88      | 107.37   |
| 42  | 2     | 301 | A86  | O4-C38-C39  | 3.78  | 117.82      | 111.09   |
| 42  | 7     | 301 | A86  | O4-C38-C39  | 3.77  | 117.82      | 111.09   |
| 44  | p     | 611 | DD6  | C9-C10-C11  | -3.77 | 121.99      | 127.28   |
| 42  | P     | 610 | A86  | O1-C20-C15  | -3.77 | 57.71       | 59.23    |
| 42  | 9     | 203 | A86  | O4-C38-O5   | -3.76 | 115.72      | 122.99   |
| 42  | 3     | 302 | A86  | O1-C15-C20  | -3.76 | 56.26       | 59.45    |
| 42  | p     | 610 | A86  | C21-C20-C15 | -3.75 | 111.24      | 123.35   |
| 42  | 4     | 202 | A86  | C23-C16-C22 | -3.74 | 101.93      | 107.37   |
| 42  | p     | 610 | A86  | O1-C20-C15  | -3.74 | 57.72       | 59.23    |
| 42  | P     | 610 | A86  | C21-C20-C15 | -3.74 | 111.27      | 123.35   |
| 42  | 8     | 302 | A86  | O1-C15-C20  | -3.74 | 56.28       | 59.45    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 207 | CLA  | CAA-C2A-C3A | -3.74 | 107.65      | 116.23   |
| 31  | p     | 603 | CLA  | CAA-C2A-C3A | -3.74 | 107.66      | 116.23   |
| 42  | 9     | 202 | A86  | O1-C20-C21  | -3.73 | 110.88      | 115.05   |
| 31  | 4     | 207 | CLA  | CAA-C2A-C3A | -3.73 | 107.68      | 116.23   |
| 39  | H     | 102 | DGD  | O3G-C3G-C2G | -3.73 | 101.75      | 110.82   |
| 34  | b     | 501 | SQD  | O9-S-O7     | -3.72 | 101.72      | 113.82   |
| 39  | h     | 102 | DGD  | O3G-C3G-C2G | -3.72 | 101.77      | 110.82   |
| 34  | B     | 523 | SQD  | O9-S-O7     | -3.72 | 101.73      | 113.82   |
| 42  | 9     | 202 | A86  | C23-C16-C22 | -3.72 | 101.97      | 107.37   |
| 31  | P     | 603 | CLA  | CAA-C2A-C3A | -3.71 | 107.73      | 116.23   |
| 44  | 8     | 303 | DD6  | C37-C36-C35 | 3.70  | 121.22      | 114.42   |
| 44  | 3     | 303 | DD6  | C37-C36-C35 | 3.70  | 121.22      | 114.42   |
| 42  | 4     | 202 | A86  | O1-C20-C21  | -3.69 | 110.92      | 115.05   |
| 44  | 2     | 304 | DD6  | O1-C20-C19  | 3.69  | 116.95      | 113.49   |
| 42  | 1     | 202 | A86  | C35-C34-C33 | -3.68 | 103.28      | 109.89   |
| 42  | 6     | 202 | A86  | C35-C34-C33 | -3.67 | 103.29      | 109.89   |
| 42  | 9     | 201 | A86  | C25-C26-C27 | -3.66 | 122.14      | 127.28   |
| 42  | 7     | 301 | A86  | O4-C34-C33  | 3.66  | 117.00      | 107.64   |
| 42  | 2     | 301 | A86  | O4-C34-C33  | 3.66  | 117.00      | 107.64   |
| 44  | 7     | 304 | DD6  | O1-C20-C19  | 3.66  | 116.92      | 113.49   |
| 42  | 0     | 317 | A86  | C41-C32-C31 | -3.65 | 107.20      | 110.47   |
| 31  | 4     | 210 | CLA  | CAA-C2A-C3A | -3.65 | 107.87      | 116.23   |
| 42  | 4     | 201 | A86  | C25-C26-C27 | -3.64 | 122.17      | 127.28   |
| 42  | p     | 610 | A86  | C25-C26-C27 | -3.63 | 122.18      | 127.28   |
| 42  | 5     | 317 | A86  | C41-C32-C31 | -3.63 | 107.22      | 110.47   |
| 31  | 9     | 210 | CLA  | CAA-C2A-C3A | -3.62 | 107.92      | 116.23   |
| 42  | 1     | 202 | A86  | C3-C4-C5    | -3.62 | 116.11      | 123.52   |
| 42  | 3     | 302 | A86  | C21-C20-C19 | 3.62  | 118.31      | 114.24   |
| 42  | 5     | 303 | A86  | C34-O4-C38  | -3.61 | 111.47      | 117.85   |
| 42  | 6     | 202 | A86  | C3-C4-C5    | -3.60 | 116.15      | 123.52   |
| 42  | p     | 610 | A86  | O1-C15-C20  | -3.60 | 56.40       | 59.45    |
| 42  | P     | 610 | A86  | C25-C26-C27 | -3.59 | 122.24      | 127.28   |
| 42  | 0     | 303 | A86  | C34-O4-C38  | -3.58 | 111.52      | 117.85   |
| 44  | 3     | 303 | DD6  | C37-C36-C31 | -3.57 | 117.48      | 124.16   |
| 44  | 7     | 304 | DD6  | C21-C20-C19 | 3.57  | 118.25      | 114.24   |
| 31  | 8     | 314 | CLA  | CAA-C2A-C3A | -3.57 | 108.04      | 116.23   |
| 44  | 8     | 303 | DD6  | C37-C36-C31 | -3.57 | 117.48      | 124.16   |
| 42  | P     | 610 | A86  | O1-C15-C20  | -3.57 | 56.43       | 59.45    |
| 42  | P     | 610 | A86  | C3-C2-C1    | -3.56 | 122.28      | 127.28   |
| 31  | 3     | 314 | CLA  | CAA-C2A-C3A | -3.56 | 108.06      | 116.23   |
| 31  | 8     | 309 | CLA  | CAA-C2A-C3A | -3.56 | 108.06      | 116.23   |
| 31  | 1     | 201 | CLA  | O2D-CGD-O1D | -3.56 | 116.92      | 123.85   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 8     | 302 | A86  | C21-C20-C19 | 3.56  | 118.24      | 114.24   |
| 42  | 3     | 301 | A86  | O4-C38-O5   | -3.56 | 116.13      | 122.99   |
| 31  | 3     | 310 | CLA  | CAA-C2A-C3A | -3.56 | 108.08      | 116.23   |
| 42  | 8     | 301 | A86  | O4-C38-O5   | -3.55 | 116.13      | 122.99   |
| 31  | 8     | 310 | CLA  | CAA-C2A-C3A | -3.54 | 108.11      | 116.23   |
| 43  | 0     | 302 | ET4  | O40-C36-C35 | 3.54  | 116.98      | 109.75   |
| 42  | p     | 610 | A86  | C3-C2-C1    | -3.54 | 122.32      | 127.28   |
| 44  | 2     | 304 | DD6  | C21-C20-C19 | 3.54  | 118.21      | 114.24   |
| 31  | 3     | 309 | CLA  | CAA-C2A-C3A | -3.54 | 108.12      | 116.23   |
| 43  | 5     | 302 | ET4  | O40-C36-C35 | 3.54  | 116.98      | 109.75   |
| 31  | 2     | 307 | CLA  | O2D-CGD-O1D | -3.53 | 116.97      | 123.85   |
| 42  | 7     | 302 | A86  | C3-C4-C5    | -3.53 | 116.29      | 123.52   |
| 31  | 7     | 307 | CLA  | O2D-CGD-O1D | -3.53 | 116.97      | 123.85   |
| 31  | B     | 511 | CLA  | C1-C2-C3    | -3.53 | 120.42      | 126.20   |
| 31  | 6     | 201 | CLA  | O2D-CGD-O1D | -3.52 | 116.99      | 123.85   |
| 39  | C     | 519 | DGD  | O6D-C1D-O3G | -3.51 | 101.74      | 110.04   |
| 39  | c     | 519 | DGD  | O6D-C1D-O3G | -3.51 | 101.74      | 110.04   |
| 31  | 3     | 304 | CLA  | CAA-C2A-C3A | -3.51 | 108.18      | 116.23   |
| 31  | p     | 601 | CLA  | CBD-CHA-C1A | 3.51  | 132.68      | 127.38   |
| 42  | 2     | 302 | A86  | C3-C4-C5    | -3.50 | 116.35      | 123.52   |
| 31  | 8     | 304 | CLA  | CAA-C2A-C3A | -3.50 | 108.20      | 116.23   |
| 31  | b     | 512 | CLA  | C1-C2-C3    | -3.50 | 120.46      | 126.20   |
| 31  | 0     | 305 | CLA  | CMB-C2B-C1B | -3.50 | 120.09      | 125.42   |
| 43  | 0     | 302 | ET4  | C35-C34-C33 | 3.50  | 116.38      | 109.49   |
| 43  | 5     | 302 | ET4  | C35-C34-C33 | 3.49  | 116.37      | 109.49   |
| 31  | a     | 404 | CLA  | O2D-CGD-O1D | -3.49 | 117.05      | 123.85   |
| 34  | A     | 409 | SQD  | O47-C7-C8   | 3.48  | 119.00      | 111.48   |
| 31  | P     | 601 | CLA  | CBD-CHA-C1A | 3.47  | 132.62      | 127.38   |
| 34  | a     | 409 | SQD  | O47-C7-C8   | 3.47  | 118.98      | 111.48   |
| 42  | 9     | 202 | A86  | C3-C4-C5    | -3.46 | 116.43      | 123.52   |
| 31  | A     | 404 | CLA  | O2D-CGD-O1D | -3.46 | 117.11      | 123.85   |
| 31  | 5     | 305 | CLA  | CMB-C2B-C1B | -3.46 | 120.15      | 125.42   |
| 34  | B     | 523 | SQD  | O9-S-C6     | 3.45  | 111.91      | 106.76   |
| 42  | 4     | 202 | A86  | C3-C4-C5    | -3.45 | 116.45      | 123.52   |
| 44  | 6     | 203 | DD6  | C15-C14-C13 | -3.45 | 118.70      | 125.99   |
| 44  | 8     | 303 | DD6  | O1-C15-C14  | -3.44 | 107.02      | 116.88   |
| 34  | b     | 501 | SQD  | O9-S-C6     | 3.43  | 111.88      | 106.76   |
| 42  | 6     | 202 | A86  | O4-C38-C39  | 3.43  | 117.21      | 111.09   |
| 44  | 3     | 303 | DD6  | O1-C15-C14  | -3.43 | 107.05      | 116.88   |
| 44  | 1     | 203 | DD6  | C15-C14-C13 | -3.43 | 118.75      | 125.99   |
| 42  | 9     | 203 | A86  | C10-C9-C8   | -3.43 | 113.27      | 123.20   |
| 42  | 4     | 203 | A86  | C10-C9-C8   | -3.42 | 113.28      | 123.20   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 3     | 301 | A86  | C9-C10-C11  | -3.42 | 116.97      | 126.64   |
| 34  | 5     | 316 | SQD  | O47-C7-C8   | 3.42  | 118.88      | 111.48   |
| 42  | 1     | 202 | A86  | O4-C38-C39  | 3.42  | 117.18      | 111.09   |
| 31  | p     | 606 | CLA  | C3A-C2A-C1A | -3.41 | 102.81      | 106.30   |
| 34  | 0     | 316 | SQD  | O47-C7-C8   | 3.41  | 118.86      | 111.48   |
| 31  | P     | 604 | CLA  | CAA-C2A-C3A | -3.41 | 108.42      | 116.23   |
| 44  | 7     | 303 | DD6  | C15-C14-C13 | -3.41 | 118.79      | 125.99   |
| 44  | 2     | 303 | DD6  | C15-C14-C13 | -3.40 | 118.79      | 125.99   |
| 31  | P     | 605 | CLA  | CBD-CHA-C1A | 3.40  | 132.52      | 127.38   |
| 42  | 8     | 301 | A86  | C9-C10-C11  | -3.40 | 117.02      | 126.64   |
| 31  | p     | 604 | CLA  | CAA-C2A-C3A | -3.40 | 108.43      | 116.23   |
| 31  | P     | 606 | CLA  | C3A-C2A-C1A | -3.40 | 102.82      | 106.30   |
| 31  | 4     | 212 | CLA  | CAA-C2A-C3A | -3.40 | 108.44      | 116.23   |
| 31  | p     | 605 | CLA  | CBD-CHA-C1A | 3.39  | 132.49      | 127.38   |
| 31  | 9     | 212 | CLA  | CAA-C2A-C3A | -3.38 | 108.49      | 116.23   |
| 34  | A     | 411 | SQD  | O5-C5-C4    | 3.36  | 115.75      | 109.70   |
| 31  | C     | 504 | CLA  | C1-C2-C3    | -3.34 | 120.72      | 126.20   |
| 42  | 2     | 302 | A86  | C25-C26-C27 | -3.34 | 122.59      | 127.28   |
| 31  | c     | 504 | CLA  | C1-C2-C3    | -3.34 | 120.72      | 126.20   |
| 34  | B     | 522 | SQD  | O5-C5-C4    | 3.34  | 115.71      | 109.70   |
| 42  | 7     | 302 | A86  | C25-C26-C27 | -3.33 | 122.60      | 127.28   |
| 31  | P     | 607 | CLA  | C3A-C2A-C1A | -3.33 | 102.89      | 106.30   |
| 31  | 0     | 304 | CLA  | O2D-CGD-O1D | -3.33 | 117.36      | 123.85   |
| 31  | p     | 607 | CLA  | C3A-C2A-C1A | -3.32 | 102.90      | 106.30   |
| 31  | 5     | 304 | CLA  | O2D-CGD-O1D | -3.32 | 117.38      | 123.85   |
| 31  | 2     | 305 | CLA  | CAA-C2A-C3A | -3.32 | 108.61      | 116.23   |
| 34  | B     | 523 | SQD  | O47-C7-C8   | 3.31  | 118.64      | 111.48   |
| 34  | b     | 501 | SQD  | O47-C7-C8   | 3.31  | 118.64      | 111.48   |
| 31  | 7     | 305 | CLA  | CAA-C2A-C3A | -3.31 | 108.65      | 116.23   |
| 31  | 4     | 204 | CLA  | CAA-C2A-C3A | -3.30 | 108.65      | 116.23   |
| 31  | 6     | 210 | CLA  | O2D-CGD-O1D | -3.30 | 117.42      | 123.85   |
| 32  | a     | 406 | PHO  | C2B-C1B-NB  | -3.30 | 107.04      | 109.43   |
| 42  | 4     | 203 | A86  | C25-C26-C27 | -3.30 | 122.65      | 127.28   |
| 31  | 9     | 204 | CLA  | CAA-C2A-C3A | -3.29 | 108.69      | 116.23   |
| 31  | b     | 504 | CLA  | O2D-CGD-O1D | -3.29 | 117.44      | 123.85   |
| 31  | 1     | 210 | CLA  | O2D-CGD-O1D | -3.29 | 117.45      | 123.85   |
| 34  | b     | 501 | SQD  | C3-C4-C5    | 3.29  | 116.19      | 110.23   |
| 31  | B     | 503 | CLA  | O2D-CGD-O1D | -3.28 | 117.45      | 123.85   |
| 34  | B     | 523 | SQD  | C3-C4-C5    | 3.28  | 116.19      | 110.23   |
| 42  | 4     | 202 | A86  | C4-C5-C6    | -3.28 | 122.67      | 127.28   |
| 31  | P     | 602 | CLA  | CAA-C2A-C3A | -3.27 | 108.72      | 116.23   |
| 32  | A     | 406 | PHO  | C2B-C1B-NB  | -3.27 | 107.06      | 109.43   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 9     | 202 | A86  | C4-C5-C6    | -3.27 | 122.69      | 127.28   |
| 31  | p     | 602 | CLA  | CAA-C2A-C3A | -3.27 | 108.73      | 116.23   |
| 31  | Z     | 101 | CLA  | C3B-C4B-NB  | -3.27 | 107.61      | 110.53   |
| 31  | 8     | 306 | CLA  | CBD-CHA-C1A | 3.27  | 131.49      | 128.03   |
| 31  | 9     | 213 | CLA  | C3A-C2A-C1A | -3.26 | 102.96      | 106.30   |
| 31  | 4     | 213 | CLA  | C3A-C2A-C1A | -3.26 | 102.96      | 106.30   |
| 42  | 9     | 203 | A86  | C25-C26-C27 | -3.26 | 122.70      | 127.28   |
| 31  | 3     | 306 | CLA  | CBD-CHA-C1A | 3.26  | 131.48      | 128.03   |
| 31  | 4     | 206 | CLA  | CBD-CHA-C1A | 3.25  | 131.48      | 128.03   |
| 31  | p     | 602 | CLA  | O2D-CGD-O1D | -3.25 | 117.52      | 123.85   |
| 31  | 7     | 306 | CLA  | C3B-C4B-NB  | -3.23 | 107.64      | 110.53   |
| 43  | 5     | 302 | ET4  | C01-C06-C07 | 3.23  | 124.42      | 115.65   |
| 31  | 9     | 206 | CLA  | CBD-CHA-C1A | 3.23  | 131.46      | 128.03   |
| 43  | 0     | 302 | ET4  | C01-C06-C07 | 3.23  | 124.40      | 115.65   |
| 34  | B     | 522 | SQD  | O47-C7-C8   | 3.22  | 118.45      | 111.48   |
| 34  | A     | 411 | SQD  | O47-C7-C8   | 3.22  | 118.45      | 111.48   |
| 31  | B     | 504 | CLA  | O2D-CGD-O1D | -3.22 | 117.58      | 123.85   |
| 31  | P     | 602 | CLA  | O2D-CGD-O1D | -3.21 | 117.60      | 123.85   |
| 31  | z     | 101 | CLA  | C3B-C4B-NB  | -3.21 | 107.67      | 110.53   |
| 44  | 6     | 204 | DD6  | C4-C3-C2    | -3.21 | 116.96      | 123.52   |
| 31  | 2     | 306 | CLA  | C3B-C4B-NB  | -3.20 | 107.67      | 110.53   |
| 31  | 9     | 205 | CLA  | C3A-C2A-C1A | -3.20 | 103.02      | 106.30   |
| 44  | 1     | 204 | DD6  | C4-C3-C2    | -3.20 | 116.97      | 123.52   |
| 31  | b     | 505 | CLA  | O2D-CGD-O1D | -3.20 | 117.62      | 123.85   |
| 31  | w     | 202 | CLA  | O2D-CGD-O1D | -3.19 | 117.63      | 123.85   |
| 31  | W     | 202 | CLA  | O2D-CGD-O1D | -3.19 | 117.63      | 123.85   |
| 42  | 6     | 202 | A86  | O1-C15-C20  | -3.19 | 56.75       | 59.45    |
| 31  | 2     | 313 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 31  | 7     | 313 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 32  | A     | 405 | PHO  | C1-C2-C3    | -3.18 | 121.00      | 126.20   |
| 32  | a     | 405 | PHO  | C1-C2-C3    | -3.17 | 121.00      | 126.20   |
| 31  | p     | 603 | CLA  | CBD-CHA-C1A | 3.17  | 132.17      | 127.38   |
| 42  | 0     | 301 | A86  | O4-C38-O5   | -3.17 | 116.87      | 122.99   |
| 42  | 5     | 301 | A86  | O4-C38-O5   | -3.17 | 116.87      | 122.99   |
| 31  | P     | 603 | CLA  | CBD-CHA-C1A | 3.17  | 132.16      | 127.38   |
| 31  | 4     | 205 | CLA  | C3A-C2A-C1A | -3.16 | 103.06      | 106.30   |
| 31  | B     | 501 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 31  | 3     | 308 | CLA  | C3B-C4B-NB  | -3.16 | 107.71      | 110.53   |
| 31  | 1     | 215 | CLA  | CBD-CHA-C1A | 3.16  | 132.15      | 127.38   |
| 31  | a     | 407 | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 39  | C     | 518 | DGD  | O6D-C1D-O3G | -3.16 | 102.58      | 110.04   |
| 42  | 2     | 302 | A86  | O4-C38-O5   | -3.16 | 116.90      | 122.99   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | P     | 610 | A86  | C28-C27-C26 | -3.16 | 117.70      | 122.82   |
| 31  | b     | 505 | CLA  | C1-C2-C3    | -3.15 | 121.03      | 126.20   |
| 31  | 0     | 314 | CLA  | CBD-CHA-C1A | 3.15  | 132.14      | 127.38   |
| 39  | c     | 518 | DGD  | O6D-C1D-O3G | -3.15 | 102.59      | 110.04   |
| 31  | b     | 502 | CLA  | O2D-CGD-O1D | -3.15 | 117.71      | 123.85   |
| 42  | 1     | 202 | A86  | C9-C8-C6    | -3.15 | 117.72      | 126.36   |
| 31  | 6     | 215 | CLA  | CBD-CHA-C1A | 3.15  | 132.13      | 127.38   |
| 31  | B     | 504 | CLA  | C1-C2-C3    | -3.15 | 121.04      | 126.20   |
| 32  | a     | 406 | PHO  | O1D-CGD-CBD | 3.15  | 129.50      | 124.72   |
| 32  | A     | 405 | PHO  | C2B-C1B-NB  | -3.15 | 107.16      | 109.43   |
| 31  | P     | 606 | CLA  | C3B-C4B-NB  | -3.14 | 107.72      | 110.53   |
| 31  | A     | 407 | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 31  | W     | 202 | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 31  | p     | 606 | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 31  | 9     | 206 | CLA  | C3A-C2A-C1A | -3.14 | 103.09      | 106.30   |
| 32  | A     | 406 | PHO  | O1D-CGD-CBD | 3.14  | 129.48      | 124.72   |
| 42  | 7     | 302 | A86  | O4-C38-O5   | -3.13 | 116.94      | 122.99   |
| 42  | 6     | 202 | A86  | C9-C8-C6    | -3.13 | 117.77      | 126.36   |
| 42  | p     | 610 | A86  | C28-C27-C26 | -3.13 | 117.74      | 122.82   |
| 31  | 8     | 308 | CLA  | C3B-C4B-NB  | -3.13 | 107.73      | 110.53   |
| 34  | A     | 409 | SQD  | O9-S-C6     | 3.13  | 111.43      | 106.76   |
| 42  | 1     | 202 | A86  | O1-C15-C20  | -3.13 | 56.80       | 59.45    |
| 31  | 7     | 305 | CLA  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |
| 31  | w     | 202 | CLA  | C3B-C4B-NB  | -3.12 | 107.74      | 110.53   |
| 31  | 3     | 311 | CLA  | CAA-C2A-C3A | -3.12 | 109.08      | 116.23   |
| 31  | 5     | 314 | CLA  | CBD-CHA-C1A | 3.12  | 132.09      | 127.38   |
| 31  | 7     | 313 | CLA  | CBD-CHA-C1A | 3.12  | 132.09      | 127.38   |
| 31  | 2     | 313 | CLA  | CBD-CHA-C1A | 3.12  | 132.09      | 127.38   |
| 31  | 3     | 313 | CLA  | C3B-C4B-NB  | -3.12 | 107.75      | 110.53   |
| 34  | a     | 409 | SQD  | O9-S-C6     | 3.12  | 111.41      | 106.76   |
| 31  | 8     | 310 | CLA  | C3B-C4B-NB  | -3.11 | 107.75      | 110.53   |
| 37  | y     | 101 | LMG  | O6-C1-O1    | -3.11 | 102.69      | 110.04   |
| 34  | 0     | 316 | SQD  | O9-S-C6     | 3.11  | 111.40      | 106.76   |
| 31  | 4     | 206 | CLA  | C3A-C2A-C1A | -3.11 | 103.12      | 106.30   |
| 32  | a     | 405 | PHO  | C2B-C1B-NB  | -3.11 | 107.18      | 109.43   |
| 31  | c     | 506 | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 31  | 8     | 311 | CLA  | CAA-C2A-C3A | -3.10 | 109.11      | 116.23   |
| 31  | 5     | 313 | CLA  | CBD-CHA-C1A | 3.10  | 132.06      | 127.38   |
| 31  | 2     | 305 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 37  | Y     | 101 | LMG  | O6-C1-O1    | -3.10 | 102.72      | 110.04   |
| 34  | B     | 523 | SQD  | O7-S-C6     | 3.10  | 111.39      | 106.76   |
| 31  | C     | 506 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34  | 5     | 316 | SQD  | O9-S-C6     | 3.10  | 111.38      | 106.76   |
| 34  | B     | 522 | SQD  | C4-C3-C2    | 3.10  | 116.27      | 110.83   |
| 31  | c     | 509 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 34  | b     | 501 | SQD  | O7-S-C6     | 3.10  | 111.38      | 106.76   |
| 31  | 9     | 207 | CLA  | CBD-CHA-C1A | 3.10  | 132.05      | 127.38   |
| 36  | D     | 411 | LHG  | O8-C23-C24  | 3.09  | 120.53      | 111.15   |
| 31  | C     | 514 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 31  | 1     | 216 | CLA  | CBD-CHA-C1A | 3.09  | 132.04      | 127.38   |
| 31  | b     | 517 | CLA  | C3B-C4B-NB  | -3.09 | 107.78      | 110.53   |
| 31  | 4     | 207 | CLA  | CBD-CHA-C1A | 3.09  | 132.04      | 127.38   |
| 34  | B     | 522 | SQD  | O7-S-C6     | 3.08  | 111.36      | 106.76   |
| 34  | A     | 411 | SQD  | C4-C3-C2    | 3.08  | 116.25      | 110.83   |
| 36  | d     | 411 | LHG  | O8-C23-C24  | 3.08  | 120.51      | 111.15   |
| 31  | C     | 509 | CLA  | O2D-CGD-O1D | -3.08 | 117.84      | 123.85   |
| 31  | c     | 514 | CLA  | O2D-CGD-O1D | -3.08 | 117.84      | 123.85   |
| 31  | 0     | 313 | CLA  | CBD-CHA-C1A | 3.08  | 132.03      | 127.38   |
| 31  | 7     | 316 | CLA  | O2D-CGD-O1D | -3.08 | 117.85      | 123.85   |
| 34  | A     | 411 | SQD  | O7-S-C6     | 3.08  | 111.36      | 106.76   |
| 31  | B     | 516 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 31  | 8     | 313 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 42  | 8     | 302 | A86  | C23-C16-C22 | -3.07 | 102.91      | 107.37   |
| 31  | b     | 515 | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 31  | c     | 502 | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 31  | 8     | 313 | CLA  | CBD-CHA-C1A | 3.07  | 132.01      | 127.38   |
| 31  | 6     | 216 | CLA  | CBD-CHA-C1A | 3.06  | 132.00      | 127.38   |
| 31  | 5     | 312 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 31  | 0     | 312 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 31  | B     | 514 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 31  | 2     | 316 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 44  | 6     | 204 | DD6  | C21-C20-C15 | -3.06 | 117.27      | 122.30   |
| 31  | 3     | 310 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 31  | C     | 502 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 31  | 3     | 313 | CLA  | CBD-CHA-C1A | 3.06  | 131.99      | 127.38   |
| 31  | 5     | 306 | CLA  | C3B-C4B-NB  | -3.05 | 107.80      | 110.53   |
| 31  | 4     | 204 | CLA  | C3B-C4B-NB  | -3.05 | 107.80      | 110.53   |
| 42  | 3     | 302 | A86  | C23-C16-C22 | -3.05 | 102.93      | 107.37   |
| 31  | 0     | 306 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 31  | b     | 513 | CLA  | CAA-C2A-C3A | -3.05 | 109.24      | 116.23   |
| 31  | 0     | 309 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 31  | B     | 512 | CLA  | CAA-C2A-C3A | -3.05 | 109.25      | 116.23   |
| 31  | D     | 404 | CLA  | O2D-CGD-O1D | -3.04 | 117.92      | 123.85   |
| 31  | 9     | 204 | CLA  | C3B-C4B-NB  | -3.04 | 107.81      | 110.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 44  | 8     | 303 | DD6  | C4-C3-C2    | -3.04 | 117.30      | 123.52   |
| 31  | 7     | 307 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 42  | 7     | 302 | A86  | C41-C32-C31 | -3.04 | 107.75      | 110.47   |
| 42  | 8     | 302 | A86  | C4-C3-C2    | -3.04 | 117.31      | 123.52   |
| 31  | 0     | 313 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 44  | 1     | 204 | DD6  | C21-C20-C15 | -3.03 | 117.31      | 122.30   |
| 44  | 3     | 303 | DD6  | C4-C3-C2    | -3.03 | 117.31      | 123.52   |
| 42  | 9     | 203 | A86  | C12-C11-C13 | 3.03  | 120.91      | 116.00   |
| 31  | b     | 515 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 37  | J     | 101 | LMG  | O6-C1-O1    | -3.03 | 102.89      | 110.04   |
| 31  | 2     | 312 | CLA  | CBD-CHA-C1A | 3.02  | 131.94      | 127.38   |
| 31  | C     | 508 | CLA  | O2D-CGD-O1D | -3.02 | 117.96      | 123.85   |
| 31  | 2     | 310 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 31  | B     | 510 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 42  | 2     | 302 | A86  | C41-C32-C31 | -3.02 | 107.77      | 110.47   |
| 31  | 7     | 312 | CLA  | CBD-CHA-C1A | 3.02  | 131.94      | 127.38   |
| 37  | j     | 101 | LMG  | O6-C1-O1    | -3.02 | 102.91      | 110.04   |
| 44  | P     | 611 | DD6  | C21-C20-C15 | -3.02 | 117.34      | 122.30   |
| 31  | d     | 404 | CLA  | O2D-CGD-O1D | -3.02 | 117.98      | 123.85   |
| 44  | p     | 611 | DD6  | C21-C20-C15 | -3.01 | 117.34      | 122.30   |
| 33  | B     | 517 | BCR  | C24-C23-C22 | -3.01 | 121.78      | 126.23   |
| 31  | p     | 603 | CLA  | CMB-C2B-C1B | -3.01 | 120.83      | 125.42   |
| 42  | 3     | 302 | A86  | C4-C3-C2    | -3.01 | 117.36      | 123.52   |
| 31  | B     | 514 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 37  | D     | 410 | LMG  | O6-C1-O1    | -3.01 | 102.93      | 110.04   |
| 31  | 7     | 315 | CLA  | CBD-CHA-C1A | 3.01  | 131.92      | 127.38   |
| 37  | d     | 410 | LMG  | O6-C1-O1    | -3.01 | 102.94      | 110.04   |
| 31  | 5     | 309 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 31  | 6     | 211 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 33  | b     | 518 | BCR  | C24-C23-C22 | -3.00 | 121.79      | 126.23   |
| 42  | 7     | 302 | A86  | C9-C10-C11  | -3.00 | 118.16      | 126.64   |
| 31  | P     | 603 | CLA  | CMB-C2B-C1B | -3.00 | 120.85      | 125.42   |
| 31  | 7     | 310 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 42  | 4     | 203 | A86  | C12-C11-C13 | 3.00  | 120.86      | 116.00   |
| 31  | b     | 511 | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 31  | c     | 508 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |
| 33  | c     | 516 | BCR  | C20-C21-C22 | -2.99 | 123.08      | 127.28   |
| 32  | A     | 406 | PHO  | CMB-C2B-C3B | 2.99  | 130.66      | 124.68   |
| 31  | 9     | 211 | CLA  | C3A-C2A-C1A | -2.99 | 103.24      | 106.30   |
| 31  | 0     | 304 | CLA  | CAA-C2A-C3A | -2.99 | 109.38      | 116.23   |
| 32  | a     | 406 | PHO  | CMB-C2B-C3B | 2.99  | 130.65      | 124.68   |
| 42  | 2     | 302 | A86  | C9-C10-C11  | -2.98 | 118.21      | 126.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | D     | 410 | LMG  | O6-C1-C2    | 2.98  | 116.49      | 110.37   |
| 31  | 9     | 206 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 31  | 0     | 309 | CLA  | CAA-C2A-C3A | -2.98 | 109.41      | 116.23   |
| 42  | 9     | 202 | A86  | C21-C20-C19 | 2.98  | 117.58      | 114.24   |
| 31  | 2     | 307 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 31  | 2     | 308 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 31  | 2     | 315 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 37  | d     | 410 | LMG  | O6-C1-C2    | 2.97  | 116.48      | 110.37   |
| 31  | 3     | 306 | CLA  | C3A-C4A-CHB | -2.97 | 120.27      | 123.91   |
| 31  | 1     | 211 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 31  | 5     | 309 | CLA  | CAA-C2A-C3A | -2.97 | 109.42      | 116.23   |
| 31  | c     | 503 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 31  | 5     | 304 | CLA  | CAA-C2A-C3A | -2.97 | 109.42      | 116.23   |
| 43  | 5     | 302 | ET4  | C07-C06-C05 | -2.97 | 114.71      | 121.56   |
| 31  | 8     | 306 | CLA  | C3A-C4A-CHB | -2.97 | 120.27      | 123.91   |
| 31  | 4     | 211 | CLA  | C3A-C2A-C1A | -2.97 | 103.26      | 106.30   |
| 31  | D     | 401 | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |
| 31  | d     | 401 | CLA  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 31  | B     | 515 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 35  | d     | 406 | PL9  | C7-C8-C9    | -2.96 | 121.73      | 126.83   |
| 42  | 8     | 302 | A86  | C28-C27-C26 | -2.96 | 118.02      | 122.82   |
| 31  | C     | 503 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 33  | C     | 516 | BCR  | C20-C21-C22 | -2.96 | 123.13      | 127.28   |
| 31  | 7     | 308 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 31  | 2     | 315 | CLA  | CBD-CHA-C1A | 2.96  | 131.84      | 127.38   |
| 44  | 6     | 204 | DD6  | O1-C20-C21  | -2.95 | 111.75      | 115.05   |
| 31  | b     | 508 | CLA  | CAA-C2A-C3A | -2.95 | 109.45      | 116.23   |
| 34  | a     | 409 | SQD  | O7-S-C6     | 2.95  | 111.17      | 106.76   |
| 31  | B     | 508 | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 31  | 5     | 313 | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 31  | B     | 512 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 44  | 2     | 304 | DD6  | C37-C36-C35 | 2.95  | 119.85      | 114.42   |
| 31  | B     | 507 | CLA  | CAA-C2A-C3A | -2.95 | 109.46      | 116.23   |
| 42  | 4     | 202 | A86  | C21-C20-C19 | 2.95  | 117.56      | 114.24   |
| 33  | c     | 516 | BCR  | C7-C8-C9    | -2.95 | 121.87      | 126.23   |
| 34  | A     | 409 | SQD  | O7-S-C6     | 2.95  | 111.16      | 106.76   |
| 44  | 1     | 204 | DD6  | O1-C20-C21  | -2.95 | 111.75      | 115.05   |
| 31  | 4     | 206 | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 43  | 0     | 302 | ET4  | C07-C06-C05 | -2.95 | 114.76      | 121.56   |
| 31  | C     | 510 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 31  | c     | 510 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 42  | 5     | 303 | A86  | C40-C32-C31 | -2.95 | 107.83      | 110.47   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 0     | 303 | A86  | C40-C32-C31 | -2.95 | 107.83      | 110.47   |
| 42  | 4     | 201 | A86  | C41-C32-C40 | -2.95 | 100.20      | 108.63   |
| 31  | b     | 516 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 31  | b     | 513 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 34  | 5     | 316 | SQD  | O7-S-C6     | 2.94  | 111.15      | 106.76   |
| 42  | 9     | 201 | A86  | C41-C32-C40 | -2.94 | 100.22      | 108.63   |
| 31  | 0     | 307 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 35  | D     | 406 | PL9  | C7-C8-C9    | -2.94 | 121.77      | 126.83   |
| 42  | 3     | 302 | A86  | C28-C27-C26 | -2.94 | 118.06      | 122.82   |
| 31  | 9     | 208 | CLA  | C3B-C4B-NB  | -2.93 | 107.91      | 110.53   |
| 31  | P     | 609 | CLA  | CAA-C2A-C3A | -2.93 | 109.51      | 116.23   |
| 31  | z     | 101 | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 31  | b     | 509 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 31  | 3     | 305 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 31  | 9     | 210 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 31  | P     | 608 | CLA  | C3A-C2A-C1A | -2.92 | 103.31      | 106.30   |
| 31  | 6     | 208 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 32  | A     | 406 | PHO  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 31  | 7     | 305 | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 31  | C     | 512 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 33  | C     | 516 | BCR  | C7-C8-C9    | -2.92 | 121.91      | 126.23   |
| 31  | 5     | 307 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 32  | a     | 406 | PHO  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 31  | 4     | 208 | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 31  | 8     | 305 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 42  | 8     | 302 | A86  | O4-C38-O5   | -2.92 | 117.36      | 122.99   |
| 31  | Z     | 101 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 44  | 7     | 304 | DD6  | C37-C36-C35 | 2.92  | 119.78      | 114.42   |
| 34  | 0     | 316 | SQD  | O7-S-C6     | 2.92  | 111.11      | 106.76   |
| 31  | C     | 507 | CLA  | O2D-CGD-O1D | -2.91 | 118.17      | 123.85   |
| 31  | 8     | 310 | CLA  | CHC-C1C-C2C | -2.91 | 123.56      | 129.94   |
| 31  | 6     | 214 | CLA  | CBD-CHA-C1A | 2.91  | 131.78      | 127.38   |
| 31  | 1     | 214 | CLA  | CBD-CHA-C1A | 2.91  | 131.78      | 127.38   |
| 31  | 6     | 206 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 31  | c     | 512 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 31  | 6     | 206 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 33  | b     | 518 | BCR  | C33-C5-C6   | -2.91 | 121.31      | 124.48   |
| 31  | 1     | 206 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 31  | c     | 507 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 32  | A     | 405 | PHO  | O1D-CGD-CBD | 2.91  | 129.13      | 124.72   |
| 44  | 2     | 303 | DD6  | C13-C11-C10 | 2.91  | 123.58      | 119.01   |
| 31  | 3     | 310 | CLA  | CHC-C1C-C2C | -2.91 | 123.58      | 129.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | H     | 102 | DGD  | O6D-C1D-O3G | -2.90 | 103.18      | 110.04   |
| 39  | h     | 102 | DGD  | O6D-C1D-O3G | -2.90 | 103.18      | 110.04   |
| 33  | B     | 518 | BCR  | C15-C14-C13 | -2.90 | 123.21      | 127.28   |
| 31  | b     | 506 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 31  | 7     | 309 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 31  | 1     | 216 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 31  | 0     | 307 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 31  | 1     | 208 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 31  | C     | 503 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 42  | 3     | 302 | A86  | O4-C38-O5   | -2.90 | 117.39      | 122.99   |
| 37  | B     | 520 | LMG  | O6-C1-O1    | -2.90 | 103.19      | 110.04   |
| 31  | p     | 609 | CLA  | CAA-C2A-C3A | -2.90 | 109.59      | 116.23   |
| 37  | b     | 521 | LMG  | O6-C1-O1    | -2.90 | 103.20      | 110.04   |
| 44  | 7     | 303 | DD6  | C13-C11-C10 | 2.90  | 123.56      | 119.01   |
| 37  | c     | 521 | LMG  | C8-O7-C10   | -2.89 | 110.87      | 117.80   |
| 31  | 2     | 305 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 44  | 1     | 203 | DD6  | C13-C11-C10 | 2.89  | 123.56      | 119.01   |
| 31  | 7     | 313 | CLA  | CAA-C2A-C3A | -2.89 | 109.60      | 116.23   |
| 31  | 7     | 315 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 37  | C     | 521 | LMG  | C8-O7-C10   | -2.89 | 110.87      | 117.80   |
| 31  | p     | 608 | CLA  | C3A-C2A-C1A | -2.89 | 103.34      | 106.30   |
| 33  | b     | 519 | BCR  | C15-C14-C13 | -2.89 | 123.22      | 127.28   |
| 31  | P     | 604 | CLA  | CMB-C2B-C1B | -2.89 | 121.02      | 125.42   |
| 31  | b     | 504 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | 6     | 216 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | A     | 403 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | B     | 505 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 31  | a     | 403 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 33  | k     | 101 | BCR  | C15-C16-C17 | -2.89 | 117.61      | 123.52   |
| 31  | p     | 609 | CLA  | CHB-C4A-NA  | 2.89  | 128.56      | 124.40   |
| 31  | 0     | 310 | CLA  | O2D-CGD-O1D | -2.89 | 118.23      | 123.85   |
| 42  | 9     | 202 | A86  | C9-C10-C11  | -2.88 | 118.49      | 126.64   |
| 33  | K     | 101 | BCR  | C15-C16-C17 | -2.88 | 117.62      | 123.52   |
| 31  | 2     | 314 | CLA  | CBD-CHA-C1A | 2.88  | 131.73      | 127.38   |
| 31  | 5     | 304 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 31  | 6     | 205 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 31  | 0     | 304 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 34  | 5     | 316 | SQD  | O6-C1-C2    | 2.88  | 112.65      | 108.27   |
| 44  | 6     | 203 | DD6  | C13-C11-C10 | 2.88  | 123.54      | 119.01   |
| 32  | a     | 405 | PHO  | O1D-CGD-CBD | 2.88  | 129.09      | 124.72   |
| 44  | 1     | 204 | DD6  | C25-C24-C1  | -2.88 | 118.47      | 126.36   |
| 31  | 5     | 310 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 209 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 31  | 4     | 210 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 31  | 1     | 206 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 31  | 0     | 311 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 31  | b     | 512 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 33  | B     | 517 | BCR  | C33-C5-C6   | -2.87 | 121.35      | 124.48   |
| 32  | a     | 405 | PHO  | CMB-C2B-C3B | 2.87  | 130.42      | 124.68   |
| 31  | 2     | 311 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 32  | A     | 405 | PHO  | CMB-C2B-C3B | 2.87  | 130.42      | 124.68   |
| 31  | P     | 609 | CLA  | CHB-C4A-NA  | 2.87  | 128.54      | 124.40   |
| 31  | 2     | 309 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 44  | 6     | 204 | DD6  | C25-C24-C1  | -2.87 | 118.50      | 126.36   |
| 31  | p     | 604 | CLA  | CMB-C2B-C1B | -2.87 | 121.05      | 125.42   |
| 31  | B     | 503 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 31  | 5     | 307 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 34  | B     | 522 | SQD  | O5-C1-C2    | 2.87  | 116.26      | 110.37   |
| 31  | 5     | 311 | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 34  | A     | 411 | SQD  | O5-C1-C2    | 2.86  | 116.25      | 110.37   |
| 31  | C     | 504 | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 31  | c     | 503 | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 31  | 6     | 208 | CLA  | C3B-C4B-NB  | -2.86 | 107.97      | 110.53   |
| 31  | 3     | 305 | CLA  | C3B-C4B-NB  | -2.86 | 107.97      | 110.53   |
| 42  | 4     | 202 | A86  | C9-C10-C11  | -2.86 | 118.55      | 126.64   |
| 31  | 5     | 314 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 31  | 9     | 209 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 34  | 0     | 316 | SQD  | O6-C1-C2    | 2.86  | 112.62      | 108.27   |
| 31  | 8     | 305 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 31  | 1     | 209 | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 31  | 2     | 313 | CLA  | CAA-C2A-C3A | -2.86 | 109.68      | 116.23   |
| 31  | c     | 504 | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 31  | 7     | 311 | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 39  | h     | 102 | DGD  | CDB-CCB-CBB | -2.85 | 99.94       | 114.37   |
| 39  | H     | 102 | DGD  | CDB-CCB-CBB | -2.85 | 99.95       | 114.37   |
| 31  | a     | 407 | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 31  | 1     | 208 | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 36  | d     | 412 | LHG  | O8-C23-C24  | 2.85  | 120.53      | 111.83   |
| 34  | A     | 411 | SQD  | C44-O6-C1   | 2.85  | 119.91      | 113.80   |
| 31  | 6     | 215 | CLA  | CAA-C2A-C3A | -2.85 | 109.69      | 116.23   |
| 31  | 0     | 314 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 31  | B     | 511 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 31  | c     | 511 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 31  | 7     | 311 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34  | B     | 522 | SQD  | C44-O6-C1   | 2.84  | 119.89      | 113.80   |
| 42  | 0     | 301 | A86  | C28-C27-C26 | -2.84 | 118.21      | 122.82   |
| 31  | 1     | 215 | CLA  | CAA-C2A-C3A | -2.84 | 109.72      | 116.23   |
| 31  | P     | 601 | CLA  | CHC-C1C-C2C | -2.84 | 123.73      | 129.94   |
| 36  | A     | 412 | LHG  | O8-C23-C24  | 2.84  | 120.49      | 111.83   |
| 31  | 6     | 209 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 31  | 7     | 314 | CLA  | CBD-CHA-C1A | 2.84  | 131.66      | 127.38   |
| 31  | C     | 511 | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 42  | 5     | 303 | A86  | C19-C18-C17 | -2.84 | 105.48      | 110.79   |
| 36  | a     | 411 | LHG  | O8-C23-C24  | 2.83  | 120.47      | 111.83   |
| 31  | 2     | 311 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 31  | 3     | 312 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 37  | C     | 521 | LMG  | O8-C28-C29  | 2.83  | 120.46      | 111.83   |
| 31  | p     | 601 | CLA  | CHC-C1C-C2C | -2.83 | 123.75      | 129.94   |
| 42  | 0     | 303 | A86  | C19-C18-C17 | -2.83 | 105.50      | 110.79   |
| 31  | b     | 514 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 31  | 6     | 212 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 37  | c     | 521 | LMG  | O8-C28-C29  | 2.82  | 120.44      | 111.83   |
| 31  | 1     | 212 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 31  | B     | 501 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 36  | D     | 412 | LHG  | O8-C23-C24  | 2.82  | 120.44      | 111.83   |
| 42  | 5     | 301 | A86  | C28-C27-C26 | -2.82 | 118.25      | 122.82   |
| 31  | c     | 502 | CLA  | CHB-C4A-NA  | 2.82  | 128.47      | 124.40   |
| 31  | 0     | 314 | CLA  | CAA-C2A-C3A | -2.82 | 109.77      | 116.23   |
| 31  | 0     | 313 | CLA  | CAA-C2A-C3A | -2.82 | 109.77      | 116.23   |
| 31  | A     | 407 | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 31  | B     | 510 | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 42  | 7     | 302 | A86  | C33-C32-C31 | 2.82  | 111.95      | 109.21   |
| 42  | 8     | 301 | A86  | C19-C18-C17 | 2.82  | 116.06      | 110.79   |
| 31  | 8     | 307 | CLA  | CMB-C2B-C1B | -2.82 | 121.13      | 125.42   |
| 31  | 8     | 312 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 31  | 1     | 205 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 37  | J     | 101 | LMG  | O1-C7-C8    | -2.81 | 103.98      | 110.82   |
| 31  | 4     | 208 | CLA  | C2A-C1A-CHA | 2.81  | 128.73      | 123.86   |
| 31  | 3     | 307 | CLA  | CMB-C2B-C1B | -2.81 | 121.14      | 125.42   |
| 31  | 9     | 208 | CLA  | O2D-CGD-O1D | -2.81 | 117.70      | 124.08   |
| 42  | 3     | 301 | A86  | C19-C18-C17 | 2.81  | 116.05      | 110.79   |
| 34  | B     | 522 | SQD  | O9-S-C6     | 2.81  | 110.95      | 106.76   |
| 31  | c     | 514 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 31  | 7     | 312 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 31  | B     | 506 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 31  | p     | 606 | CLA  | C4D-C3D-CAD | -2.81 | 105.06      | 108.11   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34  | b     | 501 | SQD  | O6-C1-C2    | 2.81  | 112.54      | 108.27   |
| 31  | 7     | 306 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 31  | 9     | 208 | CLA  | C2A-C1A-CHA | 2.81  | 128.73      | 123.86   |
| 33  | b     | 518 | BCR  | C15-C16-C17 | -2.81 | 117.77      | 123.52   |
| 31  | B     | 507 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 31  | C     | 513 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 31  | b     | 508 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 42  | 2     | 302 | A86  | C33-C32-C31 | 2.81  | 111.94      | 109.21   |
| 31  | b     | 511 | CLA  | C3B-C4B-NB  | -2.81 | 108.03      | 110.53   |
| 31  | b     | 507 | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 37  | j     | 101 | LMG  | O1-C7-C8    | -2.80 | 104.00      | 110.82   |
| 31  | B     | 513 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 31  | 4     | 208 | CLA  | O2D-CGD-O1D | -2.80 | 117.72      | 124.08   |
| 31  | 5     | 314 | CLA  | CAA-C2A-C3A | -2.80 | 109.80      | 116.23   |
| 31  | 5     | 313 | CLA  | CAA-C2A-C3A | -2.80 | 109.80      | 116.23   |
| 33  | B     | 517 | BCR  | C15-C16-C17 | -2.80 | 117.78      | 123.52   |
| 31  | C     | 509 | CLA  | CMB-C2B-C1B | -2.80 | 121.16      | 125.42   |
| 31  | D     | 403 | CLA  | O2D-CGD-O1D | -2.80 | 118.40      | 123.85   |
| 34  | A     | 411 | SQD  | O9-S-C6     | 2.80  | 110.94      | 106.76   |
| 31  | b     | 502 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 31  | 8     | 306 | CLA  | CHC-C1C-C2C | -2.80 | 123.82      | 129.94   |
| 31  | 0     | 306 | CLA  | O2D-CGD-O1D | -2.80 | 118.40      | 123.85   |
| 31  | b     | 517 | CLA  | O2D-CGD-O1D | -2.80 | 118.41      | 123.85   |
| 37  | d     | 409 | LMG  | C6-C5-C4    | -2.80 | 106.16      | 113.02   |
| 31  | B     | 507 | CLA  | C3B-C4B-NB  | -2.79 | 108.03      | 110.53   |
| 31  | 9     | 207 | CLA  | C3B-C4B-NB  | -2.79 | 108.03      | 110.53   |
| 37  | D     | 409 | LMG  | C6-C5-C4    | -2.79 | 106.16      | 113.02   |
| 31  | B     | 515 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | b     | 516 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | 5     | 309 | CLA  | O2D-CGD-O1D | -2.79 | 118.41      | 123.85   |
| 31  | C     | 502 | CLA  | CHB-C4A-NA  | 2.79  | 128.43      | 124.40   |
| 31  | 7     | 314 | CLA  | CAA-C2A-C3A | -2.79 | 109.83      | 116.23   |
| 31  | c     | 509 | CLA  | CMB-C2B-C1B | -2.79 | 121.17      | 125.42   |
| 31  | 2     | 306 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 31  | 2     | 312 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | P     | 606 | CLA  | C4D-C3D-CAD | -2.79 | 105.08      | 108.11   |
| 37  | m     | 102 | LMG  | O6-C1-O1    | -2.79 | 103.45      | 110.04   |
| 35  | D     | 406 | PL9  | C27-C28-C29 | -2.79 | 121.24      | 127.62   |
| 31  | C     | 514 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 31  | c     | 513 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 31  | 0     | 309 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 31  | 5     | 306 | CLA  | O2D-CGD-O1D | -2.79 | 118.43      | 123.85   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 207 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 31  | 2     | 310 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 31  | 6     | 206 | CLA  | CHB-C4A-NA  | 2.78  | 128.41      | 124.40   |
| 31  | 2     | 314 | CLA  | CAA-C2A-C3A | -2.78 | 109.85      | 116.23   |
| 42  | P     | 610 | A86  | C23-C16-C17 | -2.78 | 104.08      | 108.97   |
| 31  | 3     | 306 | CLA  | CHC-C1C-C2C | -2.78 | 123.86      | 129.94   |
| 35  | d     | 406 | PL9  | C27-C28-C29 | -2.78 | 121.27      | 127.62   |
| 34  | B     | 523 | SQD  | O6-C1-C2    | 2.78  | 112.49      | 108.27   |
| 31  | B     | 516 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 31  | c     | 511 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 37  | M     | 102 | LMG  | O6-C1-O1    | -2.77 | 103.49      | 110.04   |
| 31  | C     | 511 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 31  | p     | 601 | CLA  | CHB-C4A-NA  | 2.77  | 128.40      | 124.40   |
| 31  | B     | 508 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 31  | d     | 403 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 44  | p     | 611 | DD6  | C15-C14-C13 | -2.77 | 120.13      | 125.99   |
| 37  | M     | 101 | LMG  | O6-C1-O1    | -2.77 | 103.49      | 110.04   |
| 34  | B     | 523 | SQD  | O48-C23-C24 | 2.77  | 120.28      | 111.83   |
| 31  | 6     | 211 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 31  | 7     | 315 | CLA  | CAA-C2A-C3A | -2.77 | 109.88      | 116.23   |
| 31  | 8     | 309 | CLA  | CMA-C3A-C2A | -2.77 | 109.88      | 116.23   |
| 34  | b     | 501 | SQD  | O48-C23-C24 | 2.77  | 120.28      | 111.83   |
| 42  | p     | 610 | A86  | C23-C16-C17 | -2.77 | 104.11      | 108.97   |
| 44  | 2     | 304 | DD6  | C19-C18-C17 | 2.77  | 115.97      | 110.79   |
| 31  | A     | 404 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 31  | 2     | 315 | CLA  | CAA-C2A-C3A | -2.77 | 109.89      | 116.23   |
| 31  | c     | 508 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 34  | a     | 409 | SQD  | O5-C5-C4    | 2.77  | 114.68      | 109.70   |
| 31  | 7     | 310 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 31  | a     | 404 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 34  | A     | 409 | SQD  | O5-C5-C4    | 2.76  | 114.68      | 109.70   |
| 31  | 1     | 211 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 33  | b     | 519 | BCR  | C15-C16-C17 | -2.76 | 117.87      | 123.52   |
| 31  | b     | 508 | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 33  | B     | 518 | BCR  | C15-C16-C17 | -2.76 | 117.88      | 123.52   |
| 42  | P     | 610 | A86  | C4-C3-C2    | -2.76 | 117.88      | 123.52   |
| 31  | 3     | 309 | CLA  | CMA-C3A-C2A | -2.76 | 109.91      | 116.23   |
| 31  | 3     | 304 | CLA  | CHC-C1C-C2C | -2.76 | 123.91      | 129.94   |
| 44  | P     | 611 | DD6  | C15-C14-C13 | -2.75 | 120.17      | 125.99   |
| 31  | B     | 511 | CLA  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 31  | 6     | 216 | CLA  | CAA-C2A-C3A | -2.75 | 109.91      | 116.23   |
| 37  | m     | 101 | LMG  | O6-C1-O1    | -2.75 | 103.54      | 110.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 44  | 7     | 304 | DD6  | C19-C18-C17 | 2.75  | 115.94      | 110.79   |
| 31  | 6     | 215 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 31  | 1     | 215 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 42  | 9     | 202 | A86  | C35-C34-C33 | -2.75 | 104.94      | 109.89   |
| 31  | 5     | 312 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 31  | b     | 509 | CLA  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 31  | 8     | 304 | CLA  | CHC-C1C-C2C | -2.75 | 123.92      | 129.94   |
| 31  | 1     | 206 | CLA  | CHB-C4A-NA  | 2.75  | 128.37      | 124.40   |
| 31  | 6     | 210 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 31  | b     | 512 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 42  | 4     | 202 | A86  | C35-C34-C33 | -2.75 | 104.95      | 109.89   |
| 31  | c     | 508 | CLA  | CHB-C4A-NA  | 2.75  | 128.36      | 124.40   |
| 31  | 0     | 312 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 31  | 3     | 304 | CLA  | CHB-C4A-NA  | 2.75  | 128.36      | 124.40   |
| 31  | 6     | 207 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 31  | C     | 508 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 31  | b     | 507 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 42  | p     | 610 | A86  | C4-C3-C2    | -2.74 | 117.91      | 123.52   |
| 31  | 9     | 207 | CLA  | CHB-C4A-NA  | 2.74  | 128.36      | 124.40   |
| 31  | 6     | 205 | CLA  | CAA-C2A-C3A | -2.74 | 109.94      | 116.23   |
| 31  | 1     | 216 | CLA  | CAA-C2A-C3A | -2.74 | 109.95      | 116.23   |
| 31  | 0     | 308 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 31  | d     | 404 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 31  | 7     | 309 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 31  | 2     | 309 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 31  | 6     | 205 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 31  | D     | 404 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 31  | 6     | 213 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 31  | 1     | 213 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 31  | 6     | 212 | CLA  | CAA-C2A-C3A | -2.73 | 109.96      | 116.23   |
| 31  | 1     | 205 | CLA  | CAA-C2A-C3A | -2.73 | 109.96      | 116.23   |
| 31  | C     | 508 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 31  | 8     | 304 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 31  | 1     | 212 | CLA  | CAA-C2A-C3A | -2.73 | 109.97      | 116.23   |
| 31  | 1     | 205 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 31  | 1     | 207 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 31  | 8     | 307 | CLA  | C3B-C4B-NB  | -2.73 | 108.10      | 110.53   |
| 31  | C     | 505 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 37  | D     | 410 | LMG  | O1-C7-C8    | -2.72 | 104.20      | 110.82   |
| 31  | P     | 601 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 42  | 0     | 301 | A86  | C25-C24-C1  | -2.72 | 118.90      | 126.36   |
| 31  | 2     | 312 | CLA  | CHC-C1C-C2C | -2.72 | 123.99      | 129.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 207 | CLA  | CHB-C4A-NA  | 2.72  | 128.33      | 124.40   |
| 31  | 5     | 308 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 43  | 5     | 302 | ET4  | C42-C34-C33 | -2.72 | 105.64      | 110.52   |
| 31  | 0     | 310 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 32  | A     | 405 | PHO  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 31  | 3     | 310 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 37  | d     | 410 | LMG  | O1-C7-C8    | -2.72 | 104.21      | 110.82   |
| 39  | c     | 519 | DGD  | O5D-C6D-C5D | -2.71 | 103.30      | 109.42   |
| 42  | 5     | 301 | A86  | C25-C24-C1  | -2.71 | 118.92      | 126.36   |
| 33  | B     | 517 | BCR  | C27-C26-C25 | 2.71  | 126.37      | 122.70   |
| 39  | C     | 519 | DGD  | O5D-C6D-C5D | -2.71 | 103.31      | 109.42   |
| 31  | 4     | 210 | CLA  | CBD-CHA-C1A | 2.71  | 131.47      | 127.38   |
| 31  | c     | 505 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 44  | 1     | 204 | DD6  | C26-C25-C24 | -2.71 | 115.35      | 123.20   |
| 31  | b     | 506 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 36  | H     | 103 | LHG  | O8-C23-C24  | 2.71  | 120.09      | 111.83   |
| 33  | b     | 518 | BCR  | C27-C26-C25 | 2.71  | 126.36      | 122.70   |
| 31  | w     | 202 | CLA  | CMD-C2D-C1D | -2.71 | 119.96      | 124.73   |
| 31  | 9     | 205 | CLA  | C3B-C4B-NB  | -2.71 | 107.52      | 110.33   |
| 44  | 6     | 204 | DD6  | C26-C25-C24 | -2.70 | 115.37      | 123.20   |
| 31  | B     | 505 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 42  | 5     | 301 | A86  | C21-C20-C15 | 2.70  | 132.07      | 123.35   |
| 31  | B     | 506 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | W     | 202 | CLA  | CMD-C2D-C1D | -2.70 | 119.98      | 124.73   |
| 31  | 4     | 205 | CLA  | C3B-C4B-NB  | -2.70 | 107.53      | 110.33   |
| 31  | 7     | 312 | CLA  | CHC-C1C-C2C | -2.70 | 124.04      | 129.94   |
| 42  | 0     | 301 | A86  | C21-C20-C15 | 2.70  | 132.06      | 123.35   |
| 31  | 1     | 210 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | 9     | 210 | CLA  | CBD-CHA-C1A | 2.69  | 131.45      | 127.38   |
| 31  | 8     | 310 | CLA  | CHB-C4A-NA  | 2.69  | 128.29      | 124.40   |
| 43  | 0     | 302 | ET4  | C42-C34-C33 | -2.69 | 105.69      | 110.52   |
| 32  | a     | 405 | PHO  | O2D-CGD-O1D | -2.69 | 118.61      | 123.85   |
| 44  | 7     | 303 | DD6  | C12-C11-C10 | -2.69 | 118.46      | 122.82   |
| 44  | 6     | 203 | DD6  | C12-C11-C10 | -2.69 | 118.46      | 122.82   |
| 42  | 9     | 203 | A86  | C21-C20-C19 | 2.69  | 117.26      | 114.24   |
| 36  | h     | 103 | LHG  | O8-C23-C24  | 2.69  | 120.03      | 111.83   |
| 35  | D     | 406 | PL9  | C22-C23-C24 | -2.69 | 121.48      | 127.62   |
| 31  | C     | 506 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 33  | d     | 405 | BCR  | C27-C26-C25 | 2.68  | 126.33      | 122.70   |
| 31  | 1     | 214 | CLA  | CAA-C2A-C3A | -2.68 | 110.08      | 116.23   |
| 33  | h     | 101 | BCR  | C2-C1-C6    | 2.68  | 114.33      | 110.44   |
| 31  | P     | 603 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 0     | 317 | A86  | C23-C16-C17 | -2.68 | 104.26      | 108.97   |
| 31  | p     | 603 | CLA  | CHB-C4A-NA  | 2.68  | 128.26      | 124.40   |
| 42  | 4     | 203 | A86  | C21-C20-C19 | 2.68  | 117.25      | 114.24   |
| 44  | 1     | 203 | DD6  | C12-C11-C10 | -2.68 | 118.48      | 122.82   |
| 35  | d     | 406 | PL9  | C22-C23-C24 | -2.67 | 121.50      | 127.62   |
| 36  | B     | 521 | LHG  | C11-C10-C9  | -2.67 | 100.85      | 114.37   |
| 31  | 3     | 307 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 31  | b     | 502 | CLA  | CHB-C4A-NA  | 2.67  | 128.26      | 124.40   |
| 31  | C     | 509 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 36  | b     | 522 | LHG  | C11-C10-C9  | -2.67 | 100.86      | 114.37   |
| 42  | 4     | 202 | A86  | O4-C34-C35  | 2.67  | 114.47      | 107.64   |
| 31  | 7     | 312 | CLA  | CAA-C2A-C3A | -2.67 | 110.11      | 116.23   |
| 34  | a     | 409 | SQD  | O6-C1-C2    | 2.67  | 112.33      | 108.27   |
| 42  | 5     | 317 | A86  | C23-C16-C17 | -2.67 | 104.28      | 108.97   |
| 37  | d     | 409 | LMG  | O6-C1-O1    | -2.67 | 103.74      | 110.04   |
| 31  | 8     | 311 | CLA  | CHB-C4A-NA  | 2.67  | 128.25      | 124.40   |
| 31  | 3     | 309 | CLA  | CHB-C4A-NA  | 2.66  | 128.25      | 124.40   |
| 33  | c     | 515 | BCR  | C24-C23-C22 | -2.66 | 122.29      | 126.23   |
| 42  | 7     | 301 | A86  | C23-C16-C17 | -2.66 | 104.29      | 108.97   |
| 31  | p     | 605 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 31  | 6     | 214 | CLA  | CAA-C2A-C3A | -2.66 | 110.12      | 116.23   |
| 31  | 2     | 312 | CLA  | CAA-C2A-C3A | -2.66 | 110.12      | 116.23   |
| 34  | A     | 409 | SQD  | O6-C1-C2    | 2.66  | 112.32      | 108.27   |
| 33  | H     | 101 | BCR  | C2-C1-C6    | 2.66  | 114.31      | 110.44   |
| 31  | C     | 502 | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 44  | 2     | 303 | DD6  | C12-C11-C10 | -2.66 | 118.50      | 122.82   |
| 42  | 9     | 202 | A86  | C9-C8-C6    | -2.66 | 119.07      | 126.36   |
| 31  | B     | 504 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 31  | 5     | 310 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 42  | 9     | 202 | A86  | O4-C34-C35  | 2.66  | 114.45      | 107.64   |
| 31  | 6     | 210 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 31  | 8     | 309 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 31  | 4     | 213 | CLA  | CAB-C3B-C2B | 2.66  | 130.59      | 123.53   |
| 31  | 1     | 212 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 31  | b     | 505 | CLA  | CHB-C4A-NA  | 2.66  | 128.23      | 124.40   |
| 39  | c     | 519 | DGD  | CDB-CCB-CBB | -2.66 | 100.94      | 114.37   |
| 31  | 9     | 204 | CLA  | CBD-CHA-C1A | 2.66  | 131.39      | 127.38   |
| 42  | 5     | 303 | A86  | C33-C32-C31 | 2.65  | 111.79      | 109.21   |
| 42  | 0     | 303 | A86  | C33-C32-C31 | 2.65  | 111.79      | 109.21   |
| 33  | k     | 101 | BCR  | C33-C5-C6   | -2.65 | 121.59      | 124.48   |
| 37  | D     | 409 | LMG  | O6-C1-O1    | -2.65 | 103.78      | 110.04   |
| 42  | 4     | 202 | A86  | O4-C34-C33  | -2.65 | 100.84      | 107.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | C     | 519 | DGD  | CDB-CCB-CBB | -2.65 | 100.96      | 114.37   |
| 31  | c     | 506 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 42  | 5     | 301 | A86  | O-C13-C11   | -2.65 | 115.33      | 121.04   |
| 31  | 4     | 211 | CLA  | CAB-C3B-C2B | 2.65  | 130.58      | 123.53   |
| 42  | 0     | 301 | A86  | O-C13-C11   | -2.65 | 115.33      | 121.04   |
| 36  | b     | 522 | LHG  | O8-C23-C24  | 2.65  | 119.92      | 111.83   |
| 36  | B     | 521 | LHG  | O8-C23-C24  | 2.65  | 119.92      | 111.83   |
| 31  | P     | 603 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 42  | 4     | 202 | A86  | C9-C8-C6    | -2.65 | 119.10      | 126.36   |
| 31  | c     | 502 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 42  | 9     | 202 | A86  | O4-C34-C33  | -2.65 | 100.86      | 107.64   |
| 42  | 2     | 301 | A86  | C23-C16-C17 | -2.65 | 104.32      | 108.97   |
| 31  | 9     | 213 | CLA  | CAB-C3B-C2B | 2.65  | 130.56      | 123.53   |
| 31  | 1     | 210 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 31  | 8     | 307 | CLA  | CHB-C4A-NA  | 2.64  | 128.22      | 124.40   |
| 33  | D     | 405 | BCR  | C27-C26-C25 | 2.64  | 126.28      | 122.70   |
| 31  | 9     | 211 | CLA  | CAB-C3B-C2B | 2.64  | 130.56      | 123.53   |
| 42  | 8     | 301 | A86  | O-C13-C11   | -2.64 | 115.35      | 121.04   |
| 31  | P     | 609 | CLA  | CBD-CHA-C1A | 2.64  | 132.48      | 127.58   |
| 31  | c     | 505 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 31  | 4     | 209 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 31  | 3     | 311 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 31  | c     | 513 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 31  | 6     | 213 | CLA  | O2D-CGD-O1D | -2.64 | 118.09      | 124.08   |
| 33  | C     | 515 | BCR  | C24-C23-C22 | -2.64 | 122.33      | 126.23   |
| 39  | C     | 518 | DGD  | CDB-CCB-CBB | -2.64 | 101.03      | 114.37   |
| 31  | 9     | 209 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 31  | B     | 501 | CLA  | CHB-C4A-NA  | 2.64  | 128.20      | 124.40   |
| 42  | 3     | 301 | A86  | O-C13-C11   | -2.64 | 115.36      | 121.04   |
| 31  | p     | 603 | CLA  | C3B-C4B-NB  | -2.64 | 108.18      | 110.53   |
| 33  | C     | 515 | BCR  | C27-C26-C25 | 2.64  | 126.27      | 122.70   |
| 39  | c     | 518 | DGD  | CDB-CCB-CBB | -2.63 | 101.05      | 114.37   |
| 44  | 3     | 303 | DD6  | O1-C20-C21  | -2.63 | 112.11      | 115.05   |
| 31  | 4     | 204 | CLA  | CBD-CHA-C1A | 2.63  | 131.35      | 127.38   |
| 31  | 7     | 314 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 33  | B     | 519 | BCR  | C11-C10-C9  | -2.63 | 123.59      | 127.28   |
| 31  | p     | 609 | CLA  | CBD-CHA-C1A | 2.63  | 132.46      | 127.58   |
| 31  | 3     | 311 | CLA  | CMA-C3A-C2A | -2.63 | 110.20      | 116.23   |
| 31  | C     | 505 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 31  | 3     | 307 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 31  | P     | 605 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 33  | K     | 101 | BCR  | C33-C5-C6   | -2.62 | 121.62      | 124.48   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 2     | 314 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 39  | c     | 519 | DGD  | C3G-C2G-C1G | -2.62 | 105.67      | 111.78   |
| 31  | b     | 516 | CLA  | CHB-C4A-NA  | 2.62  | 128.19      | 124.40   |
| 39  | C     | 519 | DGD  | C3G-C2G-C1G | -2.62 | 105.67      | 111.78   |
| 31  | 1     | 213 | CLA  | O2D-CGD-O1D | -2.62 | 118.13      | 124.08   |
| 31  | C     | 512 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 31  | b     | 510 | CLA  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 31  | 8     | 311 | CLA  | CMA-C3A-C2A | -2.62 | 110.23      | 116.23   |
| 31  | B     | 509 | CLA  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 33  | c     | 515 | BCR  | C27-C26-C25 | 2.62  | 126.24      | 122.70   |
| 31  | p     | 601 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 31  | B     | 514 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 31  | 6     | 212 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 31  | 0     | 305 | CLA  | O2D-CGD-O1D | -2.61 | 118.76      | 123.85   |
| 33  | a     | 408 | BCR  | C27-C26-C25 | 2.61  | 126.23      | 122.70   |
| 31  | 7     | 316 | CLA  | CAA-C2A-C3A | -2.61 | 110.24      | 116.23   |
| 36  | a     | 412 | LHG  | C11-C10-C9  | -2.61 | 101.17      | 114.37   |
| 44  | 2     | 303 | DD6  | C21-C20-C15 | -2.61 | 118.00      | 122.30   |
| 31  | 2     | 316 | CLA  | CAA-C2A-C3A | -2.61 | 110.25      | 116.23   |
| 44  | p     | 611 | DD6  | C37-C36-C35 | 2.61  | 119.22      | 114.42   |
| 36  | A     | 413 | LHG  | C11-C10-C9  | -2.61 | 101.18      | 114.37   |
| 31  | D     | 404 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 31  | b     | 515 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 31  | c     | 509 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 31  | A     | 407 | CLA  | C1-C2-C3    | -2.60 | 121.93      | 126.20   |
| 42  | P     | 610 | A86  | C41-C32-C40 | 2.60  | 116.09      | 108.63   |
| 44  | 1     | 203 | DD6  | C21-C20-C15 | -2.60 | 118.02      | 122.30   |
| 31  | p     | 602 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 42  | p     | 610 | A86  | C41-C32-C40 | 2.60  | 116.09      | 108.63   |
| 31  | 5     | 308 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 42  | 0     | 303 | A86  | C41-C32-C31 | -2.60 | 108.14      | 110.47   |
| 31  | b     | 513 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 31  | B     | 515 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 31  | c     | 514 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 31  | 0     | 311 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 44  | 8     | 303 | DD6  | O1-C20-C21  | -2.60 | 112.14      | 115.05   |
| 31  | a     | 407 | CLA  | C1-C2-C3    | -2.60 | 121.94      | 126.20   |
| 31  | C     | 514 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 31  | a     | 407 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 44  | P     | 611 | DD6  | C37-C36-C35 | 2.60  | 119.20      | 114.42   |
| 42  | 3     | 301 | A86  | C8-C6-C5    | 2.60  | 123.09      | 119.01   |
| 33  | b     | 520 | BCR  | C11-C10-C9  | -2.59 | 123.64      | 127.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 305 | CLA  | O2D-CGD-O1D | -2.59 | 118.80      | 123.85   |
| 31  | p     | 608 | CLA  | CAB-C3B-C2B | 2.59  | 130.43      | 123.53   |
| 31  | 1     | 214 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | D     | 403 | CLA  | CMB-C2B-C3B | 2.59  | 130.42      | 123.53   |
| 31  | P     | 608 | CLA  | CAB-C3B-C2B | 2.59  | 130.42      | 123.53   |
| 31  | 0     | 305 | CLA  | CMB-C2B-C3B | 2.59  | 132.65      | 126.55   |
| 31  | d     | 404 | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 31  | C     | 513 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | P     | 602 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | d     | 403 | CLA  | CMB-C2B-C3B | 2.59  | 130.42      | 123.53   |
| 31  | C     | 512 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 31  | C     | 507 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | 5     | 309 | CLA  | CHB-C4A-NA  | 2.59  | 128.13      | 124.40   |
| 44  | 1     | 204 | DD6  | C32-C33-C34 | -2.59 | 107.92      | 113.59   |
| 31  | B     | 502 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | c     | 512 | CLA  | CHB-C4A-NA  | 2.59  | 128.13      | 124.40   |
| 33  | H     | 101 | BCR  | C27-C26-C25 | 2.59  | 126.20      | 122.70   |
| 31  | C     | 505 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 31  | b     | 514 | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 31  | 4     | 209 | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 31  | B     | 512 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 44  | 6     | 204 | DD6  | C9-C8-C6    | -2.58 | 119.28      | 126.36   |
| 31  | A     | 407 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 31  | B     | 513 | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 33  | c     | 515 | BCR  | C15-C16-C17 | -2.58 | 118.24      | 123.52   |
| 31  | B     | 516 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 31  | 5     | 311 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 42  | 5     | 303 | A86  | C41-C32-C31 | -2.58 | 108.16      | 110.47   |
| 31  | P     | 601 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 31  | 6     | 210 | CLA  | CAA-C2A-C3A | -2.58 | 106.03      | 113.00   |
| 33  | B     | 518 | BCR  | C27-C26-C25 | 2.58  | 126.19      | 122.70   |
| 44  | 6     | 204 | DD6  | C32-C33-C34 | -2.58 | 107.94      | 113.59   |
| 42  | 4     | 203 | A86  | C26-C25-C24 | -2.58 | 115.74      | 123.20   |
| 31  | b     | 503 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 33  | C     | 515 | BCR  | C15-C16-C17 | -2.58 | 118.25      | 123.52   |
| 42  | 8     | 301 | A86  | C8-C6-C5    | 2.57  | 123.06      | 119.01   |
| 42  | 7     | 301 | A86  | C9-C10-C11  | -2.57 | 119.36      | 126.64   |
| 31  | 6     | 214 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 42  | 2     | 301 | A86  | C9-C10-C11  | -2.57 | 119.37      | 126.64   |
| 31  | b     | 514 | CLA  | C1-C2-C3    | -2.57 | 121.98      | 126.20   |
| 31  | c     | 510 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 44  | 6     | 203 | DD6  | C21-C20-C15 | -2.57 | 118.07      | 122.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 44  | 8     | 303 | DD6  | C26-C25-C24 | -2.57 | 115.75      | 123.20   |
| 31  | b     | 513 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 31  | 5     | 305 | CLA  | CMB-C2B-C3B | 2.57  | 132.59      | 126.55   |
| 31  | P     | 604 | CLA  | CHB-C4A-NA  | 2.57  | 128.10      | 124.40   |
| 31  | 3     | 312 | CLA  | O2D-CGD-O1D | -2.57 | 118.26      | 124.08   |
| 37  | 5     | 315 | LMG  | O6-C1-O1    | -2.57 | 103.98      | 110.04   |
| 42  | 7     | 302 | A86  | C25-C24-C1  | -2.57 | 119.33      | 126.36   |
| 31  | 9     | 209 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 31  | B     | 512 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 31  | 0     | 311 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 31  | 2     | 316 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 31  | b     | 517 | CLA  | CHB-C4A-NA  | 2.57  | 128.10      | 124.40   |
| 31  | B     | 513 | CLA  | C1-C2-C3    | -2.56 | 122.00      | 126.20   |
| 33  | K     | 101 | BCR  | C27-C26-C25 | 2.56  | 126.17      | 122.70   |
| 31  | C     | 510 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 31  | D     | 401 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 31  | d     | 401 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 44  | 7     | 303 | DD6  | C21-C20-C15 | -2.56 | 118.08      | 122.30   |
| 31  | 1     | 211 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 31  | 4     | 212 | CLA  | CMB-C2B-C3B | 2.56  | 130.34      | 123.53   |
| 37  | B     | 520 | LMG  | O1-C1-C2    | -2.56 | 104.38      | 108.27   |
| 33  | b     | 519 | BCR  | C27-C26-C25 | 2.56  | 126.17      | 122.70   |
| 44  | 1     | 203 | DD6  | O1-C20-C21  | -2.56 | 112.18      | 115.05   |
| 43  | 0     | 302 | ET4  | C08-C09-C10 | 2.56  | 123.04      | 119.01   |
| 31  | 8     | 305 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 31  | c     | 505 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 44  | 1     | 204 | DD6  | C9-C8-C6    | -2.56 | 119.34      | 126.36   |
| 33  | A     | 408 | BCR  | C27-C26-C25 | 2.56  | 126.16      | 122.70   |
| 33  | k     | 101 | BCR  | C27-C26-C25 | 2.56  | 126.16      | 122.70   |
| 31  | c     | 507 | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 37  | b     | 521 | LMG  | O1-C1-C2    | -2.56 | 104.39      | 108.27   |
| 37  | d     | 410 | LMG  | O1-C1-C2    | -2.56 | 104.39      | 108.27   |
| 42  | 9     | 203 | A86  | C26-C25-C24 | -2.56 | 115.79      | 123.20   |
| 31  | 8     | 305 | CLA  | O2D-CGD-O1D | -2.56 | 118.28      | 124.08   |
| 42  | 2     | 302 | A86  | C25-C24-C1  | -2.56 | 119.35      | 126.36   |
| 43  | 5     | 302 | ET4  | C08-C09-C10 | 2.56  | 123.03      | 119.01   |
| 31  | 9     | 210 | CLA  | CMB-C2B-C1B | -2.56 | 121.53      | 125.42   |
| 31  | 8     | 312 | CLA  | O2D-CGD-O1D | -2.56 | 118.28      | 124.08   |
| 44  | 3     | 303 | DD6  | C26-C25-C24 | -2.56 | 115.79      | 123.20   |
| 31  | 4     | 210 | CLA  | CMB-C2B-C1B | -2.56 | 121.53      | 125.42   |
| 31  | 4     | 210 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 31  | 0     | 309 | CLA  | CHB-C4A-NA  | 2.55  | 128.09      | 124.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | 0     | 315 | LMG  | O6-C1-O1    | -2.55 | 104.01      | 110.04   |
| 31  | D     | 404 | CLA  | CHB-C4A-NA  | 2.55  | 128.09      | 124.40   |
| 33  | C     | 517 | BCR  | C33-C5-C6   | -2.55 | 121.70      | 124.48   |
| 33  | h     | 101 | BCR  | C27-C26-C25 | 2.55  | 126.15      | 122.70   |
| 31  | 9     | 212 | CLA  | CMB-C2B-C3B | 2.55  | 130.31      | 123.53   |
| 31  | b     | 503 | CLA  | CMB-C2B-C1B | -2.55 | 121.54      | 125.42   |
| 31  | 7     | 316 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 31  | 1     | 210 | CLA  | CAA-C2A-C3A | -2.55 | 106.11      | 113.00   |
| 31  | c     | 512 | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 31  | P     | 603 | CLA  | CMB-C2B-C3B | 2.55  | 132.54      | 126.55   |
| 44  | 2     | 304 | DD6  | C37-C36-C31 | -2.55 | 119.40      | 124.16   |
| 33  | c     | 517 | BCR  | C33-C5-C6   | -2.55 | 121.71      | 124.48   |
| 42  | 9     | 203 | A86  | C28-C27-C26 | -2.55 | 118.69      | 122.82   |
| 31  | 0     | 308 | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 42  | 5     | 317 | A86  | C9-C10-C11  | -2.54 | 119.45      | 126.64   |
| 36  | B     | 521 | LHG  | C20-C19-C18 | -2.54 | 101.52      | 114.37   |
| 44  | 8     | 303 | DD6  | C3-C2-C1    | -2.54 | 123.71      | 127.28   |
| 31  | 7     | 308 | CLA  | CAB-C3B-C2B | 2.54  | 130.28      | 123.53   |
| 31  | B     | 508 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 31  | d     | 404 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 37  | D     | 410 | LMG  | O1-C1-C2    | -2.54 | 104.42      | 108.27   |
| 36  | b     | 522 | LHG  | C20-C19-C18 | -2.54 | 101.53      | 114.37   |
| 31  | 8     | 306 | CLA  | CAB-C3B-C2B | 2.54  | 130.28      | 123.53   |
| 42  | 0     | 317 | A86  | C9-C10-C11  | -2.54 | 119.46      | 126.64   |
| 33  | B     | 519 | BCR  | C33-C5-C6   | -2.54 | 121.71      | 124.48   |
| 33  | b     | 520 | BCR  | C33-C5-C6   | -2.54 | 121.71      | 124.48   |
| 42  | 8     | 302 | A86  | C3-C4-C5    | -2.54 | 118.33      | 123.52   |
| 31  | 9     | 210 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 44  | 7     | 303 | DD6  | O1-C20-C21  | -2.54 | 112.21      | 115.05   |
| 31  | b     | 509 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 31  | p     | 603 | CLA  | CMB-C2B-C3B | 2.54  | 132.52      | 126.55   |
| 31  | c     | 504 | CLA  | C3B-C4B-NB  | -2.54 | 108.27      | 110.53   |
| 31  | 3     | 311 | CLA  | C3B-C4B-NB  | -2.54 | 108.27      | 110.53   |
| 33  | c     | 515 | BCR  | C15-C14-C13 | -2.54 | 123.72      | 127.28   |
| 44  | P     | 611 | DD6  | C25-C24-C1  | -2.54 | 119.41      | 126.36   |
| 31  | D     | 401 | CLA  | C1-C2-C3    | -2.53 | 122.04      | 126.20   |
| 34  | A     | 409 | SQD  | O48-C23-C24 | 2.53  | 119.56      | 111.83   |
| 31  | p     | 602 | CLA  | O2D-CGD-CBD | 2.53  | 115.66      | 111.23   |
| 44  | 2     | 303 | DD6  | O1-C20-C21  | -2.53 | 112.22      | 115.05   |
| 31  | b     | 507 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 31  | 6     | 214 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 31  | 1     | 214 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 306 | CLA  | CAB-C3B-C2B | 2.53  | 130.26      | 123.53   |
| 31  | P     | 602 | CLA  | O2D-CGD-CBD | 2.53  | 115.65      | 111.23   |
| 31  | 5     | 313 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 37  | j     | 101 | LMG  | C38-C37-C36 | -2.53 | 101.59      | 114.37   |
| 31  | 3     | 313 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 37  | J     | 101 | LMG  | C38-C37-C36 | -2.53 | 101.60      | 114.37   |
| 31  | 5     | 311 | CLA  | C3B-C4B-NB  | -2.53 | 108.28      | 110.53   |
| 31  | 1     | 213 | CLA  | CAA-C2A-C3A | -2.53 | 110.44      | 116.23   |
| 34  | a     | 409 | SQD  | O48-C23-C24 | 2.52  | 119.53      | 111.83   |
| 31  | 3     | 305 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 31  | 3     | 305 | CLA  | O2D-CGD-O1D | -2.52 | 118.35      | 124.08   |
| 31  | 0     | 313 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 31  | d     | 401 | CLA  | C1-C2-C3    | -2.52 | 122.06      | 126.20   |
| 31  | B     | 502 | CLA  | CMB-C2B-C1B | -2.52 | 121.58      | 125.42   |
| 42  | 8     | 302 | A86  | C26-C25-C24 | -2.52 | 115.89      | 123.20   |
| 33  | k     | 101 | BCR  | C24-C23-C22 | -2.52 | 122.50      | 126.23   |
| 31  | B     | 507 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 42  | 4     | 203 | A86  | C28-C27-C26 | -2.52 | 118.73      | 122.82   |
| 42  | 3     | 302 | A86  | C26-C25-C24 | -2.52 | 115.90      | 123.20   |
| 31  | C     | 510 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 31  | C     | 504 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 31  | 2     | 308 | CLA  | CAB-C3B-C2B | 2.52  | 130.22      | 123.53   |
| 33  | K     | 101 | BCR  | C24-C23-C22 | -2.52 | 122.51      | 126.23   |
| 31  | p     | 604 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 31  | 6     | 210 | CLA  | O2D-CGD-CBD | 2.52  | 115.63      | 111.23   |
| 41  | V     | 201 | HEM  | C4D-ND-C1D  | 2.52  | 108.19      | 105.21   |
| 31  | 9     | 211 | CLA  | CMB-C2B-C3B | 2.51  | 130.22      | 123.53   |
| 31  | 6     | 213 | CLA  | CAA-C2A-C3A | -2.51 | 110.46      | 116.23   |
| 42  | 3     | 302 | A86  | C3-C4-C5    | -2.51 | 118.38      | 123.52   |
| 44  | p     | 611 | DD6  | C25-C24-C1  | -2.51 | 119.47      | 126.36   |
| 44  | 6     | 203 | DD6  | O1-C20-C21  | -2.51 | 112.24      | 115.05   |
| 31  | a     | 403 | CLA  | CHB-C4A-NA  | 2.51  | 128.03      | 124.40   |
| 31  | 9     | 212 | CLA  | CAB-C3B-C2B | 2.51  | 130.20      | 123.53   |
| 44  | 7     | 303 | DD6  | C-C1-C2     | -2.51 | 118.75      | 122.82   |
| 44  | 2     | 303 | DD6  | C-C1-C2     | -2.51 | 118.75      | 122.82   |
| 31  | 3     | 314 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 31  | 0     | 307 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 36  | D     | 407 | LHG  | C11-C10-C9  | -2.51 | 101.69      | 114.37   |
| 31  | 5     | 307 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 31  | 8     | 313 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 33  | C     | 516 | BCR  | C11-C10-C9  | -2.51 | 123.76      | 127.28   |
| 44  | 3     | 303 | DD6  | C3-C2-C1    | -2.51 | 123.76      | 127.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 41  | v     | 201 | HEM  | C4D-ND-C1D  | 2.51  | 108.17      | 105.21   |
| 31  | A     | 403 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 31  | 6     | 211 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 33  | C     | 515 | BCR  | C15-C14-C13 | -2.50 | 123.77      | 127.28   |
| 31  | 4     | 212 | CLA  | CAB-C3B-C2B | 2.50  | 130.18      | 123.53   |
| 44  | 7     | 304 | DD6  | C37-C36-C31 | -2.50 | 119.48      | 124.16   |
| 34  | a     | 409 | SQD  | O8-S-C6     | 2.50  | 110.80      | 105.97   |
| 33  | c     | 516 | BCR  | C11-C10-C9  | -2.50 | 123.77      | 127.28   |
| 31  | B     | 516 | CLA  | C1-C2-C3    | -2.50 | 122.10      | 126.20   |
| 36  | d     | 407 | LHG  | C11-C10-C9  | -2.50 | 101.72      | 114.37   |
| 31  | 1     | 210 | CLA  | O2D-CGD-CBD | 2.50  | 115.60      | 111.23   |
| 31  | b     | 508 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 31  | 4     | 211 | CLA  | CMB-C2B-C3B | 2.50  | 130.17      | 123.53   |
| 31  | d     | 401 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 44  | 7     | 303 | DD6  | C28-C27-C26 | -2.50 | 119.33      | 124.18   |
| 31  | B     | 506 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 39  | c     | 518 | DGD  | O5D-C6D-C5D | -2.49 | 103.80      | 109.42   |
| 31  | D     | 401 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 35  | a     | 410 | PL9  | C7-C8-C9    | -2.49 | 122.54      | 126.83   |
| 42  | 9     | 201 | A86  | C12-C11-C13 | 2.49  | 120.04      | 116.00   |
| 31  | b     | 517 | CLA  | C1-C2-C3    | -2.49 | 122.11      | 126.20   |
| 35  | A     | 410 | PL9  | C7-C8-C9    | -2.49 | 122.54      | 126.83   |
| 31  | 1     | 201 | CLA  | O2D-CGD-CBD | 2.49  | 115.58      | 111.23   |
| 39  | C     | 518 | DGD  | O5D-C6D-C5D | -2.49 | 103.81      | 109.42   |
| 44  | 2     | 303 | DD6  | C28-C27-C26 | -2.49 | 119.35      | 124.18   |
| 31  | c     | 504 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 31  | 9     | 212 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 36  | d     | 407 | LHG  | O8-C23-C24  | 2.49  | 119.42      | 111.83   |
| 31  | C     | 504 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 44  | 1     | 203 | DD6  | C-C1-C2     | -2.49 | 118.78      | 122.82   |
| 37  | d     | 408 | LMG  | O6-C1-O1    | -2.49 | 104.17      | 110.04   |
| 31  | P     | 604 | CLA  | CMB-C2B-C3B | 2.49  | 132.40      | 126.55   |
| 31  | 9     | 204 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 31  | p     | 604 | CLA  | CMB-C2B-C3B | 2.49  | 132.40      | 126.55   |
| 31  | 1     | 216 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 34  | A     | 409 | SQD  | O8-S-C6     | 2.49  | 110.77      | 105.97   |
| 31  | b     | 511 | CLA  | CHB-C4A-NA  | 2.48  | 127.99      | 124.40   |
| 31  | 6     | 212 | CLA  | CHB-C4A-NA  | 2.48  | 127.99      | 124.40   |
| 35  | d     | 406 | PL9  | C20-C19-C21 | 2.48  | 119.54      | 115.23   |
| 31  | c     | 510 | CLA  | C1-C2-C3    | -2.48 | 122.13      | 126.20   |
| 31  | b     | 506 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | b     | 510 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 314 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | 2     | 305 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 39  | H     | 102 | DGD  | C1D-C2D-C3D | -2.48 | 104.79      | 110.01   |
| 37  | D     | 408 | LMG  | O6-C1-O1    | -2.48 | 104.18      | 110.04   |
| 31  | c     | 510 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | B     | 505 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | c     | 509 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 31  | C     | 510 | CLA  | C1-C2-C3    | -2.48 | 122.13      | 126.20   |
| 44  | 1     | 203 | DD6  | C28-C27-C26 | -2.48 | 119.37      | 124.18   |
| 31  | 9     | 208 | CLA  | CHA-C1A-NA  | -2.48 | 120.78      | 126.39   |
| 31  | 1     | 215 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 37  | m     | 101 | LMG  | O1-C7-C8    | -2.48 | 104.79      | 110.82   |
| 44  | 6     | 203 | DD6  | C-C1-C2     | -2.48 | 118.80      | 122.82   |
| 31  | c     | 503 | CLA  | C1-C2-C3    | -2.48 | 122.14      | 126.20   |
| 31  | 7     | 309 | CLA  | CMB-C2B-C1B | -2.48 | 121.65      | 125.42   |
| 31  | 2     | 309 | CLA  | CMB-C2B-C1B | -2.48 | 121.65      | 125.42   |
| 33  | c     | 517 | BCR  | C15-C16-C17 | -2.48 | 118.45      | 123.52   |
| 31  | 3     | 312 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 34  | B     | 523 | SQD  | C44-O6-C1   | 2.47  | 119.10      | 113.80   |
| 36  | D     | 407 | LHG  | O8-C23-C24  | 2.47  | 119.38      | 111.83   |
| 31  | C     | 503 | CLA  | C1-C2-C3    | -2.47 | 122.14      | 126.20   |
| 42  | 3     | 302 | A86  | C10-C9-C8   | -2.47 | 116.03      | 123.20   |
| 31  | 6     | 216 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 31  | C     | 509 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 39  | h     | 102 | DGD  | C1D-C2D-C3D | -2.47 | 104.81      | 110.01   |
| 31  | 6     | 201 | CLA  | CMB-C2B-C3B | 2.47  | 130.10      | 123.53   |
| 31  | 6     | 215 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 42  | 8     | 302 | A86  | C10-C9-C8   | -2.47 | 116.04      | 123.20   |
| 31  | 6     | 201 | CLA  | O2D-CGD-CBD | 2.47  | 115.55      | 111.23   |
| 44  | 6     | 203 | DD6  | C28-C27-C26 | -2.47 | 119.38      | 124.18   |
| 34  | 0     | 316 | SQD  | O48-C23-C24 | 2.47  | 119.37      | 111.83   |
| 31  | 4     | 204 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | B     | 509 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 33  | c     | 517 | BCR  | C24-C23-C22 | -2.47 | 122.58      | 126.23   |
| 31  | 7     | 312 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | b     | 514 | CLA  | CMB-C2B-C1B | -2.47 | 121.66      | 125.42   |
| 31  | 1     | 208 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 31  | 3     | 311 | CLA  | O2D-CGD-O1D | -2.47 | 118.48      | 124.08   |
| 31  | 8     | 311 | CLA  | O2D-CGD-O1D | -2.47 | 118.48      | 124.08   |
| 33  | C     | 517 | BCR  | C15-C16-C17 | -2.46 | 118.48      | 123.52   |
| 31  | 7     | 305 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 44  | 1     | 203 | DD6  | C37-C36-C31 | -2.46 | 119.55      | 124.16   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 306 | CLA  | CMB-C2B-C3B | 2.46  | 130.08      | 123.53   |
| 35  | D     | 406 | PL9  | C20-C19-C21 | 2.46  | 119.50      | 115.23   |
| 42  | 0     | 301 | A86  | C36-C31-C32 | -2.46 | 117.25      | 119.70   |
| 33  | a     | 408 | BCR  | C33-C5-C6   | -2.46 | 121.80      | 124.48   |
| 31  | p     | 602 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 8     | 311 | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 37  | M     | 101 | LMG  | O1-C7-C8    | -2.46 | 104.84      | 110.82   |
| 31  | P     | 609 | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 34  | 5     | 316 | SQD  | O48-C23-C24 | 2.46  | 119.33      | 111.83   |
| 31  | B     | 510 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 5     | 312 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 4     | 208 | CLA  | CHA-C1A-NA  | -2.46 | 120.82      | 126.39   |
| 31  | 6     | 208 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | 1     | 207 | CLA  | CMB-C2B-C3B | 2.46  | 130.06      | 123.53   |
| 31  | a     | 404 | CLA  | O2D-CGD-CBD | 2.46  | 115.53      | 111.23   |
| 42  | 9     | 201 | A86  | C35-C34-C33 | -2.46 | 105.47      | 109.89   |
| 31  | P     | 607 | CLA  | CMB-C2B-C3B | 2.46  | 130.06      | 123.53   |
| 31  | 1     | 201 | CLA  | CMB-C2B-C3B | 2.46  | 130.06      | 123.53   |
| 35  | d     | 406 | PL9  | C12-C13-C14 | -2.46 | 122.00      | 127.62   |
| 34  | b     | 501 | SQD  | C44-O6-C1   | 2.46  | 119.06      | 113.80   |
| 31  | 2     | 313 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 37  | M     | 101 | LMG  | C40-C39-C38 | -2.45 | 101.96      | 114.37   |
| 31  | 4     | 212 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 37  | m     | 101 | LMG  | C40-C39-C38 | -2.45 | 101.96      | 114.37   |
| 31  | B     | 511 | CLA  | CMB-C2B-C1B | -2.45 | 121.68      | 125.42   |
| 31  | b     | 512 | CLA  | CMB-C2B-C1B | -2.45 | 121.68      | 125.42   |
| 35  | D     | 406 | PL9  | C12-C13-C14 | -2.45 | 122.01      | 127.62   |
| 31  | C     | 513 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 31  | c     | 513 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 33  | C     | 517 | BCR  | C24-C23-C22 | -2.45 | 122.61      | 126.23   |
| 31  | B     | 513 | CLA  | CMB-C2B-C1B | -2.45 | 121.69      | 125.42   |
| 33  | A     | 408 | BCR  | C33-C5-C6   | -2.45 | 121.81      | 124.48   |
| 33  | b     | 518 | BCR  | C15-C14-C13 | -2.45 | 123.84      | 127.28   |
| 42  | 4     | 201 | A86  | C12-C11-C13 | 2.45  | 119.97      | 116.00   |
| 44  | 7     | 303 | DD6  | C37-C36-C31 | -2.45 | 119.58      | 124.16   |
| 31  | 3     | 309 | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 42  | 4     | 201 | A86  | C35-C34-C33 | -2.45 | 105.49      | 109.89   |
| 35  | D     | 406 | PL9  | C37-C38-C39 | -2.45 | 122.02      | 127.62   |
| 31  | 0     | 312 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 31  | 1     | 212 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 33  | B     | 517 | BCR  | C15-C14-C13 | -2.45 | 123.85      | 127.28   |
| 31  | b     | 514 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 403 | CLA  | CMB-C2B-C1B | -2.45 | 121.69      | 125.42   |
| 31  | p     | 607 | CLA  | CMB-C2B-C3B | 2.45  | 130.03      | 123.53   |
| 31  | 8     | 312 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 31  | 6     | 207 | CLA  | CMB-C2B-C3B | 2.44  | 130.03      | 123.53   |
| 44  | 2     | 303 | DD6  | C37-C36-C31 | -2.44 | 119.59      | 124.16   |
| 31  | 0     | 314 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 31  | 8     | 306 | CLA  | CMB-C2B-C3B | 2.44  | 130.02      | 123.53   |
| 31  | P     | 602 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 42  | P     | 610 | A86  | O-C13-C11   | -2.44 | 115.78      | 121.04   |
| 33  | K     | 101 | BCR  | C15-C14-C13 | -2.44 | 123.86      | 127.28   |
| 31  | a     | 403 | CLA  | CMB-C2B-C1B | -2.44 | 121.70      | 125.42   |
| 31  | C     | 511 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 44  | 6     | 203 | DD6  | C37-C36-C31 | -2.44 | 119.60      | 124.16   |
| 31  | 5     | 308 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 33  | k     | 101 | BCR  | C15-C14-C13 | -2.44 | 123.86      | 127.28   |
| 34  | B     | 523 | SQD  | C4-C3-C2    | 2.44  | 115.11      | 110.83   |
| 31  | A     | 404 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | c     | 503 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | b     | 504 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | 7     | 310 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 31  | 2     | 310 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 39  | h     | 102 | DGD  | C3G-C2G-C1G | -2.44 | 106.11      | 111.78   |
| 33  | b     | 520 | BCR  | C24-C23-C22 | -2.44 | 122.63      | 126.23   |
| 31  | 5     | 305 | CLA  | C3B-C4B-NB  | -2.44 | 108.36      | 110.53   |
| 31  | p     | 608 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 31  | 1     | 207 | CLA  | C3B-C4B-NB  | -2.43 | 107.80      | 110.33   |
| 31  | c     | 507 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 31  | 0     | 310 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 31  | 1     | 201 | CLA  | CAB-C3B-C2B | 2.43  | 130.00      | 123.53   |
| 31  | P     | 604 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 31  | 6     | 209 | CLA  | CAB-C3B-C2B | 2.43  | 129.99      | 123.53   |
| 35  | d     | 406 | PL9  | C37-C38-C39 | -2.43 | 122.06      | 127.62   |
| 31  | 7     | 313 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 33  | B     | 519 | BCR  | C24-C23-C22 | -2.43 | 122.64      | 126.23   |
| 35  | a     | 410 | PL9  | O2-C1-C6    | 2.43  | 124.34      | 120.48   |
| 31  | 0     | 308 | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 31  | w     | 202 | CLA  | CMD-C2D-C3D | 2.43  | 133.25      | 127.69   |
| 31  | C     | 514 | CLA  | CMB-C2B-C1B | -2.43 | 121.72      | 125.42   |
| 31  | 7     | 315 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 31  | 2     | 315 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 31  | A     | 404 | CLA  | O2D-CGD-CBD | 2.43  | 115.47      | 111.23   |
| 31  | p     | 604 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 201 | CLA  | CAB-C3B-C2B | 2.42  | 129.98      | 123.53   |
| 31  | 4     | 208 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 39  | H     | 102 | DGD  | C3G-C2G-C1G | -2.42 | 106.13      | 111.78   |
| 31  | c     | 514 | CLA  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 31  | 5     | 314 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 44  | 6     | 204 | DD6  | C37-C36-C35 | 2.42  | 118.87      | 114.42   |
| 34  | b     | 501 | SQD  | C4-C3-C2    | 2.42  | 115.08      | 110.83   |
| 31  | 8     | 309 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 33  | C     | 516 | BCR  | C15-C14-C13 | -2.42 | 123.88      | 127.28   |
| 31  | B     | 513 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 31  | p     | 604 | CLA  | O2D-CGD-O1D | -2.42 | 118.59      | 124.08   |
| 31  | P     | 604 | CLA  | O2D-CGD-O1D | -2.42 | 118.59      | 124.08   |
| 31  | 1     | 201 | CLA  | C3B-C4B-NB  | -2.42 | 107.82      | 110.33   |
| 31  | 1     | 209 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 31  | 5     | 307 | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 31  | 0     | 307 | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 31  | c     | 511 | CLA  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 41  | v     | 201 | HEM  | CAA-C2A-C1A | 2.42  | 129.66      | 124.94   |
| 31  | a     | 404 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 31  | 1     | 209 | CLA  | CAB-C3B-C2B | 2.42  | 129.95      | 123.53   |
| 31  | p     | 609 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 37  | J     | 101 | LMG  | O3-C3-C2    | -2.42 | 104.68      | 110.38   |
| 42  | 7     | 301 | A86  | O4-C34-C35  | 2.41  | 113.82      | 107.64   |
| 42  | 2     | 301 | A86  | O4-C34-C35  | 2.41  | 113.82      | 107.64   |
| 31  | 8     | 314 | CLA  | C3B-C4B-NB  | -2.41 | 107.82      | 110.33   |
| 31  | p     | 607 | CLA  | CAB-C3B-C2B | 2.41  | 129.95      | 123.53   |
| 33  | c     | 516 | BCR  | C27-C26-C25 | 2.41  | 125.97      | 122.70   |
| 42  | 6     | 202 | A86  | C26-C25-C24 | -2.41 | 116.21      | 123.20   |
| 42  | p     | 610 | A86  | O-C13-C11   | -2.41 | 115.84      | 121.04   |
| 36  | d     | 407 | LHG  | C20-C19-C18 | -2.41 | 102.17      | 114.37   |
| 31  | 7     | 314 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | 0     | 304 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 36  | D     | 407 | LHG  | C20-C19-C18 | -2.41 | 102.18      | 114.37   |
| 31  | B     | 509 | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 44  | 7     | 304 | DD6  | C26-C25-C24 | -2.41 | 116.21      | 123.20   |
| 44  | 2     | 304 | DD6  | C26-C25-C24 | -2.41 | 116.21      | 123.20   |
| 31  | P     | 607 | CLA  | CAB-C3B-C2B | 2.41  | 129.94      | 123.53   |
| 31  | 6     | 207 | CLA  | C3B-C4B-NB  | -2.41 | 107.83      | 110.33   |
| 31  | 6     | 214 | CLA  | CMA-C3A-C2A | -2.41 | 110.70      | 116.23   |
| 31  | C     | 503 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | 5     | 310 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 31  | 1     | 205 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 208 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 37  | j     | 101 | LMG  | O3-C3-C2    | -2.41 | 104.70      | 110.38   |
| 42  | 0     | 303 | A86  | C-C1-C2     | -2.41 | 118.92      | 122.82   |
| 35  | A     | 410 | PL9  | O2-C1-C6    | 2.41  | 124.31      | 120.48   |
| 31  | 3     | 314 | CLA  | C3B-C4B-NB  | -2.41 | 107.83      | 110.33   |
| 31  | 1     | 214 | CLA  | CMA-C3A-C2A | -2.41 | 110.71      | 116.23   |
| 37  | W     | 201 | LMG  | C38-C37-C36 | -2.41 | 102.21      | 114.37   |
| 37  | w     | 201 | LMG  | C38-C37-C36 | -2.41 | 102.21      | 114.37   |
| 42  | 5     | 303 | A86  | C-C1-C2     | -2.40 | 118.92      | 122.82   |
| 41  | V     | 201 | HEM  | CAA-C2A-C1A | 2.40  | 129.63      | 124.94   |
| 32  | a     | 405 | PHO  | C2D-C1D-ND  | -2.40 | 107.69      | 109.43   |
| 42  | 5     | 301 | A86  | C36-C31-C32 | -2.40 | 117.31      | 119.70   |
| 31  | 6     | 207 | CLA  | CAB-C3B-C2B | 2.40  | 129.92      | 123.53   |
| 31  | z     | 101 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 31  | W     | 202 | CLA  | CMD-C2D-C3D | 2.40  | 133.19      | 127.69   |
| 44  | 7     | 304 | DD6  | C-C1-C24    | 2.40  | 121.75      | 118.09   |
| 31  | 2     | 312 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 33  | c     | 516 | BCR  | C15-C14-C13 | -2.40 | 123.91      | 127.28   |
| 35  | D     | 406 | PL9  | O2-C1-C6    | 2.40  | 124.30      | 120.48   |
| 31  | 5     | 306 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 31  | 0     | 306 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 31  | C     | 507 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 37  | M     | 101 | LMG  | C38-C37-C36 | -2.40 | 102.25      | 114.37   |
| 31  | c     | 509 | CLA  | O2D-CGD-CBD | 2.40  | 115.42      | 111.23   |
| 42  | 4     | 201 | A86  | C41-C32-C33 | 2.40  | 120.41      | 109.06   |
| 31  | 9     | 213 | CLA  | CMB-C2B-C3B | 2.40  | 129.90      | 123.53   |
| 35  | d     | 406 | PL9  | O2-C1-C6    | 2.40  | 124.29      | 120.48   |
| 37  | m     | 101 | LMG  | C38-C37-C36 | -2.40 | 102.26      | 114.37   |
| 31  | 6     | 205 | CLA  | CHB-C4A-NA  | 2.39  | 127.86      | 124.40   |
| 31  | 0     | 305 | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 31  | P     | 608 | CLA  | CMB-C2B-C3B | 2.39  | 129.89      | 123.53   |
| 37  | D     | 408 | LMG  | O3-C3-C2    | -2.39 | 104.73      | 110.38   |
| 31  | B     | 503 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 31  | 1     | 211 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |
| 42  | 9     | 201 | A86  | C41-C32-C33 | 2.39  | 120.39      | 109.06   |
| 33  | C     | 516 | BCR  | C27-C26-C25 | 2.39  | 125.94      | 122.70   |
| 44  | 1     | 204 | DD6  | C37-C36-C35 | 2.39  | 118.82      | 114.42   |
| 36  | d     | 411 | LHG  | C11-C10-C9  | -2.39 | 102.28      | 114.37   |
| 31  | P     | 608 | CLA  | O2D-CGD-O1D | -2.39 | 118.66      | 124.08   |
| 31  | b     | 510 | CLA  | C3B-C4B-NB  | -2.39 | 108.40      | 110.53   |
| 31  | C     | 509 | CLA  | O2D-CGD-CBD | 2.39  | 115.41      | 111.23   |
| 31  | 6     | 211 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | D     | 409 | LMG  | O1-C7-C8    | -2.39 | 105.01      | 110.82   |
| 31  | 7     | 307 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 31  | 2     | 314 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 36  | D     | 411 | LHG  | C11-C10-C9  | -2.39 | 102.30      | 114.37   |
| 31  | 8     | 307 | CLA  | CMB-C2B-C3B | 2.39  | 132.16      | 126.55   |
| 31  | 7     | 308 | CLA  | CMB-C2B-C3B | 2.39  | 129.87      | 123.53   |
| 41  | v     | 201 | HEM  | C3D-C4D-ND  | -2.38 | 107.56      | 110.17   |
| 31  | 2     | 306 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 31  | p     | 607 | CLA  | C3B-C4B-NB  | -2.38 | 107.85      | 110.33   |
| 33  | B     | 518 | BCR  | C33-C5-C6   | -2.38 | 121.88      | 124.48   |
| 31  | 2     | 308 | CLA  | CMB-C2B-C3B | 2.38  | 129.87      | 123.53   |
| 36  | A     | 412 | LHG  | C11-C10-C9  | -2.38 | 102.32      | 114.37   |
| 36  | a     | 411 | LHG  | C11-C10-C9  | -2.38 | 102.32      | 114.37   |
| 31  | 2     | 307 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 41  | V     | 201 | HEM  | C3D-C4D-ND  | -2.38 | 107.56      | 110.17   |
| 31  | 3     | 307 | CLA  | CMB-C2B-C3B | 2.38  | 132.15      | 126.55   |
| 31  | Z     | 101 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 37  | d     | 408 | LMG  | O3-C3-C2    | -2.38 | 104.76      | 110.38   |
| 31  | d     | 403 | CLA  | CAB-C3B-C2B | 2.38  | 129.86      | 123.53   |
| 33  | c     | 517 | BCR  | C15-C14-C13 | -2.38 | 123.94      | 127.28   |
| 31  | 6     | 201 | CLA  | C3B-C4B-NB  | -2.38 | 107.86      | 110.33   |
| 31  | B     | 511 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 42  | 1     | 202 | A86  | C26-C25-C24 | -2.38 | 116.31      | 123.20   |
| 40  | D     | 402 | BCT  | O3-C-O1     | -2.38 | 113.59      | 119.68   |
| 31  | P     | 607 | CLA  | C3B-C4B-NB  | -2.38 | 107.86      | 110.33   |
| 44  | 2     | 304 | DD6  | C-C1-C24    | 2.38  | 121.72      | 118.09   |
| 31  | B     | 514 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 42  | 5     | 317 | A86  | C9-C8-C6    | -2.38 | 119.85      | 126.36   |
| 42  | 0     | 317 | A86  | C9-C8-C6    | -2.38 | 119.85      | 126.36   |
| 31  | 1     | 207 | CLA  | CAB-C3B-C2B | 2.37  | 129.84      | 123.53   |
| 31  | a     | 403 | CLA  | O2D-CGD-CBD | 2.37  | 115.38      | 111.23   |
| 31  | D     | 403 | CLA  | CAB-C3B-C2B | 2.37  | 129.84      | 123.53   |
| 32  | A     | 405 | PHO  | C2D-C1D-ND  | -2.37 | 107.72      | 109.43   |
| 44  | 7     | 303 | DD6  | C7-C6-C5    | -2.37 | 118.97      | 122.82   |
| 31  | 5     | 304 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | P     | 608 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 31  | p     | 602 | CLA  | CMB-C2B-C1B | -2.37 | 121.81      | 125.42   |
| 31  | A     | 403 | CLA  | O2D-CGD-CBD | 2.37  | 115.37      | 111.23   |
| 31  | P     | 602 | CLA  | CMB-C2B-C1B | -2.37 | 121.81      | 125.42   |
| 33  | C     | 517 | BCR  | C15-C14-C13 | -2.37 | 123.96      | 127.28   |
| 31  | 7     | 306 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 37  | d     | 409 | LMG  | O1-C7-C8    | -2.37 | 105.06      | 110.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 209 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 31  | 1     | 209 | CLA  | CMB-C2B-C3B | 2.36  | 129.82      | 123.53   |
| 31  | b     | 515 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 31  | p     | 608 | CLA  | O2D-CGD-O1D | -2.36 | 118.72      | 124.08   |
| 33  | b     | 519 | BCR  | C33-C5-C6   | -2.36 | 121.91      | 124.48   |
| 44  | 2     | 303 | DD6  | C7-C6-C5    | -2.36 | 118.99      | 122.82   |
| 31  | 0     | 308 | CLA  | O2A-CGA-O1A | -2.36 | 117.72      | 123.63   |
| 40  | d     | 402 | BCT  | O3-C-O1     | -2.36 | 113.63      | 119.68   |
| 31  | 4     | 213 | CLA  | CMB-C2B-C3B | 2.36  | 129.81      | 123.53   |
| 31  | 6     | 209 | CLA  | CMB-C2B-C3B | 2.36  | 129.81      | 123.53   |
| 37  | w     | 201 | LMG  | C40-C39-C38 | -2.36 | 102.44      | 114.37   |
| 31  | 8     | 314 | CLA  | CAB-C3B-C2B | 2.36  | 129.80      | 123.53   |
| 31  | p     | 608 | CLA  | CMB-C2B-C3B | 2.36  | 129.80      | 123.53   |
| 31  | b     | 503 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 37  | Y     | 101 | LMG  | C38-C37-C36 | -2.35 | 102.46      | 114.37   |
| 31  | b     | 512 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 37  | W     | 201 | LMG  | C40-C39-C38 | -2.35 | 102.47      | 114.37   |
| 33  | C     | 515 | BCR  | C11-C10-C9  | -2.35 | 123.98      | 127.28   |
| 37  | y     | 101 | LMG  | C38-C37-C36 | -2.35 | 102.49      | 114.37   |
| 36  | A     | 412 | LHG  | C27-C26-C25 | -2.35 | 102.50      | 114.37   |
| 36  | a     | 411 | LHG  | C27-C26-C25 | -2.35 | 102.50      | 114.37   |
| 31  | 6     | 201 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 31  | 2     | 316 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 31  | B     | 504 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 31  | 3     | 314 | CLA  | CAB-C3B-C2B | 2.34  | 129.76      | 123.53   |
| 31  | 6     | 213 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 31  | c     | 506 | CLA  | CMB-C2B-C1B | -2.34 | 121.85      | 125.42   |
| 37  | b     | 521 | LMG  | O3-C3-C2    | -2.34 | 104.86      | 110.38   |
| 44  | 6     | 203 | DD6  | C7-C6-C5    | -2.34 | 119.02      | 122.82   |
| 31  | 5     | 308 | CLA  | O2A-CGA-O1A | -2.34 | 117.78      | 123.63   |
| 31  | 8     | 304 | CLA  | C3B-C4B-NB  | -2.34 | 107.90      | 110.33   |
| 42  | 2     | 301 | A86  | C26-C25-C24 | -2.34 | 116.42      | 123.20   |
| 31  | b     | 505 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 31  | C     | 506 | CLA  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |
| 31  | B     | 502 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 31  | 7     | 316 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 37  | 5     | 315 | LMG  | C38-C37-C36 | -2.33 | 102.56      | 114.37   |
| 37  | 0     | 315 | LMG  | C38-C37-C36 | -2.33 | 102.56      | 114.37   |
| 42  | 7     | 301 | A86  | C26-C25-C24 | -2.33 | 116.44      | 123.20   |
| 37  | B     | 520 | LMG  | O3-C3-C2    | -2.33 | 104.87      | 110.38   |
| 37  | M     | 102 | LMG  | O2-C2-C1    | -2.33 | 104.52      | 110.08   |
| 31  | 6     | 209 | CLA  | C3B-C4B-NB  | -2.33 | 107.91      | 110.33   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 1     | 209 | CLA  | C3B-C4B-NB  | -2.33 | 107.91      | 110.33   |
| 33  | b     | 519 | BCR  | C11-C10-C9  | -2.33 | 124.01      | 127.28   |
| 31  | B     | 504 | CLA  | O2D-CGD-CBD | 2.33  | 115.31      | 111.23   |
| 44  | 1     | 203 | DD6  | C7-C6-C5    | -2.33 | 119.04      | 122.82   |
| 35  | A     | 410 | PL9  | C21-C22-C23 | -2.33 | 107.51      | 112.57   |
| 31  | 1     | 201 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 37  | m     | 102 | LMG  | O2-C2-C1    | -2.33 | 104.52      | 110.08   |
| 31  | C     | 507 | CLA  | CMB-C2B-C1B | -2.33 | 121.88      | 125.42   |
| 33  | B     | 518 | BCR  | C11-C10-C9  | -2.33 | 124.02      | 127.28   |
| 33  | c     | 515 | BCR  | C11-C10-C9  | -2.33 | 124.02      | 127.28   |
| 31  | c     | 507 | CLA  | CMB-C2B-C1B | -2.33 | 121.88      | 125.42   |
| 42  | 9     | 203 | A86  | O-C13-C11   | -2.33 | 116.03      | 121.04   |
| 31  | C     | 510 | CLA  | O2A-CGA-O1A | -2.33 | 117.81      | 123.63   |
| 39  | C     | 518 | DGD  | C3G-C2G-C1G | -2.33 | 106.36      | 111.78   |
| 35  | a     | 410 | PL9  | C21-C22-C23 | -2.32 | 107.52      | 112.57   |
| 39  | c     | 518 | DGD  | C3G-C2G-C1G | -2.32 | 106.36      | 111.78   |
| 31  | C     | 506 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 31  | c     | 510 | CLA  | O2A-CGA-O1A | -2.32 | 117.81      | 123.63   |
| 31  | 3     | 304 | CLA  | C3B-C4B-NB  | -2.32 | 107.92      | 110.33   |
| 36  | d     | 407 | LHG  | C27-C26-C25 | -2.32 | 102.63      | 114.37   |
| 36  | d     | 407 | LHG  | C18-C17-C16 | -2.32 | 102.64      | 114.37   |
| 36  | D     | 407 | LHG  | C27-C26-C25 | -2.32 | 102.64      | 114.37   |
| 36  | D     | 407 | LHG  | C18-C17-C16 | -2.32 | 102.65      | 114.37   |
| 31  | b     | 505 | CLA  | O2D-CGD-CBD | 2.32  | 115.28      | 111.23   |
| 31  | 7     | 311 | CLA  | CMB-C2B-C1B | -2.32 | 121.89      | 125.42   |
| 31  | 2     | 308 | CLA  | CHB-C4A-NA  | 2.32  | 127.74      | 124.40   |
| 31  | 1     | 213 | CLA  | CHB-C4A-NA  | 2.32  | 127.74      | 124.40   |
| 42  | 7     | 301 | A86  | C9-C8-C6    | -2.32 | 120.01      | 126.36   |
| 42  | 4     | 203 | A86  | O-C13-C11   | -2.32 | 116.05      | 121.04   |
| 39  | c     | 520 | DGD  | O1G-C1A-C2A | 2.32  | 118.89      | 111.83   |
| 31  | 2     | 309 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 31  | 8     | 304 | CLA  | CAB-C3B-C2B | 2.31  | 129.68      | 123.53   |
| 39  | C     | 520 | DGD  | O1G-C1A-C2A | 2.31  | 118.89      | 111.83   |
| 31  | 7     | 308 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 31  | b     | 513 | CLA  | CMA-C3A-C2A | -2.31 | 110.93      | 116.23   |
| 31  | B     | 512 | CLA  | CMA-C3A-C2A | -2.31 | 110.93      | 116.23   |
| 35  | d     | 406 | PL9  | O1-C4-C3    | -2.31 | 118.30      | 120.73   |
| 31  | 5     | 308 | CLA  | CHB-C4A-NA  | 2.30  | 127.73      | 124.40   |
| 42  | 5     | 303 | A86  | O1-C15-C20  | -2.30 | 57.50       | 59.45    |
| 31  | A     | 403 | CLA  | O2D-CGD-O1D | -2.30 | 119.36      | 123.85   |
| 31  | 3     | 304 | CLA  | CAB-C3B-C2B | 2.30  | 129.66      | 123.53   |
| 33  | D     | 405 | BCR  | C15-C16-C17 | -2.30 | 118.81      | 123.52   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | 0     | 315 | LMG  | C40-C39-C38 | -2.30 | 102.73      | 114.37   |
| 33  | d     | 405 | BCR  | C15-C16-C17 | -2.30 | 118.81      | 123.52   |
| 37  | M     | 101 | LMG  | O2-C2-C1    | -2.30 | 104.59      | 110.08   |
| 36  | B     | 521 | LHG  | C18-C17-C16 | -2.30 | 102.74      | 114.37   |
| 36  | b     | 522 | LHG  | C18-C17-C16 | -2.30 | 102.74      | 114.37   |
| 31  | c     | 506 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 37  | 5     | 315 | LMG  | C40-C39-C38 | -2.30 | 102.75      | 114.37   |
| 42  | 2     | 301 | A86  | C9-C8-C6    | -2.30 | 120.06      | 126.36   |
| 37  | m     | 101 | LMG  | O2-C2-C1    | -2.30 | 104.60      | 110.08   |
| 42  | 6     | 202 | A86  | C25-C24-C1  | -2.30 | 120.07      | 126.36   |
| 44  | 1     | 203 | DD6  | C9-C8-C6    | -2.30 | 120.07      | 126.36   |
| 44  | 6     | 203 | DD6  | C9-C8-C6    | -2.29 | 120.07      | 126.36   |
| 34  | A     | 411 | SQD  | O48-C23-C24 | 2.29  | 118.82      | 111.83   |
| 42  | 8     | 302 | A86  | C36-C31-C32 | -2.29 | 117.42      | 119.70   |
| 31  | d     | 403 | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 31  | a     | 403 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 34  | B     | 522 | SQD  | O48-C23-C24 | 2.29  | 118.81      | 111.83   |
| 37  | W     | 201 | LMG  | O7-C10-O9   | -2.29 | 118.36      | 123.70   |
| 42  | 4     | 202 | A86  | C23-C16-C17 | -2.29 | 104.95      | 108.97   |
| 31  | 2     | 312 | CLA  | C1C-NC-C4C  | 2.28  | 107.72      | 106.68   |
| 42  | 9     | 202 | A86  | C23-C16-C17 | -2.28 | 104.96      | 108.97   |
| 33  | a     | 408 | BCR  | C15-C14-C13 | -2.28 | 124.08      | 127.28   |
| 31  | c     | 511 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 44  | 7     | 303 | DD6  | C9-C8-C6    | -2.28 | 120.11      | 126.36   |
| 31  | 3     | 306 | CLA  | C3B-C4B-NB  | -2.28 | 107.96      | 110.33   |
| 31  | 0     | 308 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 31  | D     | 403 | CLA  | C3B-C4B-NB  | -2.28 | 107.96      | 110.33   |
| 31  | B     | 506 | CLA  | O2A-CGA-O1A | -2.28 | 117.93      | 123.63   |
| 39  | h     | 102 | DGD  | CBB-CAB-C9B | -2.28 | 102.86      | 114.37   |
| 31  | 7     | 311 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 34  | B     | 522 | SQD  | C1-C2-C3    | 2.28  | 114.80      | 110.01   |
| 42  | 0     | 303 | A86  | O1-C15-C20  | -2.28 | 57.52       | 59.45    |
| 31  | D     | 403 | CLA  | CHB-C4A-NA  | 2.28  | 127.68      | 124.40   |
| 44  | p     | 611 | DD6  | C28-C27-C26 | -2.28 | 119.76      | 124.18   |
| 42  | 1     | 202 | A86  | C25-C24-C1  | -2.27 | 120.13      | 126.36   |
| 37  | d     | 410 | LMG  | O3-C3-C2    | -2.27 | 105.02      | 110.38   |
| 37  | M     | 101 | LMG  | O1-C1-C2    | -2.27 | 104.82      | 108.27   |
| 37  | M     | 102 | LMG  | O3-C3-C2    | -2.27 | 105.02      | 110.38   |
| 33  | C     | 515 | BCR  | C7-C8-C9    | -2.27 | 122.88      | 126.23   |
| 31  | 2     | 311 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 34  | A     | 411 | SQD  | C1-C2-C3    | 2.27  | 114.79      | 110.01   |
| 33  | A     | 408 | BCR  | C15-C14-C13 | -2.27 | 124.09      | 127.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | D     | 410 | LMG  | O3-C3-C2    | -2.27 | 105.03      | 110.38   |
| 33  | C     | 516 | BCR  | C33-C5-C6   | -2.27 | 122.01      | 124.48   |
| 33  | c     | 516 | BCR  | C33-C5-C6   | -2.27 | 122.01      | 124.48   |
| 37  | m     | 102 | LMG  | O1-C7-C8    | -2.27 | 105.30      | 110.82   |
| 39  | H     | 102 | DGD  | CBB-CAB-C9B | -2.27 | 102.90      | 114.37   |
| 34  | 0     | 316 | SQD  | O8-S-C6     | 2.27  | 110.35      | 105.97   |
| 37  | w     | 201 | LMG  | O7-C10-O9   | -2.27 | 118.40      | 123.70   |
| 31  | 8     | 306 | CLA  | C3B-C4B-NB  | -2.27 | 107.97      | 110.33   |
| 39  | C     | 519 | DGD  | O3E-C3E-C2E | -2.27 | 105.03      | 110.38   |
| 31  | 7     | 309 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 31  | 4     | 205 | CLA  | CAB-C3B-C2B | 2.27  | 129.56      | 123.53   |
| 44  | 2     | 303 | DD6  | C9-C8-C6    | -2.27 | 120.15      | 126.36   |
| 44  | P     | 611 | DD6  | C28-C27-C26 | -2.27 | 119.78      | 124.18   |
| 31  | b     | 507 | CLA  | O2A-CGA-O1A | -2.27 | 117.96      | 123.63   |
| 31  | d     | 403 | CLA  | C3B-C4B-NB  | -2.27 | 107.98      | 110.33   |
| 31  | 2     | 311 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 37  | D     | 408 | LMG  | C1-C2-C3    | -2.26 | 105.25      | 110.01   |
| 31  | C     | 511 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 31  | b     | 503 | CLA  | CMB-C2B-C3B | 2.26  | 131.87      | 126.55   |
| 37  | Y     | 101 | LMG  | O2-C2-C1    | -2.26 | 104.68      | 110.08   |
| 33  | B     | 519 | BCR  | C28-C27-C26 | -2.26 | 110.02      | 114.06   |
| 37  | m     | 101 | LMG  | O1-C1-C2    | -2.26 | 104.84      | 108.27   |
| 37  | M     | 102 | LMG  | O1-C7-C8    | -2.26 | 105.32      | 110.82   |
| 31  | 8     | 314 | CLA  | CMA-C3A-C2A | -2.26 | 111.05      | 116.23   |
| 31  | 4     | 213 | CLA  | C3B-C4B-NB  | -2.26 | 107.98      | 110.33   |
| 37  | y     | 101 | LMG  | O2-C2-C1    | -2.26 | 104.69      | 110.08   |
| 31  | 6     | 207 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 37  | b     | 521 | LMG  | O1-C7-C8    | -2.26 | 105.32      | 110.82   |
| 31  | c     | 512 | CLA  | CMB-C2B-C1B | -2.26 | 121.98      | 125.42   |
| 37  | Y     | 101 | LMG  | C40-C39-C38 | -2.26 | 102.96      | 114.37   |
| 31  | 9     | 205 | CLA  | CAB-C3B-C2B | 2.26  | 129.53      | 123.53   |
| 34  | 5     | 316 | SQD  | O8-S-C6     | 2.26  | 110.33      | 105.97   |
| 39  | c     | 519 | DGD  | O3E-C3E-C2E | -2.26 | 105.06      | 110.38   |
| 35  | D     | 406 | PL9  | O1-C4-C3    | -2.25 | 118.35      | 120.73   |
| 42  | 0     | 303 | A86  | C9-C8-C6    | -2.25 | 120.18      | 126.36   |
| 31  | 3     | 314 | CLA  | CMA-C3A-C2A | -2.25 | 111.06      | 116.23   |
| 31  | 9     | 213 | CLA  | C3B-C4B-NB  | -2.25 | 107.99      | 110.33   |
| 42  | 4     | 202 | A86  | O-C13-C11   | -2.25 | 116.19      | 121.04   |
| 31  | W     | 202 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 42  | 5     | 303 | A86  | C9-C8-C6    | -2.25 | 120.18      | 126.36   |
| 37  | D     | 409 | LMG  | O1-C1-C2    | -2.25 | 104.85      | 108.27   |
| 31  | 7     | 305 | CLA  | O2D-CGD-CBD | 2.25  | 115.17      | 111.23   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 2     | 305 | CLA  | O2D-CGD-CBD | 2.25  | 115.17      | 111.23   |
| 37  | B     | 520 | LMG  | O1-C7-C8    | -2.25 | 105.34      | 110.82   |
| 31  | w     | 202 | CLA  | O2D-CGD-CBD | 2.25  | 115.17      | 111.23   |
| 37  | d     | 409 | LMG  | O1-C1-C2    | -2.25 | 104.85      | 108.27   |
| 31  | 7     | 308 | CLA  | C3B-C4B-NB  | -2.25 | 107.99      | 110.33   |
| 31  | B     | 502 | CLA  | CMB-C2B-C3B | 2.25  | 131.84      | 126.55   |
| 33  | b     | 520 | BCR  | C28-C27-C26 | -2.25 | 110.04      | 114.06   |
| 37  | y     | 101 | LMG  | C40-C39-C38 | -2.25 | 103.00      | 114.37   |
| 37  | d     | 408 | LMG  | C1-C2-C3    | -2.25 | 105.28      | 110.01   |
| 42  | 3     | 302 | A86  | C36-C31-C32 | -2.25 | 117.47      | 119.70   |
| 33  | C     | 515 | BCR  | C33-C5-C6   | -2.25 | 122.03      | 124.48   |
| 31  | 1     | 207 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 34  | A     | 411 | SQD  | O8-S-C6     | 2.24  | 110.31      | 105.97   |
| 44  | 7     | 304 | DD6  | C3-C4-C5    | -2.24 | 118.93      | 123.52   |
| 37  | w     | 201 | LMG  | O3-C3-C2    | -2.24 | 105.09      | 110.38   |
| 37  | m     | 102 | LMG  | O3-C3-C2    | -2.24 | 105.09      | 110.38   |
| 31  | 7     | 310 | CLA  | C1-C2-C3    | -2.24 | 122.52      | 126.20   |
| 31  | 2     | 310 | CLA  | C1-C2-C3    | -2.24 | 122.52      | 126.20   |
| 31  | 2     | 314 | CLA  | CMB-C2B-C1B | -2.24 | 122.01      | 125.42   |
| 42  | 3     | 301 | A86  | C4-C3-C2    | -2.24 | 118.93      | 123.52   |
| 33  | h     | 101 | BCR  | C7-C8-C9    | -2.24 | 122.92      | 126.23   |
| 31  | W     | 202 | CLA  | O2D-CGD-CBD | 2.24  | 115.15      | 111.23   |
| 31  | 6     | 208 | CLA  | O2A-CGA-O1A | -2.24 | 118.02      | 123.63   |
| 41  | V     | 201 | HEM  | C2A-C1A-NA  | -2.24 | 107.67      | 110.15   |
| 37  | J     | 101 | LMG  | O1-C1-C2    | -2.24 | 104.87      | 108.27   |
| 31  | 0     | 309 | CLA  | CMA-C3A-C2A | -2.24 | 111.10      | 116.23   |
| 31  | 0     | 310 | CLA  | C1-C2-C3    | -2.24 | 122.53      | 126.20   |
| 44  | 2     | 303 | DD6  | C37-C36-C35 | 2.24  | 118.54      | 114.42   |
| 43  | 5     | 302 | ET4  | C28-C13-C14 | -2.24 | 119.19      | 122.82   |
| 42  | 8     | 301 | A86  | C26-C25-C24 | -2.24 | 116.72      | 123.20   |
| 44  | 2     | 304 | DD6  | C3-C4-C5    | -2.24 | 118.94      | 123.52   |
| 35  | A     | 410 | PL9  | C20-C19-C21 | 2.24  | 119.11      | 115.23   |
| 31  | 5     | 310 | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |
| 33  | c     | 515 | BCR  | C7-C8-C9    | -2.24 | 122.93      | 126.23   |
| 34  | B     | 522 | SQD  | O8-S-C6     | 2.24  | 110.29      | 105.97   |
| 42  | 3     | 301 | A86  | C26-C25-C24 | -2.24 | 116.72      | 123.20   |
| 31  | w     | 202 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 31  | C     | 509 | CLA  | CMB-C2B-C3B | 2.23  | 131.81      | 126.55   |
| 42  | 3     | 301 | A86  | C41-C32-C40 | 2.23  | 115.03      | 108.63   |
| 31  | 2     | 310 | CLA  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 37  | j     | 101 | LMG  | O2-C2-C1    | -2.23 | 104.75      | 110.08   |
| 31  | p     | 606 | CLA  | CHB-C1B-NB  | 2.23  | 127.40      | 124.05   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | a     | 410 | PL9  | C20-C19-C21 | 2.23  | 119.10      | 115.23   |
| 37  | Y     | 101 | LMG  | O1-C7-C8    | -2.23 | 105.39      | 110.82   |
| 37  | J     | 101 | LMG  | O2-C2-C1    | -2.23 | 104.76      | 110.08   |
| 31  | c     | 509 | CLA  | CMB-C2B-C3B | 2.23  | 131.80      | 126.55   |
| 42  | 8     | 301 | A86  | C4-C3-C2    | -2.23 | 118.95      | 123.52   |
| 31  | C     | 504 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 31  | P     | 606 | CLA  | CHB-C1B-NB  | 2.23  | 127.40      | 124.05   |
| 31  | C     | 512 | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 33  | d     | 405 | BCR  | C2-C1-C6    | 2.23  | 113.68      | 110.44   |
| 42  | 8     | 301 | A86  | C41-C32-C40 | 2.23  | 115.02      | 108.63   |
| 31  | 1     | 208 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 31  | 4     | 210 | CLA  | CMB-C2B-C3B | 2.23  | 131.79      | 126.55   |
| 31  | 7     | 310 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 31  | 2     | 308 | CLA  | C3B-C4B-NB  | -2.23 | 108.01      | 110.33   |
| 37  | W     | 201 | LMG  | O3-C3-C2    | -2.23 | 105.12      | 110.38   |
| 31  | 0     | 310 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 31  | 4     | 213 | CLA  | CHB-C1B-NB  | 2.23  | 127.39      | 124.05   |
| 33  | H     | 101 | BCR  | C24-C23-C22 | -2.23 | 122.94      | 126.23   |
| 31  | C     | 502 | CLA  | C1-C2-C3    | -2.23 | 122.55      | 126.20   |
| 37  | Y     | 101 | LMG  | O1-C1-C2    | -2.23 | 104.89      | 108.27   |
| 37  | j     | 101 | LMG  | O1-C1-C2    | -2.23 | 104.89      | 108.27   |
| 37  | y     | 101 | LMG  | O1-C7-C8    | -2.23 | 105.40      | 110.82   |
| 31  | C     | 510 | CLA  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 42  | 9     | 202 | A86  | C19-C18-C17 | -2.23 | 106.63      | 110.79   |
| 37  | y     | 101 | LMG  | O1-C1-C2    | -2.22 | 104.89      | 108.27   |
| 42  | 9     | 202 | A86  | O-C13-C11   | -2.22 | 116.25      | 121.04   |
| 31  | B     | 516 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 31  | 3     | 306 | CLA  | CHB-C4A-NA  | 2.22  | 127.59      | 124.43   |
| 42  | 3     | 301 | A86  | C9-C8-C6    | -2.22 | 120.27      | 126.36   |
| 33  | c     | 515 | BCR  | C33-C5-C6   | -2.22 | 122.06      | 124.48   |
| 42  | 8     | 301 | A86  | C9-C8-C6    | -2.22 | 120.27      | 126.36   |
| 31  | p     | 608 | CLA  | CAC-C3C-C4C | 2.22  | 127.68      | 124.79   |
| 39  | C     | 518 | DGD  | C1D-C2D-C3D | -2.22 | 105.34      | 110.01   |
| 31  | c     | 504 | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 33  | H     | 101 | BCR  | C7-C8-C9    | -2.22 | 122.95      | 126.23   |
| 31  | 9     | 208 | CLA  | CAA-C2A-C3A | -2.22 | 111.14      | 116.23   |
| 39  | c     | 518 | DGD  | C1D-C2D-C3D | -2.22 | 105.34      | 110.01   |
| 31  | 5     | 309 | CLA  | CMA-C3A-C2A | -2.22 | 111.14      | 116.23   |
| 33  | c     | 516 | BCR  | C15-C16-C17 | -2.22 | 118.98      | 123.52   |
| 31  | 7     | 314 | CLA  | CMB-C2B-C1B | -2.22 | 122.04      | 125.42   |
| 35  | a     | 410 | PL9  | O1-C4-C3    | -2.22 | 118.39      | 120.73   |
| 44  | 1     | 203 | DD6  | C37-C36-C35 | 2.22  | 118.50      | 114.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 9     | 203 | A86  | C3-C4-C5    | -2.22 | 118.98      | 123.52   |
| 31  | b     | 517 | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 44  | 7     | 303 | DD6  | C37-C36-C35 | 2.22  | 118.50      | 114.42   |
| 31  | 3     | 309 | CLA  | O2D-CGD-O1D | -2.22 | 119.05      | 124.08   |
| 42  | 5     | 317 | A86  | C12-C11-C13 | 2.22  | 119.59      | 116.00   |
| 42  | 0     | 317 | A86  | C12-C11-C13 | 2.22  | 119.59      | 116.00   |
| 37  | w     | 201 | LMG  | O2-C2-C1    | -2.22 | 104.79      | 110.08   |
| 42  | 4     | 203 | A86  | C3-C4-C5    | -2.22 | 118.98      | 123.52   |
| 44  | 3     | 303 | DD6  | C21-C20-C15 | -2.22 | 118.66      | 122.30   |
| 31  | c     | 510 | CLA  | CMB-C2B-C1B | -2.22 | 122.05      | 125.42   |
| 44  | 8     | 303 | DD6  | C28-C27-C26 | -2.22 | 119.88      | 124.18   |
| 31  | 9     | 210 | CLA  | CMB-C2B-C3B | 2.21  | 131.76      | 126.55   |
| 31  | 5     | 310 | CLA  | C1-C2-C3    | -2.21 | 122.57      | 126.20   |
| 31  | 8     | 309 | CLA  | O2D-CGD-O1D | -2.21 | 119.06      | 124.08   |
| 42  | 0     | 317 | A86  | O4-C34-C35  | 2.21  | 113.30      | 107.64   |
| 42  | 3     | 302 | A86  | C40-C32-C31 | 2.21  | 112.45      | 110.47   |
| 31  | 9     | 212 | CLA  | C3B-C4B-NB  | -2.21 | 108.03      | 110.33   |
| 42  | 0     | 303 | A86  | C25-C26-C27 | -2.21 | 124.18      | 127.28   |
| 31  | 9     | 213 | CLA  | CHB-C1B-NB  | 2.21  | 127.36      | 124.05   |
| 33  | A     | 408 | BCR  | C24-C23-C22 | -2.21 | 122.97      | 126.23   |
| 37  | m     | 101 | LMG  | O3-C3-C2    | -2.21 | 105.17      | 110.38   |
| 31  | 6     | 212 | CLA  | CMB-C2B-C1B | -2.21 | 122.06      | 125.42   |
| 31  | 4     | 208 | CLA  | CAA-C2A-C3A | -2.21 | 111.17      | 116.23   |
| 42  | 7     | 301 | A86  | C12-C11-C13 | 2.21  | 119.58      | 116.00   |
| 33  | C     | 516 | BCR  | C15-C16-C17 | -2.21 | 119.01      | 123.52   |
| 39  | c     | 518 | DGD  | C4E-C3E-C2E | -2.21 | 106.96      | 110.83   |
| 42  | 6     | 202 | A86  | C12-C11-C13 | 2.20  | 119.57      | 116.00   |
| 31  | c     | 502 | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 44  | 6     | 203 | DD6  | C37-C36-C35 | 2.20  | 118.47      | 114.42   |
| 42  | 5     | 303 | A86  | C25-C26-C27 | -2.20 | 124.19      | 127.28   |
| 43  | 0     | 302 | ET4  | C28-C13-C14 | -2.20 | 119.25      | 122.82   |
| 42  | 5     | 317 | A86  | O4-C34-C35  | 2.20  | 113.27      | 107.64   |
| 33  | h     | 101 | BCR  | C24-C23-C22 | -2.20 | 122.98      | 126.23   |
| 33  | D     | 405 | BCR  | C2-C1-C6    | 2.20  | 113.64      | 110.44   |
| 39  | h     | 102 | DGD  | CAB-C9B-C8B | -2.20 | 103.25      | 114.37   |
| 33  | b     | 520 | BCR  | C27-C26-C25 | 2.20  | 125.68      | 122.70   |
| 31  | A     | 407 | CLA  | CMB-C2B-C1B | -2.20 | 122.07      | 125.42   |
| 31  | 3     | 314 | CLA  | CMB-C2B-C3B | 2.20  | 129.38      | 123.53   |
| 31  | 4     | 212 | CLA  | C3B-C4B-NB  | -2.20 | 108.05      | 110.33   |
| 41  | v     | 201 | HEM  | C2A-C1A-NA  | -2.20 | 107.71      | 110.15   |
| 31  | 8     | 314 | CLA  | CMB-C2B-C3B | 2.20  | 129.37      | 123.53   |
| 37  | d     | 409 | LMG  | O3-C3-C2    | -2.20 | 105.20      | 110.38   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | C     | 518 | DGD  | C4E-C3E-C2E | -2.20 | 106.97      | 110.83   |
| 44  | 8     | 303 | DD6  | C21-C20-C15 | -2.20 | 118.69      | 122.30   |
| 37  | D     | 410 | LMG  | O7-C10-O9   | -2.20 | 118.57      | 123.70   |
| 37  | W     | 201 | LMG  | O2-C2-C1    | -2.20 | 104.84      | 110.08   |
| 37  | M     | 101 | LMG  | O3-C3-C2    | -2.19 | 105.20      | 110.38   |
| 31  | 1     | 212 | CLA  | CMB-C2B-C1B | -2.19 | 122.08      | 125.42   |
| 33  | a     | 408 | BCR  | C24-C23-C22 | -2.19 | 122.99      | 126.23   |
| 31  | 4     | 213 | CLA  | CBD-CHA-C1A | 2.19  | 130.36      | 128.03   |
| 39  | H     | 102 | DGD  | CAB-C9B-C8B | -2.19 | 103.29      | 114.37   |
| 42  | 4     | 202 | A86  | C33-C32-C31 | -2.19 | 107.08      | 109.21   |
| 33  | b     | 520 | BCR  | C15-C14-C13 | -2.19 | 124.21      | 127.28   |
| 44  | 3     | 303 | DD6  | C28-C27-C26 | -2.19 | 119.93      | 124.18   |
| 31  | P     | 608 | CLA  | CAC-C3C-C4C | 2.19  | 127.64      | 124.79   |
| 31  | 2     | 312 | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 33  | h     | 101 | BCR  | C3-C4-C5    | -2.19 | 110.15      | 114.06   |
| 33  | d     | 405 | BCR  | C7-C8-C9    | -2.19 | 123.00      | 126.23   |
| 31  | C     | 513 | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 31  | 8     | 306 | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.43   |
| 36  | b     | 522 | LHG  | C27-C26-C25 | -2.19 | 103.31      | 114.37   |
| 42  | 4     | 202 | A86  | C19-C18-C17 | -2.19 | 106.70      | 110.79   |
| 42  | 5     | 317 | A86  | C26-C25-C24 | -2.19 | 116.87      | 123.20   |
| 37  | d     | 410 | LMG  | O7-C10-O9   | -2.19 | 118.59      | 123.70   |
| 31  | c     | 513 | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 31  | 1     | 211 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 31  | 8     | 308 | CLA  | CHB-C1B-NB  | 2.18  | 127.33      | 124.05   |
| 42  | 0     | 317 | A86  | C26-C25-C24 | -2.18 | 116.87      | 123.20   |
| 42  | 0     | 303 | A86  | C9-C10-C11  | -2.18 | 120.47      | 126.64   |
| 37  | b     | 521 | LMG  | O2-C2-C1    | -2.18 | 104.87      | 110.08   |
| 33  | H     | 101 | BCR  | C3-C4-C5    | -2.18 | 110.16      | 114.06   |
| 31  | 7     | 312 | CLA  | CMB-C2B-C1B | -2.18 | 122.10      | 125.42   |
| 31  | a     | 403 | CLA  | CMB-C2B-C3B | 2.18  | 131.68      | 126.55   |
| 37  | B     | 520 | LMG  | O2-C2-C1    | -2.18 | 104.88      | 110.08   |
| 42  | 8     | 302 | A86  | C40-C32-C31 | 2.18  | 112.42      | 110.47   |
| 37  | w     | 201 | LMG  | O6-C1-O1    | -2.18 | 104.89      | 110.04   |
| 37  | W     | 201 | LMG  | O6-C1-O1    | -2.18 | 104.89      | 110.04   |
| 31  | A     | 403 | CLA  | CMB-C2B-C3B | 2.18  | 131.68      | 126.55   |
| 35  | A     | 410 | PL9  | O1-C4-C3    | -2.18 | 118.43      | 120.73   |
| 36  | B     | 521 | LHG  | C27-C26-C25 | -2.18 | 103.36      | 114.37   |
| 37  | d     | 408 | LMG  | C6-C5-C4    | -2.18 | 107.68      | 113.02   |
| 31  | C     | 514 | CLA  | CMB-C2B-C3B | 2.18  | 131.67      | 126.55   |
| 31  | 9     | 213 | CLA  | CBD-CHA-C1A | 2.18  | 130.34      | 128.03   |
| 37  | D     | 409 | LMG  | O3-C3-C2    | -2.17 | 105.25      | 110.38   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 44  | 2     | 304 | DD6  | C8-C6-C5    | 2.17  | 122.43      | 119.01   |
| 42  | 5     | 303 | A86  | C9-C10-C11  | -2.17 | 120.50      | 126.64   |
| 31  | a     | 407 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 42  | 5     | 301 | A86  | O-C13-C14   | -2.17 | 117.31      | 121.76   |
| 42  | 5     | 303 | A86  | C12-C11-C13 | 2.17  | 119.52      | 116.00   |
| 42  | 1     | 202 | A86  | C12-C11-C13 | 2.17  | 119.52      | 116.00   |
| 37  | D     | 408 | LMG  | O2-C2-C1    | -2.17 | 104.90      | 110.08   |
| 33  | B     | 519 | BCR  | C15-C14-C13 | -2.17 | 124.23      | 127.28   |
| 33  | D     | 405 | BCR  | C7-C8-C9    | -2.17 | 123.02      | 126.23   |
| 39  | C     | 518 | DGD  | CAB-C9B-C8B | -2.17 | 103.40      | 114.37   |
| 42  | 9     | 202 | A86  | C33-C32-C31 | -2.17 | 107.10      | 109.21   |
| 31  | b     | 509 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 42  | 0     | 301 | A86  | O-C13-C14   | -2.17 | 117.31      | 121.76   |
| 31  | c     | 514 | CLA  | CMB-C2B-C3B | 2.17  | 131.65      | 126.55   |
| 42  | 3     | 302 | A86  | C-C1-C24    | 2.17  | 121.40      | 118.09   |
| 33  | d     | 405 | BCR  | C33-C5-C6   | -2.17 | 122.12      | 124.48   |
| 32  | A     | 406 | PHO  | C1-C2-C3    | -2.17 | 122.65      | 126.20   |
| 33  | d     | 405 | BCR  | C24-C23-C22 | -2.17 | 123.03      | 126.23   |
| 39  | c     | 518 | DGD  | CAB-C9B-C8B | -2.17 | 103.42      | 114.37   |
| 33  | D     | 405 | BCR  | C24-C23-C22 | -2.17 | 123.03      | 126.23   |
| 37  | y     | 101 | LMG  | O8-C28-O10  | -2.17 | 118.21      | 123.63   |
| 37  | D     | 408 | LMG  | C6-C5-C4    | -2.17 | 107.70      | 113.02   |
| 37  | d     | 408 | LMG  | O2-C2-C1    | -2.16 | 104.92      | 110.08   |
| 42  | 8     | 302 | A86  | C-C1-C24    | 2.16  | 121.39      | 118.09   |
| 31  | 6     | 211 | CLA  | O2A-CGA-O1A | -2.16 | 118.21      | 123.63   |
| 42  | 2     | 301 | A86  | C12-C11-C13 | 2.16  | 119.51      | 116.00   |
| 33  | B     | 519 | BCR  | C27-C26-C25 | 2.16  | 125.63      | 122.70   |
| 31  | b     | 516 | CLA  | C1-C2-C3    | -2.16 | 122.65      | 126.20   |
| 33  | b     | 520 | BCR  | C20-C21-C22 | -2.16 | 124.25      | 127.28   |
| 31  | 9     | 206 | CLA  | CHB-C4A-NA  | 2.16  | 127.52      | 124.40   |
| 31  | 3     | 308 | CLA  | CHB-C1B-NB  | 2.16  | 127.29      | 124.05   |
| 33  | H     | 101 | BCR  | C15-C16-C17 | -2.16 | 119.10      | 123.52   |
| 37  | y     | 101 | LMG  | O3-C3-C2    | -2.16 | 105.28      | 110.38   |
| 31  | d     | 403 | CLA  | CAA-CBA-CGA | -2.16 | 107.08      | 113.21   |
| 42  | 3     | 302 | A86  | O-C13-C11   | -2.16 | 116.39      | 121.04   |
| 31  | 6     | 210 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 31  | 1     | 210 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 37  | Y     | 101 | LMG  | O3-C3-C2    | -2.16 | 105.29      | 110.38   |
| 31  | a     | 407 | CLA  | O2D-CGD-CBD | 2.16  | 115.00      | 111.23   |
| 33  | B     | 517 | BCR  | C7-C8-C9    | -2.16 | 123.04      | 126.23   |
| 31  | b     | 514 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 37  | d     | 409 | LMG  | O7-C10-O9   | -2.16 | 118.67      | 123.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | D     | 403 | CLA  | CAA-CBA-CGA | -2.16 | 107.09      | 113.21   |
| 31  | 7     | 312 | CLA  | C1C-NC-C4C  | 2.15  | 107.66      | 106.68   |
| 37  | D     | 409 | LMG  | O7-C10-O9   | -2.15 | 118.67      | 123.70   |
| 31  | c     | 502 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 32  | a     | 406 | PHO  | C1-C2-C3    | -2.15 | 122.67      | 126.20   |
| 31  | B     | 508 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 31  | b     | 514 | CLA  | CMB-C2B-C3B | 2.15  | 131.61      | 126.55   |
| 31  | a     | 404 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 34  | 0     | 316 | SQD  | O5-C5-C4    | 2.15  | 113.58      | 109.70   |
| 37  | b     | 521 | LMG  | C6-C5-C4    | -2.15 | 107.73      | 113.02   |
| 33  | b     | 518 | BCR  | C7-C8-C9    | -2.15 | 123.05      | 126.23   |
| 33  | c     | 517 | BCR  | C11-C10-C9  | -2.15 | 124.26      | 127.28   |
| 44  | 1     | 203 | DD6  | C24-C1-C2   | 2.15  | 122.39      | 119.01   |
| 34  | 5     | 316 | SQD  | O5-C5-C4    | 2.15  | 113.57      | 109.70   |
| 31  | 4     | 206 | CLA  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 31  | B     | 513 | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 37  | Y     | 101 | LMG  | O8-C28-O10  | -2.15 | 118.25      | 123.63   |
| 42  | 2     | 301 | A86  | C3-C4-C5    | -2.15 | 119.12      | 123.52   |
| 44  | 8     | 303 | DD6  | C12-C11-C10 | -2.15 | 119.34      | 122.82   |
| 31  | A     | 407 | CLA  | O2D-CGD-CBD | 2.15  | 114.98      | 111.23   |
| 37  | w     | 201 | LMG  | C1-C2-C3    | -2.15 | 105.49      | 110.01   |
| 42  | 8     | 302 | A86  | O-C13-C11   | -2.15 | 116.42      | 121.04   |
| 42  | 7     | 301 | A86  | C3-C4-C5    | -2.15 | 119.13      | 123.52   |
| 31  | A     | 404 | CLA  | O2A-CGA-O1A | -2.14 | 118.26      | 123.63   |
| 31  | b     | 506 | CLA  | C1-C2-C3    | -2.14 | 122.68      | 126.20   |
| 31  | B     | 515 | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 44  | P     | 611 | DD6  | C37-C36-C31 | -2.14 | 120.15      | 124.16   |
| 31  | C     | 502 | CLA  | O2A-CGA-O1A | -2.14 | 118.27      | 123.63   |
| 37  | B     | 520 | LMG  | C6-C5-C4    | -2.14 | 107.76      | 113.02   |
| 33  | h     | 101 | BCR  | C15-C16-C17 | -2.14 | 119.14      | 123.52   |
| 31  | B     | 512 | CLA  | CMB-C2B-C1B | -2.14 | 122.16      | 125.42   |
| 42  | 0     | 303 | A86  | C12-C11-C13 | 2.14  | 119.47      | 116.00   |
| 31  | b     | 513 | CLA  | CMB-C2B-C1B | -2.14 | 122.16      | 125.42   |
| 31  | B     | 505 | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 31  | P     | 608 | CLA  | C3B-C4B-NB  | -2.14 | 108.11      | 110.33   |
| 31  | C     | 506 | CLA  | O2D-CGD-CBD | 2.14  | 114.97      | 111.23   |
| 42  | 3     | 302 | A86  | C23-C16-C17 | -2.14 | 105.21      | 108.97   |
| 35  | a     | 410 | PL9  | O2-C1-C2    | -2.14 | 116.97      | 121.83   |
| 44  | 7     | 304 | DD6  | C8-C6-C5    | 2.14  | 122.37      | 119.01   |
| 42  | 9     | 202 | A86  | C26-C25-C24 | -2.14 | 117.01      | 123.20   |
| 31  | c     | 506 | CLA  | O2D-CGD-CBD | 2.14  | 114.97      | 111.23   |
| 31  | p     | 601 | CLA  | CMA-C3A-C2A | -2.14 | 111.33      | 116.23   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | B     | 519 | BCR  | C20-C21-C22 | -2.14 | 124.28      | 127.28   |
| 31  | p     | 608 | CLA  | C3B-C4B-NB  | -2.13 | 108.11      | 110.33   |
| 42  | 4     | 202 | A86  | C26-C25-C24 | -2.13 | 117.01      | 123.20   |
| 31  | B     | 513 | CLA  | CMB-C2B-C3B | 2.13  | 131.57      | 126.55   |
| 42  | 7     | 302 | A86  | C-C1-C2     | -2.13 | 119.36      | 122.82   |
| 42  | 8     | 302 | A86  | C23-C16-C17 | -2.13 | 105.22      | 108.97   |
| 39  | c     | 519 | DGD  | O2D-C2D-C1D | -2.13 | 104.99      | 110.08   |
| 37  | D     | 409 | LMG  | O2-C2-C1    | -2.13 | 104.99      | 110.08   |
| 39  | c     | 518 | DGD  | O2D-C2D-C1D | -2.13 | 104.99      | 110.08   |
| 42  | 2     | 302 | A86  | C-C1-C2     | -2.13 | 119.36      | 122.82   |
| 35  | A     | 410 | PL9  | O2-C1-C2    | -2.13 | 116.98      | 121.83   |
| 39  | C     | 519 | DGD  | CAB-C9B-C8B | -2.13 | 103.59      | 114.37   |
| 39  | C     | 519 | DGD  | C5B-C4B-C3B | -2.13 | 103.60      | 114.37   |
| 31  | a     | 407 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 31  | 9     | 213 | CLA  | CMB-C2B-C1B | -2.13 | 122.18      | 125.42   |
| 39  | C     | 519 | DGD  | O2D-C2D-C1D | -2.13 | 105.00      | 110.08   |
| 42  | 4     | 201 | A86  | C4-C3-C2    | -2.13 | 119.16      | 123.52   |
| 39  | c     | 519 | DGD  | C5B-C4B-C3B | -2.13 | 103.61      | 114.37   |
| 39  | c     | 519 | DGD  | CAB-C9B-C8B | -2.13 | 103.61      | 114.37   |
| 37  | W     | 201 | LMG  | C1-C2-C3    | -2.13 | 105.53      | 110.01   |
| 36  | D     | 412 | LHG  | C27-C26-C25 | -2.13 | 103.61      | 114.37   |
| 33  | C     | 517 | BCR  | C27-C26-C25 | 2.13  | 125.58      | 122.70   |
| 39  | C     | 518 | DGD  | O2D-C2D-C1D | -2.13 | 105.01      | 110.08   |
| 37  | d     | 409 | LMG  | O2-C2-C1    | -2.13 | 105.01      | 110.08   |
| 37  | 0     | 315 | LMG  | C42-C41-C40 | -2.12 | 103.63      | 114.37   |
| 44  | 2     | 303 | DD6  | C24-C1-C2   | 2.12  | 122.35      | 119.01   |
| 33  | C     | 517 | BCR  | C11-C10-C9  | -2.12 | 124.30      | 127.28   |
| 31  | 1     | 206 | CLA  | CMC-C2C-C1C | 2.12  | 128.35      | 125.03   |
| 33  | b     | 519 | BCR  | C24-C23-C22 | -2.12 | 123.09      | 126.23   |
| 36  | d     | 412 | LHG  | C27-C26-C25 | -2.12 | 103.64      | 114.37   |
| 44  | 7     | 303 | DD6  | C24-C1-C2   | 2.12  | 122.35      | 119.01   |
| 42  | 7     | 302 | A86  | C26-C25-C24 | -2.12 | 117.06      | 123.20   |
| 31  | A     | 407 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 44  | p     | 611 | DD6  | C37-C36-C31 | -2.12 | 120.20      | 124.16   |
| 44  | 3     | 303 | DD6  | C12-C11-C10 | -2.12 | 119.38      | 122.82   |
| 31  | 6     | 206 | CLA  | CMC-C2C-C1C | 2.12  | 128.34      | 125.03   |
| 33  | B     | 518 | BCR  | C24-C23-C22 | -2.12 | 123.10      | 126.23   |
| 42  | 2     | 302 | A86  | C26-C25-C24 | -2.12 | 117.06      | 123.20   |
| 37  | 5     | 315 | LMG  | O3-C3-C2    | -2.12 | 105.39      | 110.38   |
| 44  | 6     | 203 | DD6  | C24-C1-C2   | 2.12  | 122.34      | 119.01   |
| 39  | C     | 519 | DGD  | C1D-C2D-C3D | -2.12 | 105.56      | 110.01   |
| 37  | 0     | 315 | LMG  | O3-C3-C2    | -2.12 | 105.39      | 110.38   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | 5     | 315 | LMG  | C42-C41-C40 | -2.12 | 103.68      | 114.37   |
| 37  | y     | 101 | LMG  | C3-C4-C5    | -2.11 | 106.40      | 110.23   |
| 44  | p     | 611 | DD6  | C7-C6-C5    | -2.11 | 119.39      | 122.82   |
| 42  | 0     | 301 | A86  | C41-C32-C31 | -2.11 | 108.58      | 110.47   |
| 39  | C     | 520 | DGD  | C2G-O2G-C1B | -2.11 | 112.74      | 117.80   |
| 36  | D     | 411 | LHG  | C18-C17-C16 | -2.11 | 103.69      | 114.37   |
| 39  | c     | 520 | DGD  | C2G-O2G-C1B | -2.11 | 112.74      | 117.80   |
| 37  | Y     | 101 | LMG  | C3-C4-C5    | -2.11 | 106.41      | 110.23   |
| 39  | C     | 519 | DGD  | CBB-CAB-C9B | -2.11 | 103.70      | 114.37   |
| 33  | D     | 405 | BCR  | C33-C5-C6   | -2.11 | 122.18      | 124.48   |
| 31  | c     | 504 | CLA  | CMB-C2B-C1B | -2.11 | 122.21      | 125.42   |
| 36  | d     | 411 | LHG  | C18-C17-C16 | -2.11 | 103.70      | 114.37   |
| 31  | b     | 512 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 31  | P     | 601 | CLA  | CMA-C3A-C2A | -2.11 | 111.40      | 116.23   |
| 42  | 9     | 201 | A86  | C4-C3-C2    | -2.11 | 119.21      | 123.52   |
| 31  | C     | 510 | CLA  | CMB-C2B-C3B | 2.11  | 131.50      | 126.55   |
| 31  | c     | 506 | CLA  | CMB-C2B-C3B | 2.11  | 131.50      | 126.55   |
| 39  | c     | 519 | DGD  | CBB-CAB-C9B | -2.11 | 103.72      | 114.37   |
| 31  | 7     | 316 | CLA  | CMB-C2B-C1B | -2.10 | 122.21      | 125.42   |
| 37  | 0     | 315 | LMG  | O2-C2-C1    | -2.10 | 105.06      | 110.08   |
| 31  | d     | 401 | CLA  | O2D-CGD-CBD | 2.10  | 114.91      | 111.23   |
| 42  | 6     | 202 | A86  | C7-C6-C8    | 2.10  | 121.30      | 118.09   |
| 31  | D     | 401 | CLA  | O2D-CGD-CBD | 2.10  | 114.91      | 111.23   |
| 31  | p     | 602 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 42  | 0     | 303 | A86  | C4-C3-C2    | -2.10 | 119.22      | 123.52   |
| 39  | c     | 519 | DGD  | C1D-C2D-C3D | -2.10 | 105.59      | 110.01   |
| 31  | a     | 403 | CLA  | C1-C2-C3    | -2.10 | 122.75      | 126.20   |
| 31  | 9     | 213 | CLA  | CHD-C4C-NC  | 2.10  | 127.49      | 124.23   |
| 31  | B     | 511 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 31  | C     | 506 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 31  | c     | 510 | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 33  | b     | 518 | BCR  | C11-C10-C9  | -2.10 | 124.33      | 127.28   |
| 33  | b     | 520 | BCR  | C29-C30-C25 | 2.10  | 113.49      | 110.44   |
| 31  | 2     | 307 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 32  | A     | 405 | PHO  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 31  | P     | 602 | CLA  | CMB-C2B-C3B | 2.10  | 131.48      | 126.55   |
| 42  | 5     | 303 | A86  | C26-C25-C24 | -2.09 | 117.13      | 123.20   |
| 42  | 0     | 303 | A86  | C26-C25-C24 | -2.09 | 117.13      | 123.20   |
| 31  | 0     | 305 | CLA  | CHB-C4A-NA  | 2.09  | 127.42      | 124.40   |
| 31  | 7     | 315 | CLA  | CMA-C3A-C2A | -2.09 | 111.43      | 116.23   |
| 31  | Z     | 101 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 31  | B     | 503 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 405 | PHO  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 31  | z     | 101 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 31  | 0     | 304 | CLA  | CMA-C3A-C2A | -2.09 | 111.44      | 116.23   |
| 37  | 5     | 315 | LMG  | O2-C2-C1    | -2.09 | 105.09      | 110.08   |
| 31  | 7     | 309 | CLA  | CMB-C2B-C3B | 2.09  | 131.47      | 126.55   |
| 31  | 2     | 309 | CLA  | CMB-C2B-C3B | 2.09  | 131.47      | 126.55   |
| 44  | P     | 611 | DD6  | C7-C6-C5    | -2.09 | 119.43      | 122.82   |
| 44  | 7     | 303 | DD6  | C8-C6-C5    | 2.09  | 122.30      | 119.01   |
| 31  | b     | 504 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 31  | 5     | 305 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 31  | 9     | 211 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 33  | d     | 405 | BCR  | C11-C10-C9  | -2.09 | 124.35      | 127.28   |
| 34  | b     | 501 | SQD  | C1-O5-C5    | 2.09  | 117.80      | 113.72   |
| 42  | 1     | 202 | A86  | C7-C6-C8    | 2.09  | 121.28      | 118.09   |
| 31  | C     | 504 | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 37  | m     | 101 | LMG  | O7-C10-O9   | -2.09 | 118.83      | 123.70   |
| 31  | b     | 509 | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 34  | B     | 523 | SQD  | C1-O5-C5    | 2.09  | 117.80      | 113.72   |
| 31  | 4     | 211 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 31  | 2     | 315 | CLA  | CMA-C3A-C2A | -2.09 | 111.45      | 116.23   |
| 33  | B     | 517 | BCR  | C11-C10-C9  | -2.08 | 124.35      | 127.28   |
| 44  | 6     | 204 | DD6  | C37-C36-C31 | -2.08 | 120.26      | 124.16   |
| 33  | D     | 405 | BCR  | C11-C10-C9  | -2.08 | 124.36      | 127.28   |
| 44  | p     | 611 | DD6  | C-C1-C2     | -2.08 | 119.44      | 122.82   |
| 33  | B     | 519 | BCR  | C29-C30-C25 | 2.08  | 113.46      | 110.44   |
| 31  | 9     | 205 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 39  | c     | 518 | DGD  | O3E-C3E-C2E | -2.08 | 105.47      | 110.38   |
| 39  | h     | 102 | DGD  | O3E-C3E-C2E | -2.08 | 105.47      | 110.38   |
| 36  | A     | 412 | LHG  | C5-O7-C7    | -2.08 | 112.82      | 117.80   |
| 31  | A     | 403 | CLA  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 44  | 2     | 303 | DD6  | C8-C6-C5    | 2.08  | 122.28      | 119.01   |
| 39  | h     | 102 | DGD  | O2D-C2D-C1D | -2.08 | 105.12      | 110.08   |
| 31  | 4     | 213 | CLA  | CHD-C4C-NC  | 2.08  | 127.46      | 124.23   |
| 44  | P     | 611 | DD6  | C32-C33-C34 | -2.08 | 109.03      | 113.59   |
| 31  | P     | 607 | CLA  | C4D-CHA-C1A | 2.08  | 123.72      | 121.24   |
| 33  | c     | 517 | BCR  | C27-C26-C25 | 2.08  | 125.51      | 122.70   |
| 39  | H     | 102 | DGD  | O2D-C2D-C1D | -2.08 | 105.12      | 110.08   |
| 31  | c     | 503 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 37  | M     | 101 | LMG  | O7-C10-O9   | -2.08 | 118.85      | 123.70   |
| 31  | B     | 508 | CLA  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 35  | d     | 406 | PL9  | O2-C1-C2    | -2.08 | 117.11      | 121.83   |
| 37  | d     | 408 | LMG  | O7-C10-O9   | -2.07 | 118.85      | 123.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 515 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 35  | D     | 406 | PL9  | O2-C1-C2    | -2.07 | 117.11      | 121.83   |
| 42  | p     | 610 | A86  | C41-C32-C33 | -2.07 | 99.24       | 109.06   |
| 31  | 2     | 316 | CLA  | CMB-C2B-C1B | -2.07 | 122.26      | 125.42   |
| 39  | C     | 518 | DGD  | O3E-C3E-C2E | -2.07 | 105.49      | 110.38   |
| 36  | d     | 407 | LHG  | C5-O7-C7    | -2.07 | 112.83      | 117.80   |
| 31  | 4     | 205 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 42  | P     | 610 | A86  | C41-C32-C33 | -2.07 | 99.24       | 109.06   |
| 42  | 5     | 303 | A86  | C4-C3-C2    | -2.07 | 119.28      | 123.52   |
| 31  | 4     | 213 | CLA  | CMB-C2B-C1B | -2.07 | 122.26      | 125.42   |
| 31  | b     | 516 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 31  | 9     | 213 | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 33  | C     | 517 | BCR  | C28-C27-C26 | -2.07 | 110.36      | 114.06   |
| 44  | P     | 611 | DD6  | C-C1-C2     | -2.07 | 119.46      | 122.82   |
| 37  | y     | 101 | LMG  | O7-C10-O9   | -2.07 | 118.86      | 123.70   |
| 41  | f     | 101 | HEM  | C4D-ND-C1D  | 2.07  | 107.66      | 105.21   |
| 31  | D     | 401 | CLA  | CMB-C2B-C1B | -2.07 | 122.27      | 125.42   |
| 37  | b     | 521 | LMG  | O7-C10-O9   | -2.07 | 118.87      | 123.70   |
| 31  | 4     | 213 | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 36  | D     | 407 | LHG  | C5-O7-C7    | -2.07 | 112.85      | 117.80   |
| 42  | 9     | 201 | A86  | C9-C8-C6    | -2.07 | 120.69      | 126.36   |
| 44  | p     | 611 | DD6  | C32-C33-C34 | -2.07 | 109.06      | 113.59   |
| 42  | 4     | 201 | A86  | C9-C8-C6    | -2.07 | 120.70      | 126.36   |
| 39  | H     | 102 | DGD  | O3E-C3E-C2E | -2.07 | 105.50      | 110.38   |
| 36  | a     | 411 | LHG  | C5-O7-C7    | -2.07 | 112.85      | 117.80   |
| 31  | 5     | 304 | CLA  | CMA-C3A-C2A | -2.07 | 111.49      | 116.23   |
| 41  | F     | 101 | HEM  | C4D-ND-C1D  | 2.07  | 107.65      | 105.21   |
| 44  | 6     | 203 | DD6  | C8-C6-C5    | 2.06  | 122.26      | 119.01   |
| 33  | A     | 408 | BCR  | C15-C16-C17 | -2.06 | 119.29      | 123.52   |
| 44  | 1     | 204 | DD6  | C37-C36-C31 | -2.06 | 120.30      | 124.16   |
| 31  | 7     | 309 | CLA  | O2A-CGA-O1A | -2.06 | 118.46      | 123.63   |
| 42  | 5     | 301 | A86  | C41-C32-C31 | -2.06 | 108.62      | 110.47   |
| 37  | c     | 521 | LMG  | O7-C10-O9   | -2.06 | 118.88      | 123.70   |
| 39  | h     | 102 | DGD  | C5B-C4B-C3B | -2.06 | 103.94      | 114.37   |
| 37  | Y     | 101 | LMG  | O7-C10-O9   | -2.06 | 118.88      | 123.70   |
| 31  | b     | 510 | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 31  | 8     | 308 | CLA  | C2A-C1A-CHA | 2.06  | 124.87      | 122.46   |
| 33  | a     | 408 | BCR  | C15-C16-C17 | -2.06 | 119.30      | 123.52   |
| 42  | 4     | 202 | A86  | C12-C11-C13 | 2.06  | 119.34      | 116.00   |
| 31  | 7     | 313 | CLA  | CMA-C3A-C2A | -2.06 | 111.50      | 116.23   |
| 31  | b     | 508 | CLA  | O1D-CGD-CBD | 2.06  | 128.58      | 124.52   |
| 31  | 2     | 313 | CLA  | CMA-C3A-C2A | -2.06 | 111.51      | 116.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | H     | 102 | DGD  | C5B-C4B-C3B | -2.05 | 103.98      | 114.37   |
| 42  | 3     | 302 | A86  | C12-C11-C13 | 2.05  | 119.33      | 116.00   |
| 44  | 1     | 203 | DD6  | C8-C6-C5    | 2.05  | 122.24      | 119.01   |
| 31  | 2     | 312 | CLA  | CMA-C3A-C2A | -2.05 | 111.52      | 116.23   |
| 42  | 8     | 302 | A86  | C12-C11-C13 | 2.05  | 119.33      | 116.00   |
| 37  | B     | 520 | LMG  | O7-C10-O9   | -2.05 | 118.90      | 123.70   |
| 37  | D     | 408 | LMG  | O7-C10-O9   | -2.05 | 118.90      | 123.70   |
| 42  | 8     | 302 | A86  | C9-C10-C11  | -2.05 | 120.83      | 126.64   |
| 31  | 2     | 309 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 31  | C     | 503 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 42  | 3     | 302 | A86  | C9-C10-C11  | -2.05 | 120.84      | 126.64   |
| 35  | a     | 410 | PL9  | C12-C13-C14 | -2.05 | 122.93      | 127.62   |
| 42  | 2     | 301 | A86  | C25-C26-C27 | -2.05 | 124.40      | 127.28   |
| 42  | 9     | 203 | A86  | C34-O4-C38  | 2.05  | 121.46      | 117.85   |
| 42  | 5     | 317 | A86  | C25-C26-C27 | -2.05 | 124.41      | 127.28   |
| 42  | 0     | 317 | A86  | C25-C26-C27 | -2.05 | 124.41      | 127.28   |
| 31  | 7     | 307 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 31  | b     | 510 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 41  | V     | 201 | HEM  | C1B-NB-C4B  | 2.05  | 107.63      | 105.21   |
| 31  | B     | 509 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 31  | 7     | 312 | CLA  | CMA-C3A-C2A | -2.05 | 111.54      | 116.23   |
| 31  | B     | 507 | CLA  | O1D-CGD-CBD | 2.04  | 128.55      | 124.52   |
| 37  | C     | 521 | LMG  | O7-C10-O9   | -2.04 | 118.92      | 123.70   |
| 31  | 0     | 314 | CLA  | CMA-C3A-C2A | -2.04 | 111.54      | 116.23   |
| 31  | d     | 401 | CLA  | CMB-C2B-C1B | -2.04 | 122.31      | 125.42   |
| 31  | A     | 407 | CLA  | CMB-C2B-C3B | 2.04  | 131.35      | 126.55   |
| 42  | 7     | 301 | A86  | C25-C26-C27 | -2.04 | 124.42      | 127.28   |
| 31  | 7     | 311 | CLA  | CMB-C2B-C3B | 2.04  | 131.35      | 126.55   |
| 35  | A     | 410 | PL9  | C12-C13-C14 | -2.04 | 122.95      | 127.62   |
| 31  | p     | 607 | CLA  | C4D-CHA-C1A | 2.04  | 123.68      | 121.24   |
| 31  | p     | 606 | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 42  | 9     | 202 | A86  | C12-C11-C13 | 2.04  | 119.30      | 116.00   |
| 44  | p     | 611 | DD6  | C9-C8-C6    | -2.04 | 120.78      | 126.36   |
| 42  | 2     | 302 | A86  | C23-C16-C17 | -2.04 | 105.39      | 108.97   |
| 31  | B     | 509 | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 31  | D     | 403 | CLA  | O2A-CGA-O1A | -2.04 | 118.54      | 123.63   |
| 31  | B     | 506 | CLA  | CMB-C2B-C1B | -2.04 | 122.32      | 125.42   |
| 31  | 3     | 304 | CLA  | CMA-C3A-C2A | -2.04 | 111.56      | 116.23   |
| 33  | B     | 518 | BCR  | C7-C8-C9    | -2.03 | 123.22      | 126.23   |
| 43  | 5     | 302 | ET4  | C34-C35-C36 | -2.03 | 109.13      | 113.59   |
| 33  | c     | 517 | BCR  | C28-C27-C26 | -2.03 | 110.43      | 114.06   |
| 44  | P     | 611 | DD6  | C9-C8-C6    | -2.03 | 120.79      | 126.36   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 42  | 5     | 303 | A86  | O4-C38-O5   | -2.03 | 119.07      | 122.99   |
| 44  | 2     | 304 | DD6  | C3-C2-C1    | -2.03 | 124.43      | 127.28   |
| 31  | a     | 407 | CLA  | CMB-C2B-C3B | 2.03  | 131.32      | 126.55   |
| 35  | d     | 406 | PL9  | C32-C33-C34 | -2.03 | 122.98      | 127.62   |
| 35  | D     | 406 | PL9  | C32-C33-C34 | -2.03 | 122.98      | 127.62   |
| 31  | P     | 606 | CLA  | CHB-C4A-NA  | 2.03  | 127.33      | 124.40   |
| 33  | C     | 515 | BCR  | C2-C1-C6    | 2.03  | 113.38      | 110.44   |
| 33  | c     | 517 | BCR  | C7-C8-C9    | -2.03 | 123.24      | 126.23   |
| 43  | 0     | 302 | ET4  | C34-C35-C36 | -2.03 | 109.15      | 113.59   |
| 33  | c     | 516 | BCR  | C28-C27-C26 | -2.03 | 110.44      | 114.06   |
| 31  | 0     | 307 | CLA  | O2A-CGA-O1A | -2.02 | 118.56      | 123.63   |
| 31  | p     | 609 | CLA  | CMB-C2B-C1B | -2.02 | 122.34      | 125.42   |
| 37  | Y     | 101 | LMG  | C6-C5-C4    | -2.02 | 108.05      | 113.02   |
| 31  | B     | 512 | CLA  | CMB-C2B-C3B | 2.02  | 131.31      | 126.55   |
| 33  | b     | 519 | BCR  | C7-C8-C9    | -2.02 | 123.24      | 126.23   |
| 31  | b     | 513 | CLA  | CMB-C2B-C3B | 2.02  | 131.31      | 126.55   |
| 31  | C     | 506 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 41  | v     | 201 | HEM  | C1B-NB-C4B  | 2.02  | 107.60      | 105.21   |
| 31  | d     | 403 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 32  | a     | 406 | PHO  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 33  | C     | 516 | BCR  | C28-C27-C26 | -2.02 | 110.45      | 114.06   |
| 31  | 8     | 304 | CLA  | CMA-C3A-C2A | -2.02 | 111.60      | 116.23   |
| 36  | h     | 103 | LHG  | C11-C10-C9  | -2.02 | 104.16      | 114.37   |
| 33  | A     | 408 | BCR  | C11-C10-C9  | -2.02 | 124.44      | 127.28   |
| 31  | C     | 513 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 42  | 7     | 302 | A86  | C23-C16-C17 | -2.02 | 105.42      | 108.97   |
| 31  | B     | 515 | CLA  | O2D-CGD-CBD | 2.02  | 114.76      | 111.23   |
| 31  | 1     | 210 | CLA  | C2A-C1A-CHA | 2.02  | 127.37      | 123.87   |
| 31  | b     | 507 | CLA  | CMB-C2B-C1B | -2.02 | 122.34      | 125.42   |
| 33  | c     | 515 | BCR  | C2-C1-C6    | 2.02  | 113.37      | 110.44   |
| 31  | 2     | 311 | CLA  | CMB-C2B-C3B | 2.02  | 131.29      | 126.55   |
| 31  | C     | 509 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 31  | 4     | 207 | CLA  | CMA-C3A-C2A | -2.02 | 111.61      | 116.23   |
| 44  | 7     | 304 | DD6  | C7-C6-C5    | -2.02 | 119.55      | 122.82   |
| 42  | P     | 610 | A86  | O2-C18-C19  | -2.02 | 105.62      | 109.75   |
| 33  | h     | 101 | BCR  | C33-C5-C6   | -2.02 | 122.28      | 124.48   |
| 31  | 5     | 307 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 42  | 4     | 201 | A86  | C19-C18-C17 | -2.02 | 107.02      | 110.79   |
| 31  | 9     | 213 | CLA  | C4D-CHA-C1A | 2.02  | 123.65      | 121.24   |
| 31  | 9     | 207 | CLA  | CMA-C3A-C2A | -2.01 | 111.61      | 116.23   |
| 31  | c     | 513 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 31  | 6     | 210 | CLA  | C2A-C1A-CHA | 2.01  | 127.36      | 123.87   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | b     | 508 | CLA  | CMB-C2B-C1B | -2.01 | 122.35      | 125.42   |
| 36  | H     | 103 | LHG  | C11-C10-C9  | -2.01 | 104.19      | 114.37   |
| 31  | 6     | 214 | CLA  | CMB-C2B-C1B | -2.01 | 122.35      | 125.42   |
| 31  | 1     | 214 | CLA  | CMB-C2B-C1B | -2.01 | 122.35      | 125.42   |
| 32  | A     | 406 | PHO  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 37  | y     | 101 | LMG  | C6-C5-C4    | -2.01 | 108.08      | 113.02   |
| 31  | p     | 609 | CLA  | O2D-CGD-CBD | 2.01  | 117.34      | 110.75   |
| 39  | c     | 519 | DGD  | C3D-C4D-C5D | -2.01 | 106.59      | 110.23   |
| 37  | M     | 101 | LMG  | C1-C2-C3    | -2.01 | 105.78      | 110.01   |
| 37  | m     | 101 | LMG  | C1-C2-C3    | -2.01 | 105.78      | 110.01   |
| 37  | d     | 408 | LMG  | O1-C7-C8    | -2.01 | 105.93      | 110.82   |
| 42  | 4     | 203 | A86  | C34-O4-C38  | 2.01  | 121.39      | 117.85   |
| 31  | 5     | 314 | CLA  | CMA-C3A-C2A | -2.01 | 111.63      | 116.23   |
| 44  | 2     | 304 | DD6  | C7-C6-C5    | -2.01 | 119.56      | 122.82   |
| 31  | b     | 504 | CLA  | O2D-CGD-CBD | 2.01  | 114.74      | 111.23   |
| 31  | 4     | 206 | CLA  | CHB-C1B-NB  | 2.01  | 127.06      | 124.05   |
| 44  | 7     | 304 | DD6  | C3-C2-C1    | -2.01 | 124.47      | 127.28   |
| 31  | c     | 506 | CLA  | O2A-CGA-O1A | -2.00 | 118.61      | 123.63   |
| 42  | 0     | 303 | A86  | O4-C38-O5   | -2.00 | 119.12      | 122.99   |
| 39  | C     | 518 | DGD  | CBB-CAB-C9B | -2.00 | 104.24      | 114.37   |
| 31  | B     | 504 | CLA  | CMB-C2B-C1B | -2.00 | 122.37      | 125.42   |
| 39  | c     | 518 | DGD  | CBB-CAB-C9B | -2.00 | 104.24      | 114.37   |
| 33  | a     | 408 | BCR  | C11-C10-C9  | -2.00 | 124.47      | 127.28   |
| 31  | c     | 509 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 39  | C     | 519 | DGD  | C3D-C4D-C5D | -2.00 | 106.60      | 110.23   |
| 31  | b     | 506 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 31  | Z     | 101 | CLA  | C1-C2-C3    | -2.00 | 122.92      | 126.20   |
| 31  | 7     | 312 | CLA  | CMB-C2B-C3B | 2.00  | 131.26      | 126.55   |
| 31  | c     | 512 | CLA  | CMB-C2B-C3B | 2.00  | 131.25      | 126.55   |
| 37  | m     | 102 | LMG  | C1-O6-C5    | -2.00 | 109.81      | 113.72   |

All (206) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | A     | 403 | CLA  | ND   |
| 31  | A     | 404 | CLA  | ND   |
| 31  | A     | 407 | CLA  | ND   |
| 31  | B     | 501 | CLA  | ND   |
| 31  | B     | 502 | CLA  | ND   |
| 31  | B     | 503 | CLA  | ND   |
| 31  | B     | 504 | CLA  | ND   |
| 31  | B     | 505 | CLA  | ND   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | B     | 506 | CLA  | ND   |
| 31  | B     | 507 | CLA  | ND   |
| 31  | B     | 508 | CLA  | ND   |
| 31  | B     | 509 | CLA  | ND   |
| 31  | B     | 510 | CLA  | ND   |
| 31  | B     | 511 | CLA  | ND   |
| 31  | B     | 512 | CLA  | ND   |
| 31  | B     | 513 | CLA  | ND   |
| 31  | B     | 514 | CLA  | ND   |
| 31  | B     | 515 | CLA  | ND   |
| 31  | B     | 516 | CLA  | ND   |
| 31  | C     | 502 | CLA  | ND   |
| 31  | C     | 503 | CLA  | ND   |
| 31  | C     | 504 | CLA  | ND   |
| 31  | C     | 505 | CLA  | ND   |
| 31  | C     | 506 | CLA  | ND   |
| 31  | C     | 507 | CLA  | ND   |
| 31  | C     | 508 | CLA  | ND   |
| 31  | C     | 509 | CLA  | ND   |
| 31  | C     | 510 | CLA  | ND   |
| 31  | C     | 511 | CLA  | ND   |
| 31  | C     | 512 | CLA  | ND   |
| 31  | C     | 513 | CLA  | ND   |
| 31  | C     | 514 | CLA  | ND   |
| 31  | D     | 401 | CLA  | ND   |
| 31  | D     | 403 | CLA  | ND   |
| 31  | D     | 404 | CLA  | ND   |
| 31  | W     | 202 | CLA  | ND   |
| 31  | Z     | 101 | CLA  | ND   |
| 31  | a     | 403 | CLA  | ND   |
| 31  | a     | 404 | CLA  | ND   |
| 31  | a     | 407 | CLA  | ND   |
| 31  | b     | 502 | CLA  | ND   |
| 31  | b     | 503 | CLA  | ND   |
| 31  | b     | 504 | CLA  | ND   |
| 31  | b     | 505 | CLA  | ND   |
| 31  | b     | 506 | CLA  | ND   |
| 31  | b     | 507 | CLA  | ND   |
| 31  | b     | 508 | CLA  | ND   |
| 31  | b     | 509 | CLA  | ND   |
| 31  | b     | 510 | CLA  | ND   |
| 31  | b     | 511 | CLA  | ND   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | b     | 512 | CLA  | ND   |
| 31  | b     | 513 | CLA  | ND   |
| 31  | b     | 514 | CLA  | ND   |
| 31  | b     | 515 | CLA  | ND   |
| 31  | b     | 516 | CLA  | ND   |
| 31  | b     | 517 | CLA  | ND   |
| 31  | c     | 502 | CLA  | ND   |
| 31  | c     | 503 | CLA  | ND   |
| 31  | c     | 504 | CLA  | ND   |
| 31  | c     | 505 | CLA  | ND   |
| 31  | c     | 506 | CLA  | ND   |
| 31  | c     | 507 | CLA  | ND   |
| 31  | c     | 508 | CLA  | ND   |
| 31  | c     | 509 | CLA  | ND   |
| 31  | c     | 510 | CLA  | ND   |
| 31  | c     | 511 | CLA  | ND   |
| 31  | c     | 512 | CLA  | ND   |
| 31  | c     | 513 | CLA  | ND   |
| 31  | c     | 514 | CLA  | ND   |
| 31  | d     | 401 | CLA  | ND   |
| 31  | d     | 403 | CLA  | ND   |
| 31  | d     | 404 | CLA  | ND   |
| 31  | w     | 202 | CLA  | ND   |
| 31  | z     | 101 | CLA  | ND   |
| 31  | 5     | 304 | CLA  | ND   |
| 31  | 5     | 305 | CLA  | ND   |
| 31  | 5     | 306 | CLA  | ND   |
| 31  | 5     | 307 | CLA  | ND   |
| 31  | 5     | 308 | CLA  | ND   |
| 31  | 5     | 309 | CLA  | ND   |
| 31  | 5     | 310 | CLA  | ND   |
| 31  | 5     | 311 | CLA  | ND   |
| 31  | 5     | 312 | CLA  | ND   |
| 31  | 5     | 313 | CLA  | ND   |
| 31  | 5     | 314 | CLA  | ND   |
| 31  | 7     | 305 | CLA  | ND   |
| 31  | 7     | 306 | CLA  | ND   |
| 31  | 7     | 307 | CLA  | ND   |
| 31  | 7     | 308 | CLA  | ND   |
| 31  | 7     | 309 | CLA  | ND   |
| 31  | 7     | 310 | CLA  | ND   |
| 31  | 7     | 311 | CLA  | ND   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 7     | 312 | CLA  | ND   |
| 31  | 7     | 313 | CLA  | ND   |
| 31  | 7     | 314 | CLA  | ND   |
| 31  | 7     | 315 | CLA  | ND   |
| 31  | 7     | 316 | CLA  | ND   |
| 31  | 6     | 201 | CLA  | ND   |
| 31  | 6     | 205 | CLA  | ND   |
| 31  | 6     | 206 | CLA  | ND   |
| 31  | 6     | 207 | CLA  | ND   |
| 31  | 6     | 208 | CLA  | ND   |
| 31  | 6     | 209 | CLA  | ND   |
| 31  | 6     | 210 | CLA  | ND   |
| 31  | 6     | 211 | CLA  | ND   |
| 31  | 6     | 212 | CLA  | ND   |
| 31  | 6     | 213 | CLA  | ND   |
| 31  | 6     | 214 | CLA  | ND   |
| 31  | 6     | 215 | CLA  | ND   |
| 31  | 6     | 216 | CLA  | ND   |
| 31  | p     | 601 | CLA  | ND   |
| 31  | p     | 602 | CLA  | ND   |
| 31  | p     | 603 | CLA  | ND   |
| 31  | p     | 604 | CLA  | ND   |
| 31  | p     | 605 | CLA  | ND   |
| 31  | p     | 606 | CLA  | ND   |
| 31  | p     | 607 | CLA  | ND   |
| 31  | p     | 608 | CLA  | ND   |
| 31  | p     | 609 | CLA  | ND   |
| 31  | 4     | 204 | CLA  | ND   |
| 31  | 4     | 205 | CLA  | ND   |
| 31  | 4     | 206 | CLA  | ND   |
| 31  | 4     | 207 | CLA  | ND   |
| 31  | 4     | 208 | CLA  | ND   |
| 31  | 4     | 209 | CLA  | ND   |
| 31  | 4     | 210 | CLA  | ND   |
| 31  | 4     | 211 | CLA  | ND   |
| 31  | 4     | 212 | CLA  | ND   |
| 31  | 4     | 213 | CLA  | ND   |
| 31  | 3     | 304 | CLA  | ND   |
| 31  | 3     | 305 | CLA  | ND   |
| 31  | 3     | 306 | CLA  | ND   |
| 31  | 3     | 307 | CLA  | ND   |
| 31  | 3     | 308 | CLA  | ND   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 3     | 309 | CLA  | ND   |
| 31  | 3     | 310 | CLA  | ND   |
| 31  | 3     | 311 | CLA  | ND   |
| 31  | 3     | 312 | CLA  | ND   |
| 31  | 3     | 313 | CLA  | ND   |
| 31  | 3     | 314 | CLA  | ND   |
| 31  | P     | 601 | CLA  | ND   |
| 31  | P     | 602 | CLA  | ND   |
| 31  | P     | 603 | CLA  | ND   |
| 31  | P     | 604 | CLA  | ND   |
| 31  | P     | 605 | CLA  | ND   |
| 31  | P     | 606 | CLA  | ND   |
| 31  | P     | 607 | CLA  | ND   |
| 31  | P     | 608 | CLA  | ND   |
| 31  | P     | 609 | CLA  | ND   |
| 31  | 9     | 204 | CLA  | ND   |
| 31  | 9     | 205 | CLA  | ND   |
| 31  | 9     | 206 | CLA  | ND   |
| 31  | 9     | 207 | CLA  | ND   |
| 31  | 9     | 208 | CLA  | ND   |
| 31  | 9     | 209 | CLA  | ND   |
| 31  | 9     | 210 | CLA  | ND   |
| 31  | 9     | 211 | CLA  | ND   |
| 31  | 9     | 212 | CLA  | ND   |
| 31  | 9     | 213 | CLA  | ND   |
| 31  | 8     | 304 | CLA  | ND   |
| 31  | 8     | 305 | CLA  | ND   |
| 31  | 8     | 306 | CLA  | ND   |
| 31  | 8     | 307 | CLA  | ND   |
| 31  | 8     | 308 | CLA  | ND   |
| 31  | 8     | 309 | CLA  | ND   |
| 31  | 8     | 310 | CLA  | ND   |
| 31  | 8     | 311 | CLA  | ND   |
| 31  | 8     | 312 | CLA  | ND   |
| 31  | 8     | 313 | CLA  | ND   |
| 31  | 8     | 314 | CLA  | ND   |
| 31  | 0     | 304 | CLA  | ND   |
| 31  | 0     | 305 | CLA  | ND   |
| 31  | 0     | 306 | CLA  | ND   |
| 31  | 0     | 307 | CLA  | ND   |
| 31  | 0     | 308 | CLA  | ND   |
| 31  | 0     | 309 | CLA  | ND   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 0     | 310 | CLA  | ND   |
| 31  | 0     | 311 | CLA  | ND   |
| 31  | 0     | 312 | CLA  | ND   |
| 31  | 0     | 313 | CLA  | ND   |
| 31  | 0     | 314 | CLA  | ND   |
| 31  | 2     | 305 | CLA  | ND   |
| 31  | 2     | 306 | CLA  | ND   |
| 31  | 2     | 307 | CLA  | ND   |
| 31  | 2     | 308 | CLA  | ND   |
| 31  | 2     | 309 | CLA  | ND   |
| 31  | 2     | 310 | CLA  | ND   |
| 31  | 2     | 311 | CLA  | ND   |
| 31  | 2     | 312 | CLA  | ND   |
| 31  | 2     | 313 | CLA  | ND   |
| 31  | 2     | 314 | CLA  | ND   |
| 31  | 2     | 315 | CLA  | ND   |
| 31  | 2     | 316 | CLA  | ND   |
| 31  | 1     | 201 | CLA  | ND   |
| 31  | 1     | 205 | CLA  | ND   |
| 31  | 1     | 206 | CLA  | ND   |
| 31  | 1     | 207 | CLA  | ND   |
| 31  | 1     | 208 | CLA  | ND   |
| 31  | 1     | 209 | CLA  | ND   |
| 31  | 1     | 210 | CLA  | ND   |
| 31  | 1     | 211 | CLA  | ND   |
| 31  | 1     | 212 | CLA  | ND   |
| 31  | 1     | 213 | CLA  | ND   |
| 31  | 1     | 214 | CLA  | ND   |
| 31  | 1     | 215 | CLA  | ND   |
| 31  | 1     | 216 | CLA  | ND   |

All (2419) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 501 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 501 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 516 | CLA  | C2B-C3B-CAB-CBB |
| 31  | B     | 516 | CLA  | C4B-C3B-CAB-CBB |
| 31  | C     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 31  | C     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 31  | C     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 31  | C     | 508 | CLA  | CHA-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | C     | 513 | CLA  | CHA-CBD-CGD-O1D |
| 31  | C     | 513 | CLA  | CHA-CBD-CGD-O2D |
| 31  | C     | 514 | CLA  | CBD-CGD-O2D-CED |
| 31  | D     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 31  | D     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 31  | Z     | 101 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 31  | b     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 31  | b     | 517 | CLA  | C2B-C3B-CAB-CBB |
| 31  | b     | 517 | CLA  | C4B-C3B-CAB-CBB |
| 31  | c     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 31  | c     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 31  | c     | 508 | CLA  | CHA-CBD-CGD-O2D |
| 31  | c     | 513 | CLA  | CHA-CBD-CGD-O1D |
| 31  | c     | 513 | CLA  | CHA-CBD-CGD-O2D |
| 31  | c     | 514 | CLA  | CBD-CGD-O2D-CED |
| 31  | d     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 31  | z     | 101 | CLA  | C2-C3-C5-C6     |
| 31  | 5     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 307 | CLA  | C6-C7-C8-C9     |
| 31  | 5     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 5     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 312 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 5     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 7     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 7     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 209 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 210 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 210 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 211 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 212 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 213 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 216 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 216 | CLA  | C4B-C3B-CAB-CBB |
| 31  | p     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | p     | 605 | CLA  | C2B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | p     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 31  | p     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 31  | p     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 4     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 204 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 4     | 207 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 4     | 209 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 209 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 308 | CLA  | C2D-C3D-CAD-OB  |
| 31  | 3     | 308 | CLA  | C4D-C3D-CAD-OB  |
| 31  | 3     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | P     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 31  | P     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 31  | P     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 31  | P     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 31  | P     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 9     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 204 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 207 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 209 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 209 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 308 | CLA  | C2D-C3D-CAD-OB  |
| 31  | 8     | 308 | CLA  | C4D-C3D-CAD-OB  |
| 31  | 8     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 312 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 312 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 0     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 307 | CLA  | C6-C7-C8-C9     |
| 31  | 0     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 0     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 0     | 312 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 0     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 2     | 311 | CLA  | CAD-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 1     | 209 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 210 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 210 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 211 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 212 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 213 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 1     | 216 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 1     | 216 | CLA  | C4B-C3B-CAB-CBB |
| 32  | A     | 406 | PHO  | C1A-C2A-CAA-CBA |
| 32  | A     | 406 | PHO  | C3A-C2A-CAA-CBA |
| 32  | a     | 406 | PHO  | C1A-C2A-CAA-CBA |
| 32  | a     | 406 | PHO  | C3A-C2A-CAA-CBA |
| 33  | B     | 519 | BCR  | C7-C8-C9-C10    |
| 33  | B     | 519 | BCR  | C21-C22-C23-C24 |
| 33  | B     | 519 | BCR  | C22-C23-C24-C25 |
| 33  | K     | 101 | BCR  | C6-C7-C8-C9     |
| 33  | K     | 101 | BCR  | C7-C8-C9-C34    |
| 33  | K     | 101 | BCR  | C11-C10-C9-C8   |
| 33  | K     | 101 | BCR  | C10-C11-C12-C13 |
| 33  | K     | 101 | BCR  | C11-C12-C13-C14 |
| 33  | K     | 101 | BCR  | C11-C12-C13-C35 |
| 33  | K     | 101 | BCR  | C12-C13-C14-C15 |
| 33  | K     | 101 | BCR  | C18-C19-C20-C21 |
| 33  | b     | 520 | BCR  | C7-C8-C9-C10    |
| 33  | b     | 520 | BCR  | C21-C22-C23-C24 |
| 33  | b     | 520 | BCR  | C22-C23-C24-C25 |
| 33  | k     | 101 | BCR  | C6-C7-C8-C9     |
| 33  | k     | 101 | BCR  | C7-C8-C9-C34    |
| 33  | k     | 101 | BCR  | C11-C10-C9-C8   |
| 33  | k     | 101 | BCR  | C10-C11-C12-C13 |
| 33  | k     | 101 | BCR  | C11-C12-C13-C14 |
| 33  | k     | 101 | BCR  | C11-C12-C13-C35 |
| 33  | k     | 101 | BCR  | C12-C13-C14-C15 |
| 33  | k     | 101 | BCR  | C18-C19-C20-C21 |
| 34  | A     | 409 | SQD  | O5-C5-C6-S      |
| 34  | A     | 411 | SQD  | C2-C1-O6-C44    |
| 34  | A     | 411 | SQD  | O5-C1-O6-C44    |
| 34  | A     | 411 | SQD  | O5-C5-C6-S      |
| 34  | B     | 522 | SQD  | C2-C1-O6-C44    |
| 34  | B     | 522 | SQD  | O5-C1-O6-C44    |
| 34  | B     | 522 | SQD  | O5-C5-C6-S      |
| 34  | B     | 523 | SQD  | C2-C1-O6-C44    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | B     | 523 | SQD  | O5-C1-O6-C44    |
| 34  | B     | 523 | SQD  | O49-C7-O47-C45  |
| 34  | B     | 523 | SQD  | C8-C7-O47-C45   |
| 34  | a     | 409 | SQD  | O5-C5-C6-S      |
| 34  | b     | 501 | SQD  | C2-C1-O6-C44    |
| 34  | b     | 501 | SQD  | O5-C1-O6-C44    |
| 34  | b     | 501 | SQD  | O49-C7-O47-C45  |
| 34  | b     | 501 | SQD  | C8-C7-O47-C45   |
| 34  | 5     | 316 | SQD  | C5-C6-S-O7      |
| 34  | 0     | 316 | SQD  | C5-C6-S-O7      |
| 35  | A     | 410 | PL9  | C12-C13-C14-C16 |
| 35  | D     | 406 | PL9  | C37-C38-C39-C41 |
| 35  | a     | 410 | PL9  | C12-C13-C14-C16 |
| 35  | d     | 406 | PL9  | C37-C38-C39-C41 |
| 36  | A     | 412 | LHG  | O1-C1-C2-C3     |
| 36  | A     | 413 | LHG  | C3-O3-P-O5      |
| 36  | A     | 413 | LHG  | C3-O3-P-O6      |
| 36  | A     | 413 | LHG  | C4-O6-P-O3      |
| 36  | A     | 413 | LHG  | C4-O6-P-O4      |
| 36  | B     | 521 | LHG  | C3-O3-P-O4      |
| 36  | B     | 521 | LHG  | C3-O3-P-O6      |
| 36  | D     | 407 | LHG  | O1-C1-C2-C3     |
| 36  | D     | 407 | LHG  | O2-C2-C3-O3     |
| 36  | D     | 411 | LHG  | C3-O3-P-O6      |
| 36  | D     | 411 | LHG  | C4-O6-P-O3      |
| 36  | D     | 411 | LHG  | C4-O6-P-O4      |
| 36  | D     | 411 | LHG  | C4-O6-P-O5      |
| 36  | D     | 411 | LHG  | O6-C4-C5-O7     |
| 36  | D     | 412 | LHG  | C4-O6-P-O3      |
| 36  | D     | 412 | LHG  | C4-O6-P-O4      |
| 36  | D     | 412 | LHG  | C4-O6-P-O5      |
| 36  | D     | 412 | LHG  | O7-C5-C6-O8     |
| 36  | H     | 103 | LHG  | C3-O3-P-O6      |
| 36  | a     | 411 | LHG  | O1-C1-C2-C3     |
| 36  | a     | 412 | LHG  | C3-O3-P-O5      |
| 36  | a     | 412 | LHG  | C3-O3-P-O6      |
| 36  | a     | 412 | LHG  | C4-O6-P-O3      |
| 36  | a     | 412 | LHG  | C4-O6-P-O4      |
| 36  | b     | 522 | LHG  | C3-O3-P-O4      |
| 36  | b     | 522 | LHG  | C3-O3-P-O6      |
| 36  | d     | 407 | LHG  | O1-C1-C2-C3     |
| 36  | d     | 407 | LHG  | O2-C2-C3-O3     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | d     | 411 | LHG  | C3-O3-P-O6      |
| 36  | d     | 411 | LHG  | C4-O6-P-O3      |
| 36  | d     | 411 | LHG  | C4-O6-P-O4      |
| 36  | d     | 411 | LHG  | C4-O6-P-O5      |
| 36  | d     | 411 | LHG  | O6-C4-C5-O7     |
| 36  | d     | 412 | LHG  | C4-O6-P-O3      |
| 36  | d     | 412 | LHG  | C4-O6-P-O4      |
| 36  | d     | 412 | LHG  | C4-O6-P-O5      |
| 36  | d     | 412 | LHG  | O7-C5-C6-O8     |
| 36  | h     | 103 | LHG  | C3-O3-P-O5      |
| 36  | h     | 103 | LHG  | C3-O3-P-O6      |
| 37  | C     | 521 | LMG  | O9-C10-O7-C8    |
| 37  | D     | 408 | LMG  | C11-C10-O7-C8   |
| 37  | D     | 409 | LMG  | C11-C10-O7-C8   |
| 37  | W     | 201 | LMG  | O6-C1-O1-C7     |
| 37  | W     | 201 | LMG  | C11-C10-O7-C8   |
| 37  | c     | 521 | LMG  | O9-C10-O7-C8    |
| 37  | d     | 408 | LMG  | C11-C10-O7-C8   |
| 37  | d     | 409 | LMG  | C11-C10-O7-C8   |
| 37  | w     | 201 | LMG  | O6-C1-O1-C7     |
| 37  | w     | 201 | LMG  | C11-C10-O7-C8   |
| 37  | 5     | 315 | LMG  | O6-C1-O1-C7     |
| 37  | 5     | 315 | LMG  | O7-C8-C9-O8     |
| 37  | 0     | 315 | LMG  | O6-C1-O1-C7     |
| 37  | 0     | 315 | LMG  | O7-C8-C9-O8     |
| 39  | C     | 519 | DGD  | C2B-C1B-O2G-C2G |
| 39  | c     | 519 | DGD  | C2B-C1B-O2G-C2G |
| 41  | V     | 201 | HEM  | C1A-C2A-CAA-CBA |
| 41  | v     | 201 | HEM  | C1A-C2A-CAA-CBA |
| 42  | 5     | 301 | A86  | C10-C11-C13-O   |
| 42  | 5     | 301 | A86  | C12-C11-C13-O   |
| 42  | 5     | 301 | A86  | C13-C14-C15-C16 |
| 42  | 5     | 301 | A86  | C13-C14-C15-O1  |
| 42  | 5     | 303 | A86  | C5-C6-C8-C9     |
| 42  | 5     | 303 | A86  | C7-C6-C8-C9     |
| 42  | 5     | 317 | A86  | C10-C11-C13-O   |
| 42  | 5     | 317 | A86  | C10-C11-C13-C14 |
| 42  | 5     | 317 | A86  | C12-C11-C13-O   |
| 42  | 5     | 317 | A86  | C12-C11-C13-C14 |
| 42  | 7     | 301 | A86  | C10-C11-C13-O   |
| 42  | 7     | 301 | A86  | C10-C11-C13-C14 |
| 42  | 7     | 301 | A86  | C12-C11-C13-O   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 42  | 7     | 301 | A86  | C12-C11-C13-C14 |
| 42  | p     | 610 | A86  | C5-C6-C8-C9     |
| 42  | p     | 610 | A86  | C7-C6-C8-C9     |
| 42  | 4     | 201 | A86  | C12-C11-C13-O   |
| 42  | 4     | 202 | A86  | C10-C11-C13-C14 |
| 42  | 4     | 202 | A86  | C12-C11-C13-C14 |
| 42  | 3     | 301 | A86  | C13-C14-C15-C16 |
| 42  | 3     | 301 | A86  | C13-C14-C15-O1  |
| 42  | 3     | 301 | A86  | C3-C4-C5-C6     |
| 42  | 3     | 301 | A86  | C5-C6-C8-C9     |
| 42  | 3     | 301 | A86  | C7-C6-C8-C9     |
| 42  | P     | 610 | A86  | C5-C6-C8-C9     |
| 42  | P     | 610 | A86  | C7-C6-C8-C9     |
| 42  | 9     | 201 | A86  | C12-C11-C13-O   |
| 42  | 9     | 202 | A86  | C10-C11-C13-C14 |
| 42  | 9     | 202 | A86  | C12-C11-C13-C14 |
| 42  | 8     | 301 | A86  | C13-C14-C15-C16 |
| 42  | 8     | 301 | A86  | C13-C14-C15-O1  |
| 42  | 8     | 301 | A86  | C3-C4-C5-C6     |
| 42  | 8     | 301 | A86  | C5-C6-C8-C9     |
| 42  | 8     | 301 | A86  | C7-C6-C8-C9     |
| 42  | 0     | 301 | A86  | C10-C11-C13-O   |
| 42  | 0     | 301 | A86  | C12-C11-C13-O   |
| 42  | 0     | 301 | A86  | C13-C14-C15-C16 |
| 42  | 0     | 301 | A86  | C13-C14-C15-O1  |
| 42  | 0     | 303 | A86  | C5-C6-C8-C9     |
| 42  | 0     | 303 | A86  | C7-C6-C8-C9     |
| 42  | 0     | 317 | A86  | C10-C11-C13-O   |
| 42  | 0     | 317 | A86  | C10-C11-C13-C14 |
| 42  | 0     | 317 | A86  | C12-C11-C13-O   |
| 42  | 0     | 317 | A86  | C12-C11-C13-C14 |
| 42  | 2     | 301 | A86  | C10-C11-C13-O   |
| 42  | 2     | 301 | A86  | C10-C11-C13-C14 |
| 42  | 2     | 301 | A86  | C12-C11-C13-O   |
| 42  | 2     | 301 | A86  | C12-C11-C13-C14 |
| 43  | 5     | 302 | ET4  | C17-C18-C19-C20 |
| 43  | 5     | 302 | ET4  | C01-C06-C07-C08 |
| 43  | 5     | 302 | ET4  | C05-C06-C07-C08 |
| 43  | 5     | 302 | ET4  | C07-C08-C09-C10 |
| 43  | 5     | 302 | ET4  | C07-C08-C09-C27 |
| 43  | 0     | 302 | ET4  | C17-C18-C19-C20 |
| 43  | 0     | 302 | ET4  | C01-C06-C07-C08 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | 0     | 302 | ET4  | C05-C06-C07-C08 |
| 43  | 0     | 302 | ET4  | C07-C08-C09-C10 |
| 43  | 0     | 302 | ET4  | C07-C08-C09-C27 |
| 44  | 7     | 304 | DD6  | C-C1-C24-C25    |
| 44  | 7     | 304 | DD6  | C2-C1-C24-C25   |
| 44  | 7     | 304 | DD6  | C13-C14-C15-C16 |
| 44  | 7     | 304 | DD6  | C13-C14-C15-C20 |
| 44  | 6     | 204 | DD6  | C12-C11-C13-C14 |
| 44  | 6     | 204 | DD6  | C1-C2-C3-C4     |
| 44  | p     | 611 | DD6  | C10-C11-C13-C14 |
| 44  | p     | 611 | DD6  | C12-C11-C13-C14 |
| 44  | P     | 611 | DD6  | C10-C11-C13-C14 |
| 44  | P     | 611 | DD6  | C12-C11-C13-C14 |
| 44  | 2     | 304 | DD6  | C-C1-C24-C25    |
| 44  | 2     | 304 | DD6  | C2-C1-C24-C25   |
| 44  | 2     | 304 | DD6  | C13-C14-C15-C16 |
| 44  | 2     | 304 | DD6  | C13-C14-C15-C20 |
| 44  | 1     | 204 | DD6  | C12-C11-C13-C14 |
| 44  | 1     | 204 | DD6  | C1-C2-C3-C4     |
| 31  | A     | 403 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 504 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 514 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 403 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 504 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 514 | CLA  | O1D-CGD-O2D-CED |
| 42  | 5     | 317 | A86  | C39-C38-O4-C34  |
| 42  | 7     | 301 | A86  | C39-C38-O4-C34  |
| 42  | 6     | 202 | A86  | C39-C38-O4-C34  |
| 42  | p     | 610 | A86  | C39-C38-O4-C34  |
| 42  | 4     | 201 | A86  | C39-C38-O4-C34  |
| 42  | 3     | 301 | A86  | C39-C38-O4-C34  |
| 42  | P     | 610 | A86  | C39-C38-O4-C34  |
| 42  | 9     | 201 | A86  | C39-C38-O4-C34  |
| 42  | 8     | 301 | A86  | C39-C38-O4-C34  |
| 42  | 0     | 317 | A86  | C39-C38-O4-C34  |
| 42  | 2     | 301 | A86  | C39-C38-O4-C34  |
| 42  | 1     | 202 | A86  | C39-C38-O4-C34  |
| 31  | 7     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 211 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 211 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 403 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 505 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 509 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 516 | CLA  | CBD-CGD-O2D-CED |
| 31  | C     | 504 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 403 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 506 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 510 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 517 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 504 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 207 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 208 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 207 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 208 | CLA  | CBD-CGD-O2D-CED |
| 37  | D     | 409 | LMG  | O10-C28-O8-C9   |
| 37  | d     | 409 | LMG  | O10-C28-O8-C9   |
| 37  | 5     | 315 | LMG  | O10-C28-O8-C9   |
| 37  | 0     | 315 | LMG  | O10-C28-O8-C9   |
| 31  | 5     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 212 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 212 | CLA  | O1D-CGD-O2D-CED |
| 42  | 3     | 302 | A86  | C39-C38-O4-C34  |
| 42  | 8     | 302 | A86  | C39-C38-O4-C34  |
| 31  | 5     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 210 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 210 | CLA  | O1D-CGD-O2D-CED |
| 37  | D     | 409 | LMG  | C29-C28-O8-C9   |
| 37  | M     | 102 | LMG  | C29-C28-O8-C9   |
| 37  | d     | 409 | LMG  | C29-C28-O8-C9   |
| 37  | m     | 102 | LMG  | C29-C28-O8-C9   |
| 37  | 5     | 315 | LMG  | C29-C28-O8-C9   |
| 37  | 0     | 315 | LMG  | C29-C28-O8-C9   |
| 31  | A     | 403 | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 502 | CLA  | O1A-CGA-O2A-C1  |
| 31  | a     | 403 | CLA  | O1A-CGA-O2A-C1  |
| 31  | b     | 503 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 0     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 0     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 2     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 32  | A     | 405 | PHO  | O1A-CGA-O2A-C1  |
| 32  | a     | 405 | PHO  | O1A-CGA-O2A-C1  |
| 37  | M     | 102 | LMG  | O10-C28-O8-C9   |
| 37  | W     | 201 | LMG  | O10-C28-O8-C9   |
| 37  | m     | 102 | LMG  | O10-C28-O8-C9   |
| 37  | w     | 201 | LMG  | O10-C28-O8-C9   |
| 39  | C     | 519 | DGD  | C4E-C5E-C6E-O5E |
| 39  | c     | 519 | DGD  | C4E-C5E-C6E-O5E |
| 42  | 5     | 317 | A86  | O5-C38-O4-C34   |
| 42  | 7     | 301 | A86  | O5-C38-O4-C34   |
| 42  | 6     | 202 | A86  | O5-C38-O4-C34   |
| 42  | p     | 610 | A86  | O5-C38-O4-C34   |
| 42  | 4     | 201 | A86  | O5-C38-O4-C34   |
| 42  | 3     | 301 | A86  | O5-C38-O4-C34   |
| 42  | P     | 610 | A86  | O5-C38-O4-C34   |
| 42  | 9     | 201 | A86  | O5-C38-O4-C34   |
| 42  | 8     | 301 | A86  | O5-C38-O4-C34   |
| 42  | 0     | 317 | A86  | O5-C38-O4-C34   |
| 42  | 2     | 301 | A86  | O5-C38-O4-C34   |
| 42  | 1     | 202 | A86  | O5-C38-O4-C34   |
| 39  | C     | 518 | DGD  | C4E-C5E-C6E-O5E |
| 39  | c     | 518 | DGD  | C4E-C5E-C6E-O5E |
| 36  | H     | 103 | LHG  | O9-C7-O7-C5     |
| 36  | h     | 103 | LHG  | O9-C7-O7-C5     |
| 37  | D     | 409 | LMG  | O9-C10-O7-C8    |
| 37  | d     | 409 | LMG  | O9-C10-O7-C8    |
| 39  | C     | 519 | DGD  | O1B-C1B-O2G-C2G |
| 39  | c     | 519 | DGD  | O1B-C1B-O2G-C2G |
| 31  | a     | 407 | CLA  | C3-C5-C6-C7     |
| 31  | 5     | 308 | CLA  | C3-C5-C6-C7     |
| 31  | 5     | 310 | CLA  | C3-C5-C6-C7     |
| 31  | 0     | 308 | CLA  | C3-C5-C6-C7     |
| 31  | 0     | 310 | CLA  | C3-C5-C6-C7     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 502 | CLA  | CBA-CGA-O2A-C1  |
| 31  | b     | 503 | CLA  | CBA-CGA-O2A-C1  |
| 32  | A     | 405 | PHO  | CBA-CGA-O2A-C1  |
| 32  | a     | 405 | PHO  | CBA-CGA-O2A-C1  |
| 37  | W     | 201 | LMG  | C29-C28-O8-C9   |
| 37  | w     | 201 | LMG  | C29-C28-O8-C9   |
| 31  | B     | 507 | CLA  | CBD-CGD-O2D-CED |
| 31  | C     | 507 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 508 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 507 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 201 | CLA  | CBD-CGD-O2D-CED |
| 31  | p     | 602 | CLA  | CBD-CGD-O2D-CED |
| 31  | P     | 602 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 201 | CLA  | CBD-CGD-O2D-CED |
| 34  | A     | 411 | SQD  | C8-C7-O47-C45   |
| 34  | B     | 522 | SQD  | C8-C7-O47-C45   |
| 36  | D     | 411 | LHG  | C8-C7-O7-C5     |
| 36  | d     | 411 | LHG  | C8-C7-O7-C5     |
| 37  | C     | 521 | LMG  | C11-C10-O7-C8   |
| 37  | c     | 521 | LMG  | C11-C10-O7-C8   |
| 31  | 5     | 307 | CLA  | C4-C3-C5-C6     |
| 31  | 0     | 307 | CLA  | C4-C3-C5-C6     |
| 31  | 5     | 307 | CLA  | C2-C3-C5-C6     |
| 31  | 0     | 307 | CLA  | C2-C3-C5-C6     |
| 31  | 6     | 207 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 207 | CLA  | O1D-CGD-O2D-CED |
| 39  | C     | 519 | DGD  | O6E-C5E-C6E-O5E |
| 39  | c     | 519 | DGD  | O6E-C5E-C6E-O5E |
| 37  | J     | 101 | LMG  | C4-C5-C6-O5     |
| 37  | j     | 101 | LMG  | C4-C5-C6-O5     |
| 31  | A     | 407 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 504 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 514 | CLA  | C3-C5-C6-C7     |
| 31  | b     | 505 | CLA  | C3-C5-C6-C7     |
| 31  | b     | 515 | CLA  | C3-C5-C6-C7     |
| 32  | A     | 405 | PHO  | C3-C5-C6-C7     |
| 32  | A     | 406 | PHO  | C3-C5-C6-C7     |
| 32  | a     | 405 | PHO  | C3-C5-C6-C7     |
| 32  | a     | 406 | PHO  | C3-C5-C6-C7     |
| 31  | A     | 403 | CLA  | CBA-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | D     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 31  | a     | 403 | CLA  | CBA-CGA-O2A-C1  |
| 31  | d     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 5     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 5     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 0     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 0     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 2     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 35  | A     | 410 | PL9  | C12-C13-C14-C15 |
| 35  | a     | 410 | PL9  | C12-C13-C14-C15 |
| 42  | p     | 610 | A86  | C11-C10-C9-C8   |
| 42  | P     | 610 | A86  | C11-C10-C9-C8   |
| 44  | 7     | 304 | DD6  | C24-C25-C26-C27 |
| 44  | 6     | 204 | DD6  | C3-C4-C5-C6     |
| 44  | 2     | 304 | DD6  | C24-C25-C26-C27 |
| 44  | 1     | 204 | DD6  | C3-C4-C5-C6     |
| 34  | A     | 411 | SQD  | O49-C7-O47-C45  |
| 34  | B     | 522 | SQD  | O49-C7-O47-C45  |
| 36  | D     | 411 | LHG  | O9-C7-O7-C5     |
| 36  | d     | 411 | LHG  | O9-C7-O7-C5     |
| 37  | D     | 410 | LMG  | O9-C10-O7-C8    |
| 37  | d     | 408 | LMG  | O9-C10-O7-C8    |
| 37  | d     | 410 | LMG  | O9-C10-O7-C8    |
| 31  | B     | 509 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 510 | CLA  | O1D-CGD-O2D-CED |
| 37  | C     | 521 | LMG  | C21-C22-C23-C24 |
| 37  | c     | 521 | LMG  | C21-C22-C23-C24 |
| 39  | C     | 518 | DGD  | O6E-C5E-C6E-O5E |
| 39  | c     | 518 | DGD  | O6E-C5E-C6E-O5E |
| 31  | B     | 505 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 506 | CLA  | O1D-CGD-O2D-CED |
| 42  | 5     | 303 | A86  | C39-C38-O4-C34  |
| 42  | 4     | 202 | A86  | C39-C38-O4-C34  |
| 42  | 3     | 302 | A86  | O5-C38-O4-C34   |
| 42  | 9     | 202 | A86  | C39-C38-O4-C34  |
| 42  | 0     | 303 | A86  | C39-C38-O4-C34  |
| 31  | 5     | 307 | CLA  | C3-C5-C6-C7     |
| 31  | 0     | 307 | CLA  | C3-C5-C6-C7     |
| 31  | 7     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 308 | CLA  | O1D-CGD-O2D-CED |
| 36  | H     | 103 | LHG  | C24-C23-O8-C6   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | h     | 103 | LHG  | C24-C23-O8-C6   |
| 37  | W     | 201 | LMG  | C4-C5-C6-O5     |
| 37  | w     | 201 | LMG  | C4-C5-C6-O5     |
| 42  | 5     | 301 | A86  | C39-C38-O4-C34  |
| 42  | 5     | 301 | A86  | O5-C38-O4-C34   |
| 42  | 5     | 303 | A86  | O5-C38-O4-C34   |
| 42  | 7     | 302 | A86  | C39-C38-O4-C34  |
| 42  | 7     | 302 | A86  | O5-C38-O4-C34   |
| 42  | 4     | 202 | A86  | O5-C38-O4-C34   |
| 42  | 4     | 203 | A86  | C39-C38-O4-C34  |
| 42  | 4     | 203 | A86  | O5-C38-O4-C34   |
| 42  | 9     | 202 | A86  | O5-C38-O4-C34   |
| 42  | 9     | 203 | A86  | C39-C38-O4-C34  |
| 42  | 9     | 203 | A86  | O5-C38-O4-C34   |
| 42  | 8     | 302 | A86  | O5-C38-O4-C34   |
| 42  | 0     | 301 | A86  | C39-C38-O4-C34  |
| 42  | 0     | 301 | A86  | O5-C38-O4-C34   |
| 42  | 0     | 303 | A86  | O5-C38-O4-C34   |
| 42  | 2     | 302 | A86  | C39-C38-O4-C34  |
| 42  | 2     | 302 | A86  | O5-C38-O4-C34   |
| 31  | 7     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 307 | CLA  | CBD-CGD-O2D-CED |
| 36  | H     | 103 | LHG  | C8-C7-O7-C5     |
| 36  | h     | 103 | LHG  | C8-C7-O7-C5     |
| 37  | D     | 410 | LMG  | C11-C10-O7-C8   |
| 37  | d     | 410 | LMG  | C11-C10-O7-C8   |
| 42  | 4     | 202 | A86  | C35-C34-O4-C38  |
| 31  | 6     | 208 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 208 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 516 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 517 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 511 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 512 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 503 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 504 | CLA  | C2-C3-C5-C6     |
| 31  | D     | 404 | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | d     | 404 | CLA  | O1A-CGA-O2A-C1  |
| 36  | H     | 103 | LHG  | O10-C23-O8-C6   |
| 36  | h     | 103 | LHG  | O10-C23-O8-C6   |
| 39  | C     | 519 | DGD  | O1A-C1A-O1G-C1G |
| 39  | c     | 519 | DGD  | O1A-C1A-O1G-C1G |
| 37  | D     | 408 | LMG  | O9-C10-O7-C8    |
| 35  | A     | 410 | PL9  | C9-C11-C12-C13  |
| 35  | A     | 410 | PL9  | C14-C16-C17-C18 |
| 35  | D     | 406 | PL9  | C39-C41-C42-C43 |
| 35  | a     | 410 | PL9  | C9-C11-C12-C13  |
| 35  | a     | 410 | PL9  | C14-C16-C17-C18 |
| 35  | d     | 406 | PL9  | C39-C41-C42-C43 |
| 42  | 9     | 202 | A86  | C35-C34-O4-C38  |
| 31  | C     | 503 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 503 | CLA  | CBD-CGD-O2D-CED |
| 37  | D     | 408 | LMG  | O6-C5-C6-O5     |
| 37  | d     | 408 | LMG  | O6-C5-C6-O5     |
| 31  | 6     | 210 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 1     | 210 | CLA  | CBA-CGA-O2A-C1  |
| 31  | C     | 512 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 512 | CLA  | CBD-CGD-O2D-CED |
| 36  | D     | 407 | LHG  | C23-C24-C25-C26 |
| 36  | d     | 407 | LHG  | C23-C24-C25-C26 |
| 37  | J     | 101 | LMG  | O6-C5-C6-O5     |
| 37  | j     | 101 | LMG  | O6-C5-C6-O5     |
| 37  | W     | 201 | LMG  | O6-C5-C6-O5     |
| 37  | w     | 201 | LMG  | O6-C5-C6-O5     |
| 35  | A     | 410 | PL9  | C17-C18-C19-C21 |
| 35  | a     | 410 | PL9  | C17-C18-C19-C21 |
| 31  | B     | 503 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 504 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 210 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 1     | 210 | CLA  | O1A-CGA-O2A-C1  |
| 37  | D     | 410 | LMG  | O10-C28-O8-C9   |
| 37  | d     | 410 | LMG  | O10-C28-O8-C9   |
| 36  | A     | 412 | LHG  | C1-C2-C3-O3     |
| 36  | D     | 407 | LHG  | C1-C2-C3-O3     |
| 36  | a     | 411 | LHG  | C1-C2-C3-O3     |
| 36  | d     | 407 | LHG  | C1-C2-C3-O3     |
| 36  | D     | 412 | LHG  | C24-C23-O8-C6   |
| 36  | d     | 412 | LHG  | C24-C23-O8-C6   |
| 37  | D     | 410 | LMG  | C29-C28-O8-C9   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | d     | 410 | LMG  | C29-C28-O8-C9   |
| 39  | C     | 519 | DGD  | C2A-C1A-O1G-C1G |
| 39  | c     | 519 | DGD  | C2A-C1A-O1G-C1G |
| 31  | Z     | 101 | CLA  | CBD-CGD-O2D-CED |
| 31  | z     | 101 | CLA  | CBD-CGD-O2D-CED |
| 36  | A     | 412 | LHG  | C32-C33-C34-C35 |
| 36  | a     | 411 | LHG  | C32-C33-C34-C35 |
| 37  | C     | 521 | LMG  | C19-C20-C21-C22 |
| 37  | c     | 521 | LMG  | C19-C20-C21-C22 |
| 37  | J     | 101 | LMG  | C17-C18-C19-C20 |
| 37  | j     | 101 | LMG  | C17-C18-C19-C20 |
| 31  | B     | 503 | CLA  | C4-C3-C5-C6     |
| 31  | b     | 504 | CLA  | C4-C3-C5-C6     |
| 31  | C     | 505 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 505 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 502 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 504 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 505 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 514 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 516 | CLA  | C6-C7-C8-C9     |
| 31  | C     | 508 | CLA  | C11-C10-C8-C9   |
| 31  | C     | 508 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 510 | CLA  | C6-C7-C8-C9     |
| 31  | b     | 503 | CLA  | C11-C12-C13-C14 |
| 31  | b     | 505 | CLA  | C14-C13-C15-C16 |
| 31  | b     | 506 | CLA  | C14-C13-C15-C16 |
| 31  | b     | 515 | CLA  | C11-C10-C8-C9   |
| 31  | b     | 517 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 508 | CLA  | C11-C10-C8-C9   |
| 31  | c     | 508 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 510 | CLA  | C6-C7-C8-C9     |
| 31  | 5     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | 7     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | 6     | 210 | CLA  | C11-C12-C13-C14 |
| 31  | 0     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | 2     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | 1     | 210 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 507 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 507 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 508 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 507 | CLA  | O1D-CGD-O2D-CED |
| 37  | 5     | 315 | LMG  | C28-C29-C30-C31 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | 0     | 315 | LMG  | C28-C29-C30-C31 |
| 36  | A     | 412 | LHG  | O2-C2-C3-O3     |
| 36  | a     | 411 | LHG  | O2-C2-C3-O3     |
| 31  | 6     | 201 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 201 | CLA  | O1D-CGD-O2D-CED |
| 33  | B     | 519 | BCR  | C37-C22-C23-C24 |
| 33  | b     | 520 | BCR  | C37-C22-C23-C24 |
| 43  | 5     | 302 | ET4  | C30-C18-C19-C20 |
| 43  | 0     | 302 | ET4  | C30-C18-C19-C20 |
| 44  | 7     | 303 | DD6  | C12-C11-C13-C14 |
| 44  | 6     | 203 | DD6  | C12-C11-C13-C14 |
| 44  | 3     | 303 | DD6  | C12-C11-C13-C14 |
| 44  | 8     | 303 | DD6  | C12-C11-C13-C14 |
| 44  | 2     | 303 | DD6  | C12-C11-C13-C14 |
| 44  | 1     | 203 | DD6  | C12-C11-C13-C14 |
| 33  | K     | 101 | BCR  | C7-C8-C9-C10    |
| 33  | k     | 101 | BCR  | C7-C8-C9-C10    |
| 44  | 7     | 303 | DD6  | C10-C11-C13-C14 |
| 44  | 6     | 203 | DD6  | C10-C11-C13-C14 |
| 44  | 6     | 204 | DD6  | C10-C11-C13-C14 |
| 44  | 2     | 303 | DD6  | C10-C11-C13-C14 |
| 44  | 1     | 203 | DD6  | C10-C11-C13-C14 |
| 44  | 1     | 204 | DD6  | C10-C11-C13-C14 |
| 41  | V     | 201 | HEM  | C3A-C2A-CAA-CBA |
| 41  | v     | 201 | HEM  | C3A-C2A-CAA-CBA |
| 36  | A     | 413 | LHG  | O6-C4-C5-O7     |
| 36  | a     | 412 | LHG  | O6-C4-C5-O7     |
| 37  | M     | 102 | LMG  | C11-C10-O7-C8   |
| 37  | m     | 102 | LMG  | C11-C10-O7-C8   |
| 37  | J     | 101 | LMG  | C23-C24-C25-C26 |
| 37  | j     | 101 | LMG  | C23-C24-C25-C26 |
| 31  | C     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 505 | CLA  | CBA-CGA-O2A-C1  |
| 37  | M     | 102 | LMG  | C28-C29-C30-C31 |
| 37  | m     | 102 | LMG  | C28-C29-C30-C31 |
| 31  | p     | 602 | CLA  | O1D-CGD-O2D-CED |
| 31  | P     | 602 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 514 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 515 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 515 | CLA  | C8-C10-C11-C12  |
| 31  | b     | 516 | CLA  | C15-C16-C17-C18 |
| 34  | A     | 409 | SQD  | C7-C8-C9-C10    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | a     | 409 | SQD  | C7-C8-C9-C10    |
| 31  | C     | 502 | CLA  | CBD-CGD-O2D-CED |
| 31  | c     | 502 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 309 | CLA  | C11-C10-C8-C7   |
| 31  | 2     | 309 | CLA  | C11-C10-C8-C7   |
| 34  | A     | 411 | SQD  | C9-C10-C11-C12  |
| 34  | B     | 522 | SQD  | C9-C10-C11-C12  |
| 39  | h     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 44  | 7     | 304 | DD6  | C1-C2-C3-C4     |
| 44  | 6     | 204 | DD6  | C11-C10-C9-C8   |
| 44  | 2     | 304 | DD6  | C1-C2-C3-C4     |
| 44  | 1     | 204 | DD6  | C11-C10-C9-C8   |
| 37  | W     | 201 | LMG  | O9-C10-O7-C8    |
| 37  | w     | 201 | LMG  | O9-C10-O7-C8    |
| 39  | H     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 31  | B     | 504 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 505 | CLA  | C15-C16-C17-C18 |
| 37  | C     | 521 | LMG  | C34-C35-C36-C37 |
| 37  | c     | 521 | LMG  | C34-C35-C36-C37 |
| 34  | 5     | 316 | SQD  | C7-C8-C9-C10    |
| 34  | 0     | 316 | SQD  | C7-C8-C9-C10    |
| 36  | A     | 413 | LHG  | C7-C8-C9-C10    |
| 36  | D     | 407 | LHG  | C7-C8-C9-C10    |
| 36  | a     | 412 | LHG  | C7-C8-C9-C10    |
| 36  | d     | 407 | LHG  | C7-C8-C9-C10    |
| 37  | D     | 410 | LMG  | C28-C29-C30-C31 |
| 37  | d     | 410 | LMG  | C28-C29-C30-C31 |
| 31  | B     | 504 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 505 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 506 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 510 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 511 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 508 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 509 | CLA  | C15-C16-C17-C18 |
| 31  | 7     | 310 | CLA  | C5-C6-C7-C8     |
| 31  | 2     | 310 | CLA  | C5-C6-C7-C8     |
| 37  | J     | 101 | LMG  | C28-C29-C30-C31 |
| 37  | j     | 101 | LMG  | C28-C29-C30-C31 |
| 39  | C     | 518 | DGD  | O6D-C1D-O3G-C3G |
| 39  | C     | 519 | DGD  | O6E-C1E-O5D-C6D |
| 39  | c     | 518 | DGD  | O6D-C1D-O3G-C3G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 39  | c     | 519 | DGD  | O6E-C1E-O5D-C6D |
| 37  | J     | 101 | LMG  | C11-C12-C13-C14 |
| 37  | j     | 101 | LMG  | C11-C12-C13-C14 |
| 31  | 5     | 307 | CLA  | C8-C10-C11-C12  |
| 31  | 0     | 307 | CLA  | C8-C10-C11-C12  |
| 31  | 6     | 209 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 209 | CLA  | CBD-CGD-O2D-CED |
| 36  | B     | 521 | LHG  | C23-C24-C25-C26 |
| 36  | b     | 522 | LHG  | C23-C24-C25-C26 |
| 31  | B     | 505 | CLA  | C5-C6-C7-C8     |
| 31  | C     | 505 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 506 | CLA  | C5-C6-C7-C8     |
| 31  | c     | 505 | CLA  | C13-C15-C16-C17 |
| 34  | 0     | 316 | SQD  | C35-C36-C37-C38 |
| 37  | c     | 521 | LMG  | C17-C18-C19-C20 |
| 37  | B     | 520 | LMG  | O6-C5-C6-O5     |
| 37  | b     | 521 | LMG  | O6-C5-C6-O5     |
| 31  | c     | 508 | CLA  | C15-C16-C17-C18 |
| 31  | 5     | 308 | CLA  | C5-C6-C7-C8     |
| 31  | 0     | 308 | CLA  | C5-C6-C7-C8     |
| 31  | 7     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 2     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 34  | 5     | 316 | SQD  | C35-C36-C37-C38 |
| 36  | D     | 412 | LHG  | C8-C7-O7-C5     |
| 36  | d     | 412 | LHG  | C8-C7-O7-C5     |
| 42  | 4     | 201 | A86  | C35-C34-O4-C38  |
| 42  | 9     | 201 | A86  | C35-C34-O4-C38  |
| 37  | C     | 521 | LMG  | C17-C18-C19-C20 |
| 37  | J     | 101 | LMG  | C19-C20-C21-C22 |
| 37  | j     | 101 | LMG  | C19-C20-C21-C22 |
| 31  | C     | 505 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 505 | CLA  | O1A-CGA-O2A-C1  |
| 37  | D     | 408 | LMG  | C10-C11-C12-C13 |
| 37  | d     | 408 | LMG  | C10-C11-C12-C13 |
| 31  | C     | 512 | CLA  | C3-C5-C6-C7     |
| 31  | c     | 512 | CLA  | C3-C5-C6-C7     |
| 44  | 7     | 304 | DD6  | C11-C10-C9-C8   |
| 44  | 7     | 304 | DD6  | C3-C4-C5-C6     |
| 44  | 2     | 304 | DD6  | C11-C10-C9-C8   |
| 44  | 2     | 304 | DD6  | C3-C4-C5-C6     |
| 31  | C     | 508 | CLA  | C15-C16-C17-C18 |
| 34  | 5     | 316 | SQD  | C31-C32-C33-C34 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 0     | 316 | SQD  | C31-C32-C33-C34 |
| 37  | C     | 521 | LMG  | C38-C39-C40-C41 |
| 37  | c     | 521 | LMG  | C38-C39-C40-C41 |
| 31  | B     | 513 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 514 | CLA  | C13-C15-C16-C17 |
| 31  | 5     | 305 | CLA  | C5-C6-C7-C8     |
| 31  | 6     | 211 | CLA  | C5-C6-C7-C8     |
| 31  | 0     | 305 | CLA  | C5-C6-C7-C8     |
| 31  | 1     | 211 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 510 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 513 | CLA  | C8-C10-C11-C12  |
| 31  | C     | 508 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 511 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 514 | CLA  | C8-C10-C11-C12  |
| 31  | c     | 508 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 403 | CLA  | C13-C15-C16-C17 |
| 31  | D     | 403 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 403 | CLA  | C13-C15-C16-C17 |
| 31  | d     | 403 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 509 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 510 | CLA  | C15-C16-C17-C18 |
| 39  | C     | 518 | DGD  | C2D-C1D-O3G-C3G |
| 39  | C     | 519 | DGD  | C2E-C1E-O5D-C6D |
| 39  | c     | 518 | DGD  | C2D-C1D-O3G-C3G |
| 39  | c     | 519 | DGD  | C2E-C1E-O5D-C6D |
| 35  | A     | 410 | PL9  | C22-C23-C24-C26 |
| 35  | a     | 410 | PL9  | C22-C23-C24-C26 |
| 36  | d     | 411 | LHG  | C7-C8-C9-C10    |
| 34  | 5     | 316 | SQD  | C27-C28-C29-C30 |
| 34  | 0     | 316 | SQD  | C27-C28-C29-C30 |
| 33  | B     | 517 | BCR  | C20-C21-C22-C37 |
| 33  | K     | 101 | BCR  | C11-C10-C9-C34  |
| 33  | K     | 101 | BCR  | C35-C13-C14-C15 |
| 33  | b     | 518 | BCR  | C20-C21-C22-C37 |
| 33  | k     | 101 | BCR  | C11-C10-C9-C34  |
| 33  | k     | 101 | BCR  | C35-C13-C14-C15 |
| 36  | D     | 411 | LHG  | C7-C8-C9-C10    |
| 31  | B     | 504 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 505 | CLA  | CBD-CGD-O2D-CED |
| 33  | C     | 516 | BCR  | C37-C22-C23-C24 |
| 33  | c     | 516 | BCR  | C37-C22-C23-C24 |
| 44  | 7     | 304 | DD6  | C7-C6-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 44  | 2     | 304 | DD6  | C7-C6-C8-C9     |
| 33  | C     | 516 | BCR  | C21-C22-C23-C24 |
| 33  | c     | 516 | BCR  | C21-C22-C23-C24 |
| 44  | 7     | 304 | DD6  | C5-C6-C8-C9     |
| 44  | 2     | 304 | DD6  | C5-C6-C8-C9     |
| 36  | A     | 413 | LHG  | O1-C1-C2-C3     |
| 36  | D     | 411 | LHG  | O1-C1-C2-C3     |
| 36  | a     | 412 | LHG  | O1-C1-C2-C3     |
| 36  | d     | 411 | LHG  | O1-C1-C2-C3     |
| 31  | 7     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 307 | CLA  | O1D-CGD-O2D-CED |
| 39  | C     | 519 | DGD  | C3G-C2G-O2G-C1B |
| 39  | c     | 519 | DGD  | C3G-C2G-O2G-C1B |
| 31  | C     | 506 | CLA  | C16-C17-C18-C19 |
| 31  | c     | 506 | CLA  | C16-C17-C18-C19 |
| 31  | B     | 511 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 512 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 308 | CLA  | O1D-CGD-O2D-CED |
| 42  | p     | 610 | A86  | C33-C34-O4-C38  |
| 42  | P     | 610 | A86  | C33-C34-O4-C38  |
| 31  | c     | 503 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 503 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 515 | CLA  | C16-C17-C18-C19 |
| 31  | C     | 506 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 516 | CLA  | C16-C17-C18-C19 |
| 31  | c     | 506 | CLA  | C16-C17-C18-C20 |
| 36  | B     | 521 | LHG  | C12-C13-C14-C15 |
| 36  | B     | 521 | LHG  | C31-C32-C33-C34 |
| 36  | D     | 411 | LHG  | C16-C17-C18-C19 |
| 36  | b     | 522 | LHG  | C12-C13-C14-C15 |
| 36  | b     | 522 | LHG  | C31-C32-C33-C34 |
| 36  | d     | 407 | LHG  | C13-C14-C15-C16 |
| 36  | d     | 411 | LHG  | C16-C17-C18-C19 |
| 37  | W     | 201 | LMG  | C30-C31-C32-C33 |
| 37  | w     | 201 | LMG  | C30-C31-C32-C33 |
| 36  | D     | 407 | LHG  | C13-C14-C15-C16 |
| 36  | D     | 407 | LHG  | C32-C33-C34-C35 |
| 36  | d     | 407 | LHG  | C32-C33-C34-C35 |
| 37  | D     | 408 | LMG  | C18-C19-C20-C21 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | J     | 101 | LMG  | C21-C22-C23-C24 |
| 37  | M     | 101 | LMG  | C33-C34-C35-C36 |
| 37  | W     | 201 | LMG  | C12-C13-C14-C15 |
| 37  | d     | 408 | LMG  | C18-C19-C20-C21 |
| 37  | j     | 101 | LMG  | C21-C22-C23-C24 |
| 37  | m     | 101 | LMG  | C33-C34-C35-C36 |
| 36  | d     | 412 | LHG  | C23-C24-C25-C26 |
| 37  | C     | 521 | LMG  | C36-C37-C38-C39 |
| 37  | c     | 521 | LMG  | C36-C37-C38-C39 |
| 37  | w     | 201 | LMG  | C12-C13-C14-C15 |
| 37  | y     | 101 | LMG  | C11-C12-C13-C14 |
| 39  | C     | 519 | DGD  | C4B-C5B-C6B-C7B |
| 39  | c     | 519 | DGD  | C4B-C5B-C6B-C7B |
| 31  | 7     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 34  | A     | 409 | SQD  | C27-C28-C29-C30 |
| 34  | a     | 409 | SQD  | C27-C28-C29-C30 |
| 37  | M     | 102 | LMG  | C34-C35-C36-C37 |
| 37  | m     | 102 | LMG  | C34-C35-C36-C37 |
| 39  | C     | 518 | DGD  | C6B-C7B-C8B-C9B |
| 34  | A     | 409 | SQD  | C14-C15-C16-C17 |
| 34  | a     | 409 | SQD  | C14-C15-C16-C17 |
| 37  | C     | 521 | LMG  | C13-C14-C15-C16 |
| 37  | D     | 409 | LMG  | C29-C30-C31-C32 |
| 37  | Y     | 101 | LMG  | C30-C31-C32-C33 |
| 37  | c     | 521 | LMG  | C13-C14-C15-C16 |
| 37  | d     | 409 | LMG  | C29-C30-C31-C32 |
| 37  | y     | 101 | LMG  | C30-C31-C32-C33 |
| 39  | c     | 518 | DGD  | C6B-C7B-C8B-C9B |
| 31  | 5     | 309 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 213 | CLA  | C4B-C3B-CAB-CBB |
| 31  | p     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 4     | 208 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 308 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | P     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 208 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 308 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 0     | 309 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 2     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 1     | 213 | CLA  | C4B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | D     | 412 | LHG  | C23-C24-C25-C26 |
| 37  | Y     | 101 | LMG  | C11-C12-C13-C14 |
| 39  | H     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 39  | h     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 31  | B     | 515 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 516 | CLA  | C16-C17-C18-C20 |
| 31  | 2     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 31  | D     | 403 | CLA  | C8-C10-C11-C12  |
| 31  | d     | 403 | CLA  | C8-C10-C11-C12  |
| 37  | Y     | 101 | LMG  | C11-C10-O7-C8   |
| 37  | y     | 101 | LMG  | C11-C10-O7-C8   |
| 37  | C     | 521 | LMG  | C32-C33-C34-C35 |
| 37  | c     | 521 | LMG  | C32-C33-C34-C35 |
| 37  | J     | 101 | LMG  | C35-C36-C37-C38 |
| 37  | d     | 408 | LMG  | C17-C18-C19-C20 |
| 37  | 5     | 315 | LMG  | C31-C32-C33-C34 |
| 37  | 0     | 315 | LMG  | C31-C32-C33-C34 |
| 34  | A     | 411 | SQD  | C7-C8-C9-C10    |
| 34  | B     | 522 | SQD  | C7-C8-C9-C10    |
| 36  | A     | 412 | LHG  | C7-C8-C9-C10    |
| 36  | a     | 411 | LHG  | C7-C8-C9-C10    |
| 37  | D     | 408 | LMG  | C17-C18-C19-C20 |
| 37  | D     | 408 | LMG  | C32-C33-C34-C35 |
| 37  | d     | 408 | LMG  | C32-C33-C34-C35 |
| 37  | j     | 101 | LMG  | C35-C36-C37-C38 |
| 31  | A     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 502 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 516 | CLA  | C3A-C2A-CAA-CBA |
| 31  | a     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 503 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 517 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 209 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 210 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 0     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 2     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 1     | 209 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 1     | 210 | CLA  | C3A-C2A-CAA-CBA |
| 31  | C     | 512 | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | c     | 512 | CLA  | O1D-CGD-O2D-CED |
| 37  | y     | 101 | LMG  | C39-C40-C41-C42 |
| 37  | Y     | 101 | LMG  | C39-C40-C41-C42 |
| 31  | A     | 403 | CLA  | C16-C17-C18-C20 |
| 31  | A     | 407 | CLA  | C11-C12-C13-C14 |
| 31  | a     | 403 | CLA  | C16-C17-C18-C20 |
| 31  | a     | 407 | CLA  | C11-C12-C13-C14 |
| 31  | 7     | 310 | CLA  | C6-C7-C8-C10    |
| 31  | 2     | 310 | CLA  | C6-C7-C8-C10    |
| 37  | Y     | 101 | LMG  | C31-C32-C33-C34 |
| 37  | y     | 101 | LMG  | C31-C32-C33-C34 |
| 34  | a     | 409 | SQD  | C11-C10-C9-C8   |
| 31  | C     | 509 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 509 | CLA  | CBA-CGA-O2A-C1  |
| 31  | D     | 403 | CLA  | C12-C13-C15-C16 |
| 34  | A     | 409 | SQD  | C11-C10-C9-C8   |
| 36  | d     | 411 | LHG  | C9-C10-C11-C12  |
| 39  | h     | 102 | DGD  | C3B-C4B-C5B-C6B |
| 31  | d     | 403 | CLA  | C12-C13-C15-C16 |
| 36  | D     | 411 | LHG  | C9-C10-C11-C12  |
| 37  | D     | 409 | LMG  | C32-C33-C34-C35 |
| 37  | J     | 101 | LMG  | C16-C17-C18-C19 |
| 37  | W     | 201 | LMG  | C35-C36-C37-C38 |
| 37  | Y     | 101 | LMG  | C12-C13-C14-C15 |
| 37  | d     | 409 | LMG  | C32-C33-C34-C35 |
| 37  | j     | 101 | LMG  | C16-C17-C18-C19 |
| 37  | w     | 201 | LMG  | C35-C36-C37-C38 |
| 37  | y     | 101 | LMG  | C12-C13-C14-C15 |
| 37  | 5     | 315 | LMG  | C29-C30-C31-C32 |
| 37  | 5     | 315 | LMG  | C30-C31-C32-C33 |
| 37  | 0     | 315 | LMG  | C29-C30-C31-C32 |
| 37  | 0     | 315 | LMG  | C30-C31-C32-C33 |
| 39  | H     | 102 | DGD  | C3B-C4B-C5B-C6B |
| 39  | H     | 102 | DGD  | C4B-C5B-C6B-C7B |
| 39  | h     | 102 | DGD  | C4B-C5B-C6B-C7B |
| 37  | Y     | 101 | LMG  | C14-C15-C16-C17 |
| 37  | y     | 101 | LMG  | C14-C15-C16-C17 |
| 37  | c     | 521 | LMG  | C11-C12-C13-C14 |
| 37  | M     | 102 | LMG  | O6-C5-C6-O5     |
| 37  | m     | 102 | LMG  | O6-C5-C6-O5     |
| 37  | C     | 521 | LMG  | C11-C12-C13-C14 |
| 37  | Y     | 101 | LMG  | C13-C14-C15-C16 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | y     | 101 | LMG  | C13-C14-C15-C16 |
| 39  | H     | 102 | DGD  | CBA-CCA-CDA-CEA |
| 39  | h     | 102 | DGD  | CBA-CCA-CDA-CEA |
| 35  | D     | 406 | PL9  | C37-C38-C39-C40 |
| 35  | d     | 406 | PL9  | C37-C38-C39-C40 |
| 34  | 5     | 316 | SQD  | C23-C24-C25-C26 |
| 34  | 0     | 316 | SQD  | C23-C24-C25-C26 |
| 31  | 5     | 309 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 31  | p     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 207 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 208 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 308 | CLA  | C2B-C3B-CAB-CBB |
| 31  | P     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 207 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 208 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 308 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 309 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 2     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 33  | B     | 517 | BCR  | C1-C6-C7-C8     |
| 33  | b     | 518 | BCR  | C1-C6-C7-C8     |
| 39  | C     | 519 | DGD  | C8B-C9B-CAB-CBB |
| 31  | B     | 514 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 515 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 206 | CLA  | CBD-CGD-O2D-CED |
| 31  | 1     | 206 | CLA  | CBD-CGD-O2D-CED |
| 37  | Y     | 101 | LMG  | C34-C35-C36-C37 |
| 37  | y     | 101 | LMG  | C34-C35-C36-C37 |
| 39  | C     | 518 | DGD  | C2B-C3B-C4B-C5B |
| 39  | c     | 518 | DGD  | C2B-C3B-C4B-C5B |
| 36  | B     | 521 | LHG  | C24-C25-C26-C27 |
| 36  | b     | 522 | LHG  | C24-C25-C26-C27 |
| 37  | J     | 101 | LMG  | C20-C21-C22-C23 |
| 37  | M     | 101 | LMG  | C38-C39-C40-C41 |
| 37  | j     | 101 | LMG  | C20-C21-C22-C23 |
| 39  | c     | 519 | DGD  | C8B-C9B-CAB-CBB |
| 37  | m     | 101 | LMG  | C38-C39-C40-C41 |
| 39  | C     | 519 | DGD  | CBA-CCA-CDA-CEA |
| 39  | c     | 519 | DGD  | CBA-CCA-CDA-CEA |
| 35  | A     | 410 | PL9  | C4-C3-C7-C8     |
| 35  | a     | 410 | PL9  | C4-C3-C7-C8     |
| 34  | A     | 409 | SQD  | C12-C13-C14-C15 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | a     | 409 | SQD  | C12-C13-C14-C15 |
| 31  | B     | 505 | CLA  | C4-C3-C5-C6     |
| 31  | b     | 506 | CLA  | C4-C3-C5-C6     |
| 37  | M     | 101 | LMG  | C31-C32-C33-C34 |
| 37  | W     | 201 | LMG  | C32-C33-C34-C35 |
| 37  | m     | 101 | LMG  | C31-C32-C33-C34 |
| 37  | w     | 201 | LMG  | C32-C33-C34-C35 |
| 33  | B     | 519 | BCR  | C18-C19-C20-C21 |
| 33  | b     | 520 | BCR  | C18-C19-C20-C21 |
| 37  | M     | 101 | LMG  | C28-C29-C30-C31 |
| 37  | m     | 101 | LMG  | C28-C29-C30-C31 |
| 31  | C     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 509 | CLA  | C6-C7-C8-C9     |
| 31  | C     | 505 | CLA  | C11-C12-C13-C14 |
| 31  | b     | 510 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 505 | CLA  | C11-C12-C13-C14 |
| 32  | A     | 405 | PHO  | C14-C13-C15-C16 |
| 32  | a     | 405 | PHO  | C14-C13-C15-C16 |
| 37  | M     | 102 | LMG  | C30-C31-C32-C33 |
| 37  | m     | 102 | LMG  | C30-C31-C32-C33 |
| 39  | H     | 102 | DGD  | CCA-CDA-CEA-CFA |
| 39  | h     | 102 | DGD  | CCA-CDA-CEA-CFA |
| 34  | 5     | 316 | SQD  | C10-C11-C12-C13 |
| 34  | 0     | 316 | SQD  | C10-C11-C12-C13 |
| 37  | 5     | 315 | LMG  | C2-C1-O1-C7     |
| 37  | 0     | 315 | LMG  | C2-C1-O1-C7     |
| 34  | 5     | 316 | SQD  | C11-C12-C13-C14 |
| 37  | m     | 101 | LMG  | C17-C18-C19-C20 |
| 34  | 0     | 316 | SQD  | C11-C12-C13-C14 |
| 37  | M     | 101 | LMG  | C17-C18-C19-C20 |
| 37  | 5     | 315 | LMG  | C33-C34-C35-C36 |
| 37  | 0     | 315 | LMG  | C33-C34-C35-C36 |
| 34  | b     | 501 | SQD  | C27-C28-C29-C30 |
| 37  | D     | 409 | LMG  | C31-C32-C33-C34 |
| 37  | d     | 409 | LMG  | C31-C32-C33-C34 |
| 43  | 5     | 302 | ET4  | C09-C10-C11-C12 |
| 43  | 0     | 302 | ET4  | C09-C10-C11-C12 |
| 34  | B     | 523 | SQD  | C27-C28-C29-C30 |
| 34  | A     | 409 | SQD  | C8-C7-O47-C45   |
| 34  | a     | 409 | SQD  | C8-C7-O47-C45   |
| 37  | B     | 520 | LMG  | C11-C10-O7-C8   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | b     | 521 | LMG  | C11-C10-O7-C8   |
| 39  | C     | 520 | DGD  | C2B-C1B-O2G-C2G |
| 39  | c     | 520 | DGD  | C2B-C1B-O2G-C2G |
| 39  | H     | 102 | DGD  | C1A-C2A-C3A-C4A |
| 39  | h     | 102 | DGD  | C1A-C2A-C3A-C4A |
| 37  | M     | 102 | LMG  | O9-C10-O7-C8    |
| 37  | m     | 102 | LMG  | O9-C10-O7-C8    |
| 36  | B     | 521 | LHG  | C32-C33-C34-C35 |
| 36  | b     | 522 | LHG  | C32-C33-C34-C35 |
| 39  | C     | 518 | DGD  | C7B-C8B-C9B-CAB |
| 39  | c     | 518 | DGD  | C7B-C8B-C9B-CAB |
| 31  | C     | 513 | CLA  | C15-C16-C17-C18 |
| 31  | c     | 513 | CLA  | C15-C16-C17-C18 |
| 37  | D     | 408 | LMG  | C16-C17-C18-C19 |
| 37  | d     | 408 | LMG  | C16-C17-C18-C19 |
| 31  | C     | 502 | CLA  | C2A-CAA-CBA-CGA |
| 31  | c     | 502 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 407 | CLA  | C11-C12-C13-C15 |
| 31  | a     | 407 | CLA  | C11-C12-C13-C15 |
| 31  | 5     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 311 | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 405 | PHO  | C4-C3-C5-C6     |
| 32  | a     | 405 | PHO  | C4-C3-C5-C6     |
| 32  | A     | 405 | PHO  | C2-C3-C5-C6     |
| 32  | a     | 405 | PHO  | C2-C3-C5-C6     |
| 42  | 6     | 202 | A86  | C35-C34-O4-C38  |
| 42  | 1     | 202 | A86  | C35-C34-O4-C38  |
| 31  | 0     | 305 | CLA  | CBD-CGD-O2D-CED |
| 39  | C     | 518 | DGD  | C5B-C6B-C7B-C8B |
| 39  | c     | 518 | DGD  | C5B-C6B-C7B-C8B |
| 36  | A     | 412 | LHG  | C27-C28-C29-C30 |
| 36  | a     | 411 | LHG  | C27-C28-C29-C30 |
| 36  | D     | 411 | LHG  | C15-C16-C17-C18 |
| 37  | m     | 102 | LMG  | C29-C30-C31-C32 |
| 37  | w     | 201 | LMG  | C31-C32-C33-C34 |
| 31  | A     | 403 | CLA  | C16-C17-C18-C19 |
| 31  | a     | 403 | CLA  | C16-C17-C18-C19 |
| 31  | 7     | 310 | CLA  | C6-C7-C8-C9     |
| 31  | 2     | 310 | CLA  | C6-C7-C8-C9     |
| 36  | d     | 411 | LHG  | C15-C16-C17-C18 |
| 37  | M     | 102 | LMG  | C29-C30-C31-C32 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | W     | 201 | LMG  | C31-C32-C33-C34 |
| 31  | C     | 509 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 509 | CLA  | O1A-CGA-O2A-C1  |
| 39  | C     | 519 | DGD  | C8A-C9A-CAA-CBA |
| 39  | c     | 519 | DGD  | C8A-C9A-CAA-CBA |
| 37  | W     | 201 | LMG  | C10-C11-C12-C13 |
| 37  | w     | 201 | LMG  | C10-C11-C12-C13 |
| 31  | C     | 509 | CLA  | C5-C6-C7-C8     |
| 31  | c     | 509 | CLA  | C5-C6-C7-C8     |
| 37  | D     | 410 | LMG  | C30-C31-C32-C33 |
| 37  | d     | 410 | LMG  | C30-C31-C32-C33 |
| 39  | c     | 520 | DGD  | C9A-CAA-CBA-CCA |
| 34  | A     | 409 | SQD  | O6-C44-C45-O47  |
| 34  | a     | 409 | SQD  | O6-C44-C45-O47  |
| 34  | A     | 409 | SQD  | C31-C32-C33-C34 |
| 34  | a     | 409 | SQD  | C31-C32-C33-C34 |
| 39  | C     | 520 | DGD  | C9A-CAA-CBA-CCA |
| 39  | H     | 102 | DGD  | C2B-C3B-C4B-C5B |
| 39  | h     | 102 | DGD  | C2B-C3B-C4B-C5B |
| 31  | C     | 506 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 506 | CLA  | CBA-CGA-O2A-C1  |
| 36  | D     | 407 | LHG  | C27-C28-C29-C30 |
| 36  | d     | 407 | LHG  | C27-C28-C29-C30 |
| 37  | M     | 101 | LMG  | C30-C31-C32-C33 |
| 37  | m     | 101 | LMG  | C30-C31-C32-C33 |
| 31  | 5     | 307 | CLA  | C10-C11-C12-C13 |
| 31  | 0     | 307 | CLA  | C10-C11-C12-C13 |
| 31  | 7     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 37  | d     | 408 | LMG  | C30-C31-C32-C33 |
| 36  | D     | 412 | LHG  | C5-C4-O6-P      |
| 36  | d     | 412 | LHG  | C5-C4-O6-P      |
| 31  | C     | 503 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 503 | CLA  | C11-C10-C8-C7   |
| 37  | D     | 408 | LMG  | C30-C31-C32-C33 |
| 37  | M     | 101 | LMG  | C19-C20-C21-C22 |
| 37  | m     | 101 | LMG  | C19-C20-C21-C22 |
| 36  | B     | 521 | LHG  | C27-C28-C29-C30 |
| 36  | b     | 522 | LHG  | C27-C28-C29-C30 |
| 31  | 6     | 210 | CLA  | C4-C3-C5-C6     |
| 31  | 1     | 210 | CLA  | C4-C3-C5-C6     |
| 41  | F     | 101 | HEM  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 41  | f     | 101 | HEM  | C2A-CAA-CBA-CGA |
| 31  | B     | 503 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 504 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 0     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 510 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 511 | CLA  | CBD-CGD-O2D-CED |
| 31  | Z     | 101 | CLA  | O1D-CGD-O2D-CED |
| 31  | z     | 101 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 506 | CLA  | C5-C6-C7-C8     |
| 31  | D     | 404 | CLA  | C10-C11-C12-C13 |
| 31  | c     | 506 | CLA  | C5-C6-C7-C8     |
| 31  | d     | 404 | CLA  | C10-C11-C12-C13 |
| 31  | C     | 505 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 505 | CLA  | C11-C10-C8-C7   |
| 37  | J     | 101 | LMG  | C18-C19-C20-C21 |
| 37  | j     | 101 | LMG  | C18-C19-C20-C21 |
| 31  | c     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 6     | 210 | CLA  | C3-C5-C6-C7     |
| 31  | 1     | 210 | CLA  | C3-C5-C6-C7     |
| 36  | d     | 407 | LHG  | C14-C15-C16-C17 |
| 34  | B     | 523 | SQD  | C9-C10-C11-C12  |
| 34  | b     | 501 | SQD  | C9-C10-C11-C12  |
| 36  | D     | 407 | LHG  | C14-C15-C16-C17 |
| 31  | A     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 501 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 516 | CLA  | C1A-C2A-CAA-CBA |
| 31  | C     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 31  | D     | 401 | CLA  | C1A-C2A-CAA-CBA |
| 31  | Z     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 503 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 517 | CLA  | C1A-C2A-CAA-CBA |
| 31  | c     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 31  | d     | 401 | CLA  | C1A-C2A-CAA-CBA |
| 31  | z     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 309 | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 36  | D     | 411 | LHG  | C10-C11-C12-C13 |
| 36  | d     | 411 | LHG  | C10-C11-C12-C13 |
| 31  | C     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 37  | D     | 409 | LMG  | C12-C13-C14-C15 |
| 37  | d     | 409 | LMG  | C12-C13-C14-C15 |
| 36  | D     | 411 | LHG  | O6-C4-C5-C6     |
| 36  | D     | 412 | LHG  | O6-C4-C5-C6     |
| 36  | d     | 411 | LHG  | O6-C4-C5-C6     |
| 36  | d     | 412 | LHG  | O6-C4-C5-C6     |
| 36  | D     | 412 | LHG  | O9-C7-O7-C5     |
| 36  | d     | 412 | LHG  | O9-C7-O7-C5     |
| 39  | C     | 520 | DGD  | O1B-C1B-O2G-C2G |
| 39  | c     | 520 | DGD  | O1B-C1B-O2G-C2G |
| 31  | B     | 504 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 506 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 508 | CLA  | C12-C13-C15-C16 |
| 31  | C     | 509 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 505 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 507 | CLA  | C11-C12-C13-C15 |
| 31  | c     | 508 | CLA  | C12-C13-C15-C16 |
| 31  | c     | 509 | CLA  | C12-C13-C15-C16 |
| 31  | 5     | 307 | CLA  | C11-C10-C8-C7   |
| 31  | 0     | 307 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 403 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 403 | CLA  | C15-C16-C17-C18 |
| 31  | 6     | 210 | CLA  | C8-C10-C11-C12  |
| 31  | 1     | 210 | CLA  | C8-C10-C11-C12  |
| 31  | 5     | 305 | CLA  | C2-C3-C5-C6     |
| 31  | 0     | 305 | CLA  | C2-C3-C5-C6     |
| 36  | D     | 412 | LHG  | O10-C23-O8-C6   |
| 36  | d     | 412 | LHG  | O10-C23-O8-C6   |
| 37  | M     | 101 | LMG  | C11-C10-O7-C8   |
| 37  | m     | 101 | LMG  | C11-C10-O7-C8   |
| 31  | 5     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 0     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 506 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 508 | CLA  | C14-C13-C15-C16 |
| 31  | C     | 511 | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | C     | 513 | CLA  | C11-C10-C8-C9   |
| 31  | b     | 507 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 508 | CLA  | C14-C13-C15-C16 |
| 31  | c     | 511 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 513 | CLA  | C11-C10-C8-C9   |
| 37  | D     | 409 | LMG  | C11-C12-C13-C14 |
| 37  | d     | 409 | LMG  | C11-C12-C13-C14 |
| 37  | 5     | 315 | LMG  | O6-C5-C6-O5     |
| 37  | 0     | 315 | LMG  | O6-C5-C6-O5     |
| 37  | 5     | 315 | LMG  | C34-C35-C36-C37 |
| 37  | 0     | 315 | LMG  | C34-C35-C36-C37 |
| 36  | D     | 407 | LHG  | C24-C23-O8-C6   |
| 36  | d     | 407 | LHG  | C24-C23-O8-C6   |
| 31  | B     | 502 | CLA  | C8-C10-C11-C12  |
| 37  | C     | 521 | LMG  | C2-C1-O1-C7     |
| 37  | c     | 521 | LMG  | C2-C1-O1-C7     |
| 34  | A     | 409 | SQD  | O6-C44-C45-C46  |
| 34  | a     | 409 | SQD  | O6-C44-C45-C46  |
| 37  | C     | 521 | LMG  | C7-C8-C9-O8     |
| 37  | D     | 409 | LMG  | O1-C7-C8-C9     |
| 37  | D     | 410 | LMG  | O1-C7-C8-C9     |
| 37  | c     | 521 | LMG  | C7-C8-C9-O8     |
| 37  | d     | 409 | LMG  | O1-C7-C8-C9     |
| 37  | d     | 410 | LMG  | O1-C7-C8-C9     |
| 37  | 5     | 315 | LMG  | C7-C8-C9-O8     |
| 37  | 0     | 315 | LMG  | C7-C8-C9-O8     |
| 31  | b     | 503 | CLA  | C8-C10-C11-C12  |
| 34  | A     | 411 | SQD  | C28-C29-C30-C31 |
| 34  | B     | 522 | SQD  | C28-C29-C30-C31 |
| 37  | D     | 408 | LMG  | C33-C34-C35-C36 |
| 37  | d     | 408 | LMG  | C33-C34-C35-C36 |
| 31  | B     | 503 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 504 | CLA  | O1D-CGD-O2D-CED |
| 32  | A     | 405 | PHO  | C13-C15-C16-C17 |
| 32  | a     | 405 | PHO  | C13-C15-C16-C17 |
| 36  | D     | 407 | LHG  | C28-C29-C30-C31 |
| 36  | d     | 407 | LHG  | C28-C29-C30-C31 |
| 31  | C     | 505 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 505 | CLA  | O1D-CGD-O2D-CED |
| 39  | C     | 519 | DGD  | C3B-C4B-C5B-C6B |
| 39  | c     | 519 | DGD  | C3B-C4B-C5B-C6B |
| 32  | A     | 406 | PHO  | CHA-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | A     | 406 | PHO  | CHA-CBD-CGD-O2D |
| 32  | a     | 406 | PHO  | CHA-CBD-CGD-O1D |
| 32  | a     | 406 | PHO  | CHA-CBD-CGD-O2D |
| 33  | B     | 519 | BCR  | C20-C21-C22-C37 |
| 33  | b     | 520 | BCR  | C20-C21-C22-C37 |
| 31  | B     | 504 | CLA  | C10-C11-C12-C13 |
| 31  | C     | 502 | CLA  | C10-C11-C12-C13 |
| 31  | b     | 505 | CLA  | C10-C11-C12-C13 |
| 31  | c     | 502 | CLA  | C10-C11-C12-C13 |
| 37  | D     | 409 | LMG  | C10-C11-C12-C13 |
| 37  | d     | 409 | LMG  | C10-C11-C12-C13 |
| 31  | C     | 506 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 506 | CLA  | O1A-CGA-O2A-C1  |
| 37  | D     | 410 | LMG  | C32-C33-C34-C35 |
| 31  | 5     | 305 | CLA  | C4-C3-C5-C6     |
| 31  | 0     | 305 | CLA  | C4-C3-C5-C6     |
| 37  | d     | 410 | LMG  | C32-C33-C34-C35 |
| 31  | B     | 505 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 506 | CLA  | C15-C16-C17-C18 |
| 33  | B     | 519 | BCR  | C7-C8-C9-C34    |
| 33  | b     | 520 | BCR  | C7-C8-C9-C34    |
| 31  | B     | 511 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 512 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 512 | CLA  | C10-C11-C12-C13 |
| 36  | D     | 407 | LHG  | C15-C16-C17-C18 |
| 44  | 3     | 303 | DD6  | C10-C11-C13-C14 |
| 44  | 8     | 303 | DD6  | C10-C11-C13-C14 |
| 42  | 7     | 301 | A86  | C35-C34-O4-C38  |
| 42  | 2     | 301 | A86  | C35-C34-O4-C38  |
| 31  | B     | 511 | CLA  | C10-C11-C12-C13 |
| 34  | A     | 411 | SQD  | C33-C34-C35-C36 |
| 34  | B     | 522 | SQD  | C33-C34-C35-C36 |
| 36  | d     | 407 | LHG  | C15-C16-C17-C18 |
| 34  | B     | 523 | SQD  | C23-C24-C25-C26 |
| 34  | b     | 501 | SQD  | C23-C24-C25-C26 |
| 36  | A     | 412 | LHG  | C23-C24-C25-C26 |
| 36  | a     | 411 | LHG  | C23-C24-C25-C26 |
| 31  | B     | 516 | CLA  | CBA-CGA-O2A-C1  |
| 31  | b     | 517 | CLA  | CBA-CGA-O2A-C1  |
| 42  | 0     | 301 | A86  | C35-C34-O4-C38  |
| 36  | B     | 521 | LHG  | C30-C31-C32-C33 |
| 36  | D     | 412 | LHG  | C28-C29-C30-C31 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | b     | 522 | LHG  | C30-C31-C32-C33 |
| 36  | d     | 412 | LHG  | C28-C29-C30-C31 |
| 37  | W     | 201 | LMG  | C17-C18-C19-C20 |
| 37  | w     | 201 | LMG  | C17-C18-C19-C20 |
| 34  | B     | 523 | SQD  | C7-C8-C9-C10    |
| 34  | b     | 501 | SQD  | C7-C8-C9-C10    |
| 39  | C     | 519 | DGD  | C1A-C2A-C3A-C4A |
| 39  | c     | 519 | DGD  | C1A-C2A-C3A-C4A |
| 37  | J     | 101 | LMG  | C15-C16-C17-C18 |
| 37  | j     | 101 | LMG  | C15-C16-C17-C18 |
| 39  | H     | 102 | DGD  | C6A-C7A-C8A-C9A |
| 39  | h     | 102 | DGD  | C6A-C7A-C8A-C9A |
| 36  | D     | 412 | LHG  | O6-C4-C5-O7     |
| 36  | d     | 412 | LHG  | O6-C4-C5-O7     |
| 37  | J     | 101 | LMG  | C32-C33-C34-C35 |
| 37  | j     | 101 | LMG  | C14-C15-C16-C17 |
| 37  | j     | 101 | LMG  | C32-C33-C34-C35 |
| 37  | 5     | 315 | LMG  | C14-C15-C16-C17 |
| 37  | 0     | 315 | LMG  | C14-C15-C16-C17 |
| 35  | D     | 406 | PL9  | C38-C39-C41-C42 |
| 35  | d     | 406 | PL9  | C38-C39-C41-C42 |
| 31  | B     | 502 | CLA  | C6-C7-C8-C10    |
| 37  | C     | 521 | LMG  | C37-C38-C39-C40 |
| 37  | J     | 101 | LMG  | C14-C15-C16-C17 |
| 37  | M     | 101 | LMG  | C15-C16-C17-C18 |
| 37  | c     | 521 | LMG  | C37-C38-C39-C40 |
| 31  | b     | 503 | CLA  | C6-C7-C8-C10    |
| 37  | M     | 101 | LMG  | C34-C35-C36-C37 |
| 37  | m     | 101 | LMG  | C15-C16-C17-C18 |
| 37  | m     | 101 | LMG  | C34-C35-C36-C37 |
| 37  | D     | 409 | LMG  | C33-C34-C35-C36 |
| 37  | d     | 409 | LMG  | C33-C34-C35-C36 |
| 37  | 5     | 315 | LMG  | O1-C7-C8-O7     |
| 37  | 0     | 315 | LMG  | O1-C7-C8-O7     |
| 42  | 5     | 301 | A86  | C35-C34-O4-C38  |
| 42  | 5     | 317 | A86  | C35-C34-O4-C38  |
| 42  | 0     | 317 | A86  | C35-C34-O4-C38  |
| 37  | 5     | 315 | LMG  | C41-C42-C43-C44 |
| 37  | 0     | 315 | LMG  | C41-C42-C43-C44 |
| 31  | 6     | 209 | CLA  | O1D-CGD-O2D-CED |
| 37  | 5     | 315 | LMG  | C16-C17-C18-C19 |
| 37  | 0     | 315 | LMG  | C16-C17-C18-C19 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | W     | 201 | LMG  | C33-C34-C35-C36 |
| 37  | w     | 201 | LMG  | C33-C34-C35-C36 |
| 37  | J     | 101 | LMG  | C37-C38-C39-C40 |
| 37  | j     | 101 | LMG  | C37-C38-C39-C40 |
| 31  | B     | 508 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 509 | CLA  | CBD-CGD-O2D-CED |
| 37  | C     | 521 | LMG  | C35-C36-C37-C38 |
| 31  | 1     | 209 | CLA  | O1D-CGD-O2D-CED |
| 37  | c     | 521 | LMG  | C35-C36-C37-C38 |
| 31  | b     | 512 | CLA  | C8-C10-C11-C12  |
| 31  | C     | 502 | CLA  | O1D-CGD-O2D-CED |
| 31  | c     | 502 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 310 | CLA  | C4-C3-C5-C6     |
| 31  | 0     | 310 | CLA  | C4-C3-C5-C6     |
| 37  | J     | 101 | LMG  | C30-C31-C32-C33 |
| 37  | j     | 101 | LMG  | C30-C31-C32-C33 |
| 37  | m     | 102 | LMG  | C11-C12-C13-C14 |
| 31  | B     | 511 | CLA  | C8-C10-C11-C12  |
| 37  | M     | 102 | LMG  | C11-C12-C13-C14 |
| 31  | C     | 503 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 503 | CLA  | C6-C7-C8-C10    |
| 36  | D     | 407 | LHG  | O1-C1-C2-O2     |
| 36  | d     | 407 | LHG  | O1-C1-C2-O2     |
| 31  | B     | 503 | CLA  | C6-C7-C8-C9     |
| 31  | C     | 506 | CLA  | C11-C12-C13-C14 |
| 31  | b     | 504 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 506 | CLA  | C11-C12-C13-C14 |
| 31  | 5     | 307 | CLA  | C11-C10-C8-C9   |
| 31  | 0     | 307 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 504 | CLA  | C5-C6-C7-C8     |
| 31  | b     | 505 | CLA  | C5-C6-C7-C8     |
| 31  | W     | 202 | CLA  | C4B-C3B-CAB-CBB |
| 31  | w     | 202 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 307 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 315 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 205 | CLA  | C4B-C3B-CAB-CBB |
| 31  | p     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | P     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 0     | 307 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 2     | 315 | CLA  | C4B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 1     | 205 | CLA  | C4B-C3B-CAB-CBB |
| 31  | C     | 503 | CLA  | C8-C10-C11-C12  |
| 31  | c     | 503 | CLA  | C8-C10-C11-C12  |
| 39  | H     | 102 | DGD  | C6B-C7B-C8B-C9B |
| 39  | h     | 102 | DGD  | C6B-C7B-C8B-C9B |
| 37  | W     | 201 | LMG  | C40-C41-C42-C43 |
| 37  | w     | 201 | LMG  | C40-C41-C42-C43 |
| 37  | w     | 201 | LMG  | C29-C30-C31-C32 |
| 36  | A     | 413 | LHG  | O6-C4-C5-C6     |
| 36  | D     | 407 | LHG  | O6-C4-C5-C6     |
| 36  | a     | 412 | LHG  | O6-C4-C5-C6     |
| 36  | d     | 407 | LHG  | O6-C4-C5-C6     |
| 37  | W     | 201 | LMG  | C29-C30-C31-C32 |
| 37  | D     | 410 | LMG  | C15-C16-C17-C18 |
| 37  | d     | 410 | LMG  | C15-C16-C17-C18 |
| 31  | B     | 503 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 504 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 516 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 502 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 506 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 511 | CLA  | C6-C7-C8-C10    |
| 31  | C     | 513 | CLA  | C11-C10-C8-C7   |
| 31  | b     | 504 | CLA  | C6-C7-C8-C10    |
| 31  | b     | 505 | CLA  | C11-C12-C13-C15 |
| 31  | b     | 517 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 502 | CLA  | C11-C12-C13-C15 |
| 31  | c     | 506 | CLA  | C11-C12-C13-C15 |
| 31  | c     | 511 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 513 | CLA  | C11-C10-C8-C7   |
| 31  | 5     | 307 | CLA  | C11-C12-C13-C15 |
| 31  | 0     | 307 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 503 | CLA  | C13-C15-C16-C17 |
| 31  | c     | 503 | CLA  | C13-C15-C16-C17 |
| 36  | B     | 521 | LHG  | C7-C8-C9-C10    |
| 36  | b     | 522 | LHG  | C7-C8-C9-C10    |
| 31  | B     | 514 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 515 | CLA  | C12-C13-C15-C16 |
| 37  | j     | 101 | LMG  | C24-C25-C26-C27 |
| 37  | J     | 101 | LMG  | C24-C25-C26-C27 |
| 31  | Z     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 31  | z     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 307 | CLA  | C3A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 8     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 515 | CLA  | C10-C11-C12-C13 |
| 39  | H     | 102 | DGD  | O2G-C1B-C2B-C3B |
| 39  | h     | 102 | DGD  | O2G-C1B-C2B-C3B |
| 31  | C     | 513 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 516 | CLA  | C10-C11-C12-C13 |
| 31  | c     | 513 | CLA  | C13-C15-C16-C17 |
| 42  | 5     | 303 | A86  | C11-C10-C9-C8   |
| 42  | 0     | 303 | A86  | C11-C10-C9-C8   |
| 31  | Z     | 101 | CLA  | C4-C3-C5-C6     |
| 31  | z     | 101 | CLA  | C4-C3-C5-C6     |
| 37  | J     | 101 | LMG  | O1-C7-C8-C9     |
| 37  | j     | 101 | LMG  | O1-C7-C8-C9     |
| 37  | 5     | 315 | LMG  | O1-C7-C8-C9     |
| 37  | 0     | 315 | LMG  | O1-C7-C8-C9     |
| 39  | C     | 518 | DGD  | O1G-C1G-C2G-C3G |
| 39  | C     | 518 | DGD  | C1G-C2G-C3G-O3G |
| 39  | c     | 518 | DGD  | O1G-C1G-C2G-C3G |
| 39  | c     | 518 | DGD  | C1G-C2G-C3G-O3G |
| 42  | 7     | 302 | A86  | C12-C11-C13-O   |
| 42  | 6     | 202 | A86  | C12-C11-C13-O   |
| 42  | 4     | 202 | A86  | C12-C11-C13-O   |
| 42  | 3     | 302 | A86  | C12-C11-C13-O   |
| 42  | 9     | 202 | A86  | C12-C11-C13-O   |
| 42  | 8     | 302 | A86  | C12-C11-C13-O   |
| 42  | 2     | 302 | A86  | C12-C11-C13-O   |
| 42  | 1     | 202 | A86  | C12-C11-C13-O   |
| 36  | D     | 412 | LHG  | C26-C27-C28-C29 |
| 36  | d     | 412 | LHG  | C26-C27-C28-C29 |
| 39  | C     | 518 | DGD  | C6A-C7A-C8A-C9A |
| 39  | c     | 518 | DGD  | C6A-C7A-C8A-C9A |
| 37  | W     | 201 | LMG  | C19-C20-C21-C22 |
| 37  | d     | 408 | LMG  | C35-C36-C37-C38 |
| 37  | D     | 408 | LMG  | C35-C36-C37-C38 |
| 37  | w     | 201 | LMG  | C19-C20-C21-C22 |
| 31  | B     | 516 | CLA  | O1A-CGA-O2A-C1  |
| 31  | b     | 517 | CLA  | O1A-CGA-O2A-C1  |
| 37  | 0     | 315 | LMG  | C32-C33-C34-C35 |
| 42  | 7     | 302 | A86  | C10-C11-C13-O   |
| 42  | 6     | 202 | A86  | C10-C11-C13-O   |
| 42  | p     | 610 | A86  | C10-C11-C13-O   |
| 42  | 4     | 201 | A86  | C10-C11-C13-O   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 42  | 4     | 202 | A86  | C10-C11-C13-O   |
| 42  | 3     | 302 | A86  | C10-C11-C13-O   |
| 42  | P     | 610 | A86  | C10-C11-C13-O   |
| 42  | 9     | 201 | A86  | C10-C11-C13-O   |
| 42  | 9     | 202 | A86  | C10-C11-C13-O   |
| 42  | 8     | 302 | A86  | C10-C11-C13-O   |
| 42  | 2     | 302 | A86  | C10-C11-C13-O   |
| 42  | 1     | 202 | A86  | C10-C11-C13-O   |
| 37  | 5     | 315 | LMG  | C32-C33-C34-C35 |
| 33  | B     | 517 | BCR  | C5-C6-C7-C8     |
| 33  | C     | 517 | BCR  | C1-C6-C7-C8     |
| 33  | b     | 518 | BCR  | C5-C6-C7-C8     |
| 33  | c     | 517 | BCR  | C1-C6-C7-C8     |
| 34  | B     | 523 | SQD  | C26-C27-C28-C29 |
| 34  | b     | 501 | SQD  | C26-C27-C28-C29 |
| 36  | B     | 521 | LHG  | C28-C29-C30-C31 |
| 37  | Y     | 101 | LMG  | C29-C30-C31-C32 |
| 37  | y     | 101 | LMG  | C29-C30-C31-C32 |
| 35  | D     | 406 | PL9  | C47-C48-C49-C51 |
| 35  | d     | 406 | PL9  | C47-C48-C49-C51 |
| 36  | B     | 521 | LHG  | C15-C16-C17-C18 |
| 36  | b     | 522 | LHG  | C15-C16-C17-C18 |
| 36  | b     | 522 | LHG  | C28-C29-C30-C31 |
| 36  | D     | 411 | LHG  | O7-C5-C6-O8     |
| 36  | d     | 411 | LHG  | O7-C5-C6-O8     |
| 37  | C     | 521 | LMG  | O1-C7-C8-O7     |
| 37  | C     | 521 | LMG  | O7-C8-C9-O8     |
| 37  | c     | 521 | LMG  | O1-C7-C8-O7     |
| 37  | c     | 521 | LMG  | O7-C8-C9-O8     |
| 39  | h     | 102 | DGD  | C4E-C5E-C6E-O5E |
| 35  | a     | 410 | PL9  | C12-C11-C9-C10  |
| 39  | H     | 102 | DGD  | C4E-C5E-C6E-O5E |
| 34  | 5     | 316 | SQD  | C12-C13-C14-C15 |
| 34  | 0     | 316 | SQD  | C12-C13-C14-C15 |
| 31  | C     | 511 | CLA  | C11-C10-C8-C9   |
| 31  | c     | 511 | CLA  | C11-C10-C8-C9   |
| 37  | D     | 410 | LMG  | C31-C32-C33-C34 |
| 37  | d     | 410 | LMG  | C31-C32-C33-C34 |
| 37  | Y     | 101 | LMG  | C17-C18-C19-C20 |
| 37  | y     | 101 | LMG  | C17-C18-C19-C20 |
| 39  | C     | 518 | DGD  | C2A-C3A-C4A-C5A |
| 39  | c     | 518 | DGD  | C2A-C3A-C4A-C5A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 37  | B     | 520 | LMG  | C4-C5-C6-O5     |
| 37  | D     | 408 | LMG  | C4-C5-C6-O5     |
| 37  | b     | 521 | LMG  | C4-C5-C6-O5     |
| 36  | A     | 412 | LHG  | O1-C1-C2-O2     |
| 36  | a     | 411 | LHG  | O1-C1-C2-O2     |
| 35  | A     | 410 | PL9  | C12-C11-C9-C10  |
| 37  | d     | 408 | LMG  | C4-C5-C6-O5     |
| 31  | b     | 505 | CLA  | O1D-CGD-O2D-CED |
| 37  | J     | 101 | LMG  | C11-C10-O7-C8   |
| 37  | j     | 101 | LMG  | C11-C10-O7-C8   |
| 31  | C     | 506 | CLA  | C15-C16-C17-C18 |
| 31  | c     | 506 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 504 | CLA  | O1D-CGD-O2D-CED |
| 36  | D     | 407 | LHG  | C9-C10-C11-C12  |
| 36  | d     | 407 | LHG  | C9-C10-C11-C12  |
| 37  | m     | 102 | LMG  | C33-C34-C35-C36 |
| 37  | M     | 102 | LMG  | C33-C34-C35-C36 |
| 39  | C     | 518 | DGD  | CDB-CEB-CFB-CGB |
| 31  | C     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 505 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 506 | CLA  | C13-C15-C16-C17 |
| 39  | c     | 518 | DGD  | CDB-CEB-CFB-CGB |
| 31  | B     | 503 | CLA  | C11-C12-C13-C15 |
| 31  | b     | 504 | CLA  | C11-C12-C13-C15 |
| 44  | p     | 611 | DD6  | C-C1-C24-C25    |
| 44  | P     | 611 | DD6  | C-C1-C24-C25    |
| 31  | B     | 514 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 510 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 511 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 513 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 515 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 510 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 511 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 513 | CLA  | C12-C13-C15-C16 |
| 32  | A     | 406 | PHO  | C6-C7-C8-C10    |
| 32  | a     | 406 | PHO  | C6-C7-C8-C10    |
| 31  | b     | 514 | CLA  | C10-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 41  | V     | 201 | HEM  | C2A-CAA-CBA-CGA |
| 41  | v     | 201 | HEM  | C2A-CAA-CBA-CGA |
| 34  | 5     | 316 | SQD  | C45-C44-O6-C1   |
| 34  | 0     | 316 | SQD  | C45-C44-O6-C1   |
| 31  | B     | 513 | CLA  | C10-C11-C12-C13 |
| 31  | 5     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | 0     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 7     | 310 | CLA  | C4-C3-C5-C6     |
| 31  | 2     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 2     | 310 | CLA  | C4-C3-C5-C6     |
| 37  | j     | 101 | LMG  | C13-C14-C15-C16 |
| 37  | J     | 101 | LMG  | C13-C14-C15-C16 |
| 37  | m     | 101 | LMG  | C16-C17-C18-C19 |
| 37  | C     | 521 | LMG  | C40-C41-C42-C43 |
| 37  | c     | 521 | LMG  | C40-C41-C42-C43 |
| 37  | M     | 101 | LMG  | C16-C17-C18-C19 |
| 37  | 0     | 315 | LMG  | C42-C43-C44-C45 |
| 37  | 5     | 315 | LMG  | C42-C43-C44-C45 |
| 34  | B     | 522 | SQD  | C16-C17-C18-C19 |
| 31  | B     | 514 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 515 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 516 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 517 | CLA  | C13-C15-C16-C17 |
| 34  | A     | 411 | SQD  | C16-C17-C18-C19 |
| 36  | D     | 407 | LHG  | O6-C4-C5-O7     |
| 36  | d     | 407 | LHG  | O6-C4-C5-O7     |
| 37  | J     | 101 | LMG  | O6-C1-O1-C7     |
| 37  | j     | 101 | LMG  | O6-C1-O1-C7     |
| 31  | 1     | 206 | CLA  | O1D-CGD-O2D-CED |
| 36  | B     | 521 | LHG  | C4-C5-C6-O8     |
| 36  | D     | 411 | LHG  | C4-C5-C6-O8     |
| 36  | D     | 412 | LHG  | C4-C5-C6-O8     |
| 36  | b     | 522 | LHG  | C4-C5-C6-O8     |
| 36  | d     | 411 | LHG  | C4-C5-C6-O8     |
| 36  | d     | 412 | LHG  | C4-C5-C6-O8     |
| 41  | V     | 201 | HEM  | C4C-C3C-CAC-CBC |
| 41  | v     | 201 | HEM  | C4C-C3C-CAC-CBC |
| 31  | c     | 508 | CLA  | C16-C17-C18-C20 |
| 37  | W     | 201 | LMG  | C37-C38-C39-C40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | w     | 201 | LMG  | C37-C38-C39-C40 |
| 39  | C     | 519 | DGD  | CCA-CDA-CEA-CFA |
| 31  | 0     | 311 | CLA  | C2C-C3C-CAC-CBC |
| 31  | 6     | 206 | CLA  | O1D-CGD-O2D-CED |
| 39  | c     | 519 | DGD  | CCA-CDA-CEA-CFA |
| 31  | d     | 404 | CLA  | C4-C3-C5-C6     |
| 35  | A     | 410 | PL9  | C15-C14-C16-C17 |
| 35  | a     | 410 | PL9  | C15-C14-C16-C17 |
| 31  | B     | 505 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 506 | CLA  | C2-C3-C5-C6     |
| 42  | 5     | 301 | A86  | C28-C27-C29-C30 |
| 42  | 0     | 301 | A86  | C28-C27-C29-C30 |
| 37  | C     | 521 | LMG  | C39-C40-C41-C42 |
| 37  | c     | 521 | LMG  | C39-C40-C41-C42 |
| 31  | 5     | 311 | CLA  | C2C-C3C-CAC-CBC |
| 34  | 5     | 316 | SQD  | O47-C45-C46-O48 |
| 34  | 0     | 316 | SQD  | O47-C45-C46-O48 |
| 36  | B     | 521 | LHG  | O7-C5-C6-O8     |
| 36  | H     | 103 | LHG  | O7-C5-C6-O8     |
| 36  | b     | 522 | LHG  | O7-C5-C6-O8     |
| 36  | h     | 103 | LHG  | O7-C5-C6-O8     |
| 37  | D     | 410 | LMG  | O1-C7-C8-O7     |
| 37  | J     | 101 | LMG  | O1-C7-C8-O7     |
| 37  | d     | 410 | LMG  | O1-C7-C8-O7     |
| 37  | j     | 101 | LMG  | O1-C7-C8-O7     |
| 39  | C     | 518 | DGD  | O1G-C1G-C2G-O2G |
| 39  | C     | 518 | DGD  | O2G-C2G-C3G-O3G |
| 39  | c     | 518 | DGD  | O1G-C1G-C2G-O2G |
| 39  | c     | 518 | DGD  | O2G-C2G-C3G-O3G |
| 31  | B     | 516 | CLA  | C11-C10-C8-C9   |
| 31  | b     | 517 | CLA  | C11-C10-C8-C9   |
| 31  | 5     | 305 | CLA  | C6-C7-C8-C9     |
| 31  | 0     | 305 | CLA  | C6-C7-C8-C9     |
| 34  | 0     | 316 | SQD  | C25-C26-C27-C28 |
| 36  | A     | 412 | LHG  | C11-C12-C13-C14 |
| 36  | a     | 411 | LHG  | C11-C12-C13-C14 |
| 36  | D     | 411 | LHG  | O10-C23-O8-C6   |
| 34  | 5     | 316 | SQD  | C25-C26-C27-C28 |
| 36  | D     | 407 | LHG  | C29-C30-C31-C32 |
| 36  | d     | 407 | LHG  | C29-C30-C31-C32 |
| 31  | C     | 513 | CLA  | C5-C6-C7-C8     |
| 31  | c     | 513 | CLA  | C5-C6-C7-C8     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | C     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 36  | d     | 411 | LHG  | O10-C23-O8-C6   |
| 31  | B     | 510 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 0     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 31  | C     | 508 | CLA  | C16-C17-C18-C20 |
| 39  | C     | 518 | DGD  | CBB-CCB-CDB-CEB |
| 39  | c     | 518 | DGD  | CBB-CCB-CDB-CEB |
| 31  | b     | 511 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 509 | CLA  | C4-C3-C5-C6     |
| 31  | D     | 404 | CLA  | C4-C3-C5-C6     |
| 31  | b     | 510 | CLA  | C4-C3-C5-C6     |
| 37  | W     | 201 | LMG  | C34-C35-C36-C37 |
| 37  | w     | 201 | LMG  | C34-C35-C36-C37 |
| 31  | C     | 509 | CLA  | C16-C17-C18-C20 |
| 31  | c     | 509 | CLA  | C16-C17-C18-C20 |
| 37  | m     | 101 | LMG  | C12-C13-C14-C15 |
| 37  | M     | 101 | LMG  | C12-C13-C14-C15 |
| 31  | b     | 509 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 508 | CLA  | O1D-CGD-O2D-CED |
| 36  | D     | 411 | LHG  | O1-C1-C2-O2     |
| 36  | d     | 411 | LHG  | O1-C1-C2-O2     |
| 33  | h     | 101 | BCR  | C7-C8-C9-C34    |
| 31  | B     | 514 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 515 | CLA  | C4B-C3B-CAB-CBB |
| 31  | Z     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 31  | b     | 515 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 516 | CLA  | C4B-C3B-CAB-CBB |
| 31  | z     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 304 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 7     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 206 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 3     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 206 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 304 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 2     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 2     | 310 | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | A     | 411 | SQD  | C24-C23-O48-C46 |
| 34  | B     | 522 | SQD  | C24-C23-O48-C46 |
| 31  | B     | 511 | CLA  | C4-C3-C5-C6     |
| 31  | b     | 512 | CLA  | C4-C3-C5-C6     |
| 44  | p     | 611 | DD6  | C2-C1-C24-C25   |
| 44  | P     | 611 | DD6  | C2-C1-C24-C25   |
| 34  | 5     | 316 | SQD  | O49-C7-O47-C45  |
| 34  | 0     | 316 | SQD  | O49-C7-O47-C45  |
| 37  | Y     | 101 | LMG  | O9-C10-O7-C8    |
| 37  | y     | 101 | LMG  | O9-C10-O7-C8    |
| 39  | C     | 518 | DGD  | C4A-C5A-C6A-C7A |
| 39  | c     | 518 | DGD  | C4A-C5A-C6A-C7A |
| 31  | B     | 516 | CLA  | C6-C7-C8-C10    |
| 31  | C     | 506 | CLA  | C6-C7-C8-C10    |
| 31  | C     | 509 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 512 | CLA  | C12-C13-C15-C16 |
| 31  | C     | 513 | CLA  | C11-C12-C13-C15 |
| 31  | D     | 404 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 517 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 506 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 509 | CLA  | C11-C12-C13-C15 |
| 31  | c     | 512 | CLA  | C12-C13-C15-C16 |
| 31  | c     | 513 | CLA  | C11-C12-C13-C15 |
| 31  | d     | 404 | CLA  | C12-C13-C15-C16 |
| 31  | 5     | 305 | CLA  | C11-C10-C8-C7   |
| 31  | 5     | 308 | CLA  | C6-C7-C8-C10    |
| 31  | 0     | 305 | CLA  | C11-C10-C8-C7   |
| 31  | 0     | 308 | CLA  | C6-C7-C8-C10    |
| 39  | c     | 519 | DGD  | C9B-CAB-CBB-CCB |
| 39  | C     | 519 | DGD  | C9B-CAB-CBB-CCB |
| 37  | M     | 102 | LMG  | C31-C32-C33-C34 |
| 39  | H     | 102 | DGD  | C7B-C8B-C9B-CAB |
| 39  | h     | 102 | DGD  | C7B-C8B-C9B-CAB |
| 37  | m     | 102 | LMG  | C31-C32-C33-C34 |
| 36  | D     | 411 | LHG  | C2-C3-O3-P      |
| 36  | d     | 411 | LHG  | C2-C3-O3-P      |
| 42  | 4     | 203 | A86  | C35-C34-O4-C38  |
| 31  | B     | 504 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 510 | CLA  | C11-C10-C8-C9   |
| 31  | C     | 513 | CLA  | C14-C13-C15-C16 |
| 31  | b     | 505 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 510 | CLA  | C11-C10-C8-C9   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | c     | 513 | CLA  | C14-C13-C15-C16 |
| 31  | 5     | 307 | CLA  | C11-C12-C13-C14 |
| 31  | 0     | 307 | CLA  | C11-C12-C13-C14 |
| 42  | 9     | 203 | A86  | C35-C34-O4-C38  |
| 36  | D     | 412 | LHG  | C29-C30-C31-C32 |
| 36  | d     | 412 | LHG  | C29-C30-C31-C32 |
| 37  | W     | 201 | LMG  | C16-C17-C18-C19 |
| 31  | A     | 404 | CLA  | C1-C2-C3-C4     |
| 31  | C     | 514 | CLA  | C1-C2-C3-C4     |
| 31  | a     | 404 | CLA  | C1-C2-C3-C4     |
| 31  | c     | 514 | CLA  | C1-C2-C3-C4     |
| 31  | 6     | 213 | CLA  | CAD-CBD-CGD-O1D |
| 31  | p     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | P     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 1     | 213 | CLA  | CAD-CBD-CGD-O1D |
| 42  | 5     | 301 | A86  | C26-C27-C29-C30 |
| 42  | 0     | 301 | A86  | C26-C27-C29-C30 |
| 37  | w     | 201 | LMG  | C16-C17-C18-C19 |
| 36  | A     | 413 | LHG  | O7-C5-C6-O8     |
| 36  | a     | 412 | LHG  | O7-C5-C6-O8     |
| 37  | D     | 409 | LMG  | O1-C7-C8-O7     |
| 37  | d     | 409 | LMG  | O1-C7-C8-O7     |
| 37  | c     | 521 | LMG  | C12-C13-C14-C15 |
| 31  | C     | 513 | CLA  | O2A-C1-C2-C3    |
| 31  | c     | 513 | CLA  | O2A-C1-C2-C3    |
| 37  | C     | 521 | LMG  | C12-C13-C14-C15 |
| 34  | B     | 523 | SQD  | C30-C31-C32-C33 |
| 34  | b     | 501 | SQD  | C30-C31-C32-C33 |
| 36  | A     | 413 | LHG  | C4-C5-C6-O8     |
| 36  | H     | 103 | LHG  | C4-C5-C6-O8     |
| 36  | a     | 412 | LHG  | C4-C5-C6-O8     |
| 36  | h     | 103 | LHG  | C4-C5-C6-O8     |
| 37  | C     | 521 | LMG  | O1-C7-C8-C9     |
| 37  | c     | 521 | LMG  | O1-C7-C8-C9     |
| 31  | c     | 505 | CLA  | C10-C11-C12-C13 |
| 31  | 6     | 210 | CLA  | C2-C3-C5-C6     |
| 31  | 1     | 210 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 509 | CLA  | CAD-CBD-CGD-O2D |
| 31  | C     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 31  | C     | 506 | CLA  | CAD-CBD-CGD-O2D |
| 31  | C     | 507 | CLA  | CAD-CBD-CGD-O2D |
| 31  | C     | 514 | CLA  | CAD-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 510 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 506 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 507 | CLA  | CAD-CBD-CGD-O2D |
| 31  | c     | 514 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 208 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 1     | 208 | CLA  | CAD-CBD-CGD-O2D |
| 42  | 5     | 317 | A86  | C13-C14-C15-C20 |
| 42  | 7     | 301 | A86  | C13-C14-C15-C20 |
| 42  | 7     | 302 | A86  | C13-C14-C15-C20 |
| 42  | p     | 610 | A86  | C13-C14-C15-C20 |
| 42  | 4     | 203 | A86  | C13-C14-C15-C20 |
| 42  | P     | 610 | A86  | C13-C14-C15-C20 |
| 42  | 9     | 203 | A86  | C13-C14-C15-C20 |
| 42  | 0     | 317 | A86  | C13-C14-C15-C20 |
| 42  | 2     | 301 | A86  | C13-C14-C15-C20 |
| 42  | 2     | 302 | A86  | C13-C14-C15-C20 |
| 31  | C     | 505 | CLA  | C10-C11-C12-C13 |
| 31  | 5     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 0     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 36  | D     | 411 | LHG  | C24-C23-O8-C6   |
| 36  | d     | 411 | LHG  | C24-C23-O8-C6   |
| 31  | 5     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 0     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 37  | m     | 101 | LMG  | C10-C11-C12-C13 |
| 34  | B     | 522 | SQD  | C14-C15-C16-C17 |
| 37  | W     | 201 | LMG  | C11-C12-C13-C14 |
| 34  | A     | 411 | SQD  | C14-C15-C16-C17 |
| 42  | 6     | 202 | A86  | C33-C34-O4-C38  |
| 31  | B     | 509 | CLA  | CAD-CBD-CGD-O1D |
| 31  | C     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 31  | C     | 506 | CLA  | CAD-CBD-CGD-O1D |
| 31  | C     | 507 | CLA  | CAD-CBD-CGD-O1D |
| 31  | C     | 514 | CLA  | CAD-CBD-CGD-O1D |
| 31  | b     | 510 | CLA  | CAD-CBD-CGD-O1D |
| 31  | c     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 31  | c     | 506 | CLA  | CAD-CBD-CGD-O1D |
| 31  | c     | 507 | CLA  | CAD-CBD-CGD-O1D |
| 31  | c     | 514 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 6     | 208 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 3     | 309 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 309 | CLA  | CHA-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 1     | 208 | CLA  | CAD-CBD-CGD-O1D |
| 33  | k     | 101 | BCR  | C20-C21-C22-C37 |
| 36  | D     | 411 | LHG  | C3-O3-P-O5      |
| 36  | H     | 103 | LHG  | C3-O3-P-O5      |
| 36  | d     | 411 | LHG  | C3-O3-P-O5      |
| 42  | 7     | 302 | A86  | C10-C11-C13-C14 |
| 42  | 6     | 202 | A86  | C10-C11-C13-C14 |
| 42  | 4     | 201 | A86  | C10-C11-C13-C14 |
| 42  | 3     | 302 | A86  | C10-C11-C13-C14 |
| 42  | 9     | 201 | A86  | C10-C11-C13-C14 |
| 42  | 8     | 302 | A86  | C10-C11-C13-C14 |
| 42  | 2     | 302 | A86  | C10-C11-C13-C14 |
| 42  | 1     | 202 | A86  | C10-C11-C13-C14 |
| 37  | w     | 201 | LMG  | C11-C12-C13-C14 |
| 37  | M     | 101 | LMG  | C10-C11-C12-C13 |
| 37  | Y     | 101 | LMG  | C33-C34-C35-C36 |
| 31  | 6     | 210 | CLA  | C15-C16-C17-C18 |
| 31  | 1     | 210 | CLA  | C15-C16-C17-C18 |
| 31  | 6     | 213 | CLA  | C2B-C3B-CAB-CBB |
| 31  | p     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 31  | P     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 1     | 213 | CLA  | C2B-C3B-CAB-CBB |
| 37  | y     | 101 | LMG  | C33-C34-C35-C36 |
| 31  | B     | 509 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 510 | CLA  | C2-C3-C5-C6     |
| 35  | D     | 406 | PL9  | C13-C14-C16-C17 |
| 35  | d     | 406 | PL9  | C13-C14-C16-C17 |
| 42  | 1     | 202 | A86  | C33-C34-O4-C38  |
| 33  | H     | 101 | BCR  | C7-C8-C9-C34    |
| 43  | 5     | 302 | ET4  | C11-C12-C13-C28 |
| 43  | 0     | 302 | ET4  | C11-C12-C13-C28 |
| 42  | 7     | 302 | A86  | C12-C11-C13-C14 |
| 42  | 4     | 201 | A86  | C12-C11-C13-C14 |
| 42  | 3     | 301 | A86  | C12-C11-C13-C14 |
| 42  | 9     | 201 | A86  | C12-C11-C13-C14 |
| 42  | 8     | 301 | A86  | C12-C11-C13-C14 |
| 42  | 2     | 302 | A86  | C12-C11-C13-C14 |
| 37  | J     | 101 | LMG  | C33-C34-C35-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 37  | j     | 101 | LMG  | C33-C34-C35-C36 |
| 42  | 7     | 302 | A86  | C35-C34-O4-C38  |
| 42  | 2     | 302 | A86  | C35-C34-O4-C38  |
| 37  | D     | 410 | LMG  | C9-C8-O7-C10    |
| 37  | d     | 410 | LMG  | C9-C8-O7-C10    |
| 31  | B     | 511 | CLA  | C2-C3-C5-C6     |
| 31  | b     | 512 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | 2     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | 2     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | C     | 509 | CLA  | C16-C17-C18-C19 |
| 31  | c     | 509 | CLA  | C16-C17-C18-C19 |
| 31  | C     | 512 | CLA  | C13-C15-C16-C17 |
| 31  | c     | 512 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 510 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 502 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 506 | CLA  | C6-C7-C8-C9     |
| 31  | C     | 513 | CLA  | C6-C7-C8-C9     |
| 31  | b     | 511 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 502 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 506 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 509 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 513 | CLA  | C6-C7-C8-C9     |
| 31  | 7     | 305 | CLA  | O1D-CGD-O2D-CED |
| 34  | b     | 501 | SQD  | C10-C11-C12-C13 |
| 31  | B     | 502 | CLA  | C11-C12-C13-C15 |
| 31  | b     | 503 | CLA  | C11-C12-C13-C15 |
| 39  | c     | 519 | DGD  | C7B-C8B-C9B-CAB |
| 34  | B     | 523 | SQD  | C10-C11-C12-C13 |
| 36  | D     | 411 | LHG  | C12-C13-C14-C15 |
| 36  | d     | 411 | LHG  | C12-C13-C14-C15 |
| 39  | C     | 519 | DGD  | C7B-C8B-C9B-CAB |
| 31  | 6     | 211 | CLA  | C6-C7-C8-C9     |
| 31  | 1     | 211 | CLA  | C6-C7-C8-C9     |
| 36  | D     | 407 | LHG  | C25-C26-C27-C28 |
| 36  | d     | 407 | LHG  | C25-C26-C27-C28 |
| 31  | B     | 504 | CLA  | C16-C17-C18-C19 |
| 31  | b     | 505 | CLA  | C16-C17-C18-C19 |
| 37  | D     | 410 | LMG  | C33-C34-C35-C36 |
| 37  | d     | 410 | LMG  | C33-C34-C35-C36 |
| 34  | A     | 409 | SQD  | C9-C10-C11-C12  |
| 34  | a     | 409 | SQD  | C9-C10-C11-C12  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 39  | c     | 519 | DGD  | C5B-C6B-C7B-C8B |
| 39  | C     | 519 | DGD  | C5B-C6B-C7B-C8B |
| 31  | c     | 510 | CLA  | C3-C5-C6-C7     |
| 31  | C     | 510 | CLA  | C3-C5-C6-C7     |
| 36  | D     | 411 | LHG  | O10-C23-C24-C25 |
| 37  | W     | 201 | LMG  | C8-C7-O1-C1     |
| 37  | w     | 201 | LMG  | C8-C7-O1-C1     |
| 39  | C     | 519 | DGD  | C5D-C6D-O5D-C1E |
| 39  | c     | 519 | DGD  | C5D-C6D-O5D-C1E |
| 31  | D     | 401 | CLA  | C11-C12-C13-C14 |
| 31  | d     | 401 | CLA  | C11-C12-C13-C14 |
| 36  | D     | 411 | LHG  | O8-C23-C24-C25  |
| 36  | d     | 411 | LHG  | O8-C23-C24-C25  |
| 44  | 3     | 303 | DD6  | C27-C29-C30-C31 |
| 31  | C     | 509 | CLA  | C11-C12-C13-C14 |
| 31  | C     | 512 | CLA  | C14-C13-C15-C16 |
| 31  | C     | 513 | CLA  | C11-C12-C13-C14 |
| 31  | D     | 404 | CLA  | C14-C13-C15-C16 |
| 31  | c     | 512 | CLA  | C14-C13-C15-C16 |
| 31  | c     | 513 | CLA  | C11-C12-C13-C14 |
| 31  | d     | 404 | CLA  | C14-C13-C15-C16 |
| 31  | 5     | 308 | CLA  | C6-C7-C8-C9     |
| 31  | 0     | 308 | CLA  | C6-C7-C8-C9     |
| 37  | C     | 521 | LMG  | C29-C28-O8-C9   |
| 37  | Y     | 101 | LMG  | C29-C28-O8-C9   |
| 37  | c     | 521 | LMG  | C29-C28-O8-C9   |
| 37  | y     | 101 | LMG  | C29-C28-O8-C9   |
| 31  | 3     | 309 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 8     | 309 | CLA  | C4B-C3B-CAB-CBB |
| 36  | D     | 407 | LHG  | C24-C25-C26-C27 |
| 36  | d     | 407 | LHG  | C24-C25-C26-C27 |
| 31  | B     | 502 | CLA  | O2A-C1-C2-C3    |
| 31  | b     | 503 | CLA  | O2A-C1-C2-C3    |
| 36  | B     | 521 | LHG  | C29-C30-C31-C32 |
| 36  | b     | 522 | LHG  | C29-C30-C31-C32 |
| 39  | H     | 102 | DGD  | C5B-C6B-C7B-C8B |
| 39  | h     | 102 | DGD  | C5B-C6B-C7B-C8B |
| 31  | B     | 511 | CLA  | C12-C13-C15-C16 |
| 34  | A     | 411 | SQD  | C12-C13-C14-C15 |
| 34  | B     | 522 | SQD  | C12-C13-C14-C15 |
| 37  | C     | 521 | LMG  | O10-C28-O8-C9   |
| 37  | c     | 521 | LMG  | O10-C28-O8-C9   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | B     | 521 | LHG  | O2-C2-C3-O3     |
| 36  | b     | 522 | LHG  | O2-C2-C3-O3     |
| 31  | b     | 512 | CLA  | C12-C13-C15-C16 |
| 42  | 3     | 301 | A86  | C35-C34-O4-C38  |
| 36  | D     | 412 | LHG  | C7-C8-C9-C10    |
| 31  | C     | 506 | CLA  | C10-C11-C12-C13 |
| 31  | c     | 506 | CLA  | C10-C11-C12-C13 |
| 39  | C     | 520 | DGD  | O1G-C1G-C2G-O2G |
| 39  | c     | 520 | DGD  | O1G-C1G-C2G-O2G |
| 31  | C     | 508 | CLA  | C4-C3-C5-C6     |
| 31  | c     | 508 | CLA  | C4-C3-C5-C6     |
| 36  | d     | 412 | LHG  | C7-C8-C9-C10    |
| 37  | D     | 408 | LMG  | C19-C20-C21-C22 |
| 37  | d     | 408 | LMG  | C19-C20-C21-C22 |
| 33  | K     | 101 | BCR  | C20-C21-C22-C37 |
| 37  | B     | 520 | LMG  | O6-C1-O1-C7     |
| 37  | b     | 521 | LMG  | O6-C1-O1-C7     |
| 31  | B     | 502 | CLA  | C10-C11-C12-C13 |
| 31  | b     | 503 | CLA  | C10-C11-C12-C13 |
| 42  | 8     | 301 | A86  | C35-C34-O4-C38  |
| 31  | 6     | 210 | CLA  | C2-C1-O2A-CGA   |
| 31  | 1     | 210 | CLA  | C2-C1-O2A-CGA   |
| 31  | C     | 506 | CLA  | C13-C15-C16-C17 |
| 31  | c     | 506 | CLA  | C13-C15-C16-C17 |
| 34  | A     | 409 | SQD  | C11-C12-C13-C14 |
| 34  | a     | 409 | SQD  | C11-C12-C13-C14 |
| 31  | 7     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 35  | A     | 410 | PL9  | C23-C24-C26-C27 |
| 35  | a     | 410 | PL9  | C23-C24-C26-C27 |
| 42  | p     | 610 | A86  | C12-C11-C13-O   |
| 42  | 3     | 301 | A86  | C12-C11-C13-O   |
| 42  | P     | 610 | A86  | C12-C11-C13-O   |
| 42  | 8     | 301 | A86  | C12-C11-C13-O   |
| 31  | B     | 505 | CLA  | C11-C10-C8-C9   |
| 31  | C     | 502 | CLA  | C14-C13-C15-C16 |
| 31  | b     | 506 | CLA  | C11-C10-C8-C9   |
| 31  | c     | 502 | CLA  | C14-C13-C15-C16 |
| 37  | C     | 521 | LMG  | C31-C32-C33-C34 |
| 37  | c     | 521 | LMG  | C31-C32-C33-C34 |
| 31  | 6     | 206 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 5     | 305 | CLA  | O2A-C1-C2-C3    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 305 | CLA  | O2A-C1-C2-C3    |
| 37  | D     | 410 | LMG  | C7-C8-O7-C10    |
| 37  | d     | 410 | LMG  | C7-C8-O7-C10    |
| 31  | 7     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 316 | CLA  | CBD-CGD-O2D-CED |
| 35  | A     | 410 | PL9  | C24-C26-C27-C28 |
| 35  | a     | 410 | PL9  | C24-C26-C27-C28 |
| 31  | 7     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 1     | 206 | CLA  | CAA-CBA-CGA-O2A |
| 37  | C     | 521 | LMG  | C18-C19-C20-C21 |
| 37  | c     | 521 | LMG  | C18-C19-C20-C21 |
| 31  | 7     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | 0     | 312 | CLA  | C2C-C3C-CAC-CBC |
| 32  | a     | 406 | PHO  | C2C-C3C-CAC-CBC |
| 37  | 5     | 315 | LMG  | C17-C18-C19-C20 |
| 37  | 0     | 315 | LMG  | C17-C18-C19-C20 |
| 31  | C     | 506 | CLA  | C2A-CAA-CBA-CGA |
| 31  | c     | 506 | CLA  | C2A-CAA-CBA-CGA |
| 32  | A     | 406 | PHO  | C2C-C3C-CAC-CBC |
| 31  | B     | 503 | CLA  | C1A-C2A-CAA-CBA |
| 31  | C     | 509 | CLA  | C1A-C2A-CAA-CBA |
| 31  | c     | 509 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 206 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 211 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 0     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 206 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 1     | 211 | CLA  | C1A-C2A-CAA-CBA |
| 42  | 4     | 203 | A86  | C10-C11-C13-O   |
| 42  | 3     | 301 | A86  | C10-C11-C13-O   |
| 42  | 9     | 203 | A86  | C10-C11-C13-O   |
| 42  | 8     | 301 | A86  | C10-C11-C13-O   |
| 31  | 5     | 312 | CLA  | C2C-C3C-CAC-CBC |
| 31  | C     | 508 | CLA  | C16-C17-C18-C19 |
| 31  | c     | 508 | CLA  | C16-C17-C18-C19 |
| 31  | 5     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 37  | Y     | 101 | LMG  | C28-C29-C30-C31 |
| 37  | y     | 101 | LMG  | C28-C29-C30-C31 |
| 36  | H     | 103 | LHG  | C12-C13-C14-C15 |
| 36  | h     | 103 | LHG  | C12-C13-C14-C15 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | A     | 412 | LHG  | C34-C35-C36-C37 |
| 36  | d     | 411 | LHG  | O10-C23-C24-C25 |
| 31  | B     | 508 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 509 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 515 | CLA  | C2B-C3B-CAB-CBB |
| 31  | W     | 202 | CLA  | C2B-C3B-CAB-CBB |
| 31  | Z     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 31  | b     | 516 | CLA  | C2B-C3B-CAB-CBB |
| 31  | w     | 202 | CLA  | C2B-C3B-CAB-CBB |
| 31  | z     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 304 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 307 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 7     | 315 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 206 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 3     | 309 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 206 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 8     | 309 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 304 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 307 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 2     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 2     | 315 | CLA  | C2B-C3B-CAB-CBB |
| 33  | A     | 408 | BCR  | C1-C6-C7-C8     |
| 33  | B     | 518 | BCR  | C23-C24-C25-C30 |
| 33  | B     | 519 | BCR  | C1-C6-C7-C8     |
| 33  | C     | 516 | BCR  | C23-C24-C25-C30 |
| 33  | C     | 517 | BCR  | C5-C6-C7-C8     |
| 33  | H     | 101 | BCR  | C23-C24-C25-C30 |
| 33  | K     | 101 | BCR  | C1-C6-C7-C8     |
| 33  | a     | 408 | BCR  | C1-C6-C7-C8     |
| 33  | b     | 519 | BCR  | C23-C24-C25-C30 |
| 33  | b     | 520 | BCR  | C1-C6-C7-C8     |
| 33  | c     | 516 | BCR  | C23-C24-C25-C30 |
| 33  | c     | 517 | BCR  | C5-C6-C7-C8     |
| 33  | h     | 101 | BCR  | C23-C24-C25-C30 |
| 33  | k     | 101 | BCR  | C1-C6-C7-C8     |
| 31  | 0     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 36  | a     | 411 | LHG  | C34-C35-C36-C37 |
| 31  | 7     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 2     | 306 | CLA  | CAA-CBA-CGA-O2A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | 0     | 316 | SQD  | C33-C34-C35-C36 |
| 31  | b     | 512 | CLA  | C15-C16-C17-C18 |
| 34  | 5     | 316 | SQD  | C33-C34-C35-C36 |
| 31  | B     | 514 | CLA  | C6-C7-C8-C10    |
| 31  | C     | 508 | CLA  | C11-C12-C13-C15 |
| 31  | b     | 515 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 508 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 511 | CLA  | C15-C16-C17-C18 |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 0     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 34  | B     | 523 | SQD  | C11-C10-C9-C8   |
| 34  | b     | 501 | SQD  | C11-C10-C9-C8   |
| 32  | A     | 405 | PHO  | C5-C6-C7-C8     |
| 32  | a     | 405 | PHO  | C5-C6-C7-C8     |
| 32  | a     | 406 | PHO  | C8-C10-C11-C12  |
| 31  | 5     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | 0     | 310 | CLA  | C2-C3-C5-C6     |
| 32  | A     | 406 | PHO  | C8-C10-C11-C12  |
| 43  | 5     | 302 | ET4  | C11-C12-C13-C14 |
| 43  | 0     | 302 | ET4  | C11-C12-C13-C14 |
| 39  | C     | 518 | DGD  | CCB-CDB-CEB-CFB |
| 39  | c     | 518 | DGD  | CCB-CDB-CEB-CFB |
| 31  | C     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 31  | c     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 0     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 36  | d     | 407 | LHG  | C12-C13-C14-C15 |
| 31  | 6     | 206 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 1     | 206 | CLA  | CAA-CBA-CGA-O1A |
| 36  | D     | 407 | LHG  | C12-C13-C14-C15 |
| 31  | D     | 404 | CLA  | C2-C3-C5-C6     |
| 31  | d     | 404 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 309 | CLA  | C2-C3-C5-C6     |
| 31  | 2     | 309 | CLA  | C2-C3-C5-C6     |
| 37  | D     | 408 | LMG  | C34-C35-C36-C37 |
| 37  | d     | 408 | LMG  | C34-C35-C36-C37 |
| 37  | Y     | 101 | LMG  | O7-C10-C11-C12  |
| 36  | A     | 412 | LHG  | C12-C13-C14-C15 |
| 39  | h     | 102 | DGD  | C8A-C9A-CAA-CBA |
| 36  | a     | 411 | LHG  | C12-C13-C14-C15 |
| 39  | H     | 102 | DGD  | C8A-C9A-CAA-CBA |
| 31  | 5     | 306 | CLA  | CAA-CBA-CGA-O2A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 32  | A     | 405 | PHO  | C15-C16-C17-C18 |
| 36  | A     | 413 | LHG  | O1-C1-C2-O2     |
| 36  | a     | 412 | LHG  | O1-C1-C2-O2     |
| 31  | 1     | 201 | CLA  | CAA-CBA-CGA-O2A |
| 37  | y     | 101 | LMG  | O7-C10-C11-C12  |
| 36  | A     | 412 | LHG  | C25-C26-C27-C28 |
| 36  | a     | 411 | LHG  | C25-C26-C27-C28 |
| 31  | C     | 503 | CLA  | C4B-C3B-CAB-CBB |
| 31  | c     | 503 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 5     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 4     | 209 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 9     | 209 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 0     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 31  | 6     | 201 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 6     | 207 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 1     | 207 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 1     | 207 | CLA  | CAA-CBA-CGA-O2A |
| 32  | a     | 405 | PHO  | C15-C16-C17-C18 |
| 31  | 6     | 207 | CLA  | CAA-CBA-CGA-O2A |
| 33  | B     | 518 | BCR  | C20-C21-C22-C37 |
| 33  | b     | 519 | BCR  | C20-C21-C22-C37 |
| 31  | C     | 503 | CLA  | C5-C6-C7-C8     |
| 34  | B     | 523 | SQD  | C25-C26-C27-C28 |
| 37  | D     | 410 | LMG  | C34-C35-C36-C37 |
| 34  | b     | 501 | SQD  | C25-C26-C27-C28 |
| 37  | d     | 410 | LMG  | C34-C35-C36-C37 |
| 31  | c     | 503 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 505 | CLA  | C8-C10-C11-C12  |
| 31  | b     | 506 | CLA  | C8-C10-C11-C12  |
| 31  | 5     | 312 | CLA  | C4C-C3C-CAC-CBC |
| 31  | B     | 503 | CLA  | C13-C15-C16-C17 |
| 31  | b     | 504 | CLA  | C13-C15-C16-C17 |
| 34  | 0     | 316 | SQD  | C32-C33-C34-C35 |
| 36  | D     | 411 | LHG  | C11-C10-C9-C8   |
| 31  | 0     | 312 | CLA  | C4C-C3C-CAC-CBC |
| 36  | d     | 411 | LHG  | C11-C10-C9-C8   |
| 31  | 6     | 201 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 1     | 201 | CLA  | CAA-CBA-CGA-O1A |
| 31  | C     | 511 | CLA  | C14-C13-C15-C16 |
| 31  | c     | 511 | CLA  | C14-C13-C15-C16 |
| 31  | 5     | 305 | CLA  | C11-C10-C8-C9   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 6     | 210 | CLA  | C14-C13-C15-C16 |
| 31  | 0     | 305 | CLA  | C11-C10-C8-C9   |
| 31  | 1     | 210 | CLA  | C14-C13-C15-C16 |
| 34  | 5     | 316 | SQD  | C32-C33-C34-C35 |
| 34  | 5     | 316 | SQD  | C5-C6-S-O8      |
| 34  | 0     | 316 | SQD  | C5-C6-S-O8      |
| 37  | 5     | 315 | LMG  | C8-C7-O1-C1     |
| 37  | 0     | 315 | LMG  | C8-C7-O1-C1     |
| 31  | B     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 509 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 508 | CLA  | C2-C1-O2A-CGA   |
| 31  | b     | 509 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 508 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 509 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 509 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 510 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 208 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 1     | 208 | CLA  | C3A-C2A-CAA-CBA |
| 36  | B     | 521 | LHG  | C33-C34-C35-C36 |
| 36  | b     | 522 | LHG  | C33-C34-C35-C36 |
| 39  | C     | 520 | DGD  | C4B-C5B-C6B-C7B |
| 39  | c     | 520 | DGD  | C4B-C5B-C6B-C7B |
| 31  | p     | 608 | CLA  | C2C-C3C-CAC-CBC |
| 31  | B     | 506 | CLA  | C8-C10-C11-C12  |
| 31  | b     | 507 | CLA  | C8-C10-C11-C12  |
| 35  | D     | 406 | PL9  | C40-C39-C41-C42 |
| 35  | d     | 406 | PL9  | C40-C39-C41-C42 |
| 44  | p     | 611 | DD6  | C13-C14-C15-O1  |
| 44  | P     | 611 | DD6  | C13-C14-C15-O1  |
| 39  | C     | 520 | DGD  | O6E-C1E-O5D-C6D |
| 39  | c     | 520 | DGD  | O6E-C1E-O5D-C6D |
| 31  | C     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 31  | c     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 39  | C     | 520 | DGD  | O1G-C1G-C2G-C3G |
| 39  | c     | 520 | DGD  | O1G-C1G-C2G-C3G |
| 31  | C     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 31  | c     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 506 | CLA  | C10-C11-C12-C13 |
| 34  | B     | 522 | SQD  | C24-C25-C26-C27 |
| 36  | D     | 407 | LHG  | C33-C34-C35-C36 |
| 36  | d     | 407 | LHG  | C33-C34-C35-C36 |
| 37  | C     | 521 | LMG  | C10-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | A     | 411 | SQD  | C24-C25-C26-C27 |
| 31  | b     | 507 | CLA  | C10-C11-C12-C13 |
| 31  | P     | 608 | CLA  | C2C-C3C-CAC-CBC |
| 37  | c     | 521 | LMG  | C10-C11-C12-C13 |
| 32  | A     | 406 | PHO  | C6-C7-C8-C9     |
| 32  | a     | 406 | PHO  | C6-C7-C8-C9     |
| 35  | A     | 410 | PL9  | C21-C22-C23-C24 |
| 35  | a     | 410 | PL9  | C21-C22-C23-C24 |
| 31  | B     | 513 | CLA  | CAA-CBA-CGA-O2A |
| 37  | M     | 101 | LMG  | O7-C10-C11-C12  |
| 37  | m     | 101 | LMG  | O7-C10-C11-C12  |
| 37  | 5     | 315 | LMG  | O7-C10-C11-C12  |
| 37  | 0     | 315 | LMG  | O7-C10-C11-C12  |
| 37  | J     | 101 | LMG  | C31-C32-C33-C34 |
| 37  | j     | 101 | LMG  | C31-C32-C33-C34 |
| 31  | 0     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 1     | 208 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 503 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 503 | CLA  | C11-C12-C13-C15 |
| 31  | C     | 508 | CLA  | C11-C10-C8-C7   |
| 31  | C     | 511 | CLA  | C12-C13-C15-C16 |
| 31  | b     | 504 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 503 | CLA  | C11-C12-C13-C15 |
| 31  | c     | 508 | CLA  | C11-C10-C8-C7   |
| 31  | c     | 511 | CLA  | C12-C13-C15-C16 |
| 31  | 5     | 307 | CLA  | C6-C7-C8-C10    |
| 31  | 6     | 210 | CLA  | C11-C12-C13-C15 |
| 31  | 6     | 210 | CLA  | C12-C13-C15-C16 |
| 31  | 0     | 307 | CLA  | C6-C7-C8-C10    |
| 31  | 1     | 210 | CLA  | C11-C12-C13-C15 |
| 31  | 1     | 210 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 502 | CLA  | C2B-C3B-CAB-CBB |
| 31  | C     | 503 | CLA  | C2B-C3B-CAB-CBB |
| 31  | C     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 31  | b     | 503 | CLA  | C2B-C3B-CAB-CBB |
| 31  | c     | 503 | CLA  | C2B-C3B-CAB-CBB |
| 31  | c     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 5     | 313 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 6     | 205 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 4     | 209 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 9     | 209 | CLA  | C2B-C3B-CAB-CBB |
| 31  | 0     | 313 | CLA  | C2B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 1     | 205 | CLA  | C2B-C3B-CAB-CBB |
| 33  | B     | 517 | BCR  | C23-C24-C25-C30 |
| 33  | B     | 518 | BCR  | C1-C6-C7-C8     |
| 33  | B     | 518 | BCR  | C23-C24-C25-C26 |
| 33  | C     | 516 | BCR  | C23-C24-C25-C26 |
| 33  | D     | 405 | BCR  | C23-C24-C25-C30 |
| 33  | H     | 101 | BCR  | C23-C24-C25-C26 |
| 33  | K     | 101 | BCR  | C23-C24-C25-C30 |
| 33  | b     | 518 | BCR  | C23-C24-C25-C30 |
| 33  | b     | 519 | BCR  | C1-C6-C7-C8     |
| 33  | b     | 519 | BCR  | C23-C24-C25-C26 |
| 33  | c     | 516 | BCR  | C23-C24-C25-C26 |
| 33  | d     | 405 | BCR  | C23-C24-C25-C30 |
| 33  | h     | 101 | BCR  | C23-C24-C25-C26 |
| 33  | k     | 101 | BCR  | C23-C24-C25-C30 |
| 31  | b     | 514 | CLA  | CAA-CBA-CGA-O2A |
| 37  | B     | 520 | LMG  | O9-C10-O7-C8    |
| 37  | b     | 521 | LMG  | O9-C10-O7-C8    |
| 31  | B     | 502 | CLA  | C5-C6-C7-C8     |
| 31  | b     | 503 | CLA  | C5-C6-C7-C8     |
| 36  | D     | 411 | LHG  | O7-C7-C8-C9     |
| 36  | d     | 411 | LHG  | O7-C7-C8-C9     |
| 41  | F     | 101 | HEM  | C4D-C3D-CAD-CBD |
| 41  | f     | 101 | HEM  | C4D-C3D-CAD-CBD |
| 31  | C     | 506 | CLA  | C4-C3-C5-C6     |
| 31  | c     | 506 | CLA  | C4-C3-C5-C6     |
| 31  | C     | 506 | CLA  | C2-C3-C5-C6     |
| 31  | c     | 506 | CLA  | C2-C3-C5-C6     |
| 39  | C     | 518 | DGD  | O1B-C1B-O2G-C2G |
| 39  | c     | 518 | DGD  | O1B-C1B-O2G-C2G |
| 31  | C     | 513 | CLA  | C2-C3-C5-C6     |
| 31  | c     | 513 | CLA  | C2-C3-C5-C6     |
| 31  | 6     | 208 | CLA  | C2A-CAA-CBA-CGA |
| 41  | F     | 101 | HEM  | CAA-CBA-CGA-O2A |
| 41  | f     | 101 | HEM  | CAA-CBA-CGA-O2A |
| 31  | b     | 512 | CLA  | C11-C12-C13-C15 |
| 34  | A     | 409 | SQD  | O47-C7-C8-C9    |
| 34  | a     | 409 | SQD  | O47-C7-C8-C9    |
| 37  | W     | 201 | LMG  | O7-C10-C11-C12  |
| 37  | W     | 201 | LMG  | O8-C28-C29-C30  |
| 37  | w     | 201 | LMG  | O7-C10-C11-C12  |
| 37  | w     | 201 | LMG  | O8-C28-C29-C30  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 511 | CLA  | C11-C12-C13-C15 |
| 41  | V     | 201 | HEM  | CAA-CBA-CGA-O2A |
| 41  | v     | 201 | HEM  | CAA-CBA-CGA-O2A |
| 39  | c     | 519 | DGD  | CAA-CBA-CCA-CDA |
| 33  | H     | 101 | BCR  | C10-C11-C12-C13 |
| 33  | h     | 101 | BCR  | C10-C11-C12-C13 |
| 31  | B     | 502 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 503 | CLA  | CAA-CBA-CGA-O2A |
| 34  | B     | 522 | SQD  | O47-C7-C8-C9    |
| 31  | C     | 508 | CLA  | C2-C3-C5-C6     |
| 31  | c     | 508 | CLA  | C2-C3-C5-C6     |
| 39  | C     | 519 | DGD  | CAA-CBA-CCA-CDA |
| 31  | 2     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 36  | H     | 103 | LHG  | C27-C28-C29-C30 |
| 36  | h     | 103 | LHG  | C27-C28-C29-C30 |
| 31  | 5     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 7     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 209 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 1     | 209 | CLA  | CAA-CBA-CGA-O1A |
| 31  | C     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 31  | c     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 34  | A     | 411 | SQD  | O47-C7-C8-C9    |
| 37  | M     | 101 | LMG  | C39-C40-C41-C42 |
| 37  | m     | 101 | LMG  | C39-C40-C41-C42 |
| 31  | 7     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 41  | V     | 201 | HEM  | CAA-CBA-CGA-O1A |
| 41  | v     | 201 | HEM  | CAA-CBA-CGA-O1A |
| 31  | A     | 407 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 509 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 514 | CLA  | C6-C7-C8-C9     |
| 31  | C     | 503 | CLA  | C14-C13-C15-C16 |
| 31  | a     | 407 | CLA  | C11-C10-C8-C9   |
| 31  | b     | 510 | CLA  | C14-C13-C15-C16 |
| 31  | b     | 515 | CLA  | C6-C7-C8-C9     |
| 31  | c     | 503 | CLA  | C14-C13-C15-C16 |
| 31  | c     | 502 | CLA  | CAA-CBA-CGA-O2A |
| 37  | Y     | 101 | LMG  | O1-C7-C8-C9     |
| 37  | y     | 101 | LMG  | O1-C7-C8-C9     |
| 37  | j     | 101 | LMG  | C34-C35-C36-C37 |
| 31  | b     | 504 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 37  | J     | 101 | LMG  | C34-C35-C36-C37 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 0     | 305 | CLA  | C10-C11-C12-C13 |
| 31  | C     | 502 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 32  | A     | 406 | PHO  | CAA-CBA-CGA-O2A |
| 32  | a     | 406 | PHO  | CAA-CBA-CGA-O2A |
| 37  | M     | 101 | LMG  | C18-C19-C20-C21 |
| 33  | D     | 405 | BCR  | C21-C22-C23-C24 |
| 33  | d     | 405 | BCR  | C21-C22-C23-C24 |
| 31  | 6     | 209 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 510 | CLA  | CAA-CBA-CGA-O2A |
| 37  | J     | 101 | LMG  | O8-C28-C29-C30  |
| 37  | m     | 101 | LMG  | C18-C19-C20-C21 |
| 31  | 5     | 305 | CLA  | C10-C11-C12-C13 |
| 35  | A     | 410 | PL9  | C17-C18-C19-C20 |
| 36  | b     | 522 | LHG  | O7-C7-C8-C9     |
| 37  | j     | 101 | LMG  | O8-C28-C29-C30  |
| 34  | 0     | 316 | SQD  | C34-C35-C36-C37 |
| 31  | 1     | 209 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 513 | CLA  | C2-C1-O2A-CGA   |
| 31  | C     | 511 | CLA  | C2-C1-O2A-CGA   |
| 31  | b     | 514 | CLA  | C2-C1-O2A-CGA   |
| 31  | c     | 511 | CLA  | C2-C1-O2A-CGA   |
| 36  | B     | 521 | LHG  | O7-C7-C8-C9     |
| 34  | 5     | 316 | SQD  | C34-C35-C36-C37 |
| 31  | C     | 510 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 510 | CLA  | C6-C7-C8-C10    |
| 39  | C     | 520 | DGD  | C3B-C4B-C5B-C6B |
| 39  | c     | 520 | DGD  | C3B-C4B-C5B-C6B |
| 31  | B     | 514 | CLA  | O1A-CGA-O2A-C1  |
| 37  | j     | 101 | LMG  | C36-C37-C38-C39 |
| 31  | 7     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 206 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 1     | 206 | CLA  | C2A-CAA-CBA-CGA |
| 37  | J     | 101 | LMG  | C36-C37-C38-C39 |
| 37  | d     | 408 | LMG  | C28-C29-C30-C31 |
| 31  | b     | 515 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 514 | CLA  | CBA-CGA-O2A-C1  |
| 31  | b     | 515 | CLA  | CBA-CGA-O2A-C1  |
| 35  | a     | 410 | PL9  | C17-C18-C19-C20 |
| 31  | 6     | 213 | CLA  | CHA-CBD-CGD-O1D |
| 31  | p     | 608 | CLA  | CHA-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | P     | 608 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 1     | 213 | CLA  | CHA-CBD-CGD-O1D |
| 37  | Y     | 101 | LMG  | O9-C10-C11-C12  |
| 37  | y     | 101 | LMG  | O9-C10-C11-C12  |
| 31  | B     | 510 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 511 | CLA  | C16-C17-C18-C20 |
| 37  | D     | 408 | LMG  | C28-C29-C30-C31 |
| 41  | F     | 101 | HEM  | CAA-CBA-CGA-O1A |
| 41  | f     | 101 | HEM  | CAA-CBA-CGA-O1A |
| 36  | A     | 412 | LHG  | C24-C25-C26-C27 |
| 37  | m     | 101 | LMG  | C11-C12-C13-C14 |
| 37  | J     | 101 | LMG  | O10-C28-C29-C30 |
| 39  | H     | 102 | DGD  | O1B-C1B-C2B-C3B |
| 39  | h     | 102 | DGD  | O1B-C1B-C2B-C3B |
| 37  | M     | 101 | LMG  | C11-C12-C13-C14 |
| 34  | A     | 411 | SQD  | C23-C24-C25-C26 |
| 31  | C     | 505 | CLA  | C6-C7-C8-C10    |
| 36  | a     | 411 | LHG  | C24-C25-C26-C27 |
| 37  | 0     | 315 | LMG  | C12-C13-C14-C15 |
| 31  | C     | 502 | CLA  | CAA-CBA-CGA-O1A |
| 32  | A     | 406 | PHO  | CAA-CBA-CGA-O1A |
| 32  | a     | 406 | PHO  | CAA-CBA-CGA-O1A |
| 37  | j     | 101 | LMG  | O10-C28-C29-C30 |
| 34  | B     | 522 | SQD  | C23-C24-C25-C26 |
| 31  | C     | 511 | CLA  | C5-C6-C7-C8     |
| 31  | c     | 511 | CLA  | C5-C6-C7-C8     |
| 37  | 5     | 315 | LMG  | C11-C12-C13-C14 |
| 37  | 5     | 315 | LMG  | C12-C13-C14-C15 |
| 37  | 0     | 315 | LMG  | C11-C12-C13-C14 |
| 31  | C     | 503 | CLA  | C11-C12-C13-C14 |
| 31  | c     | 503 | CLA  | C11-C12-C13-C14 |
| 31  | 7     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | 2     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | c     | 505 | CLA  | C6-C7-C8-C10    |
| 31  | c     | 502 | CLA  | CAA-CBA-CGA-O1A |
| 35  | D     | 406 | PL9  | C15-C14-C16-C17 |
| 35  | d     | 406 | PL9  | C15-C14-C16-C17 |
| 36  | D     | 407 | LHG  | O10-C23-C24-C25 |
| 36  | d     | 407 | LHG  | O10-C23-C24-C25 |
| 37  | W     | 201 | LMG  | O10-C28-C29-C30 |
| 31  | P     | 608 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 513 | CLA  | CAA-CBA-CGA-O1A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 514 | CLA  | CAA-CBA-CGA-O1A |
| 37  | w     | 201 | LMG  | O10-C28-C29-C30 |
| 31  | W     | 202 | CLA  | CAA-CBA-CGA-O2A |
| 31  | w     | 202 | CLA  | CAA-CBA-CGA-O2A |
| 31  | D     | 404 | CLA  | C5-C6-C7-C8     |
| 31  | d     | 404 | CLA  | C5-C6-C7-C8     |
| 31  | c     | 511 | CLA  | CAA-CBA-CGA-O1A |
| 34  | A     | 411 | SQD  | C45-C44-O6-C1   |
| 34  | B     | 522 | SQD  | C45-C44-O6-C1   |
| 34  | A     | 409 | SQD  | O49-C7-O47-C45  |
| 34  | a     | 409 | SQD  | O49-C7-O47-C45  |
| 37  | 5     | 315 | LMG  | O9-C10-C11-C12  |
| 37  | 0     | 315 | LMG  | O9-C10-C11-C12  |
| 31  | C     | 513 | CLA  | C16-C17-C18-C20 |
| 42  | 4     | 203 | A86  | C12-C11-C13-O   |
| 42  | 9     | 203 | A86  | C12-C11-C13-O   |
| 31  | B     | 502 | CLA  | CAA-CBA-CGA-O1A |
| 31  | C     | 511 | CLA  | CAA-CBA-CGA-O1A |
| 31  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 31  | C     | 511 | CLA  | C8-C10-C11-C12  |
| 31  | C     | 511 | CLA  | C15-C16-C17-C18 |
| 31  | c     | 509 | CLA  | C13-C15-C16-C17 |
| 31  | c     | 511 | CLA  | C15-C16-C17-C18 |
| 34  | B     | 523 | SQD  | O47-C7-C8-C9    |
| 34  | b     | 501 | SQD  | O47-C7-C8-C9    |
| 31  | c     | 511 | CLA  | C8-C10-C11-C12  |
| 31  | b     | 503 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 511 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 513 | CLA  | CAD-CBD-CGD-O2D |
| 31  | b     | 512 | CLA  | CAD-CBD-CGD-O2D |
| 31  | b     | 514 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 7     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 32  | A     | 405 | PHO  | CAD-CBD-CGD-O2D |
| 32  | a     | 405 | PHO  | CAD-CBD-CGD-O2D |
| 42  | 3     | 301 | A86  | C13-C14-C15-C20 |
| 42  | 3     | 302 | A86  | C13-C14-C15-C20 |
| 42  | 8     | 301 | A86  | C13-C14-C15-C20 |
| 42  | 8     | 302 | A86  | C13-C14-C15-C20 |
| 31  | 1     | 207 | CLA  | C2C-C3C-CAC-CBC |
| 37  | M     | 101 | LMG  | O8-C28-C29-C30  |
| 37  | m     | 101 | LMG  | O8-C28-C29-C30  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 6     | 207 | CLA  | C2C-C3C-CAC-CBC |
| 34  | 5     | 316 | SQD  | C26-C27-C28-C29 |
| 34  | 0     | 316 | SQD  | C26-C27-C28-C29 |
| 31  | B     | 510 | CLA  | CAA-CBA-CGA-O1A |
| 37  | D     | 410 | LMG  | O8-C28-C29-C30  |
| 37  | d     | 410 | LMG  | O8-C28-C29-C30  |
| 31  | c     | 513 | CLA  | C16-C17-C18-C20 |
| 34  | A     | 411 | SQD  | C29-C30-C31-C32 |
| 34  | B     | 522 | SQD  | C29-C30-C31-C32 |
| 37  | D     | 408 | LMG  | O7-C10-C11-C12  |
| 37  | d     | 408 | LMG  | O7-C10-C11-C12  |
| 31  | B     | 511 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 512 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 511 | CLA  | CAA-CBA-CGA-O1A |
| 39  | C     | 519 | DGD  | C4A-C5A-C6A-C7A |
| 39  | c     | 519 | DGD  | C4A-C5A-C6A-C7A |
| 31  | B     | 506 | CLA  | C15-C16-C17-C18 |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 42  | 4     | 201 | A86  | C31-C32-C33-C34-C35-C36 |
| 42  | 9     | 201 | A86  | C31-C32-C33-C34-C35-C36 |

217 monomers are involved in 516 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 7     | 309 | CLA  | 6       | 0            |
| 37  | y     | 101 | LMG  | 4       | 0            |
| 39  | C     | 518 | DGD  | 1       | 0            |
| 32  | a     | 406 | PHO  | 1       | 0            |
| 31  | B     | 505 | CLA  | 4       | 0            |
| 31  | B     | 516 | CLA  | 5       | 0            |
| 42  | 1     | 202 | A86  | 1       | 0            |
| 36  | d     | 407 | LHG  | 5       | 0            |
| 34  | B     | 522 | SQD  | 2       | 0            |
| 42  | 6     | 202 | A86  | 1       | 0            |
| 44  | 2     | 303 | DD6  | 18      | 0            |
| 31  | 2     | 305 | CLA  | 1       | 0            |
| 35  | D     | 406 | PL9  | 3       | 0            |
| 31  | C     | 502 | CLA  | 3       | 0            |
| 31  | 1     | 210 | CLA  | 5       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 8     | 314 | CLA  | 1       | 0            |
| 37  | D     | 409 | LMG  | 2       | 0            |
| 31  | 6     | 214 | CLA  | 1       | 0            |
| 37  | 5     | 315 | LMG  | 1       | 0            |
| 44  | 6     | 203 | DD6  | 1       | 0            |
| 31  | B     | 514 | CLA  | 7       | 0            |
| 31  | c     | 509 | CLA  | 5       | 0            |
| 31  | 1     | 206 | CLA  | 4       | 0            |
| 31  | 3     | 311 | CLA  | 1       | 0            |
| 31  | W     | 202 | CLA  | 1       | 0            |
| 33  | k     | 101 | BCR  | 2       | 0            |
| 36  | B     | 521 | LHG  | 4       | 0            |
| 31  | 8     | 308 | CLA  | 1       | 0            |
| 37  | J     | 101 | LMG  | 3       | 0            |
| 31  | 3     | 314 | CLA  | 1       | 0            |
| 31  | C     | 510 | CLA  | 2       | 0            |
| 31  | B     | 511 | CLA  | 1       | 0            |
| 31  | 5     | 313 | CLA  | 1       | 0            |
| 31  | z     | 101 | CLA  | 6       | 0            |
| 31  | b     | 517 | CLA  | 4       | 0            |
| 36  | a     | 412 | LHG  | 2       | 0            |
| 37  | w     | 201 | LMG  | 2       | 0            |
| 33  | b     | 518 | BCR  | 5       | 0            |
| 31  | 2     | 306 | CLA  | 5       | 0            |
| 33  | K     | 101 | BCR  | 2       | 0            |
| 37  | c     | 521 | LMG  | 4       | 0            |
| 31  | c     | 507 | CLA  | 1       | 0            |
| 31  | p     | 604 | CLA  | 5       | 0            |
| 31  | C     | 512 | CLA  | 3       | 0            |
| 44  | 1     | 203 | DD6  | 1       | 0            |
| 31  | c     | 511 | CLA  | 2       | 0            |
| 31  | 8     | 305 | CLA  | 1       | 0            |
| 31  | 1     | 211 | CLA  | 1       | 0            |
| 31  | b     | 510 | CLA  | 2       | 0            |
| 39  | c     | 518 | DGD  | 2       | 0            |
| 32  | A     | 406 | PHO  | 1       | 0            |
| 42  | 0     | 303 | A86  | 1       | 0            |
| 31  | p     | 607 | CLA  | 1       | 0            |
| 31  | 0     | 314 | CLA  | 3       | 0            |
| 36  | D     | 411 | LHG  | 2       | 0            |
| 33  | C     | 515 | BCR  | 1       | 0            |
| 34  | A     | 409 | SQD  | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | p     | 603 | CLA  | 2       | 0            |
| 31  | B     | 515 | CLA  | 2       | 0            |
| 31  | 0     | 304 | CLA  | 3       | 0            |
| 31  | b     | 515 | CLA  | 8       | 0            |
| 41  | v     | 201 | HEM  | 6       | 0            |
| 39  | c     | 520 | DGD  | 6       | 0            |
| 31  | 2     | 307 | CLA  | 3       | 0            |
| 31  | A     | 403 | CLA  | 4       | 0            |
| 31  | C     | 509 | CLA  | 5       | 0            |
| 36  | b     | 522 | LHG  | 4       | 0            |
| 31  | 7     | 310 | CLA  | 7       | 0            |
| 44  | 2     | 304 | DD6  | 6       | 0            |
| 31  | c     | 505 | CLA  | 2       | 0            |
| 31  | B     | 503 | CLA  | 2       | 0            |
| 33  | b     | 519 | BCR  | 2       | 0            |
| 33  | c     | 515 | BCR  | 2       | 0            |
| 39  | C     | 519 | DGD  | 5       | 0            |
| 31  | 3     | 305 | CLA  | 1       | 0            |
| 31  | 6     | 206 | CLA  | 4       | 0            |
| 44  | 7     | 303 | DD6  | 18      | 0            |
| 39  | C     | 520 | DGD  | 7       | 0            |
| 31  | c     | 508 | CLA  | 1       | 0            |
| 31  | 2     | 310 | CLA  | 6       | 0            |
| 34  | 5     | 316 | SQD  | 5       | 0            |
| 34  | B     | 523 | SQD  | 1       | 0            |
| 34  | b     | 501 | SQD  | 1       | 0            |
| 37  | B     | 520 | LMG  | 1       | 0            |
| 37  | m     | 101 | LMG  | 1       | 0            |
| 31  | B     | 513 | CLA  | 2       | 0            |
| 31  | 6     | 201 | CLA  | 2       | 0            |
| 39  | c     | 519 | DGD  | 5       | 0            |
| 31  | p     | 602 | CLA  | 2       | 0            |
| 31  | d     | 401 | CLA  | 1       | 0            |
| 36  | h     | 103 | LHG  | 5       | 0            |
| 31  | 6     | 210 | CLA  | 5       | 0            |
| 31  | B     | 510 | CLA  | 3       | 0            |
| 44  | P     | 611 | DD6  | 7       | 0            |
| 31  | B     | 504 | CLA  | 7       | 0            |
| 31  | 8     | 313 | CLA  | 1       | 0            |
| 31  | Z     | 101 | CLA  | 6       | 0            |
| 44  | 8     | 303 | DD6  | 1       | 0            |
| 31  | C     | 511 | CLA  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | B     | 506 | CLA  | 4       | 0            |
| 41  | f     | 101 | HEM  | 3       | 0            |
| 37  | M     | 101 | LMG  | 1       | 0            |
| 31  | 2     | 312 | CLA  | 1       | 0            |
| 31  | P     | 607 | CLA  | 1       | 0            |
| 31  | 5     | 314 | CLA  | 3       | 0            |
| 37  | j     | 101 | LMG  | 2       | 0            |
| 31  | D     | 404 | CLA  | 3       | 0            |
| 36  | D     | 407 | LHG  | 5       | 0            |
| 33  | b     | 520 | BCR  | 5       | 0            |
| 31  | b     | 509 | CLA  | 2       | 0            |
| 37  | m     | 102 | LMG  | 1       | 0            |
| 31  | c     | 510 | CLA  | 2       | 0            |
| 31  | 5     | 307 | CLA  | 3       | 0            |
| 41  | F     | 101 | HEM  | 3       | 0            |
| 31  | 3     | 308 | CLA  | 1       | 0            |
| 31  | 0     | 310 | CLA  | 1       | 0            |
| 31  | 0     | 311 | CLA  | 2       | 0            |
| 33  | c     | 517 | BCR  | 4       | 0            |
| 36  | d     | 411 | LHG  | 2       | 0            |
| 32  | a     | 405 | PHO  | 2       | 0            |
| 33  | a     | 408 | BCR  | 3       | 0            |
| 31  | 6     | 209 | CLA  | 1       | 0            |
| 31  | w     | 202 | CLA  | 1       | 0            |
| 37  | C     | 521 | LMG  | 4       | 0            |
| 31  | B     | 512 | CLA  | 2       | 0            |
| 31  | 2     | 309 | CLA  | 6       | 0            |
| 31  | 5     | 304 | CLA  | 3       | 0            |
| 39  | H     | 102 | DGD  | 4       | 0            |
| 39  | h     | 102 | DGD  | 4       | 0            |
| 31  | 8     | 312 | CLA  | 1       | 0            |
| 44  | 7     | 304 | DD6  | 7       | 0            |
| 31  | d     | 404 | CLA  | 3       | 0            |
| 31  | P     | 602 | CLA  | 2       | 0            |
| 31  | 0     | 307 | CLA  | 3       | 0            |
| 35  | a     | 410 | PL9  | 3       | 0            |
| 31  | 0     | 313 | CLA  | 1       | 0            |
| 31  | B     | 509 | CLA  | 2       | 0            |
| 37  | M     | 102 | LMG  | 1       | 0            |
| 44  | 3     | 303 | DD6  | 1       | 0            |
| 42  | 5     | 303 | A86  | 1       | 0            |
| 33  | A     | 408 | BCR  | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | a     | 411 | LHG  | 2       | 0            |
| 31  | 7     | 305 | CLA  | 1       | 0            |
| 31  | 1     | 214 | CLA  | 1       | 0            |
| 31  | C     | 507 | CLA  | 1       | 0            |
| 36  | d     | 412 | LHG  | 2       | 0            |
| 31  | P     | 604 | CLA  | 5       | 0            |
| 37  | d     | 410 | LMG  | 2       | 0            |
| 31  | 5     | 311 | CLA  | 2       | 0            |
| 31  | 5     | 305 | CLA  | 3       | 0            |
| 31  | 5     | 308 | CLA  | 6       | 0            |
| 31  | b     | 505 | CLA  | 7       | 0            |
| 33  | d     | 405 | BCR  | 1       | 0            |
| 31  | b     | 502 | CLA  | 1       | 0            |
| 35  | A     | 410 | PL9  | 3       | 0            |
| 33  | H     | 101 | BCR  | 2       | 0            |
| 31  | 3     | 310 | CLA  | 1       | 0            |
| 33  | B     | 517 | BCR  | 7       | 0            |
| 31  | b     | 503 | CLA  | 1       | 0            |
| 31  | b     | 513 | CLA  | 1       | 0            |
| 37  | D     | 410 | LMG  | 2       | 0            |
| 31  | B     | 508 | CLA  | 3       | 0            |
| 31  | c     | 512 | CLA  | 3       | 0            |
| 37  | 0     | 315 | LMG  | 1       | 0            |
| 36  | H     | 103 | LHG  | 6       | 0            |
| 34  | 0     | 316 | SQD  | 5       | 0            |
| 31  | C     | 505 | CLA  | 2       | 0            |
| 36  | A     | 412 | LHG  | 2       | 0            |
| 31  | 6     | 211 | CLA  | 2       | 0            |
| 33  | B     | 518 | BCR  | 2       | 0            |
| 33  | C     | 516 | BCR  | 1       | 0            |
| 31  | b     | 507 | CLA  | 3       | 0            |
| 31  | 3     | 313 | CLA  | 1       | 0            |
| 31  | b     | 516 | CLA  | 2       | 0            |
| 31  | b     | 511 | CLA  | 3       | 0            |
| 37  | d     | 409 | LMG  | 3       | 0            |
| 31  | 1     | 209 | CLA  | 1       | 0            |
| 31  | c     | 502 | CLA  | 3       | 0            |
| 31  | b     | 504 | CLA  | 2       | 0            |
| 31  | 7     | 306 | CLA  | 4       | 0            |
| 34  | A     | 411 | SQD  | 3       | 0            |
| 31  | 3     | 312 | CLA  | 1       | 0            |
| 36  | D     | 412 | LHG  | 2       | 0            |

*Continued on next page...*

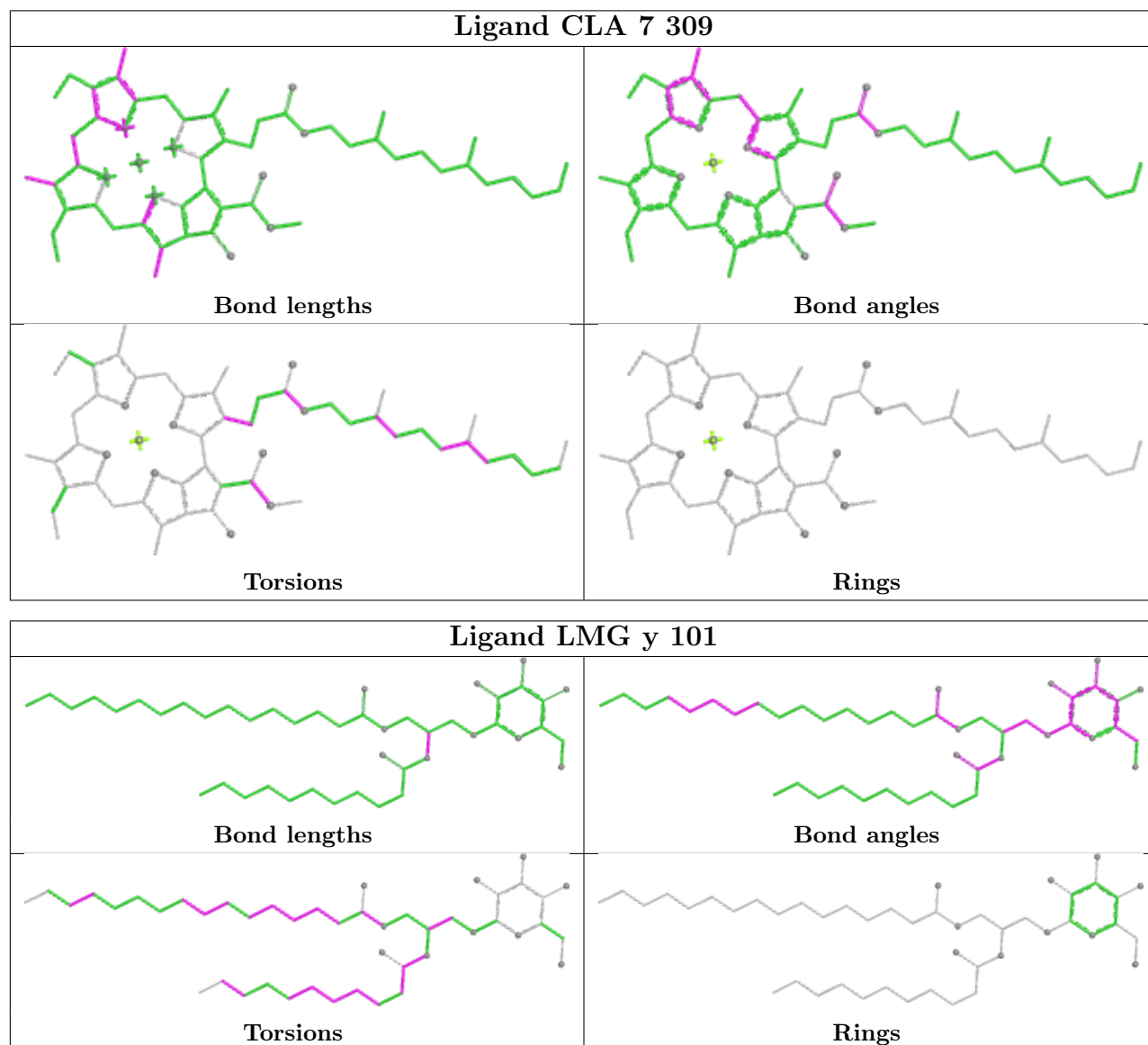


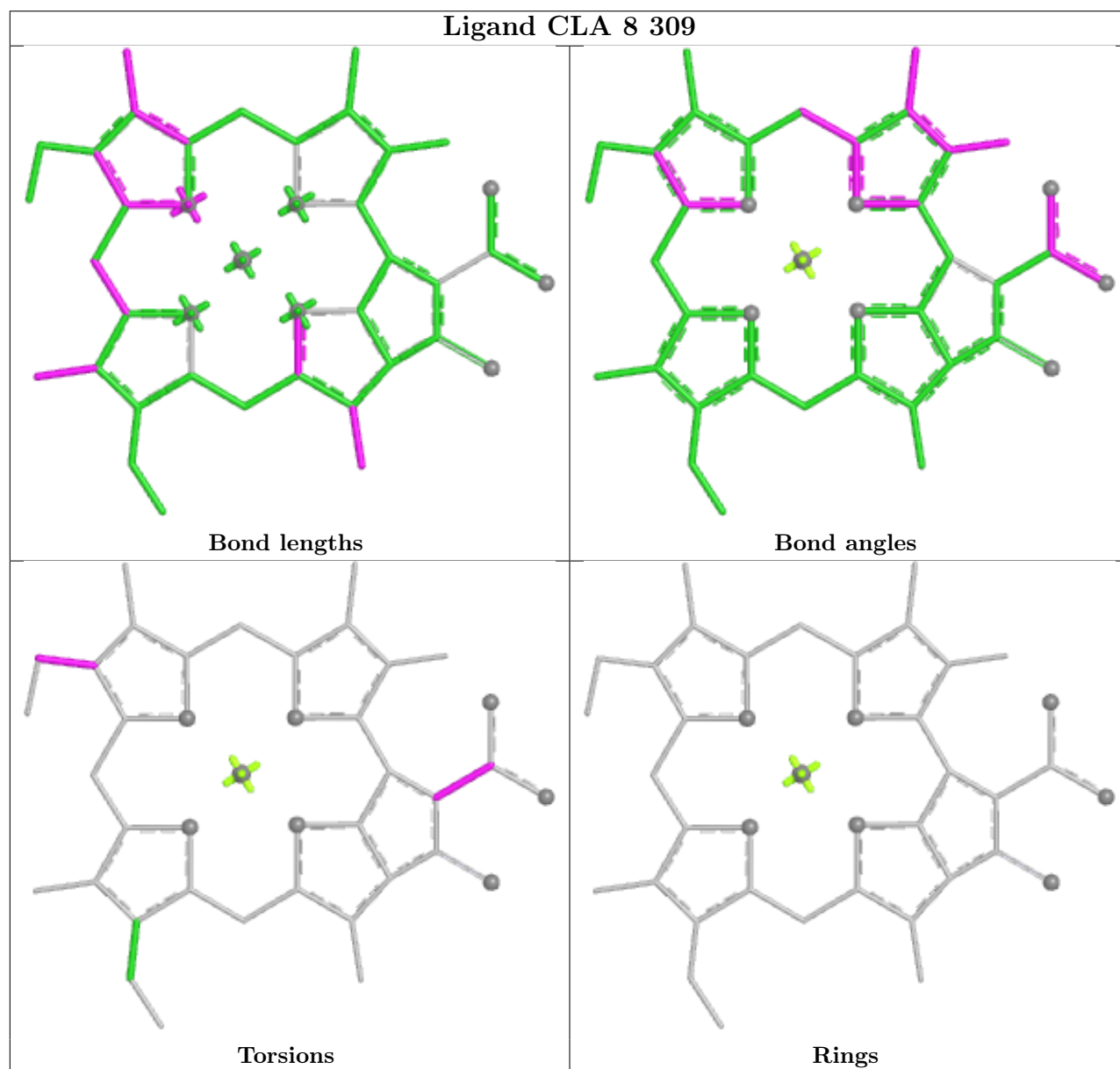
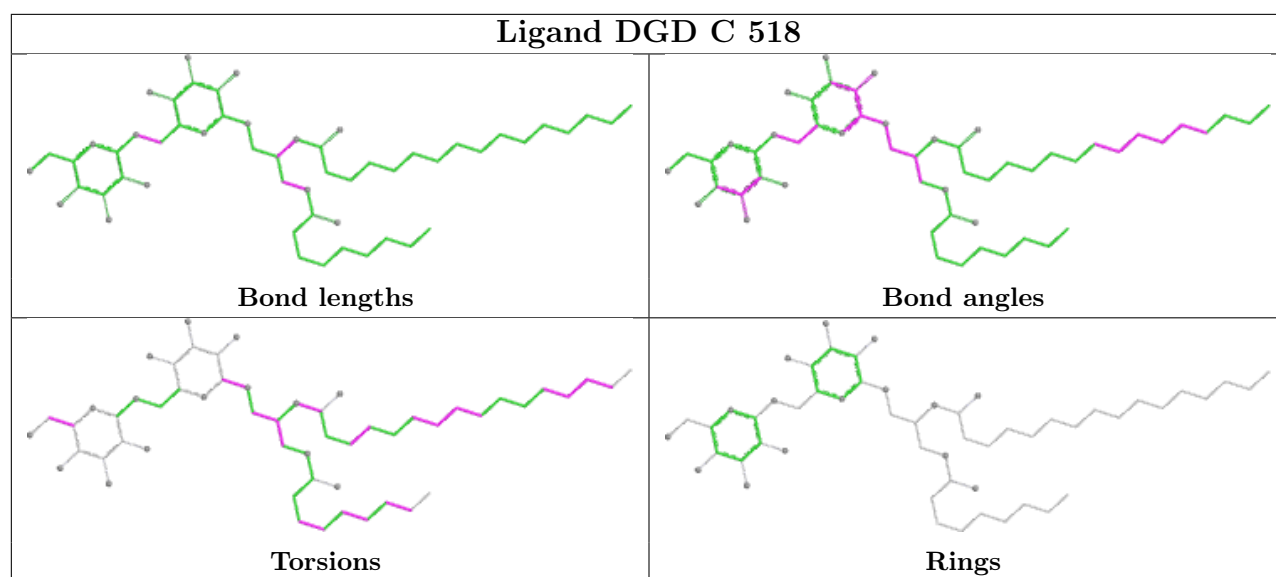
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | A     | 413 | LHG  | 2       | 0            |
| 31  | 3     | 307 | CLA  | 1       | 0            |
| 33  | c     | 516 | BCR  | 2       | 0            |
| 31  | a     | 403 | CLA  | 3       | 0            |
| 31  | 1     | 201 | CLA  | 2       | 0            |
| 44  | 6     | 204 | DD6  | 2       | 0            |
| 31  | 8     | 310 | CLA  | 1       | 0            |
| 33  | C     | 517 | BCR  | 4       | 0            |
| 35  | d     | 406 | PL9  | 4       | 0            |
| 31  | 8     | 311 | CLA  | 1       | 0            |
| 41  | V     | 201 | HEM  | 6       | 0            |
| 33  | D     | 405 | BCR  | 2       | 0            |
| 31  | c     | 506 | CLA  | 2       | 0            |
| 37  | b     | 521 | LMG  | 1       | 0            |
| 31  | 7     | 307 | CLA  | 3       | 0            |
| 31  | 7     | 312 | CLA  | 1       | 0            |
| 31  | 0     | 305 | CLA  | 3       | 0            |
| 44  | p     | 611 | DD6  | 7       | 0            |
| 31  | D     | 401 | CLA  | 1       | 0            |
| 31  | 5     | 310 | CLA  | 1       | 0            |
| 33  | B     | 519 | BCR  | 4       | 0            |
| 33  | h     | 101 | BCR  | 2       | 0            |
| 31  | 0     | 308 | CLA  | 6       | 0            |
| 31  | B     | 501 | CLA  | 1       | 0            |
| 32  | A     | 405 | PHO  | 3       | 0            |
| 31  | B     | 502 | CLA  | 1       | 0            |
| 31  | P     | 603 | CLA  | 2       | 0            |
| 31  | b     | 512 | CLA  | 1       | 0            |
| 31  | b     | 506 | CLA  | 3       | 0            |
| 37  | Y     | 101 | LMG  | 3       | 0            |
| 37  | W     | 201 | LMG  | 2       | 0            |
| 31  | C     | 506 | CLA  | 2       | 0            |
| 31  | b     | 514 | CLA  | 1       | 0            |
| 44  | 1     | 204 | DD6  | 2       | 0            |

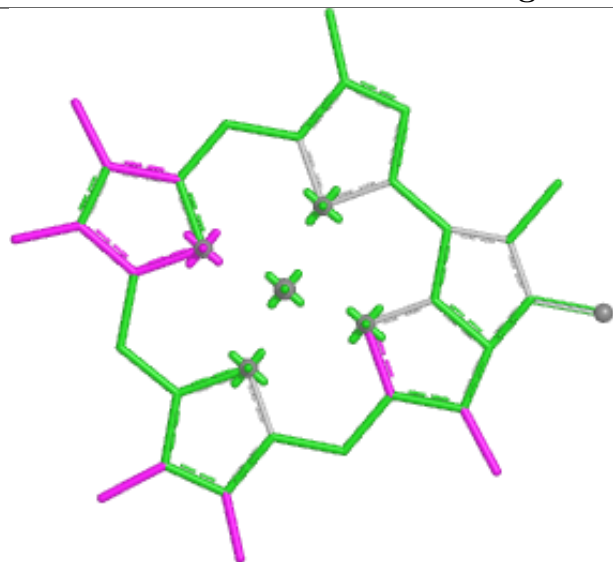
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

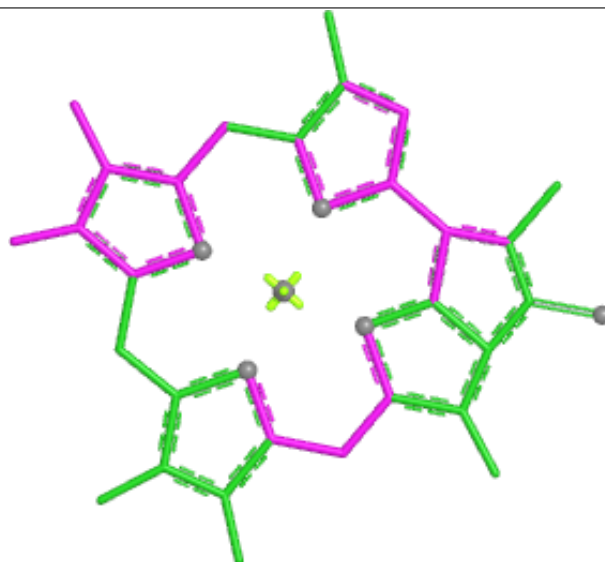




## Ligand CLA 9 213



Bond lengths



Bond angles

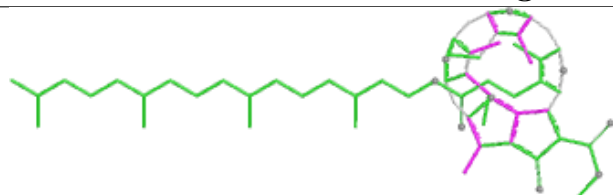


Torsions

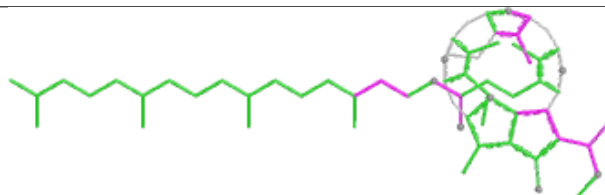


Rings

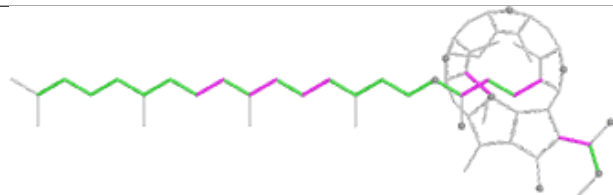
## Ligand PHO a 406



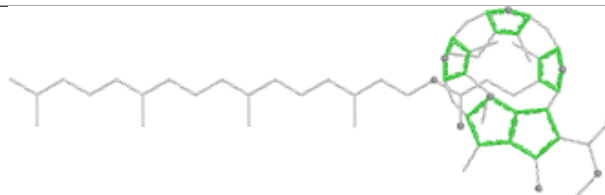
Bond lengths



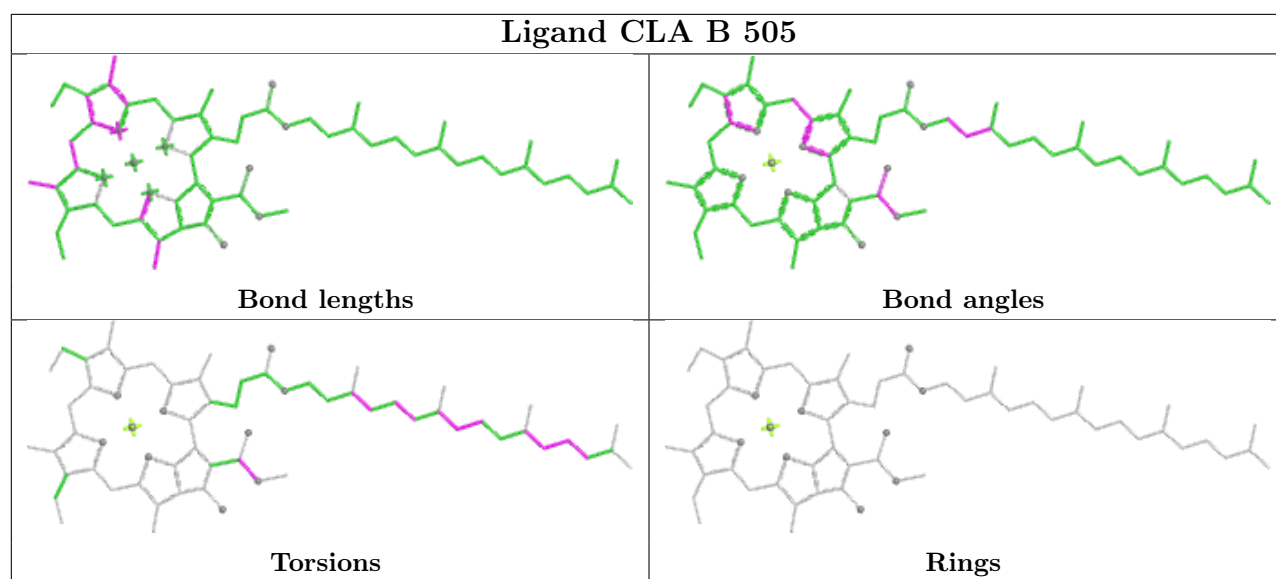
Bond angles



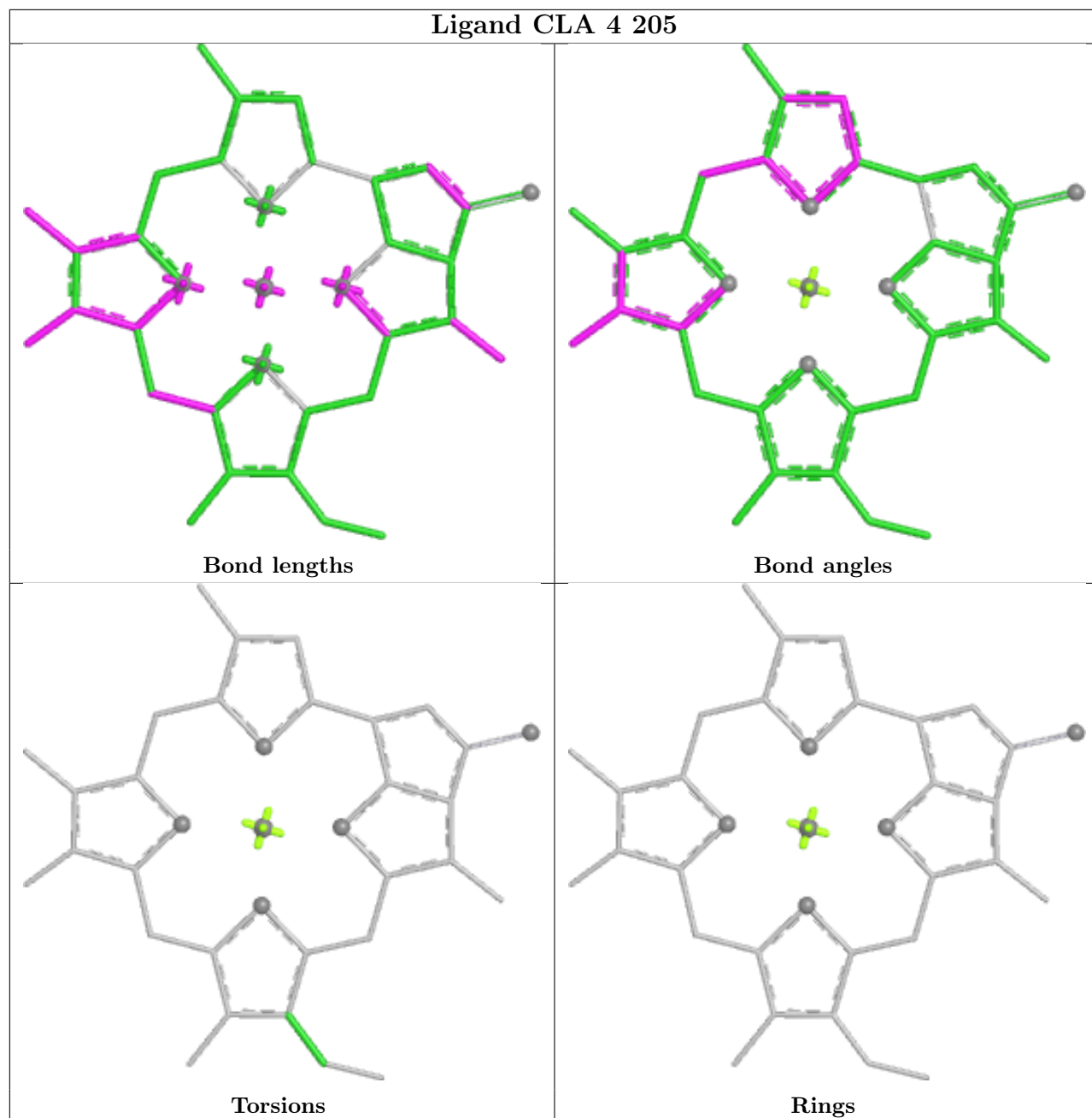
Torsions

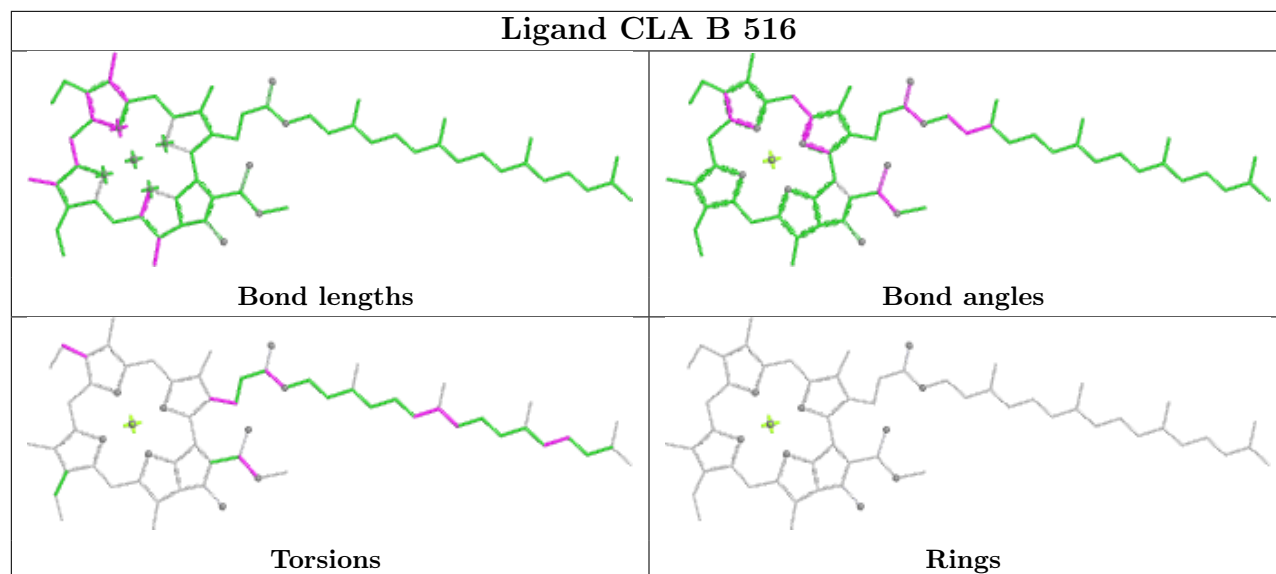
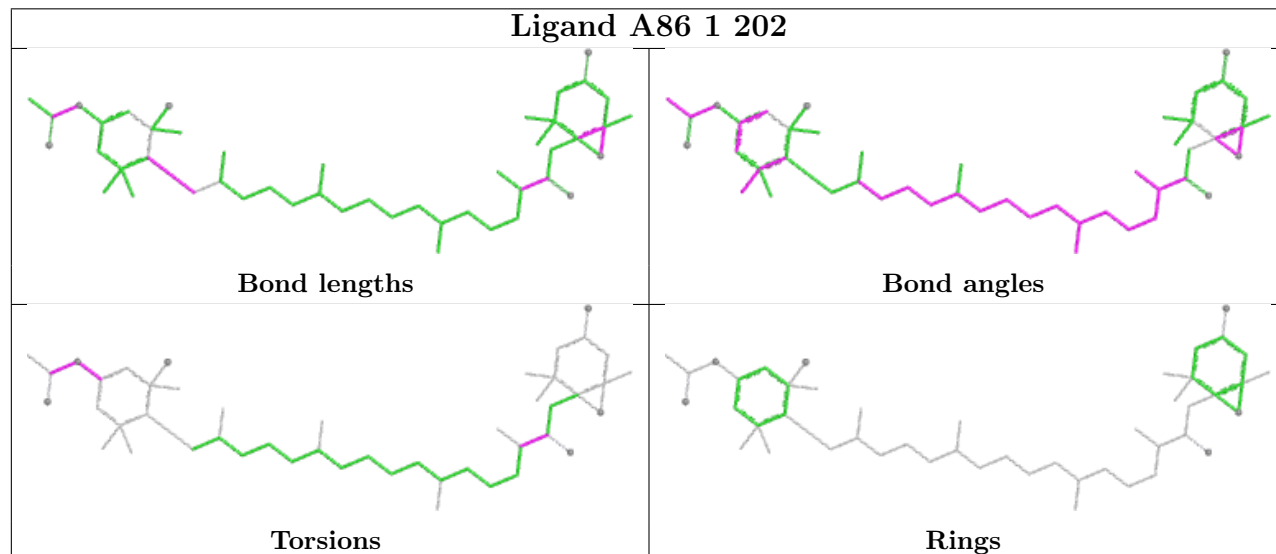


Rings

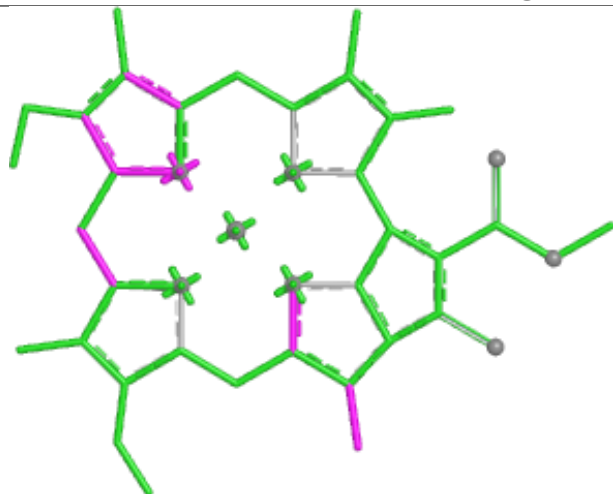


## Ligand CLA 4 205

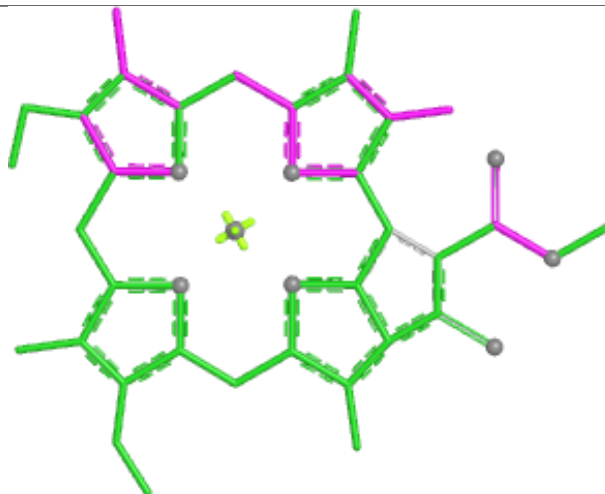


**Ligand CLA B 516****Ligand A86 1 202**

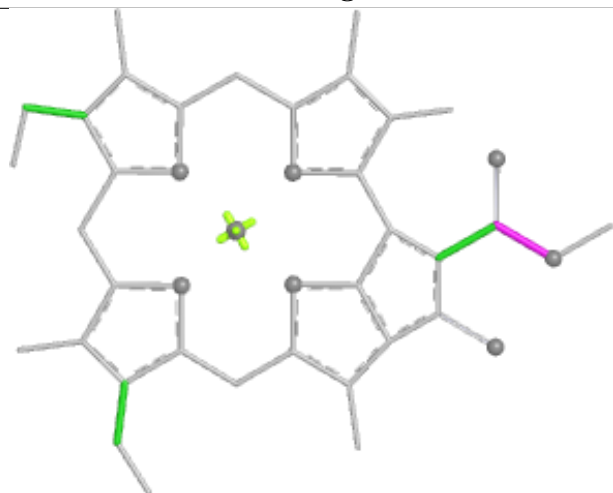
## Ligand CLA 6 212



Bond lengths



Bond angles

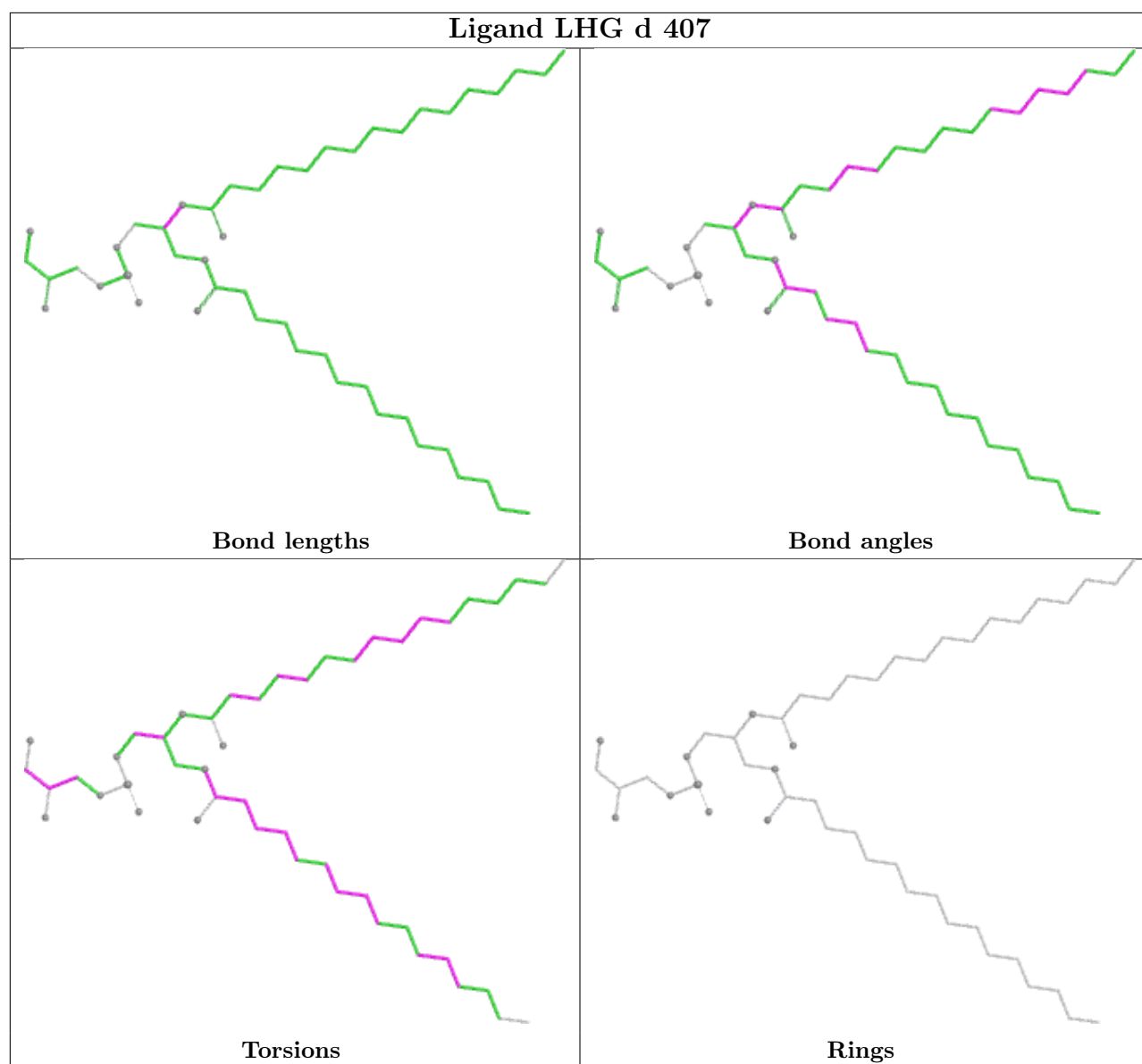


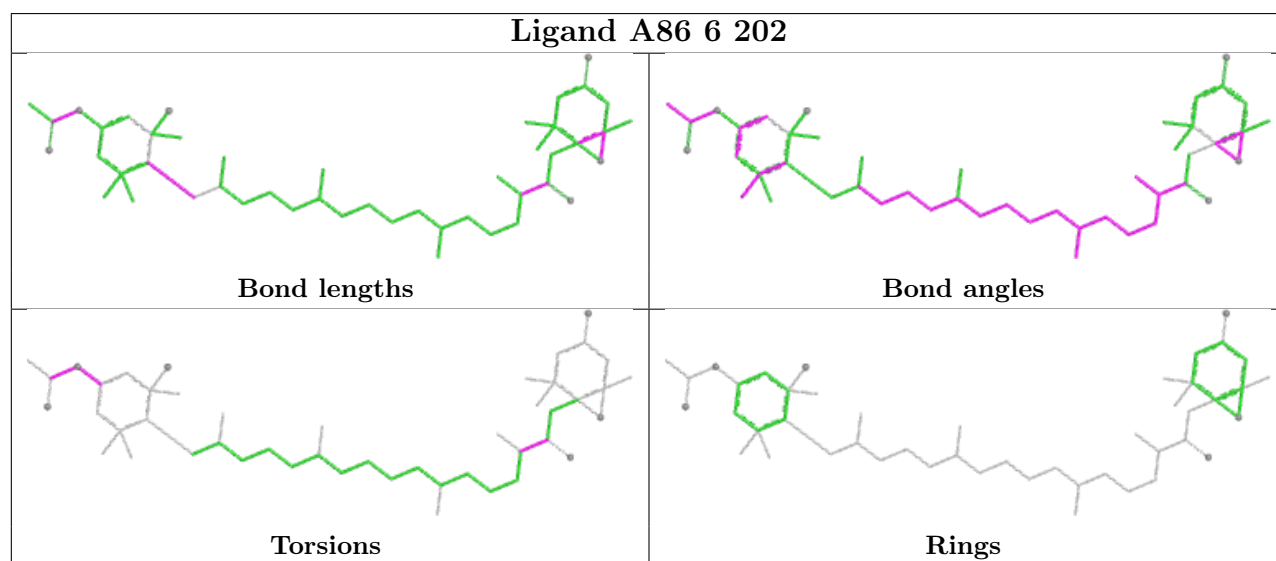
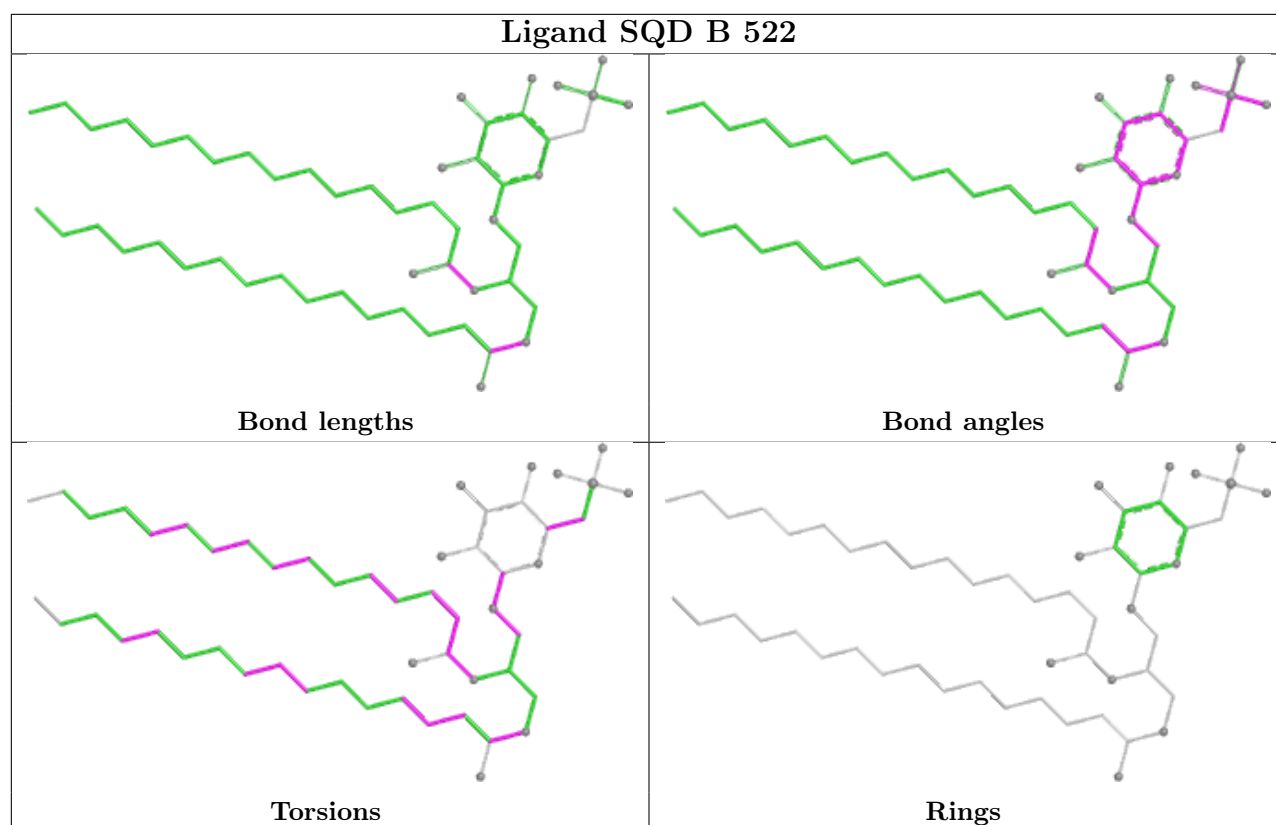
Torsions

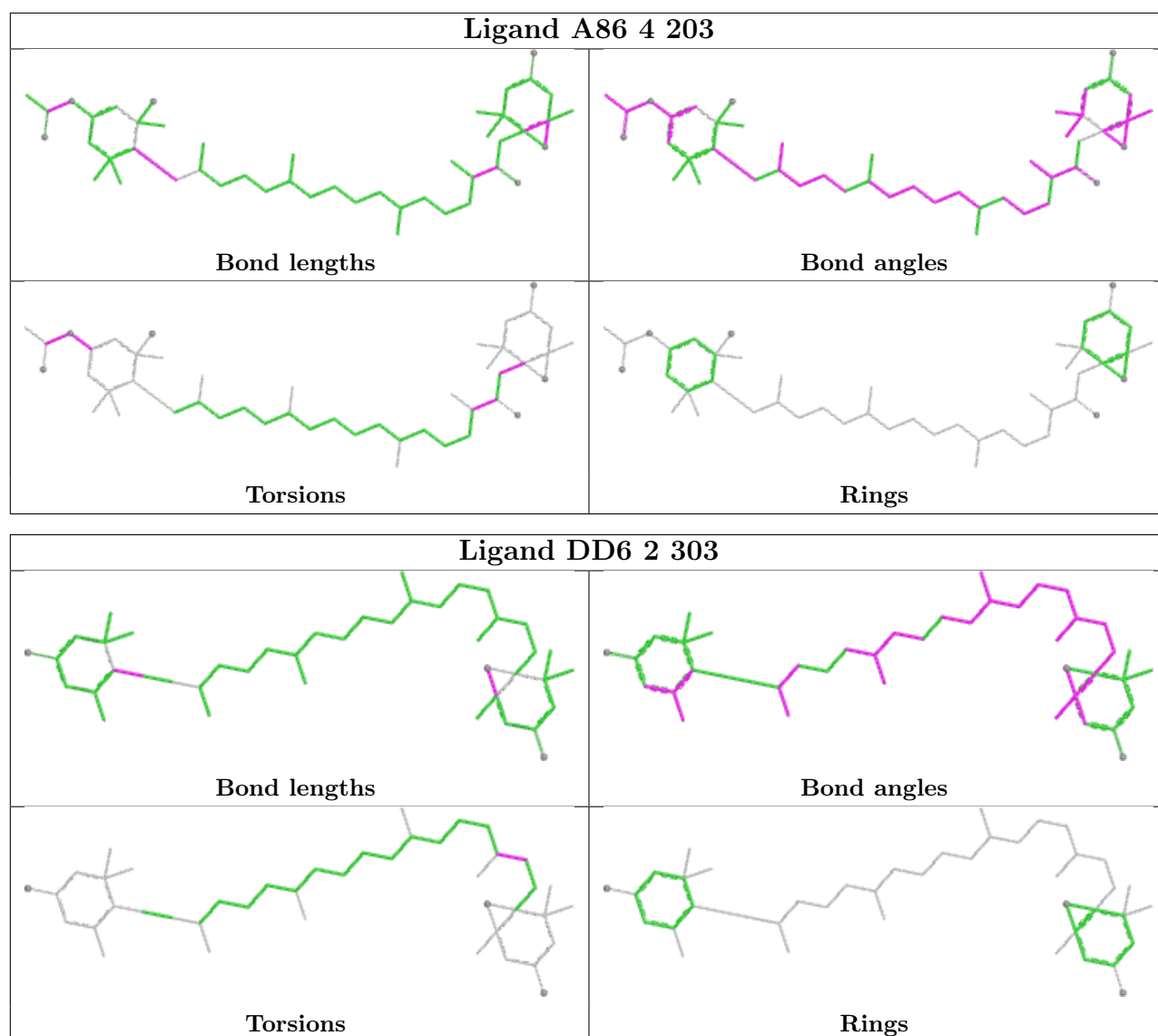


Rings

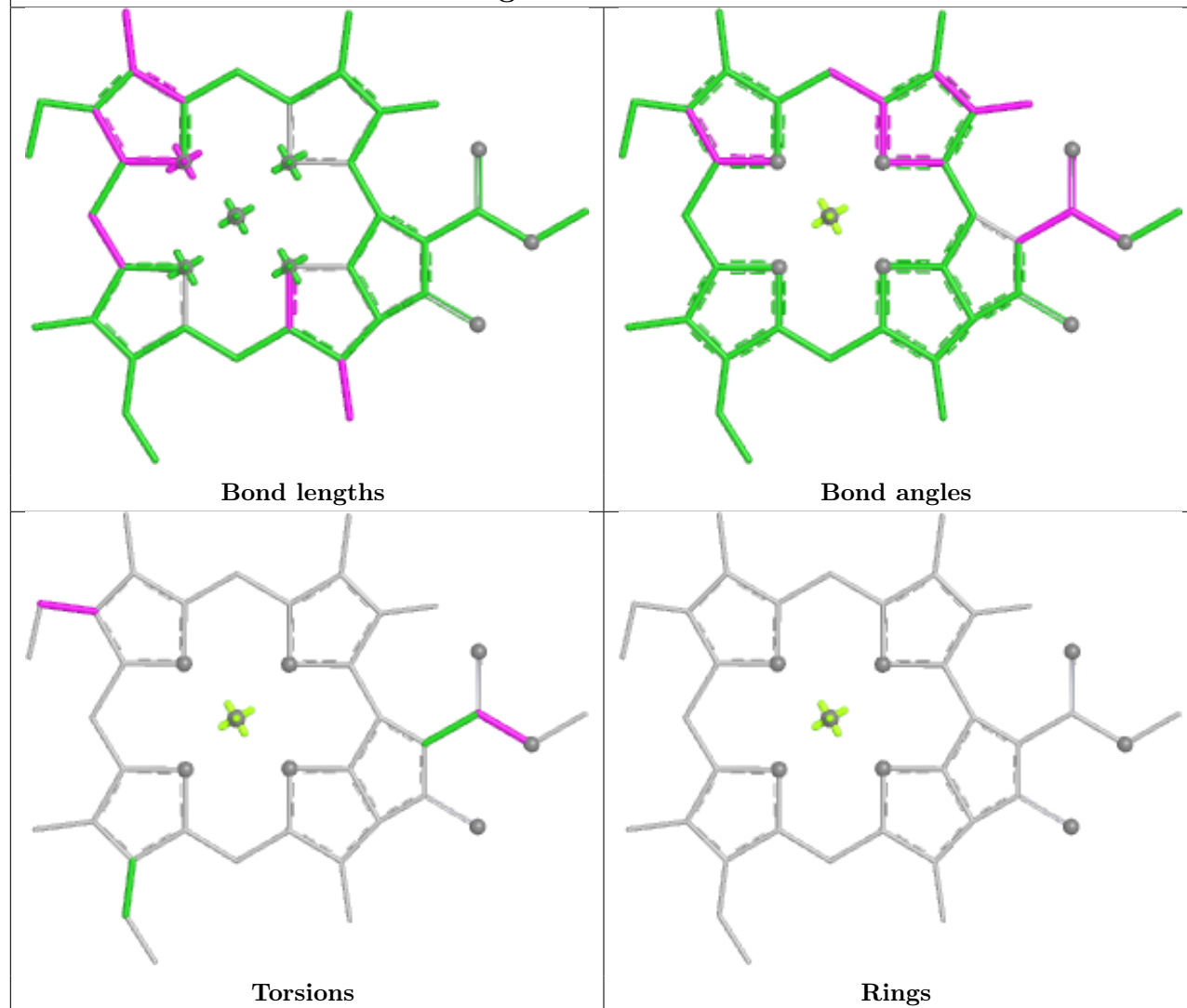




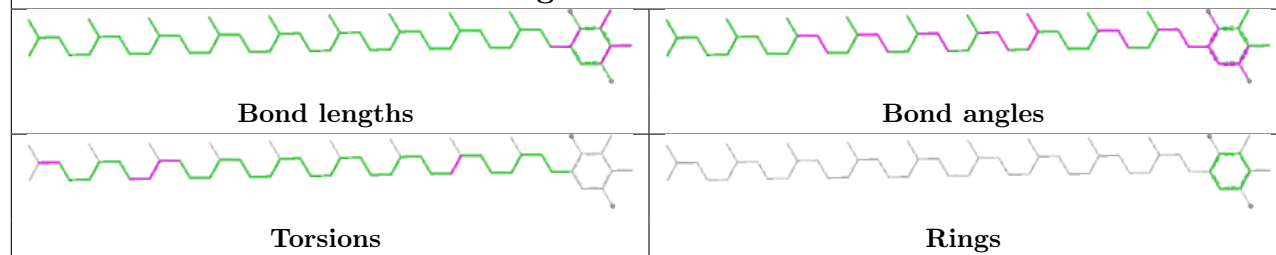


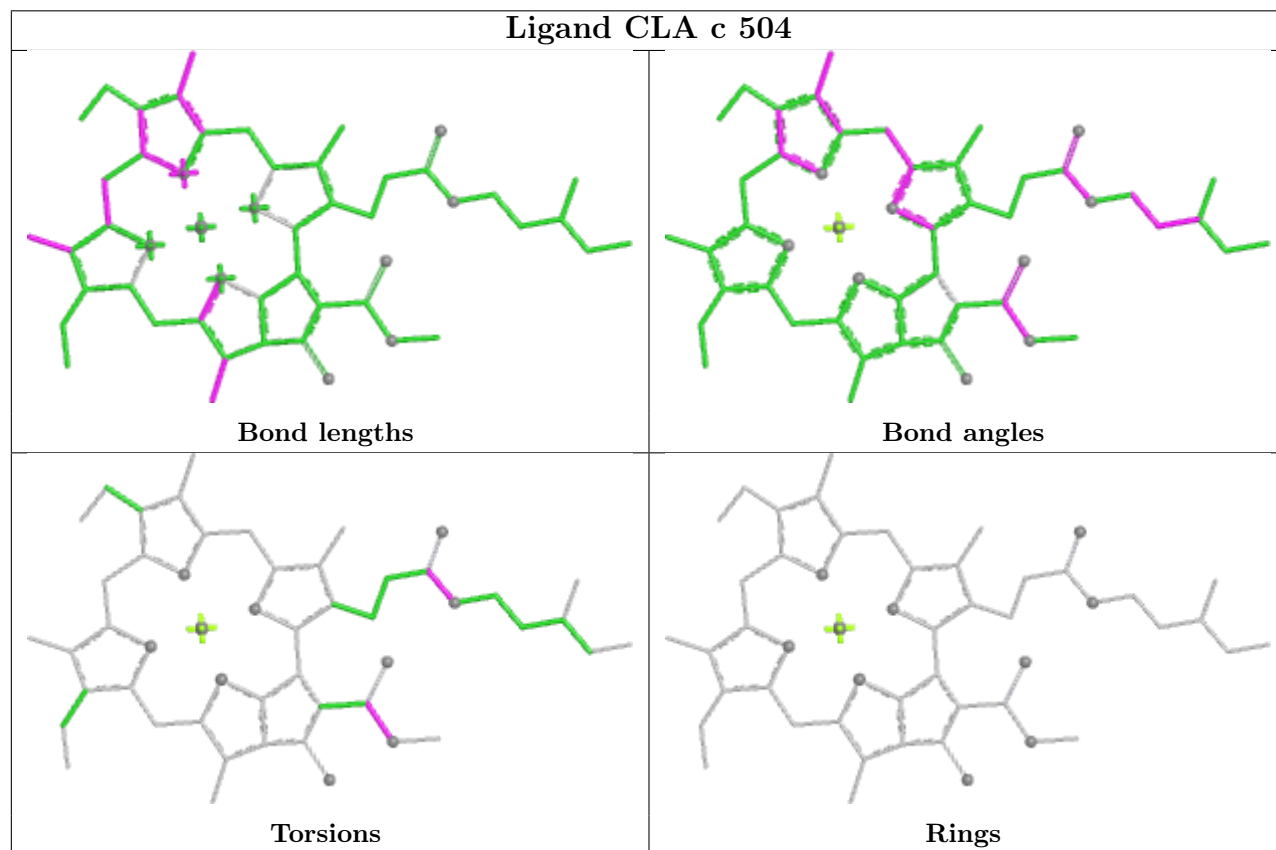
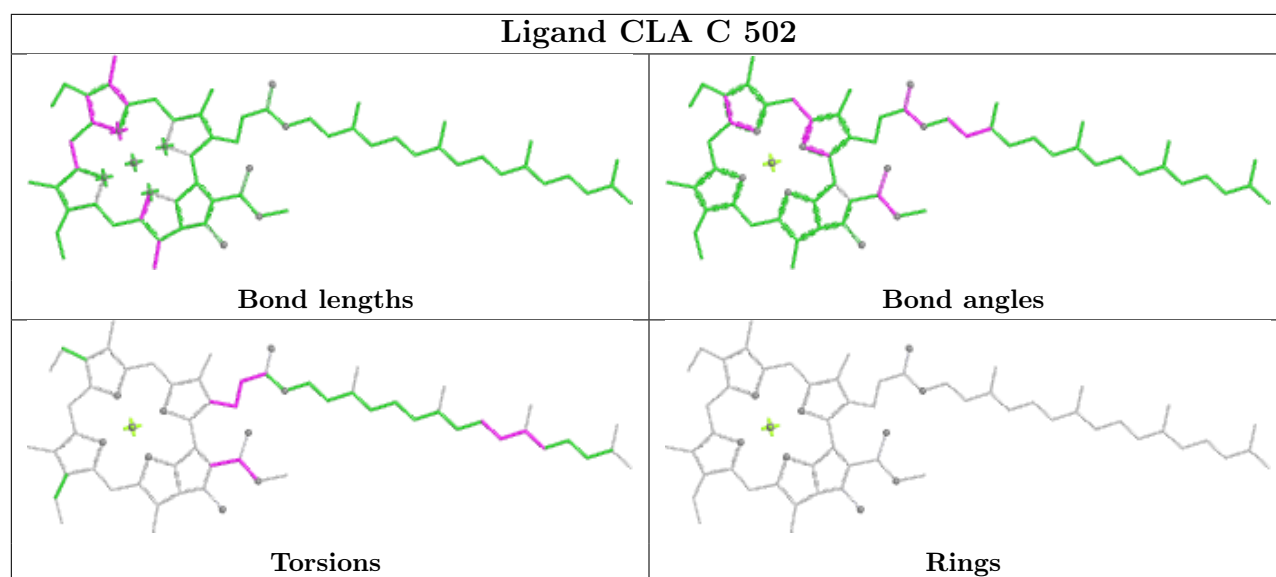


## Ligand CLA 2 305

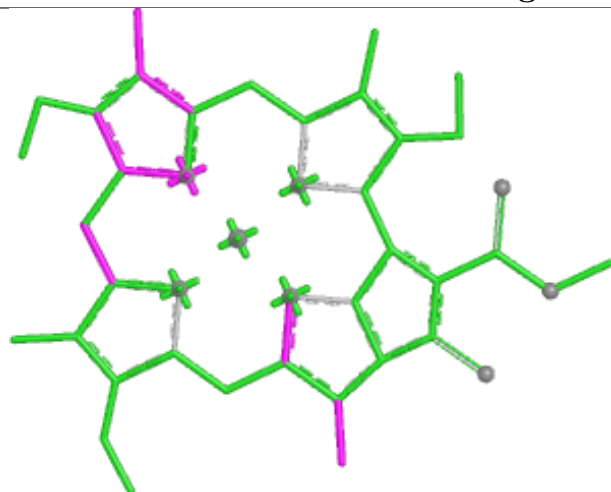


## Ligand PL9 D 406

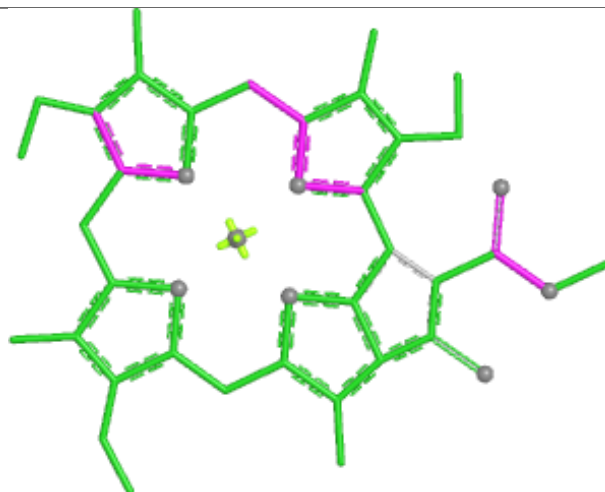




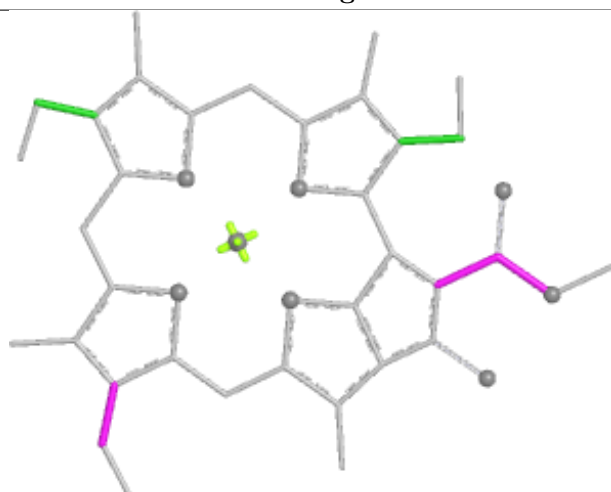
## Ligand CLA 0 312



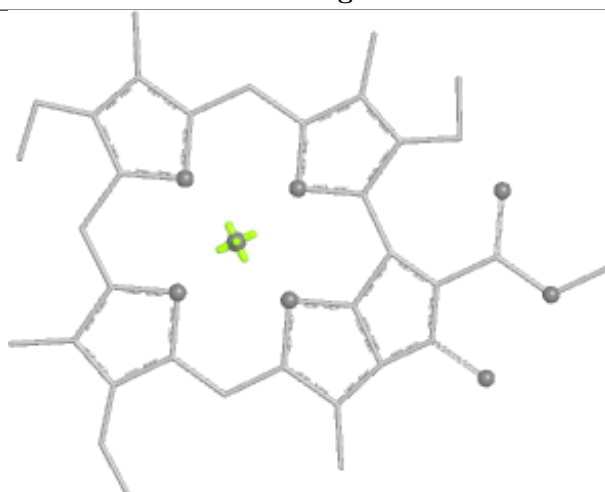
Bond lengths



Bond angles

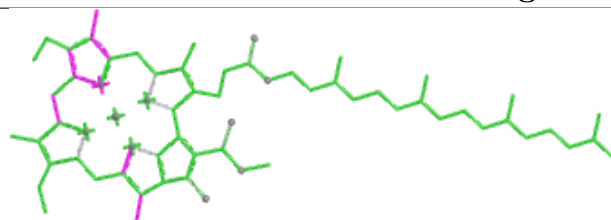


Torsions

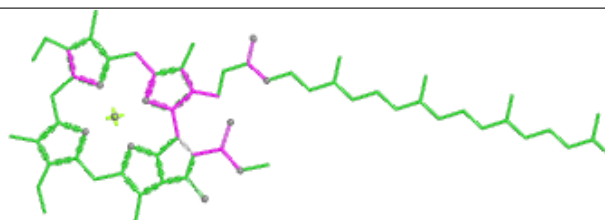


Rings

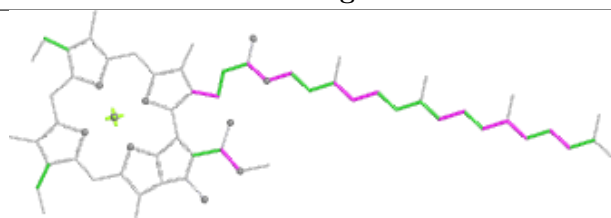
## Ligand CLA 1 210



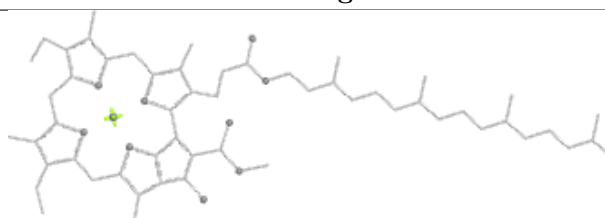
Bond lengths



Bond angles

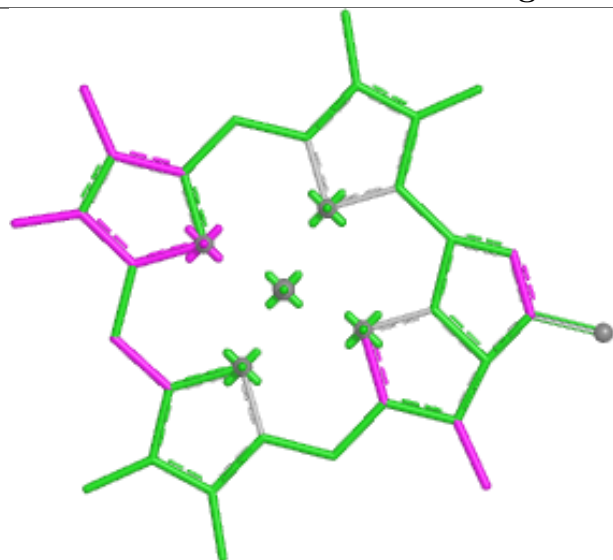


Torsions

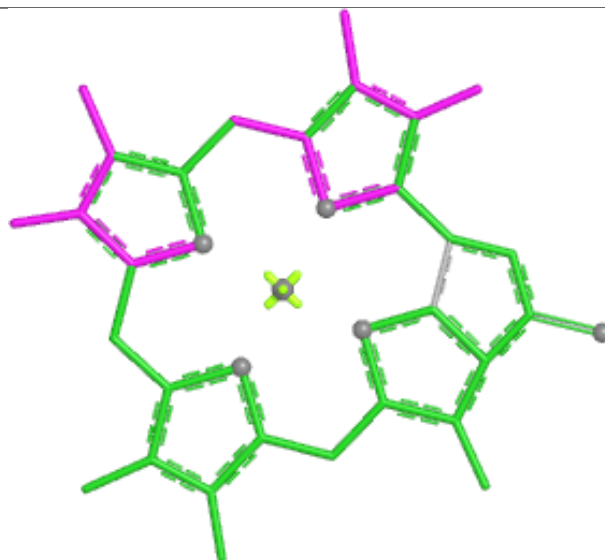


Rings

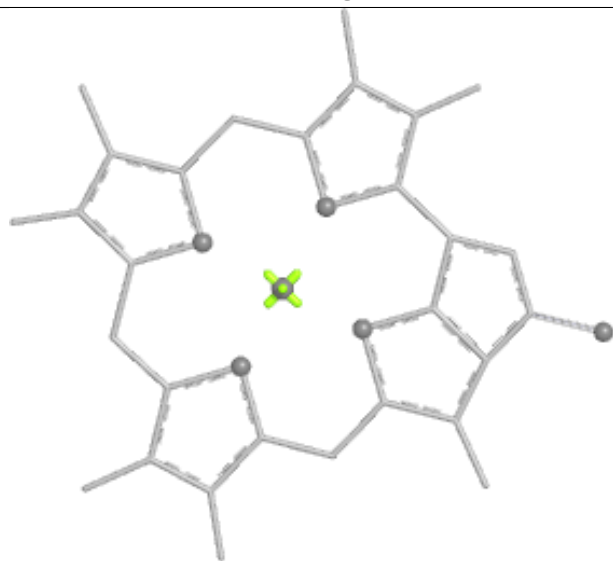
## Ligand CLA 8 314



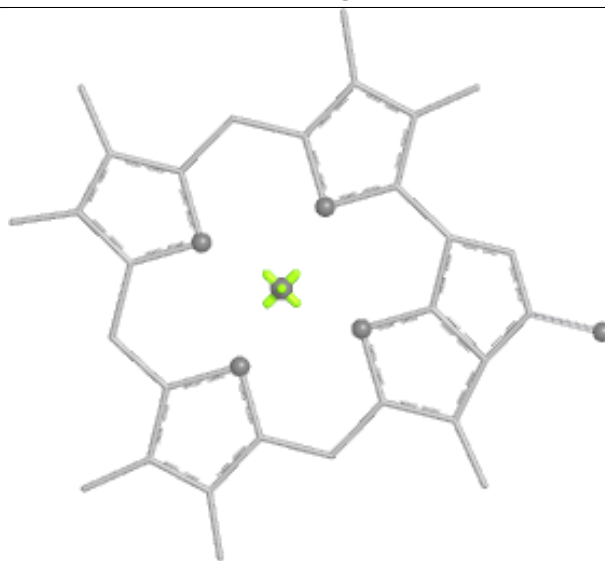
Bond lengths



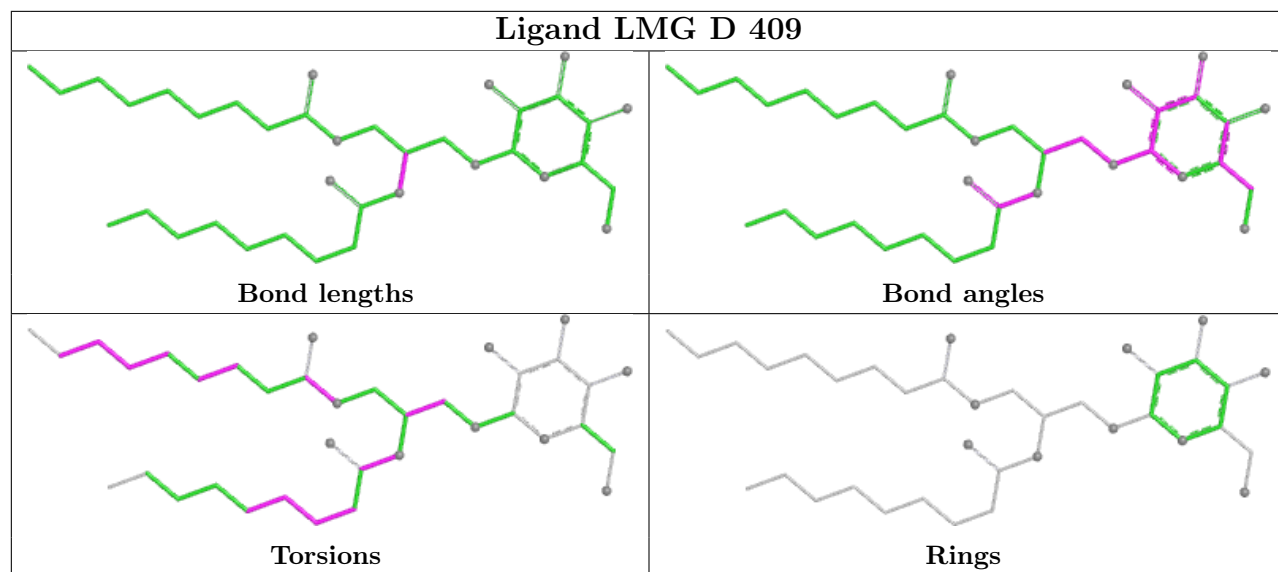
Bond angles



Torsions

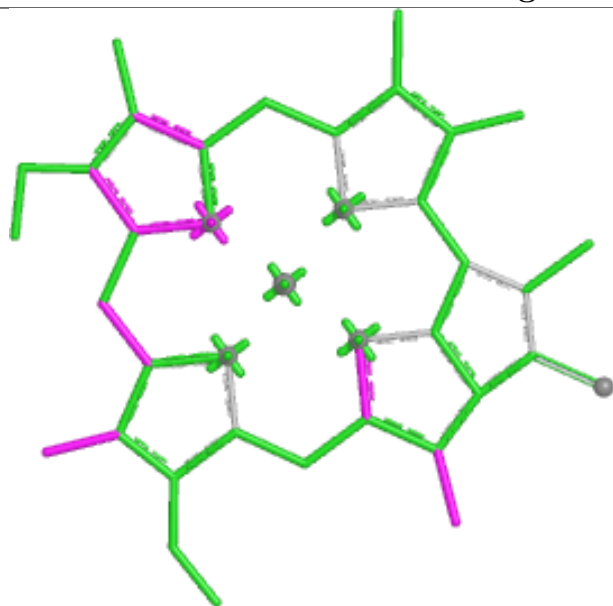


Rings

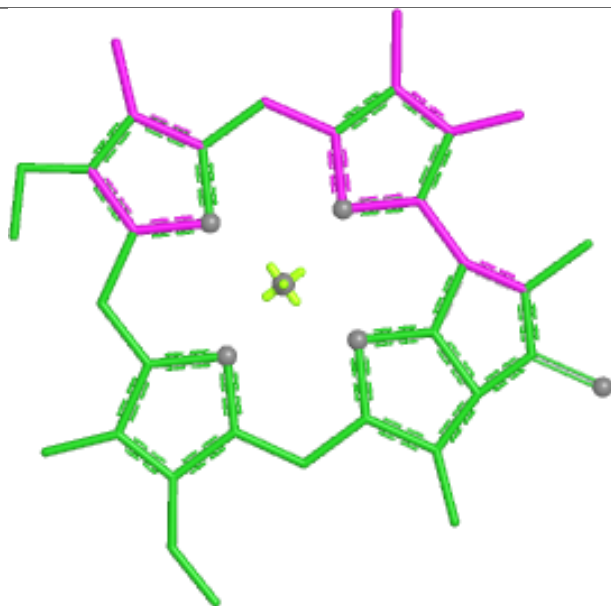




## Ligand CLA 6 214



Bond lengths



Bond angles

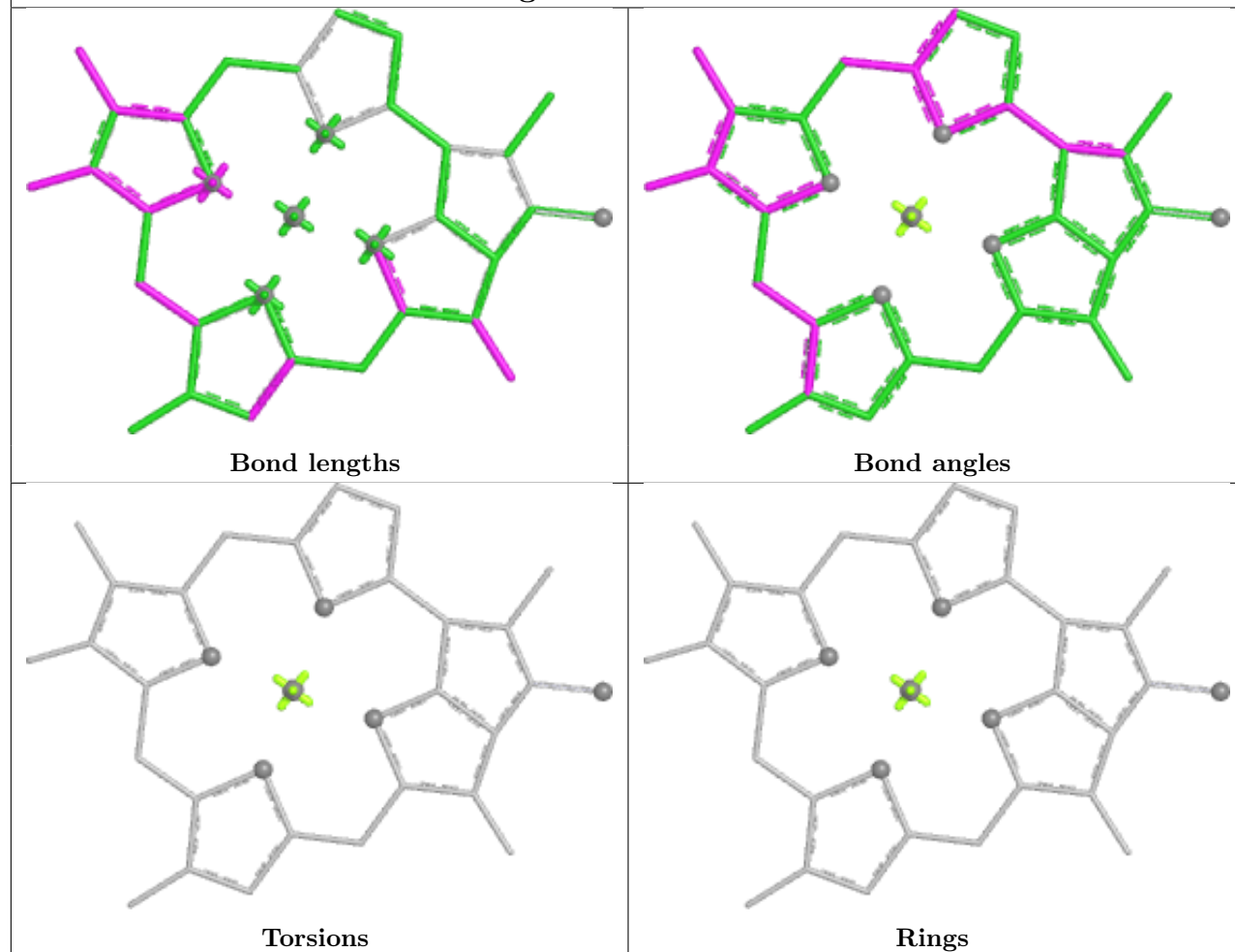


Torsions

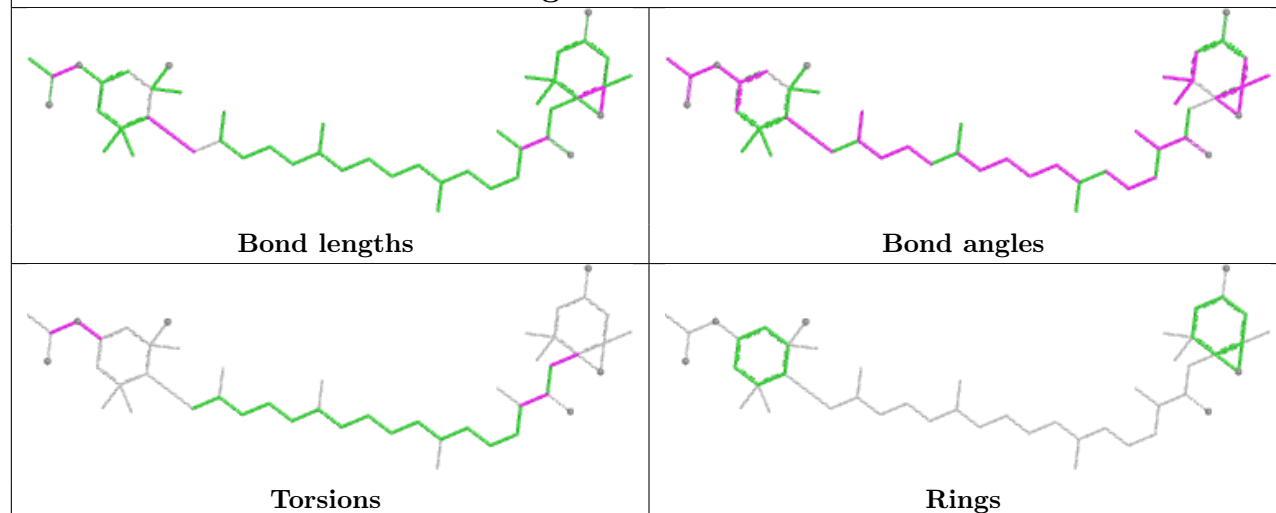


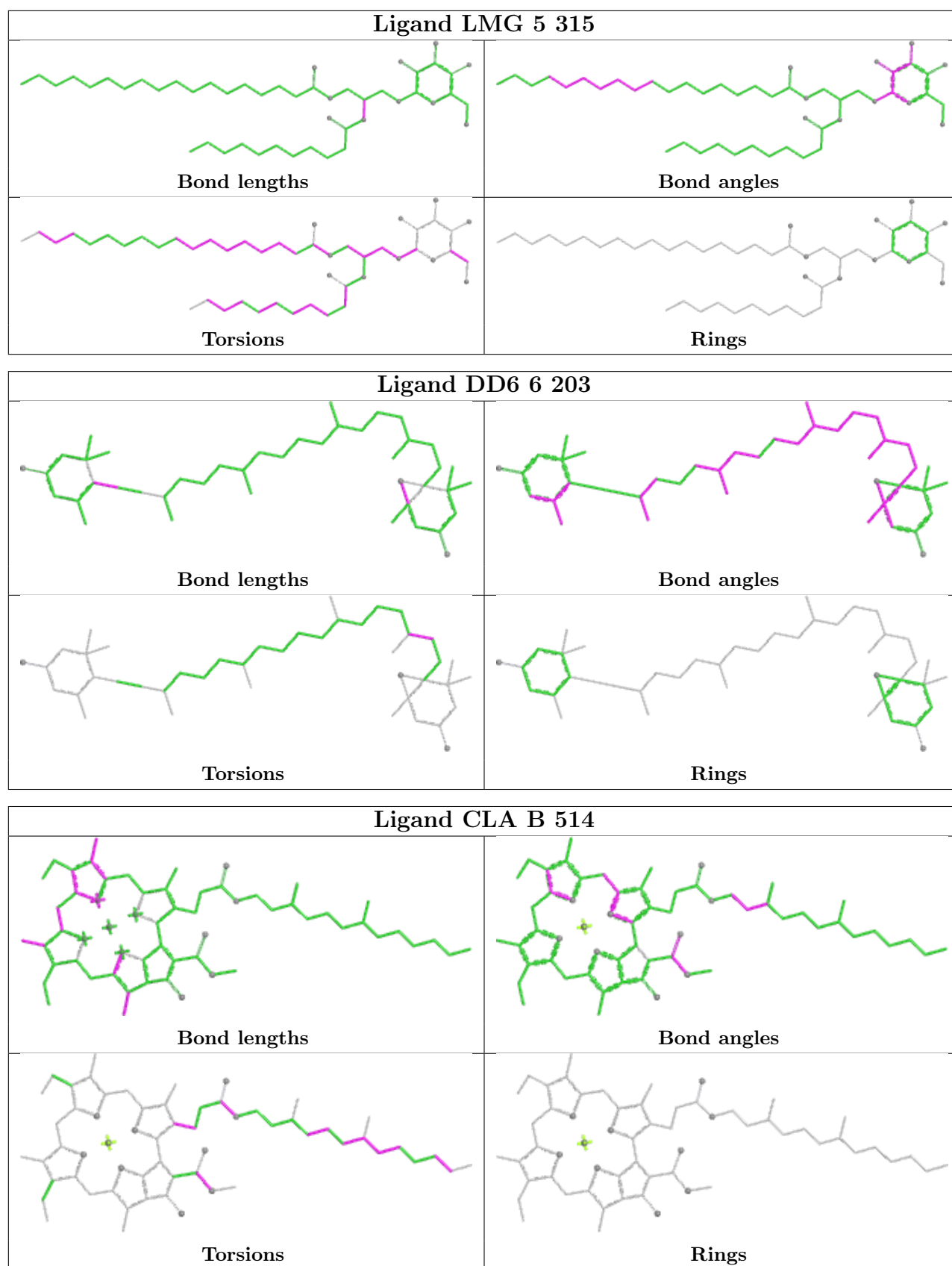
Rings

## Ligand CLA 3 306

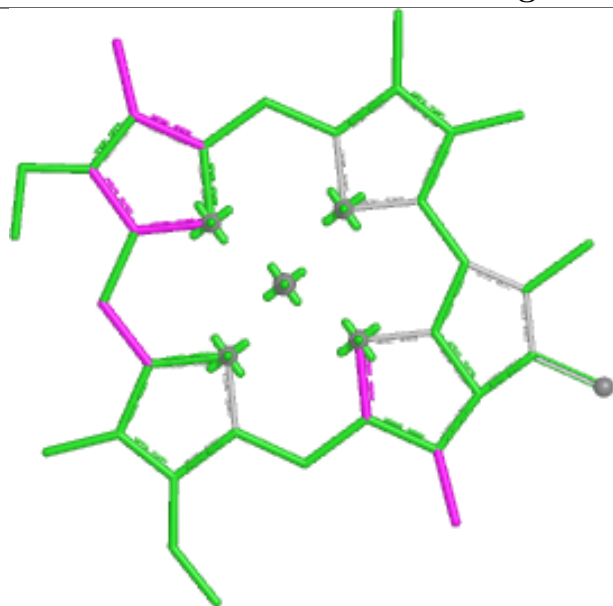


## Ligand A86 9 203

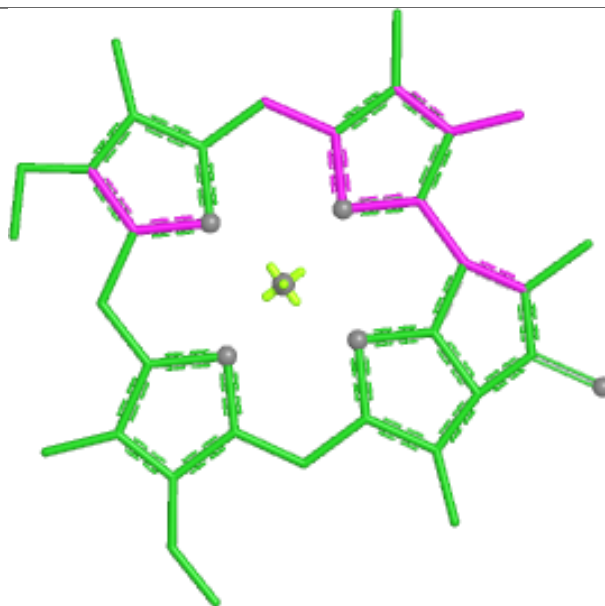




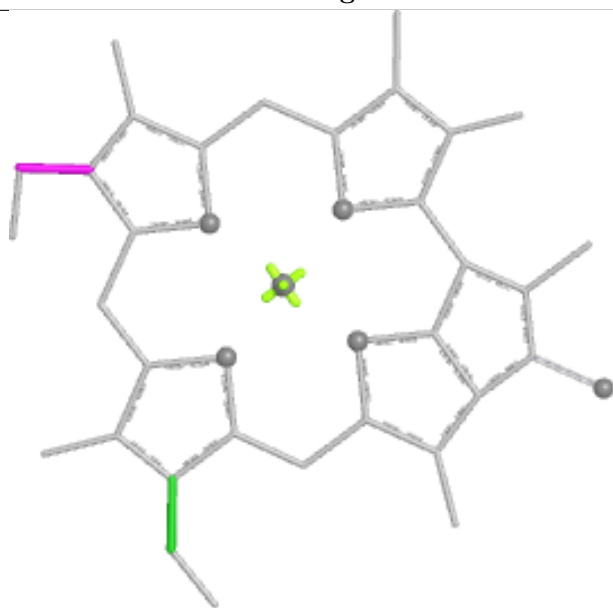
## Ligand CLA 6 216



Bond lengths



Bond angles

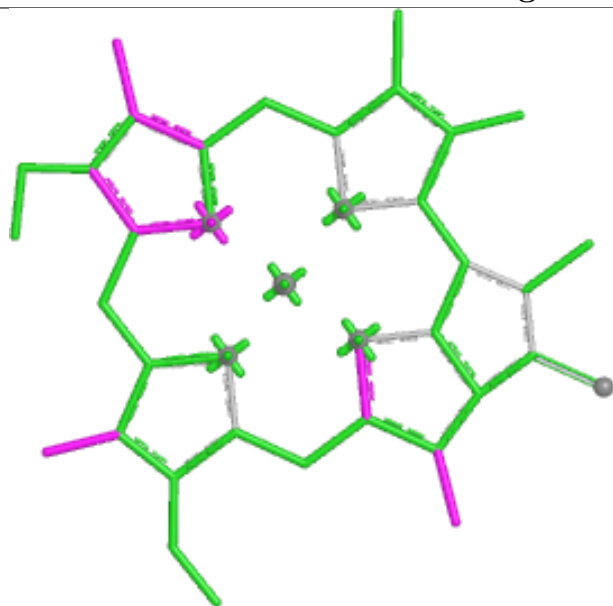


Torsions

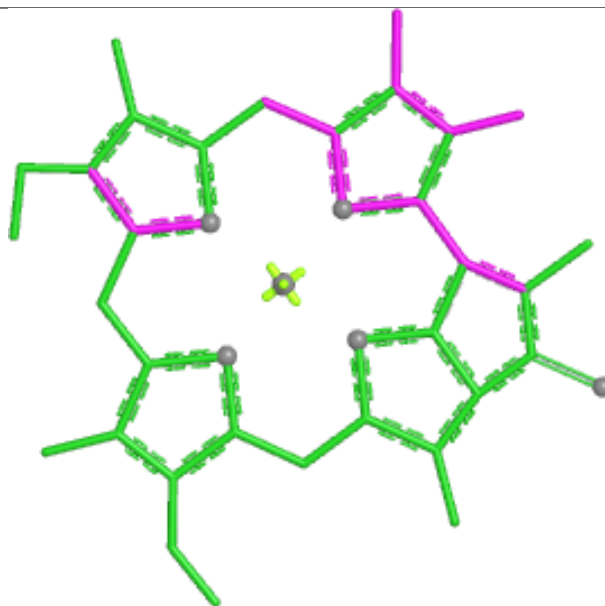


Rings

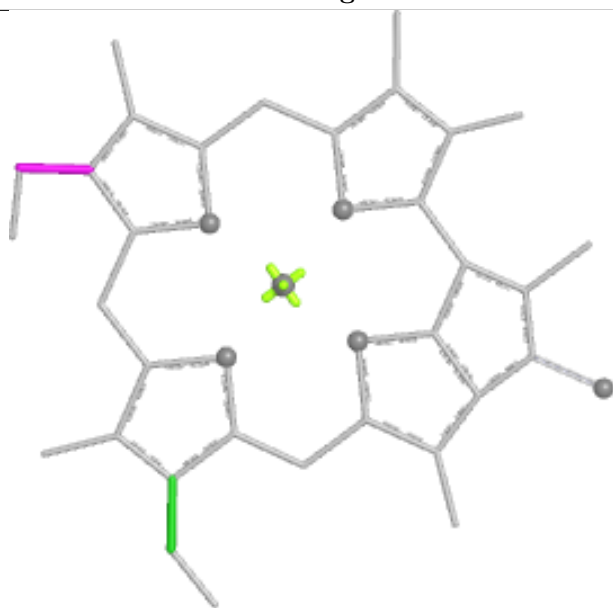
## Ligand CLA 4 207



Bond lengths



Bond angles

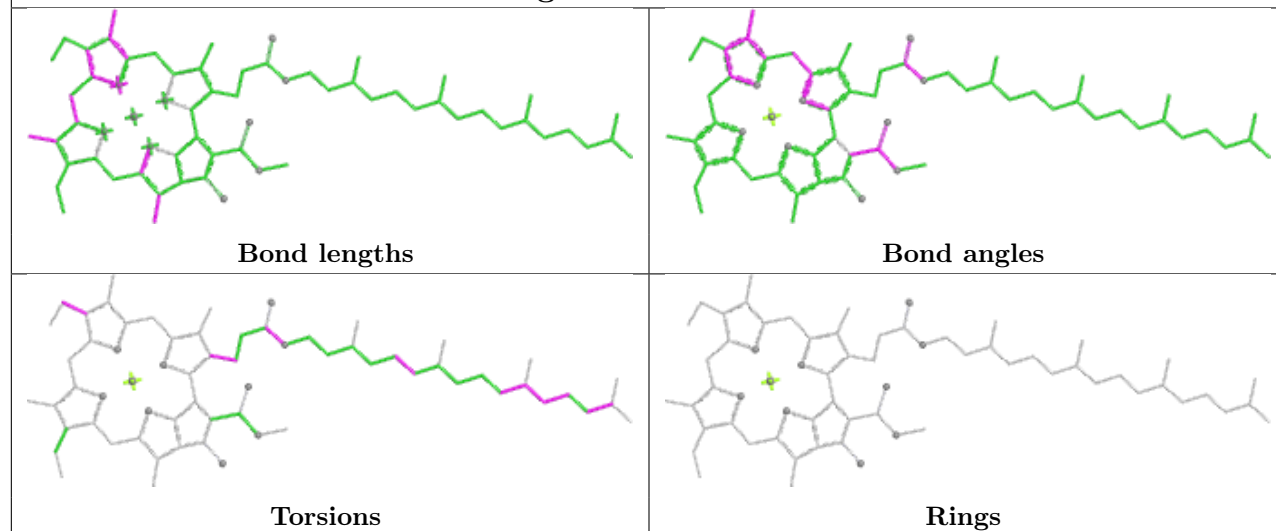


Torsions

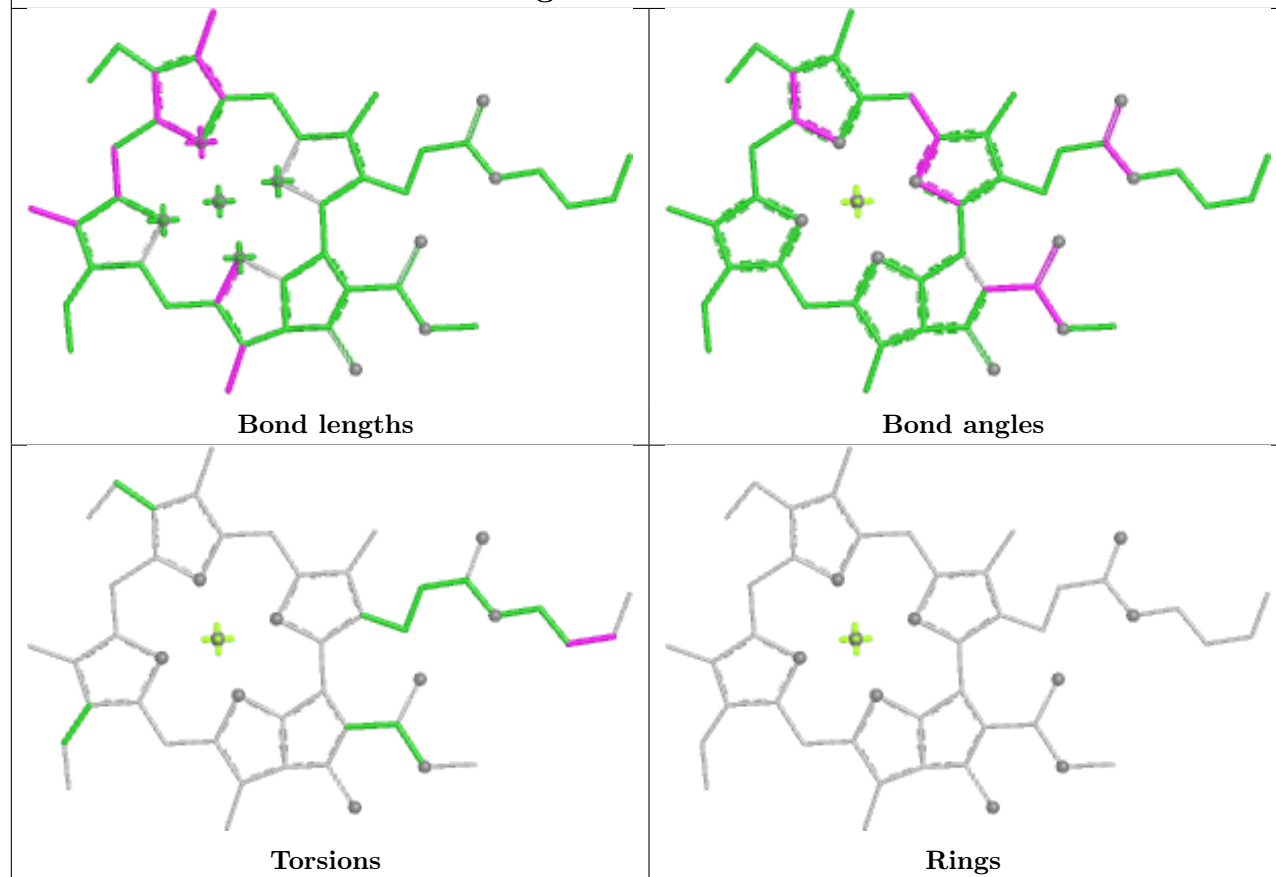


Rings

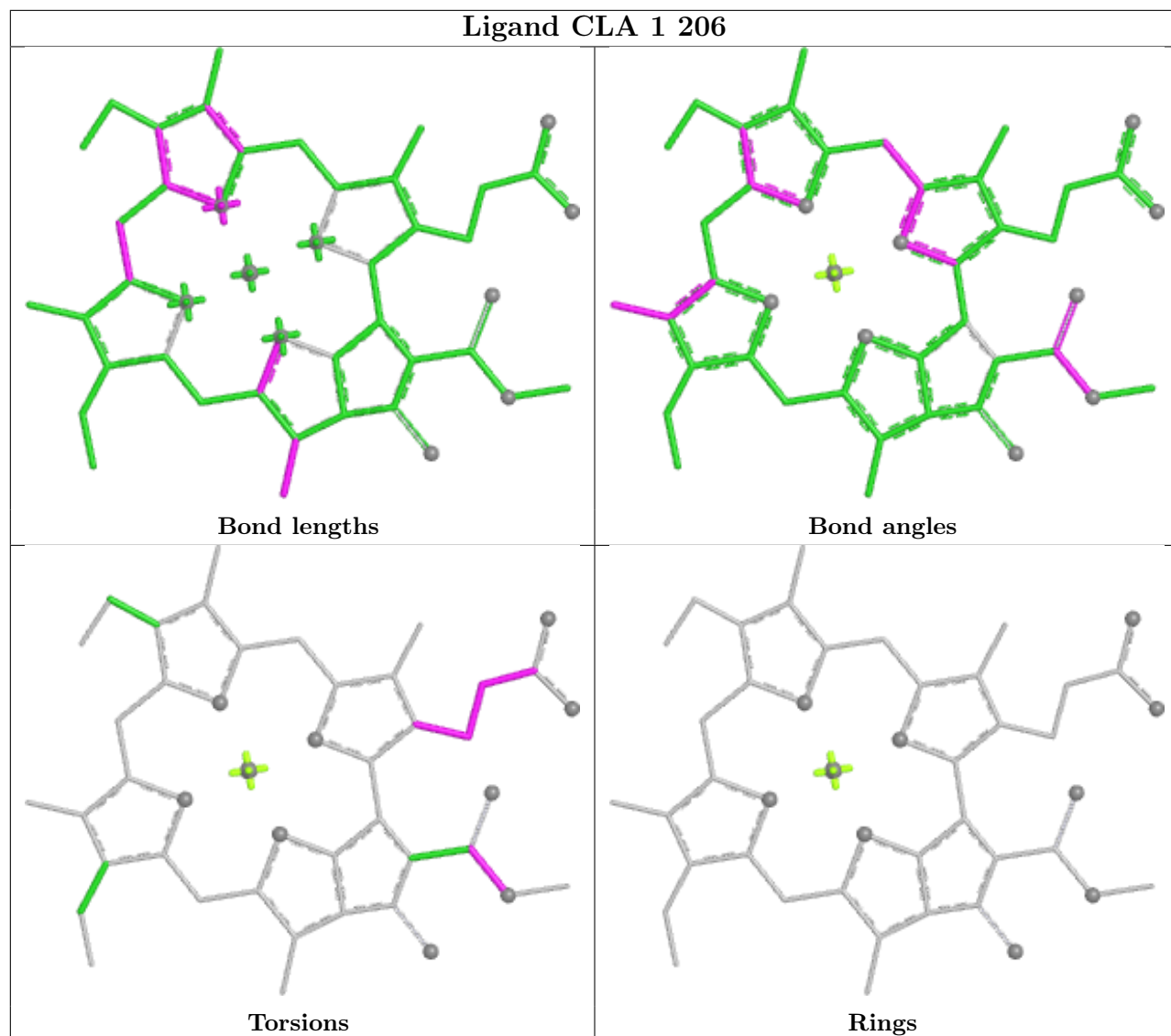
## Ligand CLA c 509



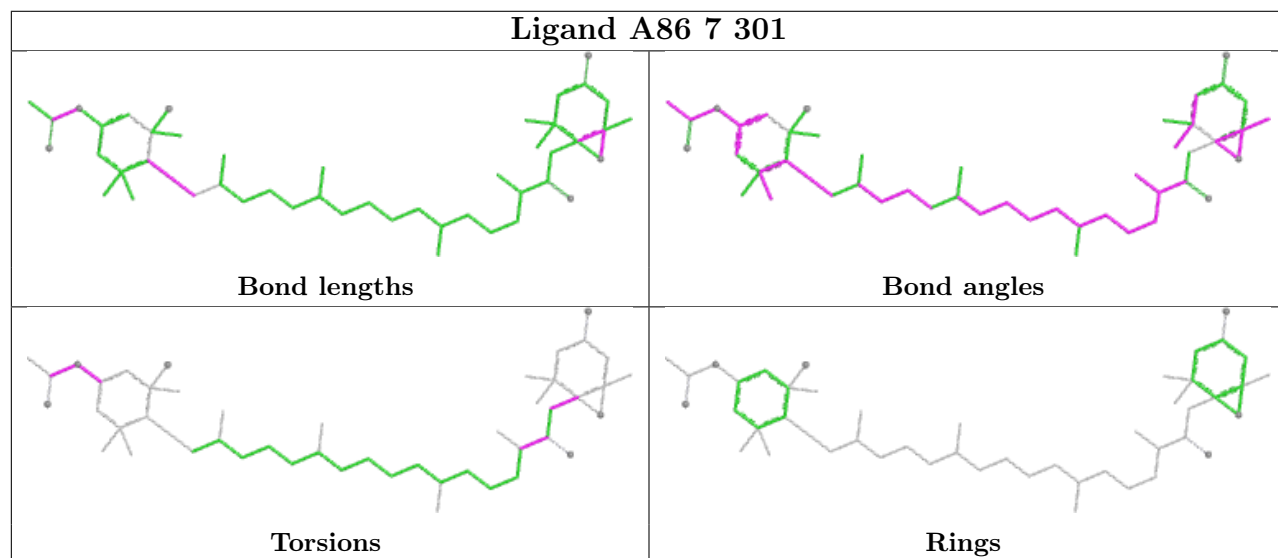
## Ligand CLA a 404

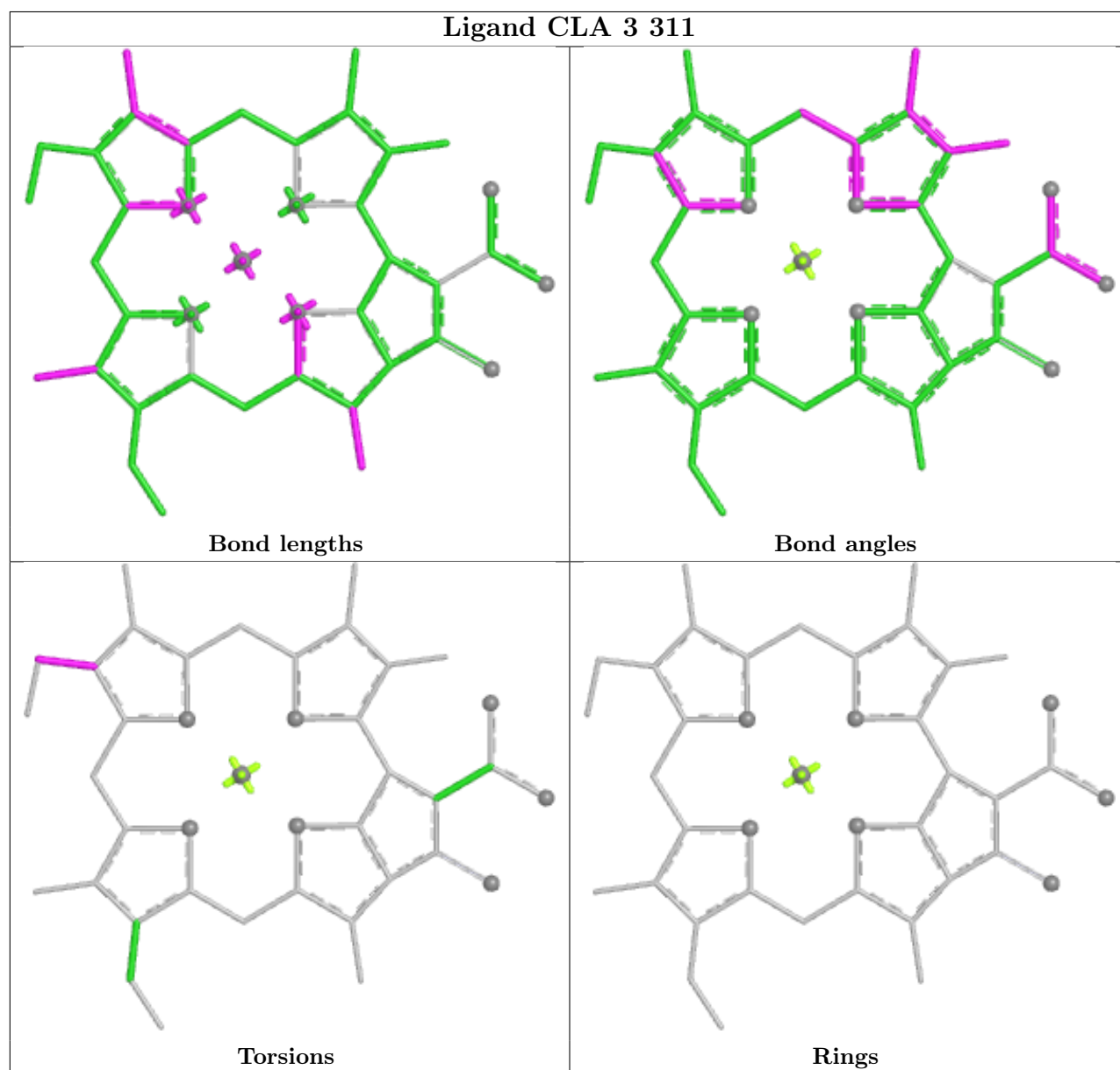
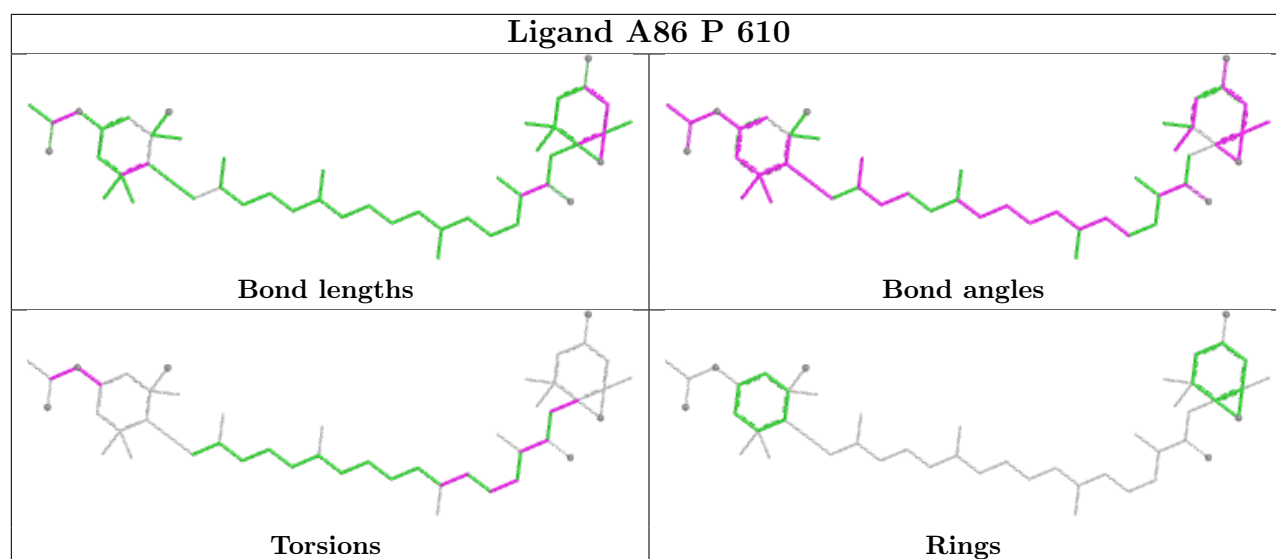


## Ligand CLA 1 206

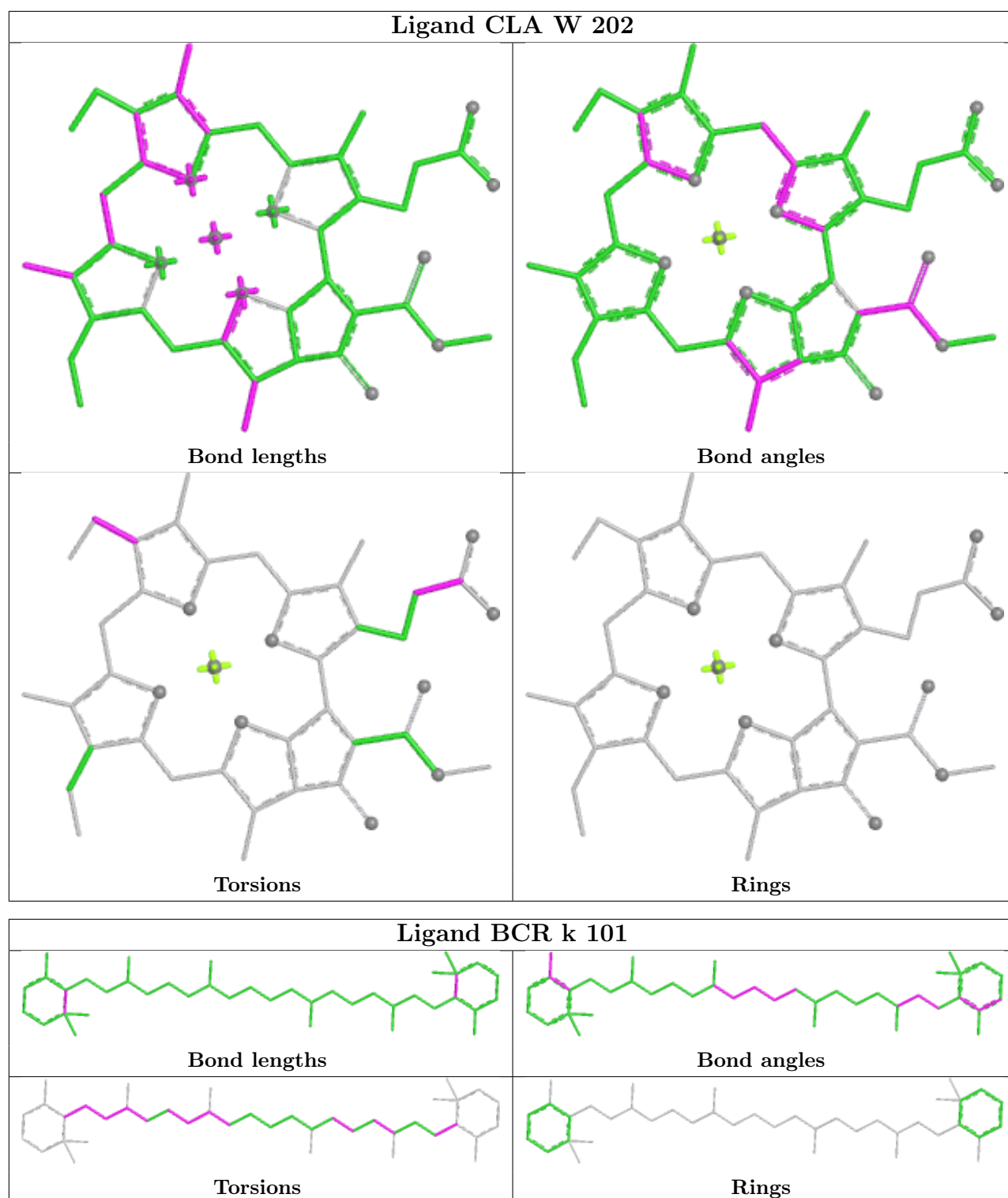


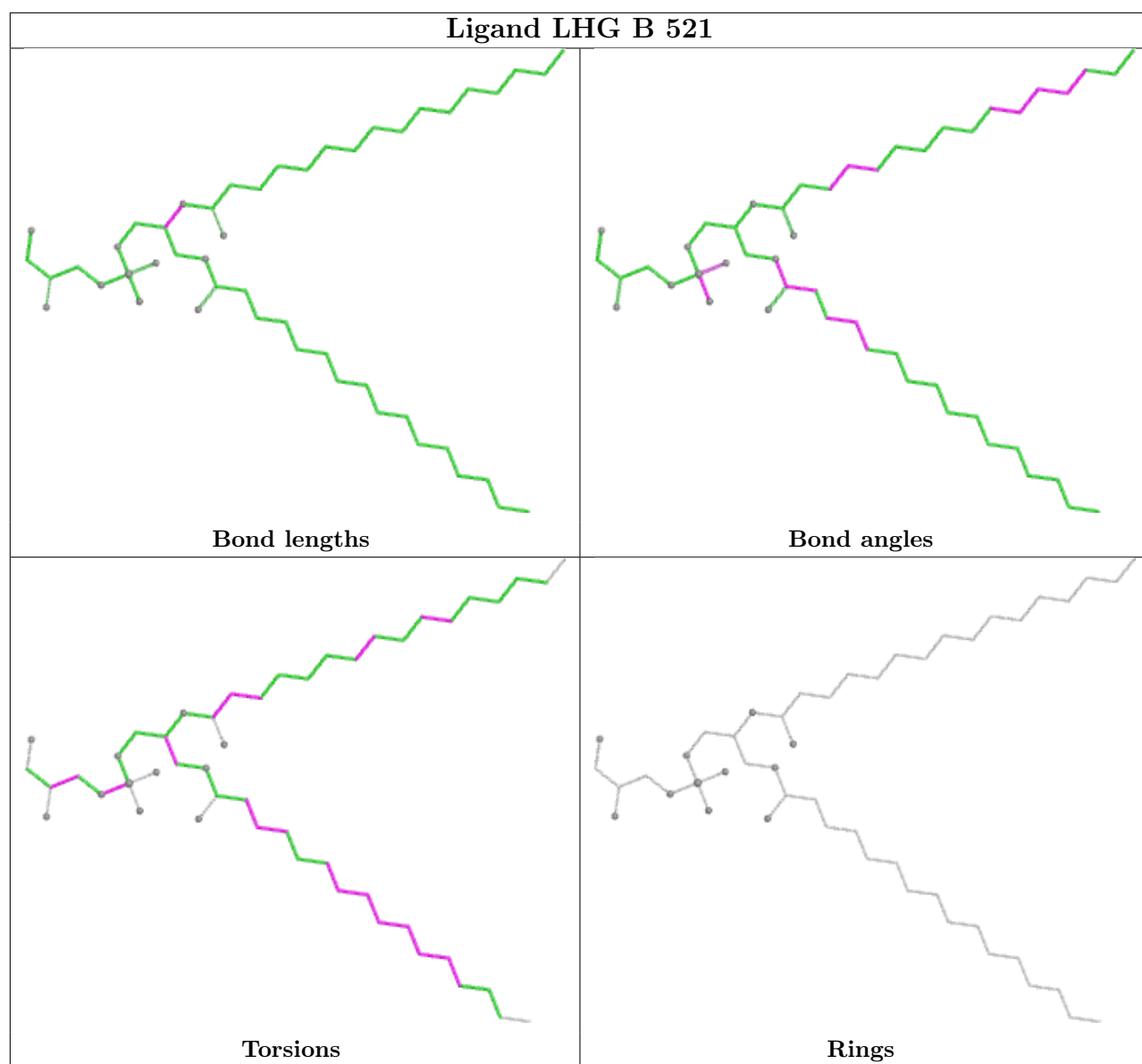
## Ligand A86 7 301



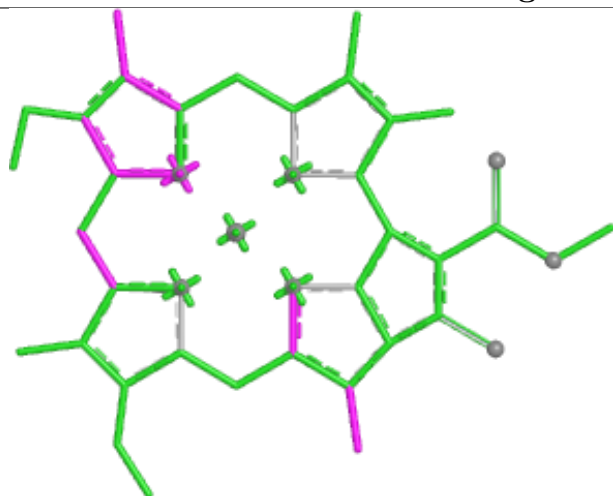




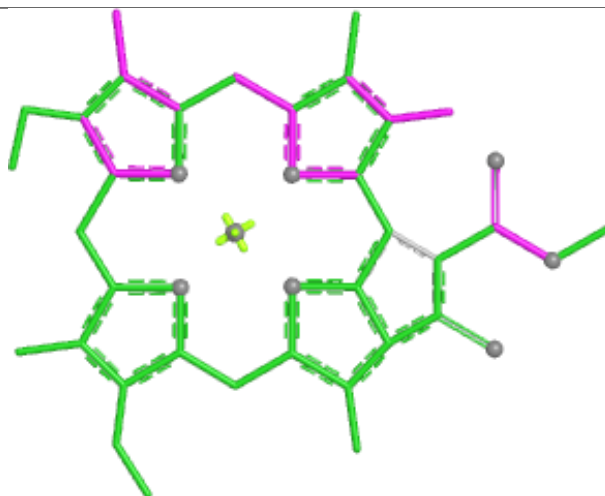




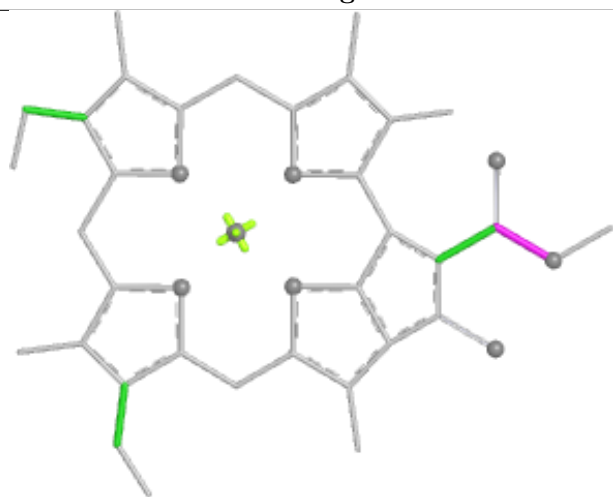
## Ligand CLA 7 316



Bond lengths



Bond angles

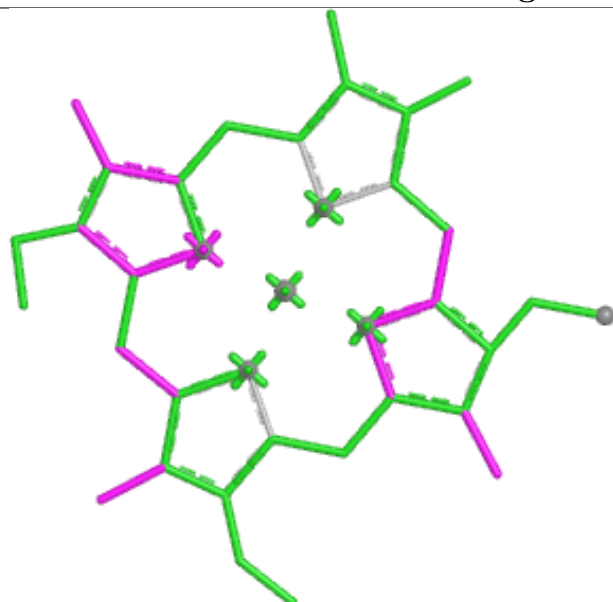


Torsions

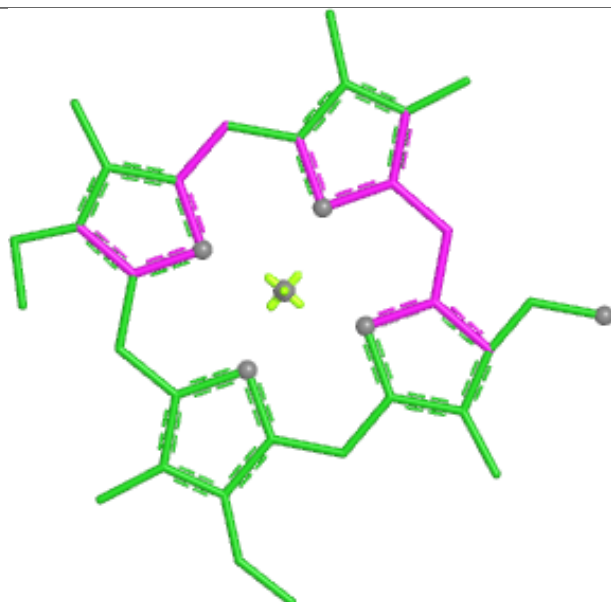


Rings

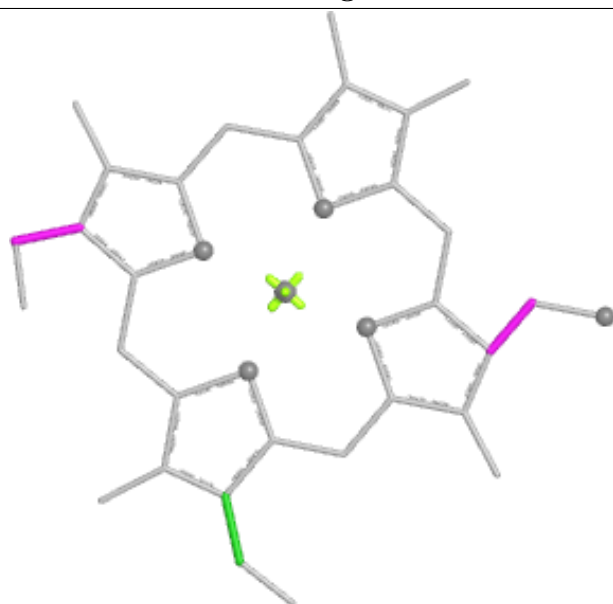
## Ligand CLA 8 308



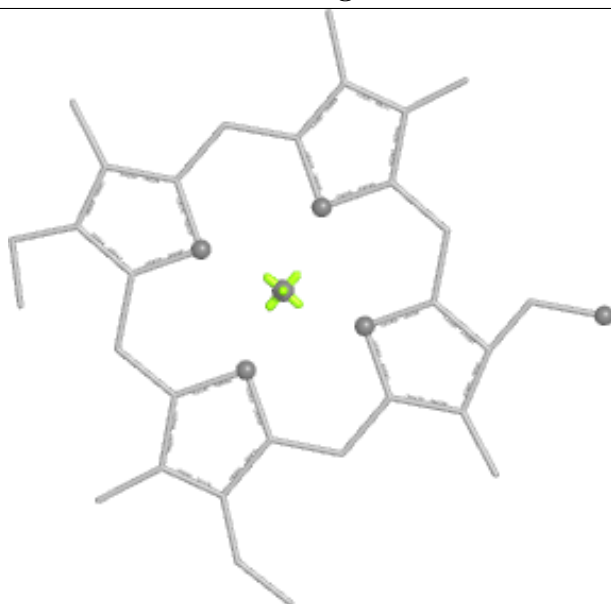
Bond lengths



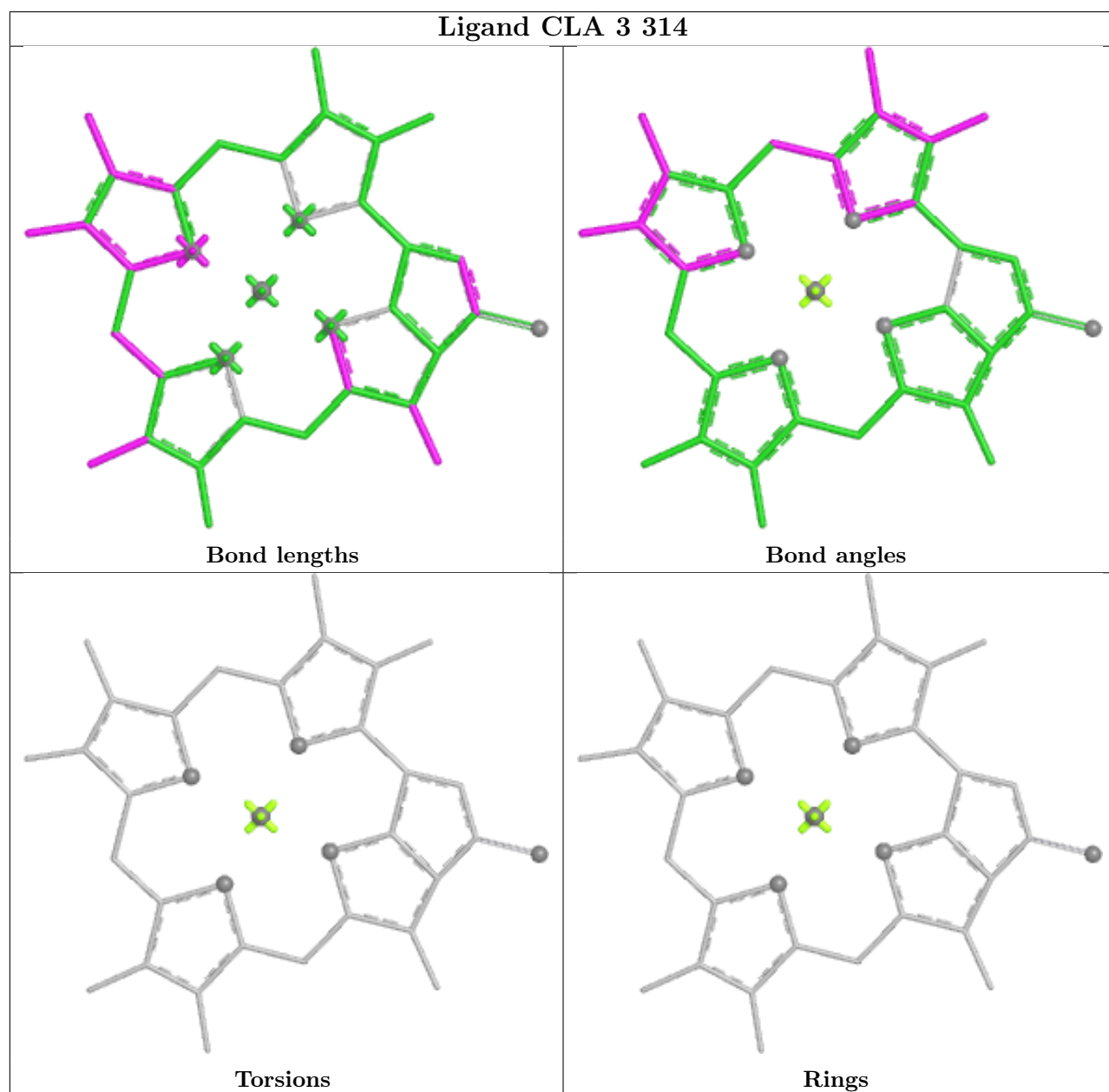
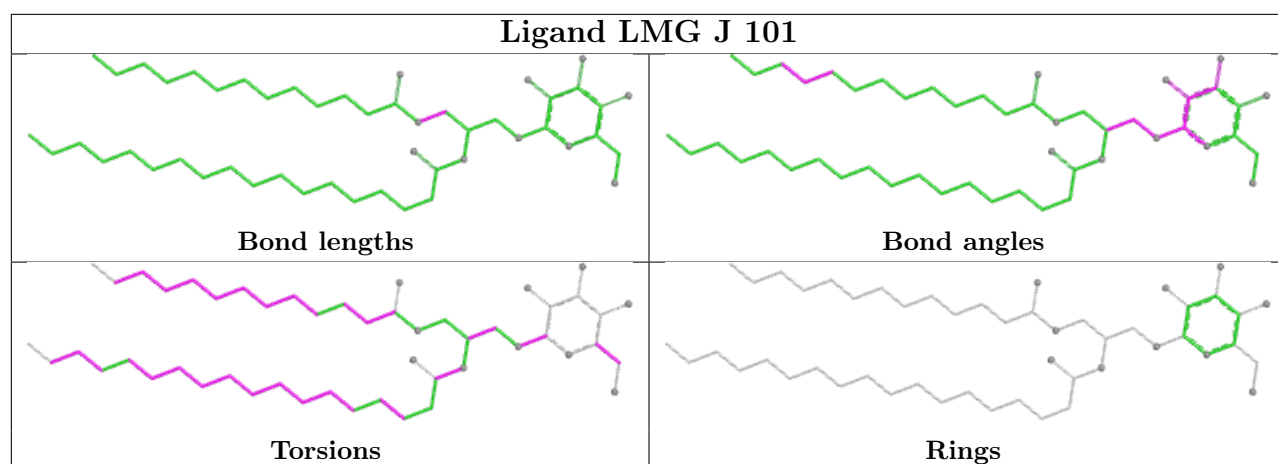
Bond angles

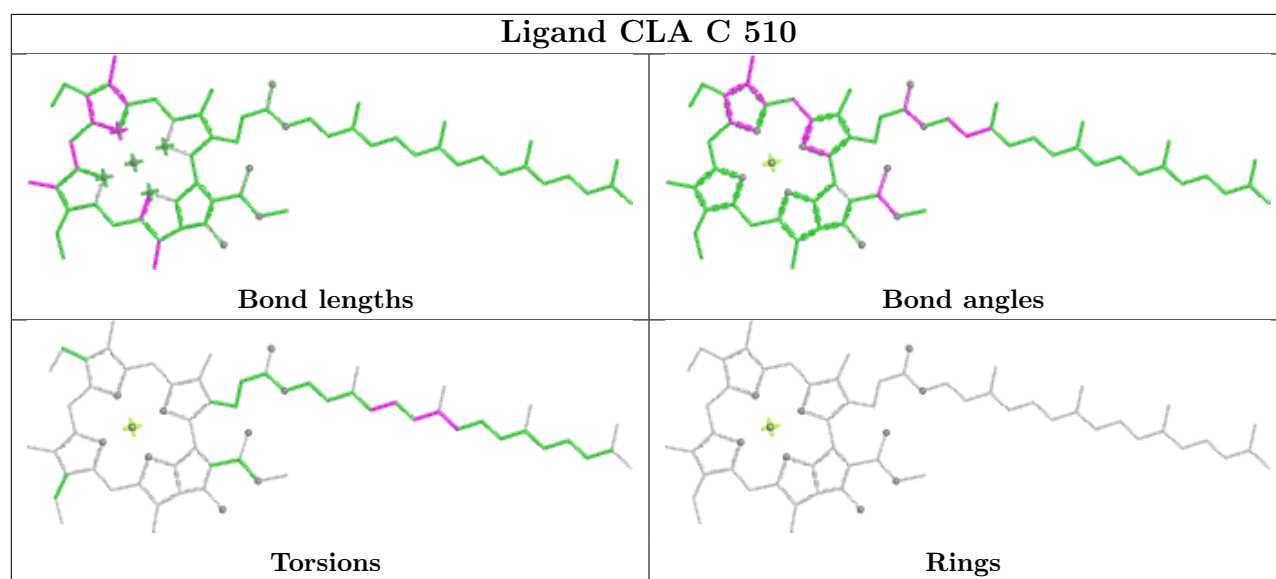


Torsions

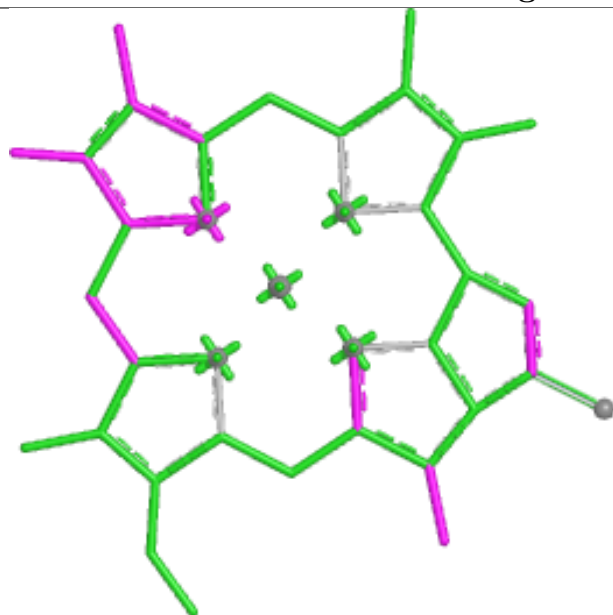


Rings

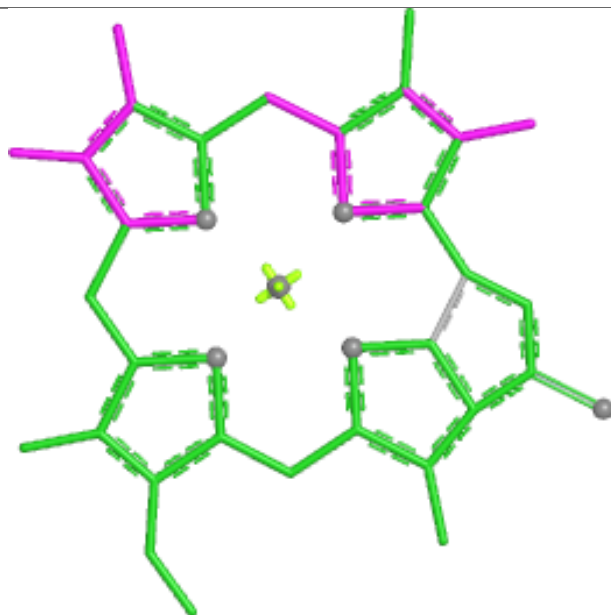




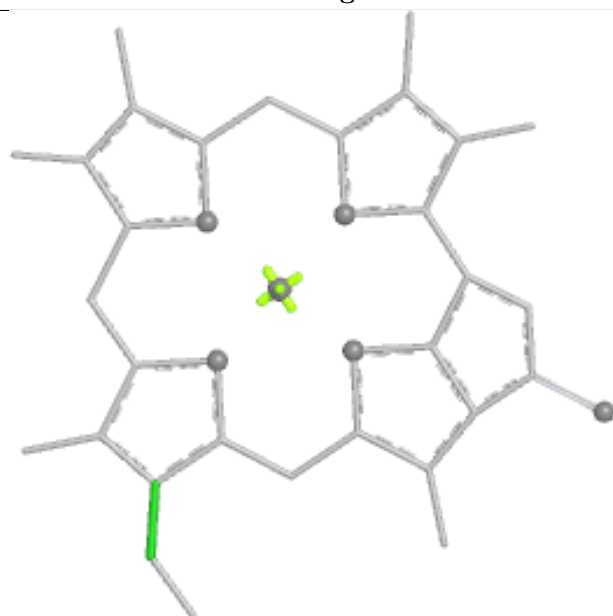
## Ligand CLA 9 212



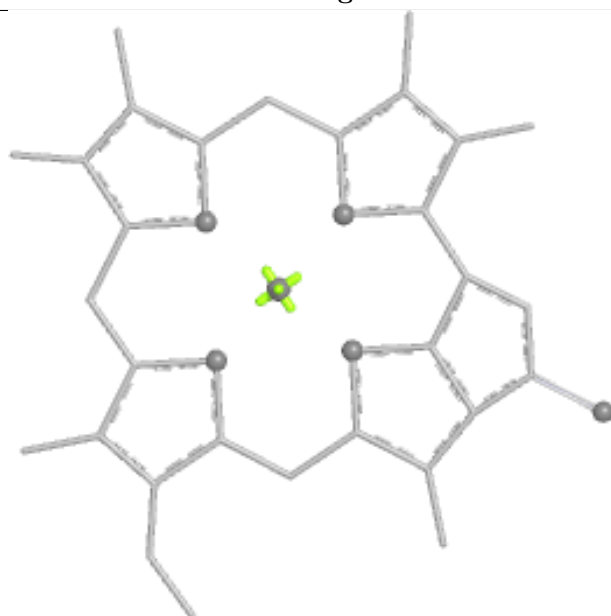
Bond lengths



Bond angles

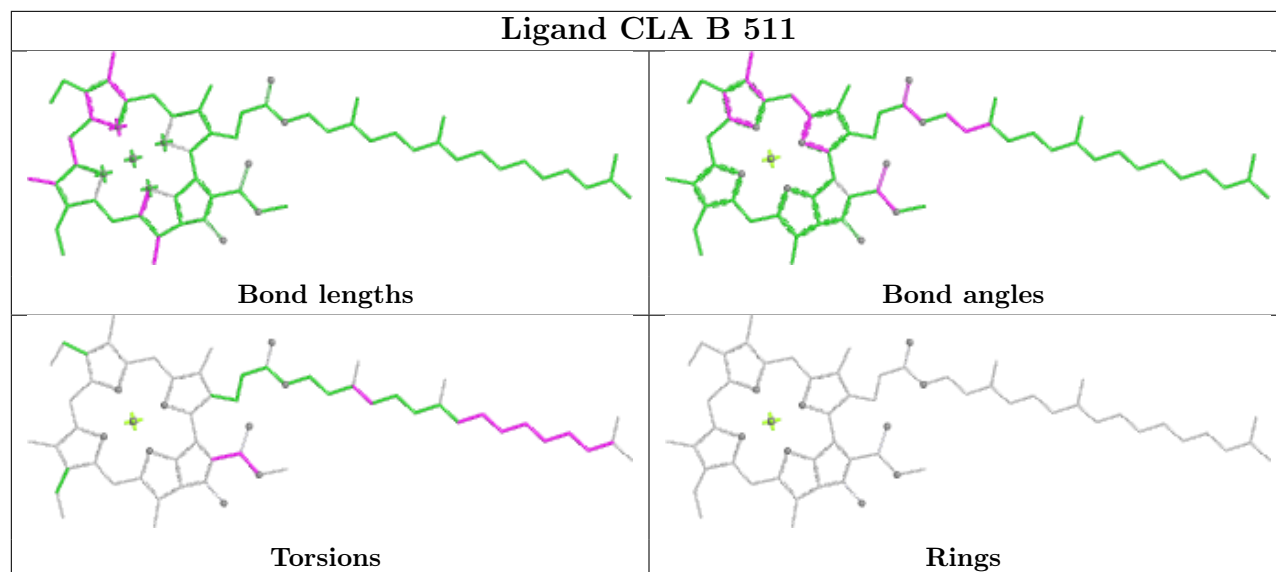


Torsions

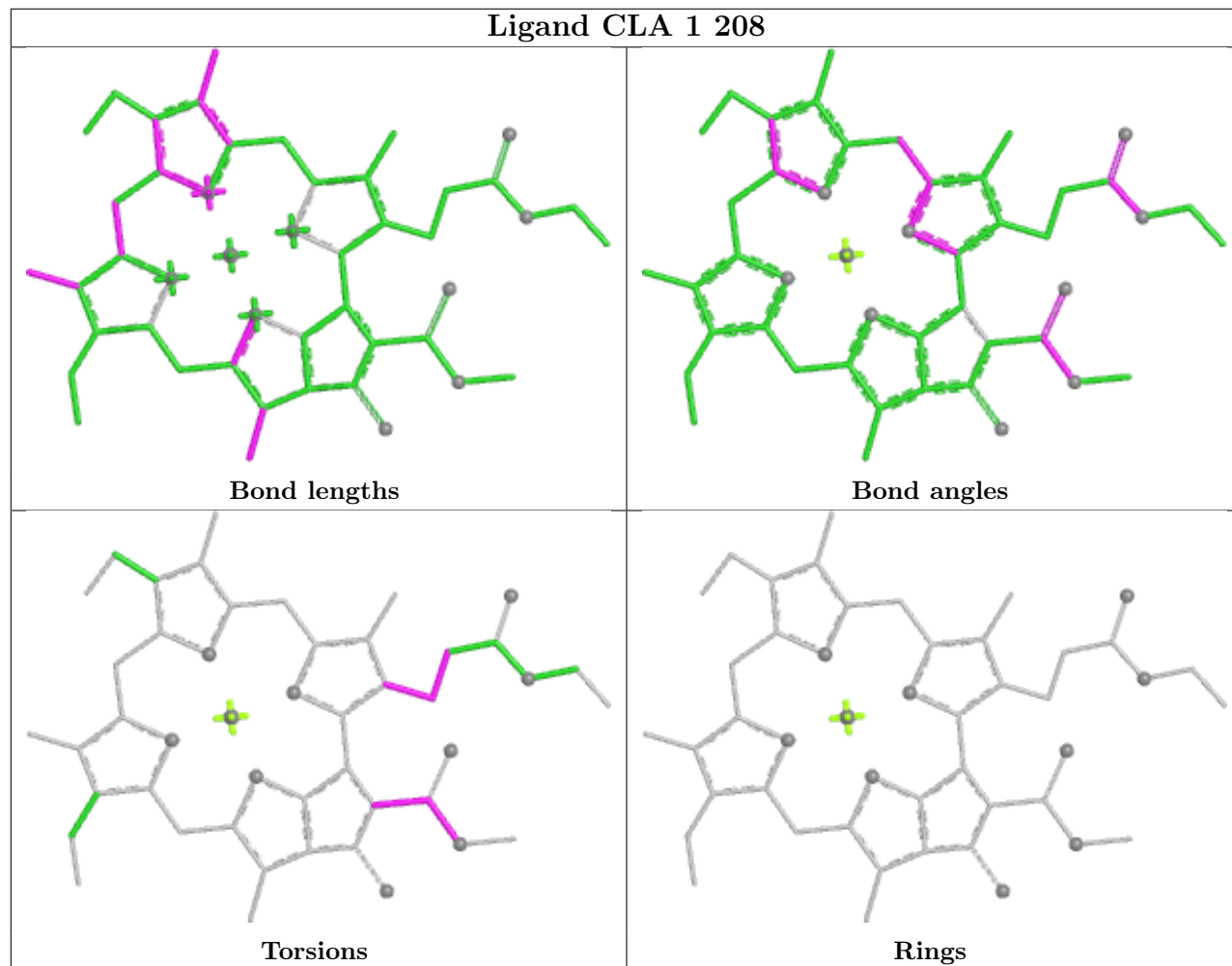


Rings

## Ligand CLA B 511

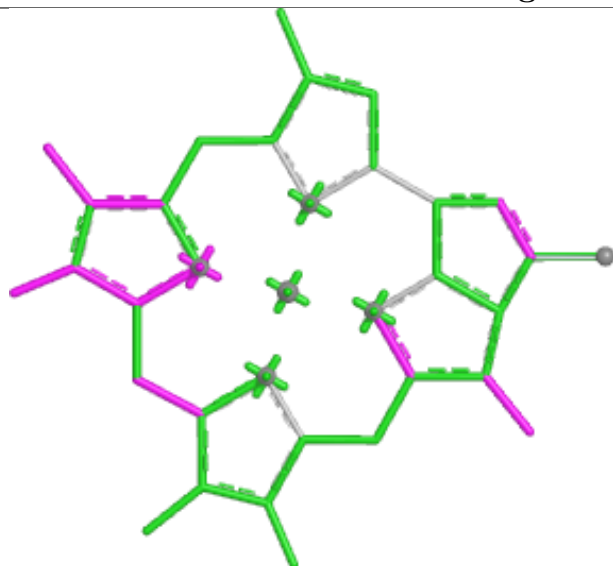


## Ligand CLA 1 208

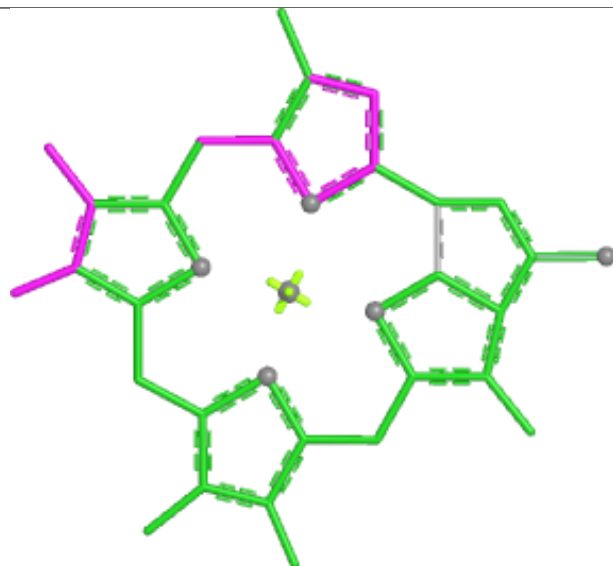




## Ligand CLA 9 211



Bond lengths



Bond angles

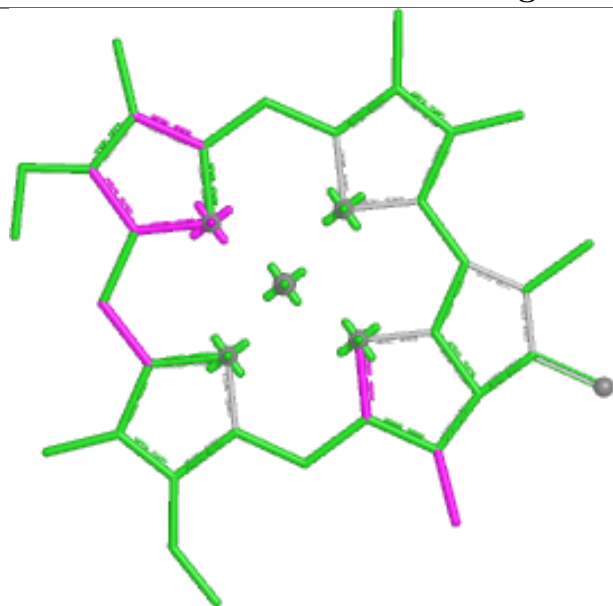


Torsions

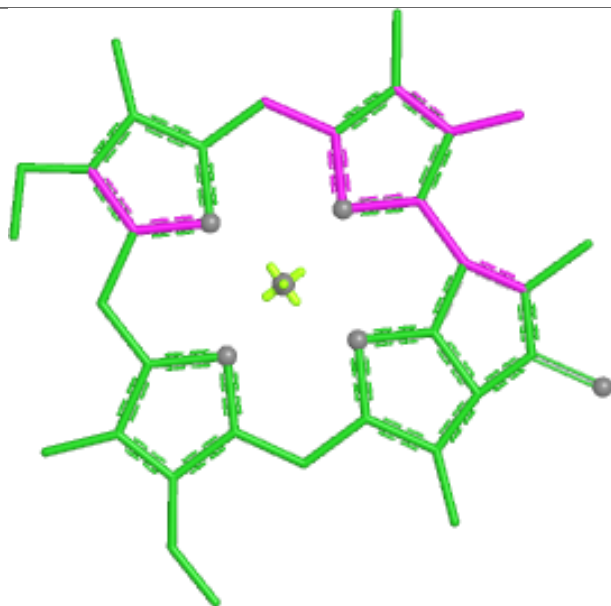


Rings

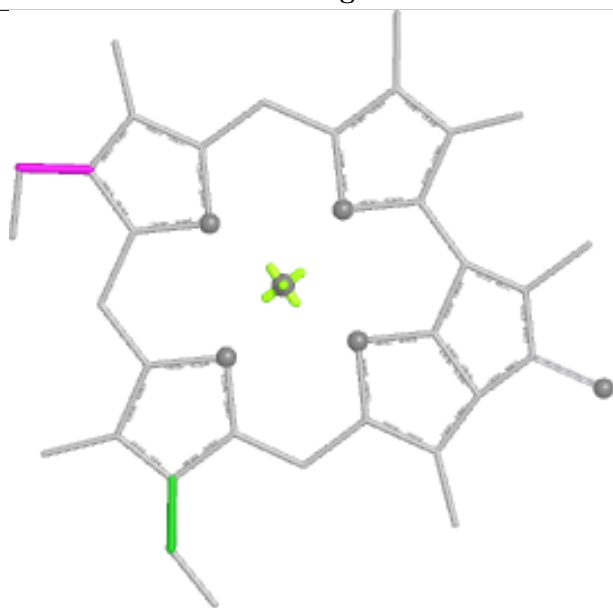
## Ligand CLA 5 313



Bond lengths



Bond angles

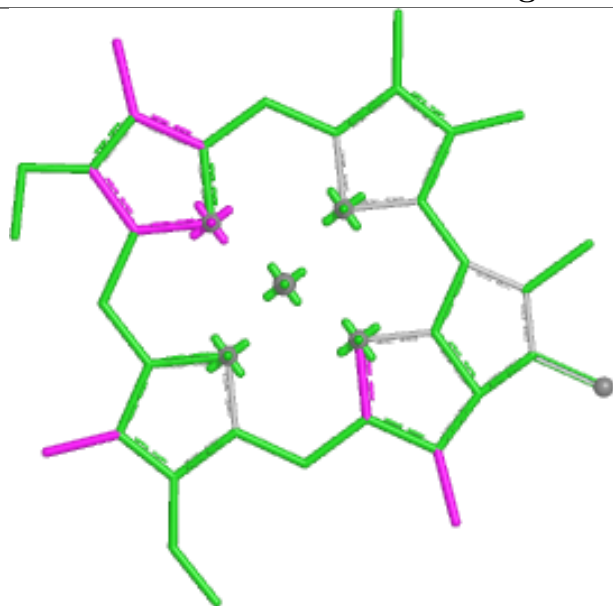


Torsions

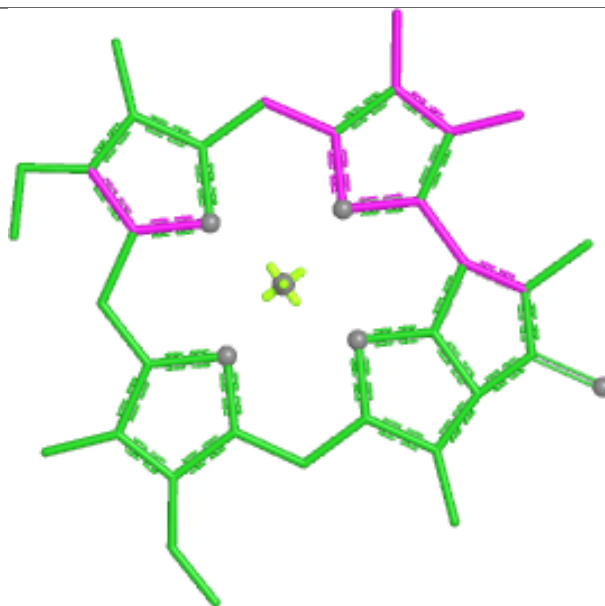


Rings

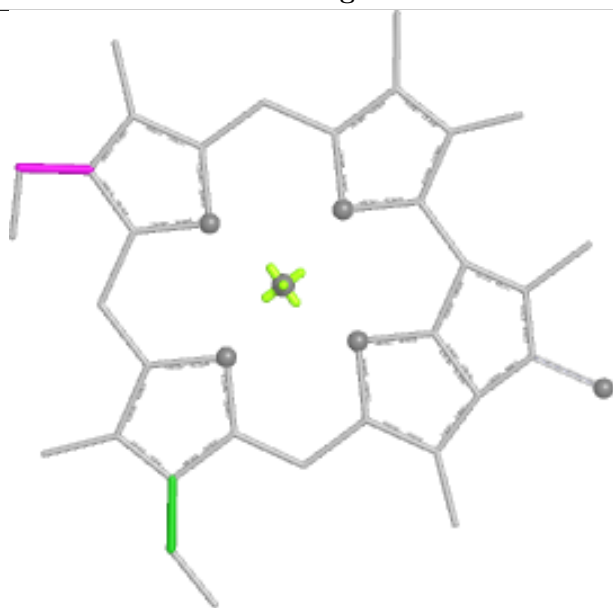
## Ligand CLA 9 207



Bond lengths



Bond angles

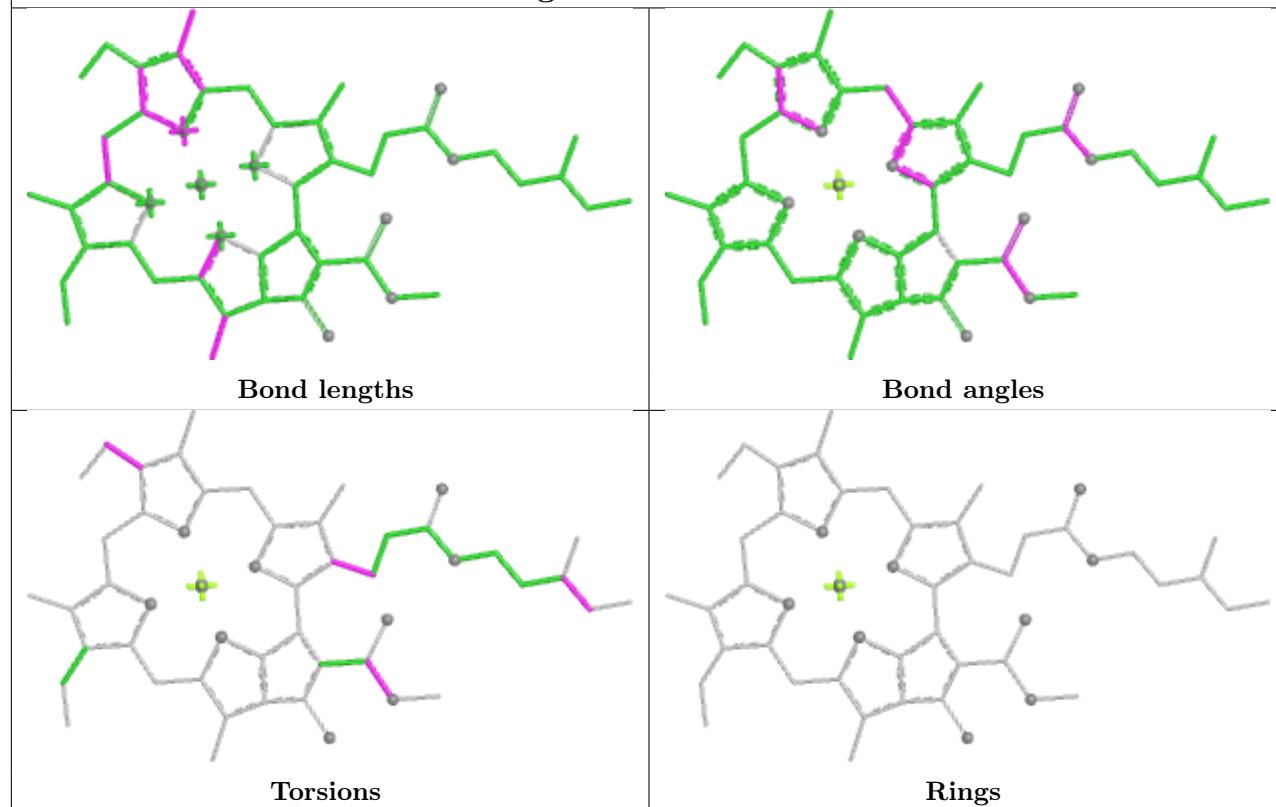


Torsions

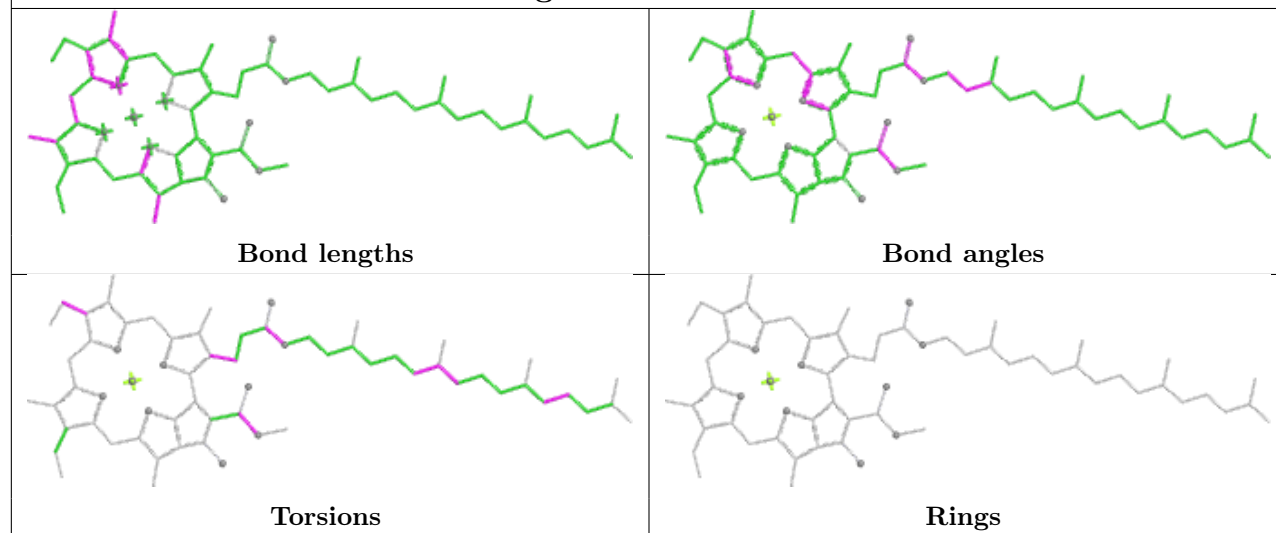


Rings

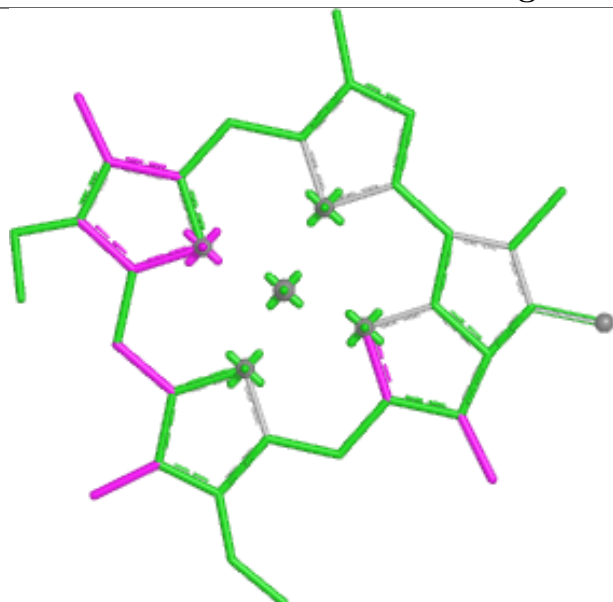
## Ligand CLA z 101



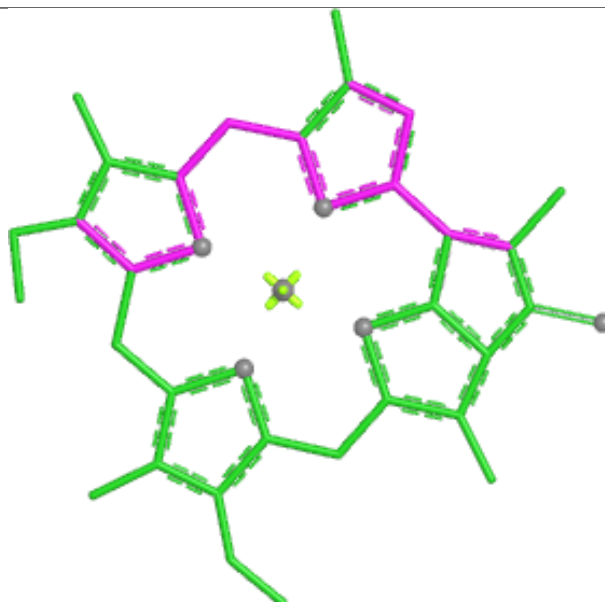
## Ligand CLA b 517



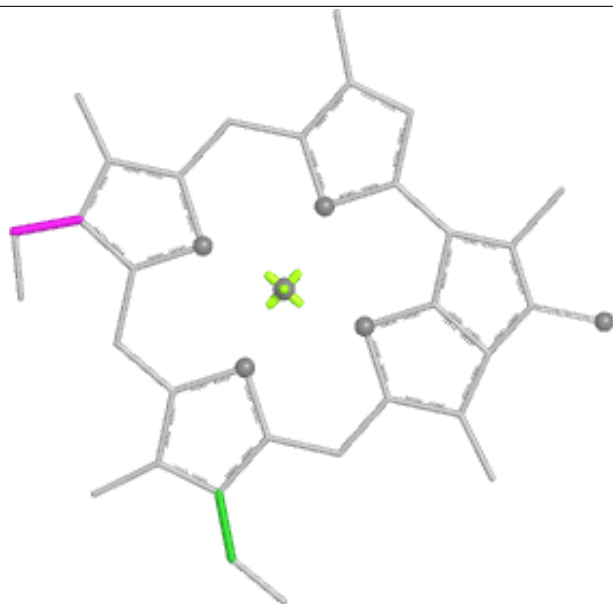
## Ligand CLA 4 206



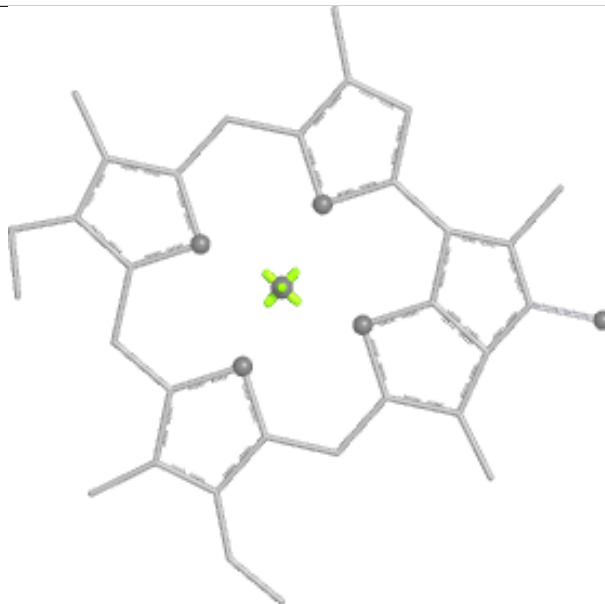
Bond lengths



Bond angles

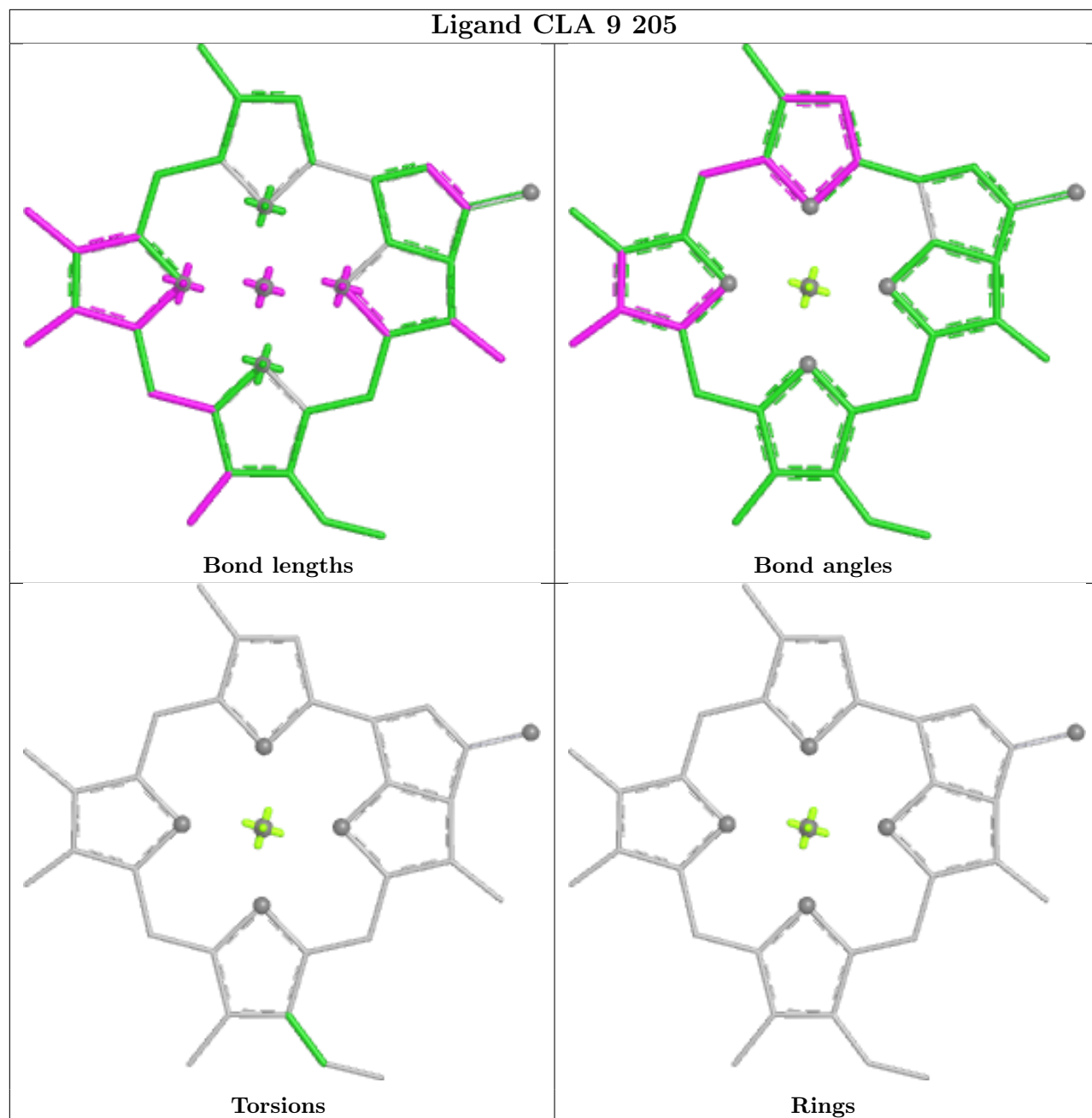


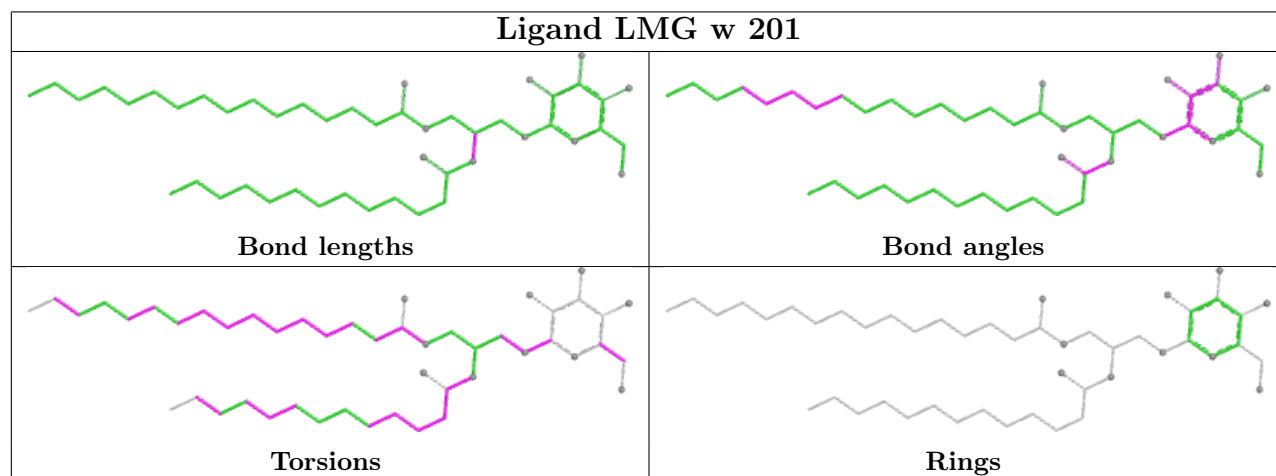
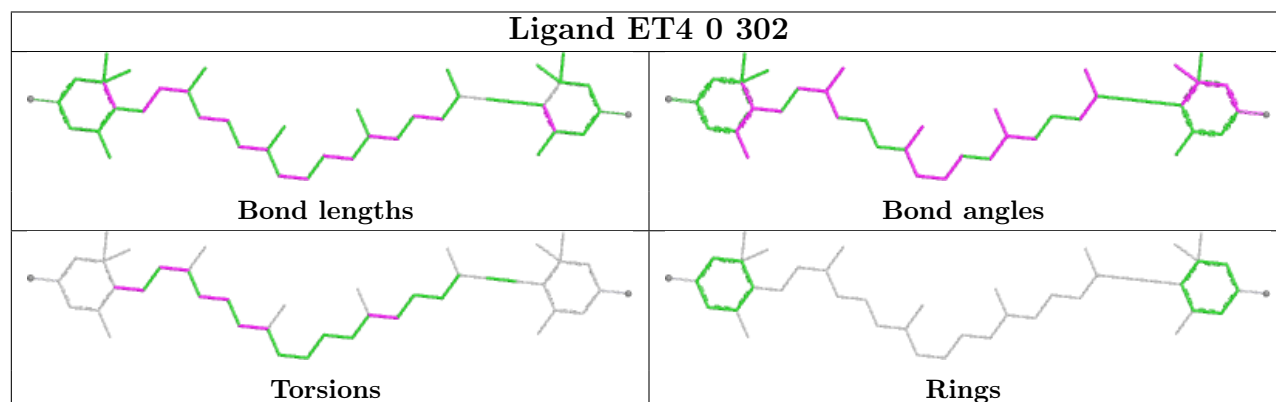
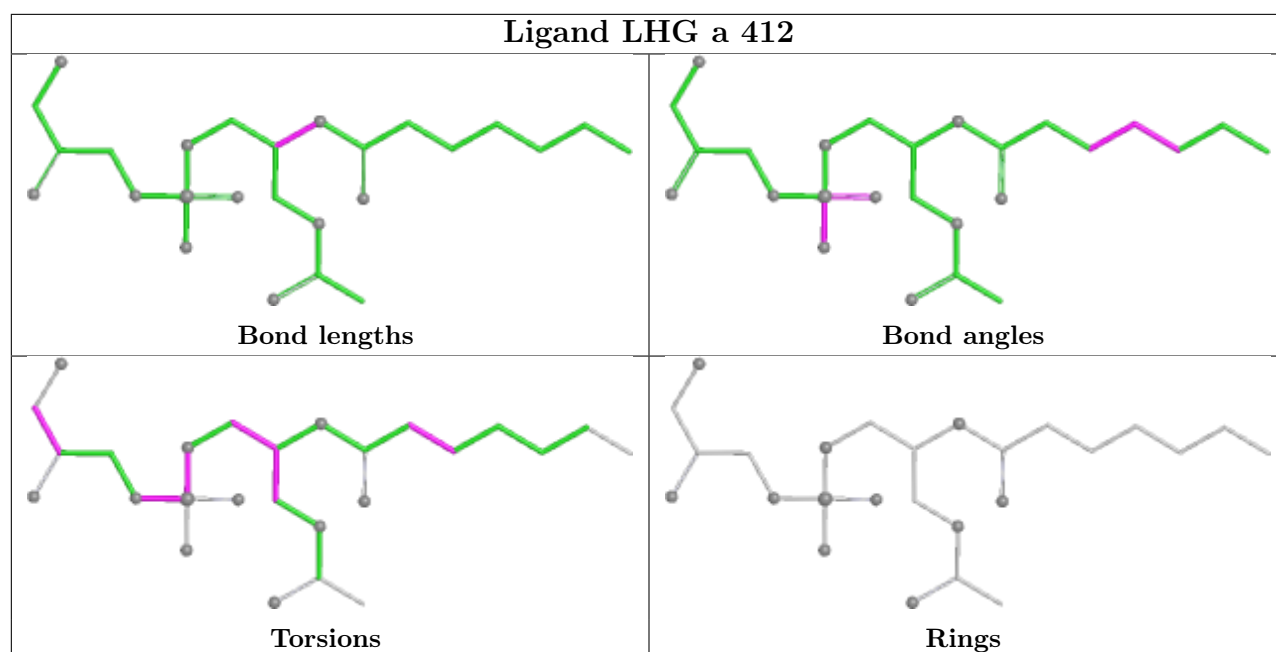
Torsions

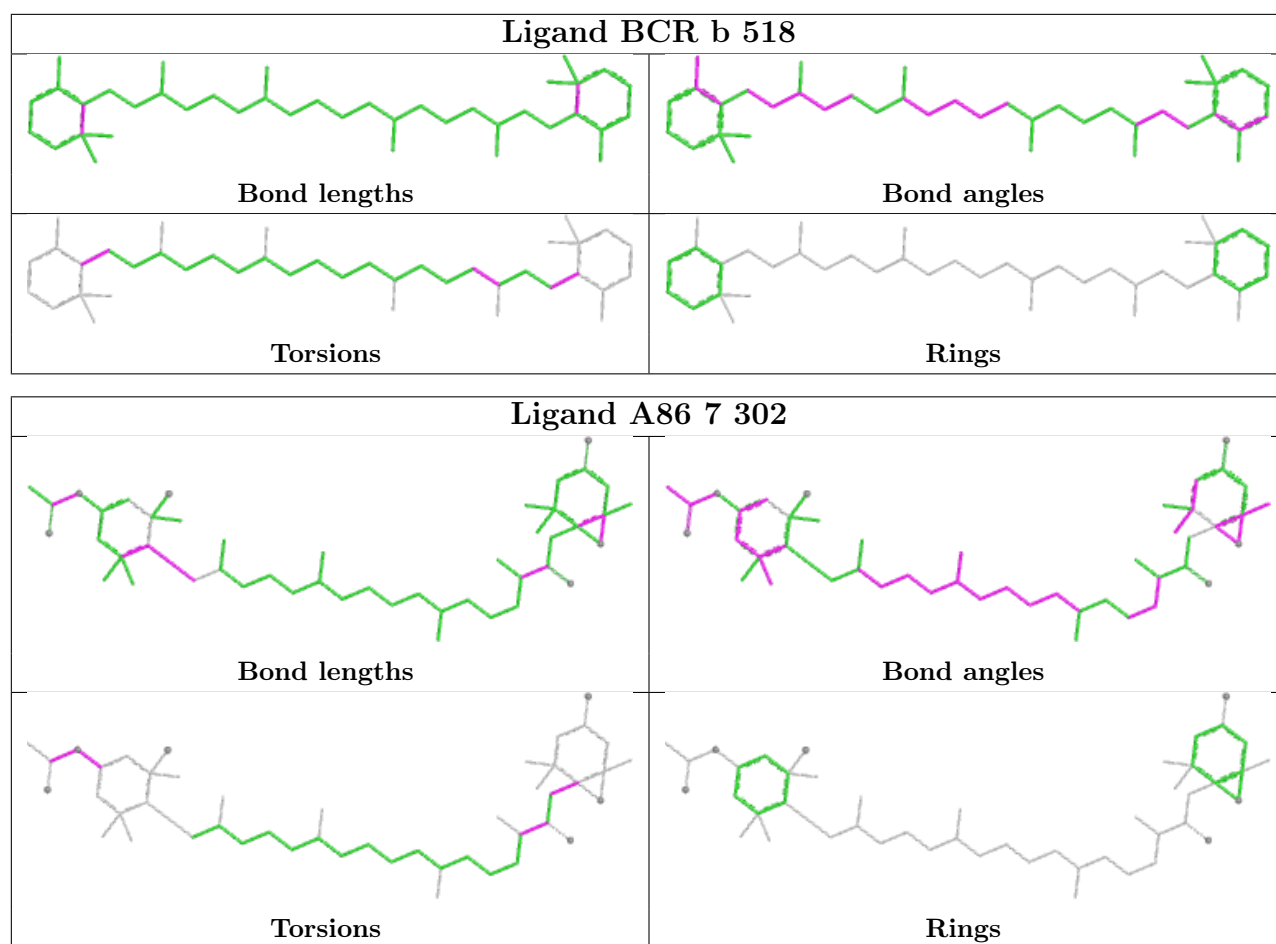


Rings

## Ligand CLA 9 205

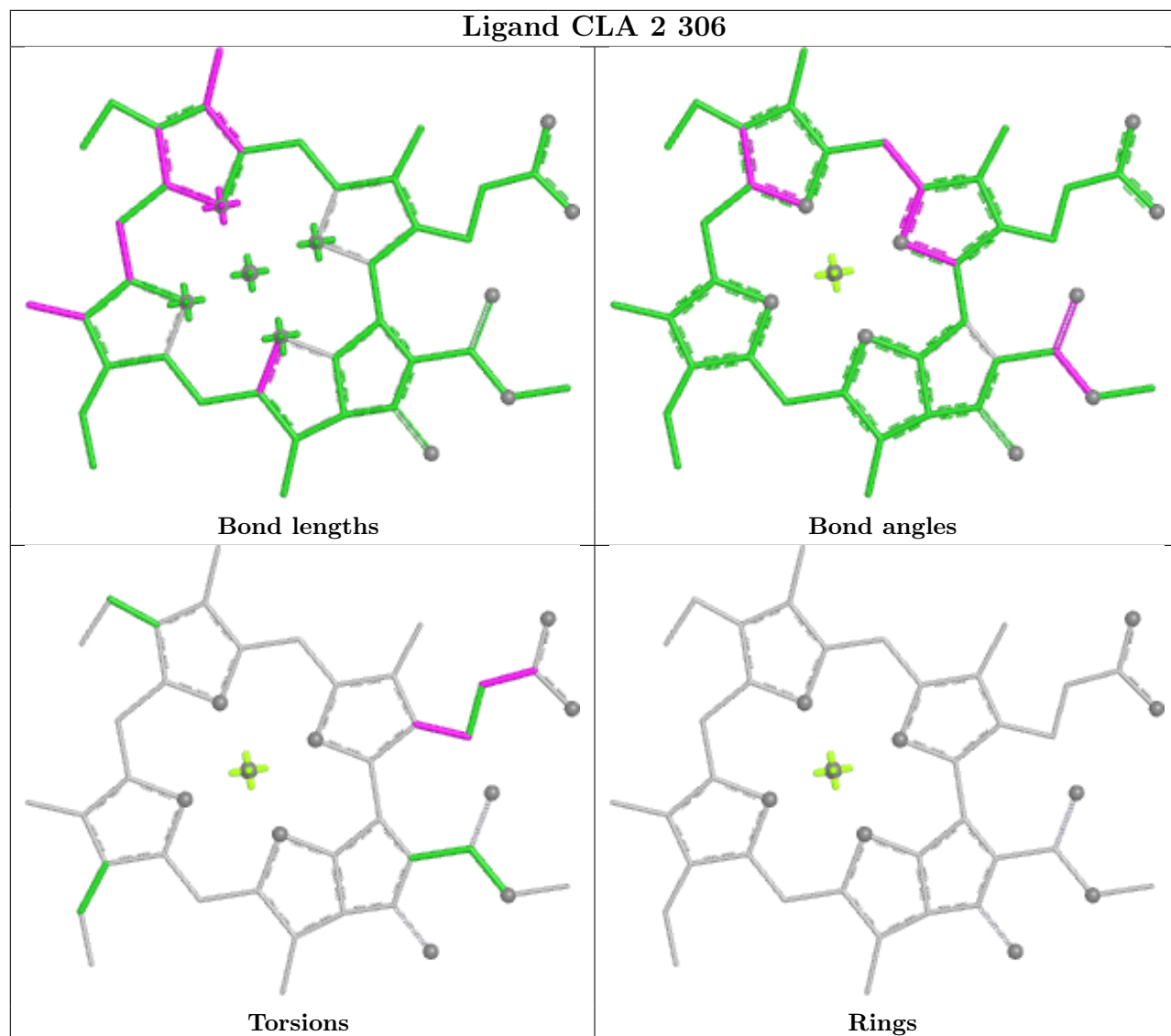


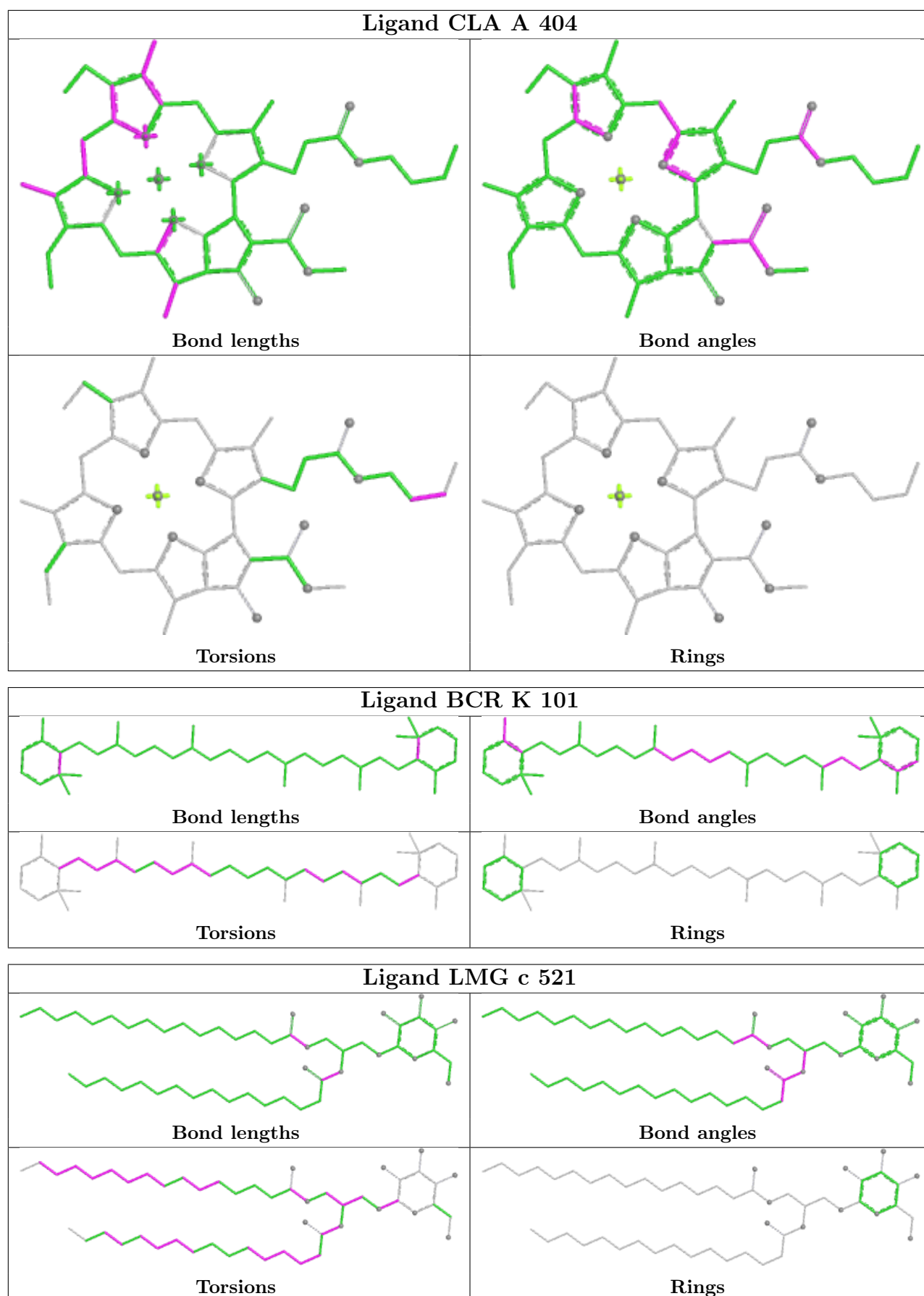




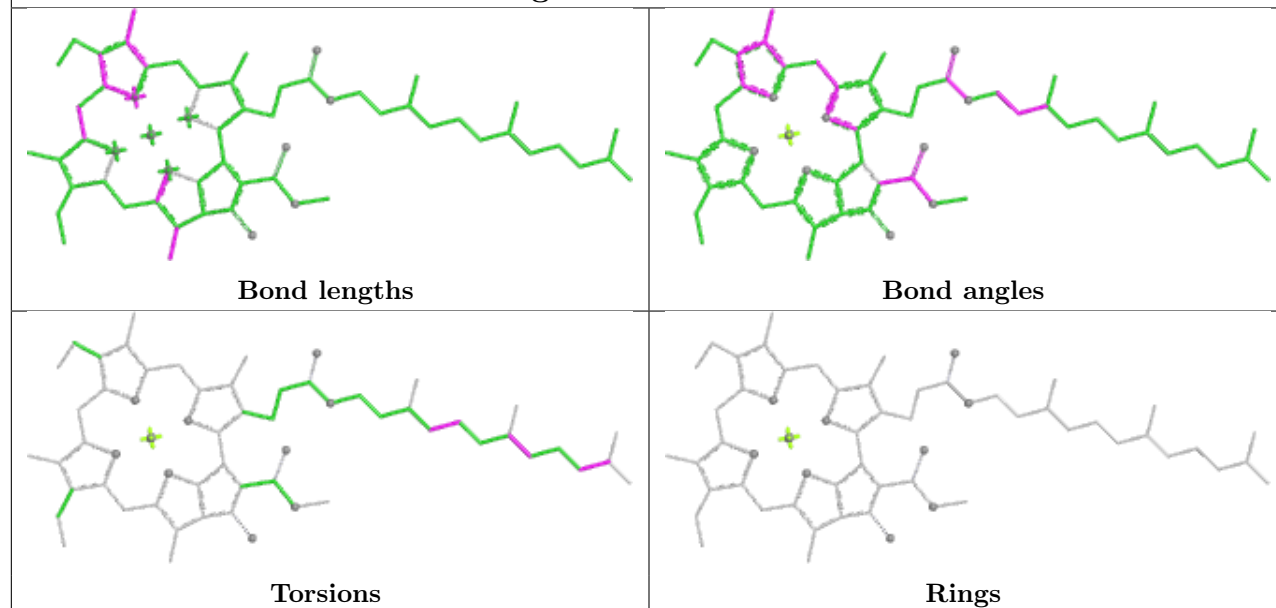


## Ligand CLA 2 306

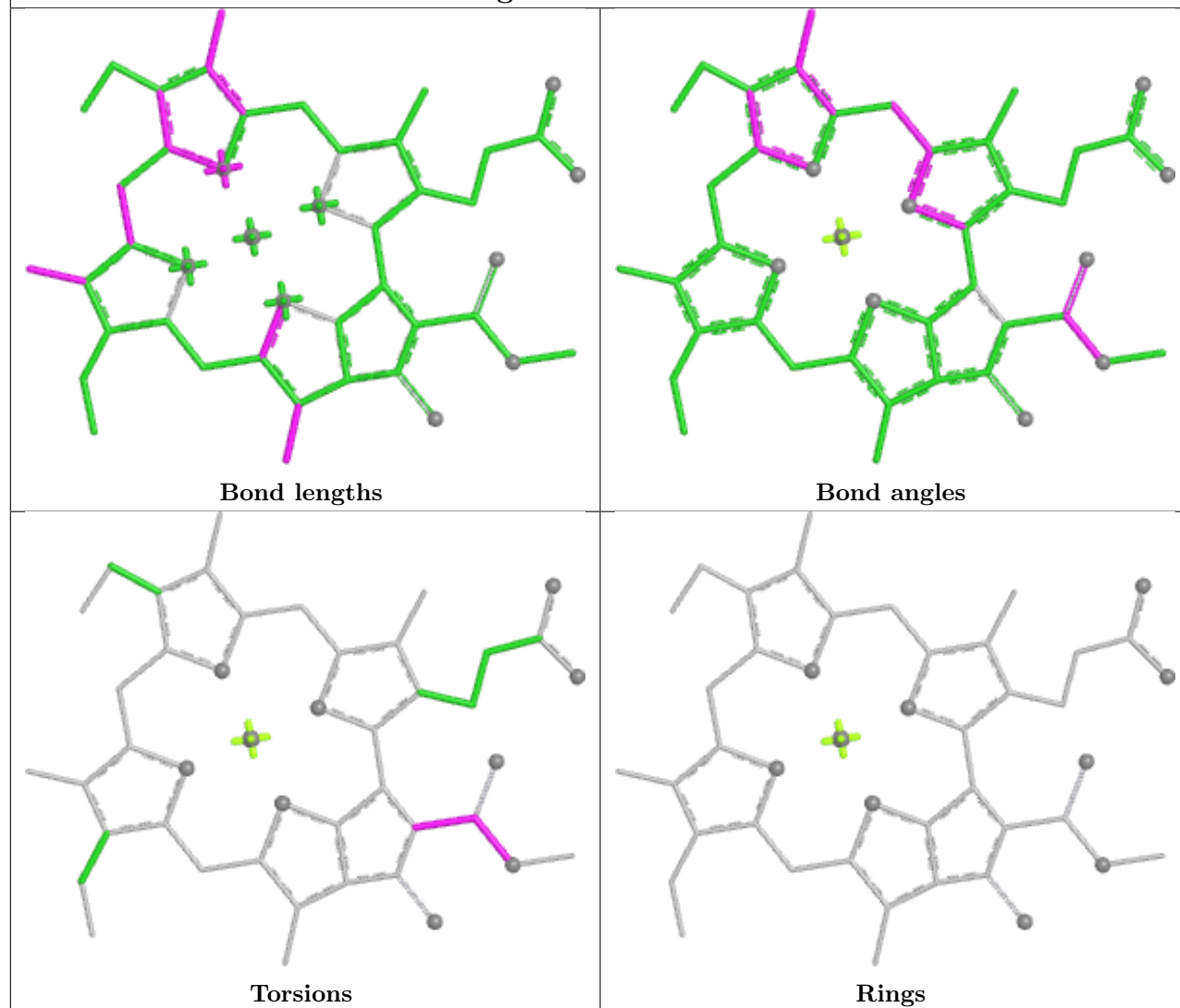


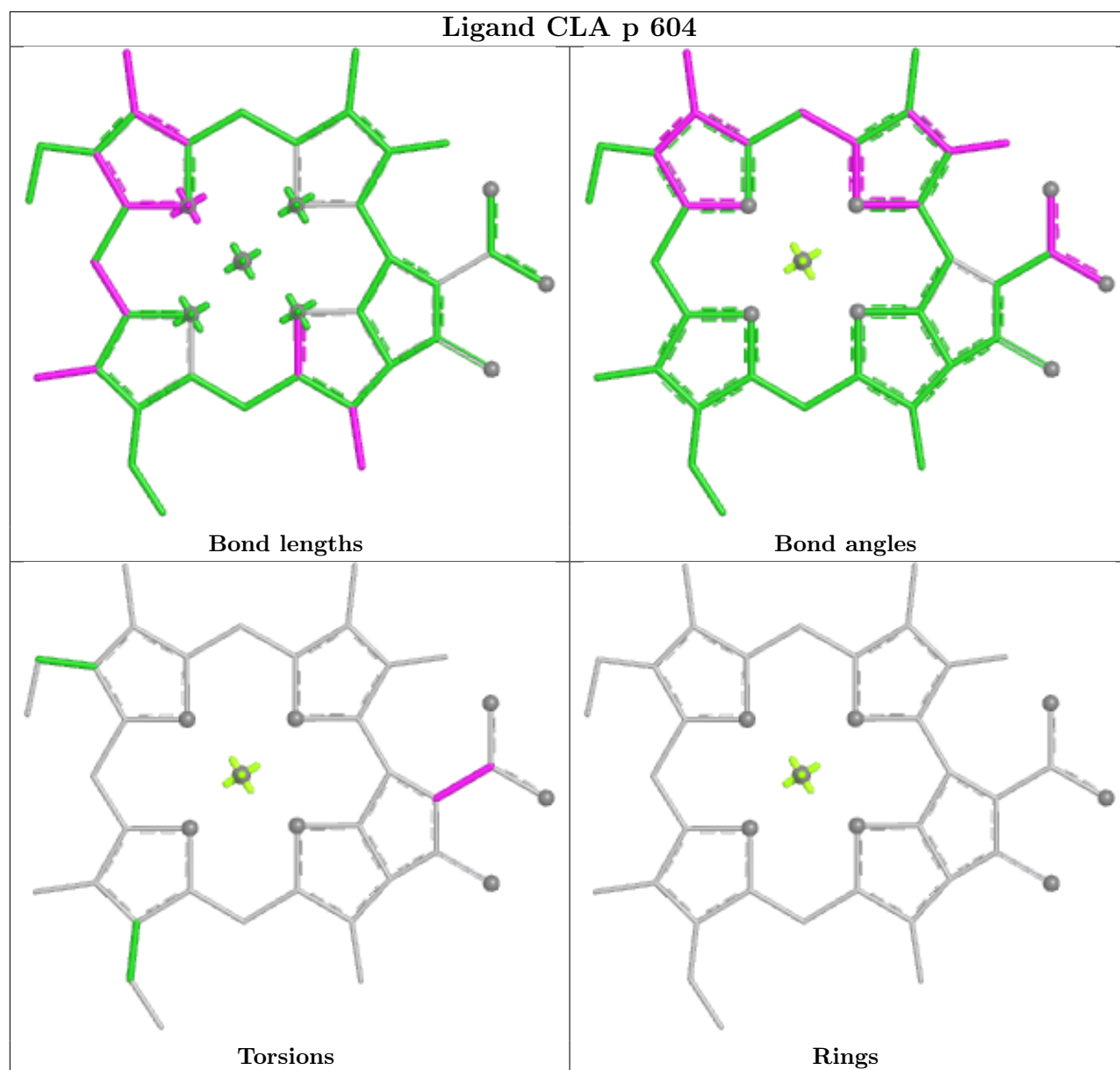
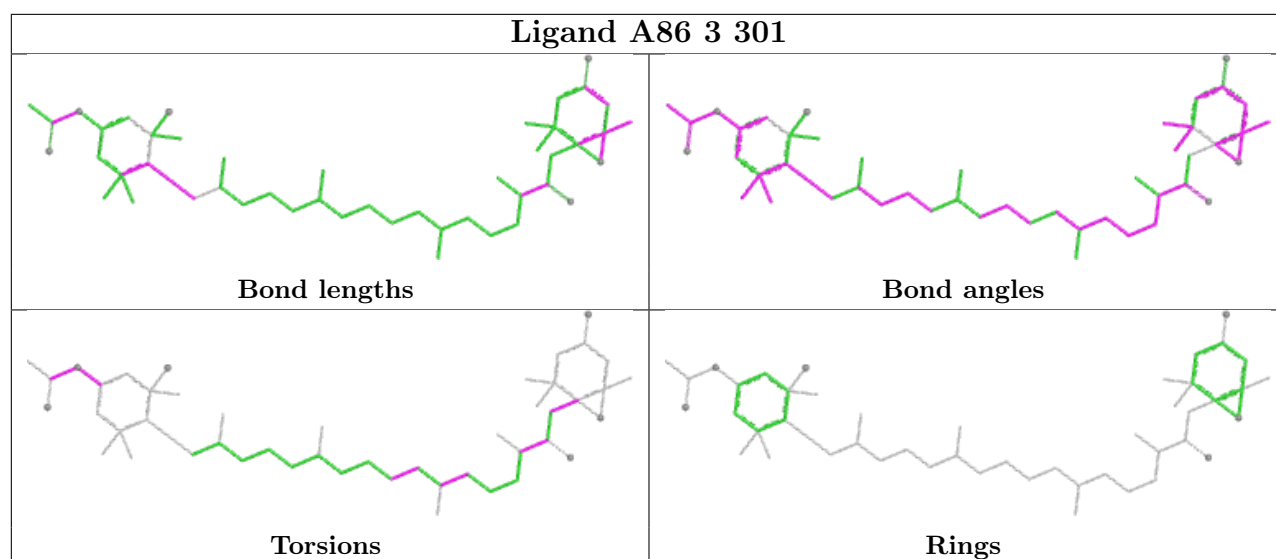


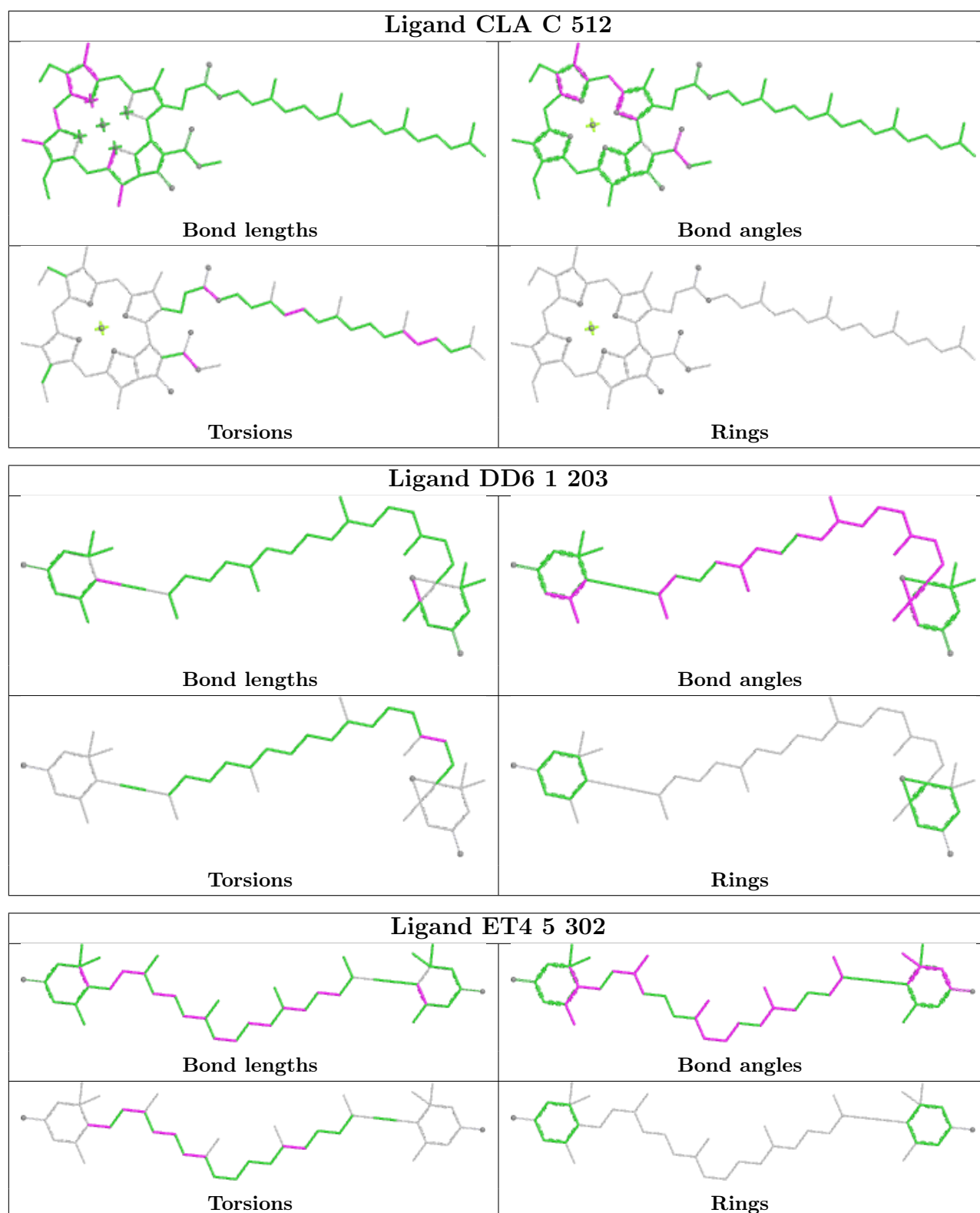
## Ligand CLA A 407



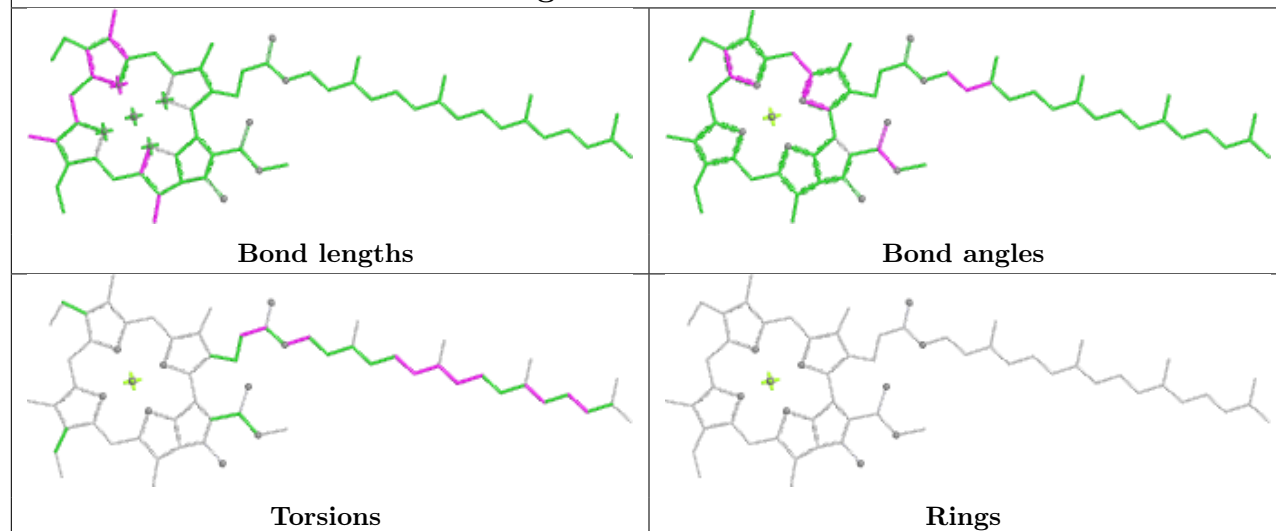
## Ligand CLA c 507



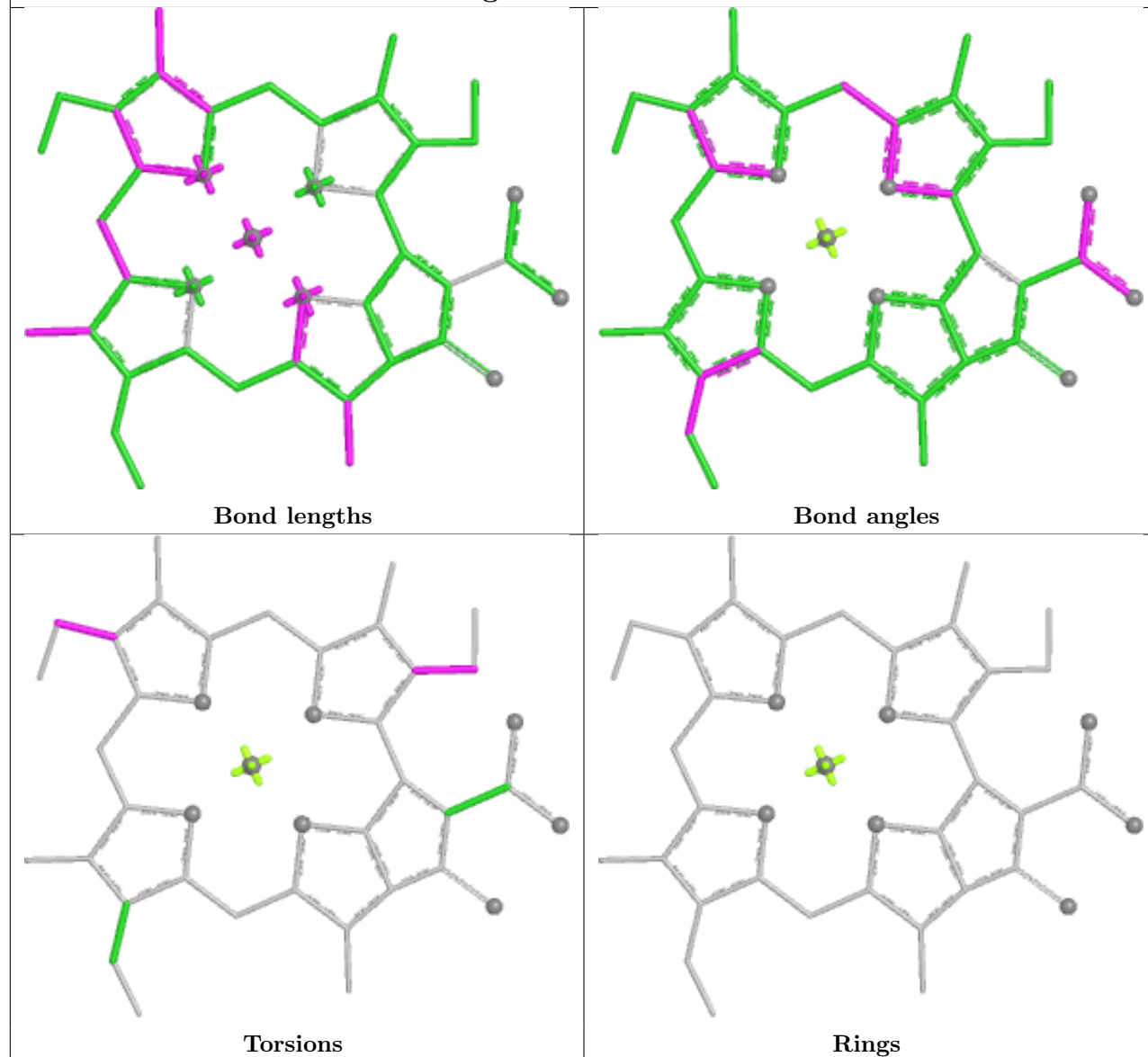




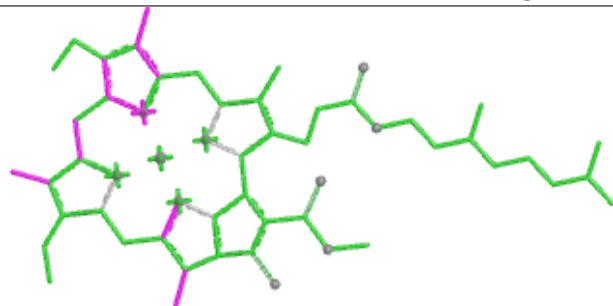
## Ligand CLA c 511



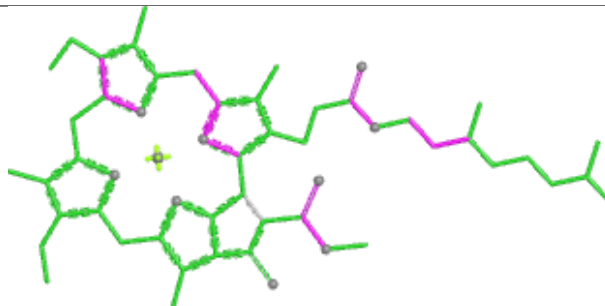
## Ligand CLA 8 305



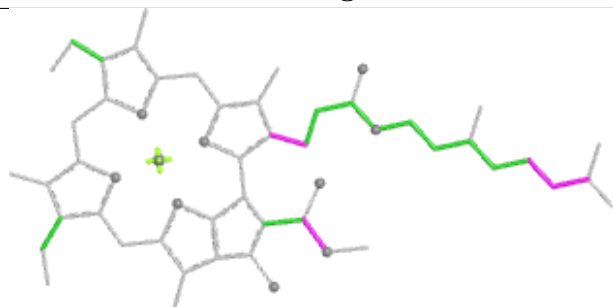
## Ligand CLA 1 211



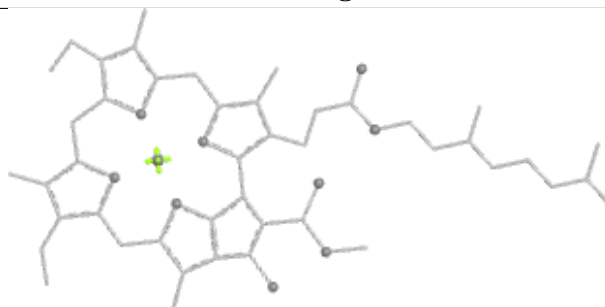
Bond lengths



Bond angles

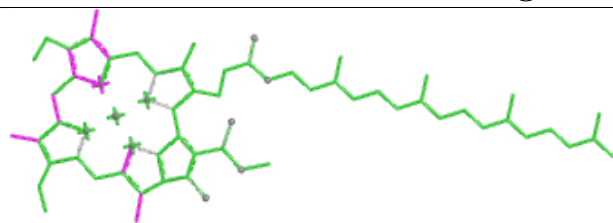


Torsions

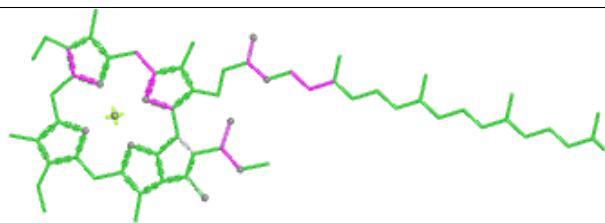


Rings

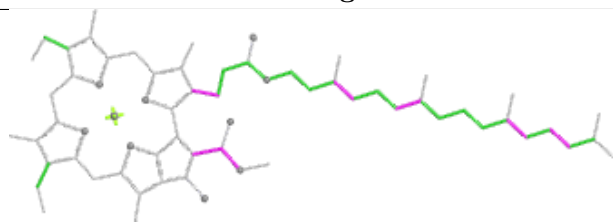
## Ligand CLA b 510



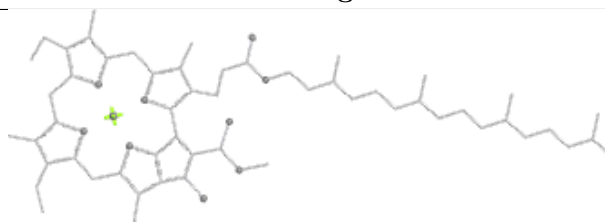
Bond lengths



Bond angles

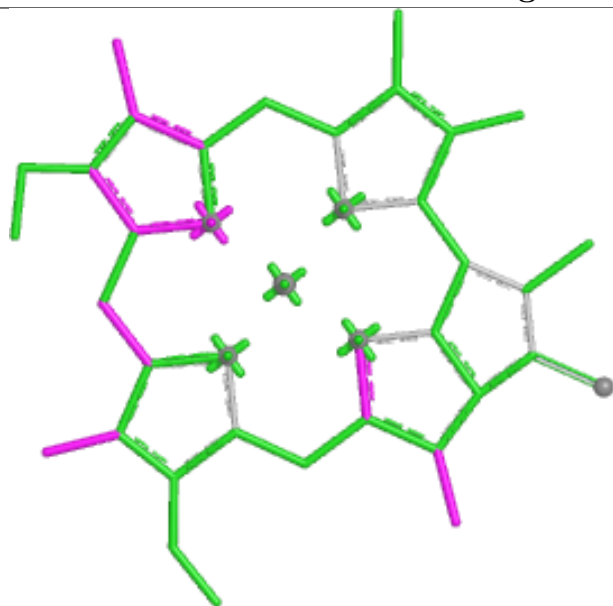


Torsions

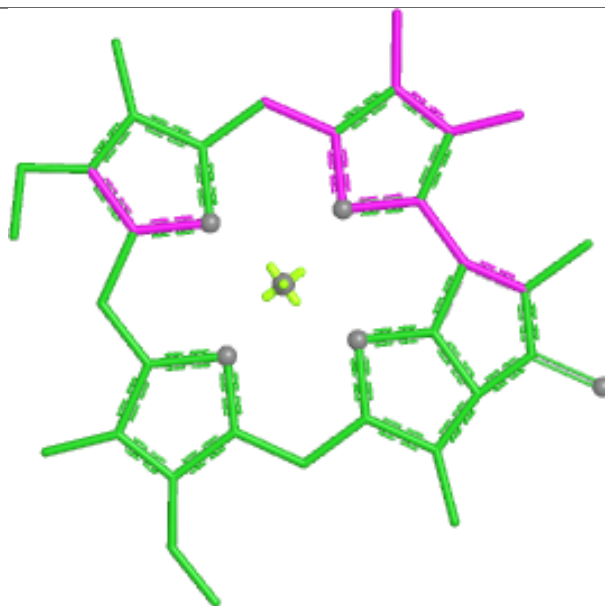


Rings

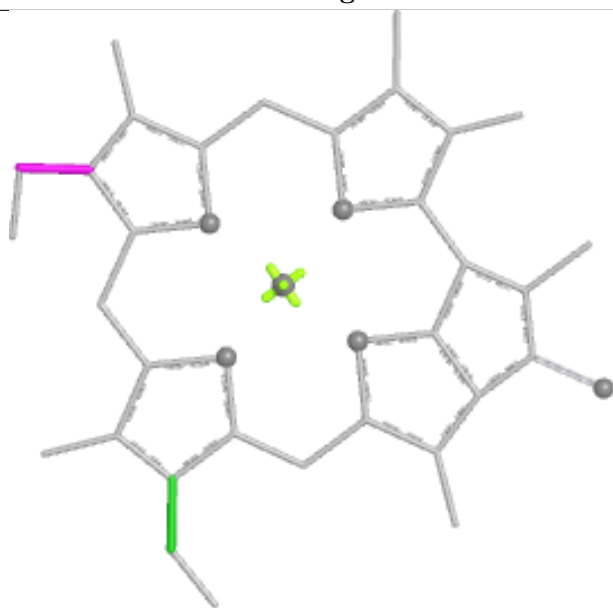
## Ligand CLA 2 315



Bond lengths



Bond angles

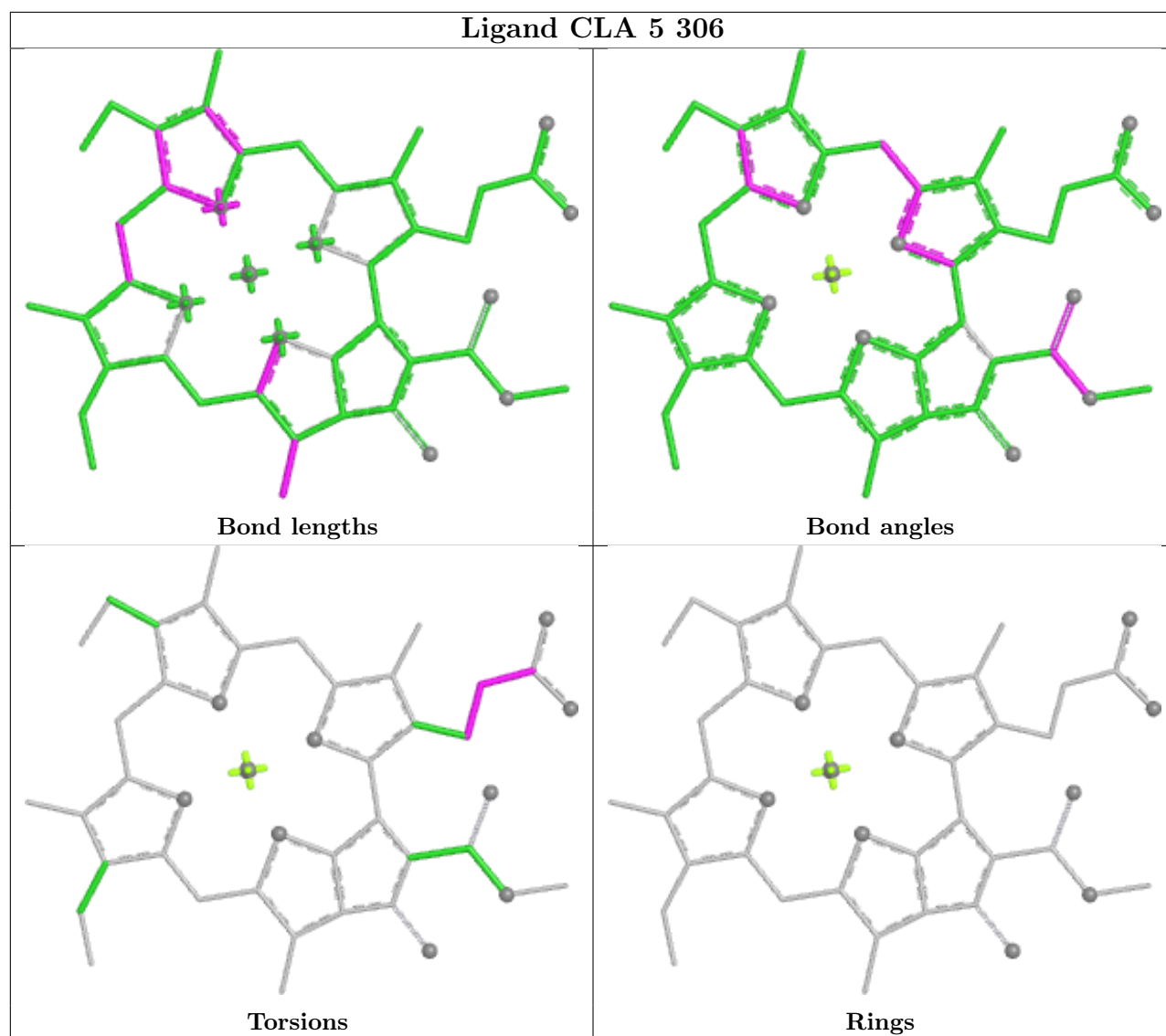
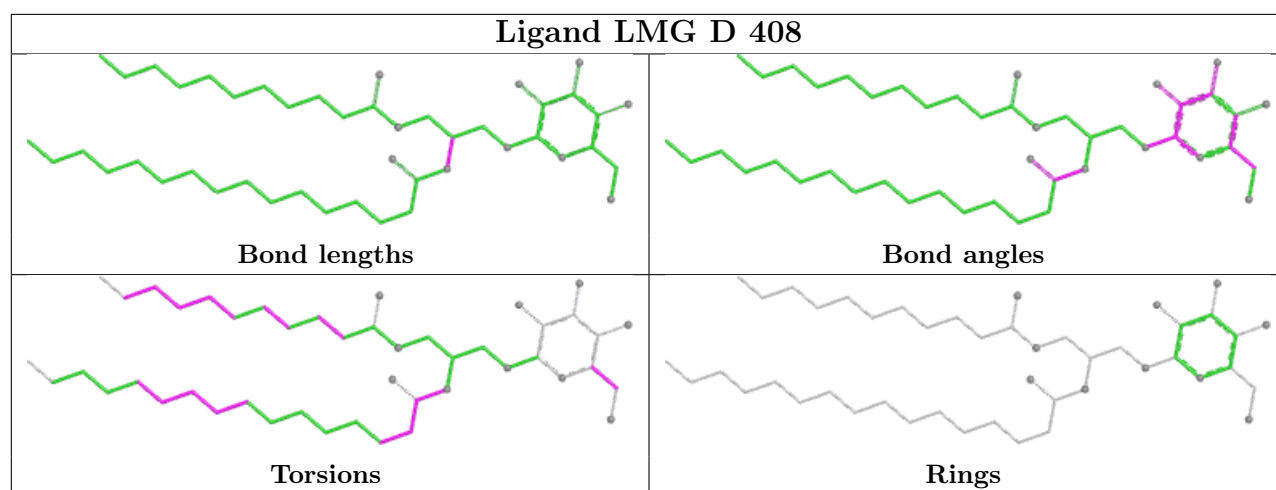


Torsions

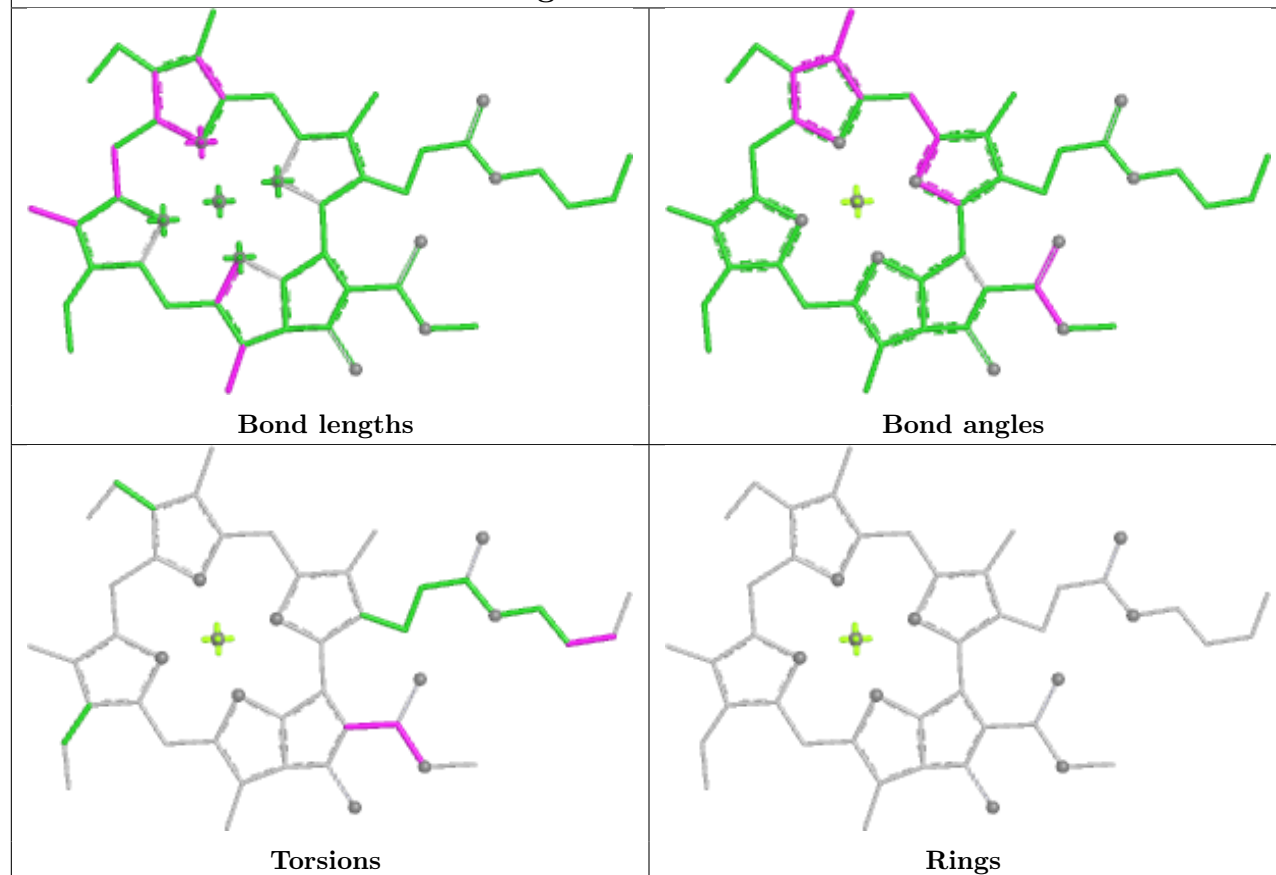


Rings

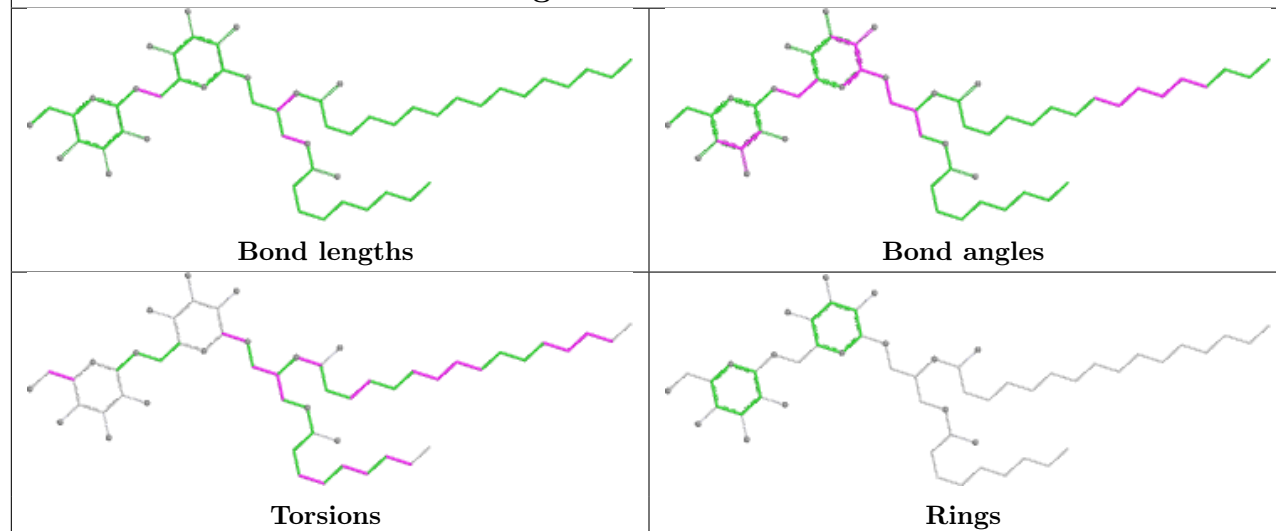


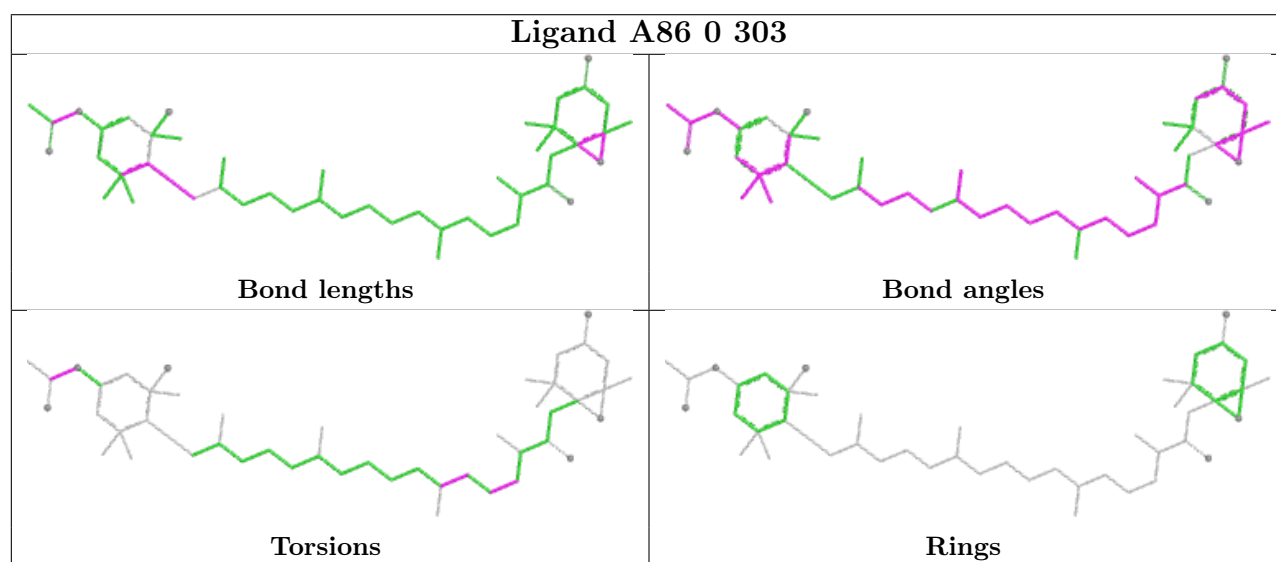
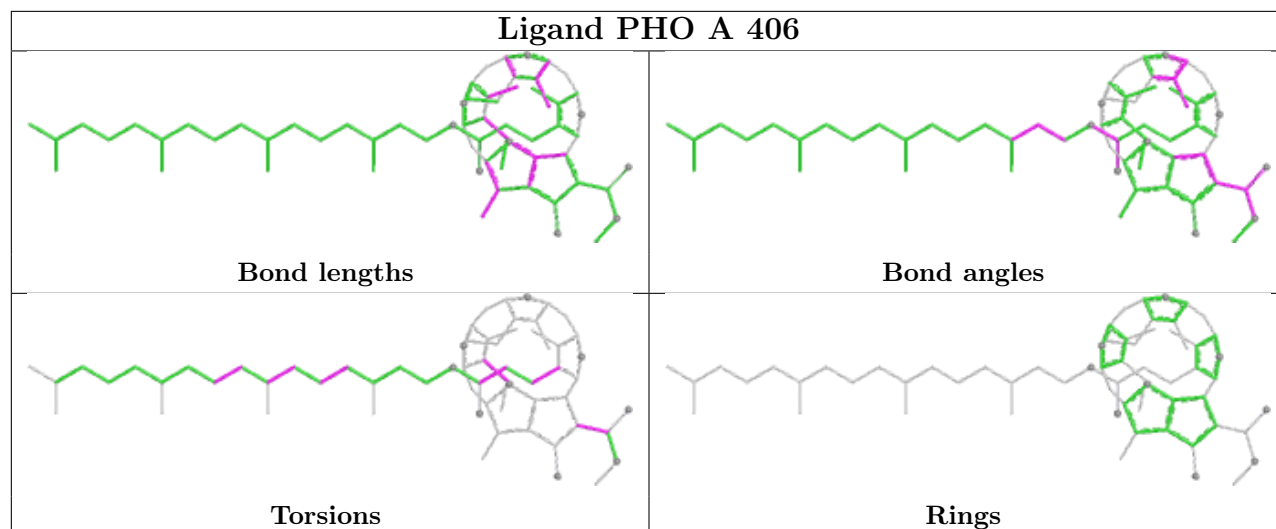


## Ligand CLA c 514

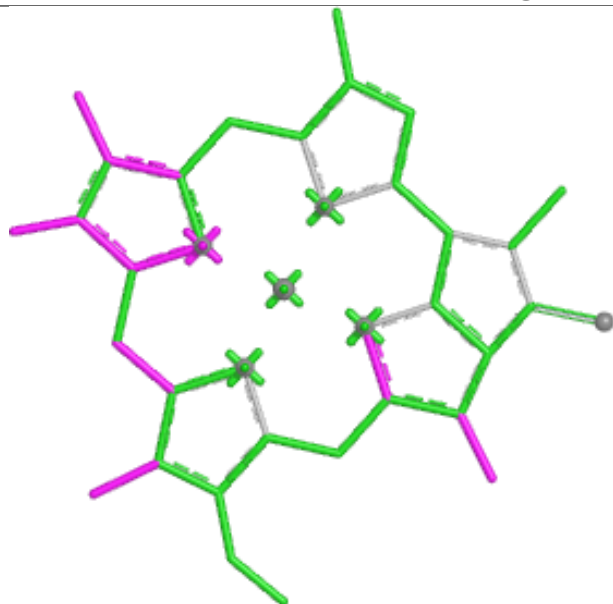


## Ligand DGD c 518

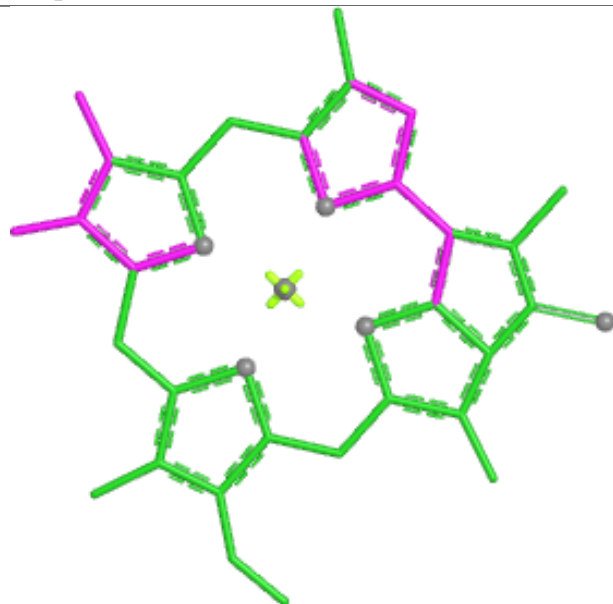




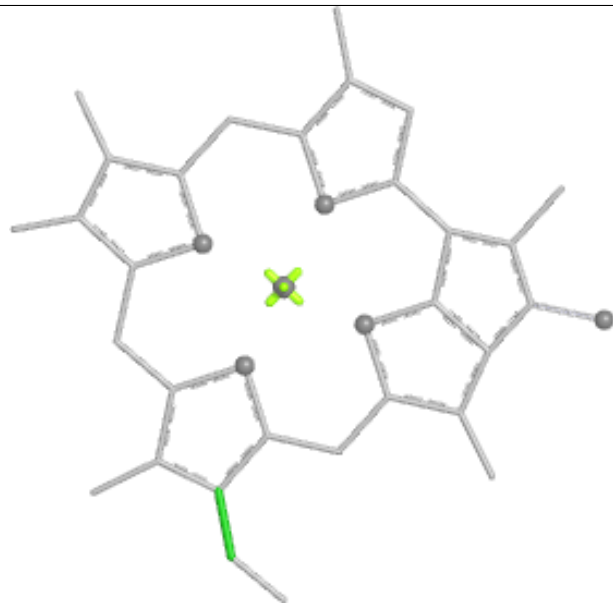
## Ligand CLA p 607



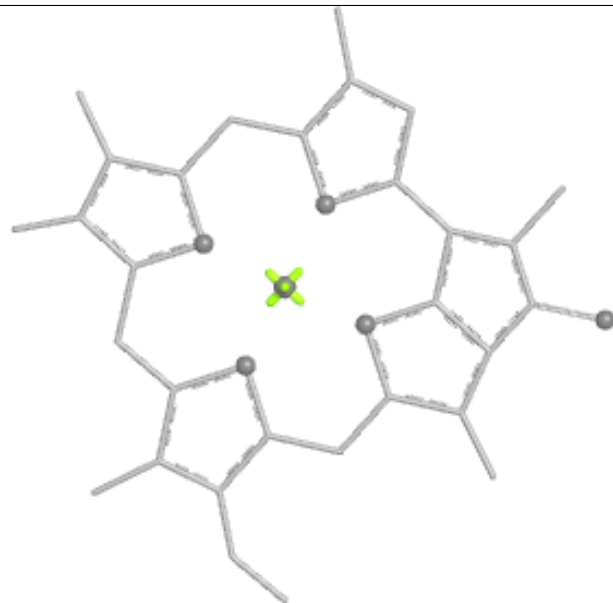
Bond lengths



Bond angles

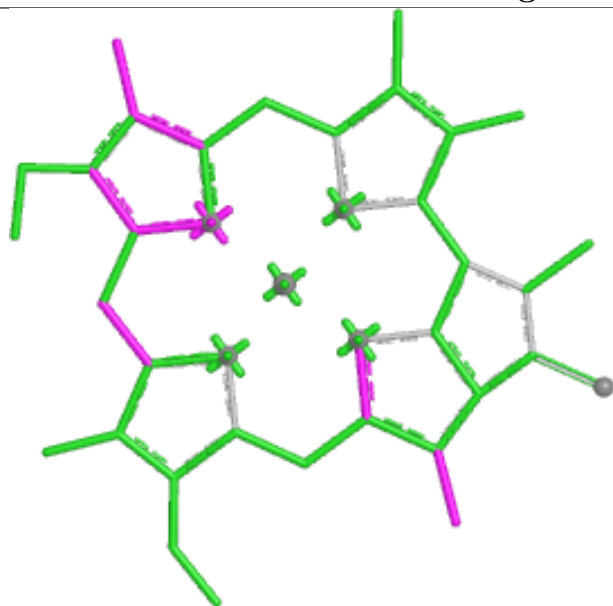


Torsions

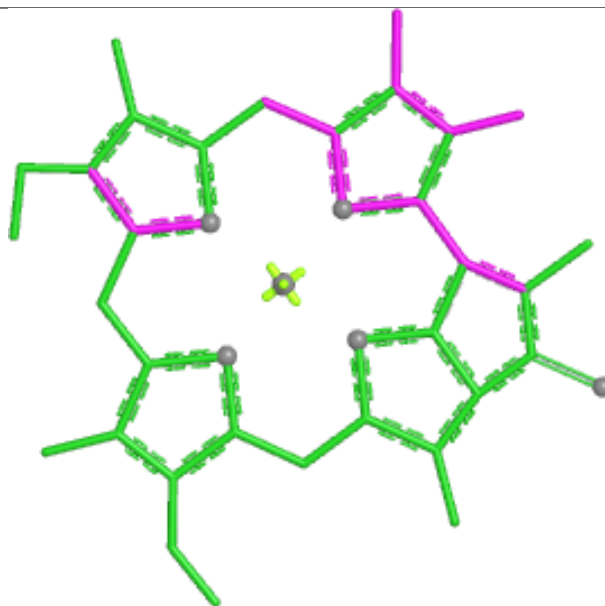


Rings

## Ligand CLA 0 314



Bond lengths



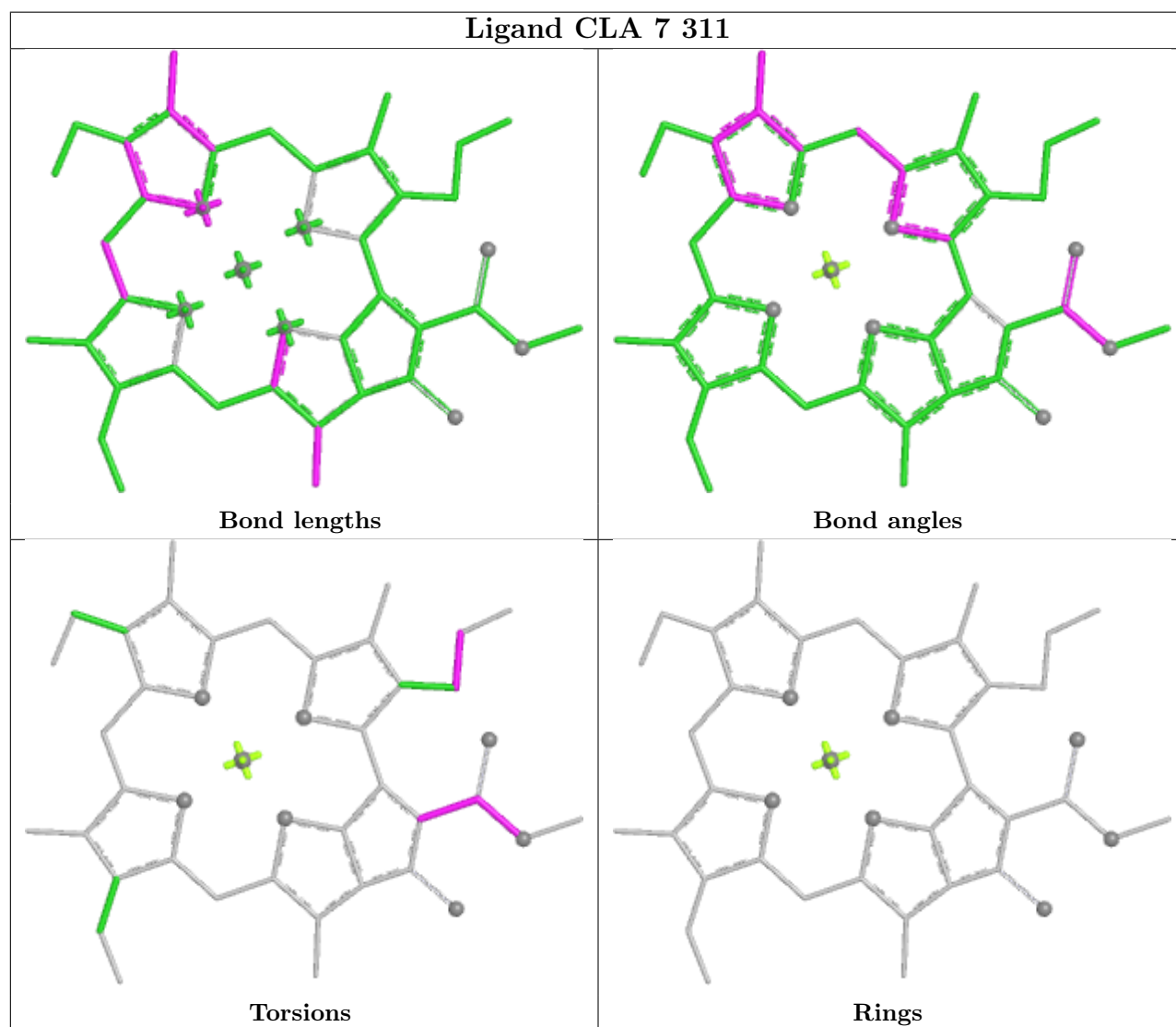
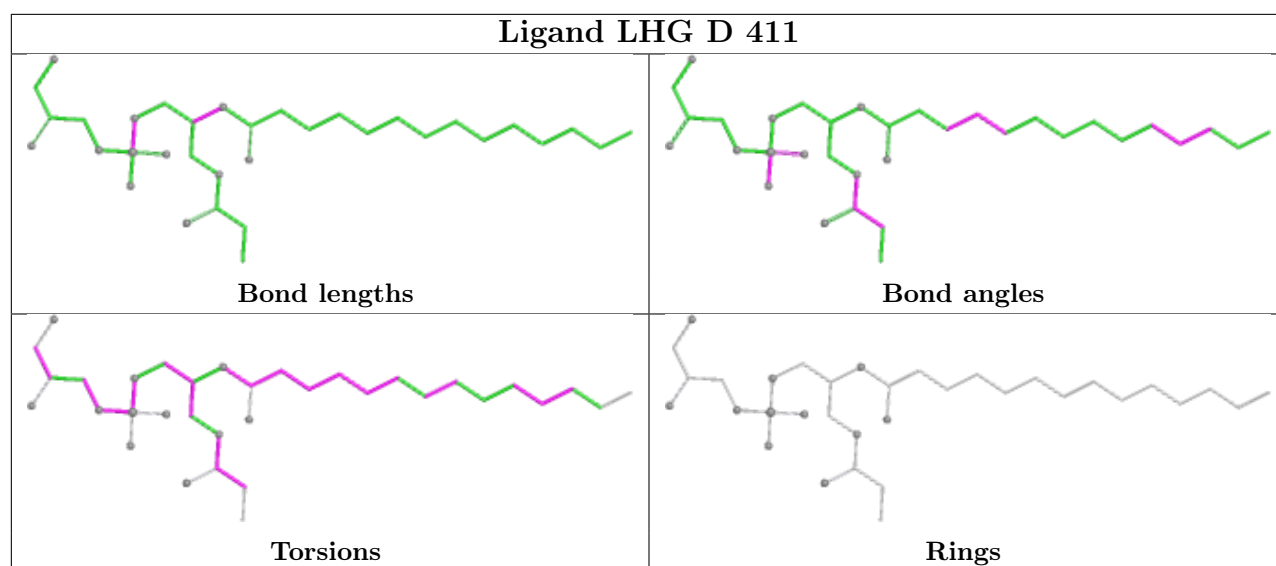
Bond angles

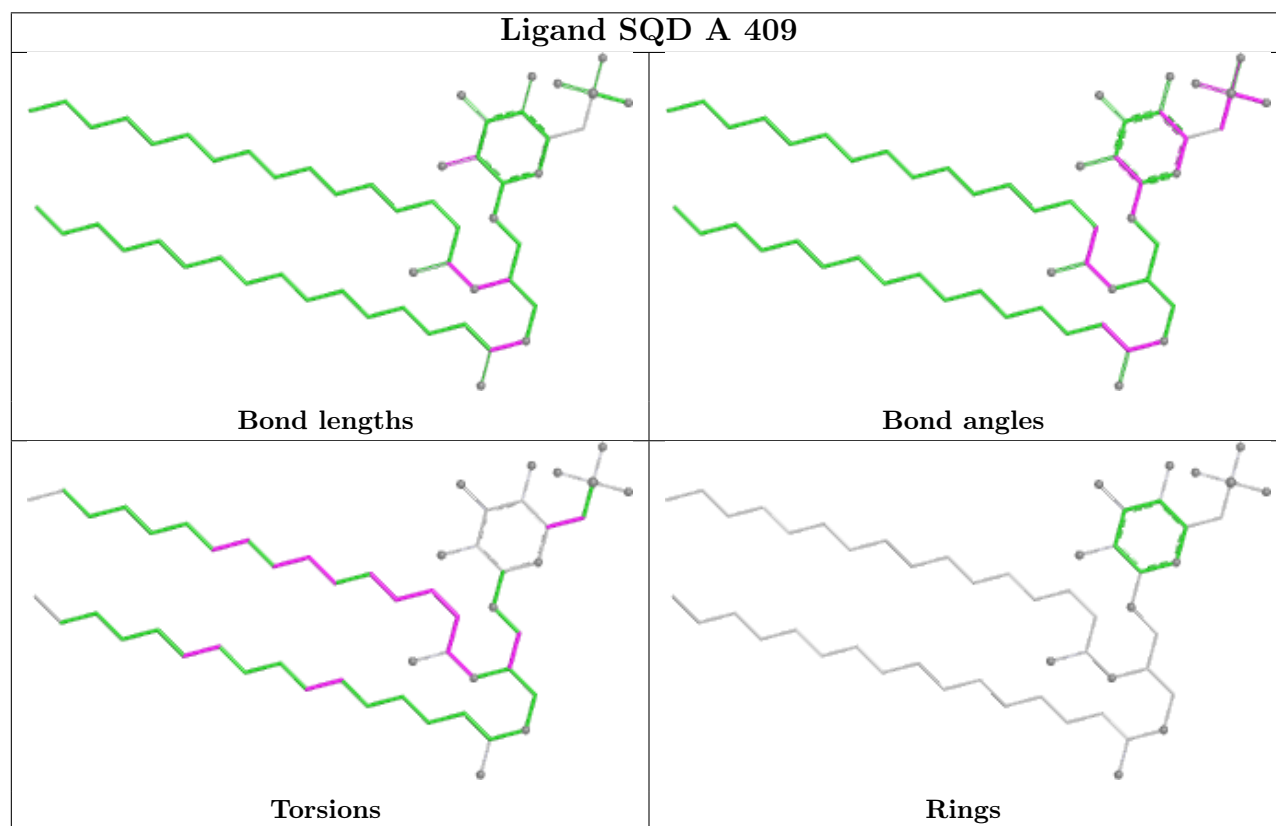
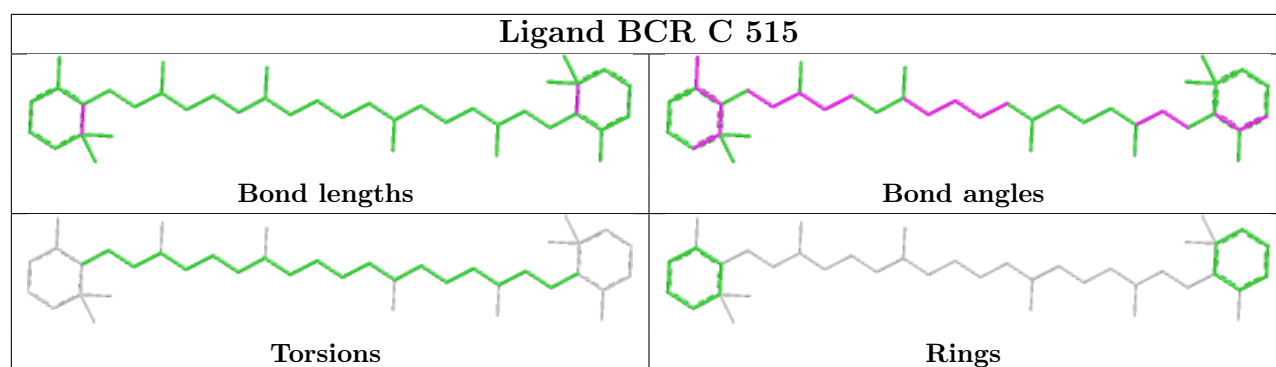


Torsions

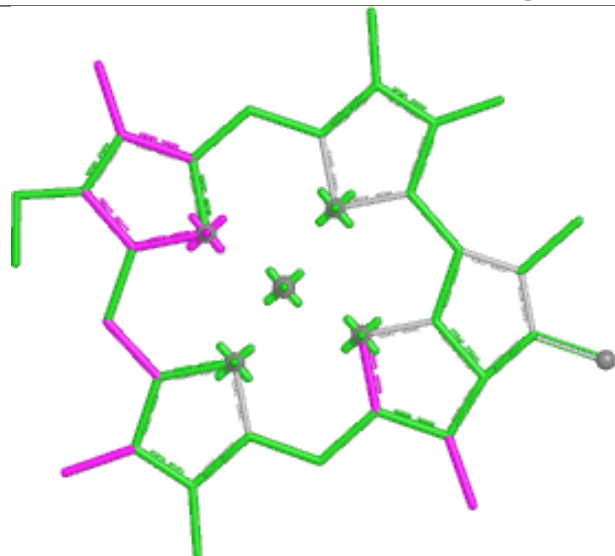


Rings

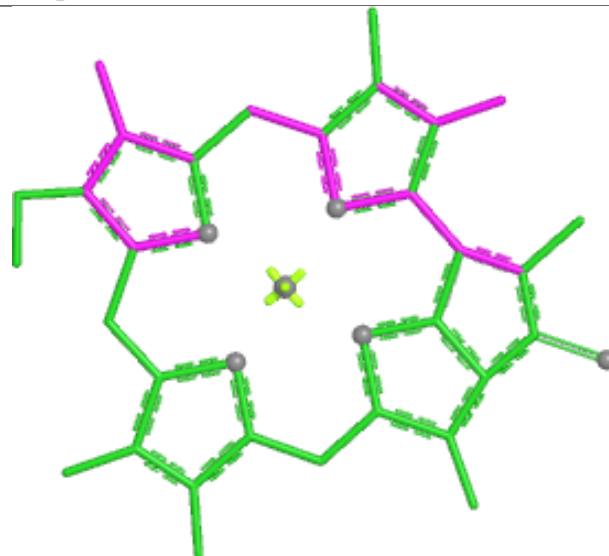




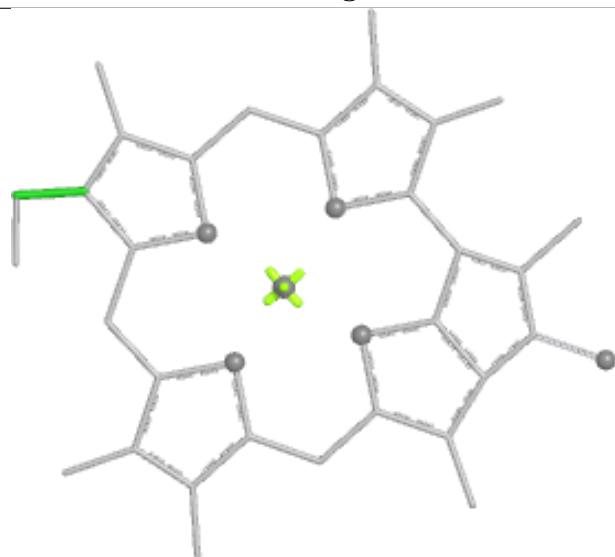
## Ligand CLA p 603



Bond lengths



Bond angles

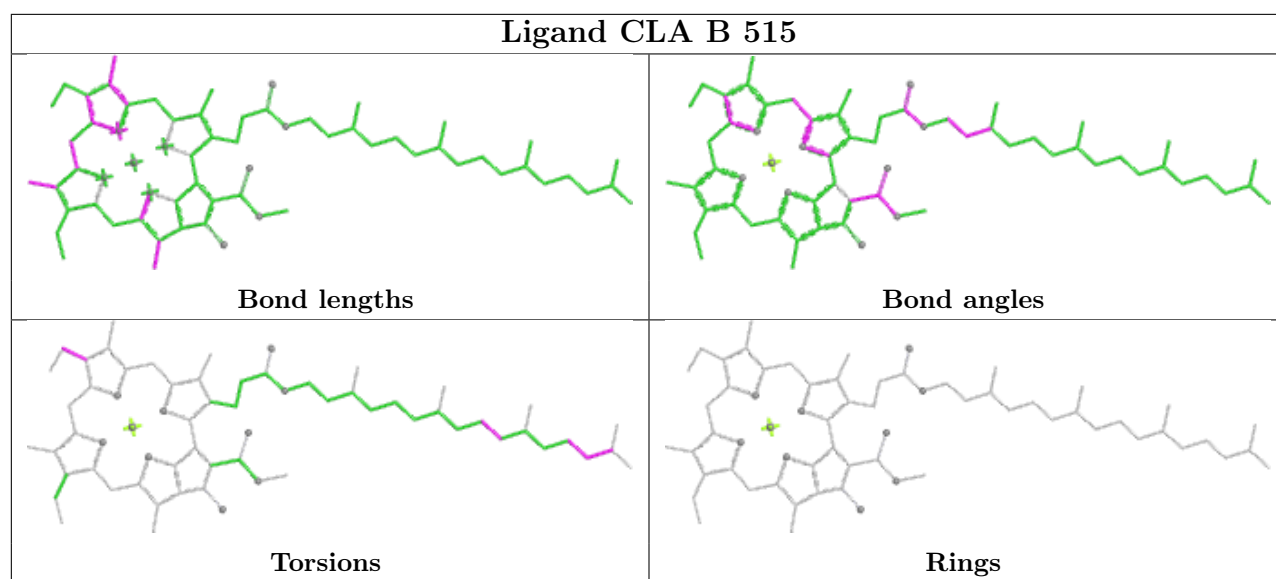


Torsions

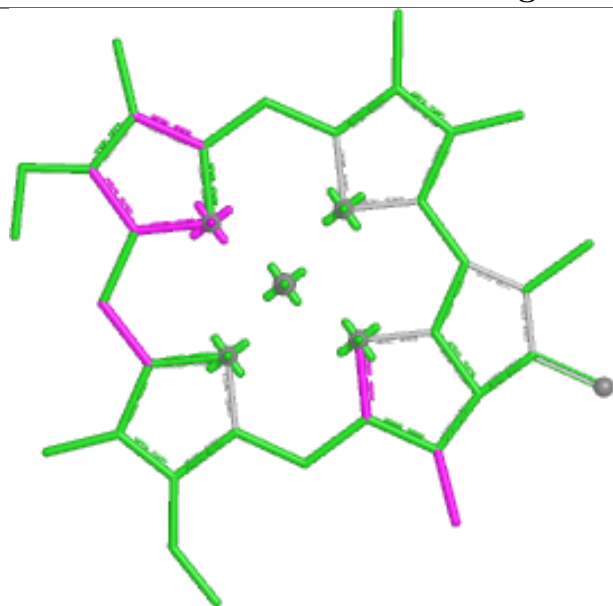


Rings

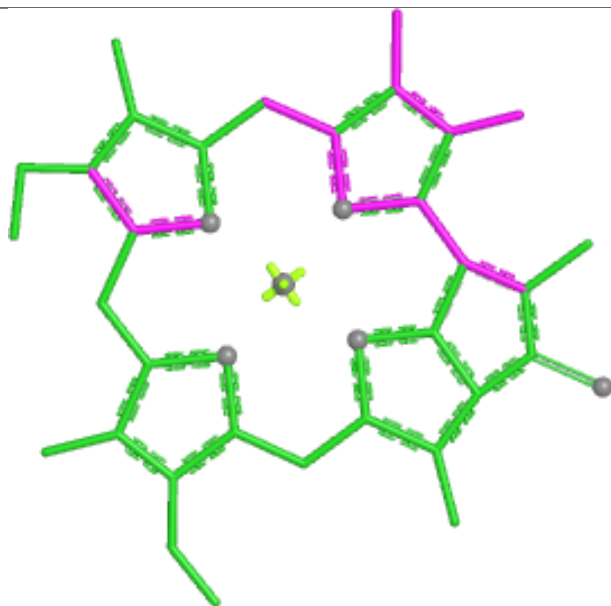




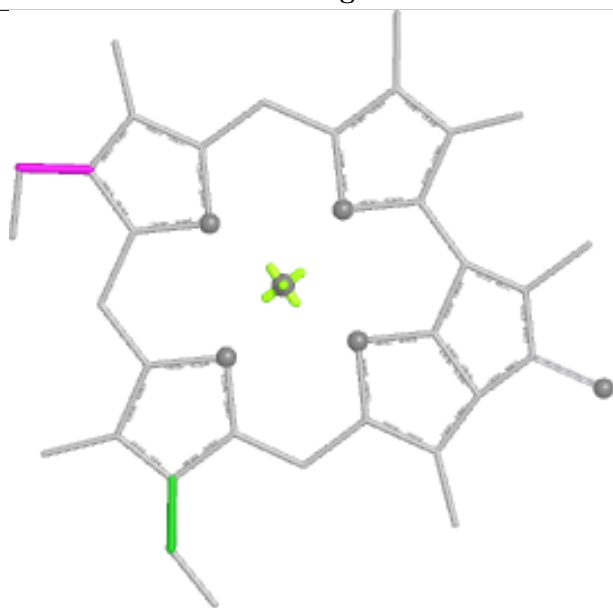
## Ligand CLA 7 313



Bond lengths



Bond angles

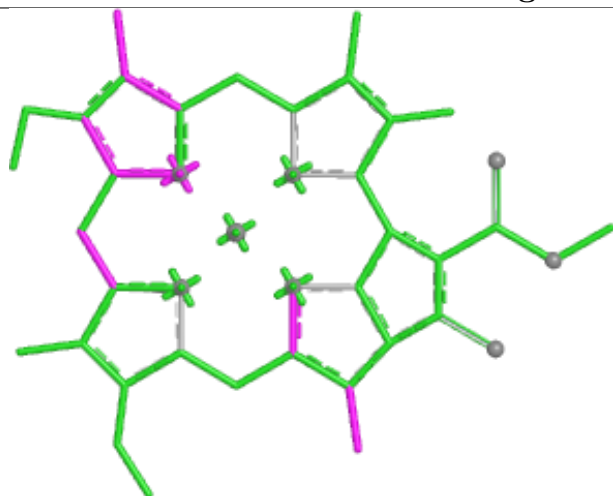


Torsions

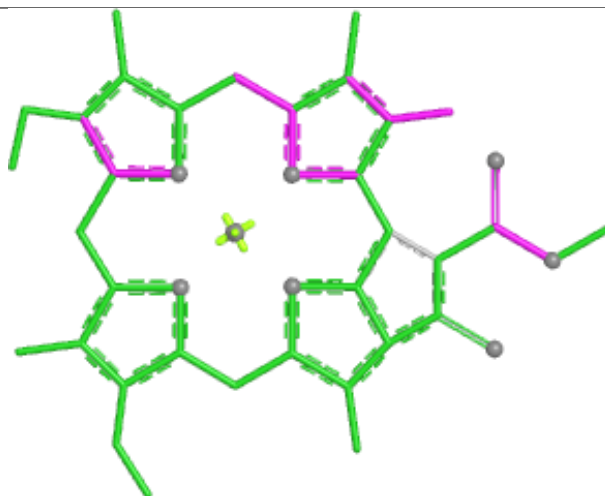


Rings

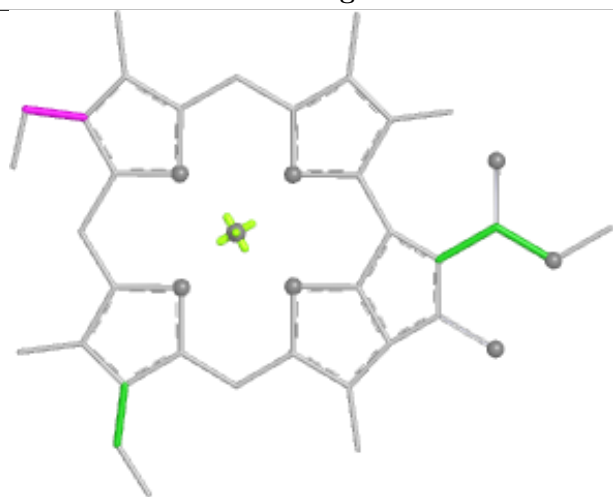
## Ligand CLA 6 205



Bond lengths



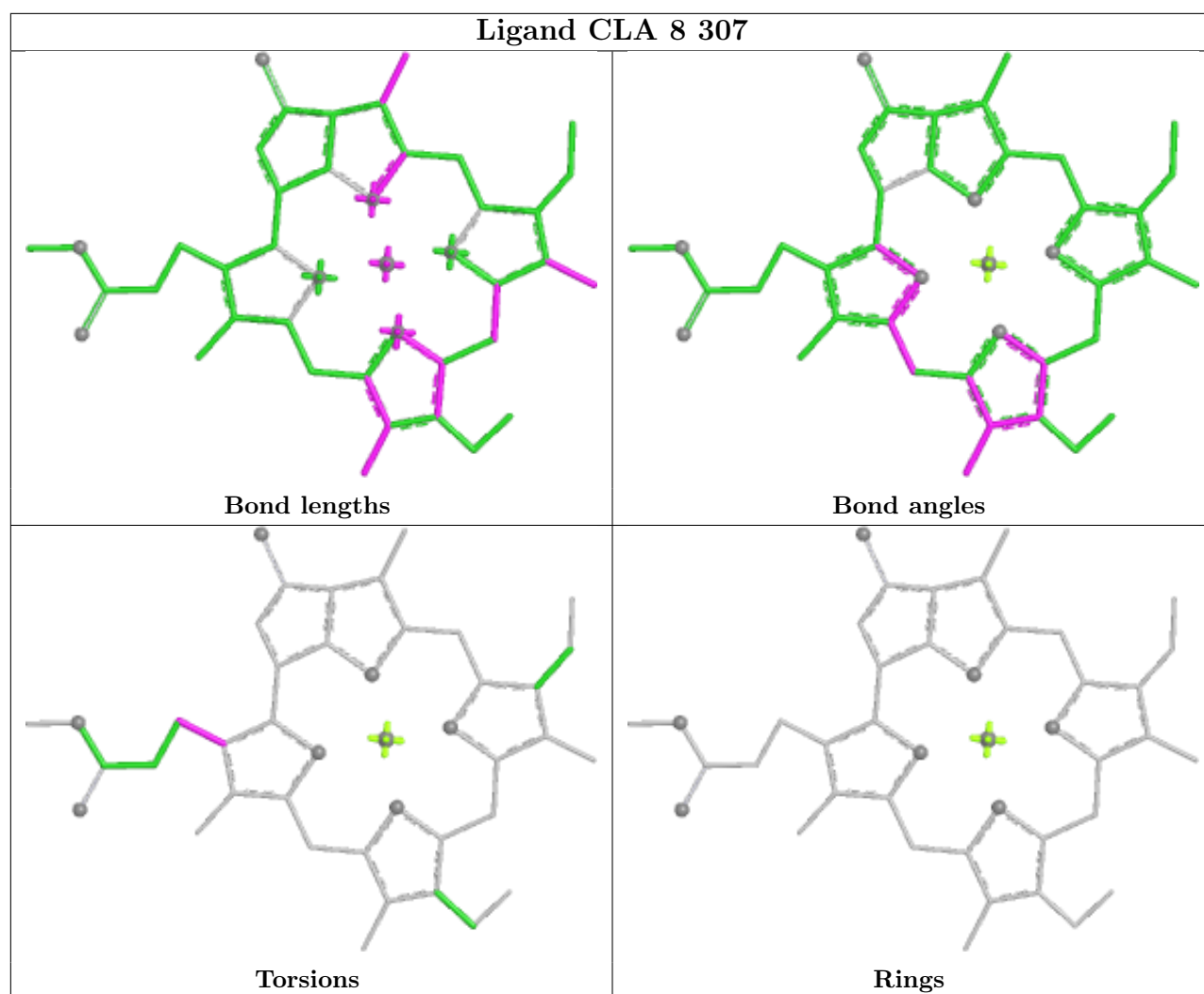
Bond angles



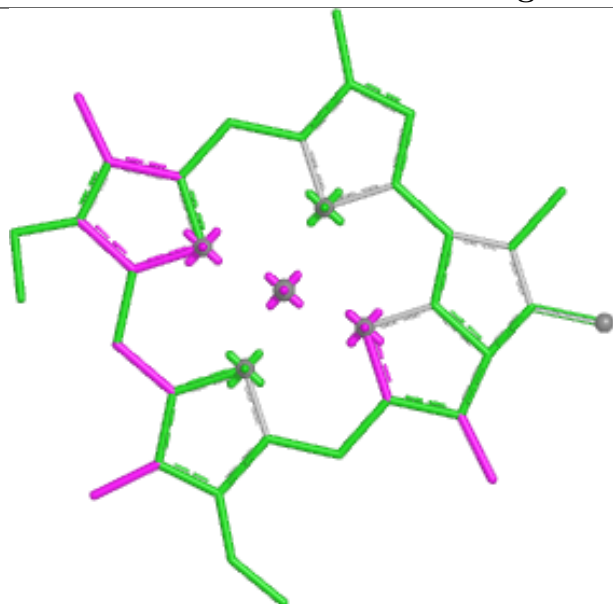
Torsions



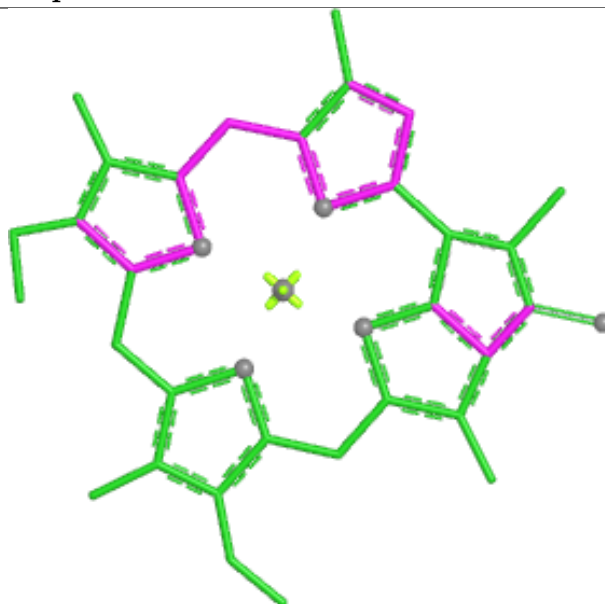
Rings



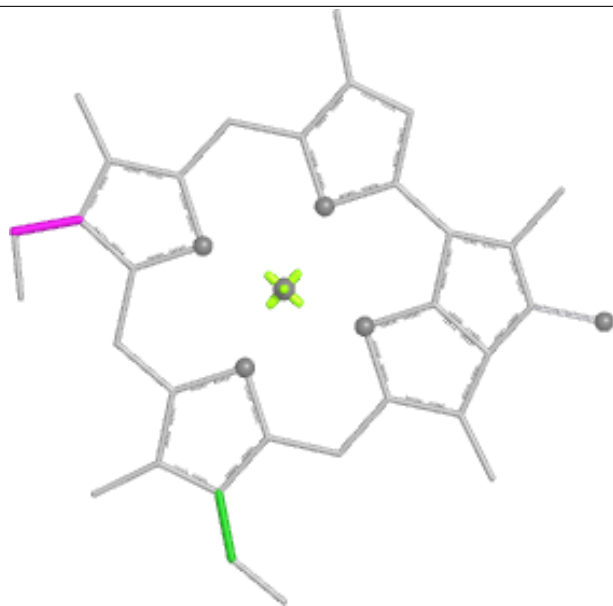
## Ligand CLA p 606



Bond lengths



Bond angles

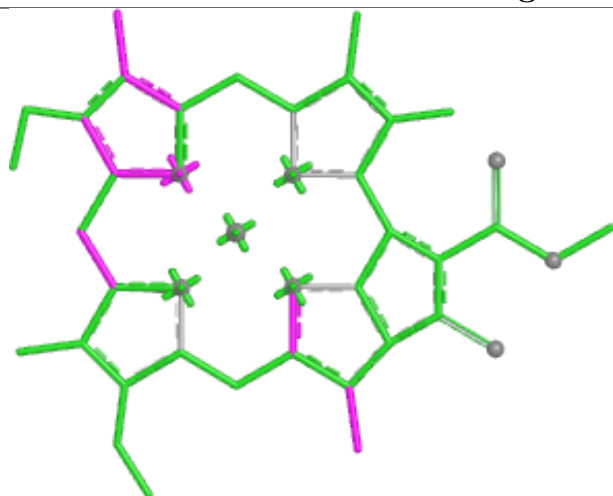


Torsions

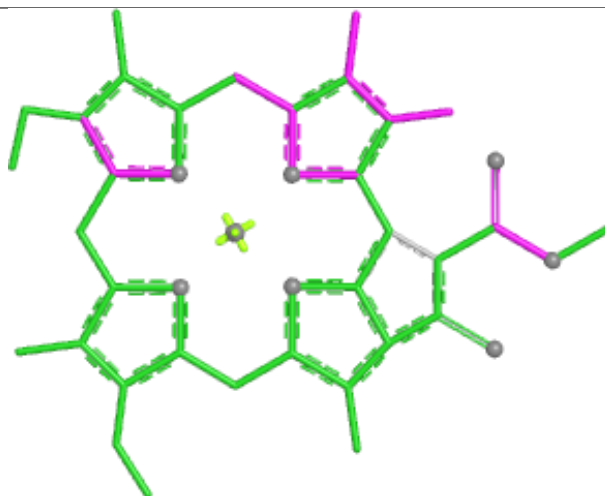


Rings

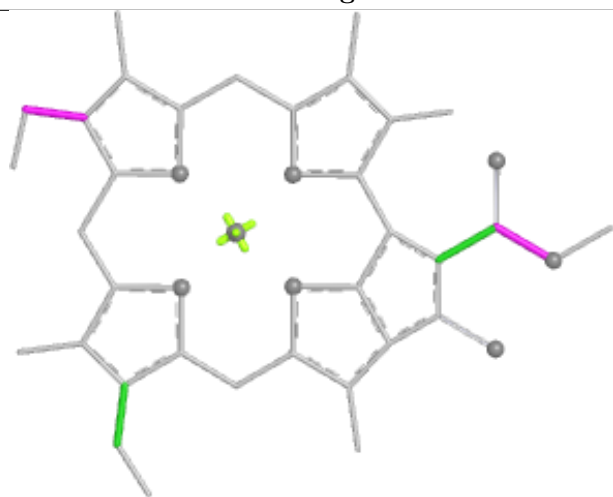
## Ligand CLA 0 304



Bond lengths



Bond angles

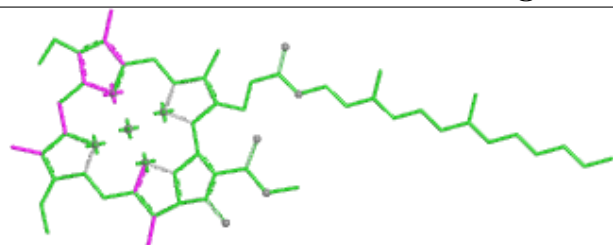


Torsions

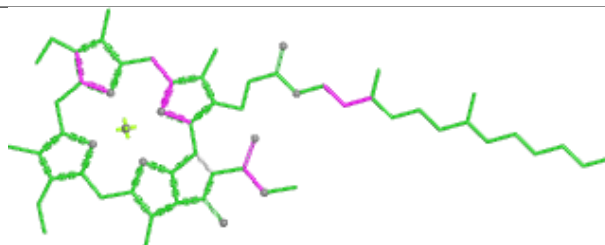


Rings

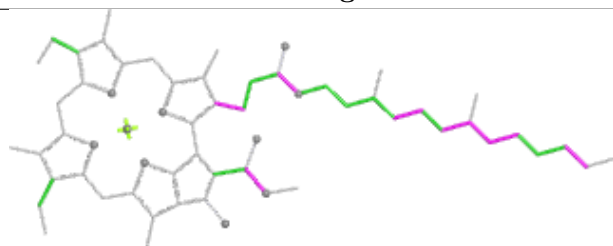
## Ligand CLA b 515



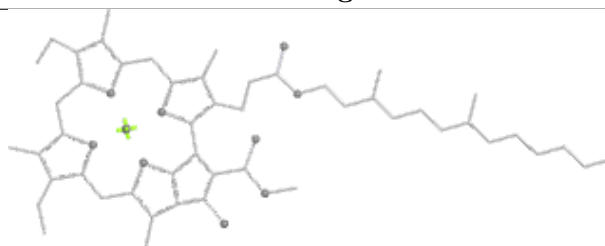
Bond lengths



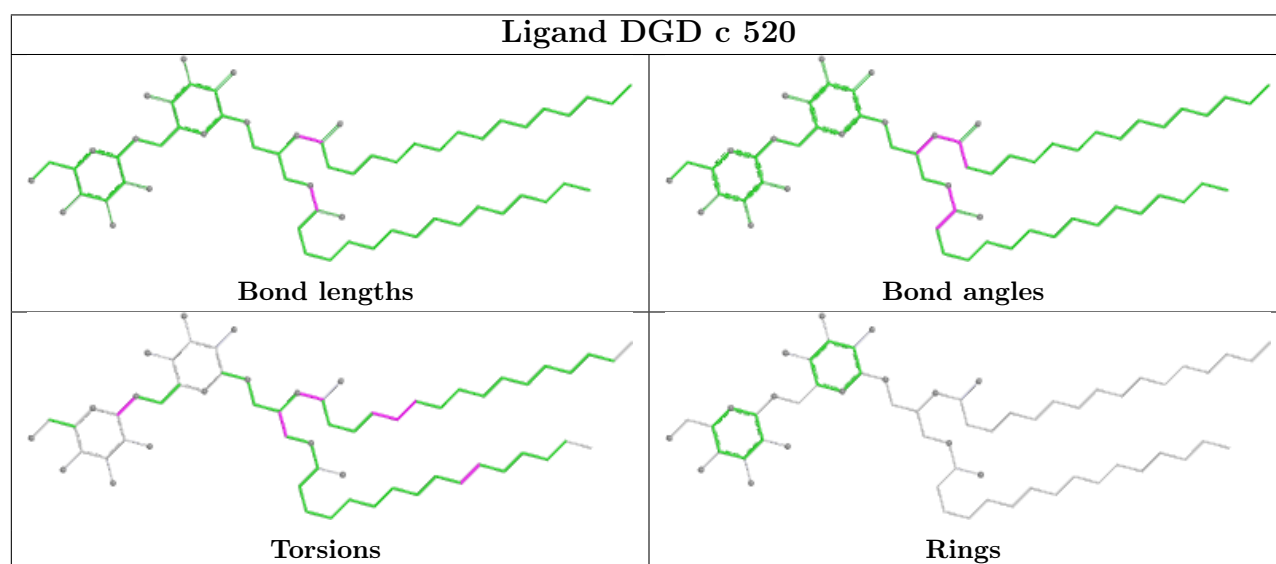
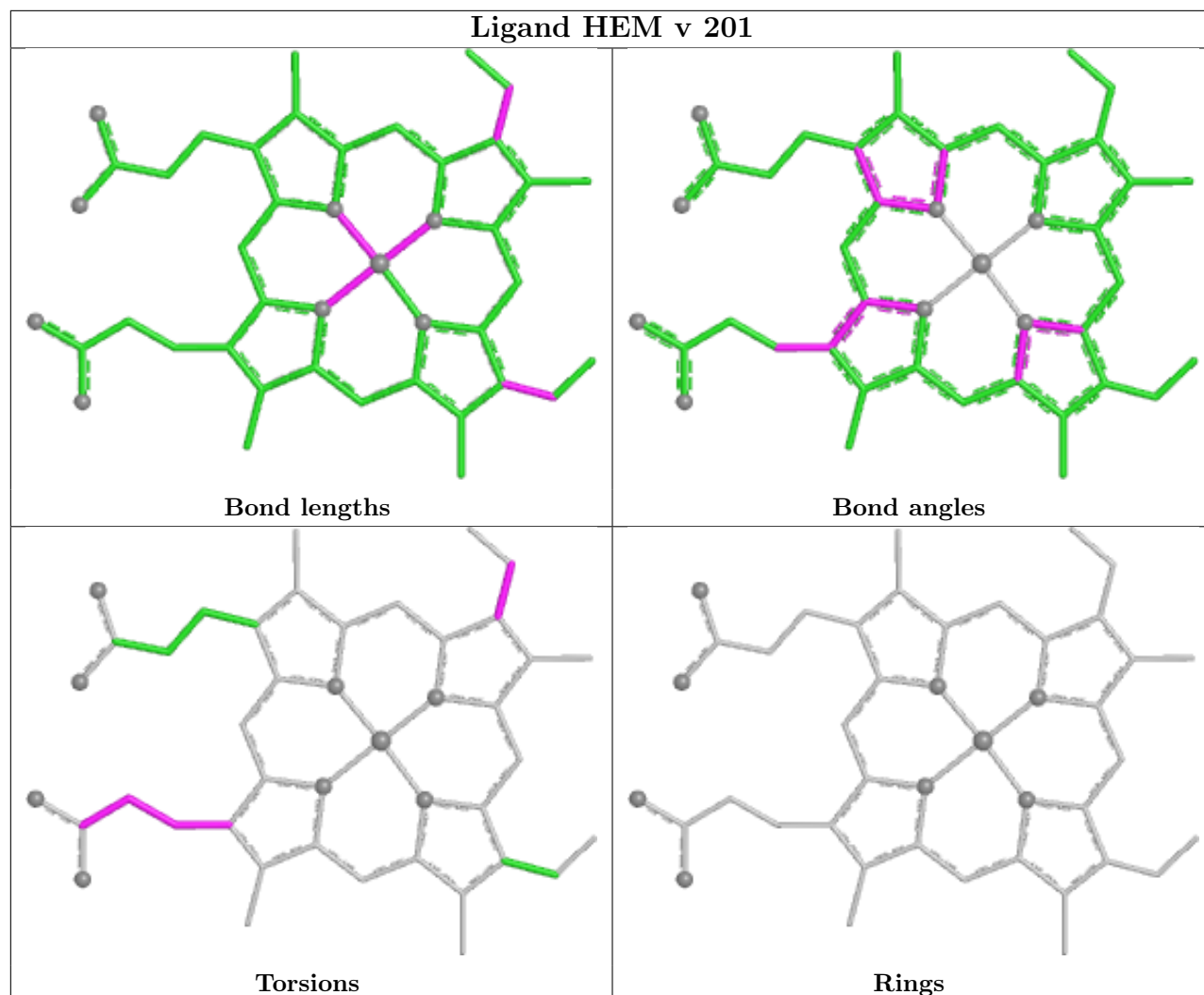
Bond angles



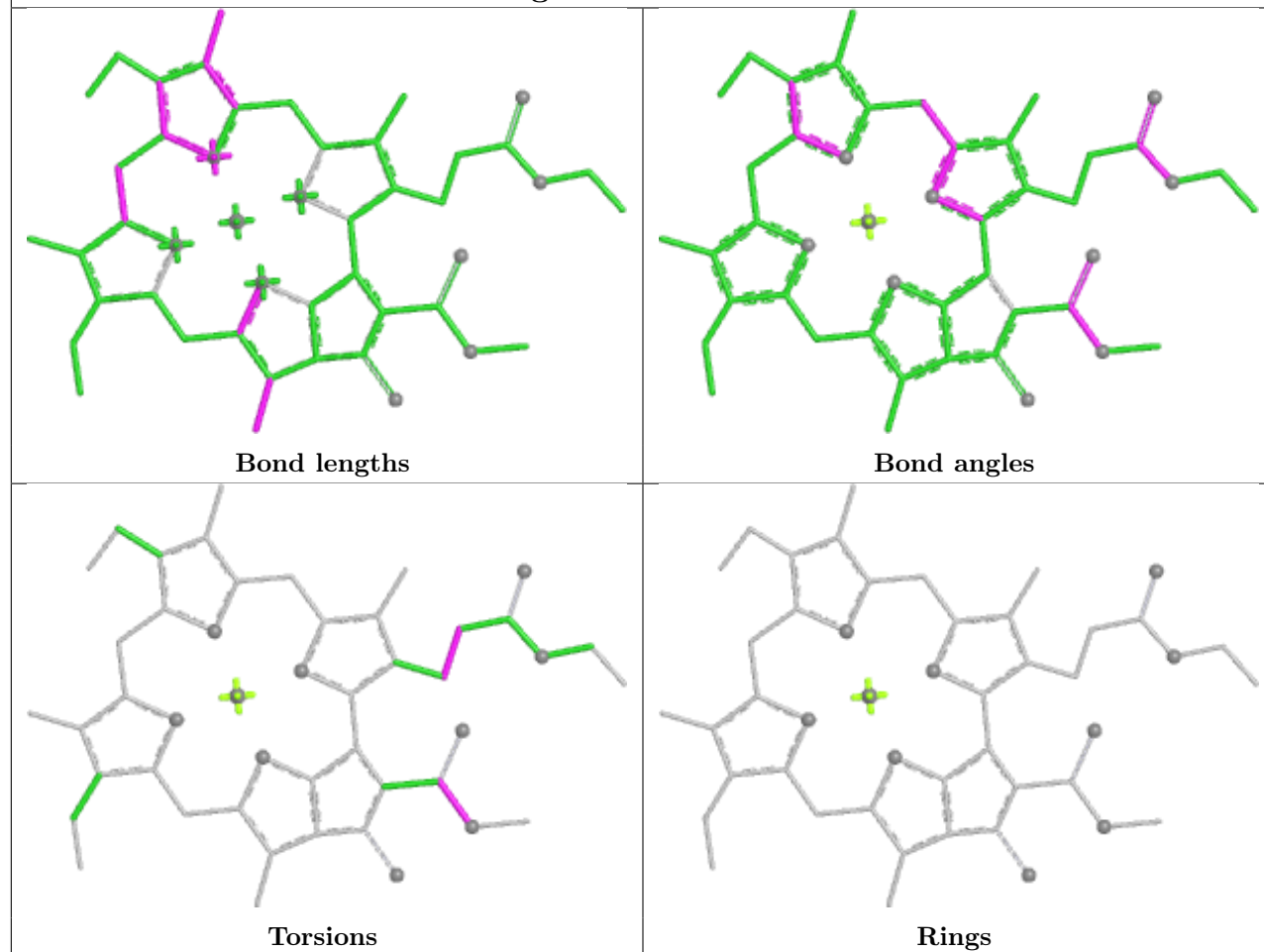
Torsions



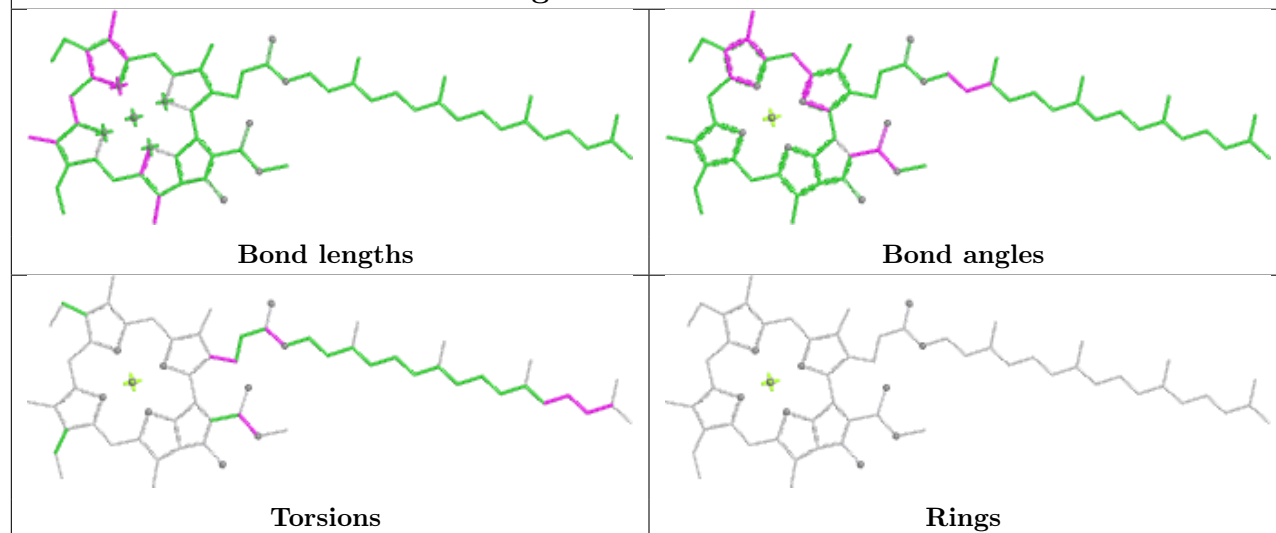
Rings



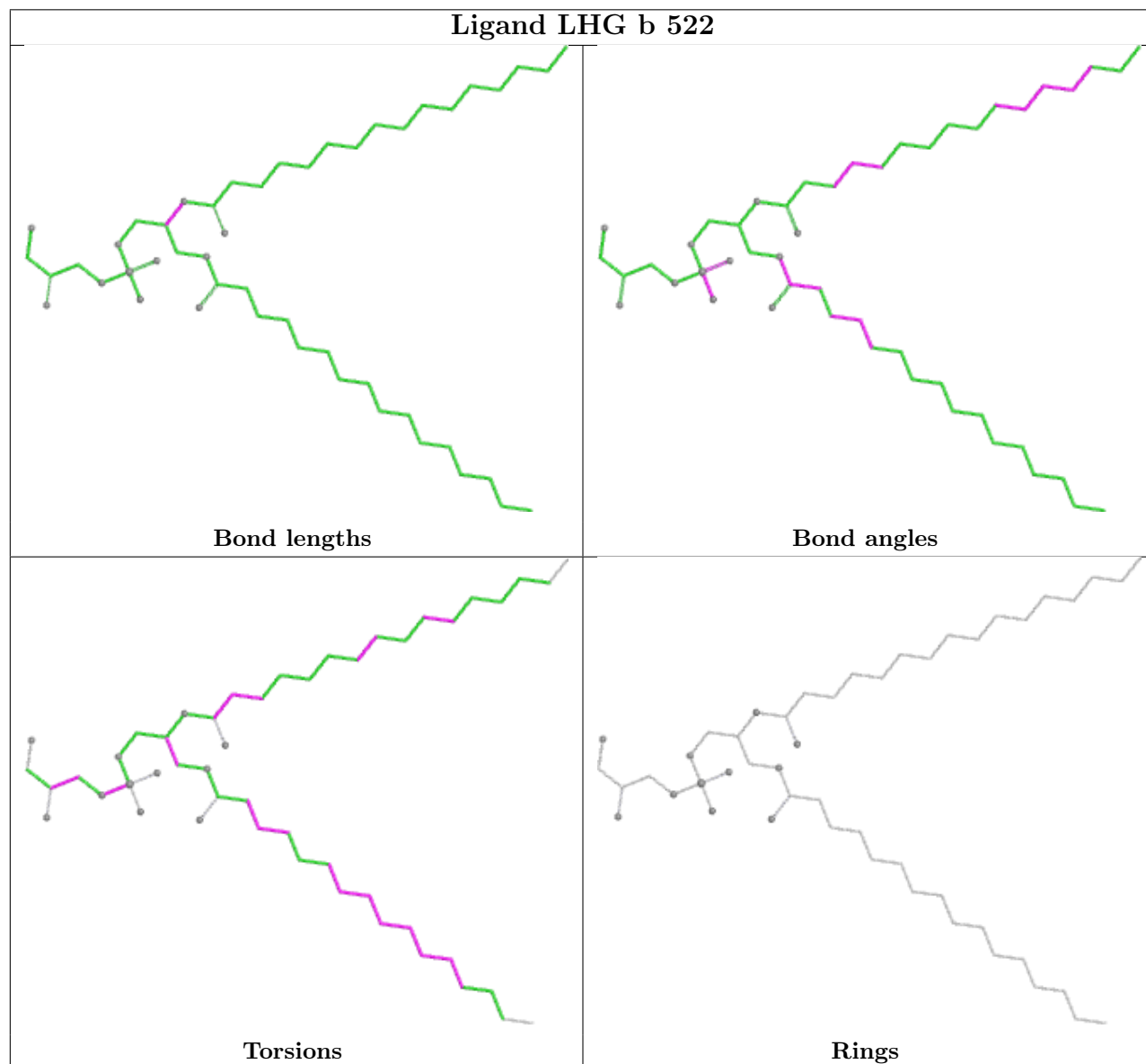
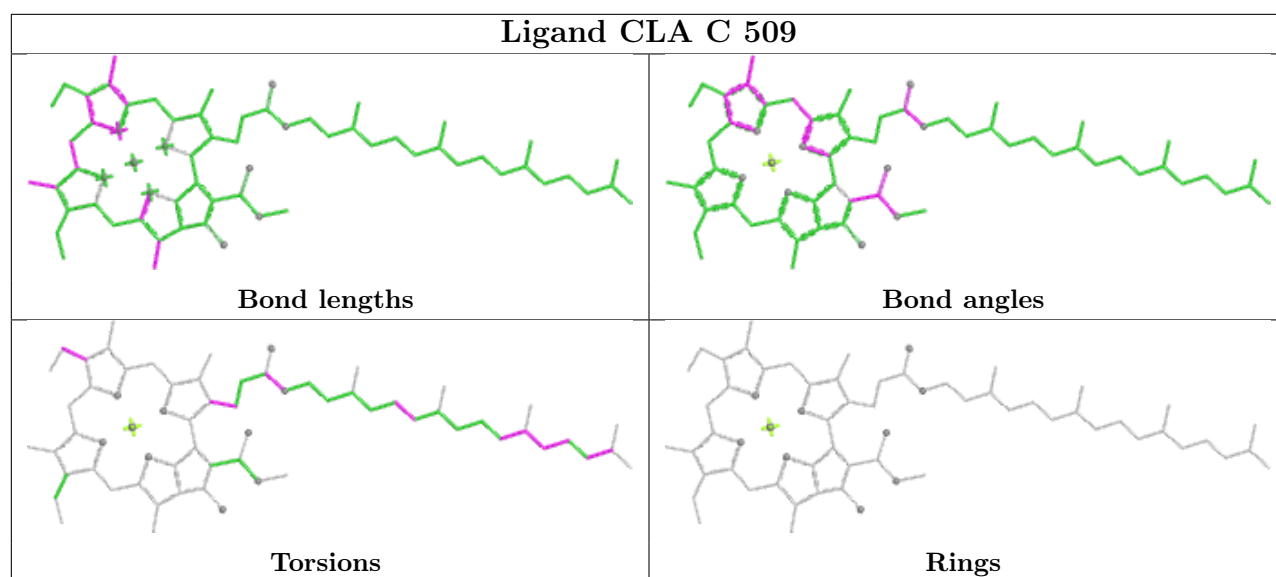
## Ligand CLA 2 307



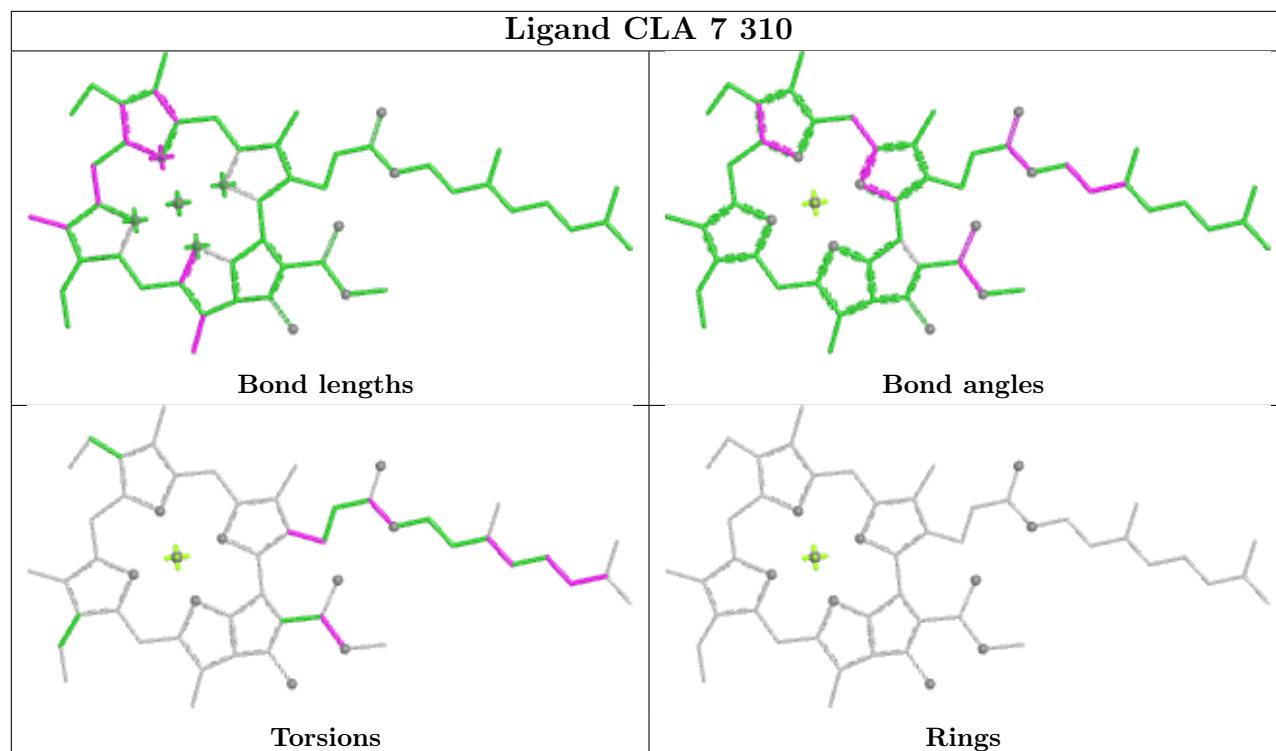
## Ligand CLA A 403



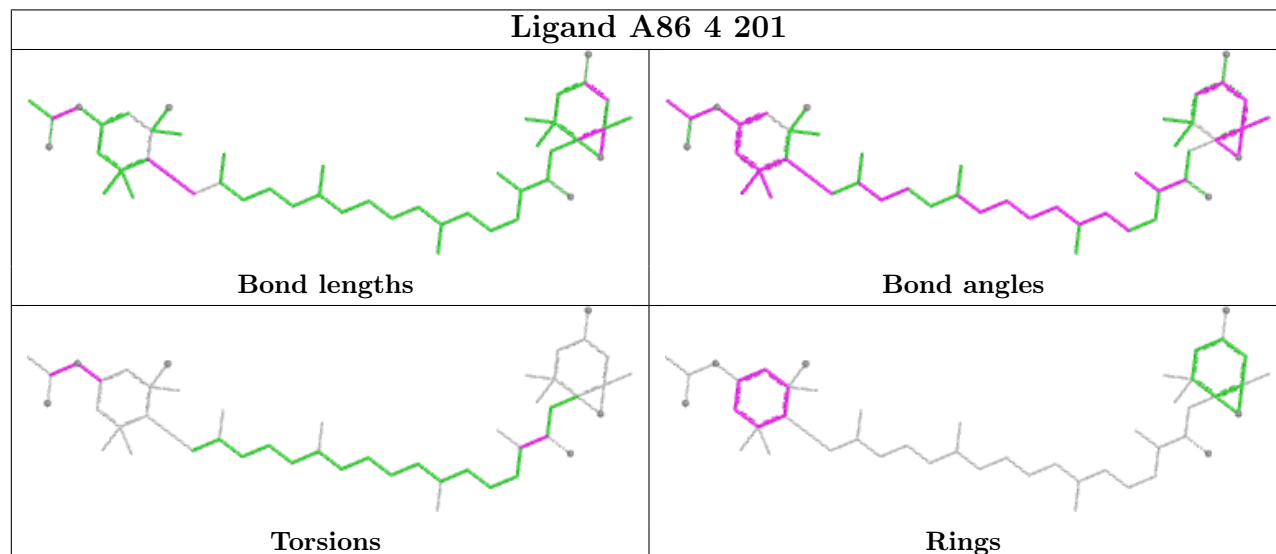




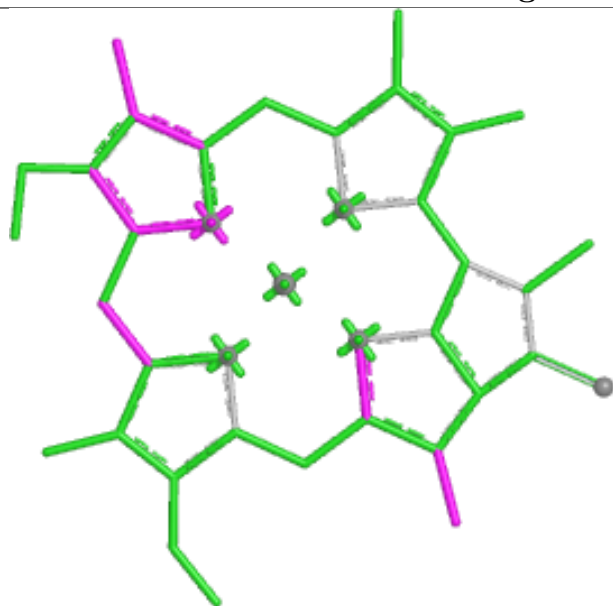
## Ligand CLA 7 310



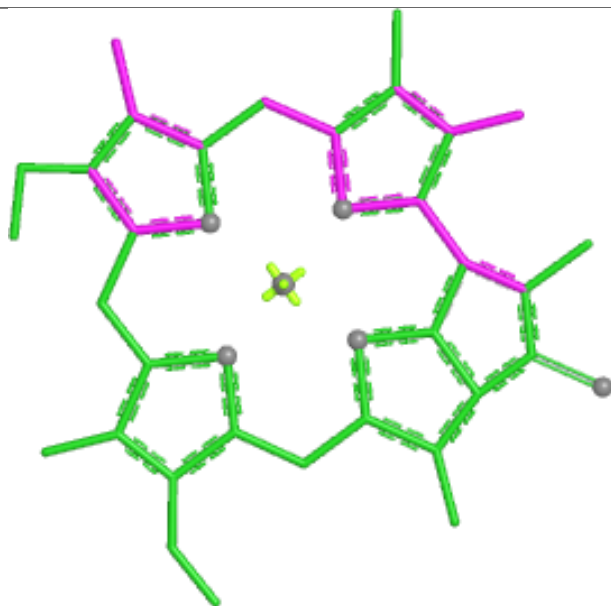
## Ligand A86 4 201



## Ligand CLA 2 314



Bond lengths



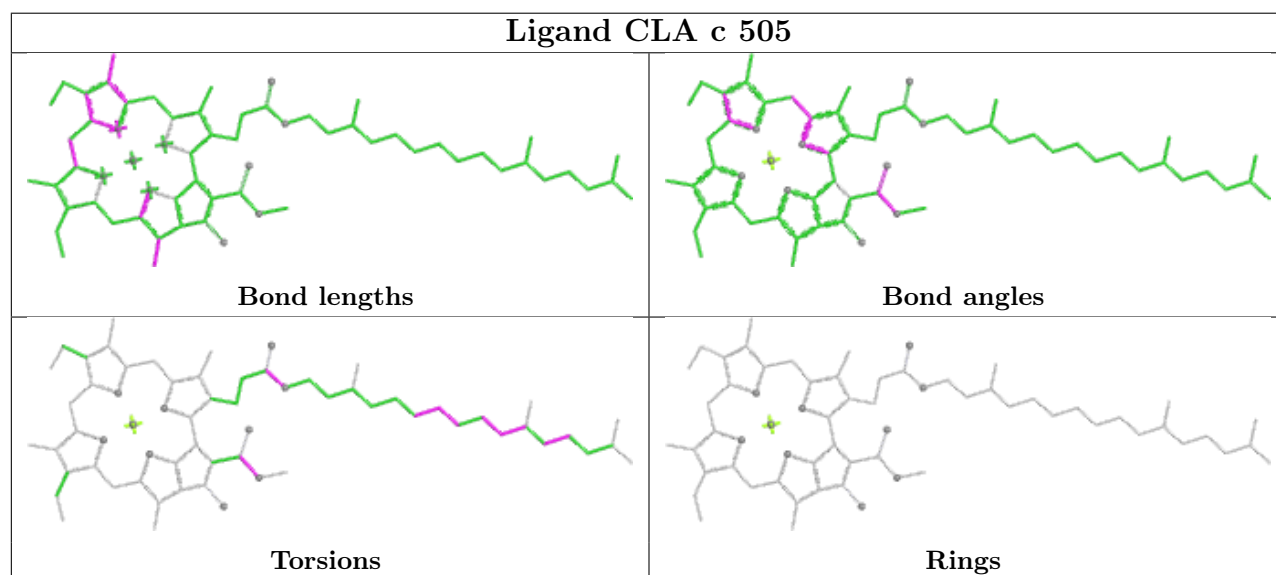
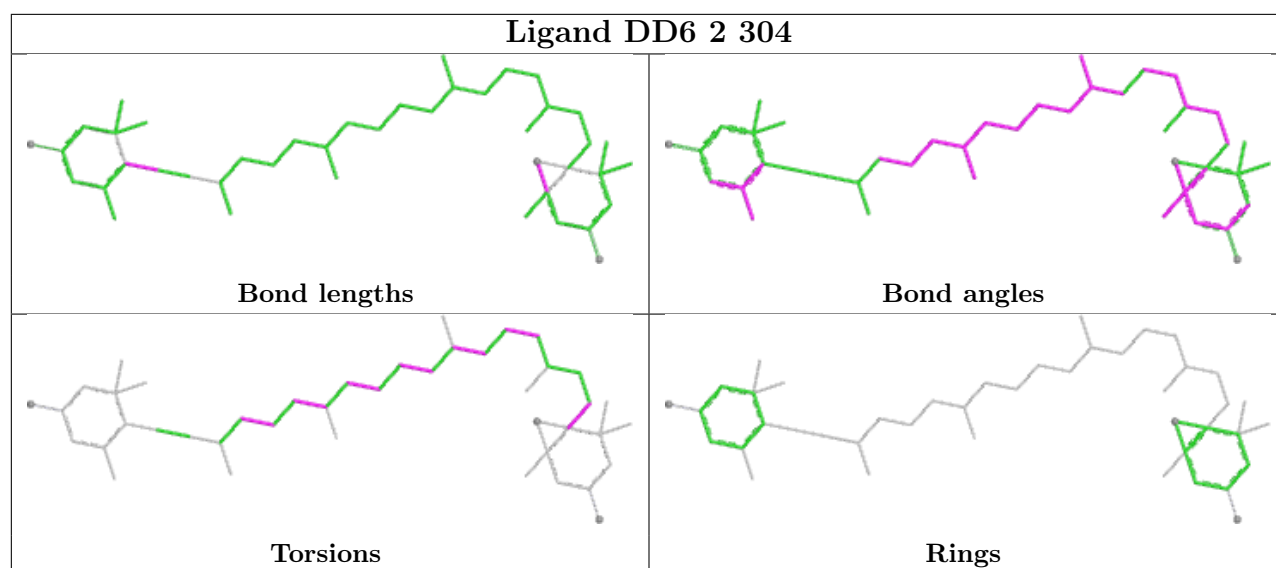
Bond angles



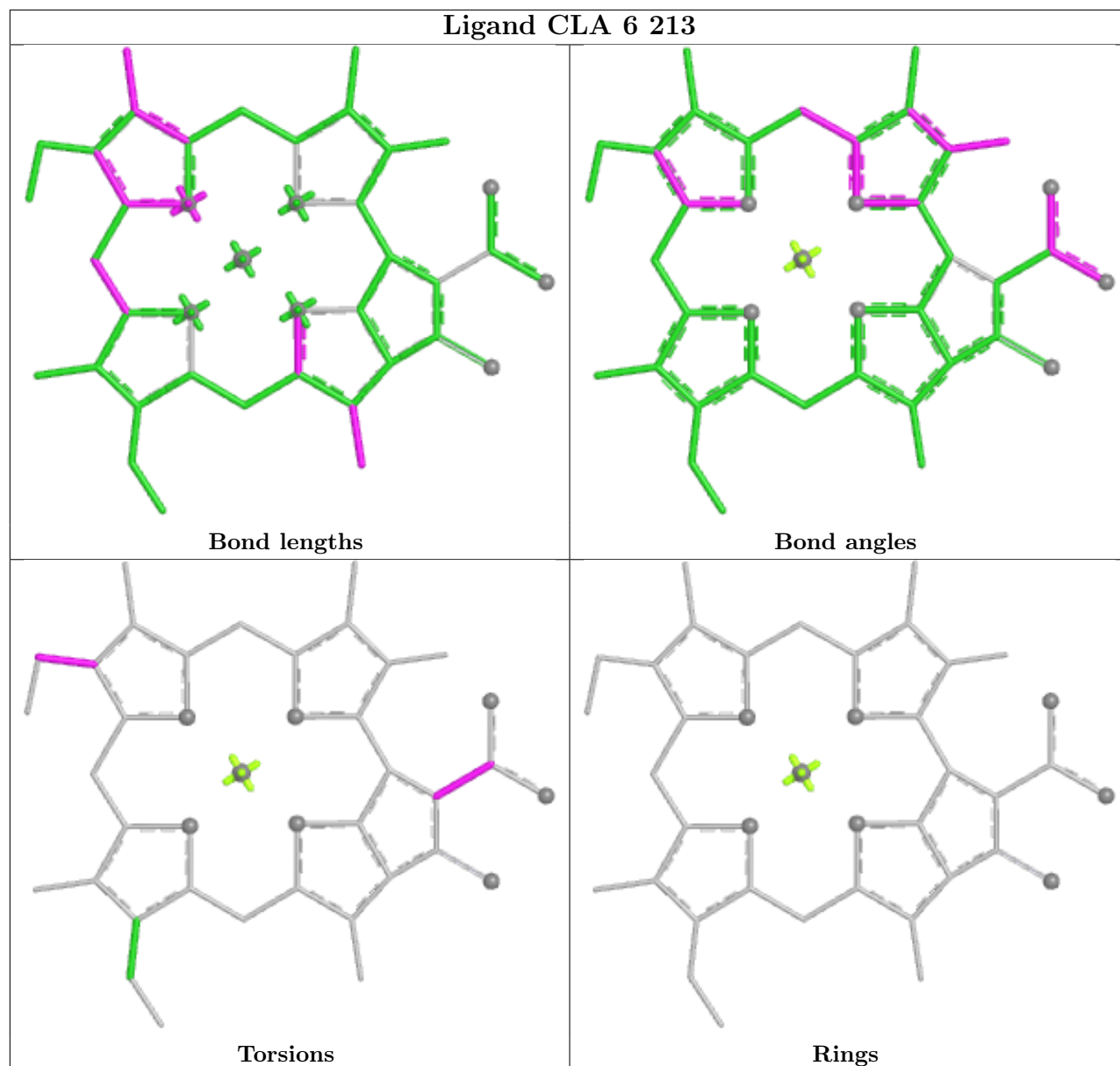
Torsions



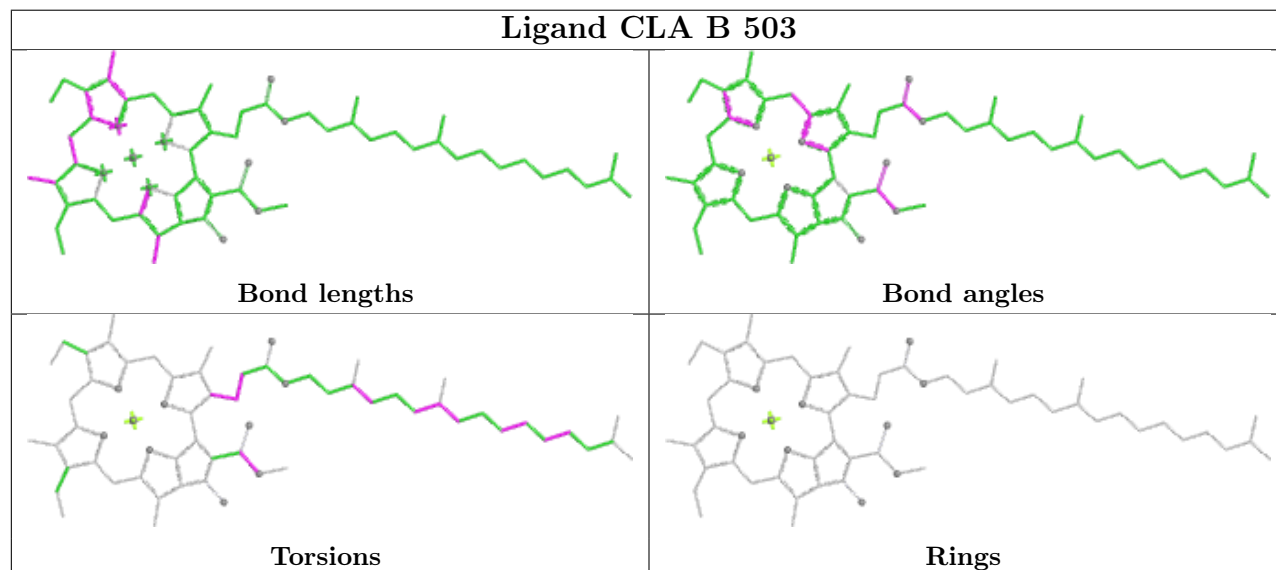
Rings



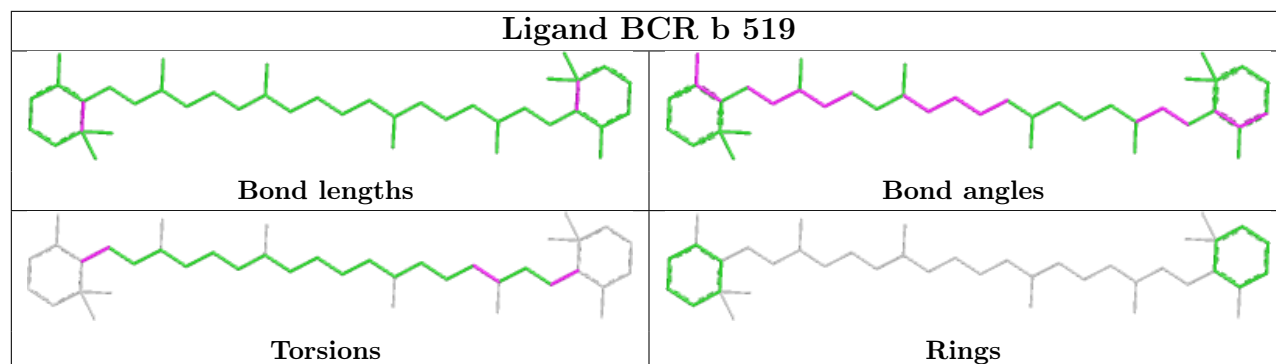
## Ligand CLA 6 213



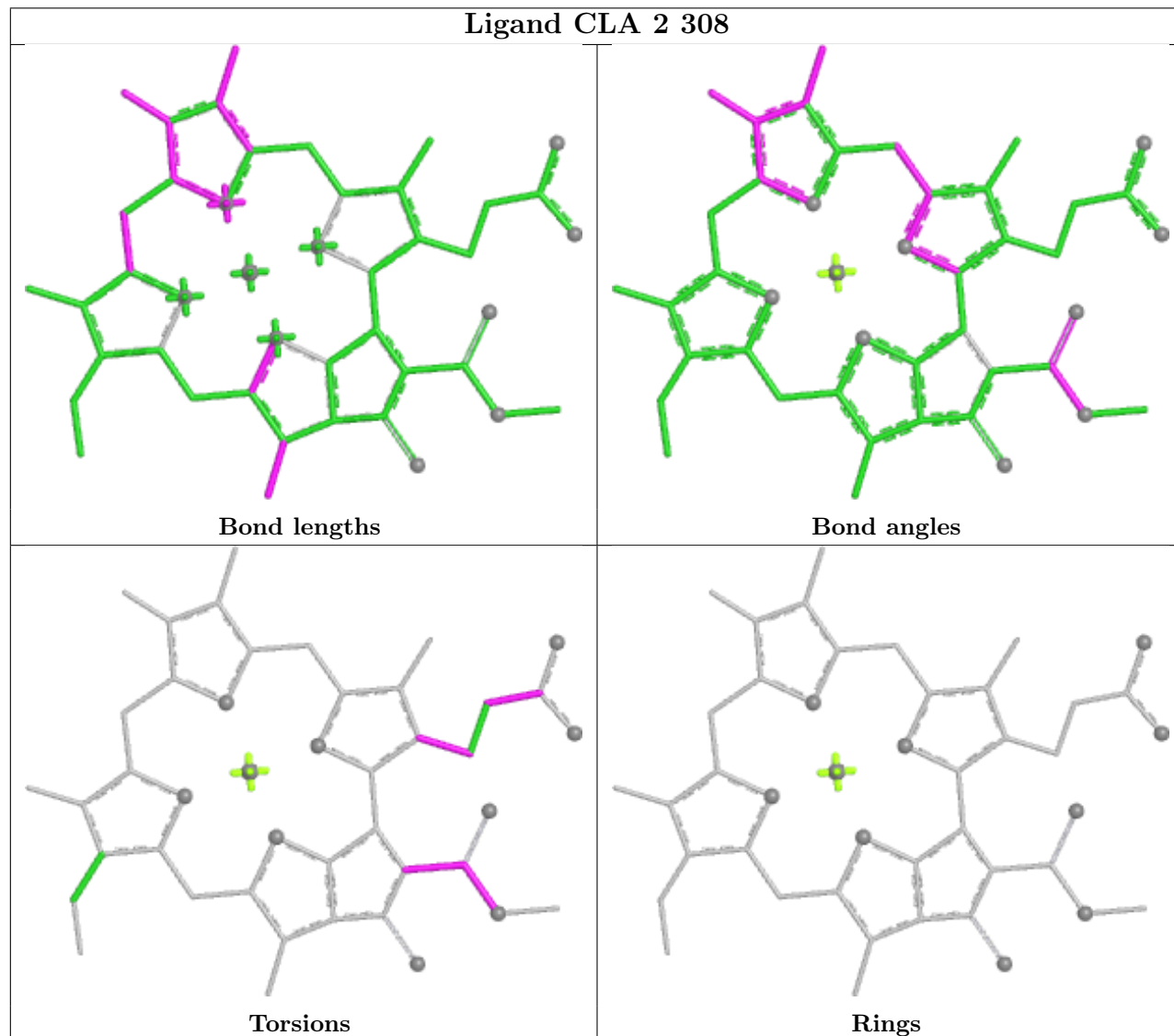
## Ligand CLA B 503



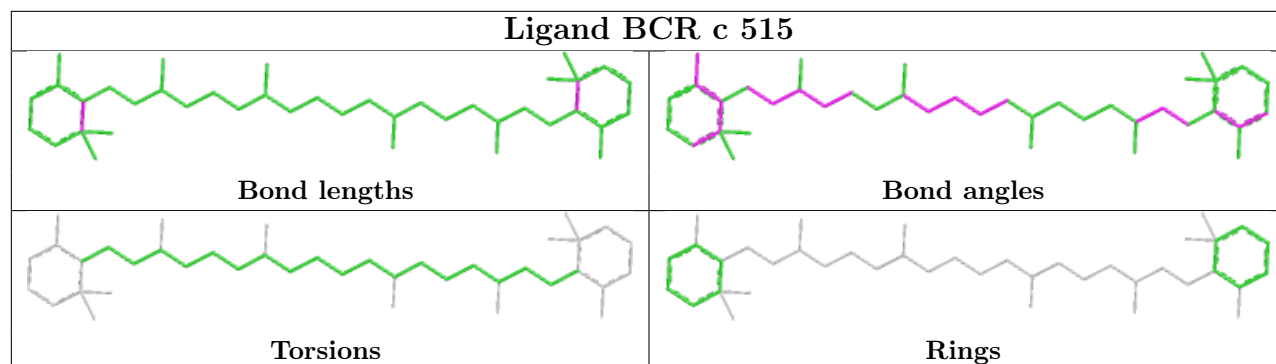
## Ligand BCR b 519



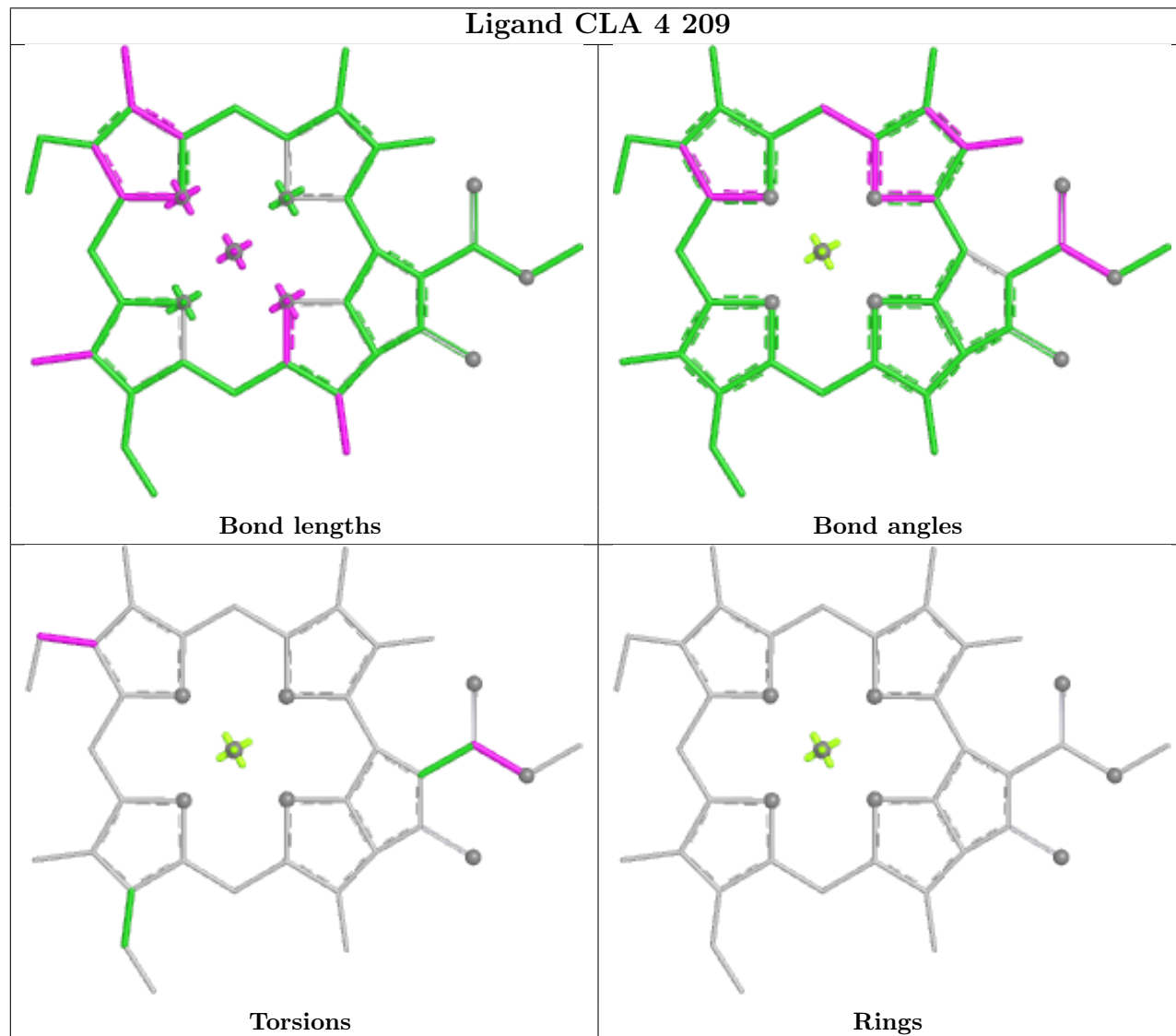
## Ligand CLA 2 308

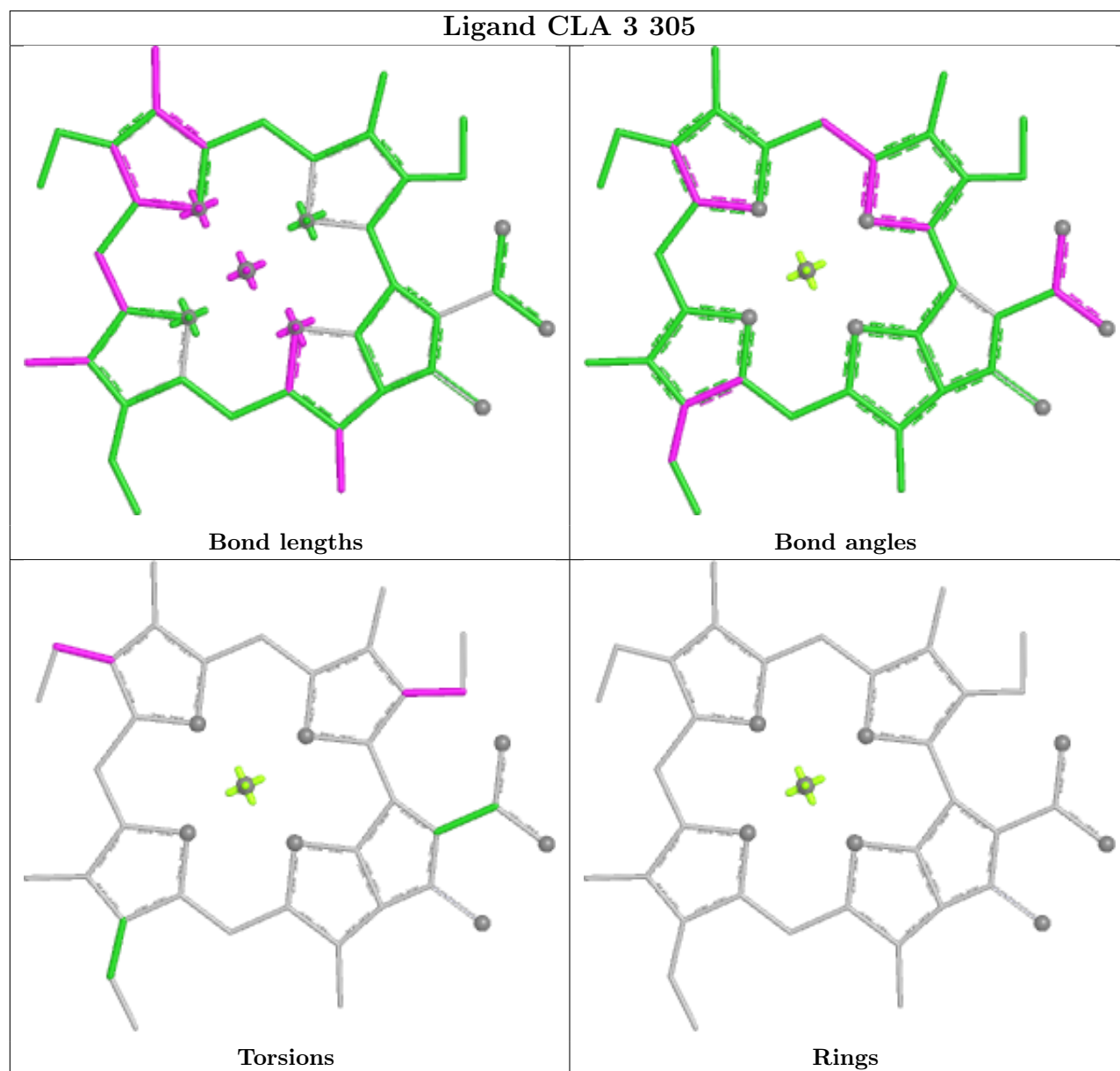
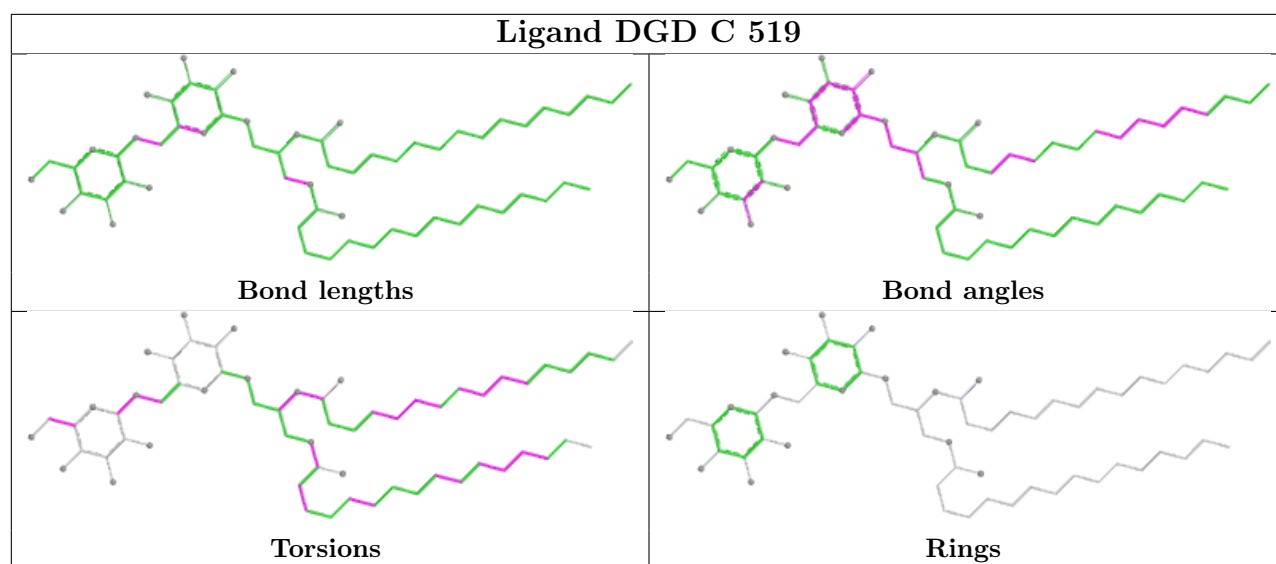


## Ligand BCR c 515



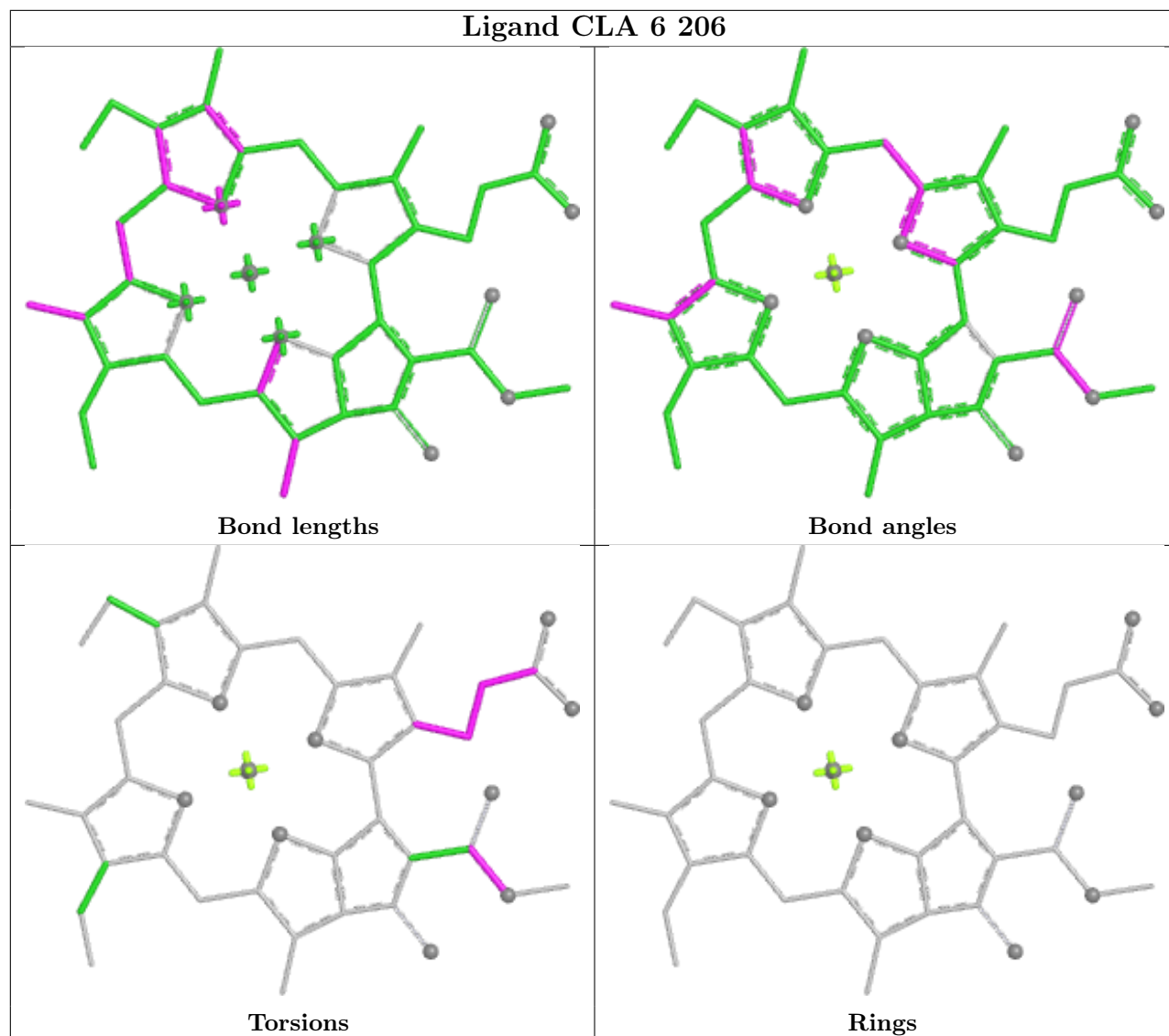
## Ligand CLA 4 209



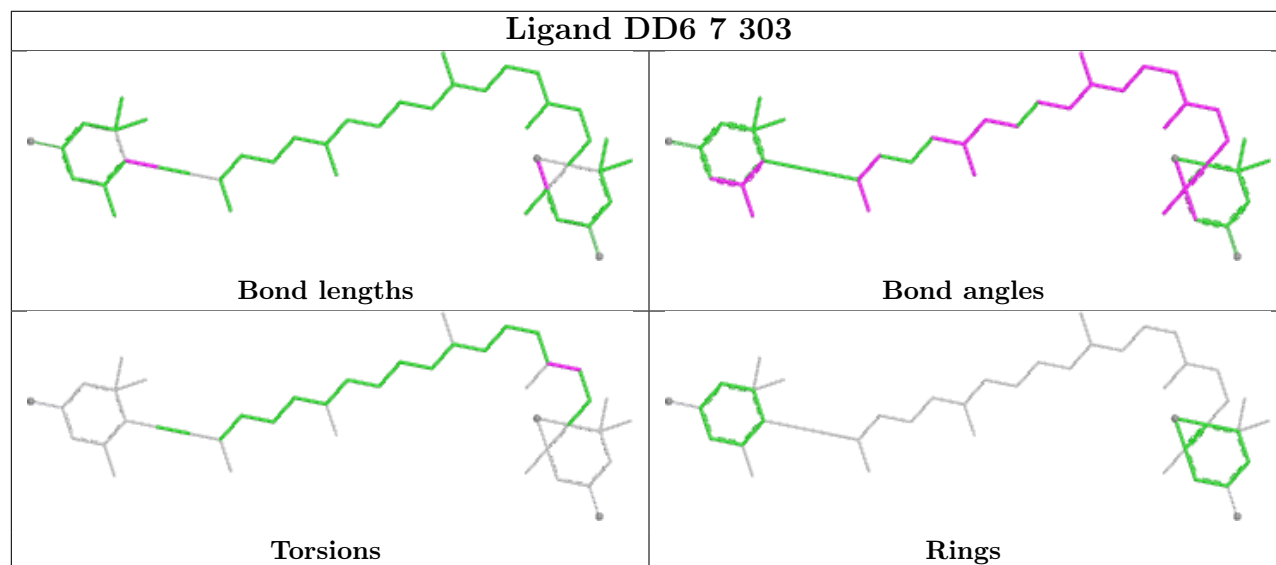


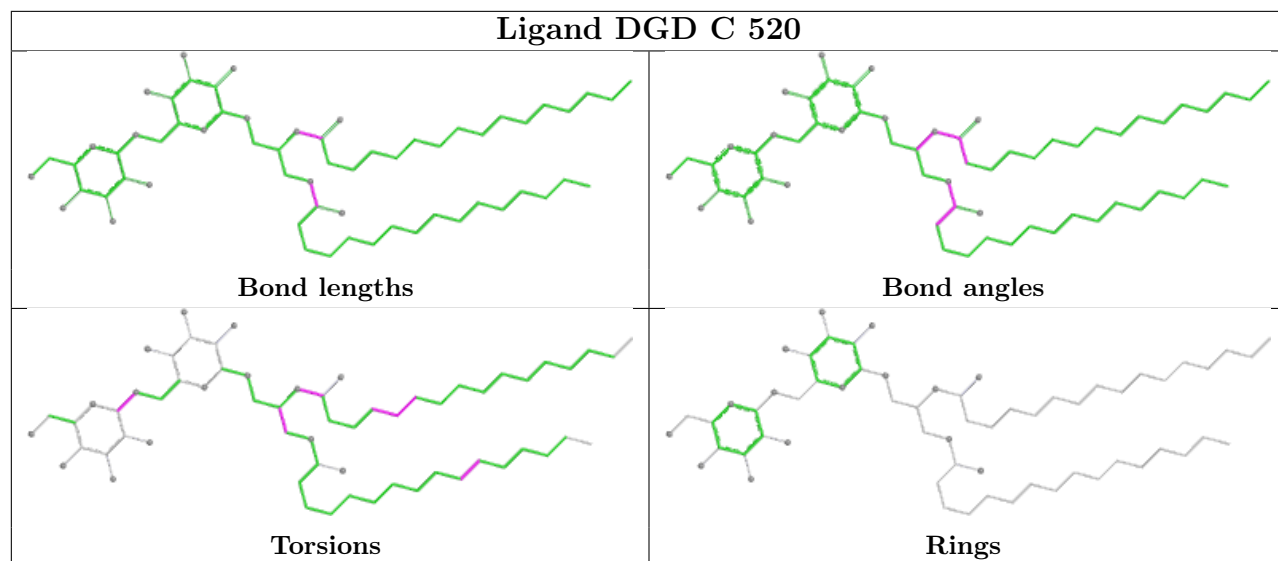


## Ligand CLA 6 206

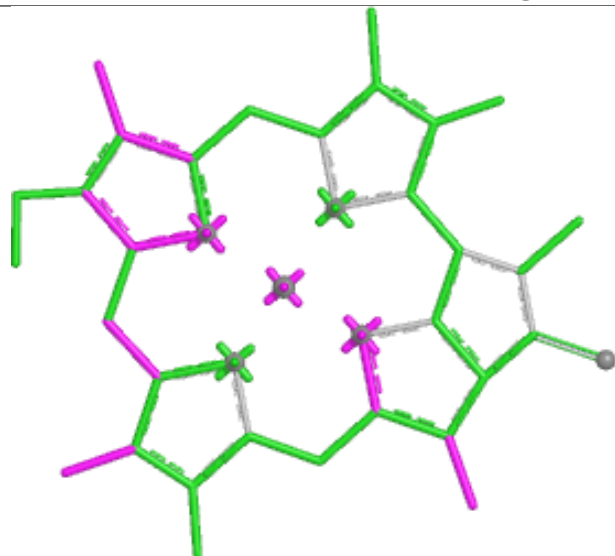


## Ligand DD6 7 303

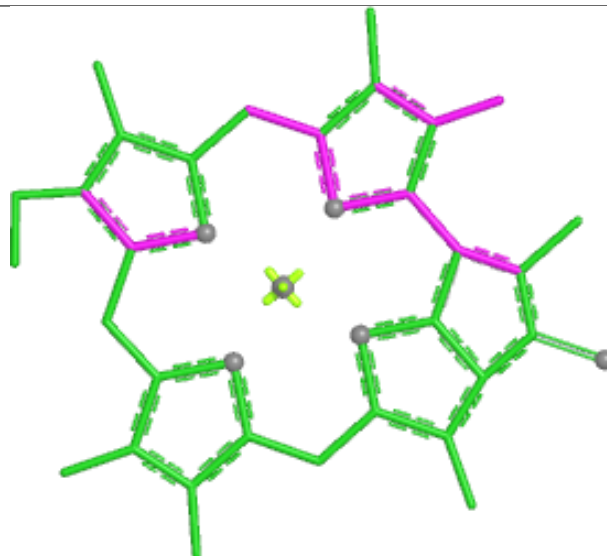




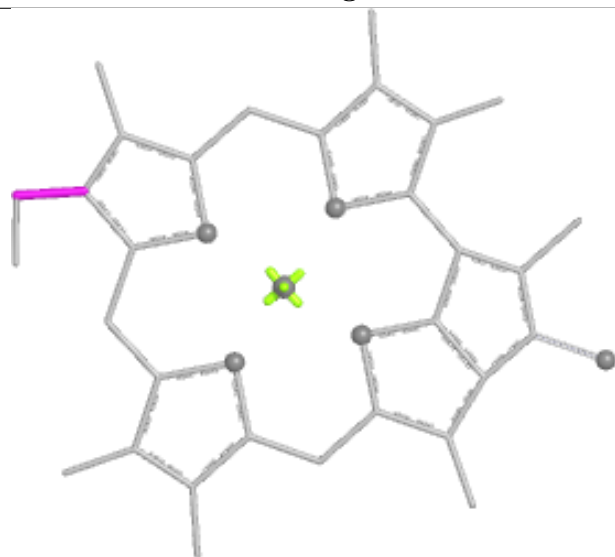
## Ligand CLA P 605



Bond lengths



Bond angles

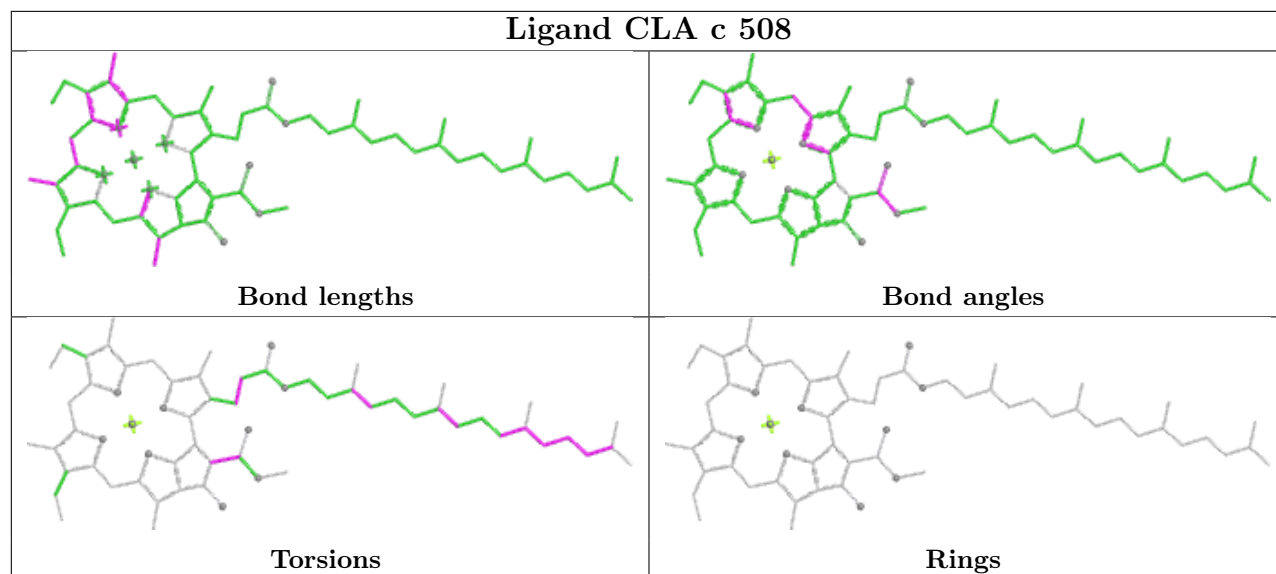


Torsions

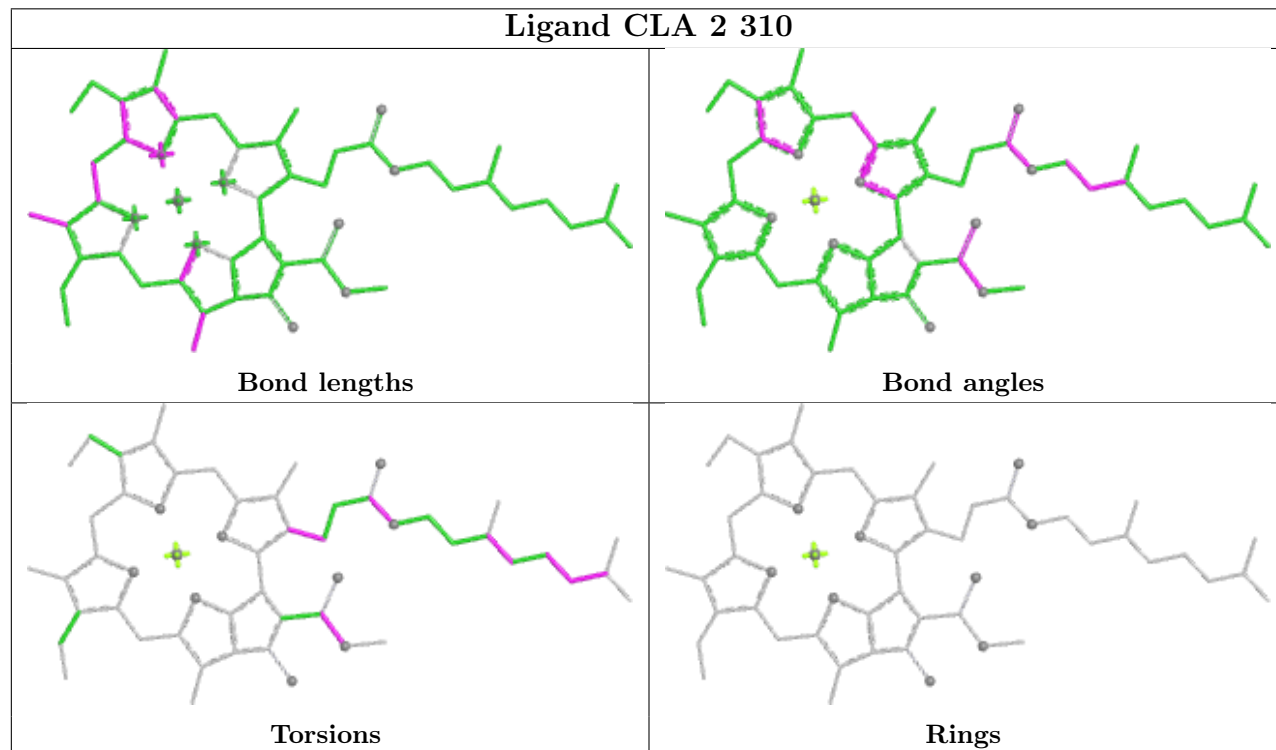


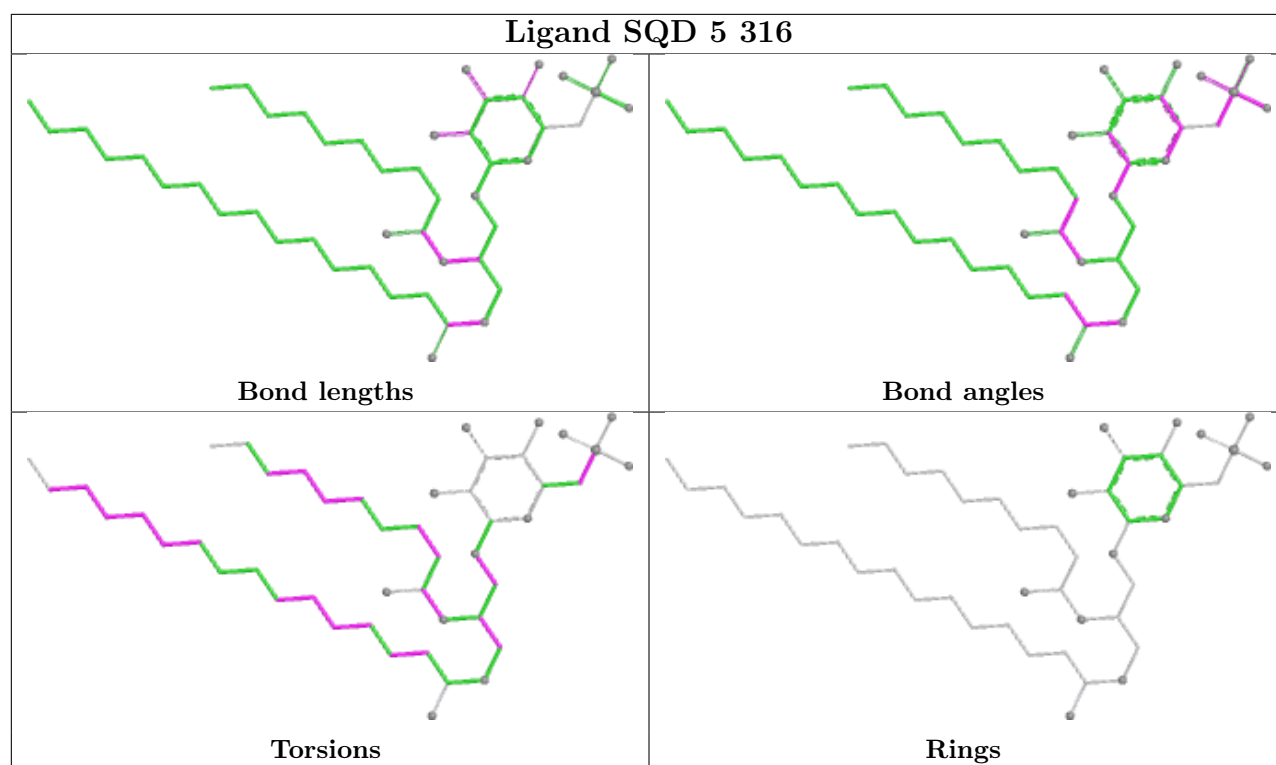
Rings

## Ligand CLA c 508

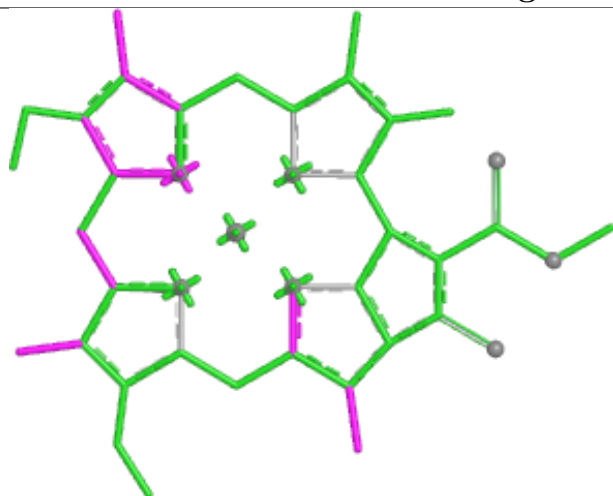


## Ligand CLA 2 310

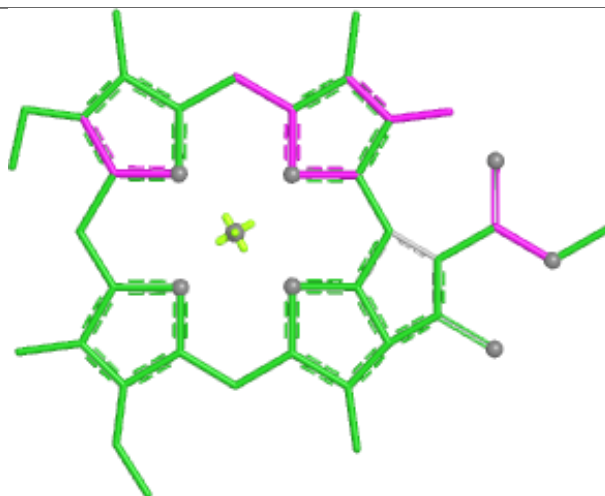




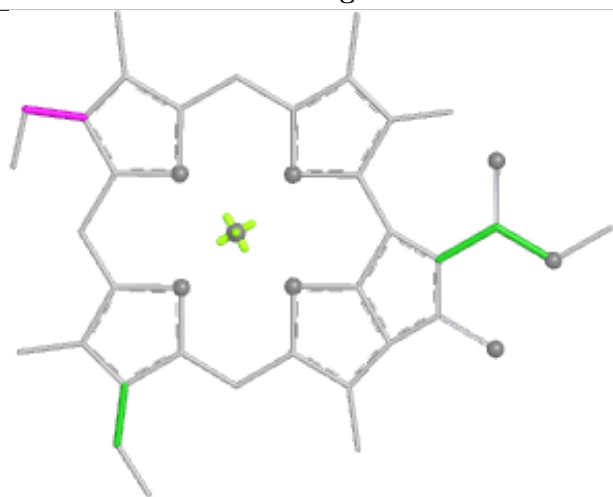
## Ligand CLA 1 205



Bond lengths



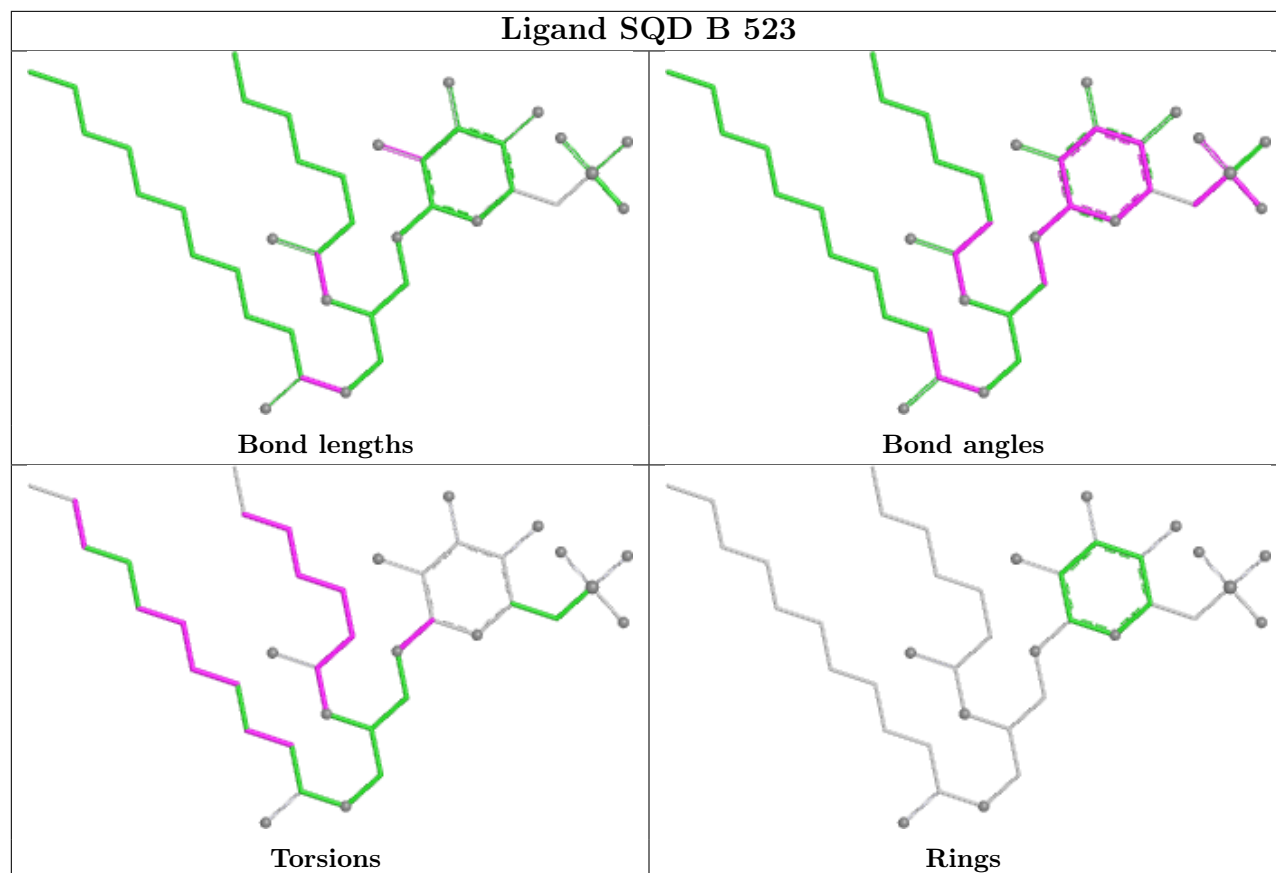
Bond angles



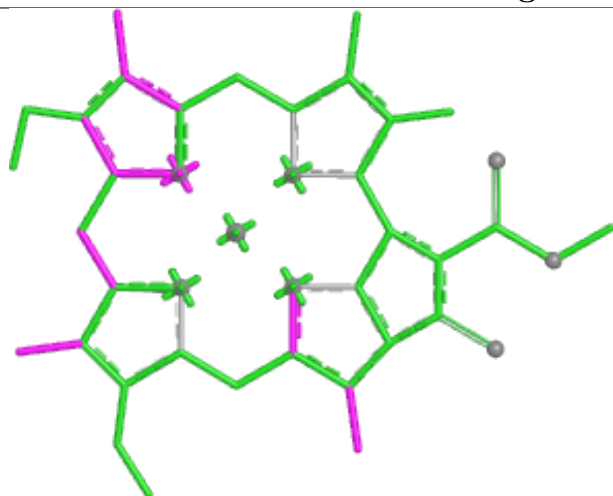
Torsions



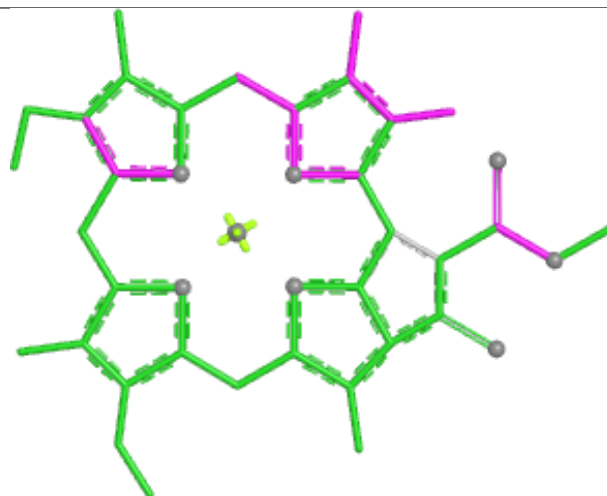
Rings



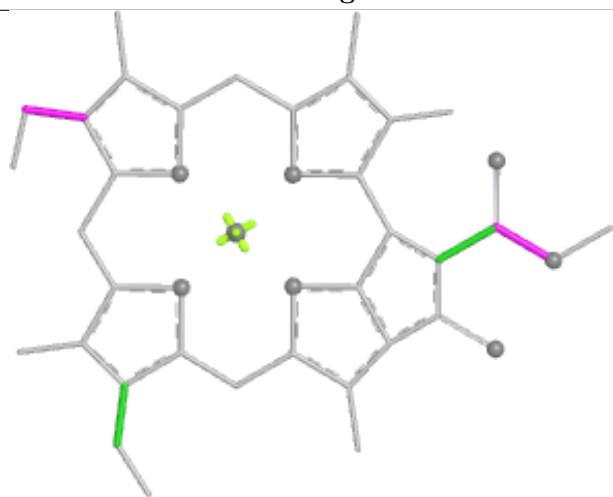
## Ligand CLA 0 309



Bond lengths



Bond angles

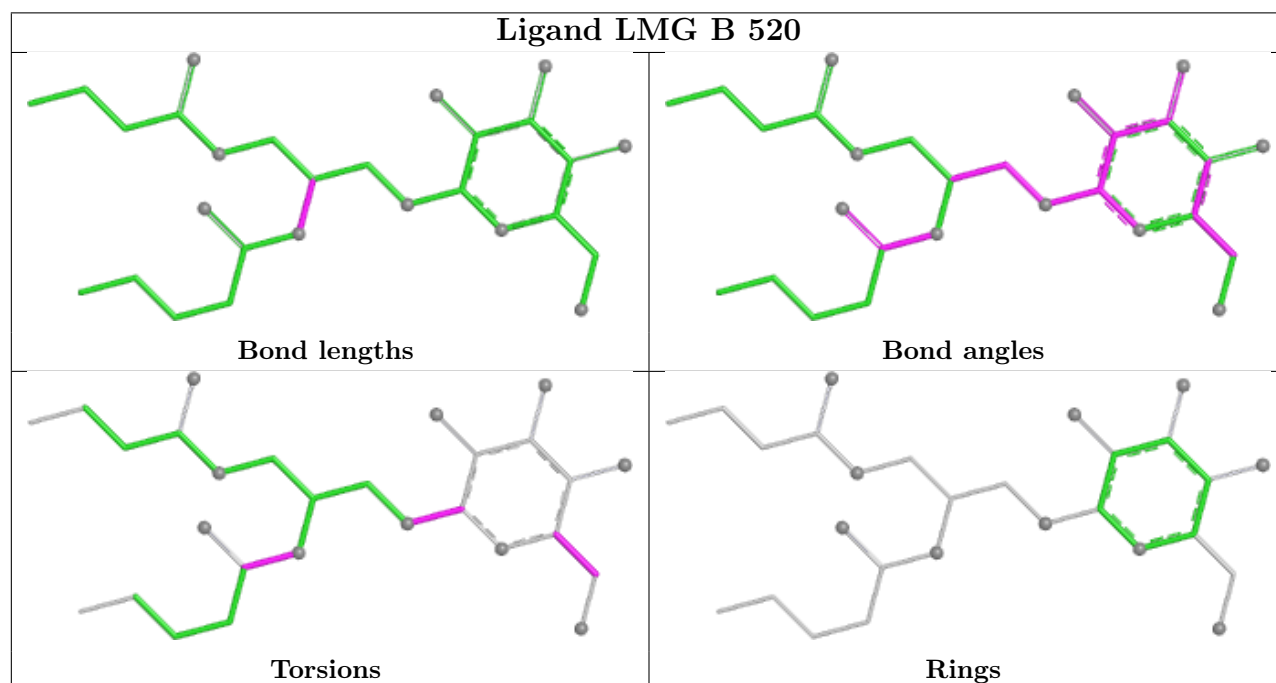
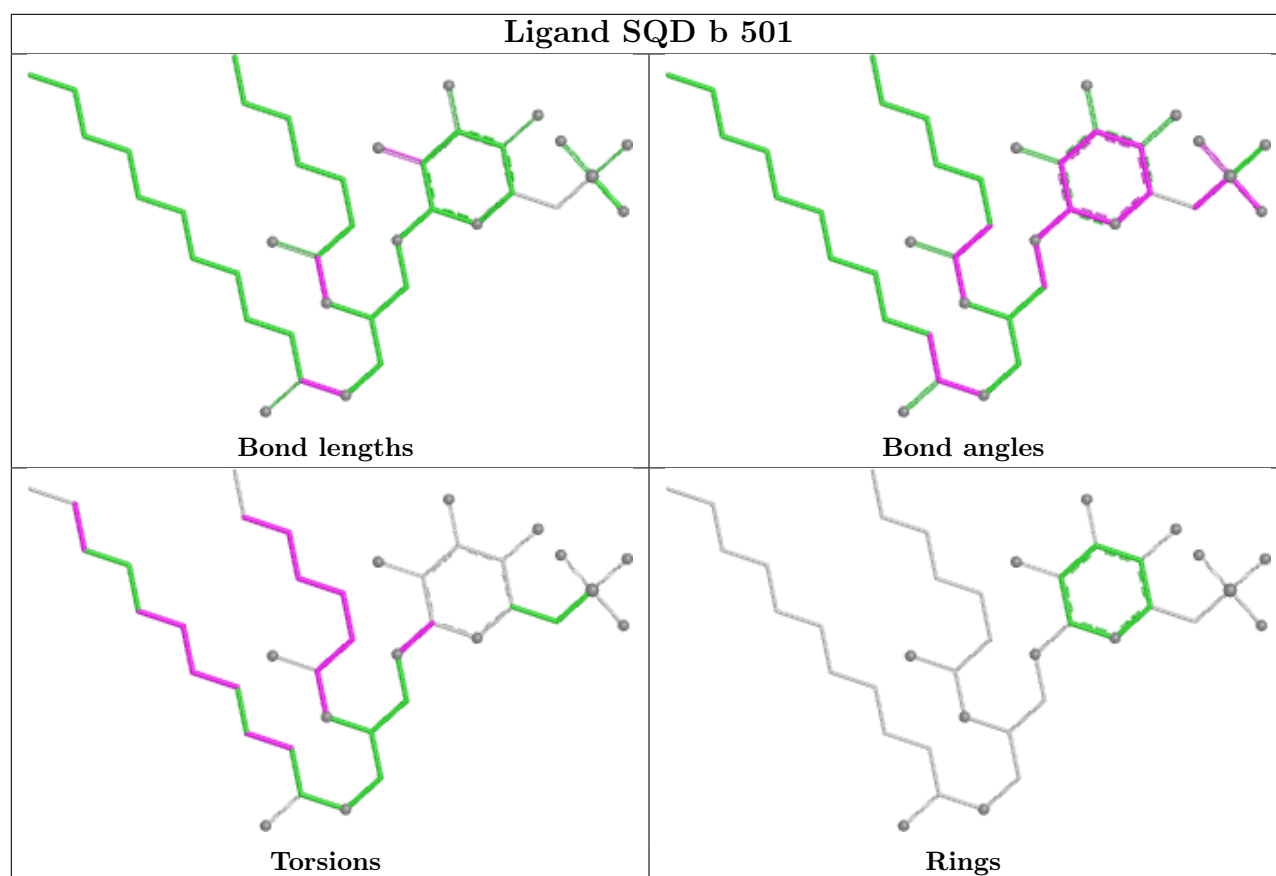


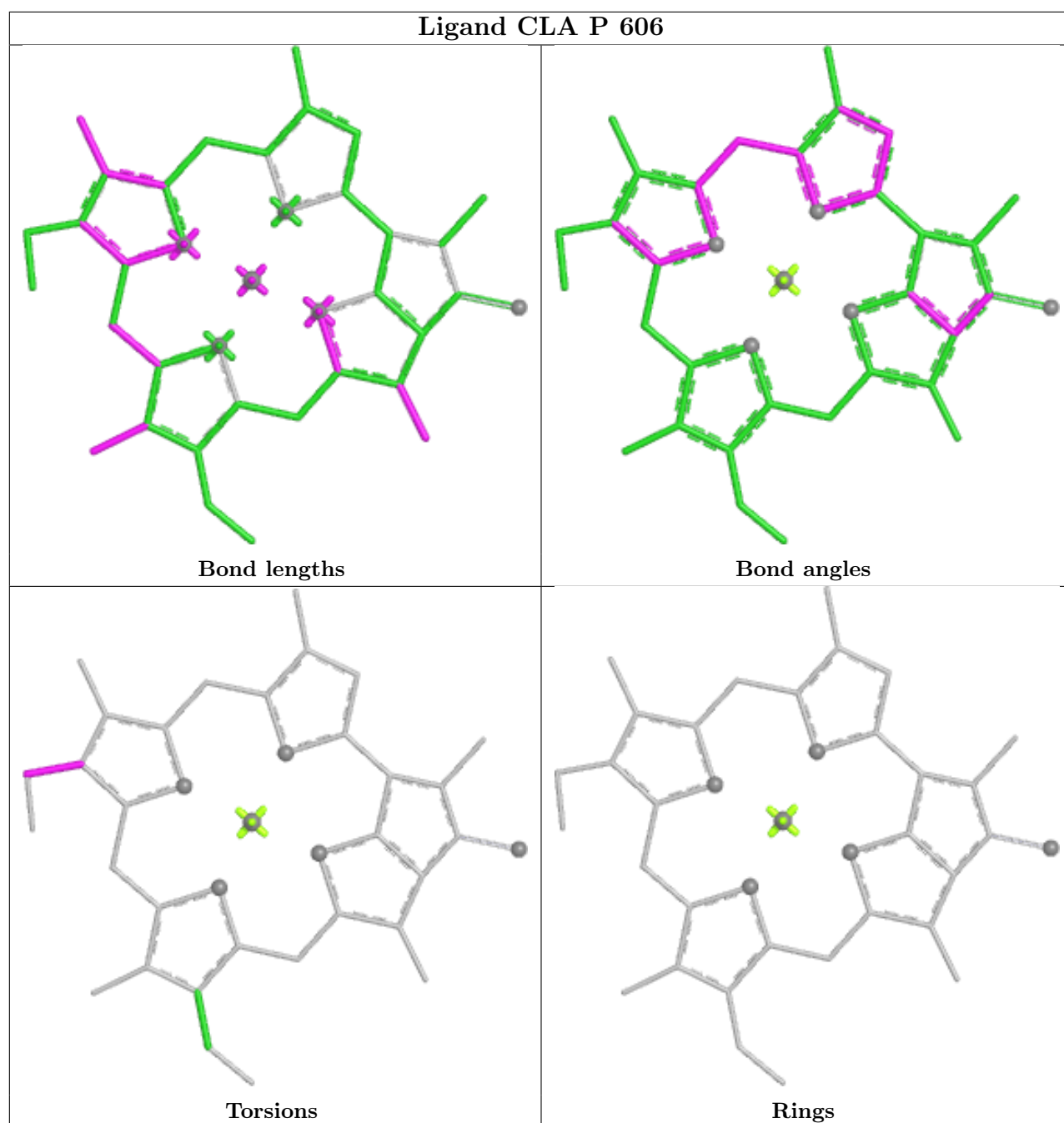
Torsions

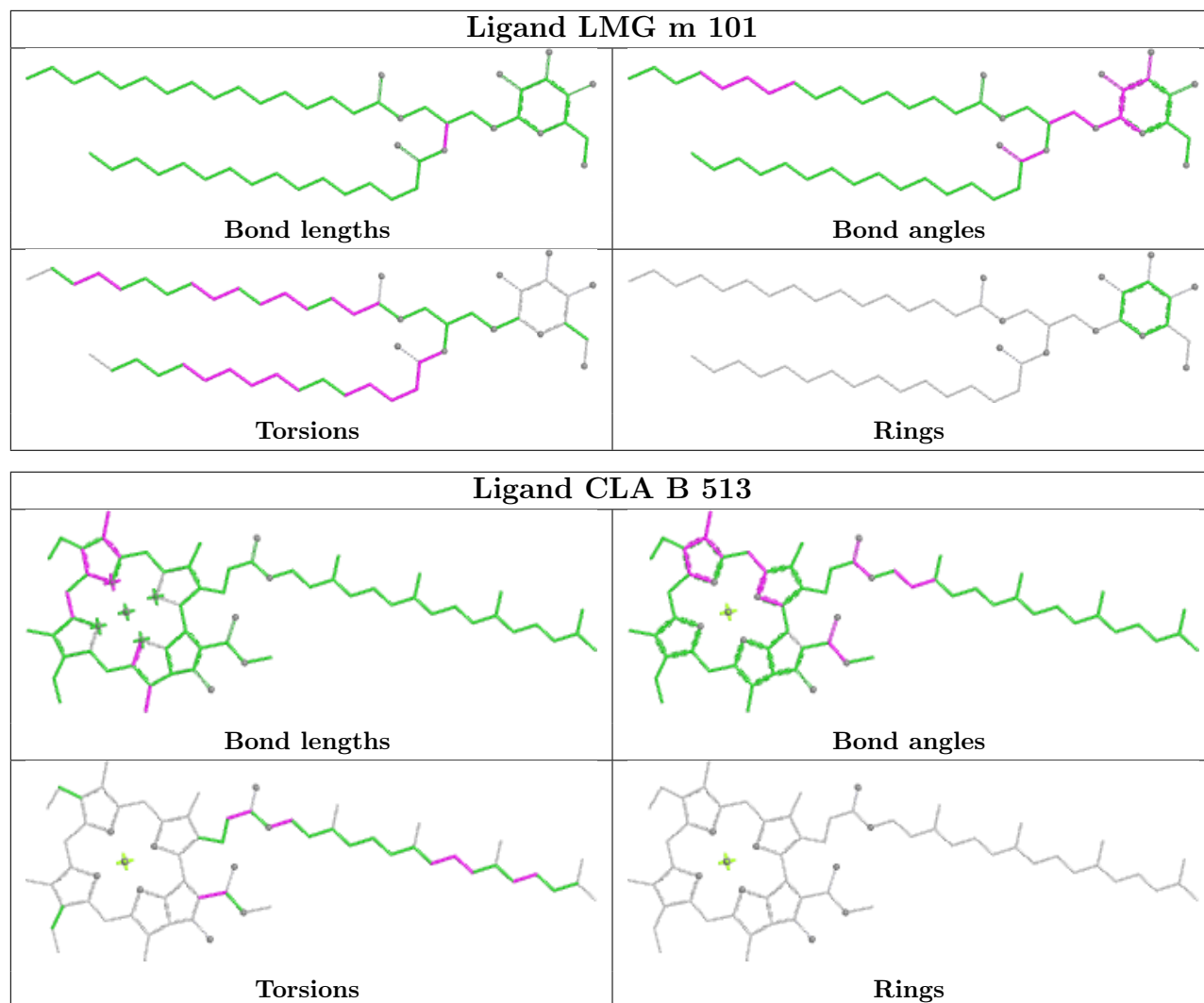


Rings

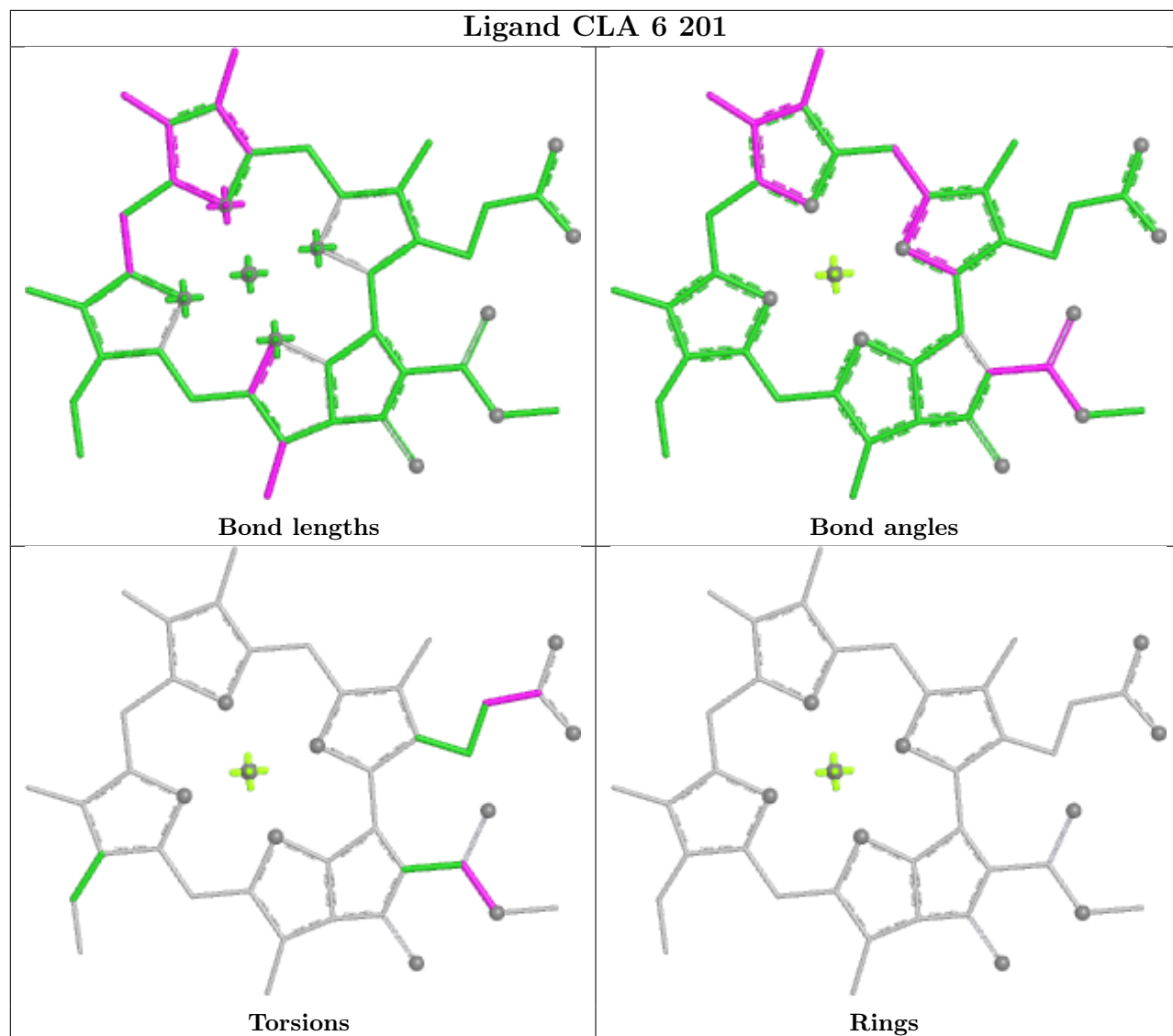


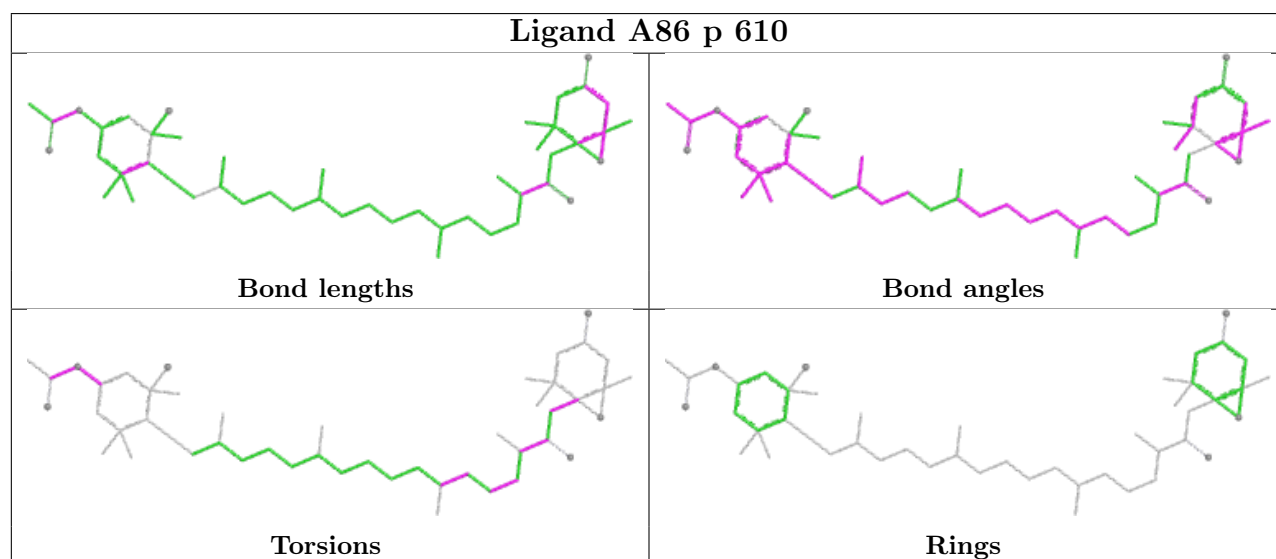
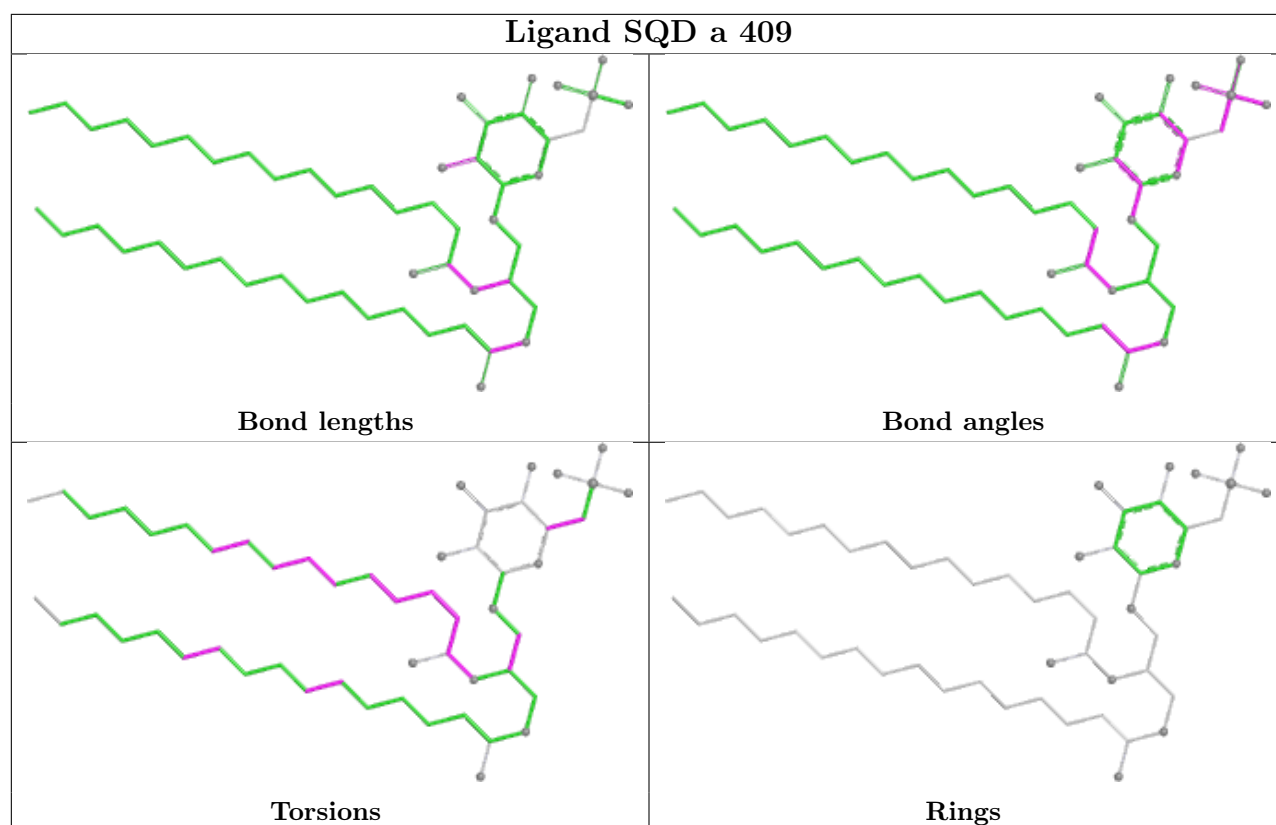




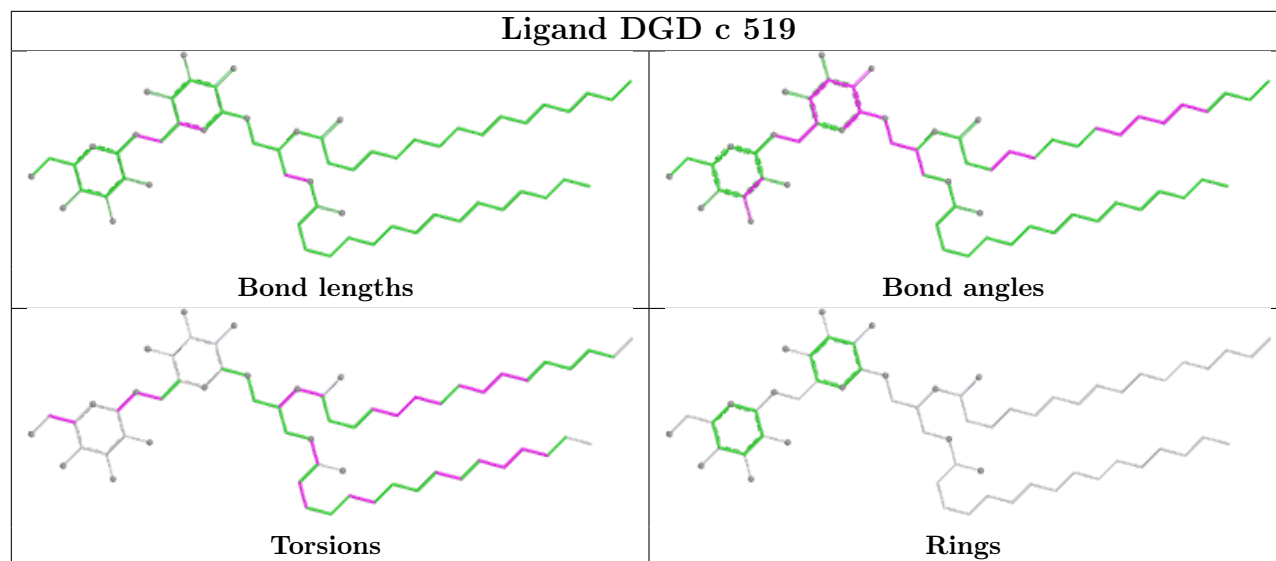


## Ligand CLA 6 201

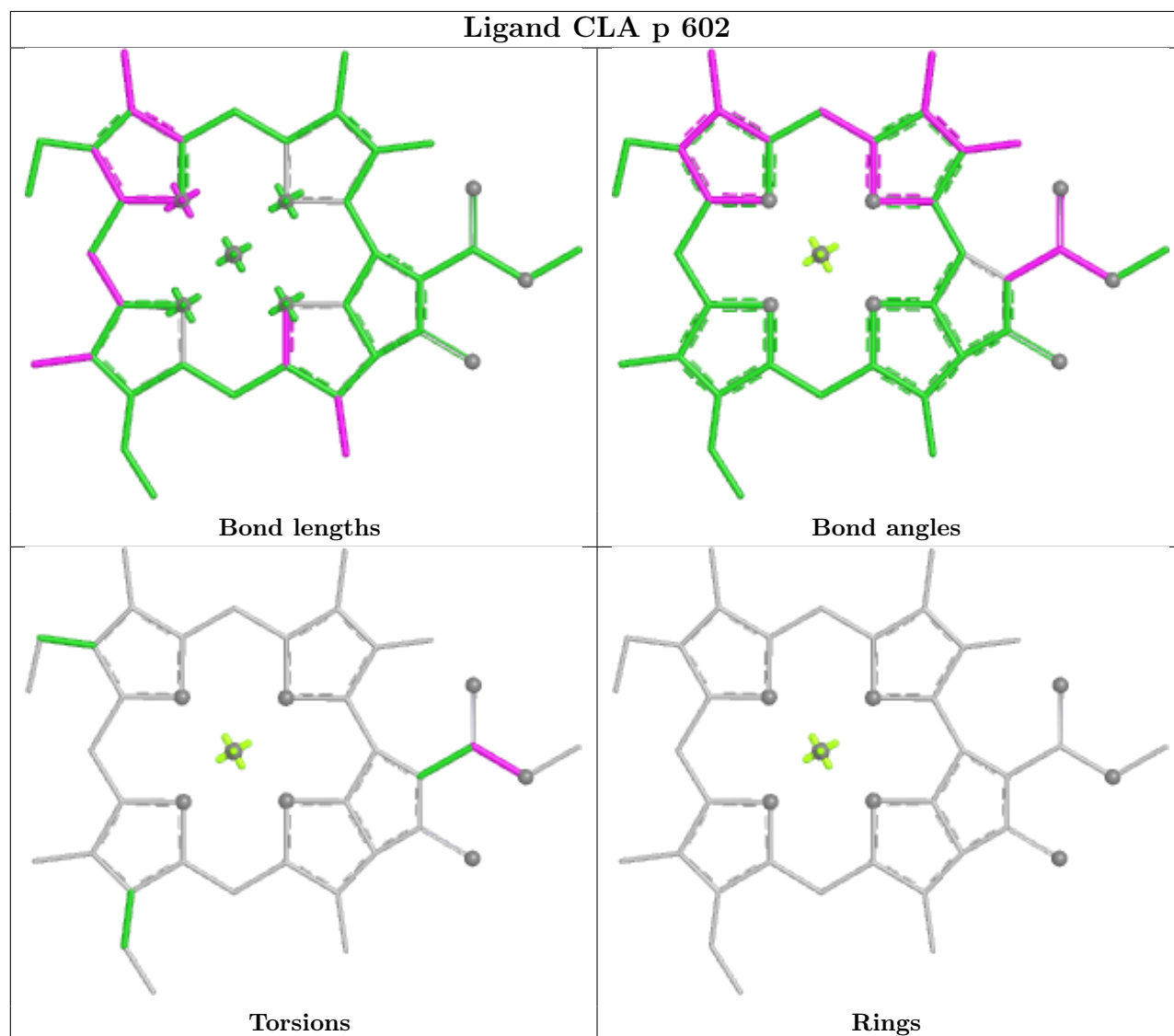




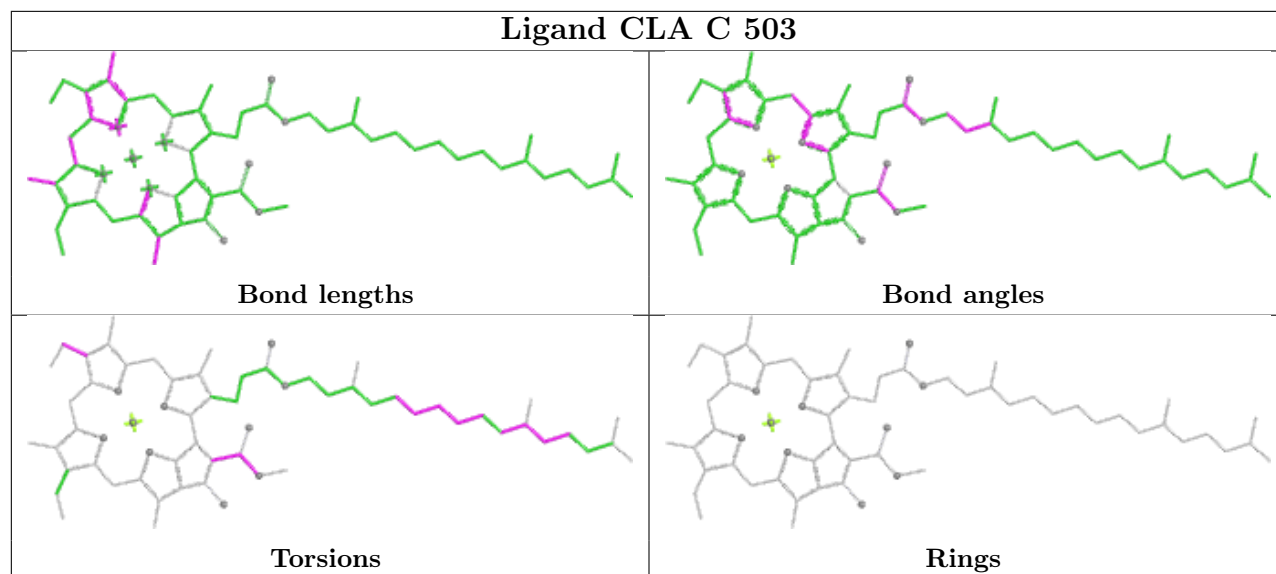
## Ligand DGD c 519



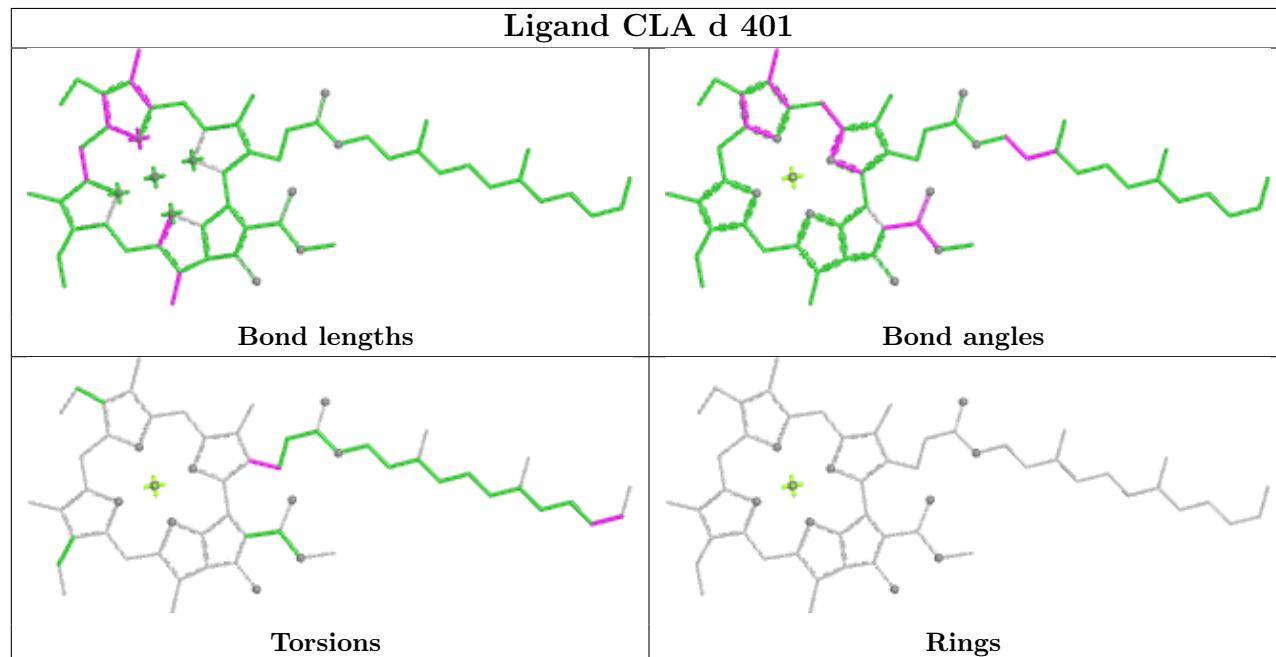
## Ligand CLA p 602

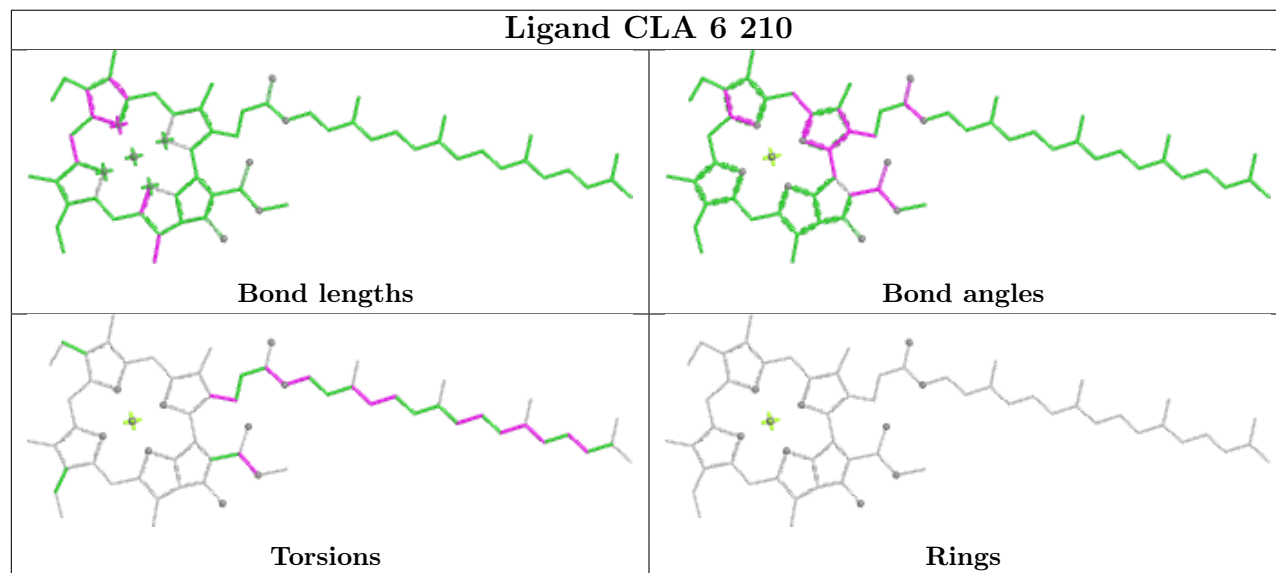
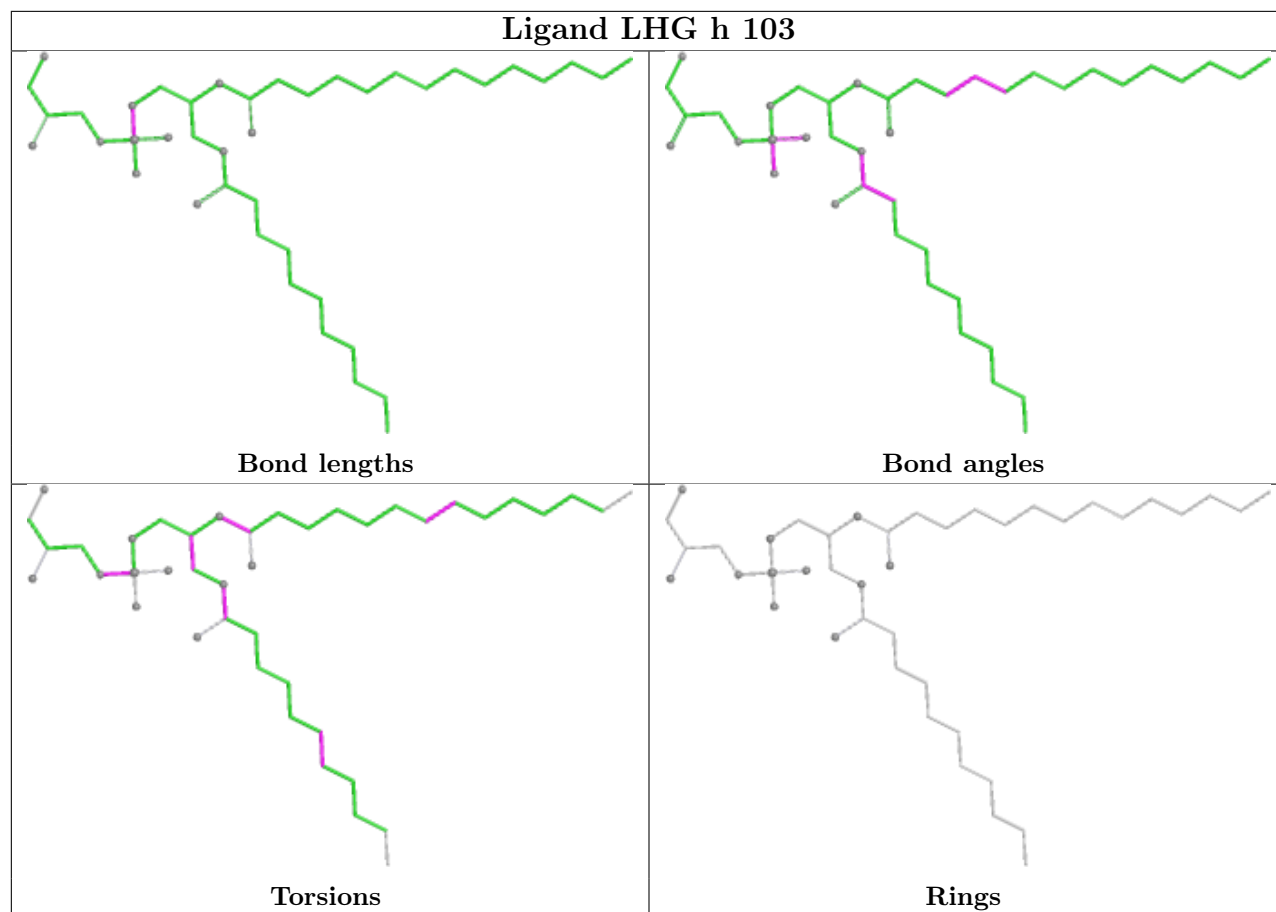


## Ligand CLA C 503

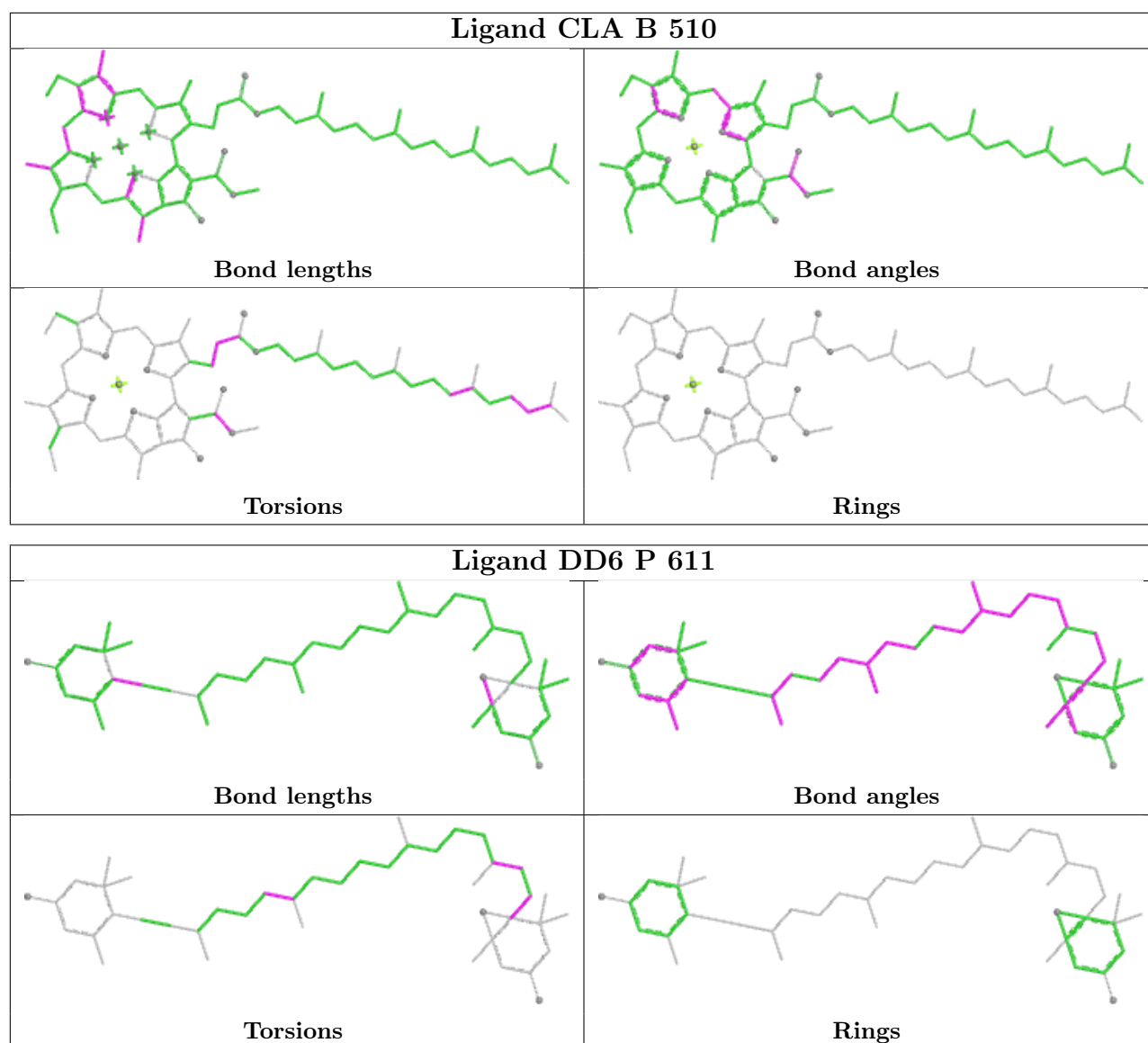


## Ligand CLA d 401

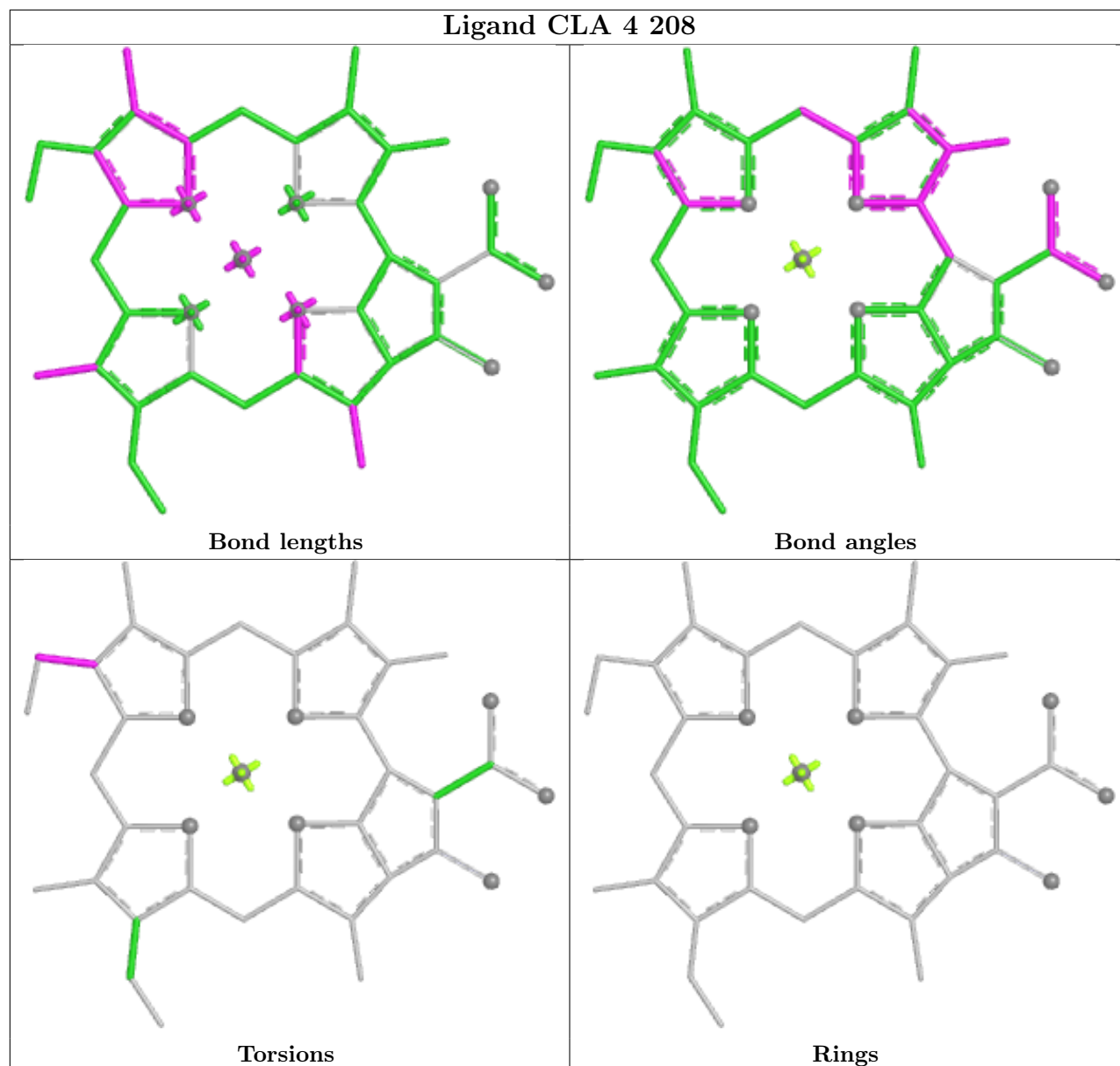




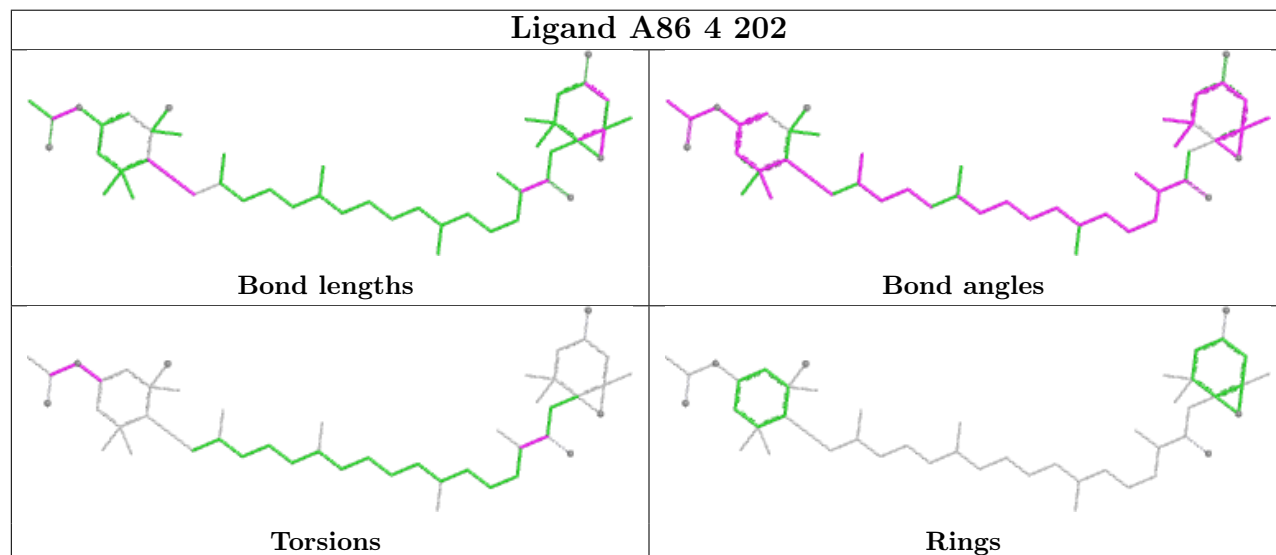




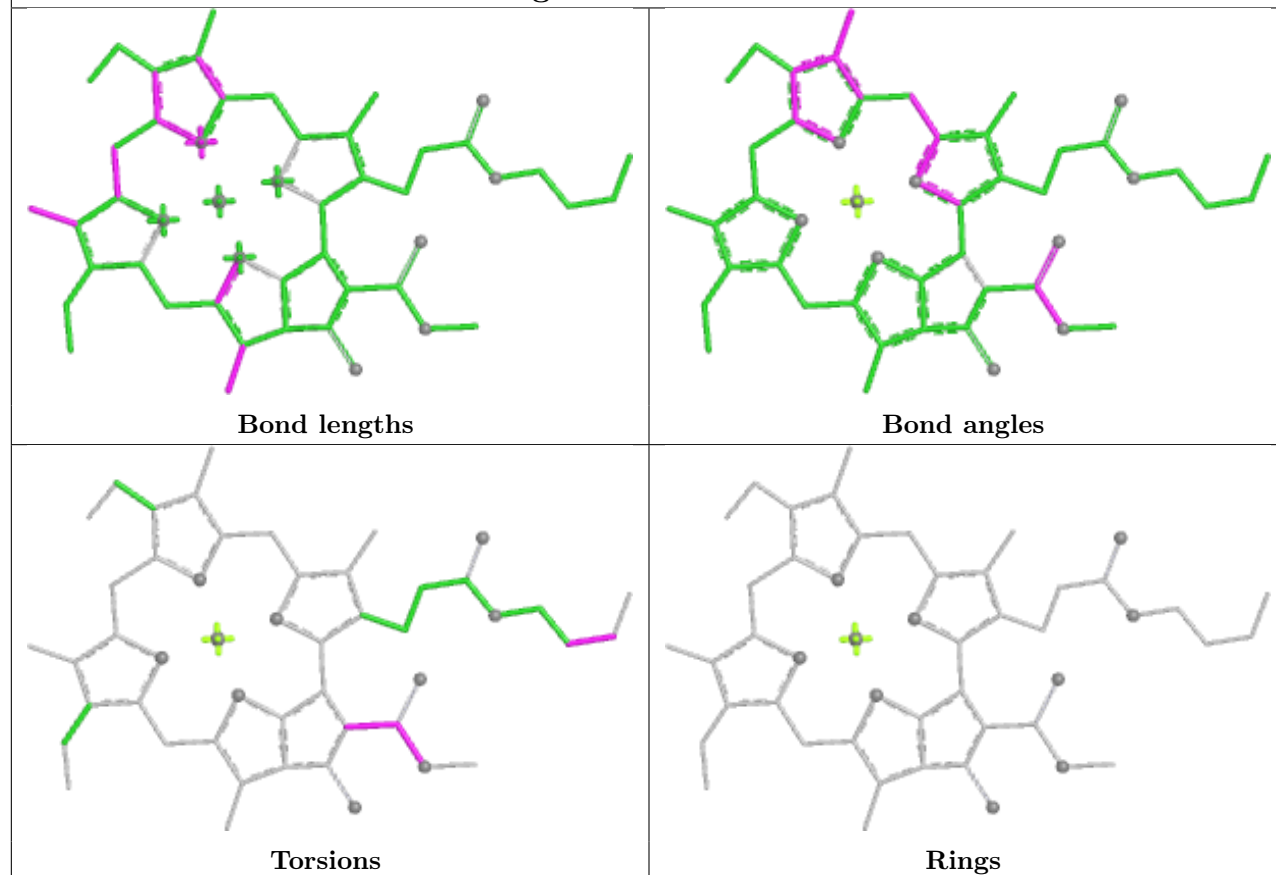
## Ligand CLA 4 208



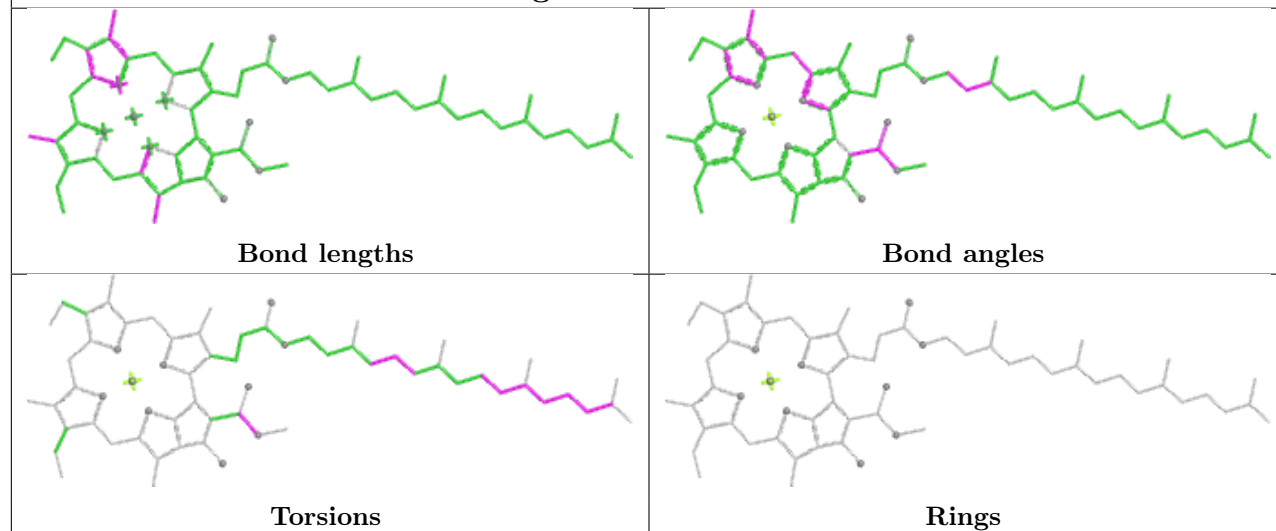
## Ligand A86 4 202



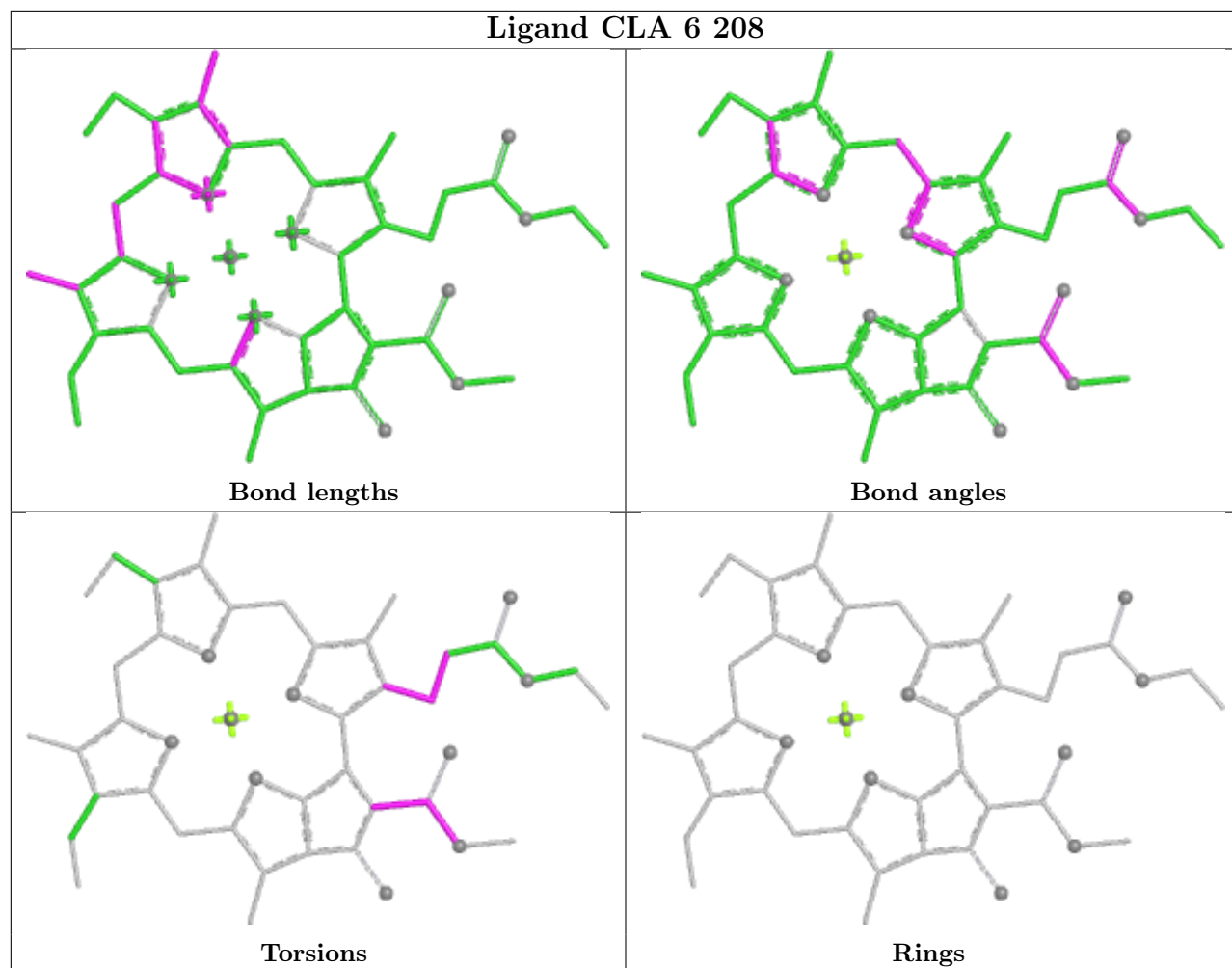
## Ligand CLA C 514



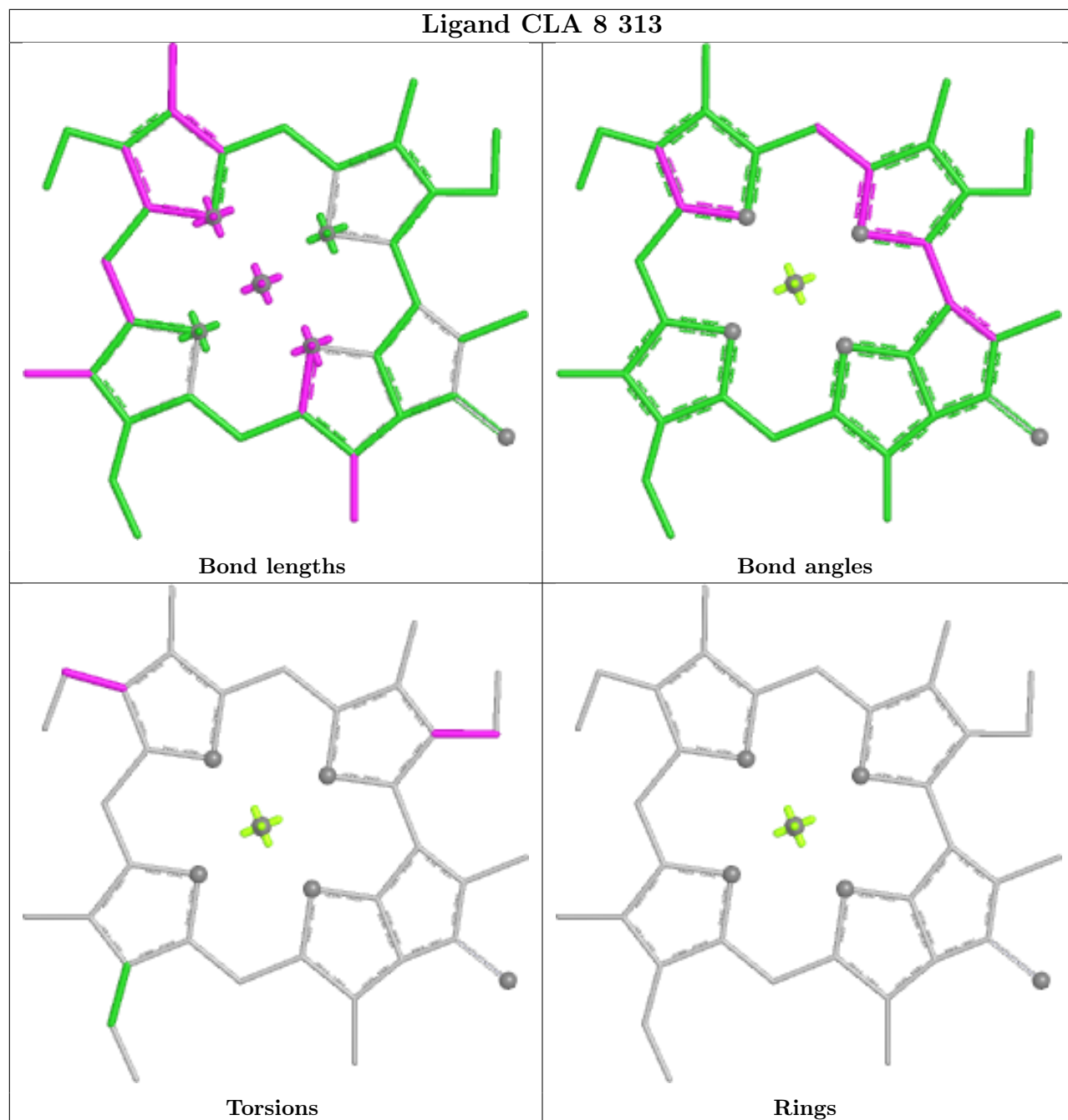
## Ligand CLA B 504

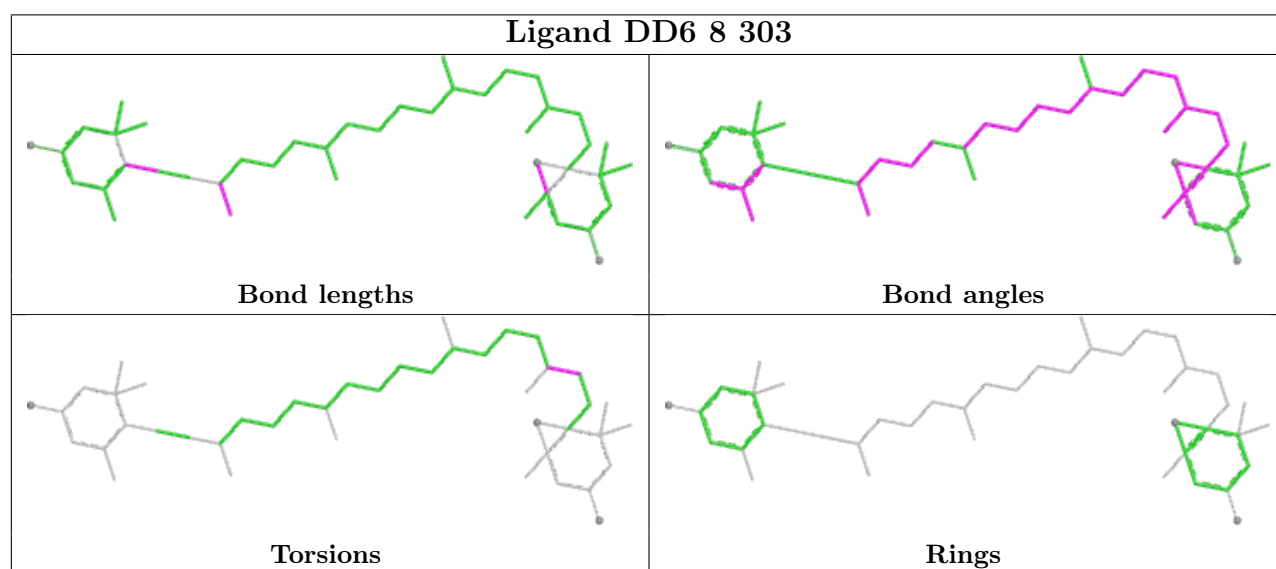
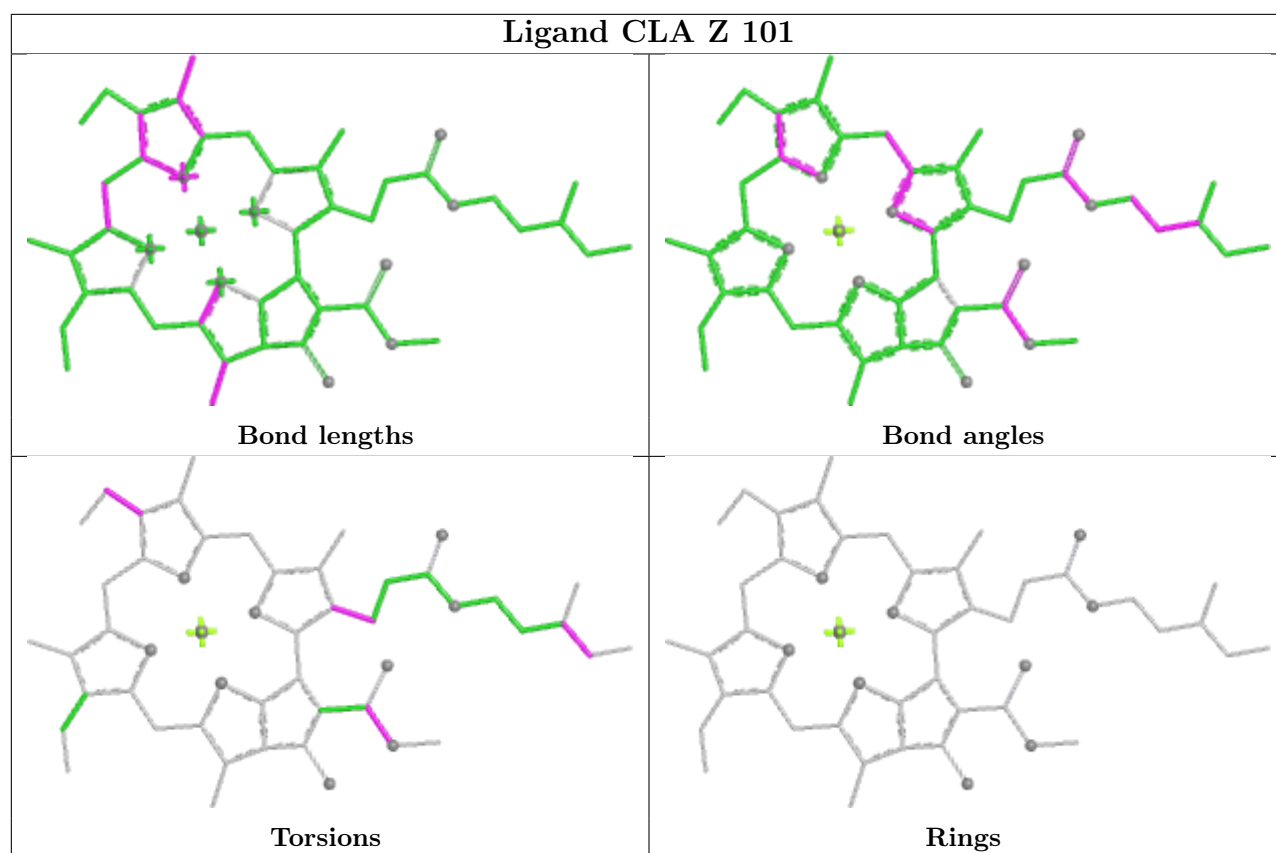


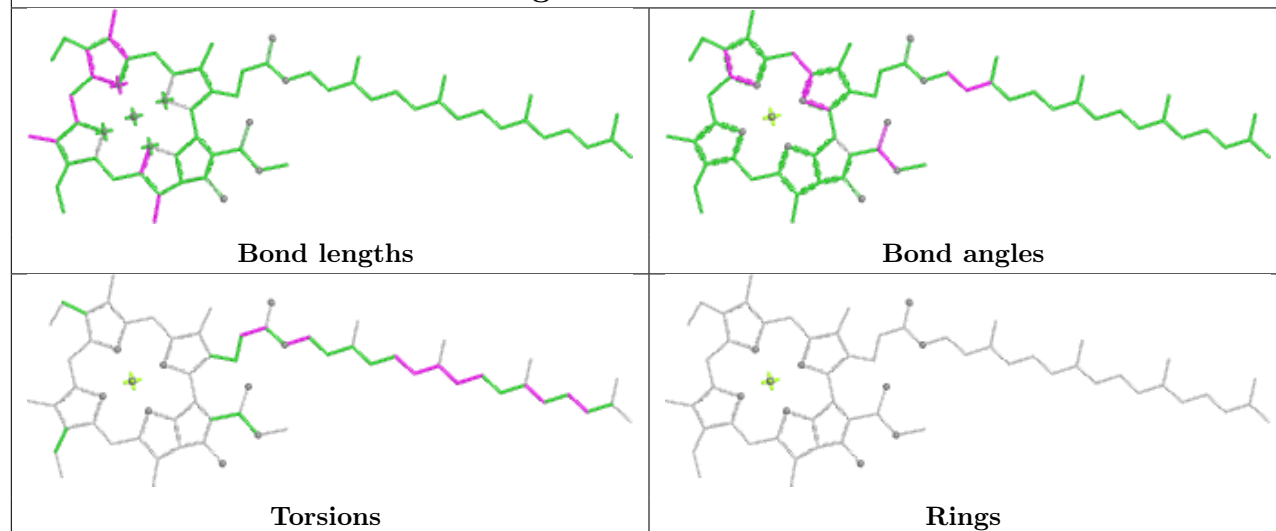
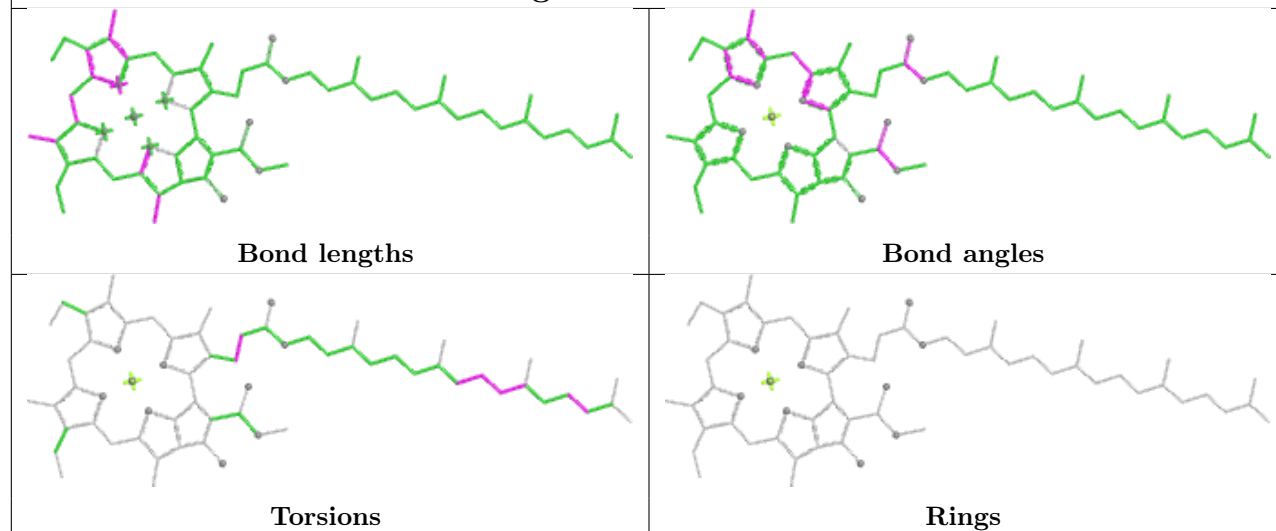
## Ligand CLA 6 208



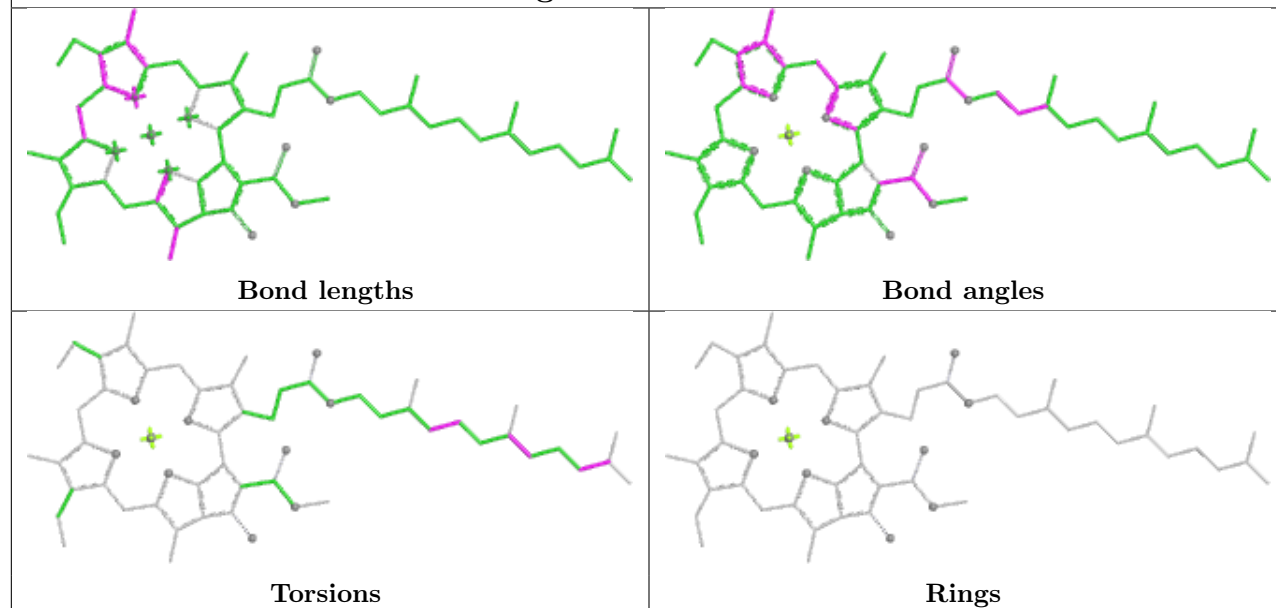
## Ligand CLA 8 313



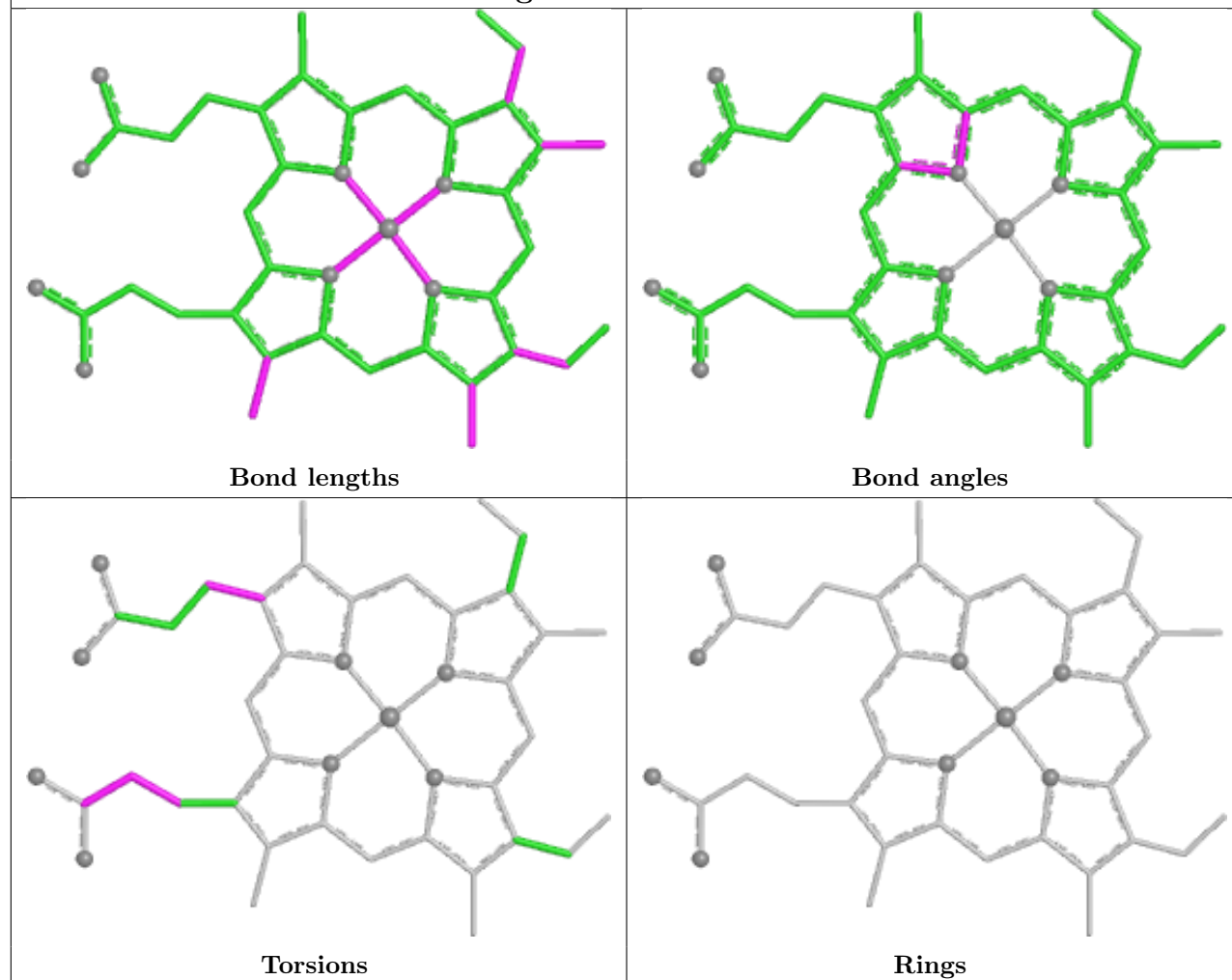


**Ligand CLA C 511****Ligand CLA B 506**

## Ligand CLA a 407

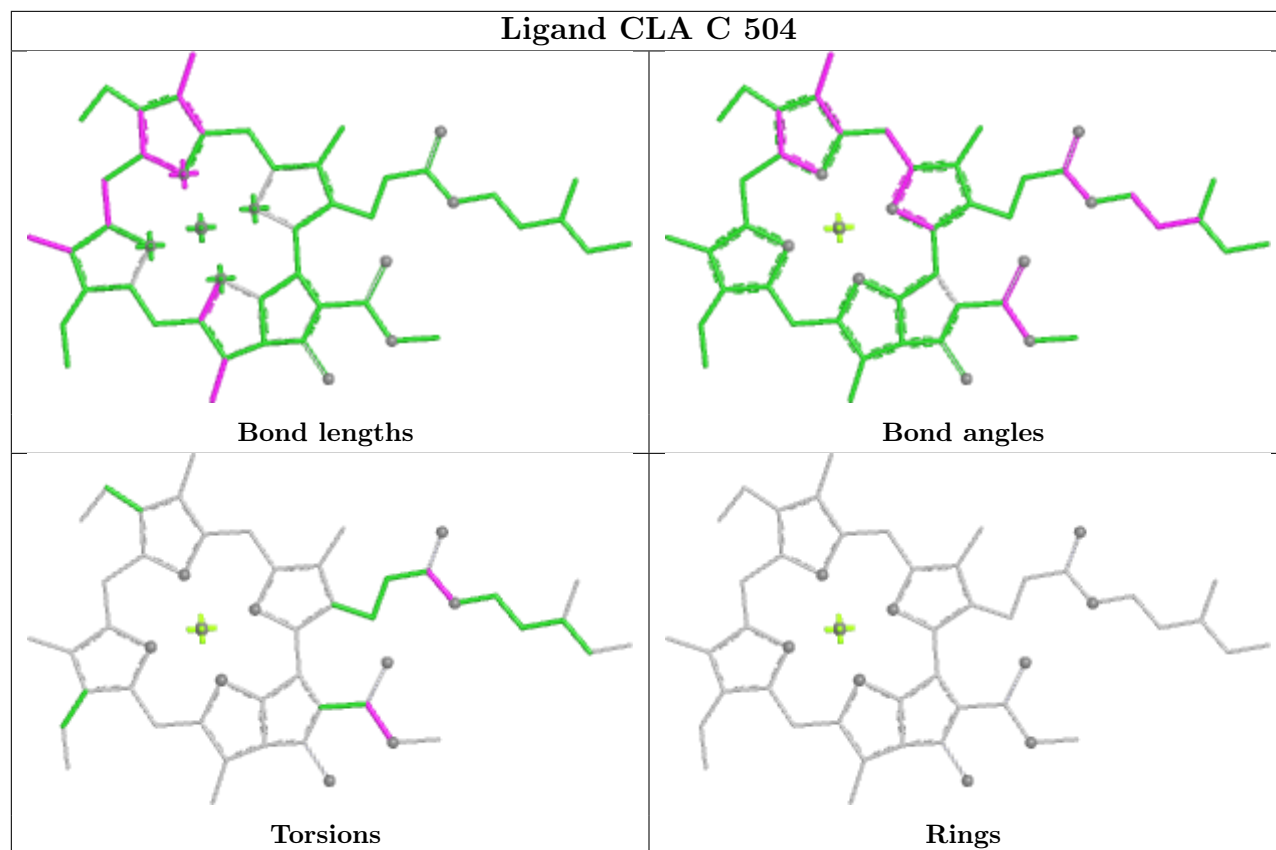


## Ligand HEM f 101

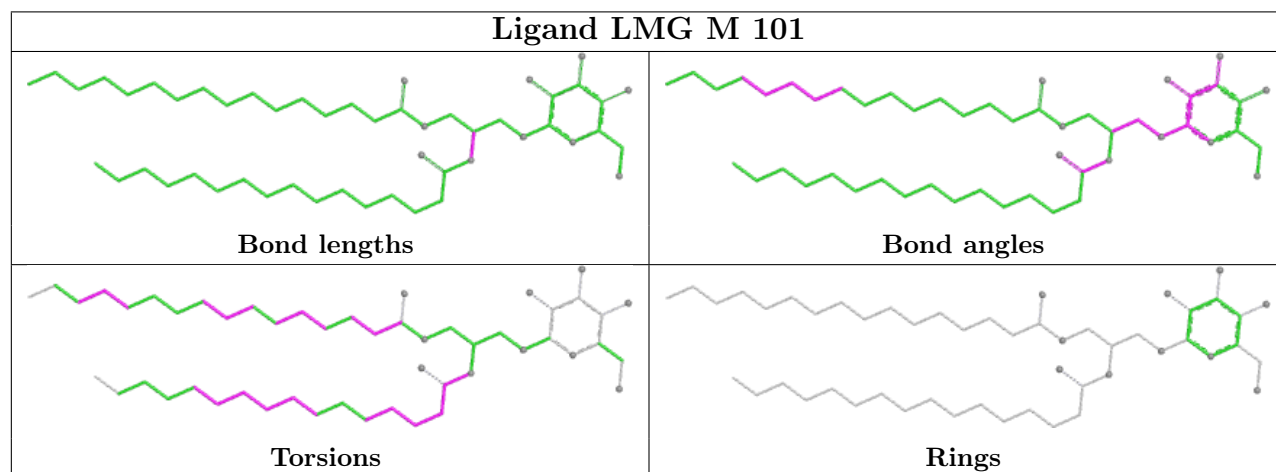




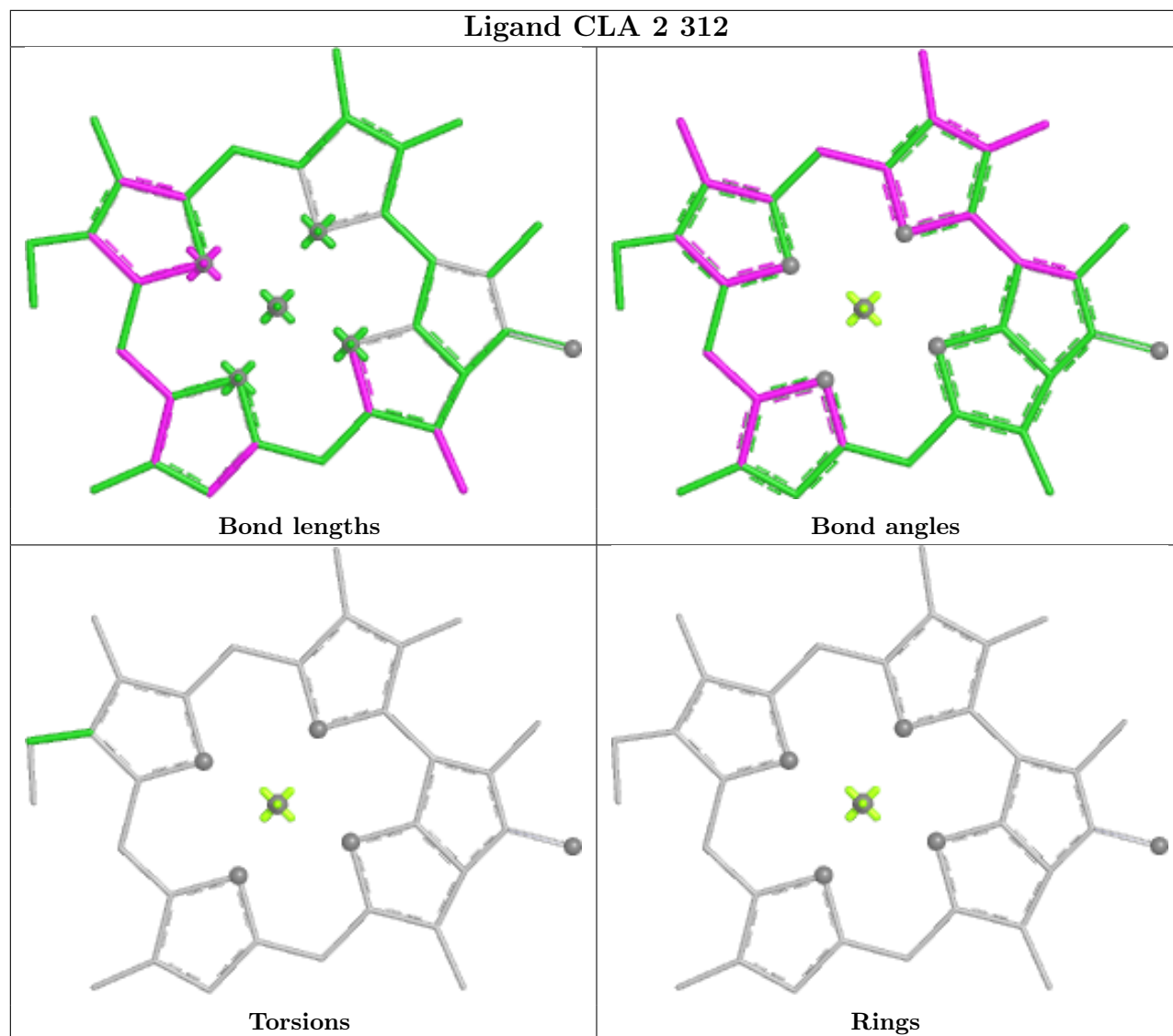
## Ligand CLA C 504



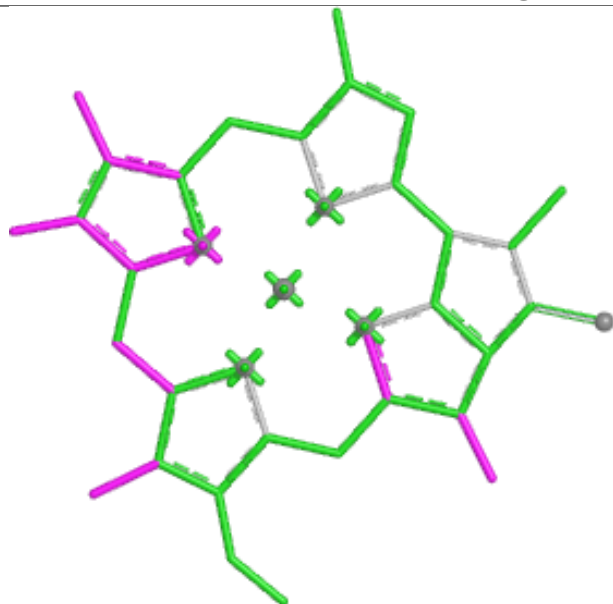
## Ligand LMG M 101



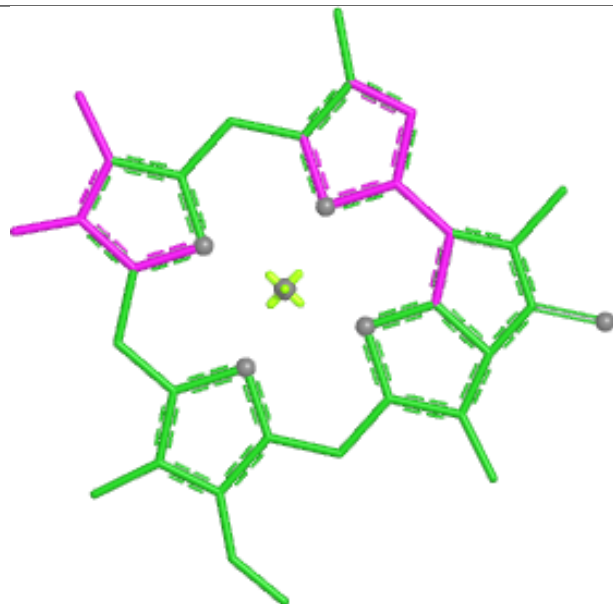
## Ligand CLA 2 312



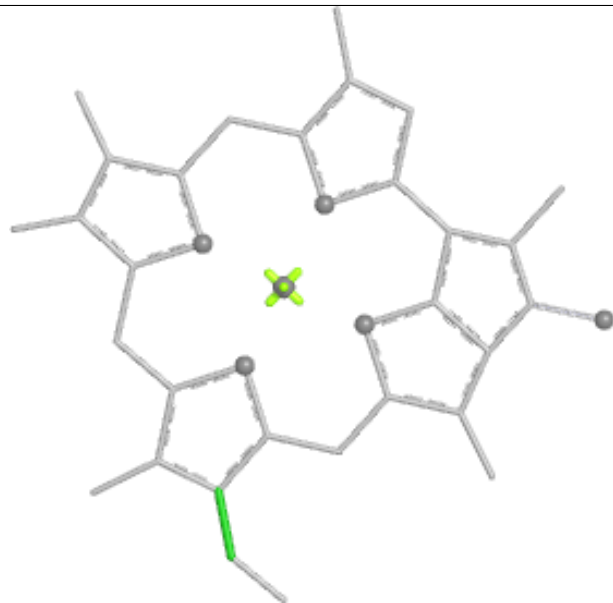
## Ligand CLA P 607



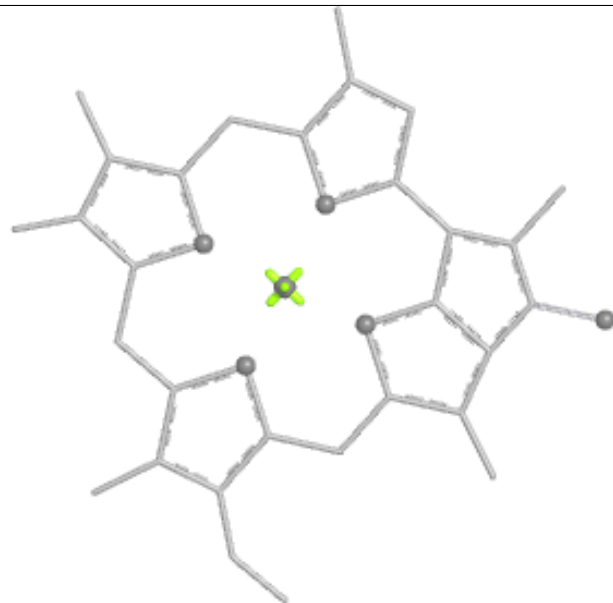
Bond lengths



Bond angles

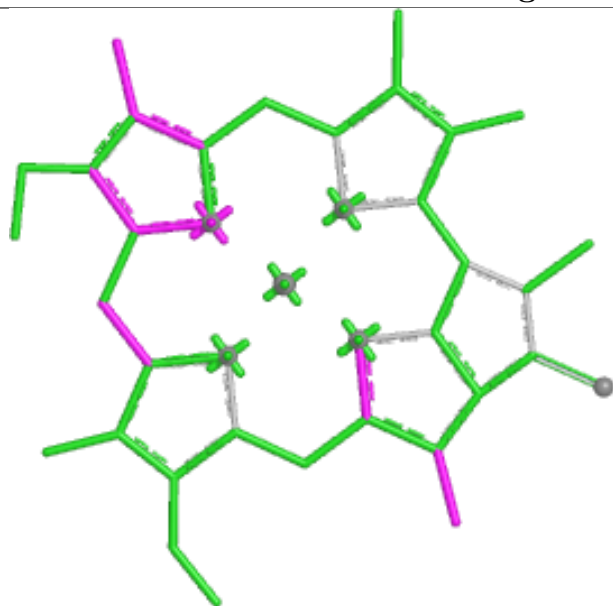


Torsions

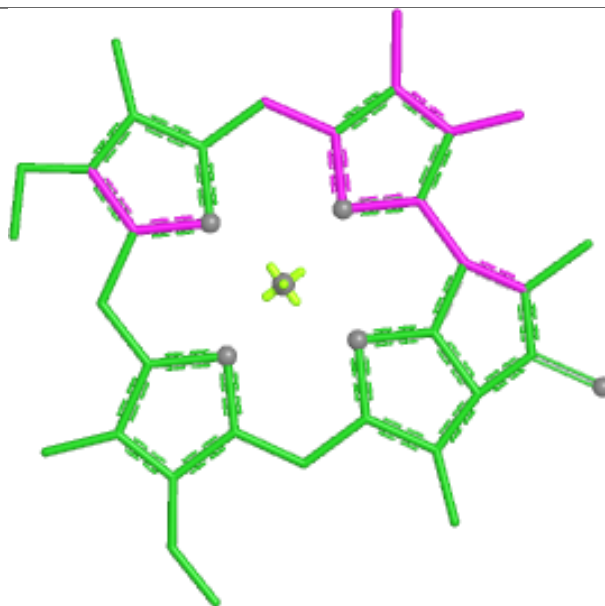


Rings

## Ligand CLA 5 314



Bond lengths



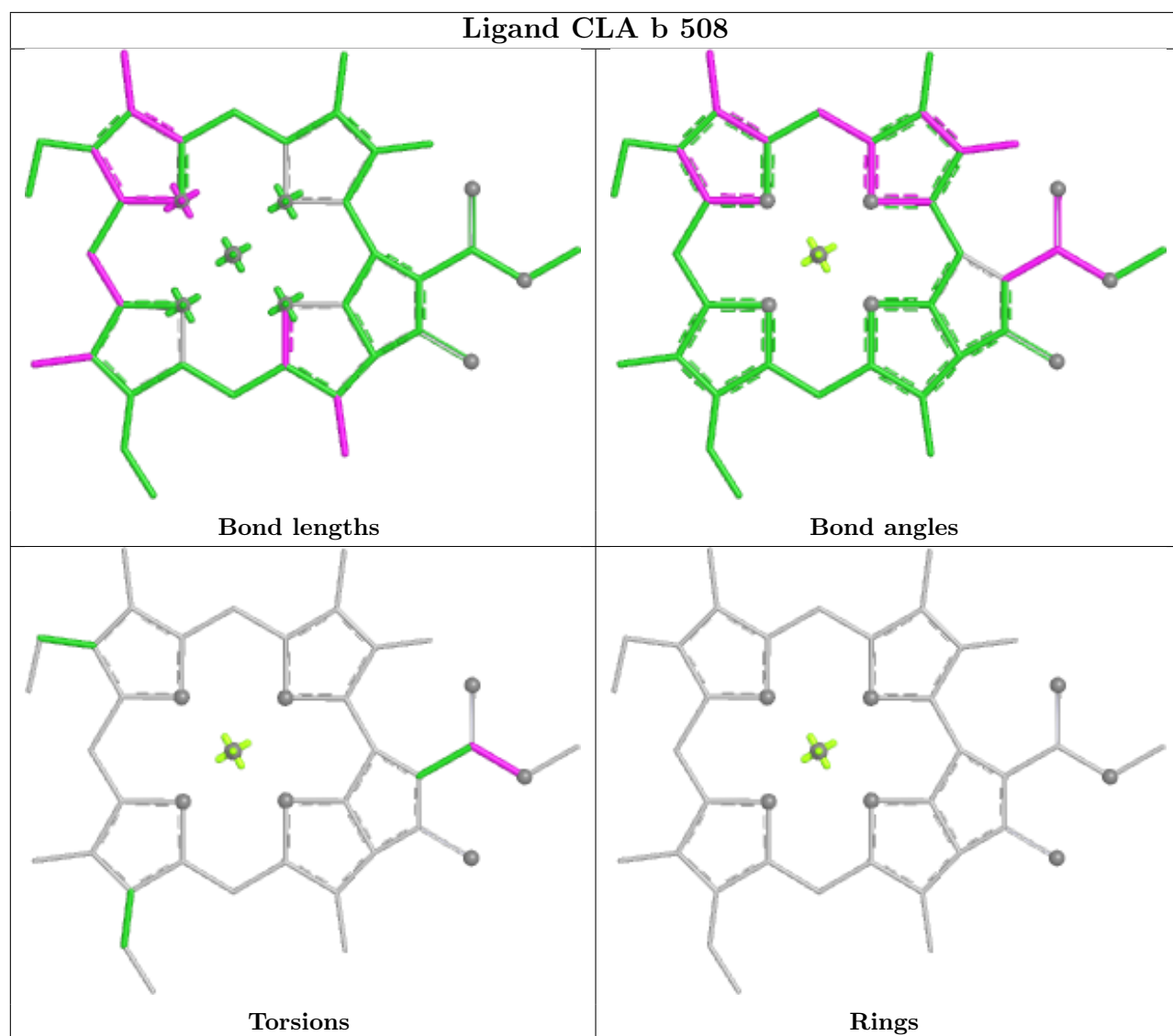
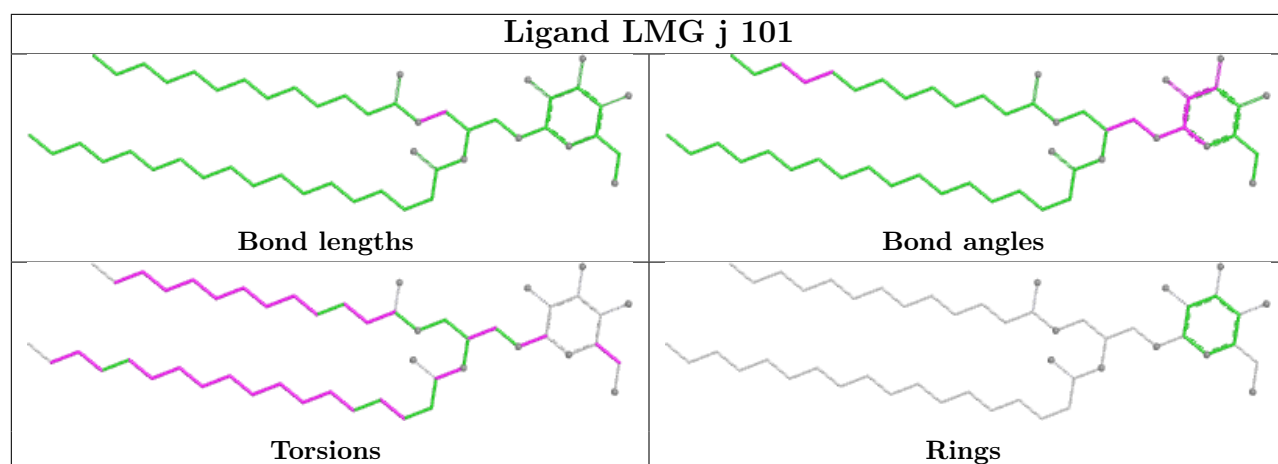
Bond angles

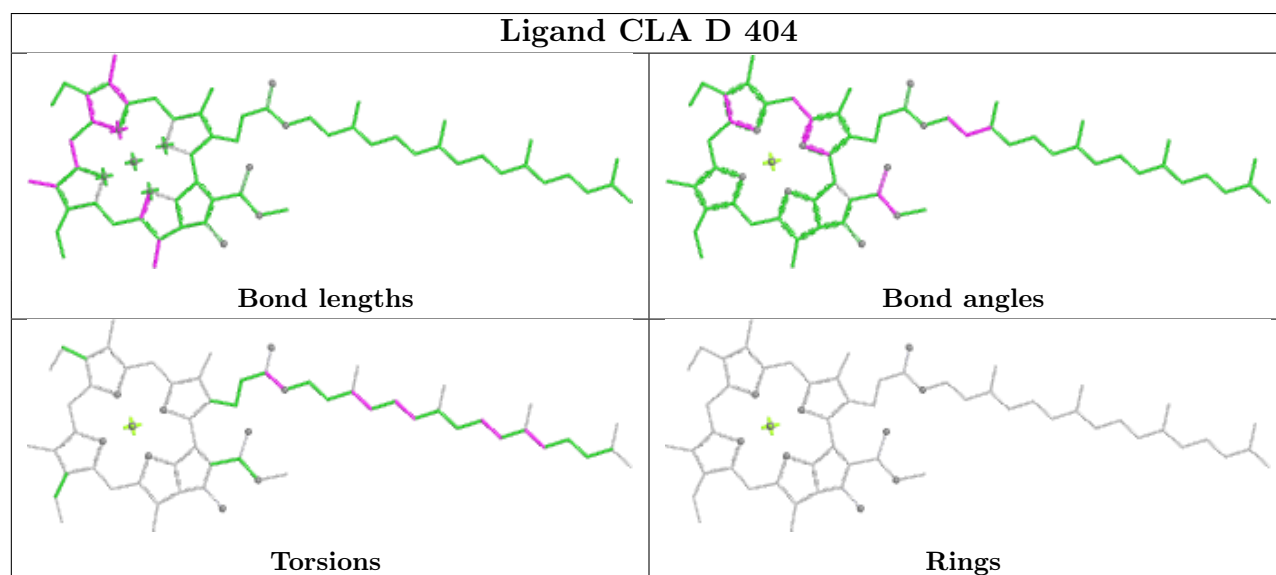
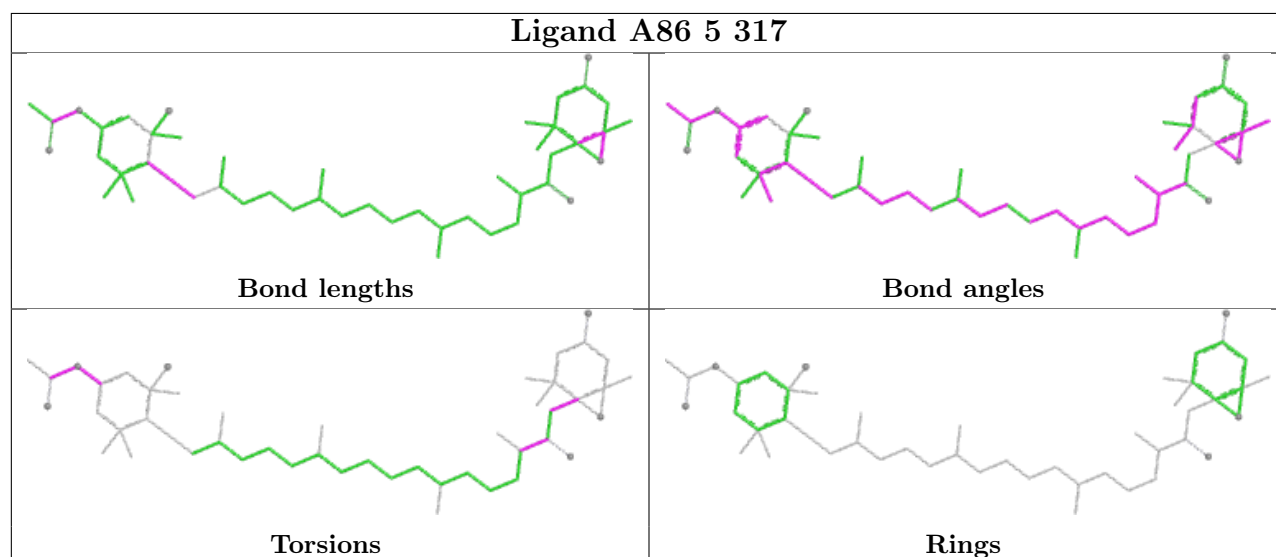
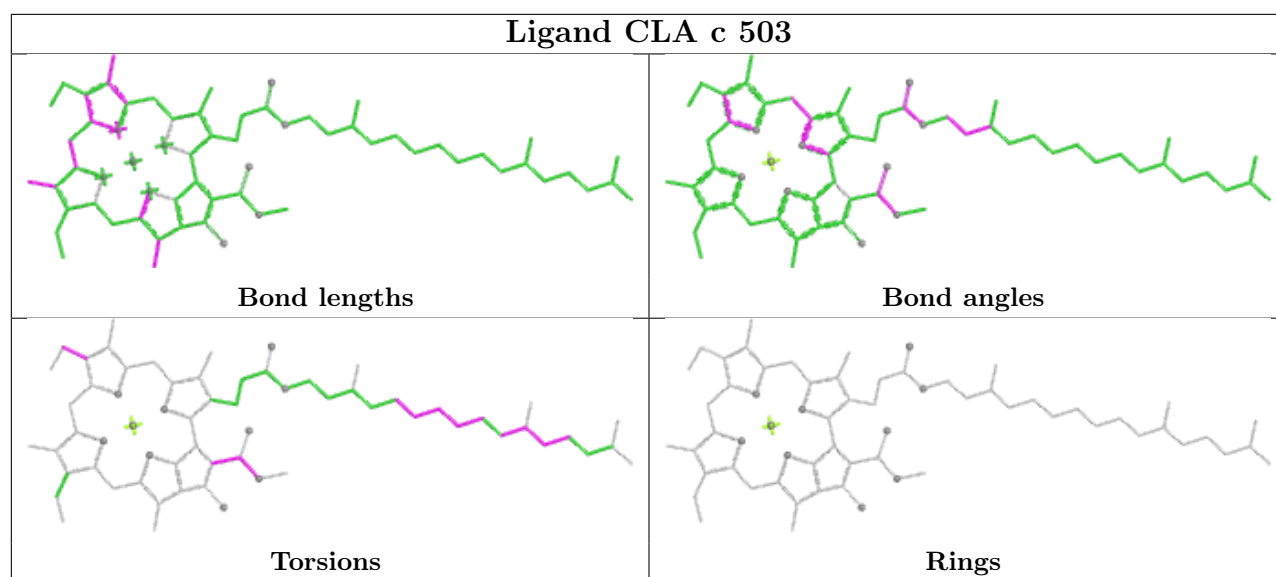


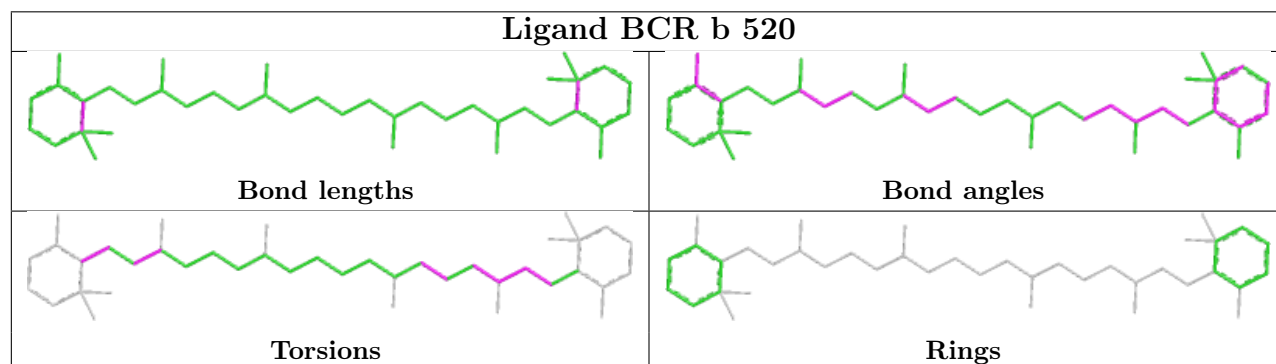
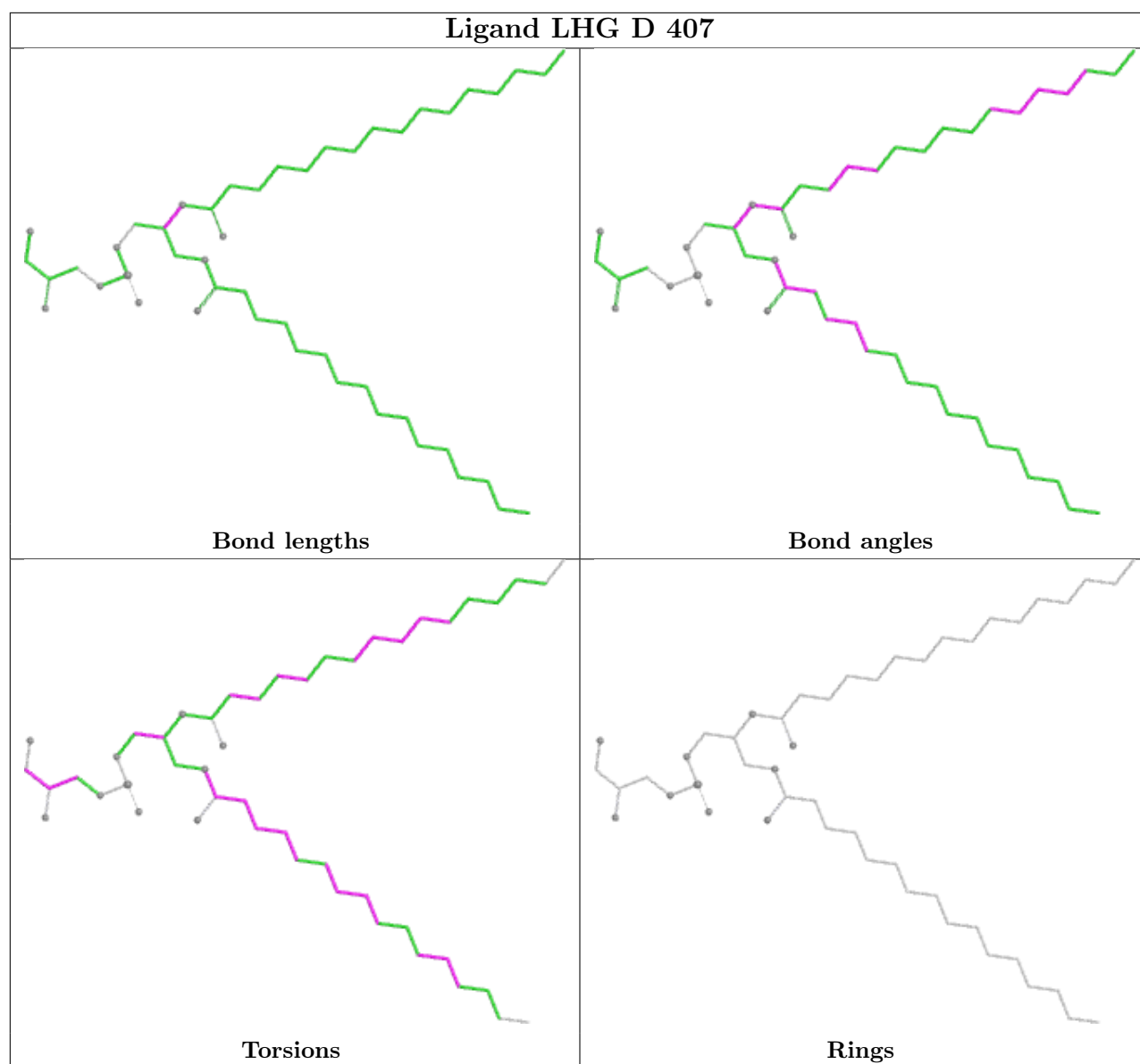
Torsions

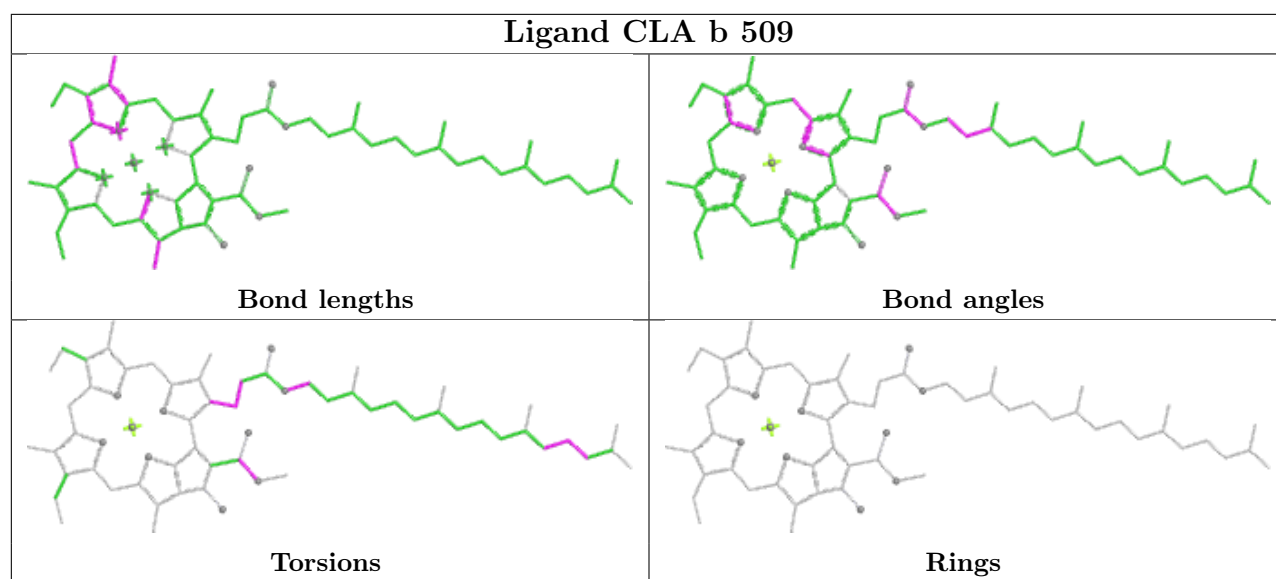


Rings



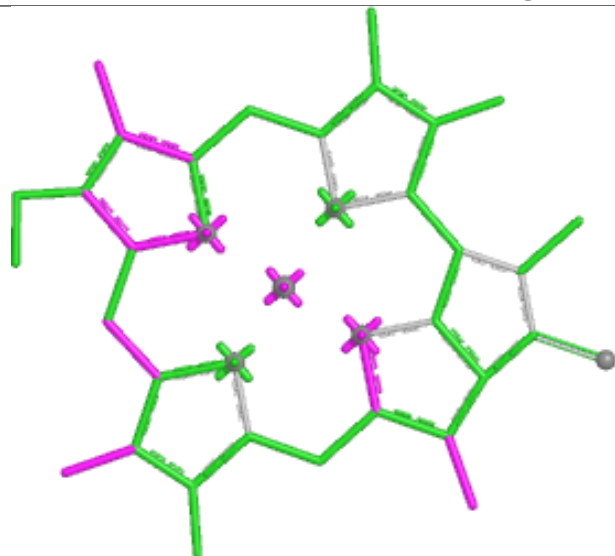




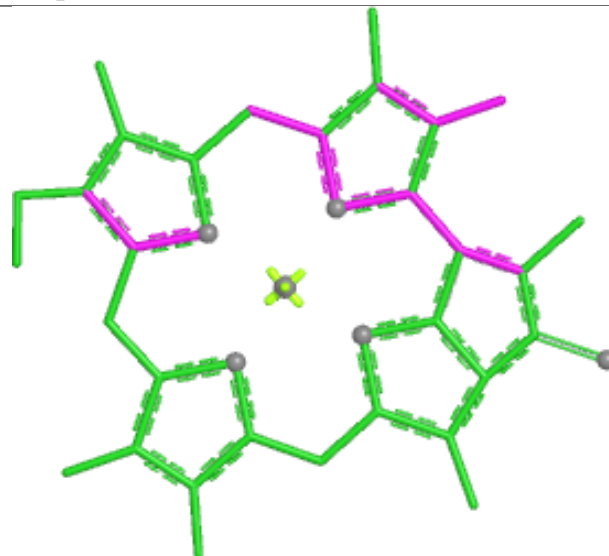




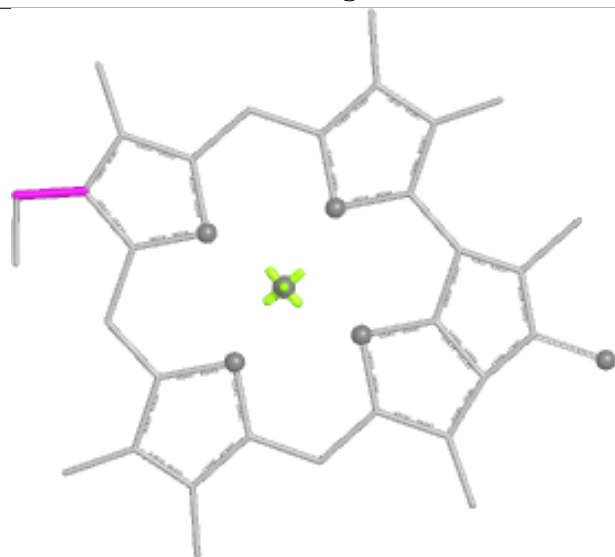
## Ligand CLA p 605



Bond lengths



Bond angles

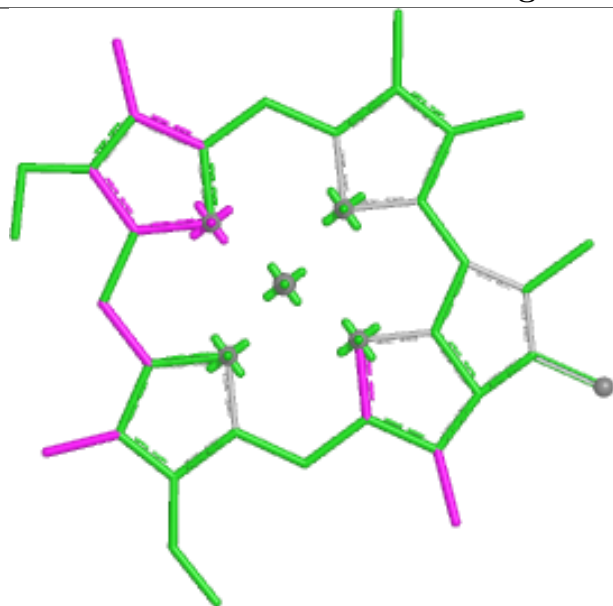


Torsions

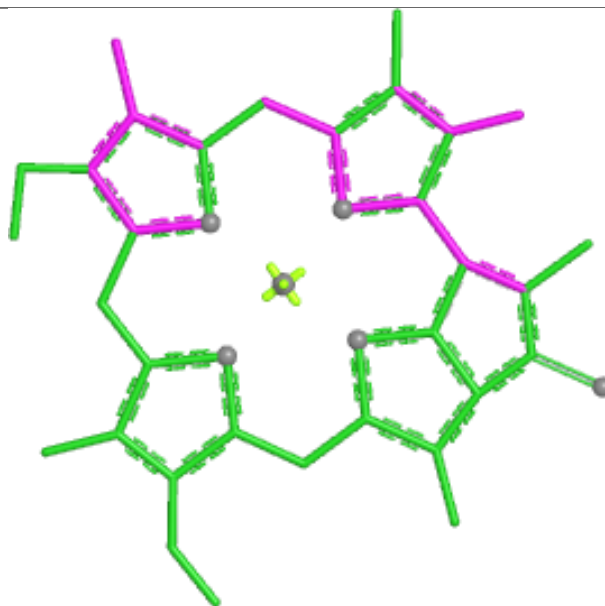


Rings

## Ligand CLA 4 210



Bond lengths



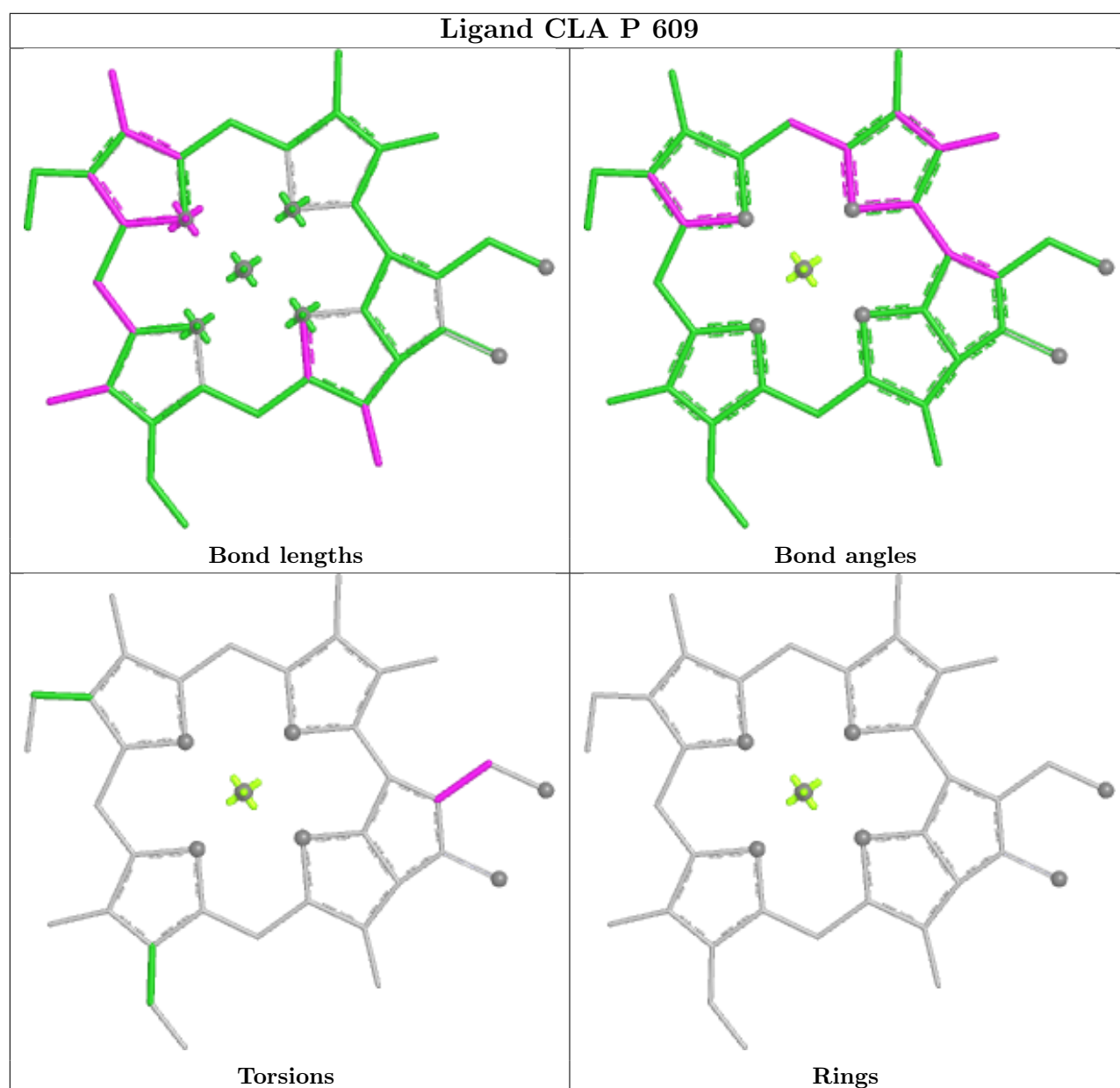
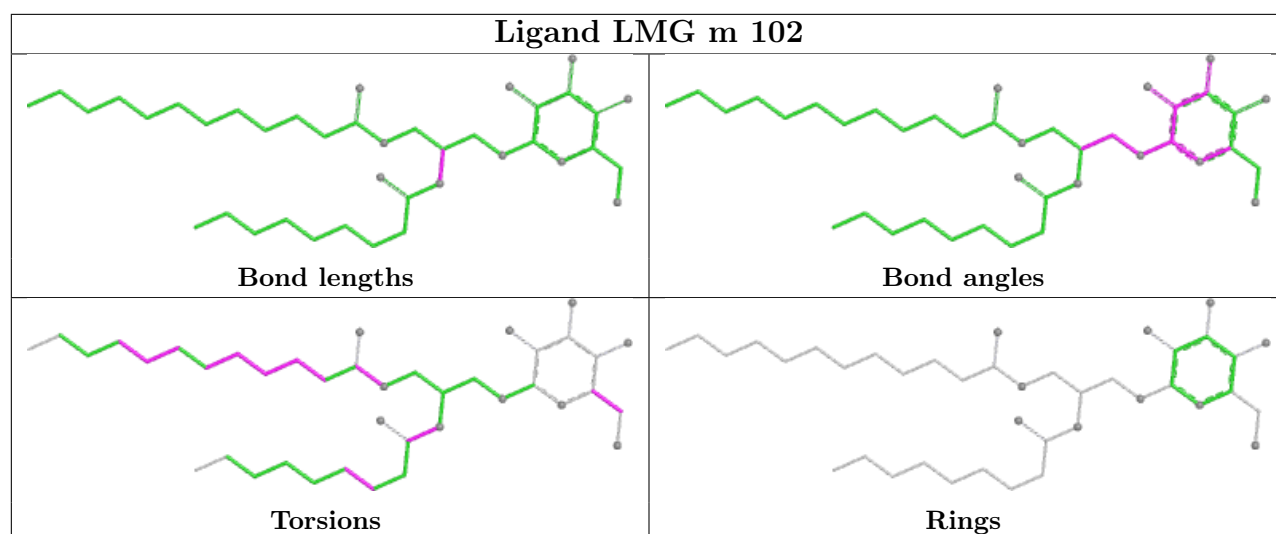
Bond angles



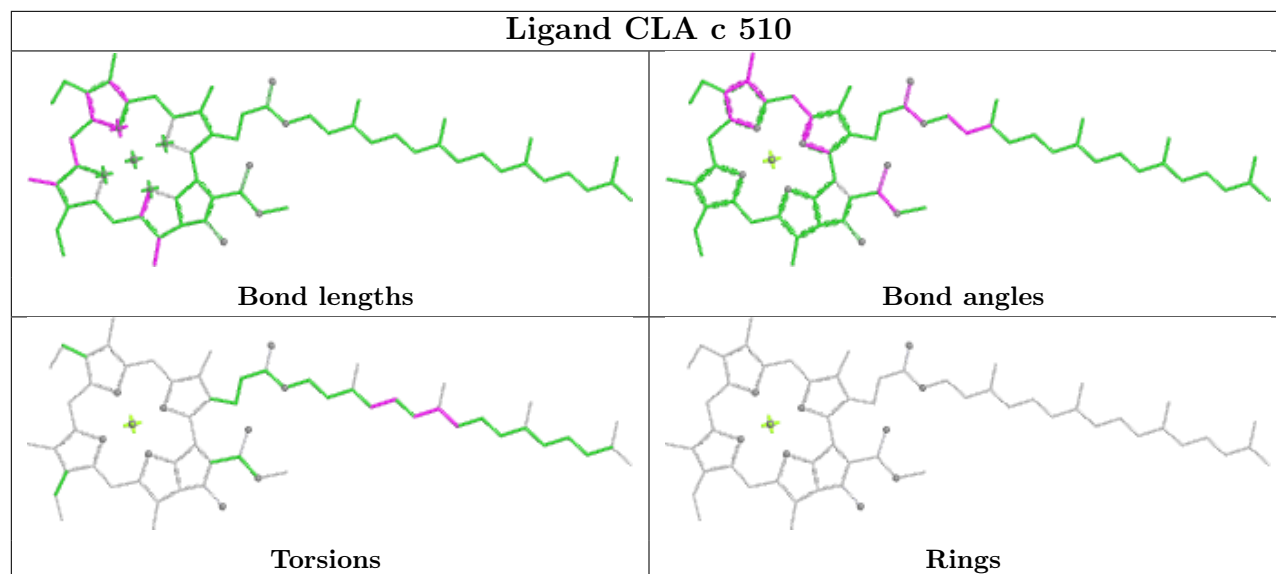
Torsions



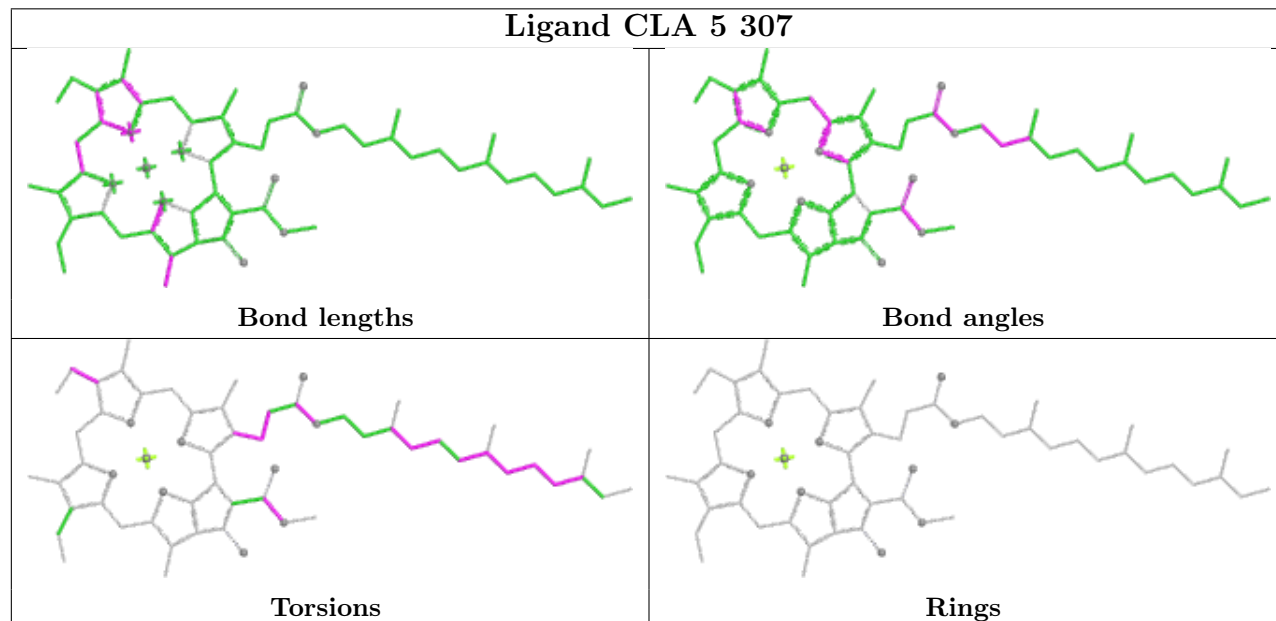
Rings

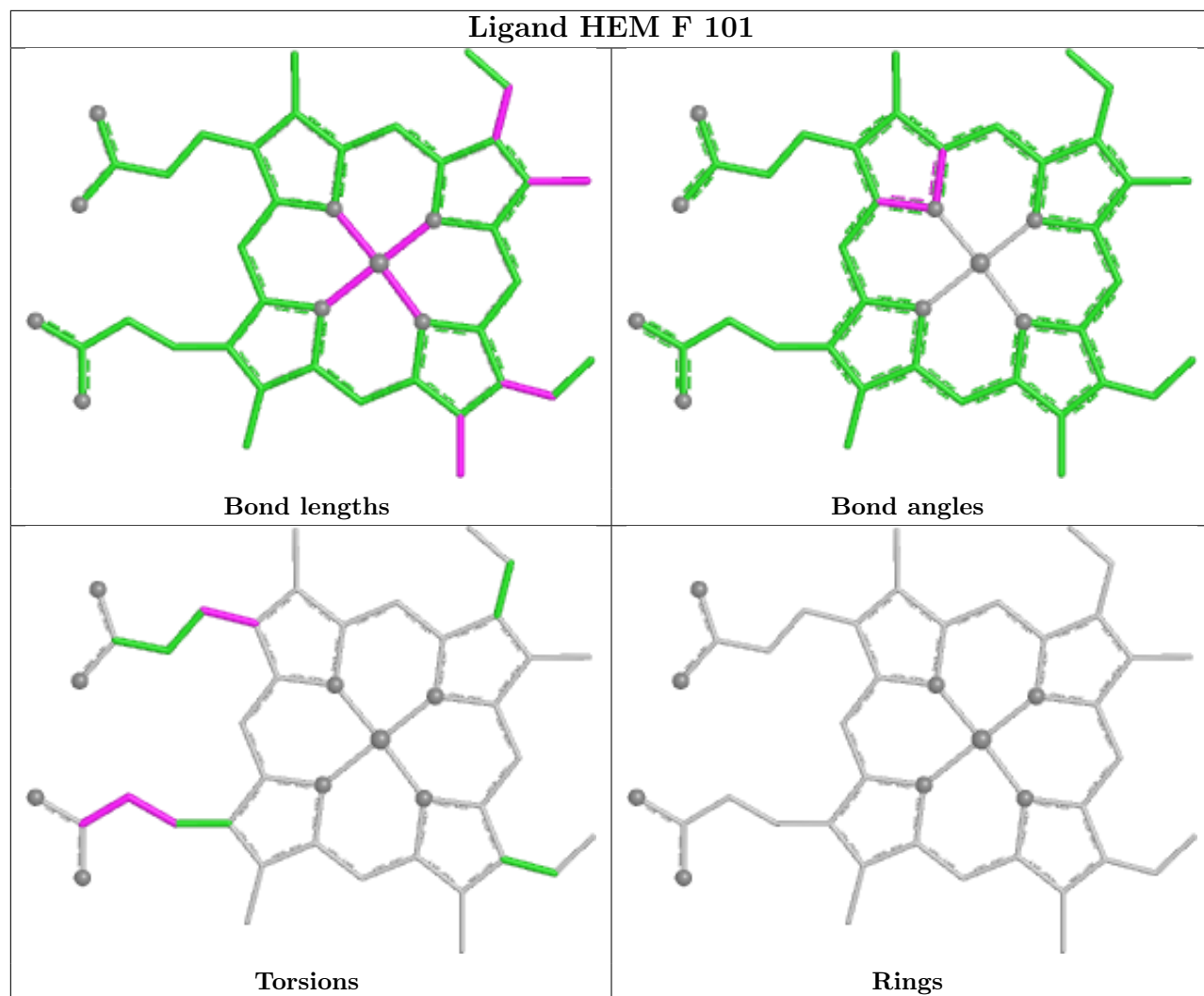


## Ligand CLA c 510

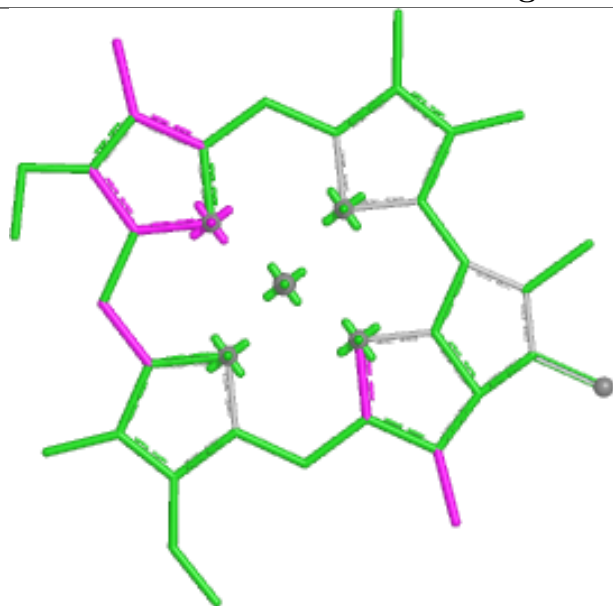


## Ligand CLA 5 307

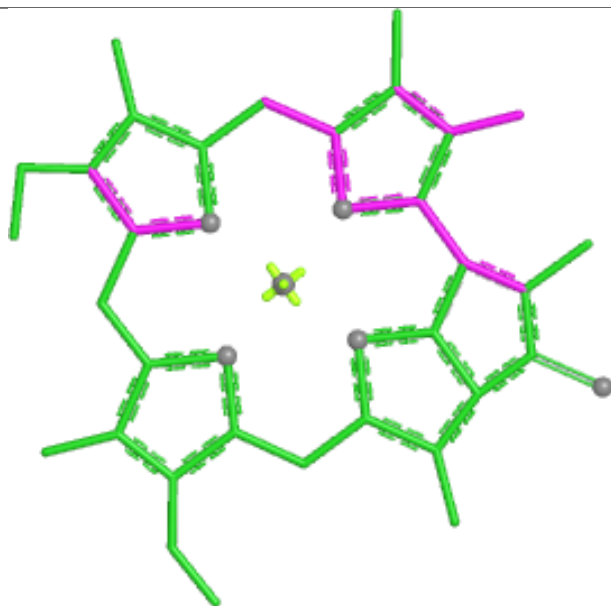




## Ligand CLA 1 215



Bond lengths



Bond angles

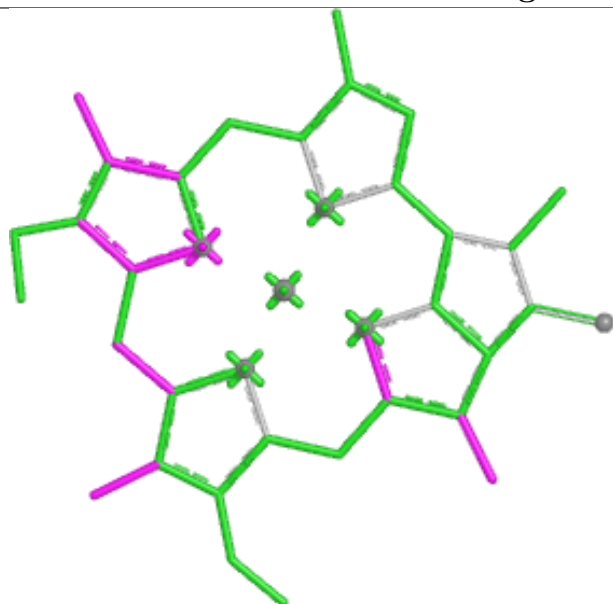


Torsions

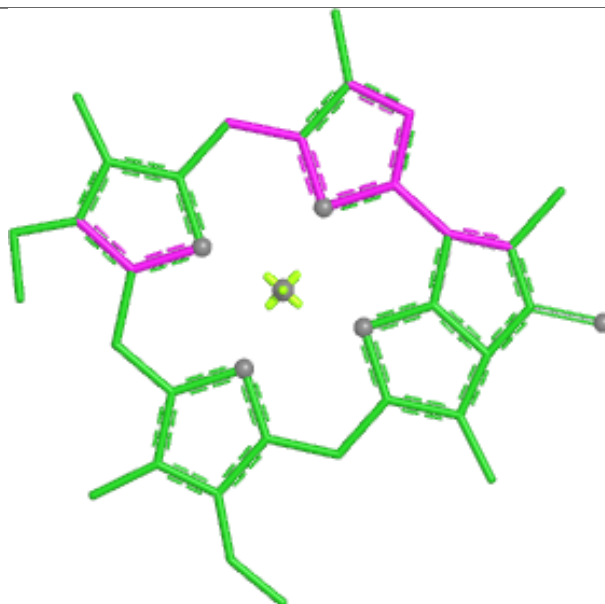


Rings

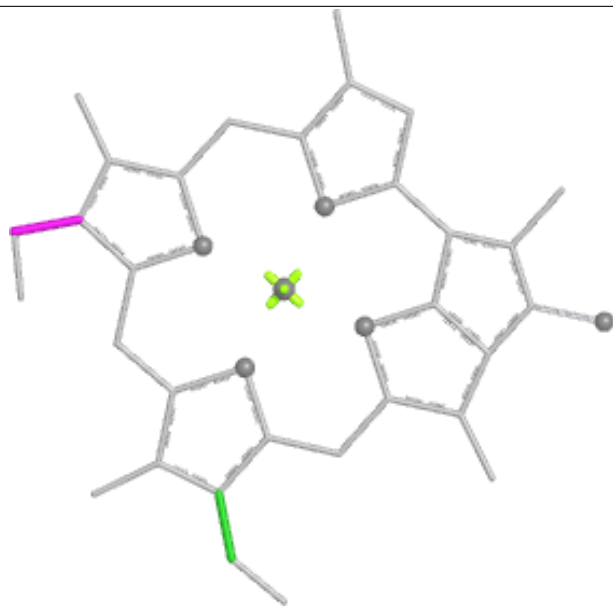
## Ligand CLA 9 206



Bond lengths



Bond angles

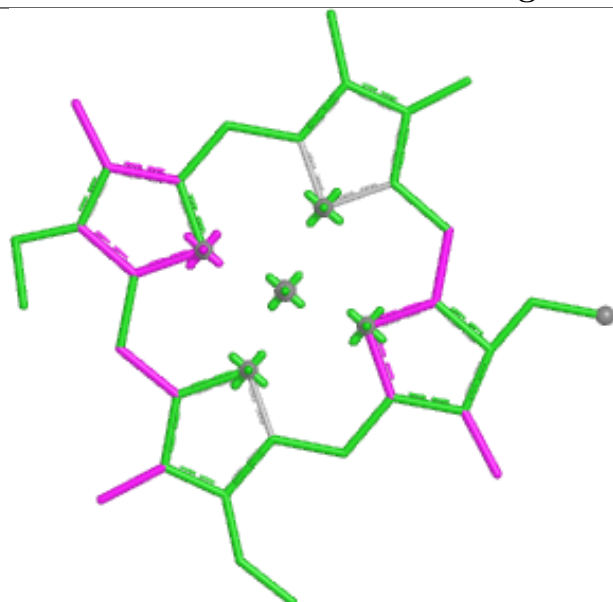


Torsions

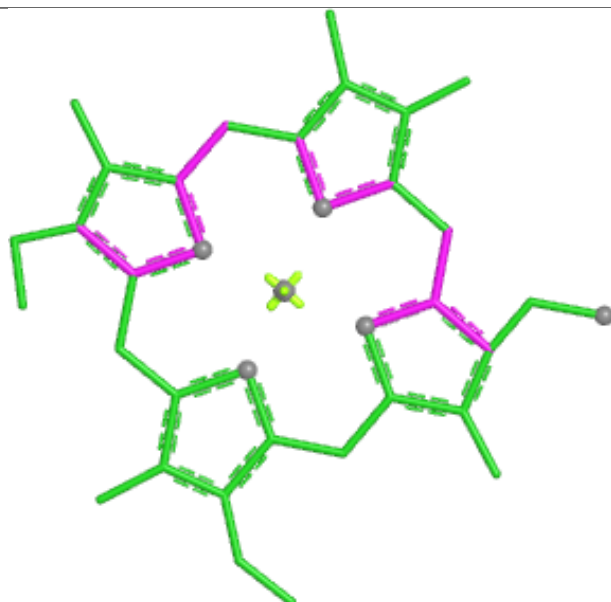


Rings

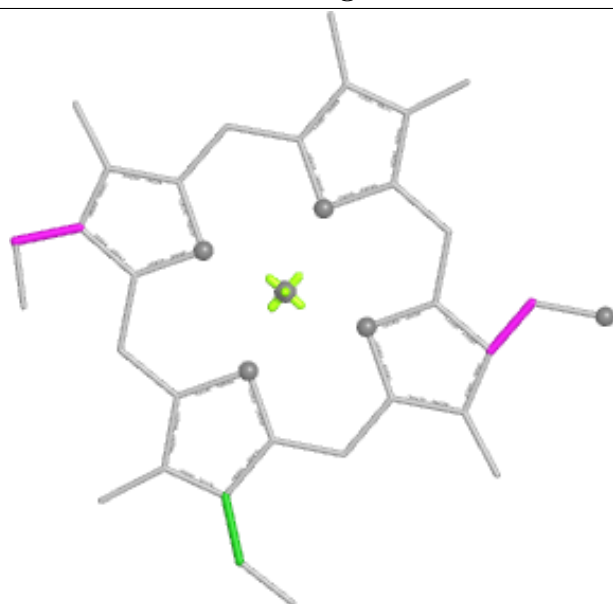
## Ligand CLA 3 308



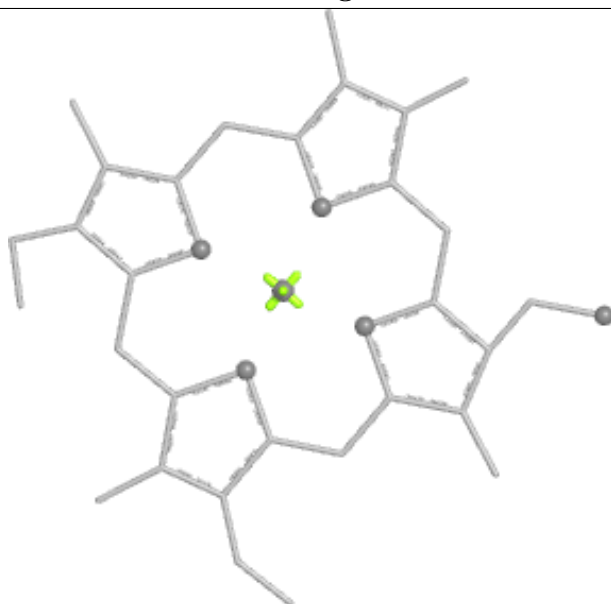
Bond lengths



Bond angles

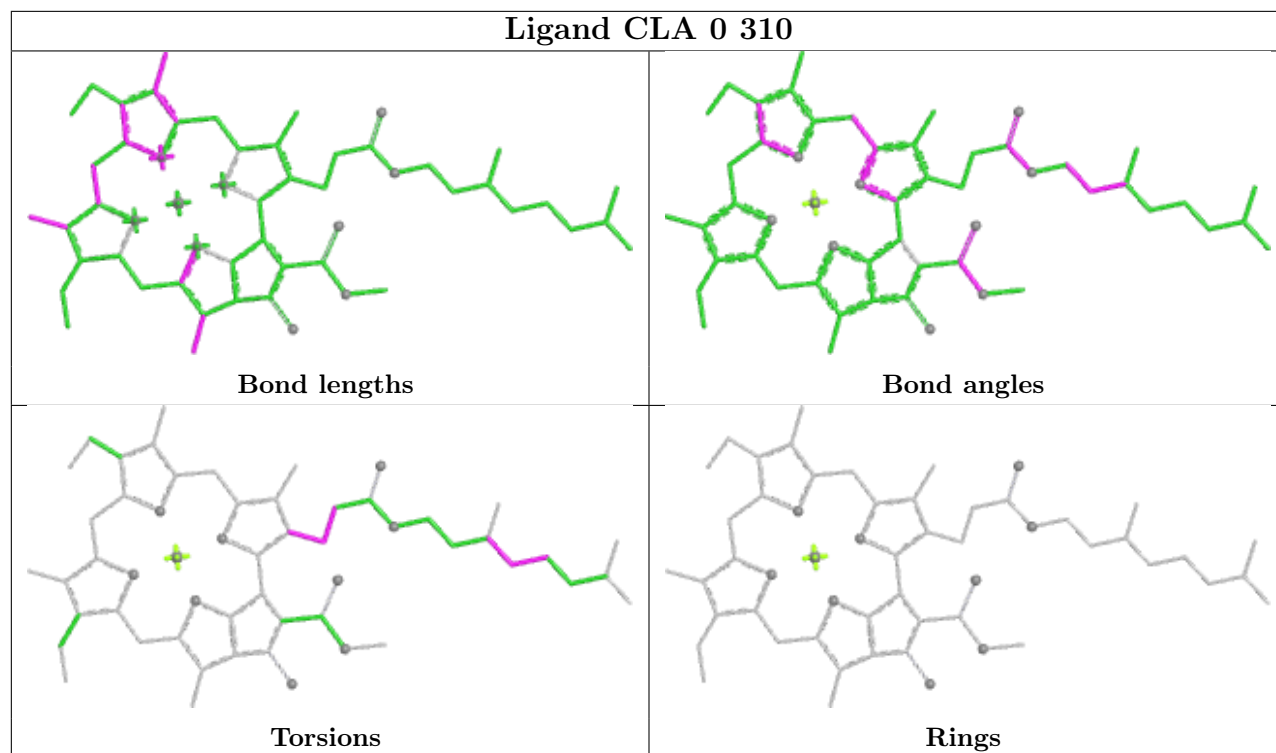
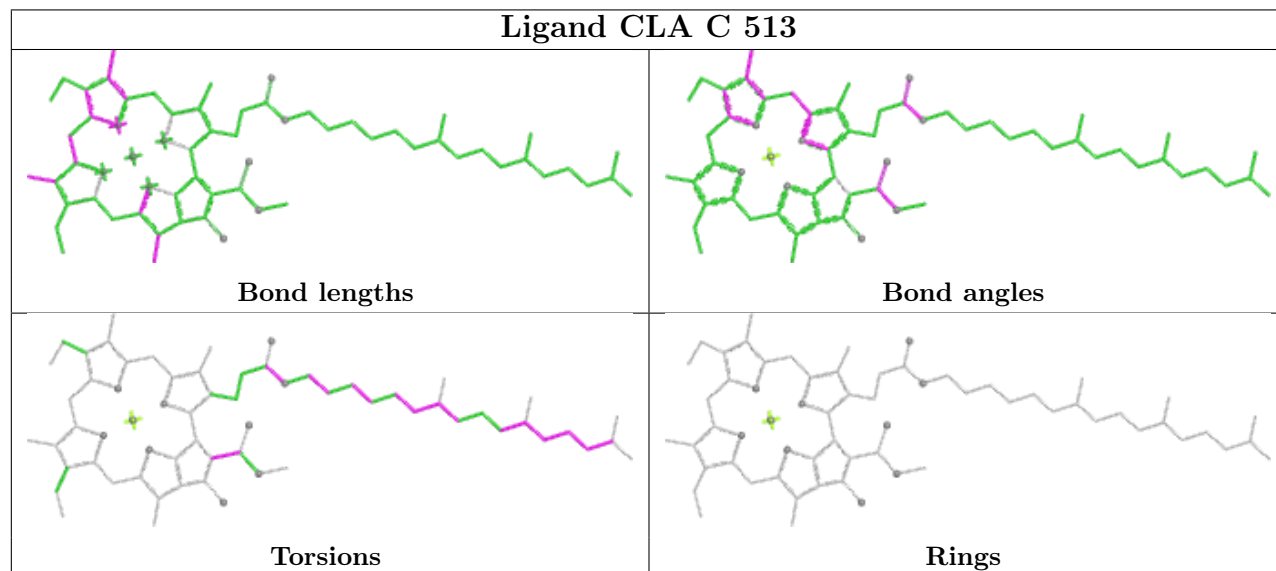


Torsions

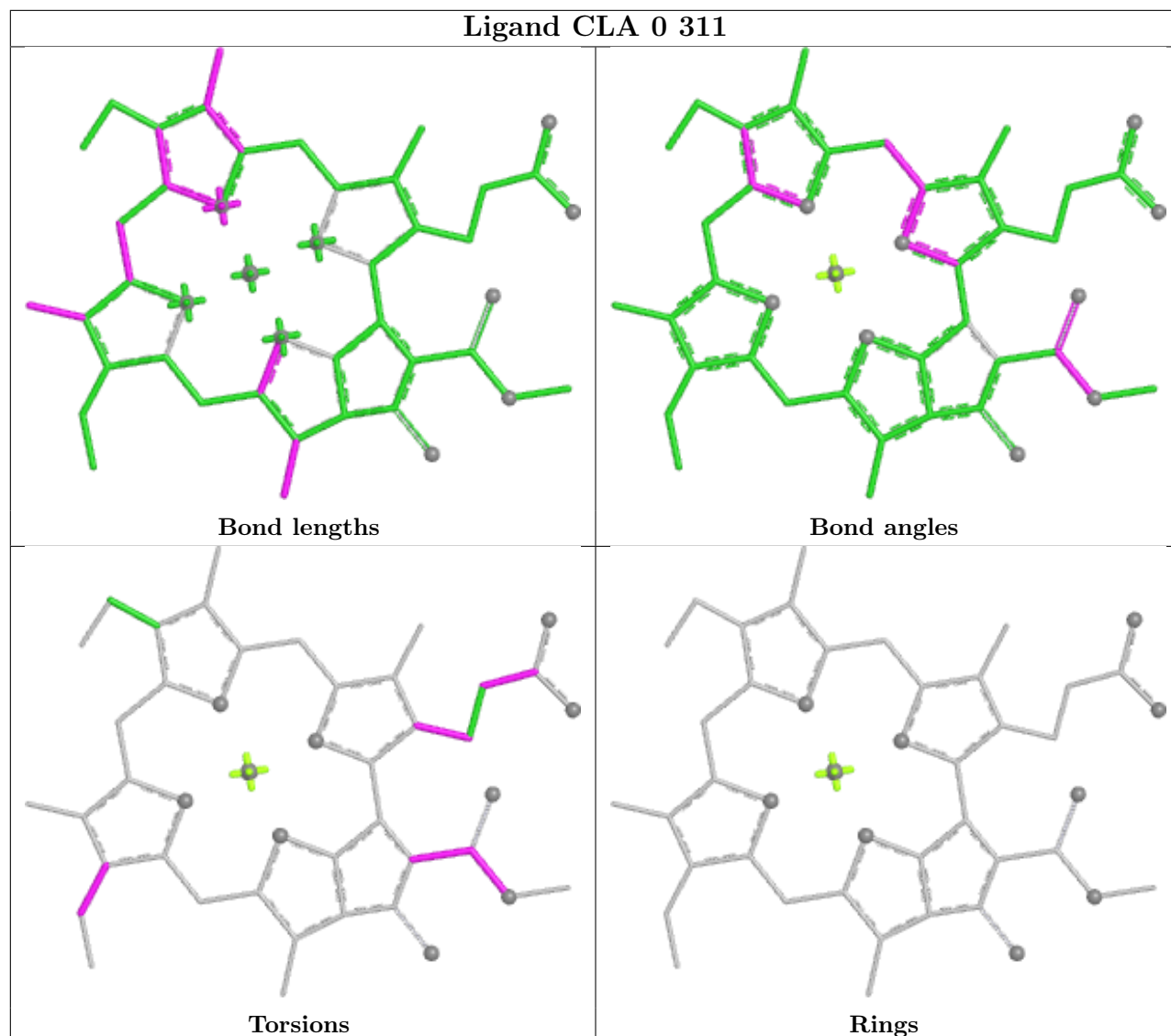


Rings

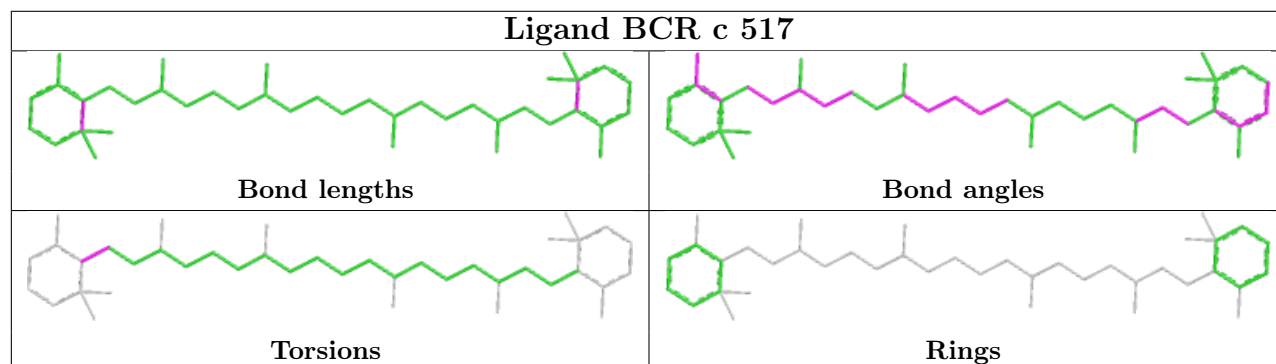


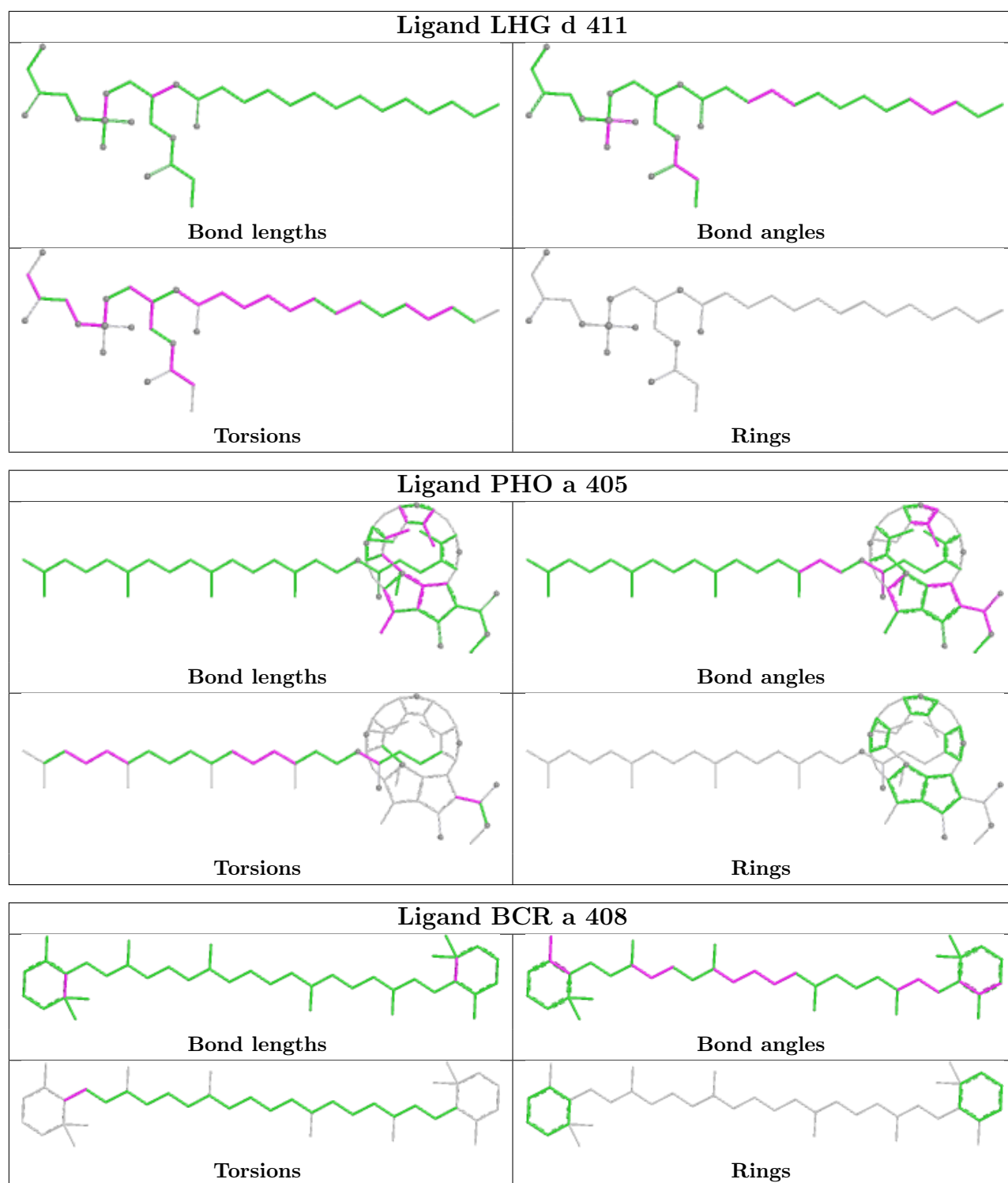
**Ligand CLA 0 310****Ligand CLA C 513**

## Ligand CLA 0 311

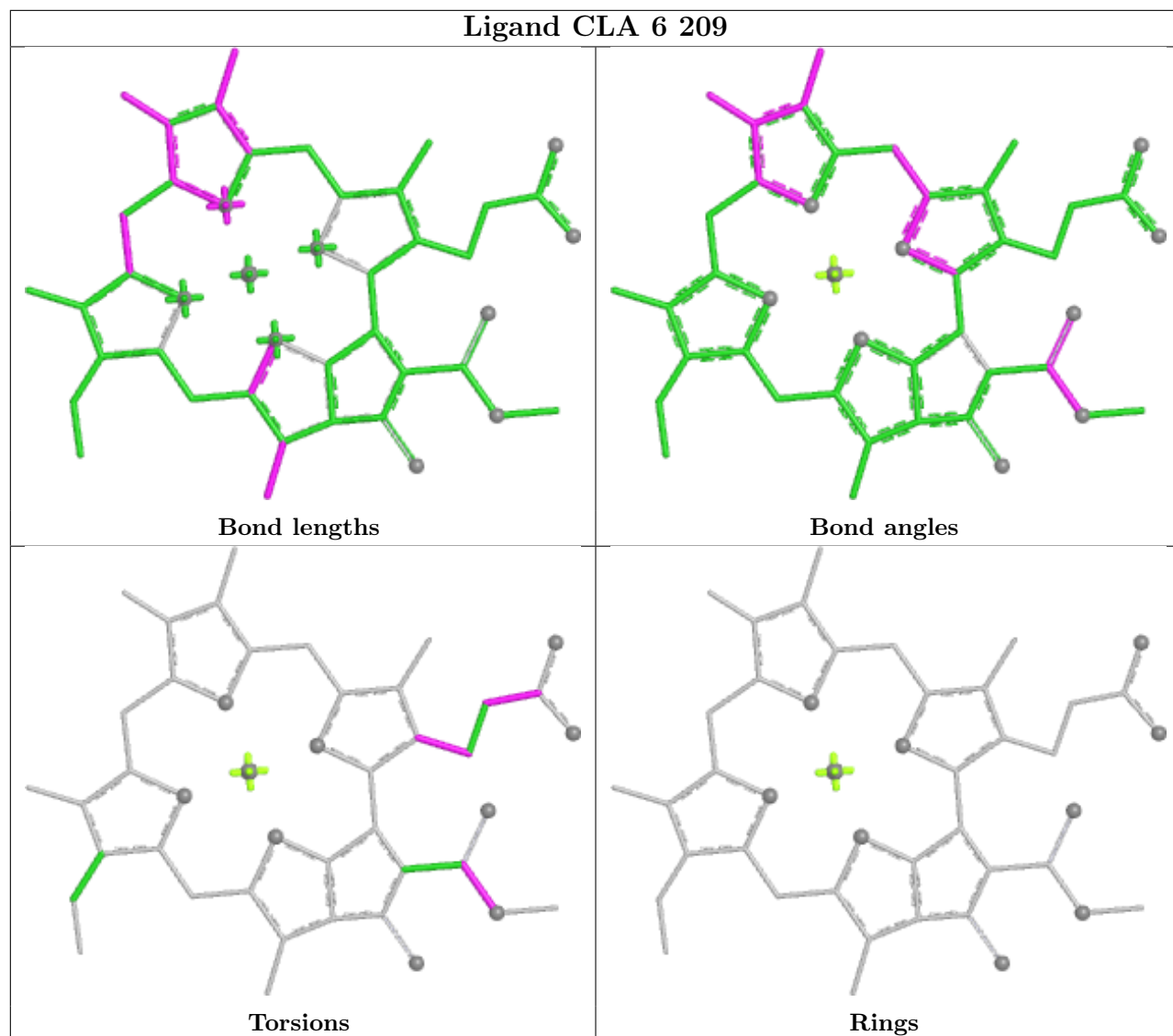


## Ligand BCR c 517

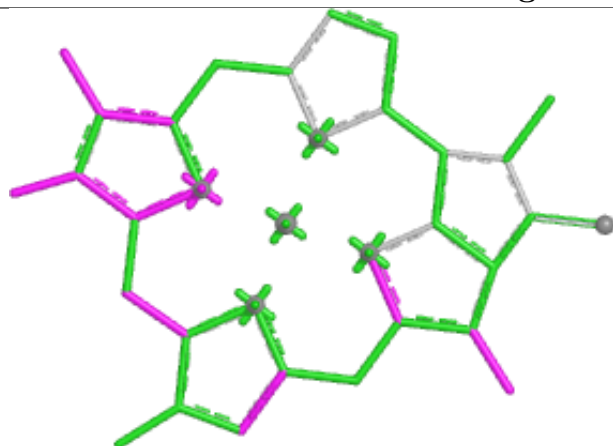




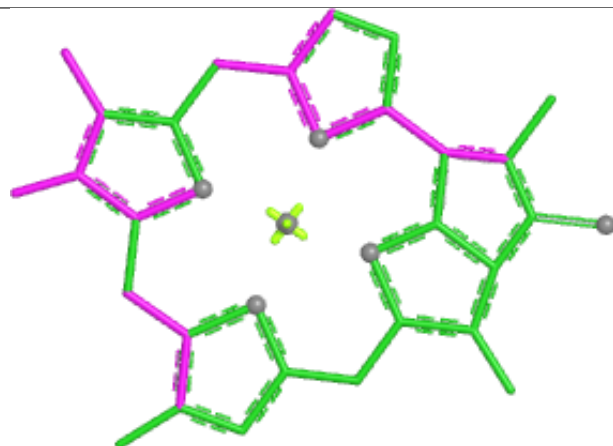
## Ligand CLA 6 209



## Ligand CLA 8 306



Bond lengths



Bond angles

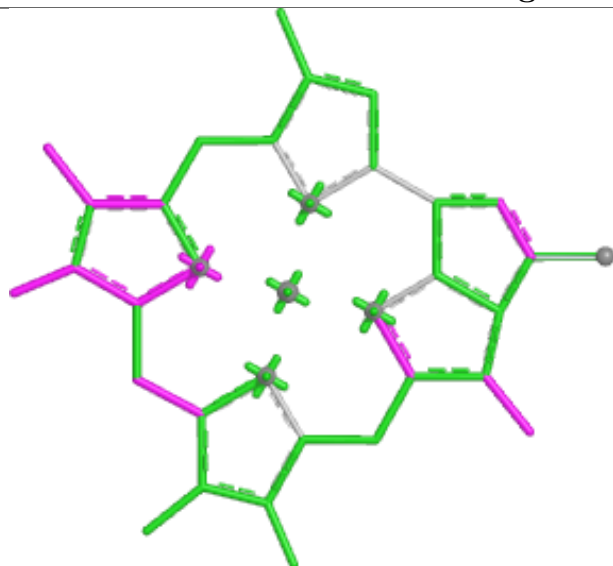


Torsions

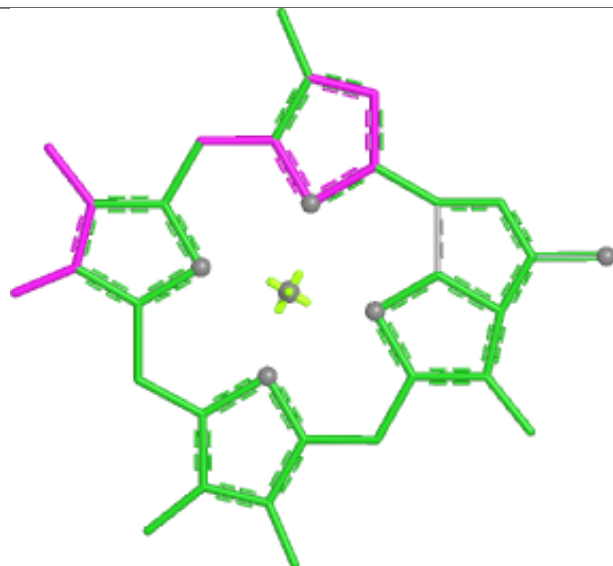


Rings

## Ligand CLA 4 211



Bond lengths



Bond angles

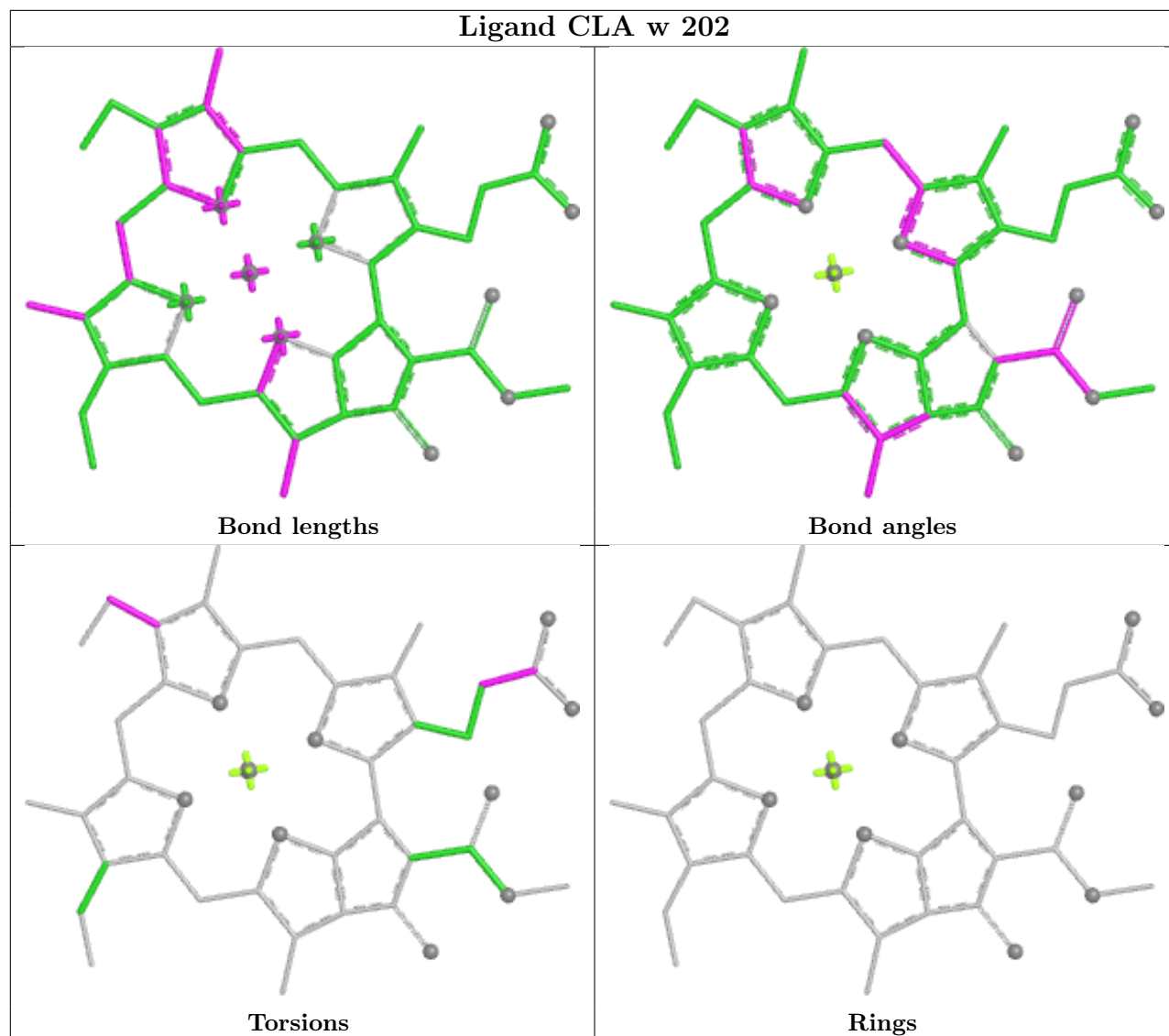


Torsions

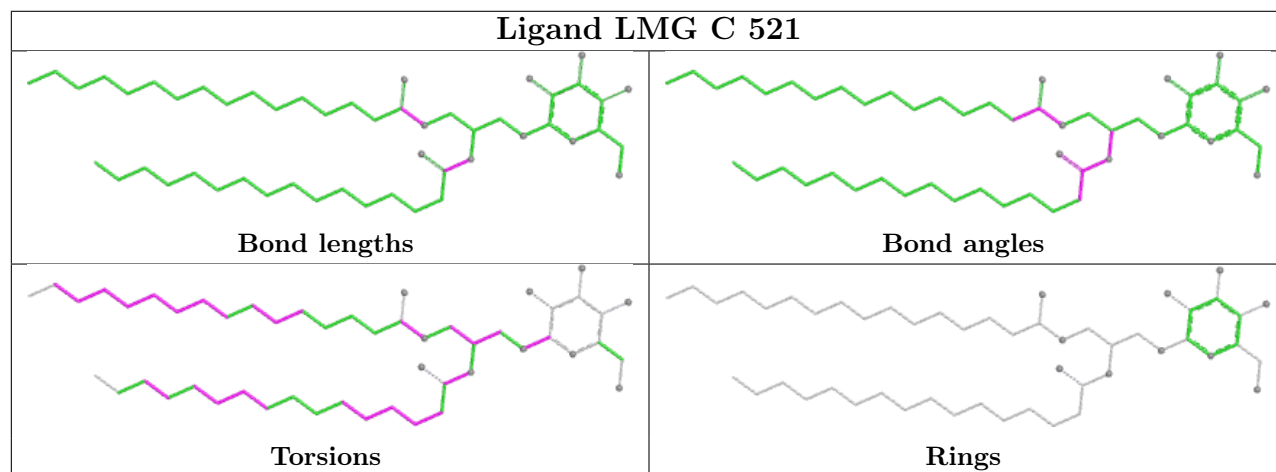


Rings

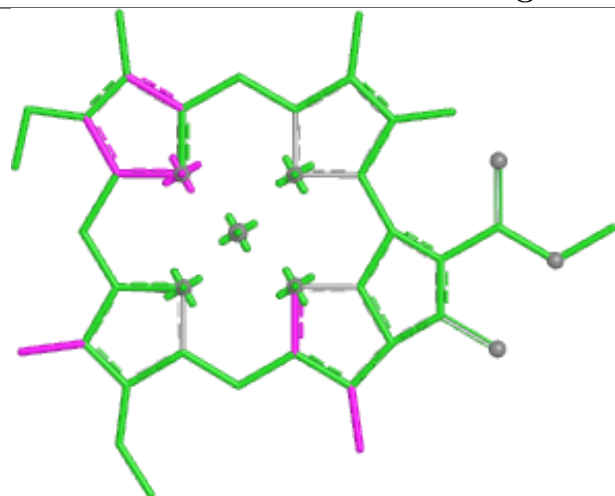
## Ligand CLA w 202



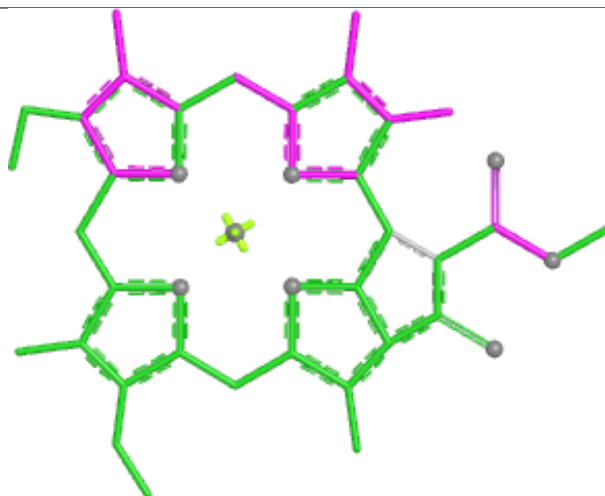
## Ligand LMG C 521



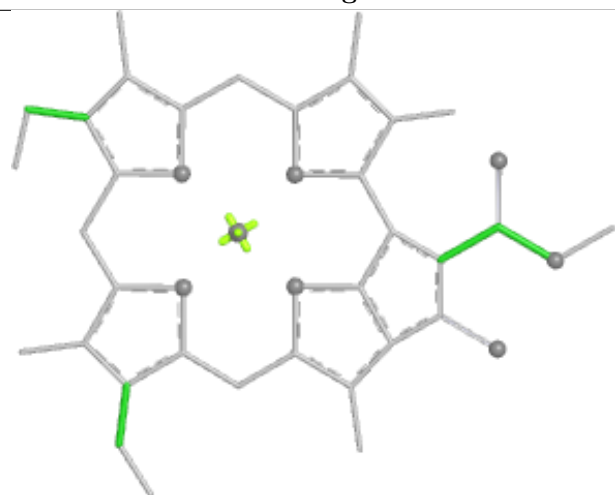
## Ligand CLA B 512



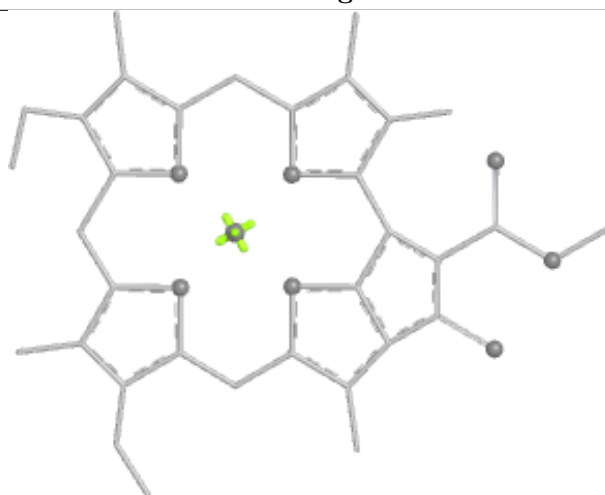
Bond lengths



Bond angles

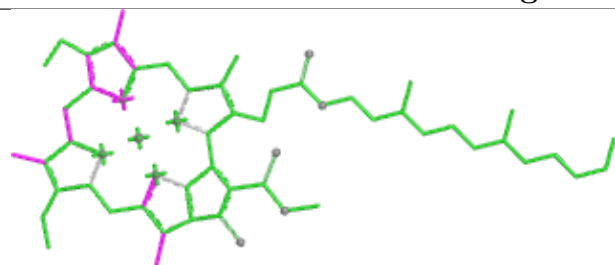


Torsions

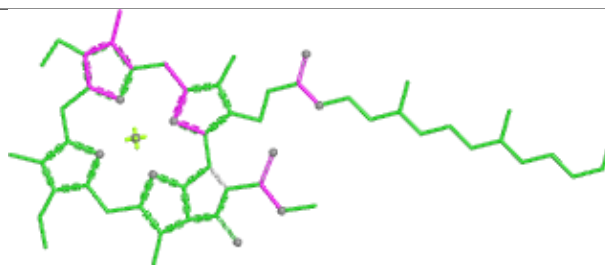


Rings

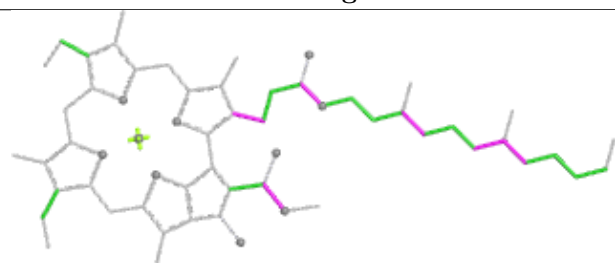
## Ligand CLA 2 309



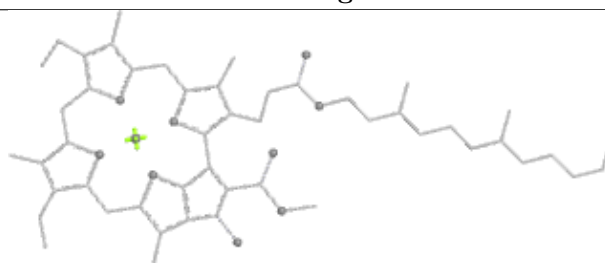
Bond lengths



Bond angles



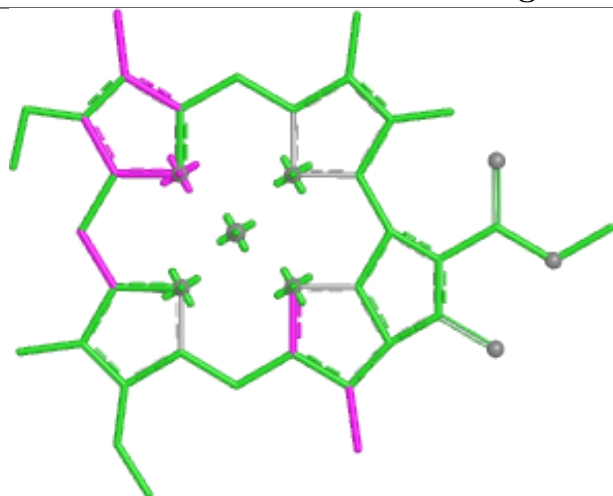
Torsions



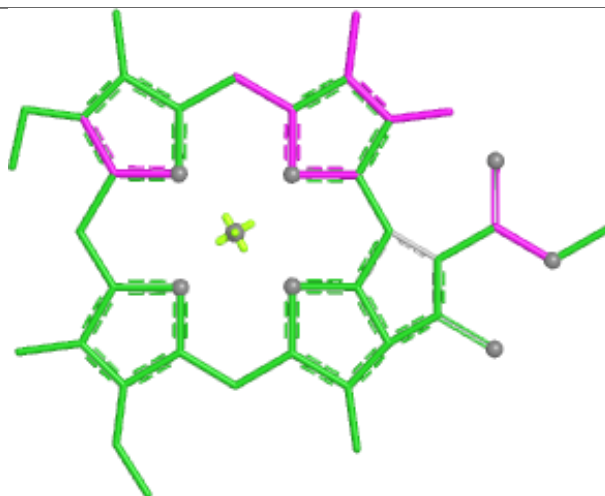
Rings



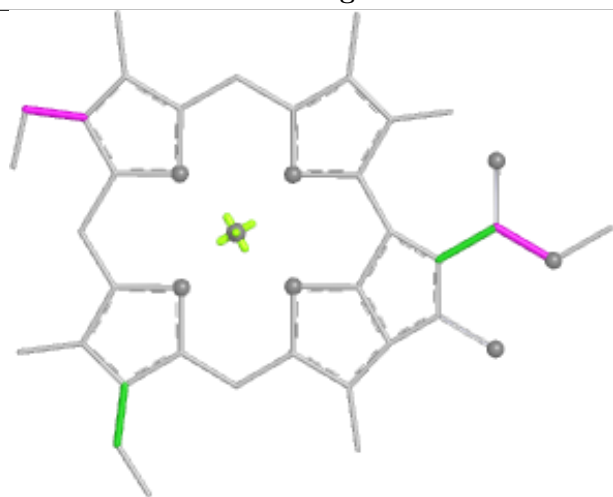
## Ligand CLA 5 304



Bond lengths



Bond angles

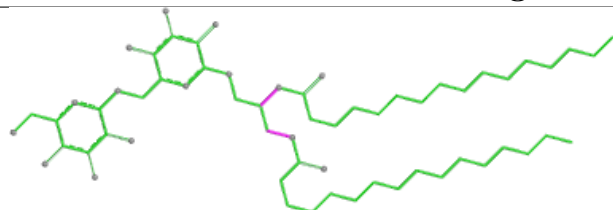


Torsions

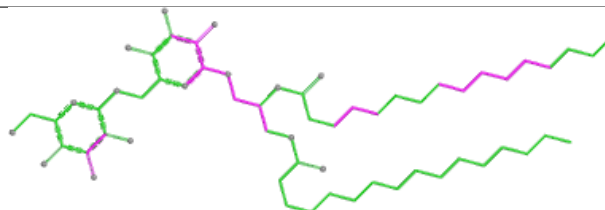


Rings

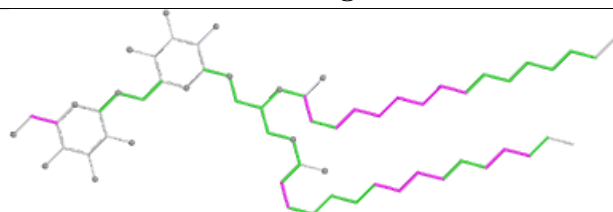
## Ligand DGD H 102



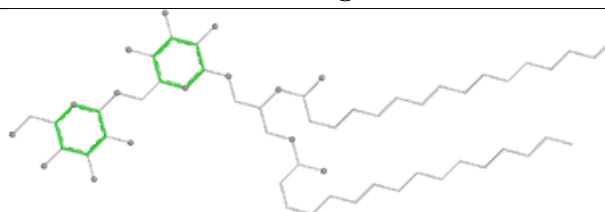
Bond lengths



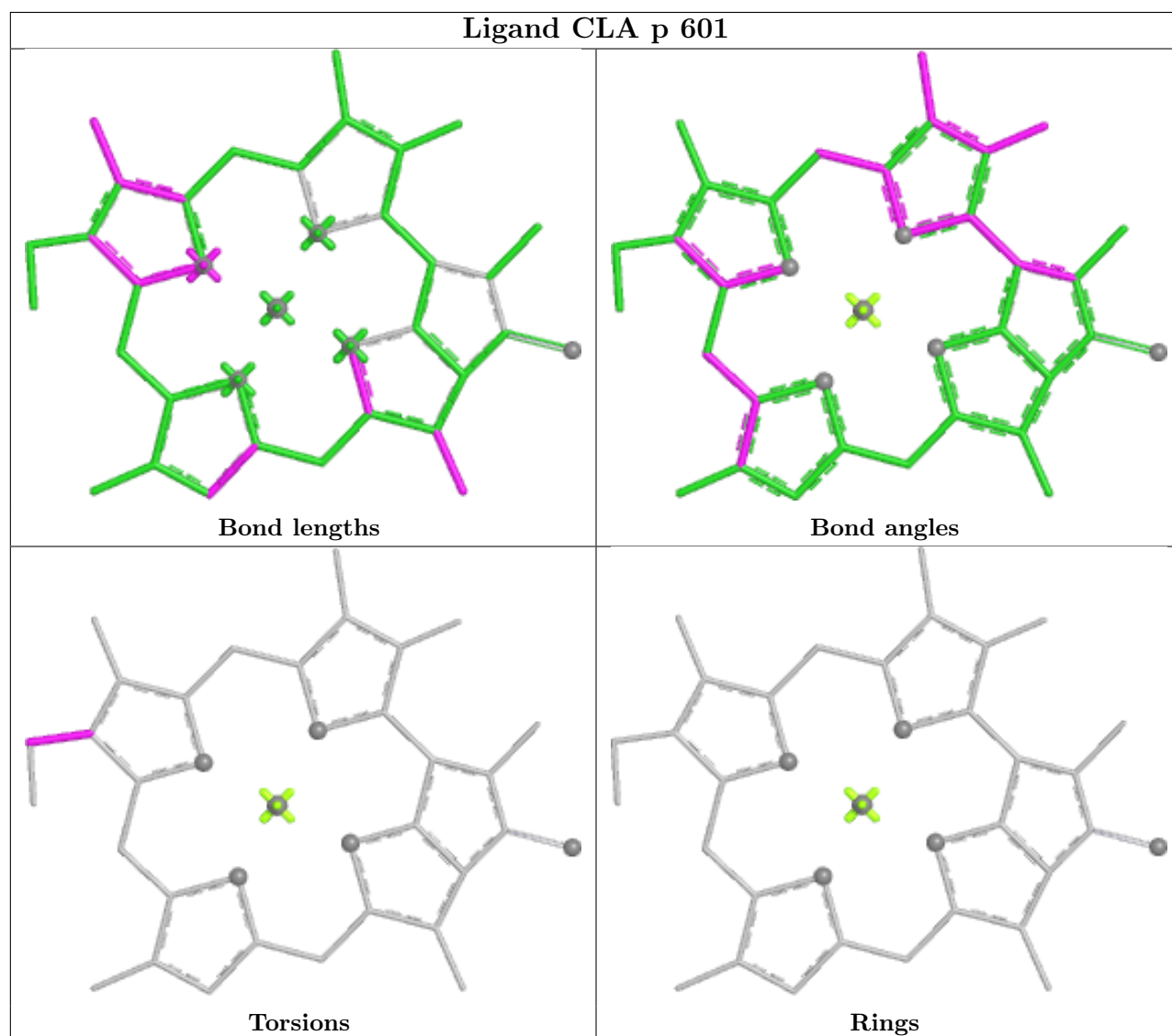
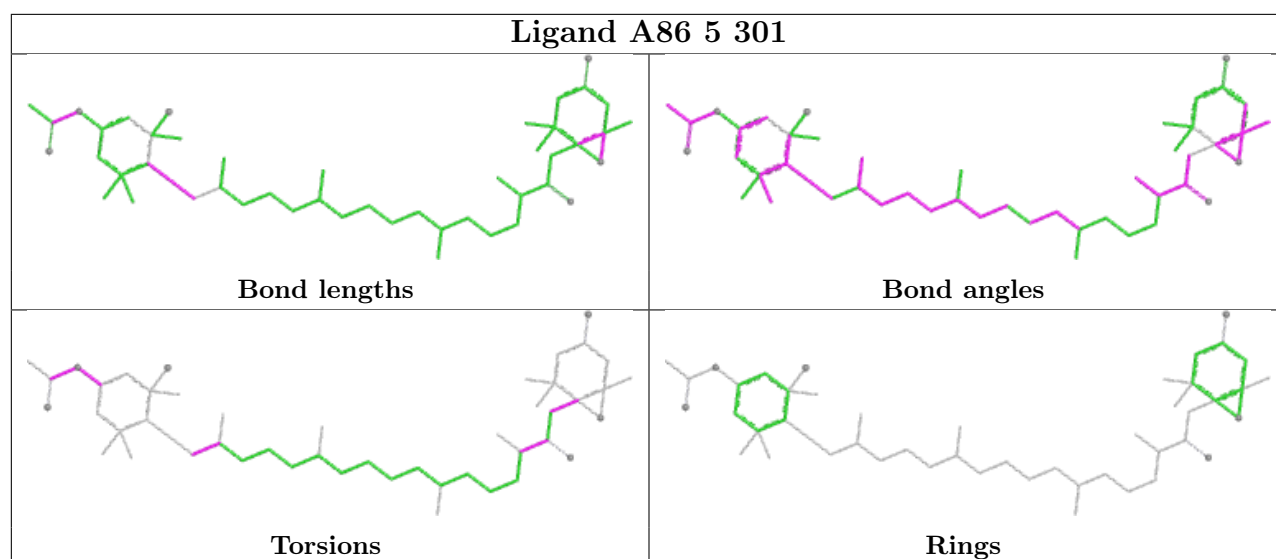
Bond angles

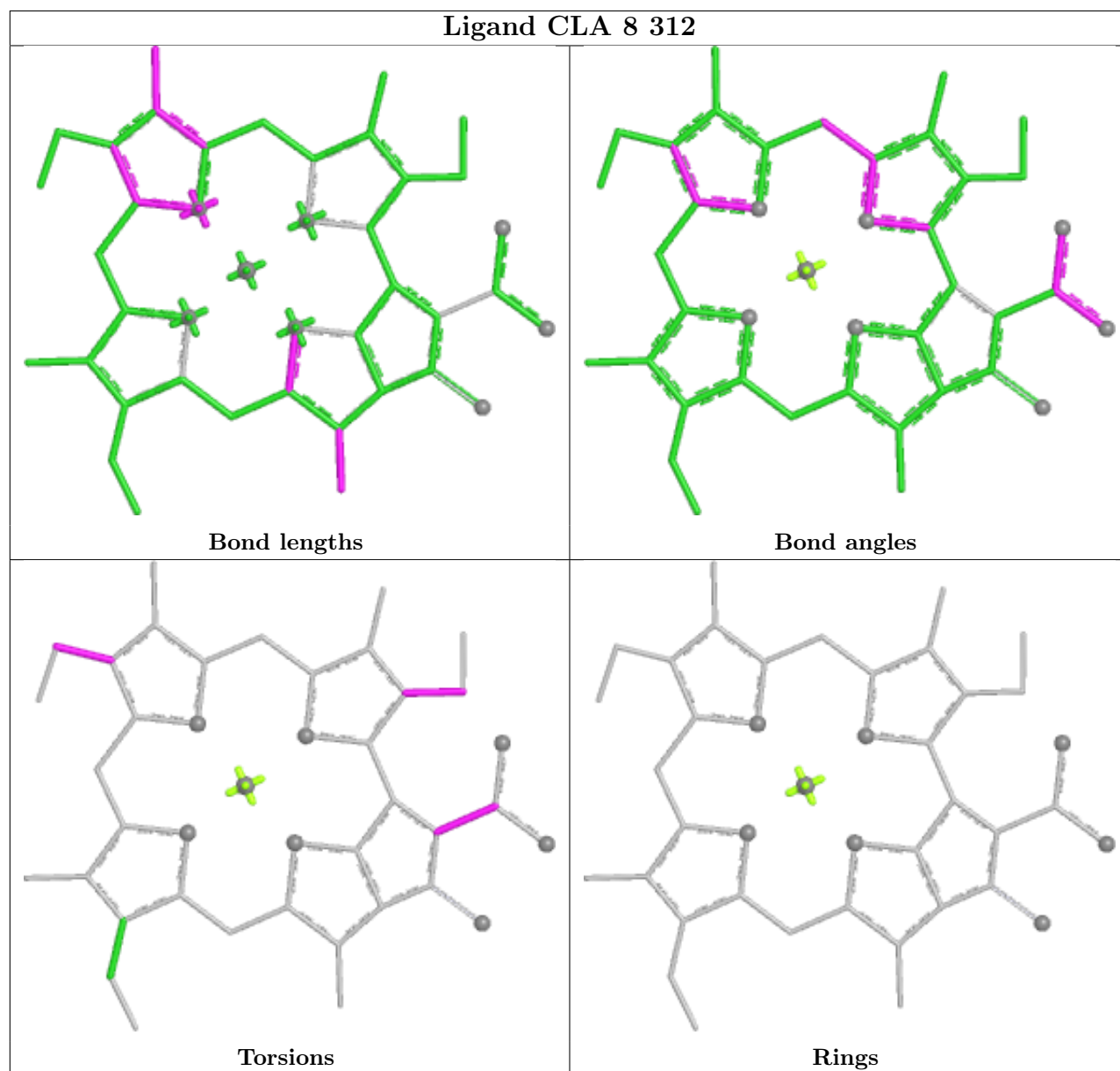
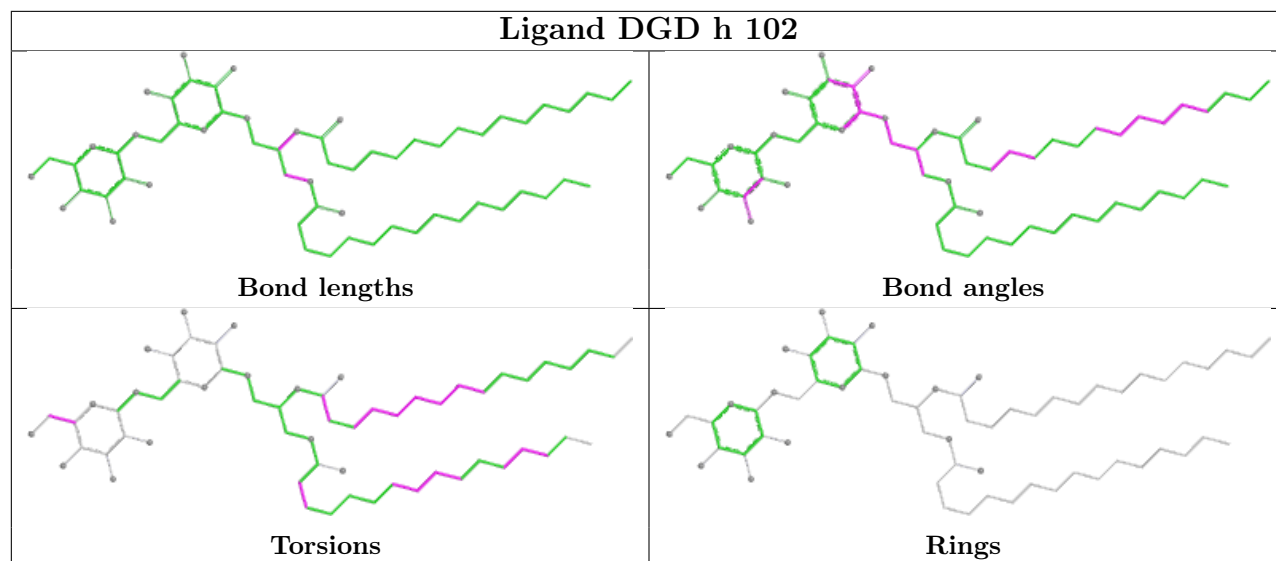


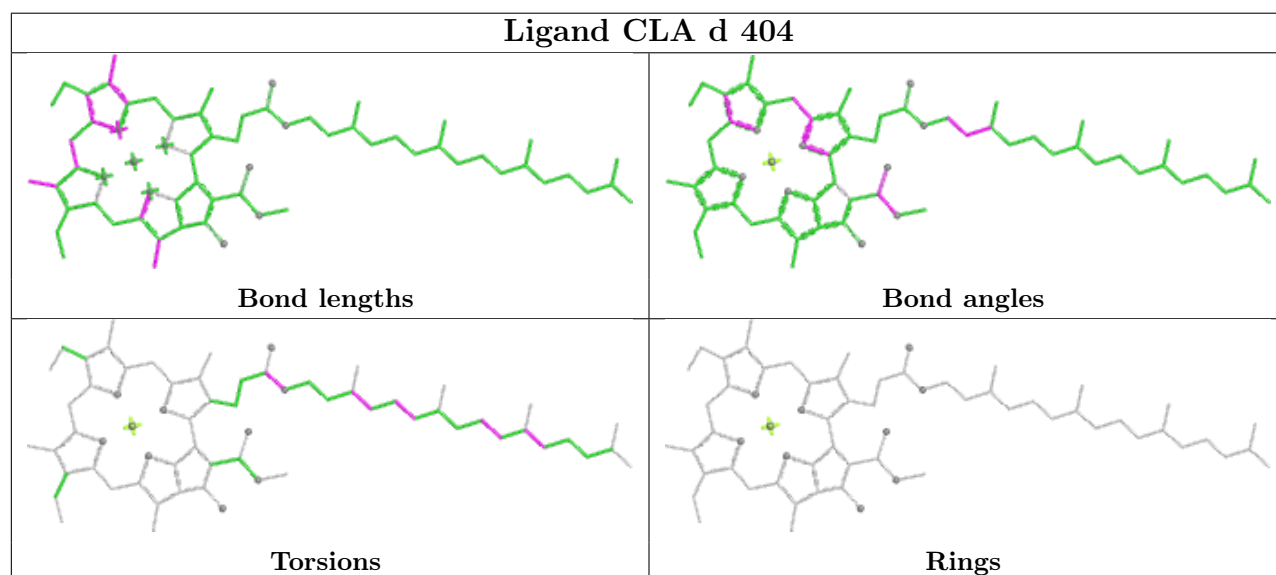
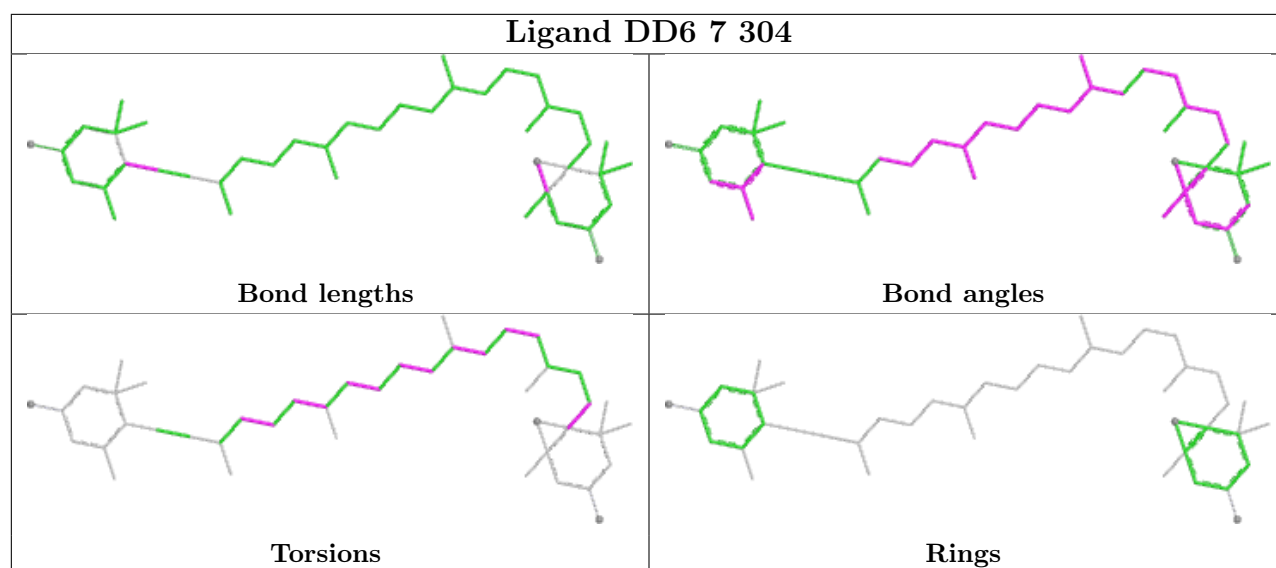
Torsions



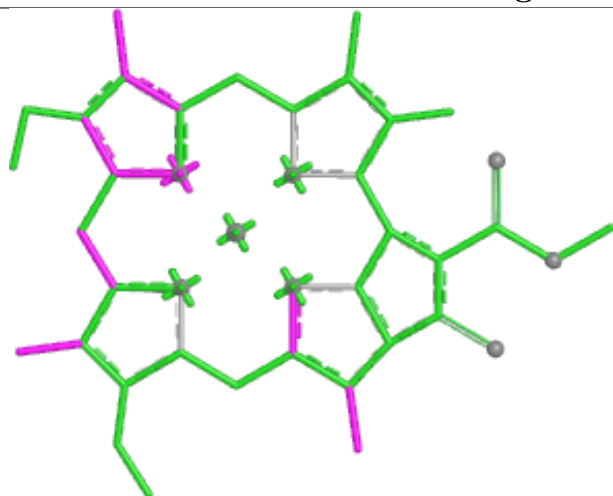
Rings



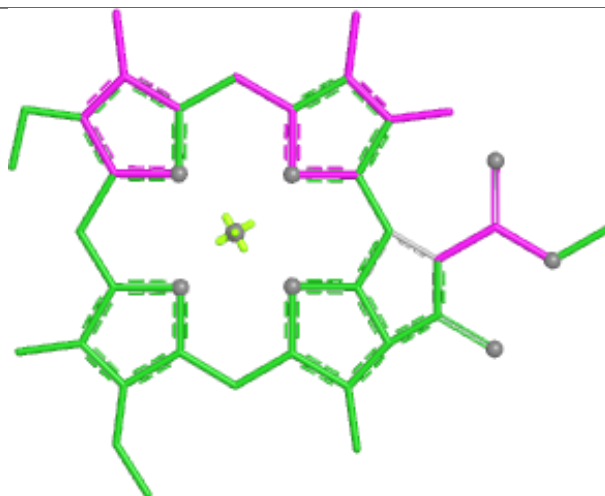




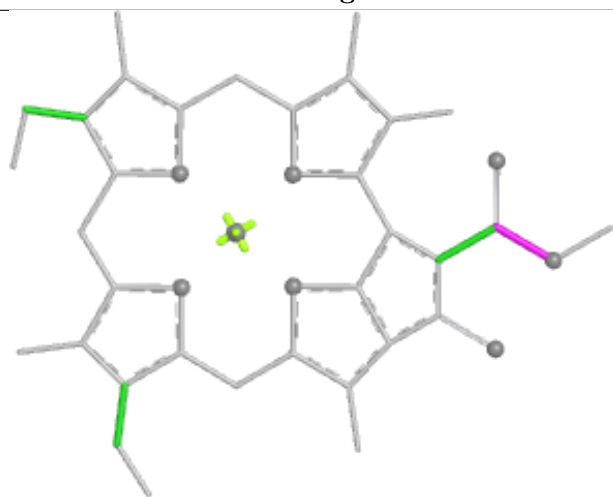
## Ligand CLA P 602



Bond lengths



Bond angles

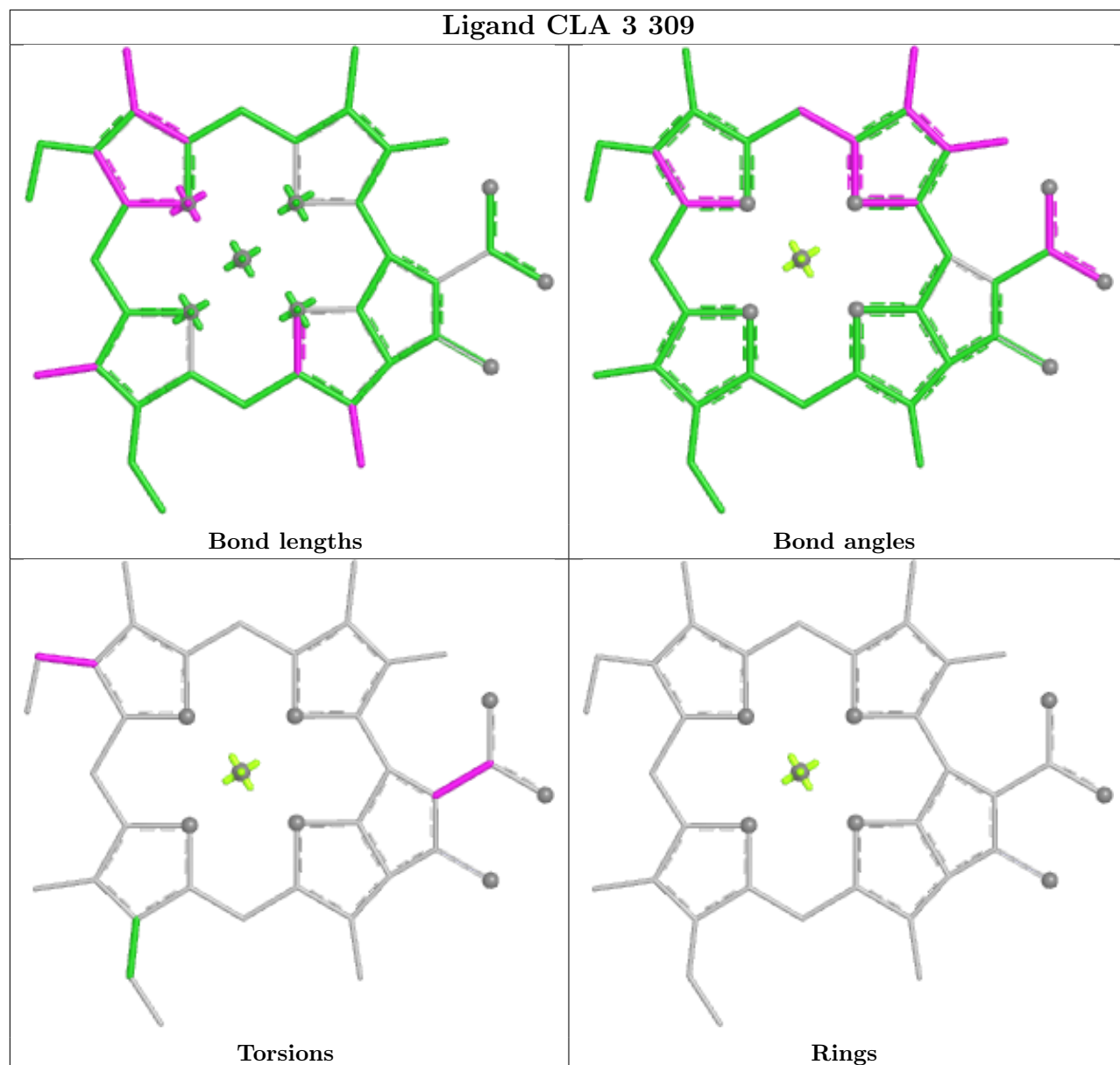


Torsions

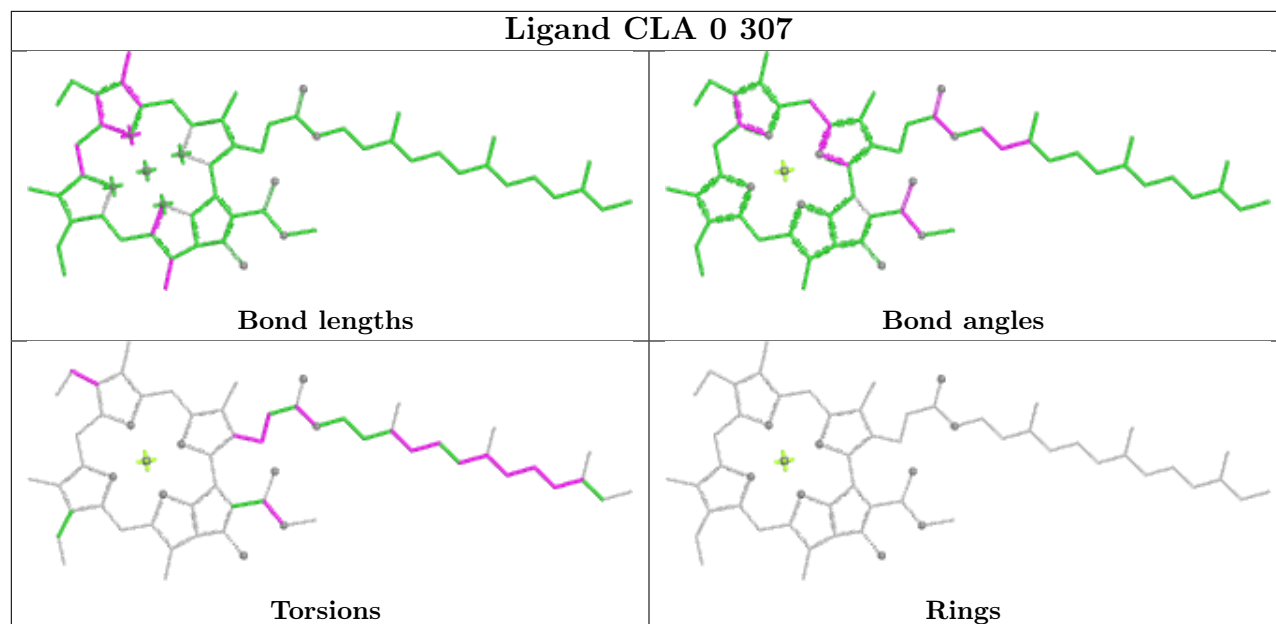


Rings

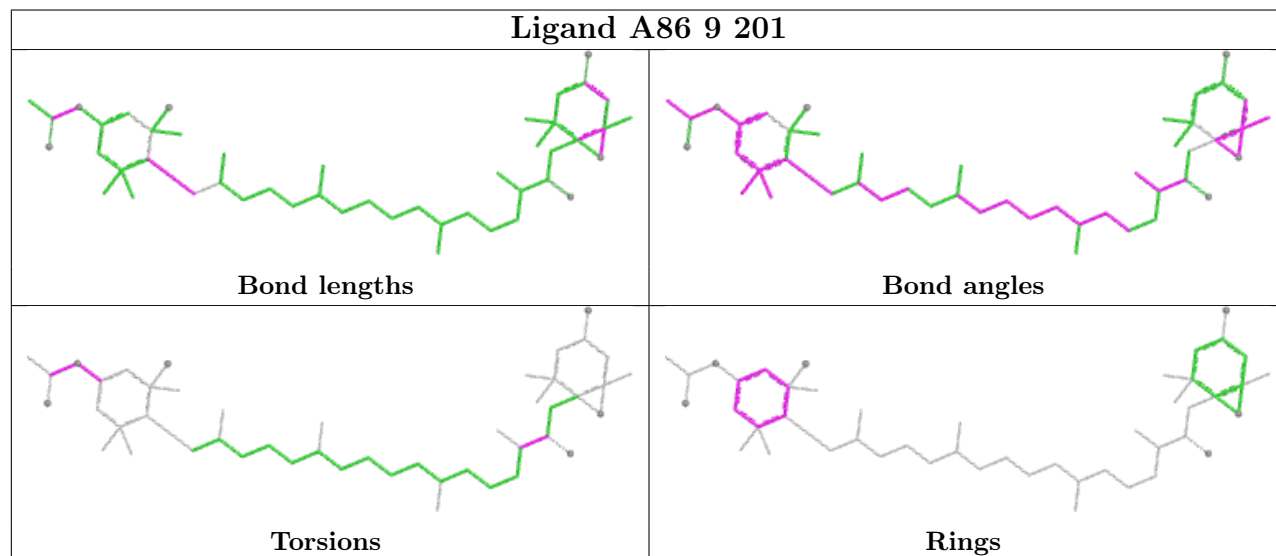
## Ligand CLA 3 309



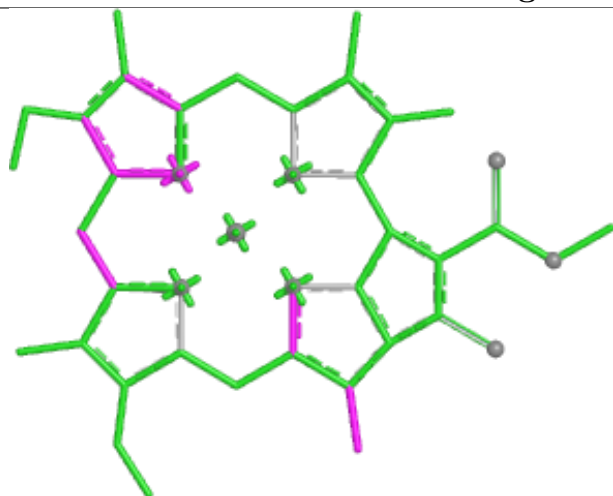
## Ligand CLA 0 307



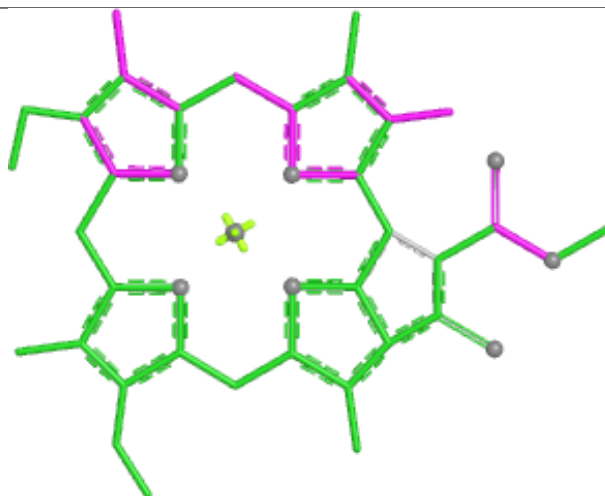
## Ligand A86 9 201



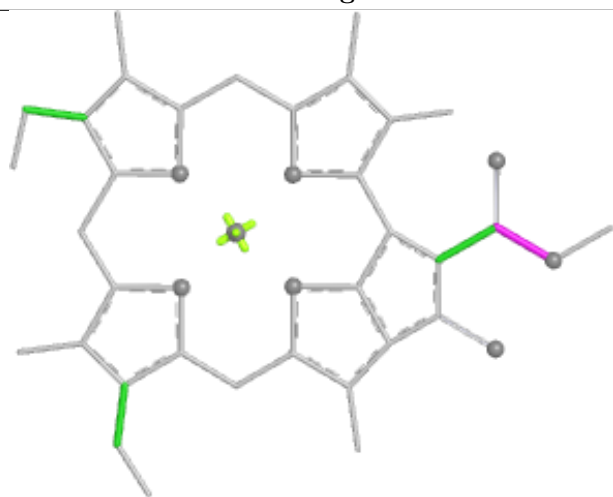
## Ligand CLA 1 212



Bond lengths



Bond angles



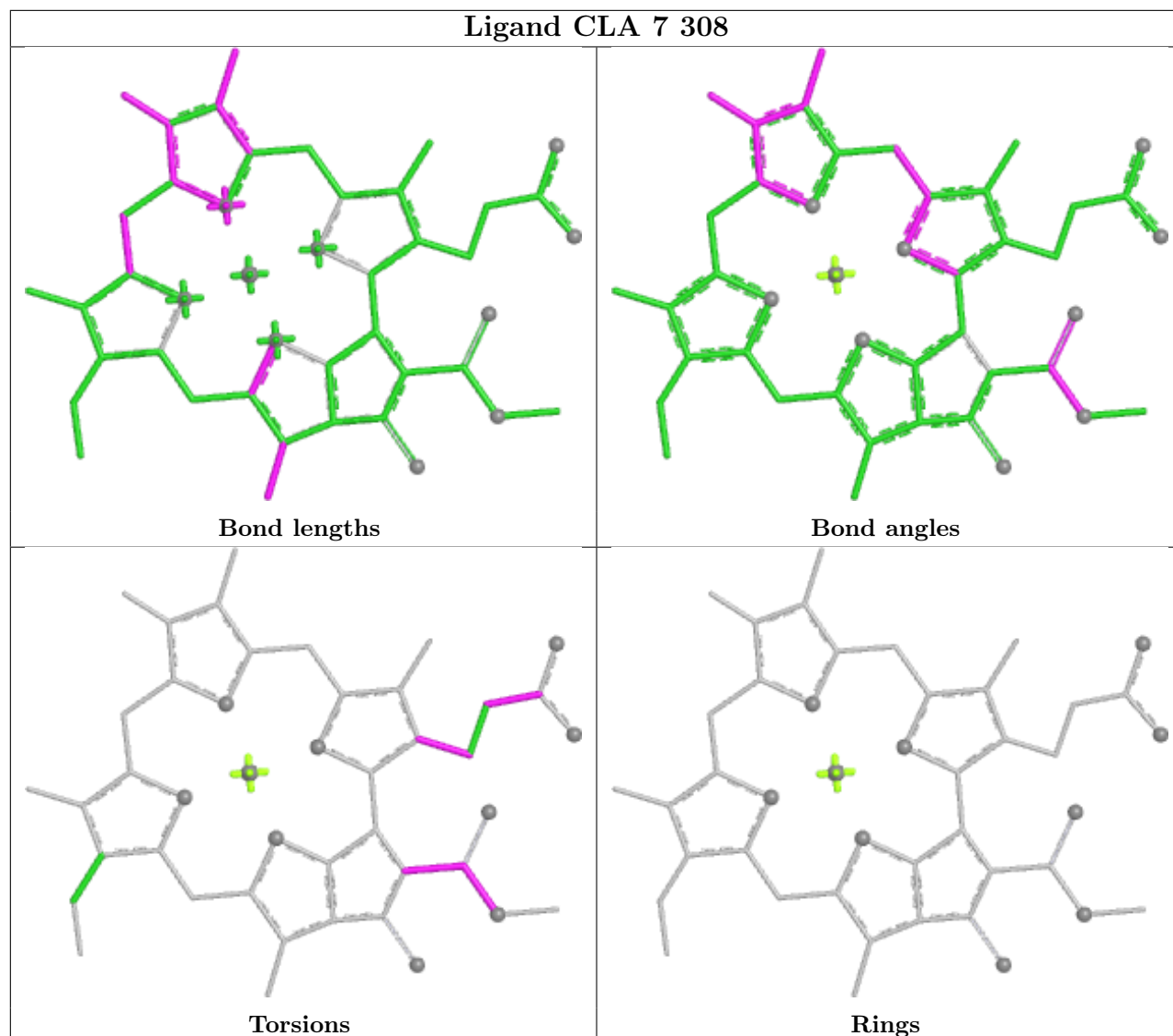
Torsions



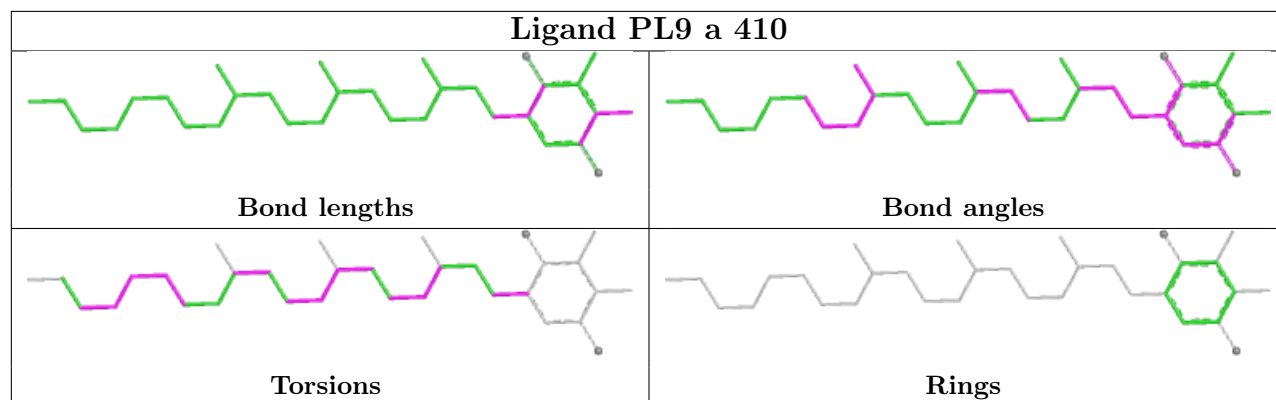
Rings



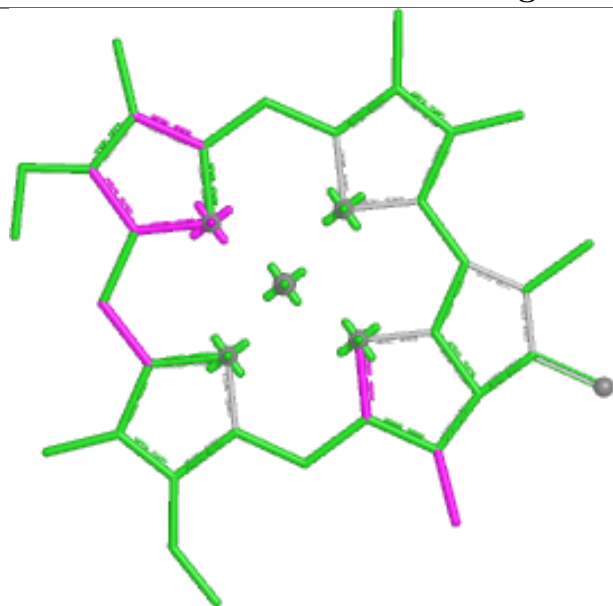
## Ligand CLA 7 308



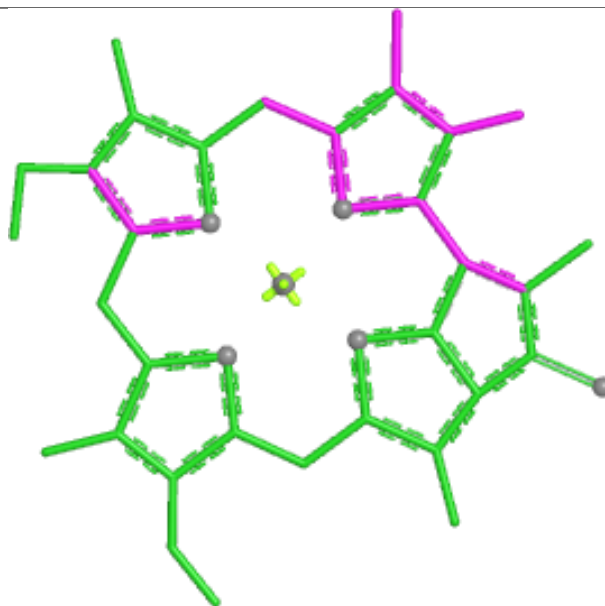
## Ligand PL9 a 410



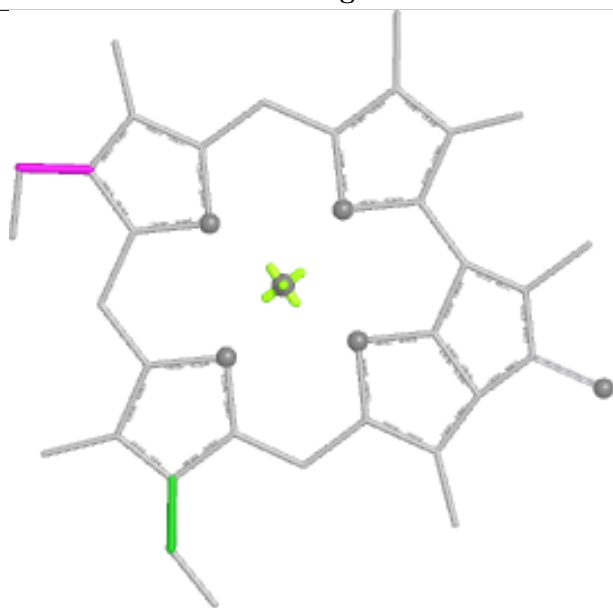
## Ligand CLA 2 313



Bond lengths



Bond angles

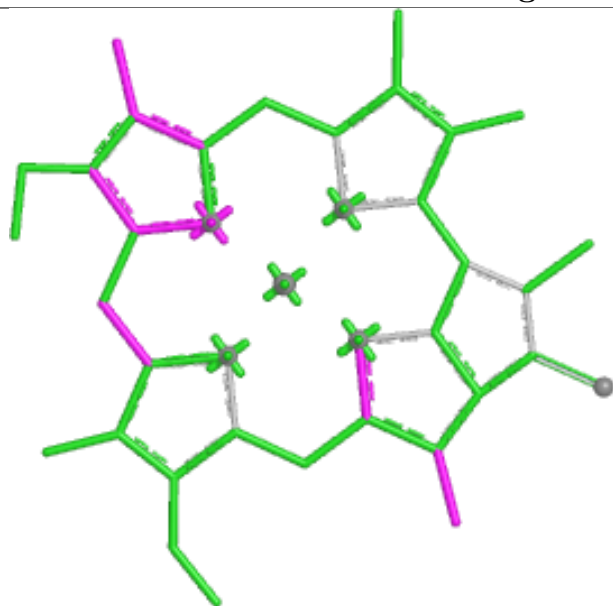


Torsions

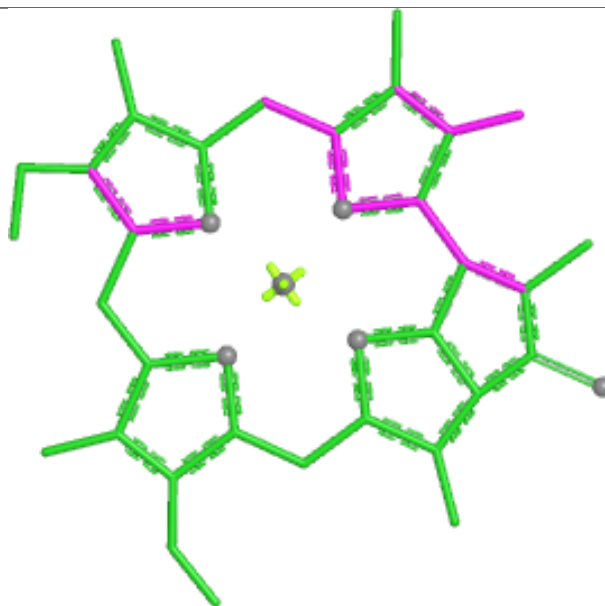


Rings

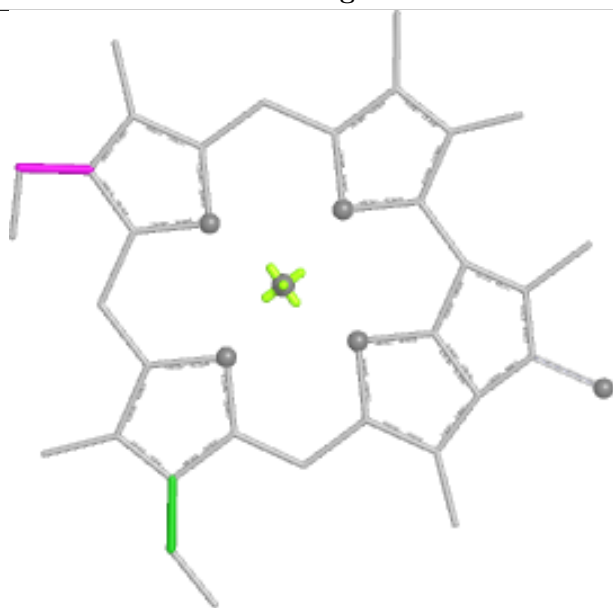
## Ligand CLA 0 313



Bond lengths



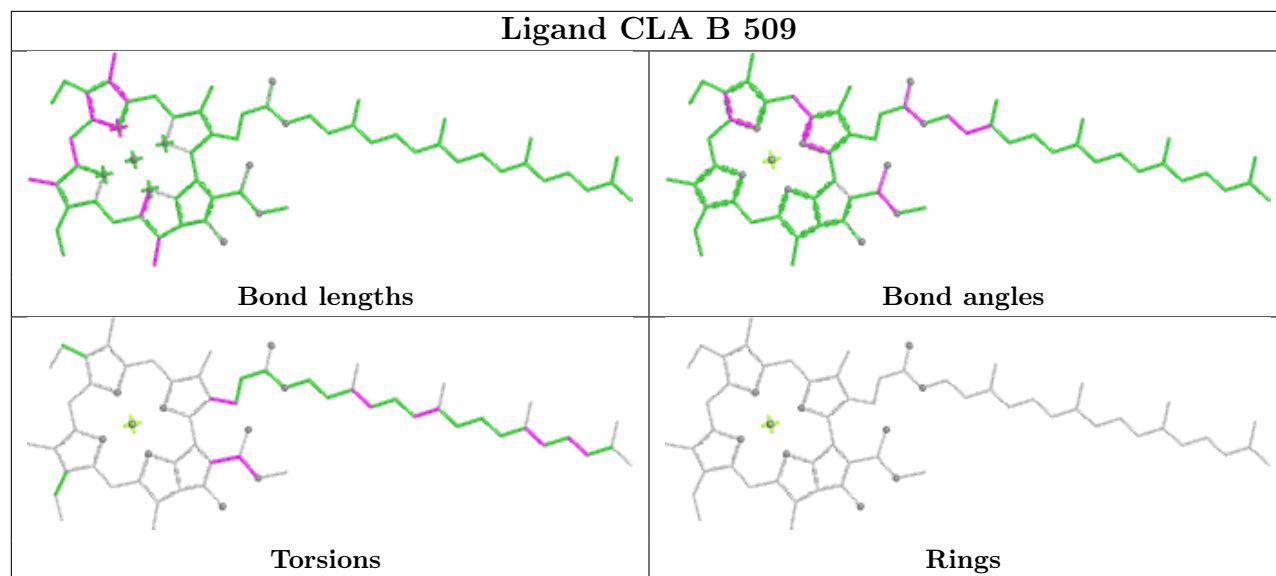
Bond angles



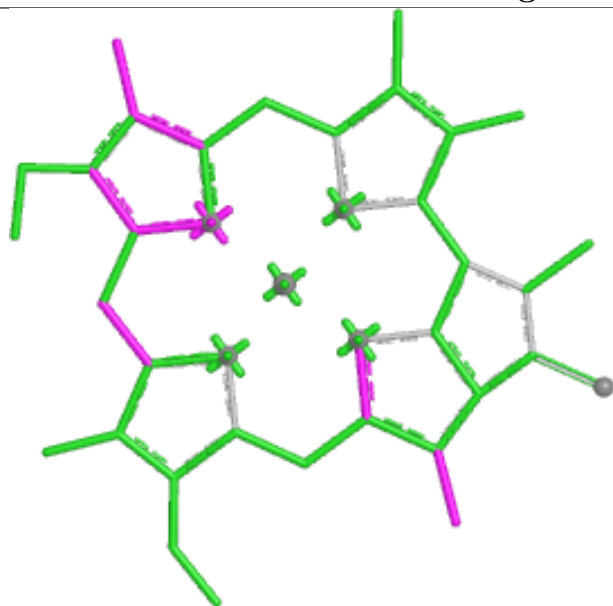
Torsions



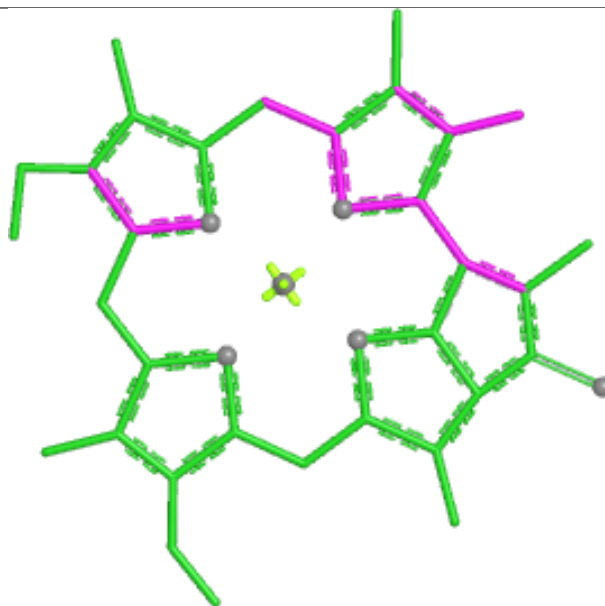
Rings



## Ligand CLA 6 215



Bond lengths



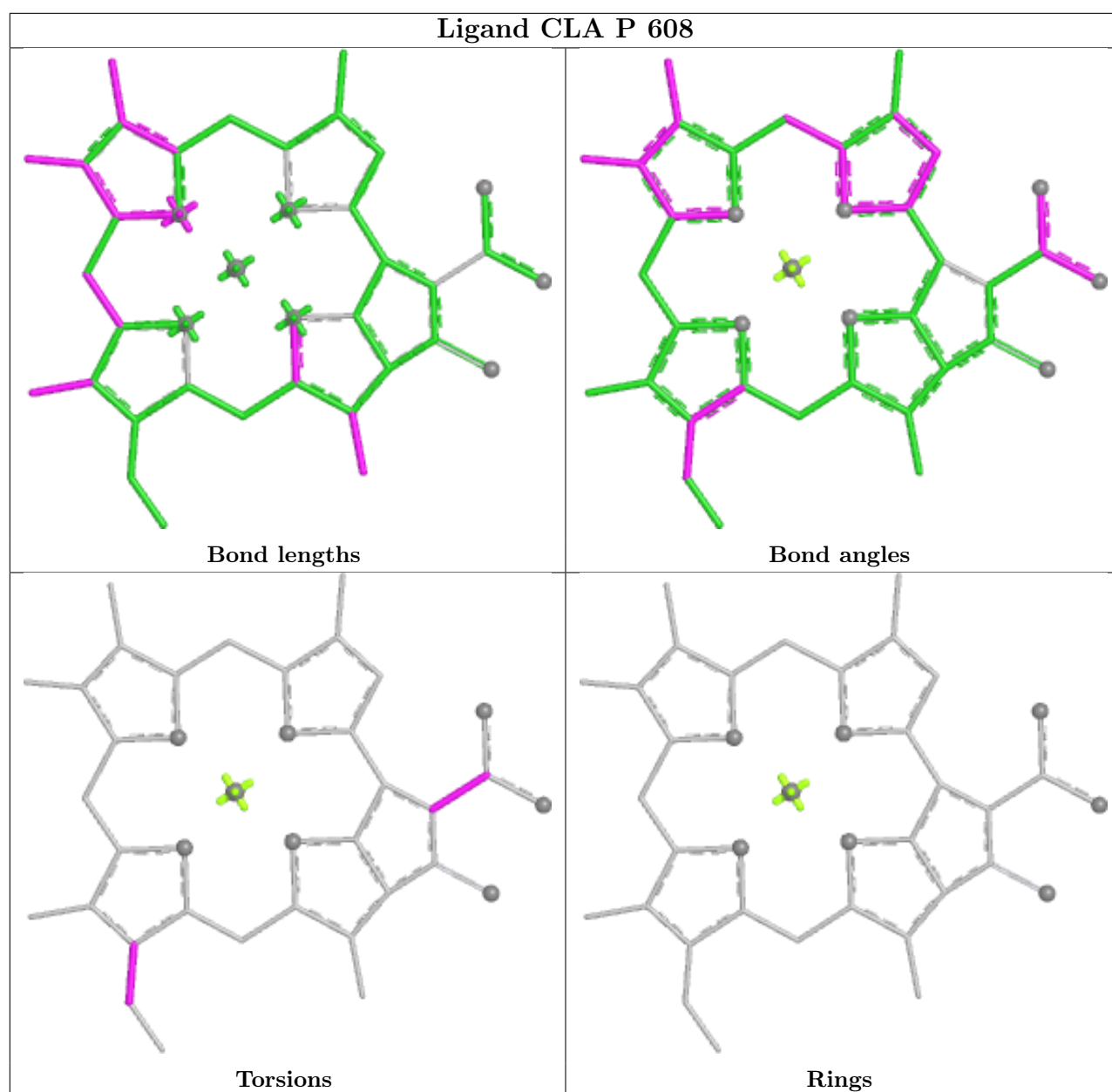
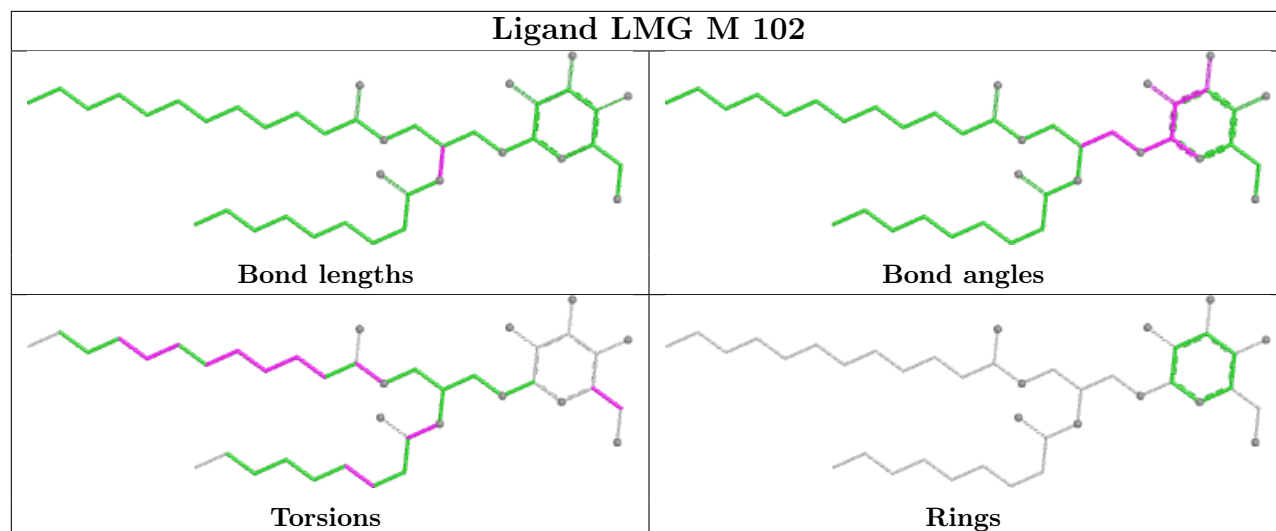
Bond angles

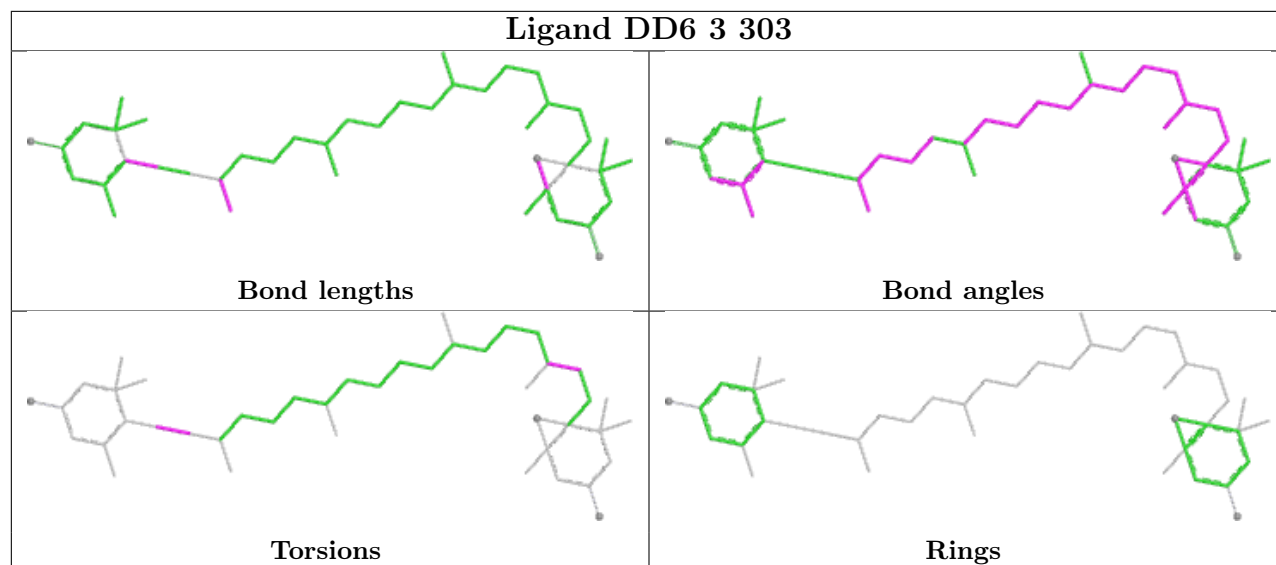
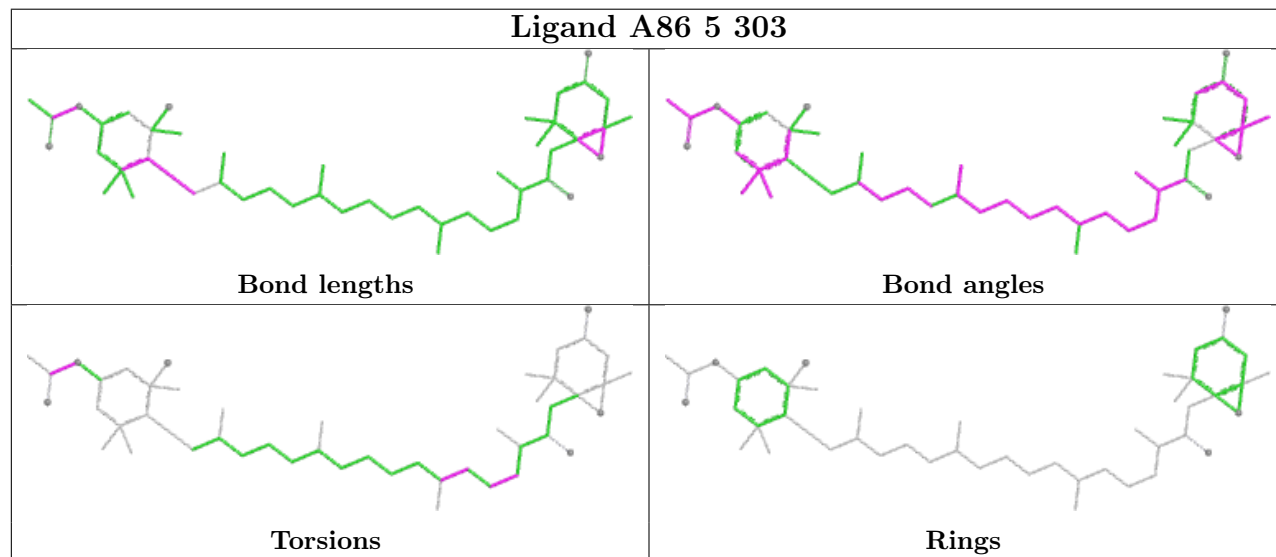


Torsions

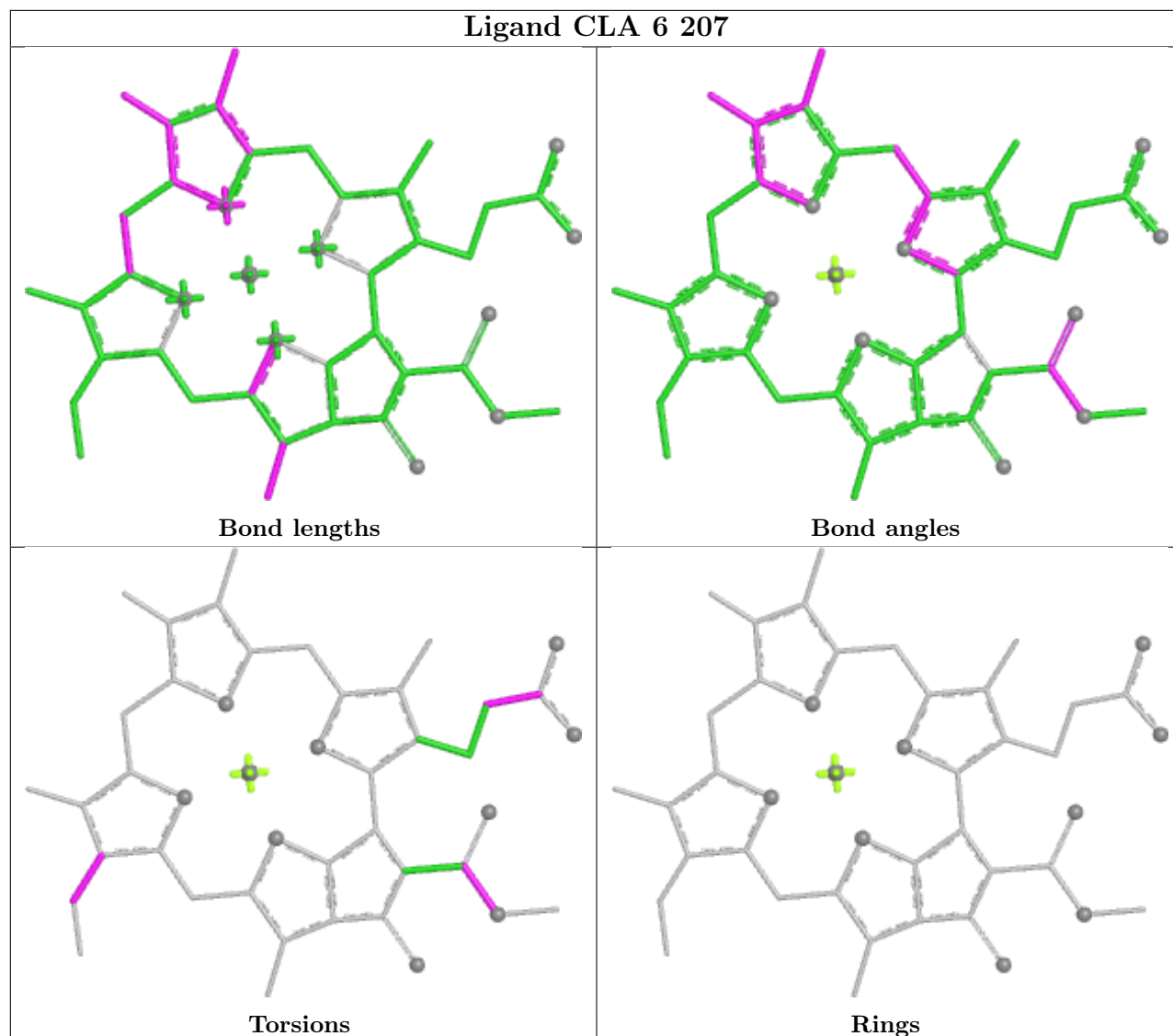


Rings

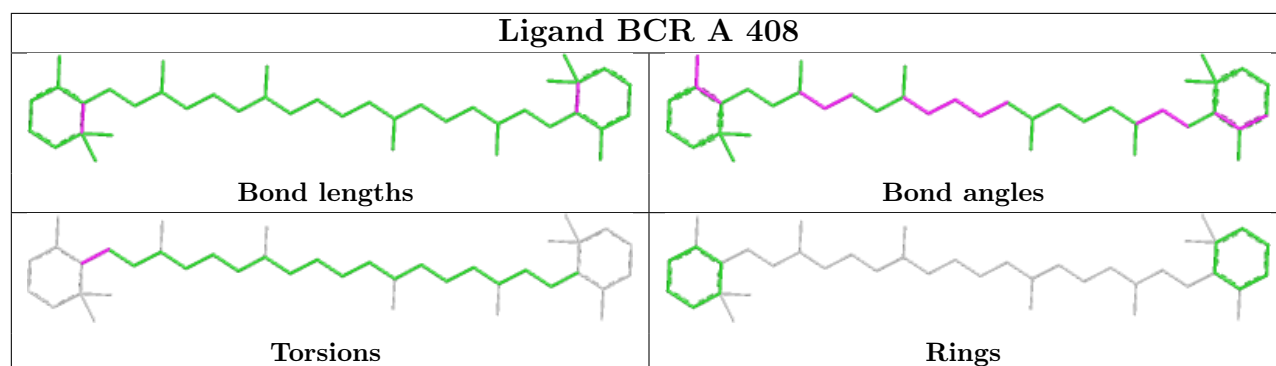


**Ligand DD6 3 303****Ligand A86 5 303**

## Ligand CLA 6 207

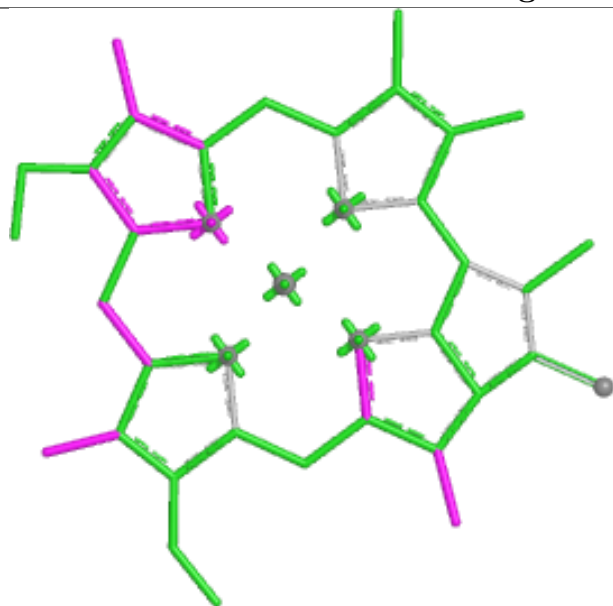


## Ligand BCR A 408

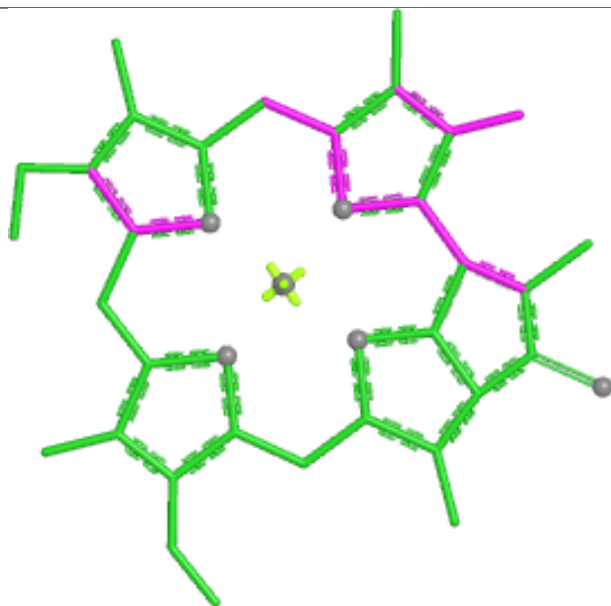




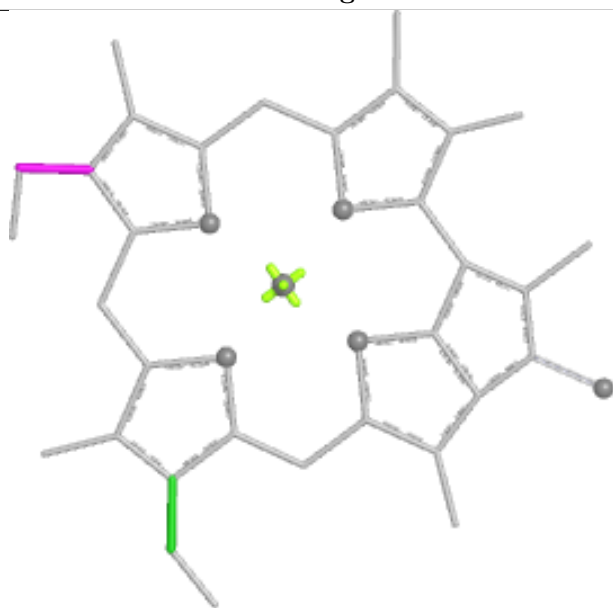
## Ligand CLA 9 204



Bond lengths



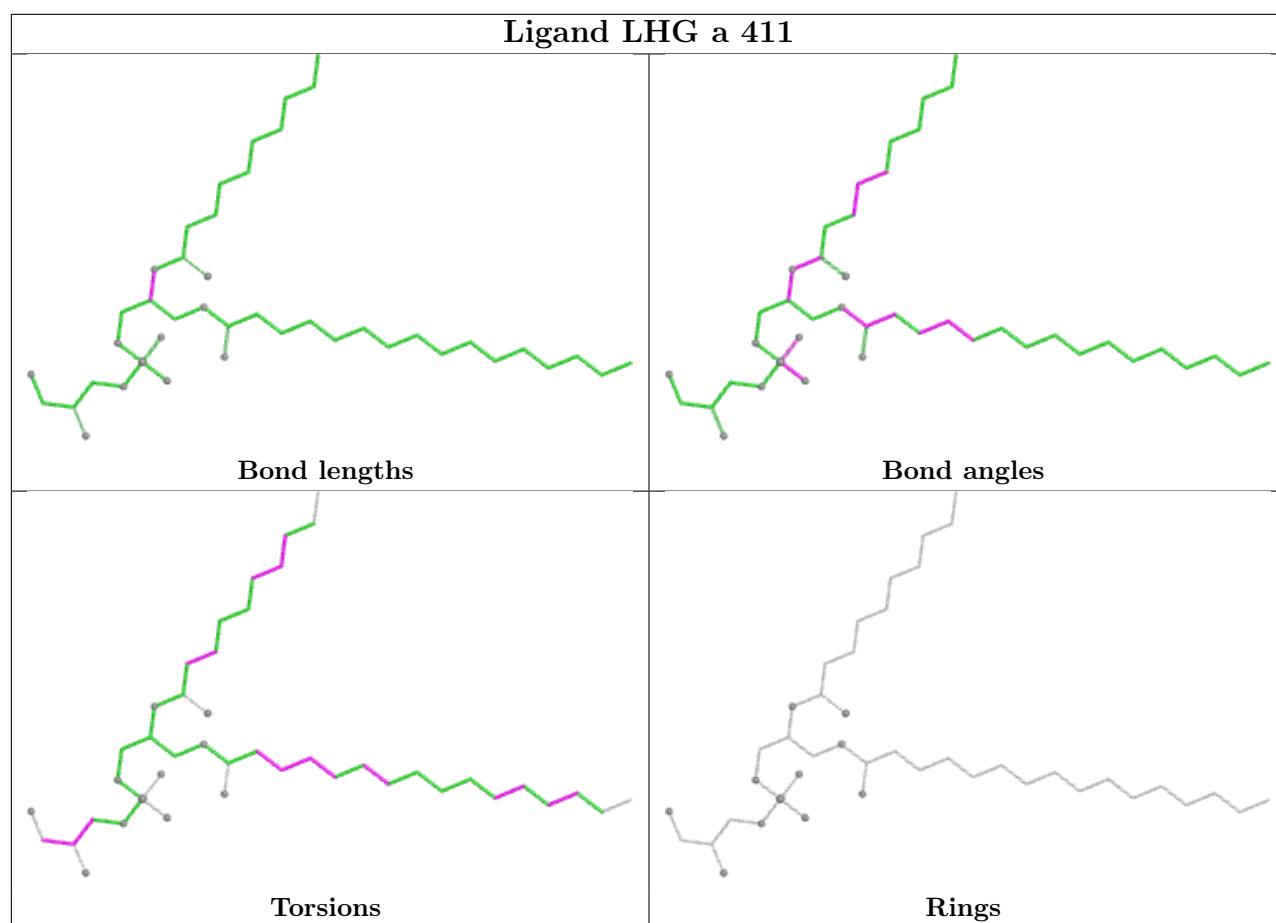
Bond angles



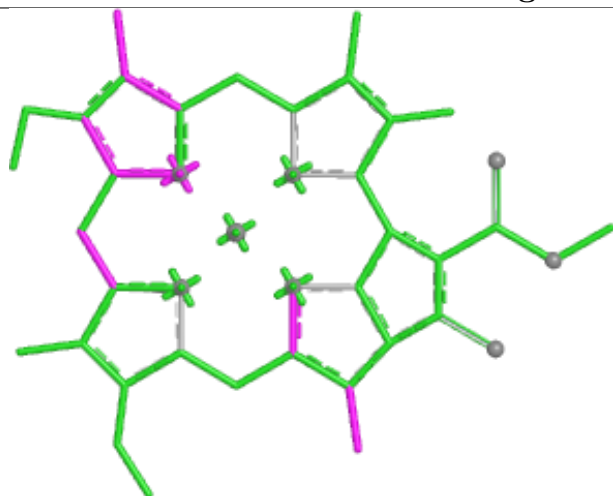
Torsions



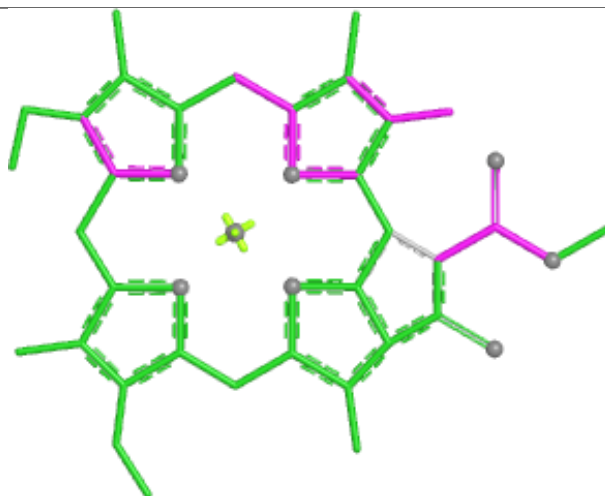
Rings



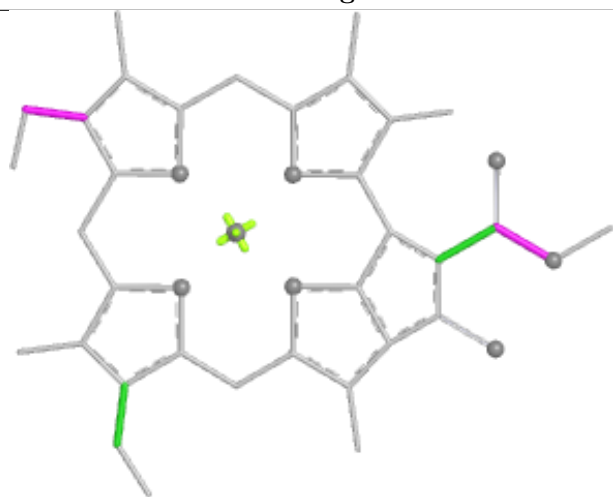
## Ligand CLA 7 305



Bond lengths



Bond angles

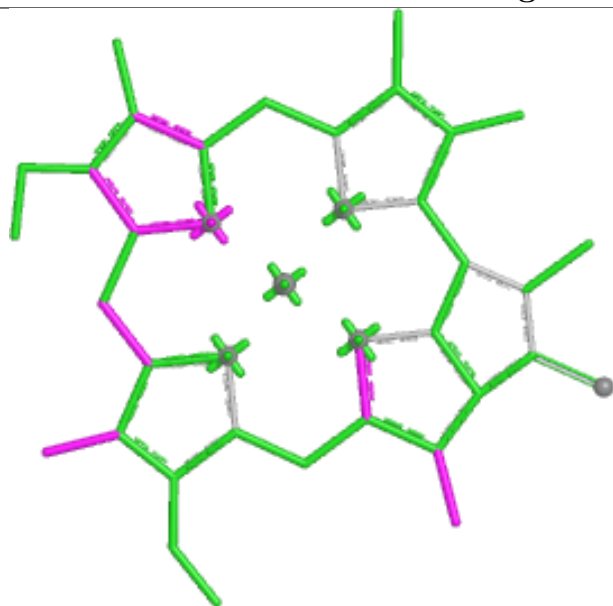


Torsions

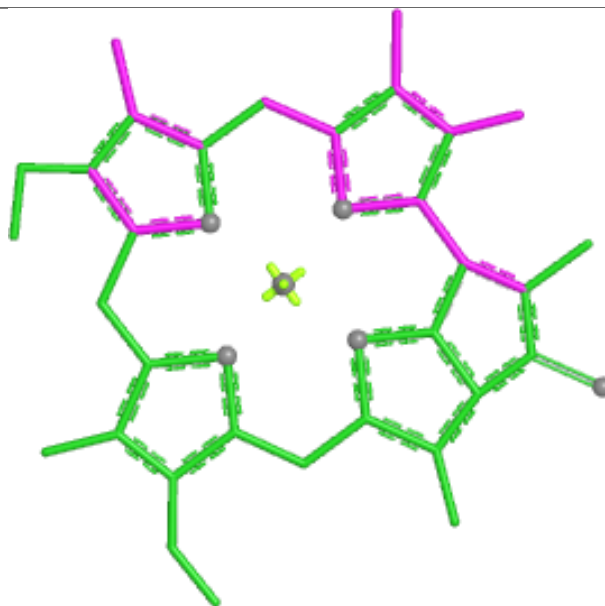


Rings

## Ligand CLA 1 214



Bond lengths



Bond angles

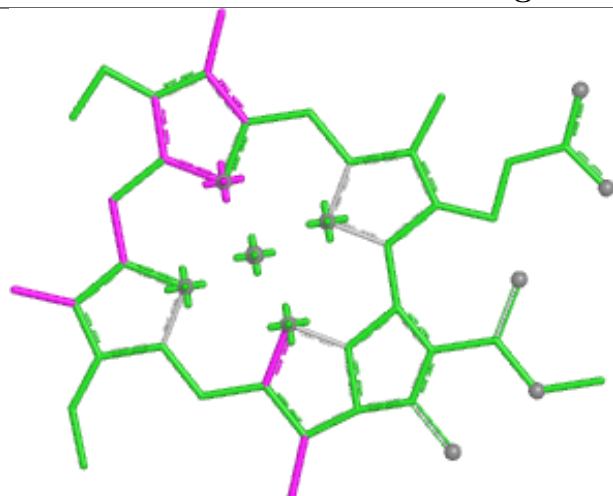


Torsions

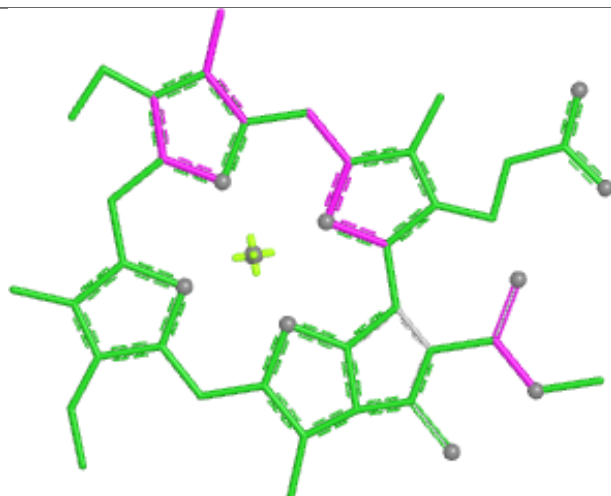


Rings

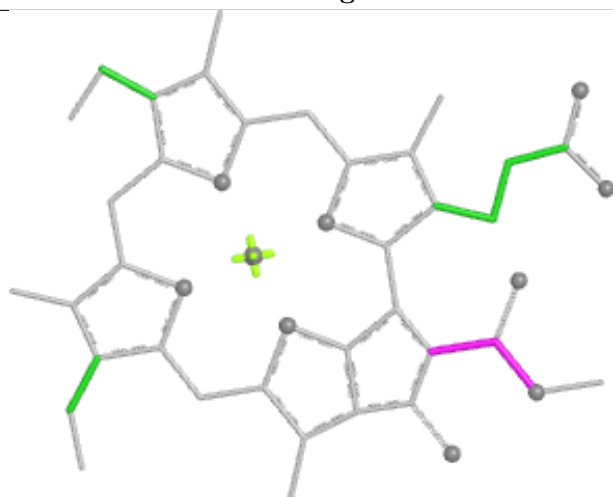
## Ligand CLA C 507



Bond lengths



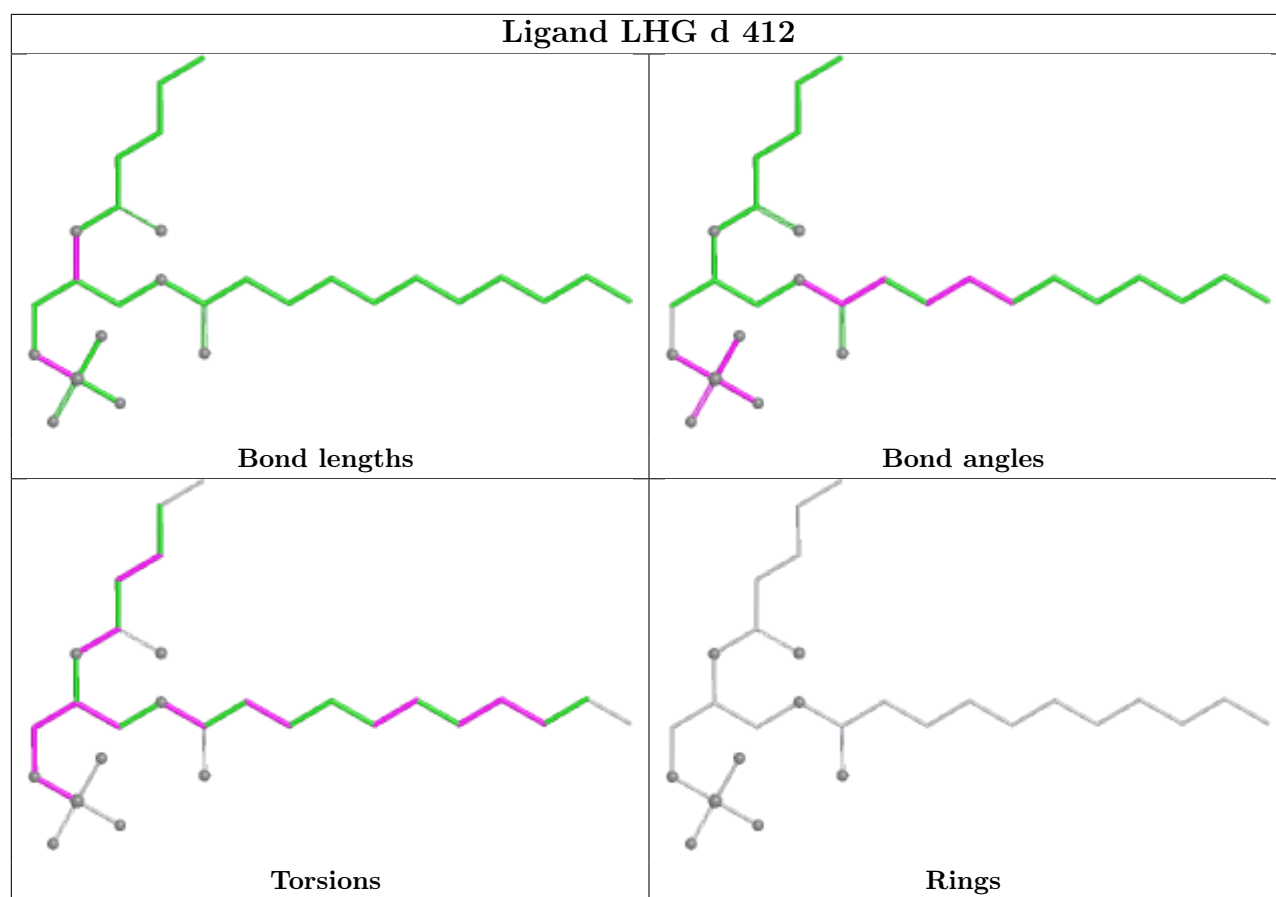
Bond angles



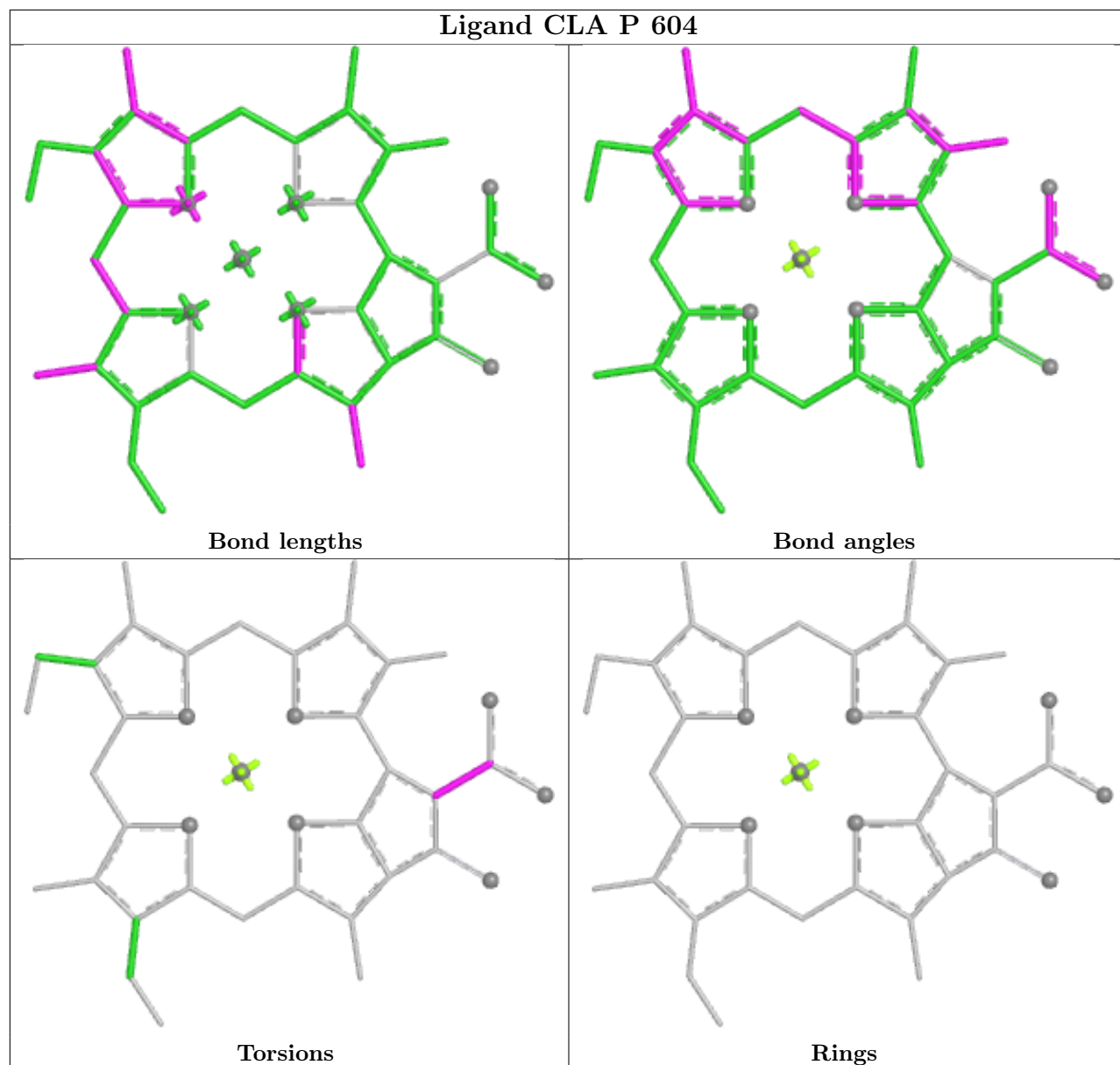
Torsions



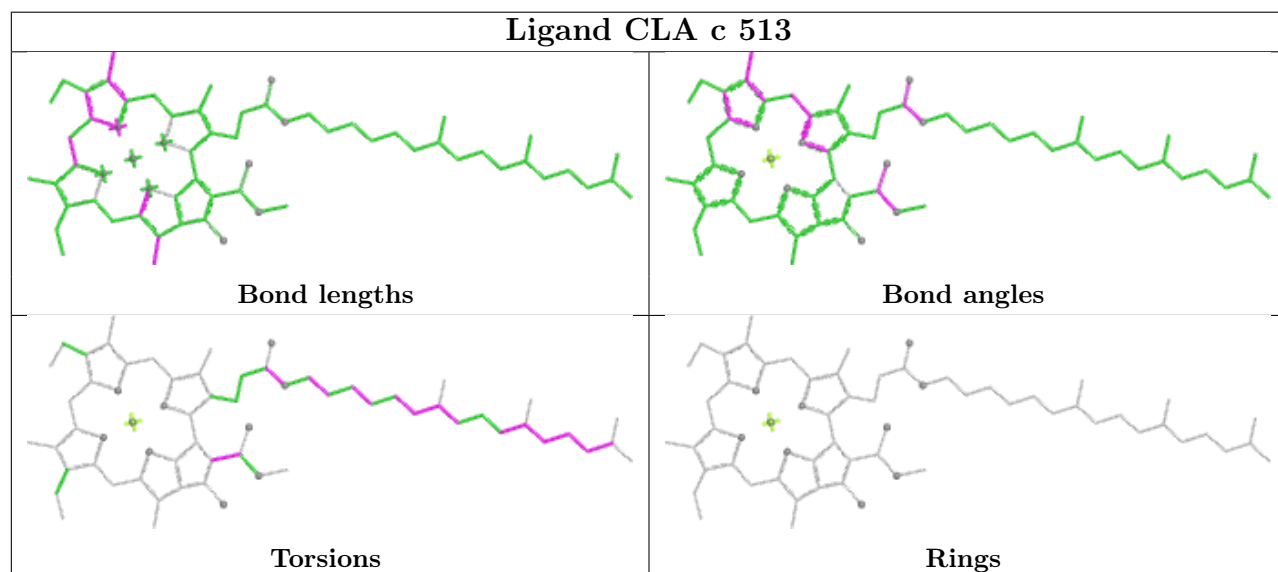
Rings

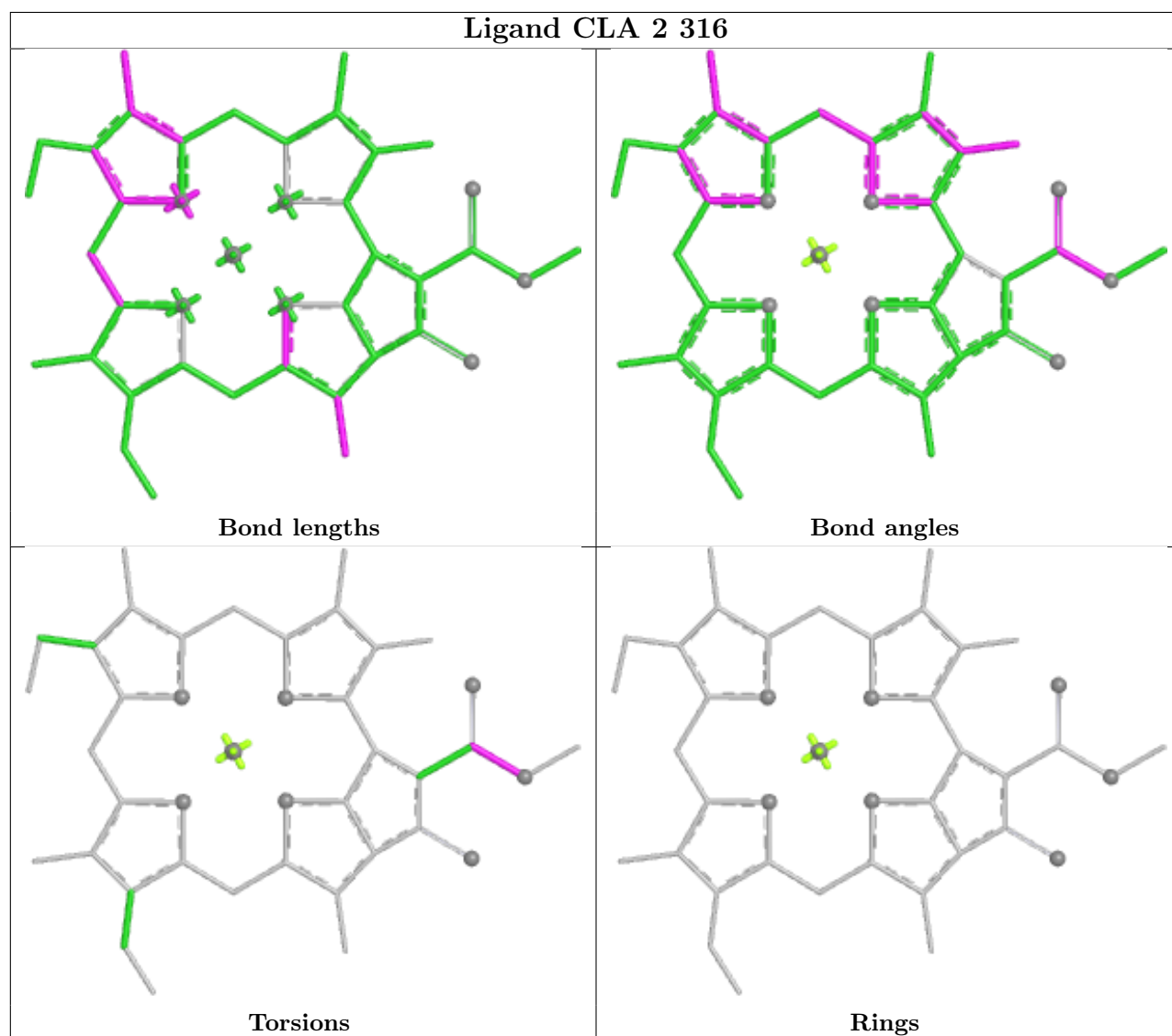
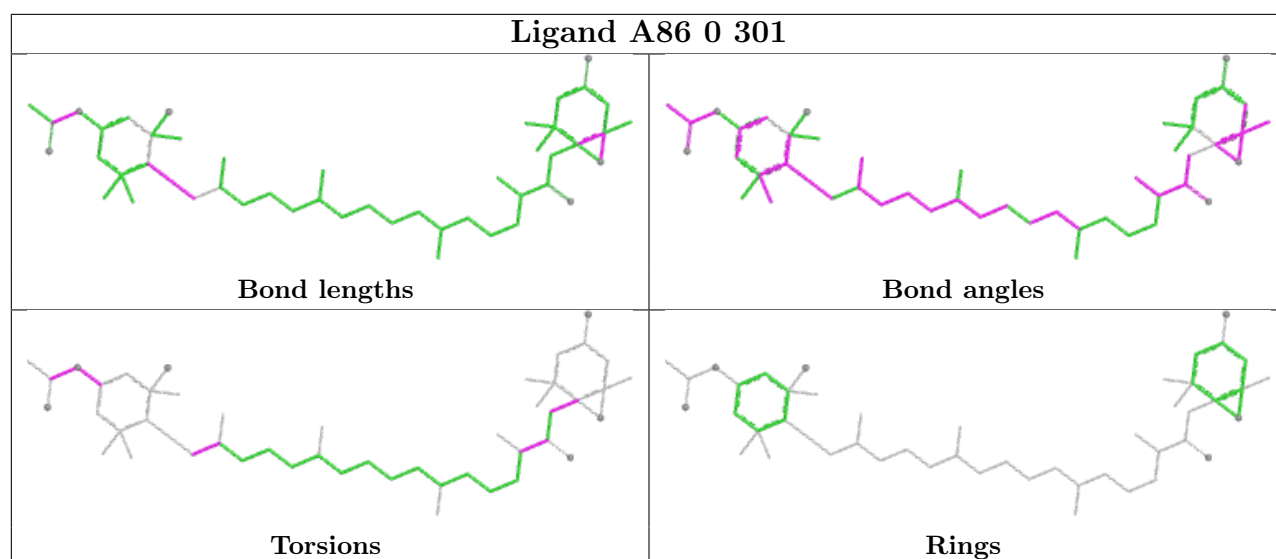


## Ligand CLA P 604

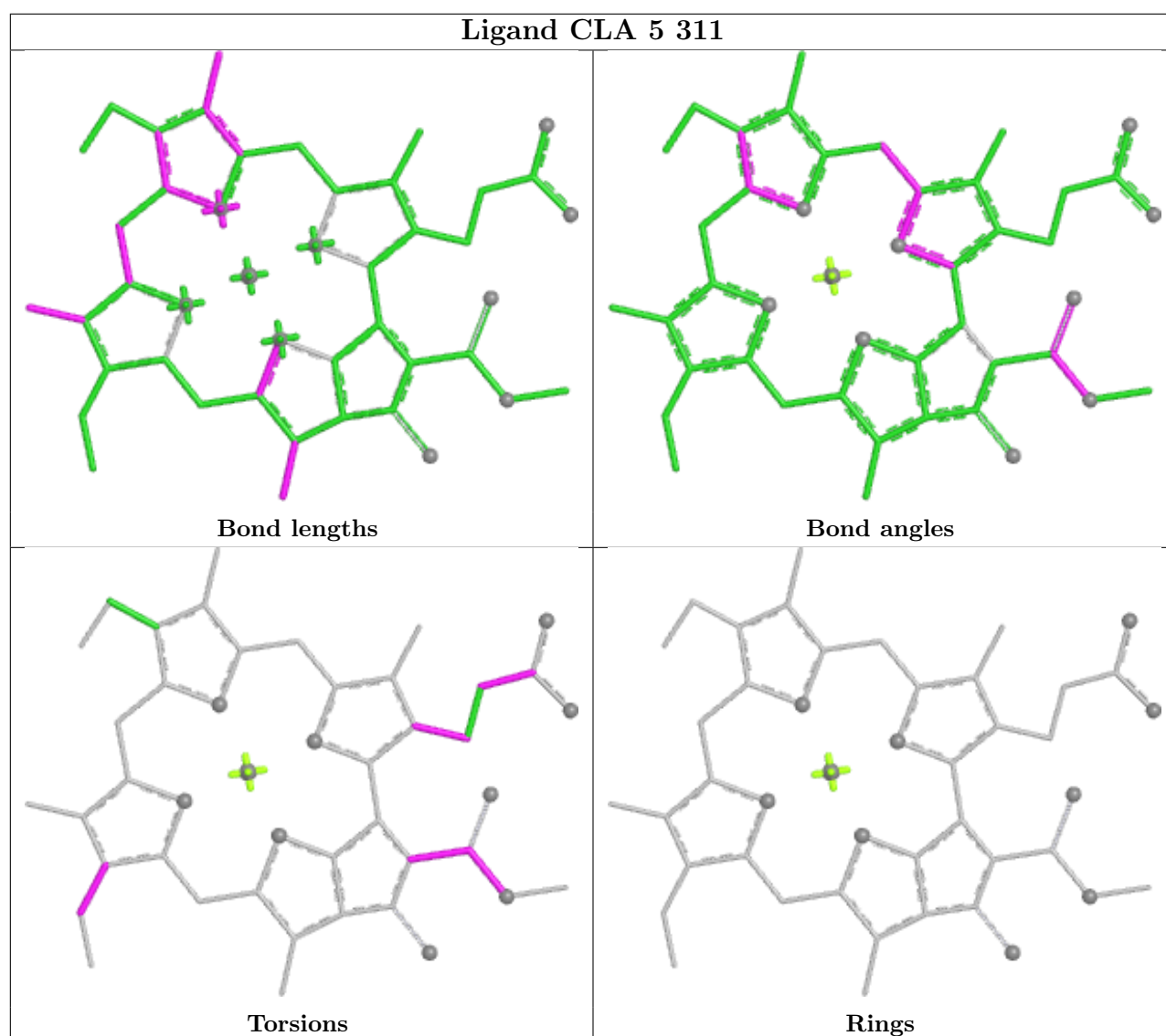
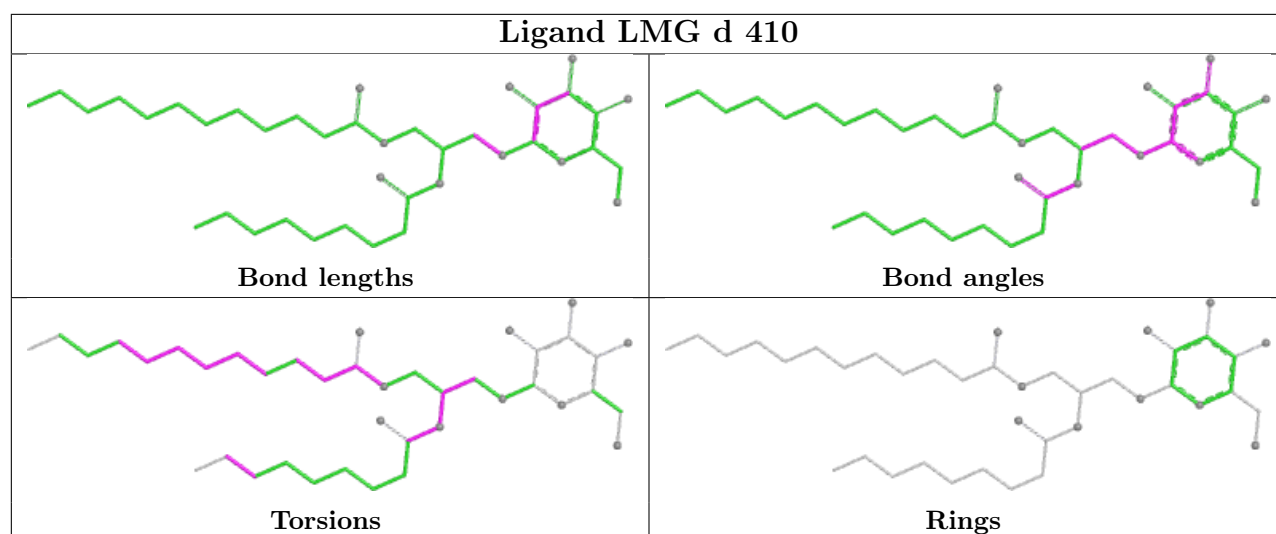


## Ligand CLA c 513

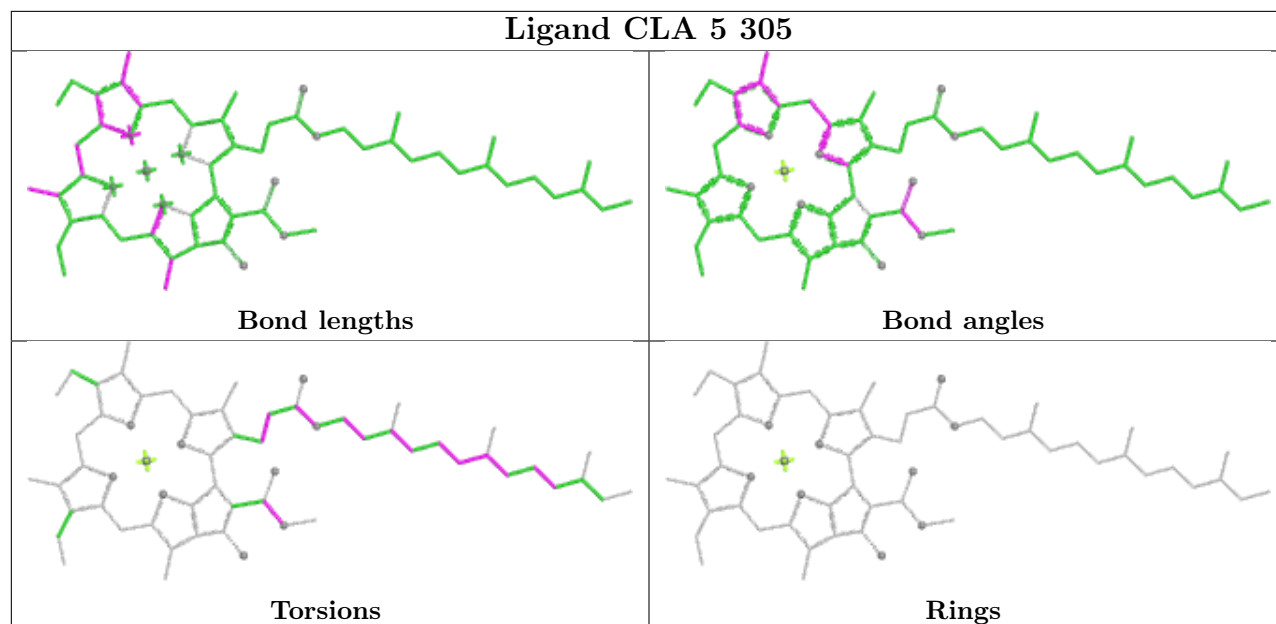




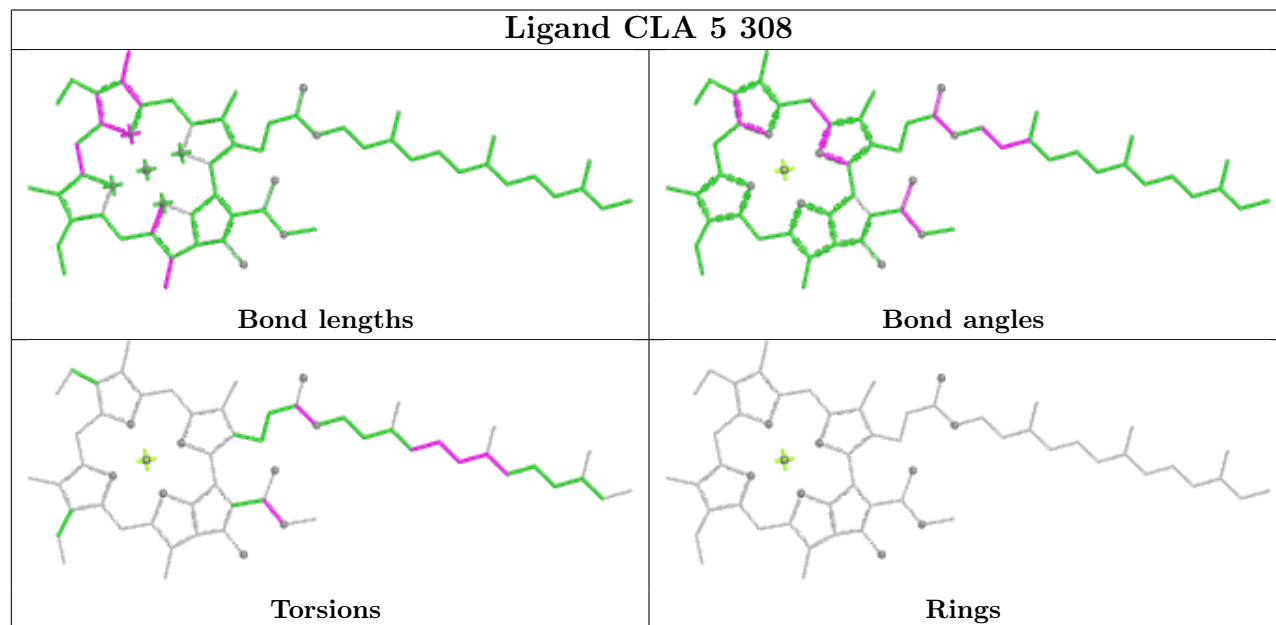




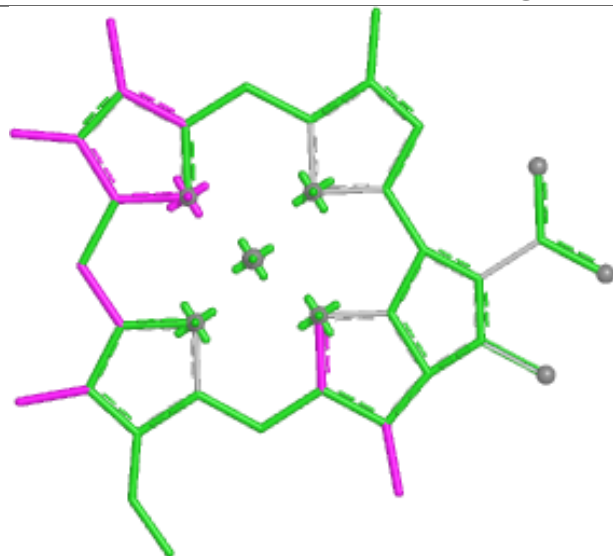
## Ligand CLA 5 305



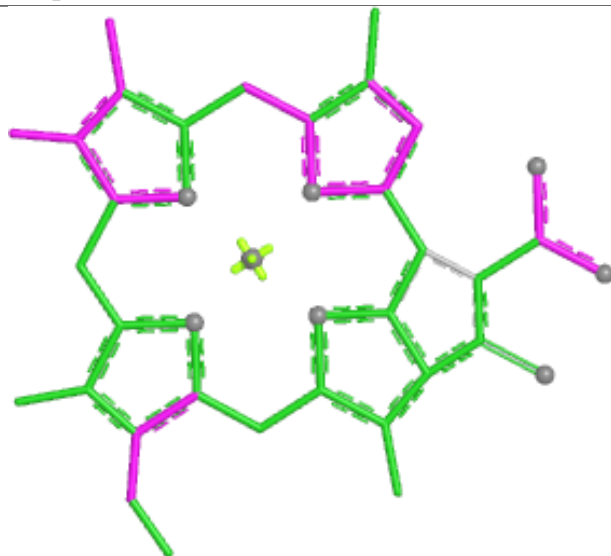
## Ligand CLA 5 308



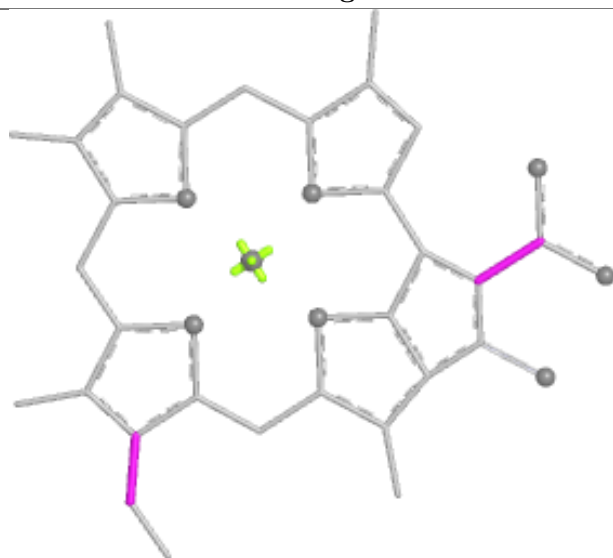
## Ligand CLA p 608



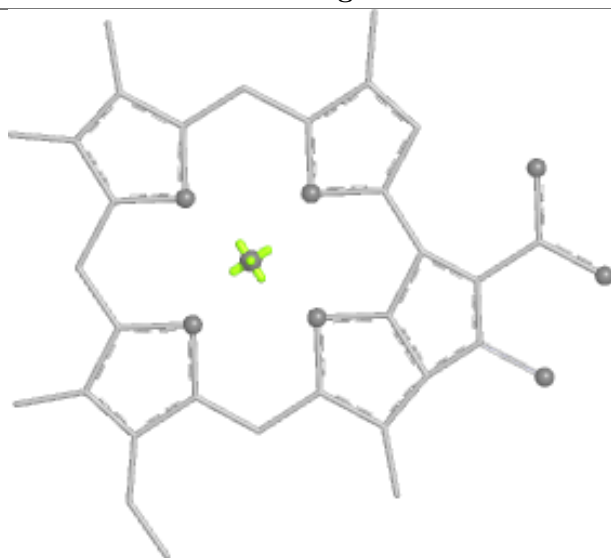
Bond lengths



Bond angles

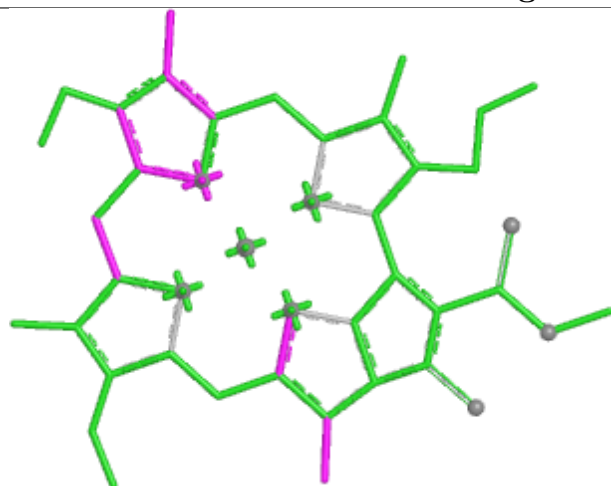


Torsions

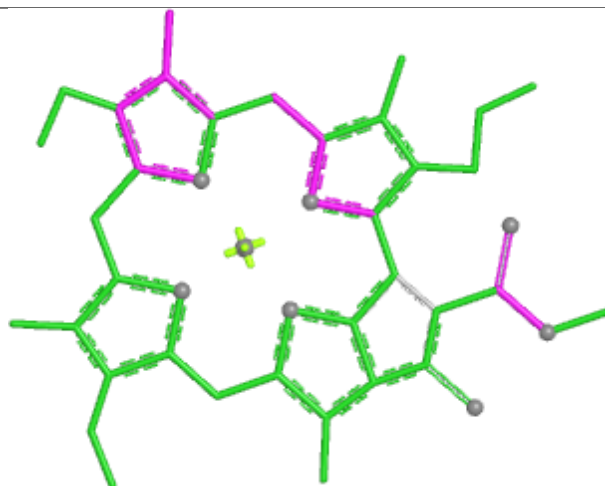


Rings

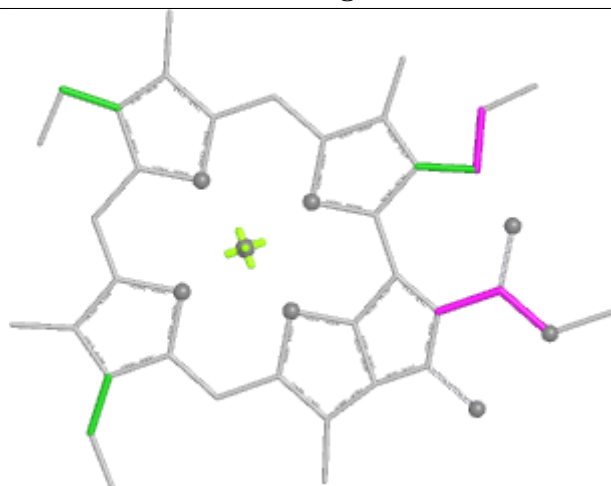
## Ligand CLA 2 311



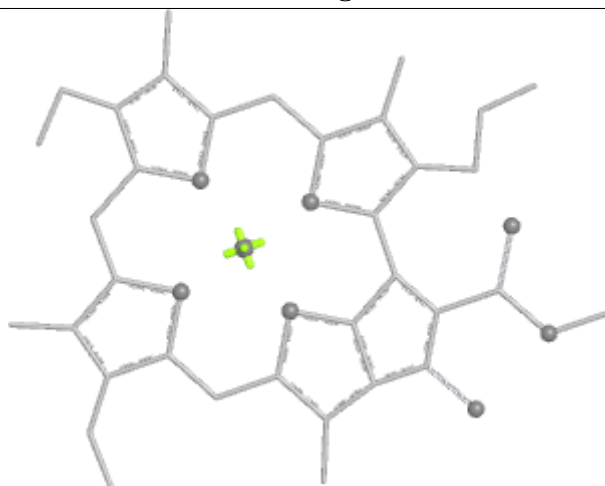
Bond lengths



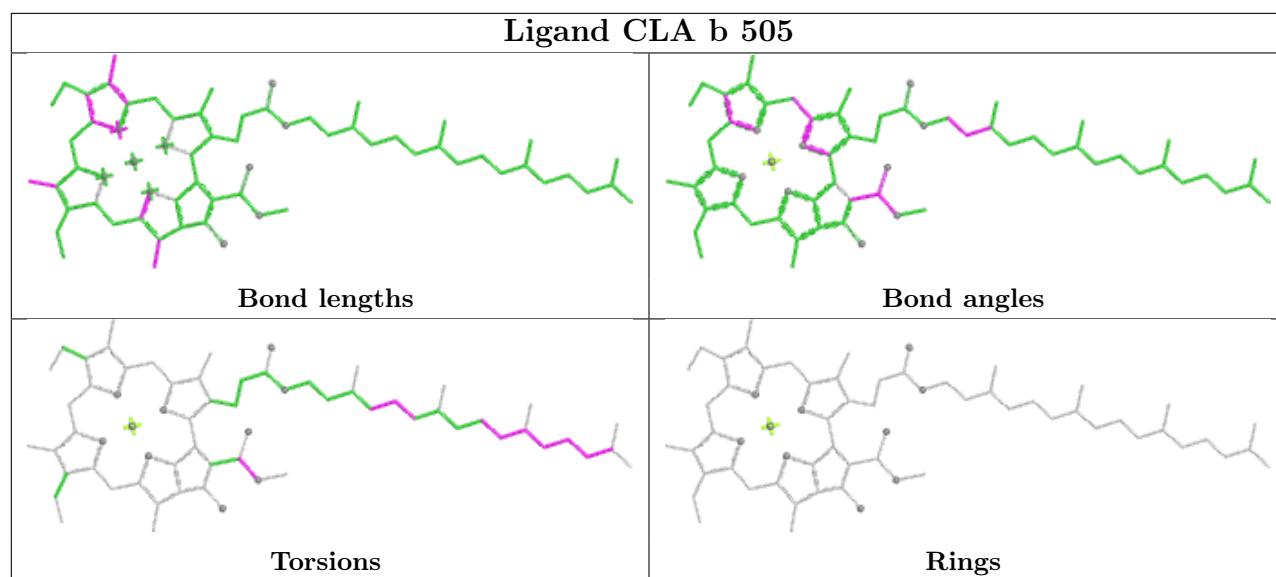
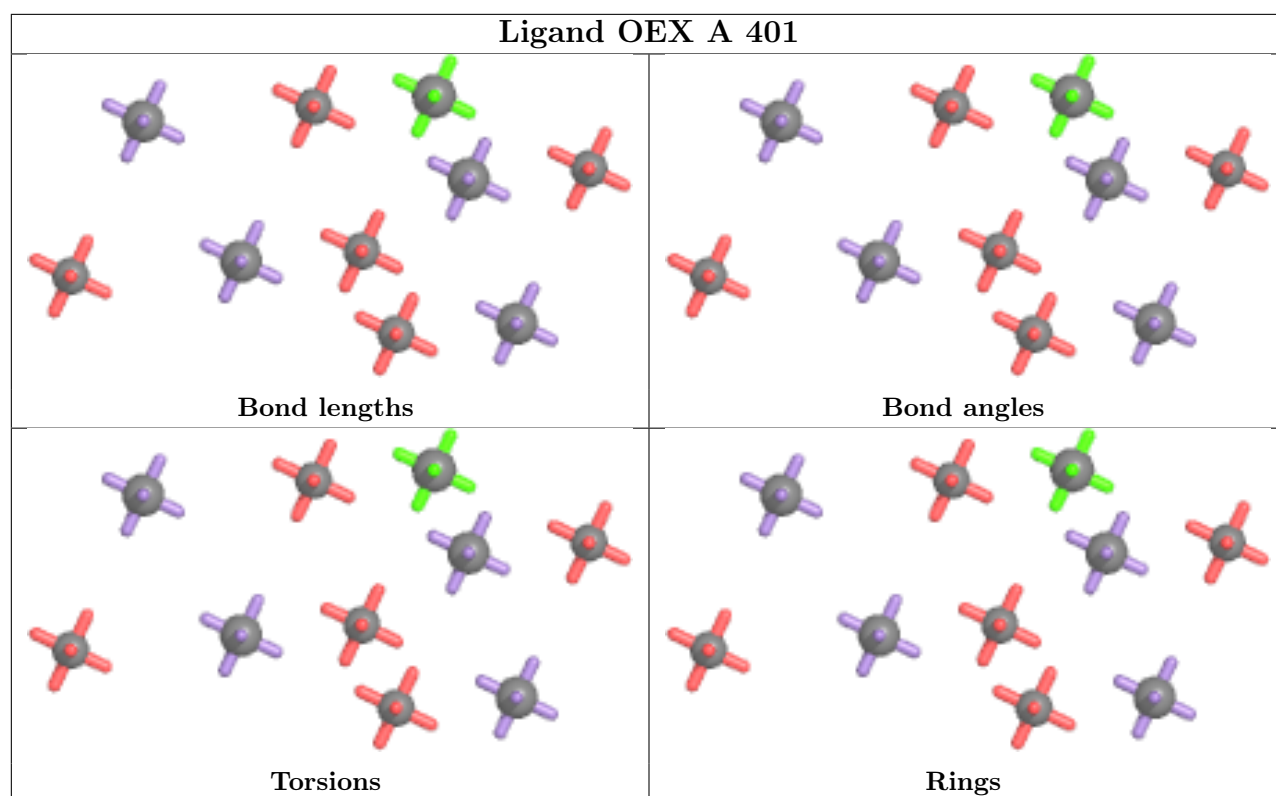
Bond angles

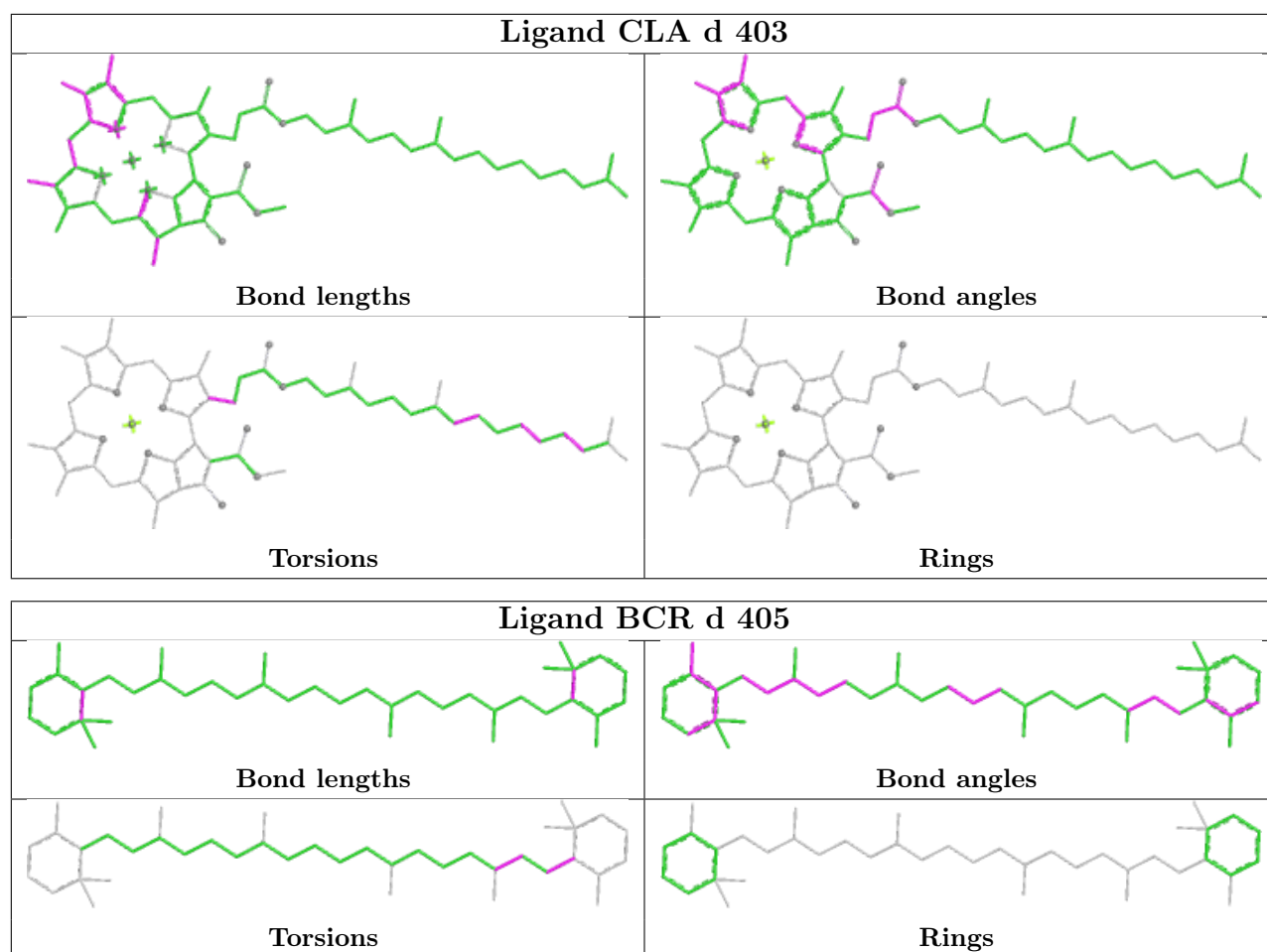


Torsions

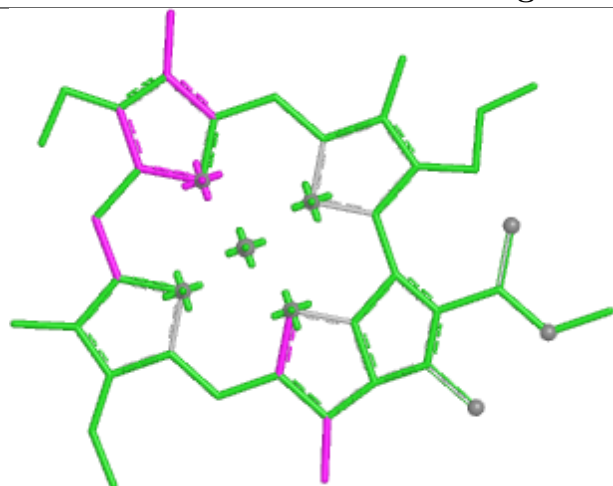


Rings

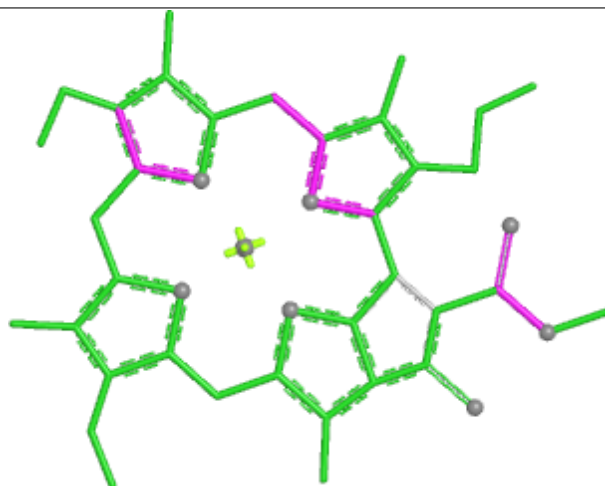




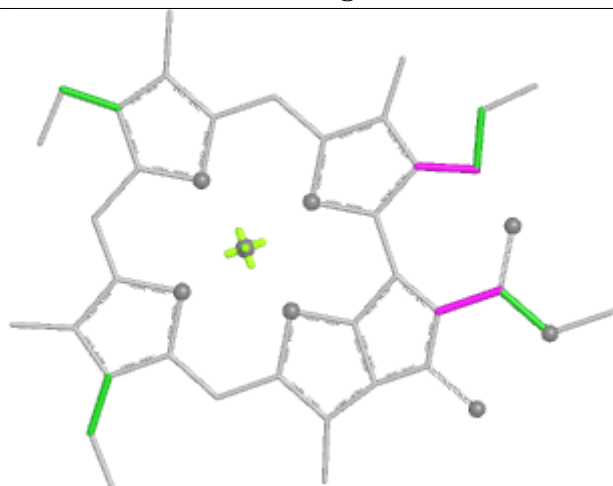
## Ligand CLA b 502



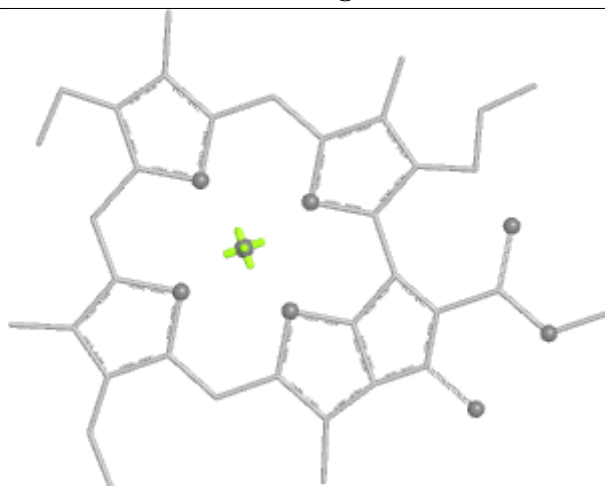
Bond lengths



Bond angles

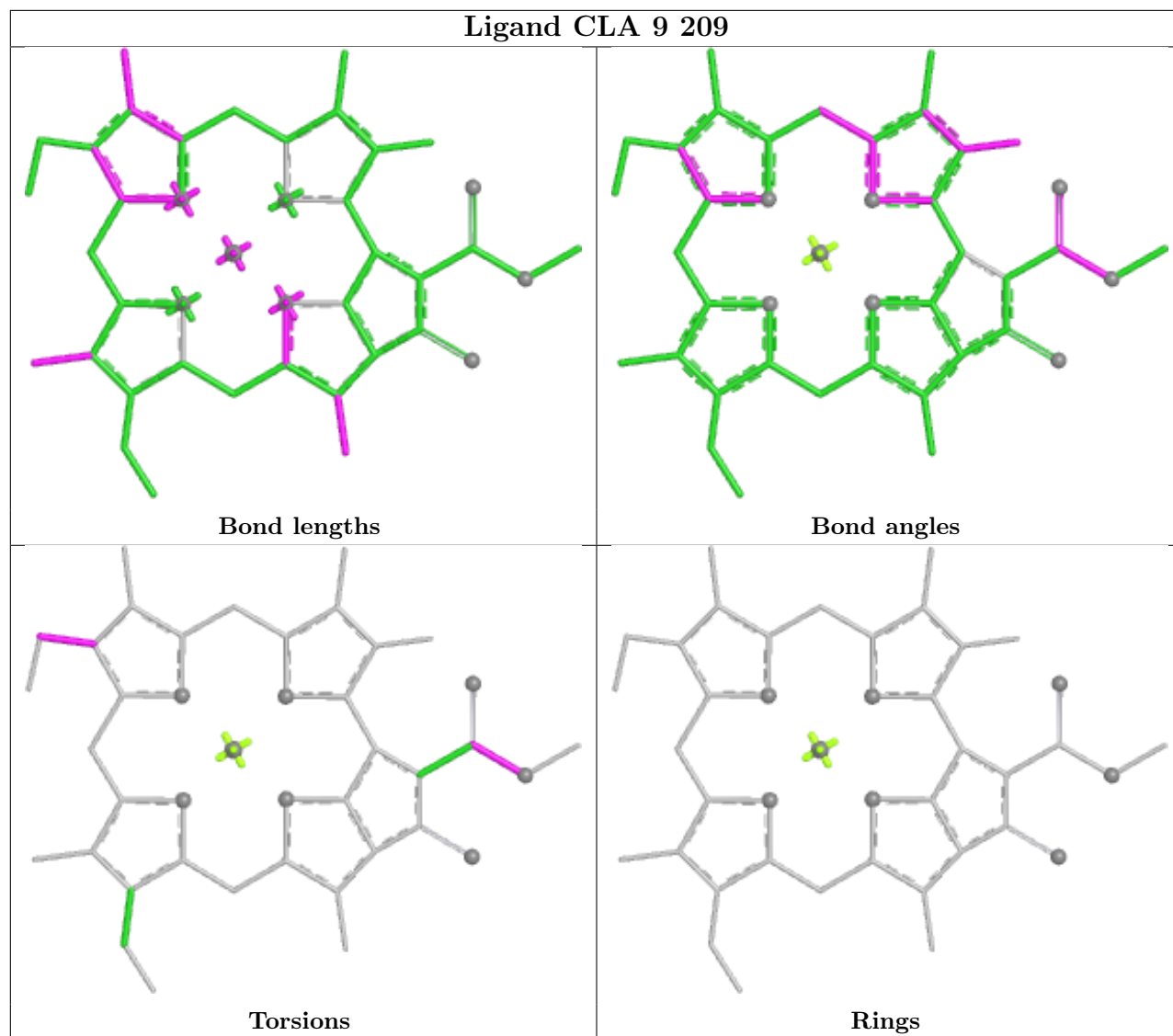


Torsions

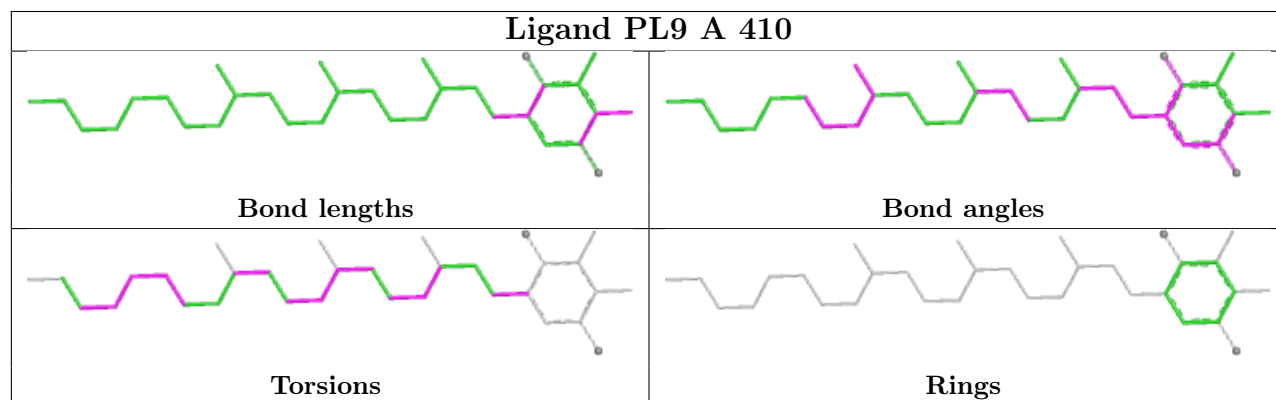


Rings

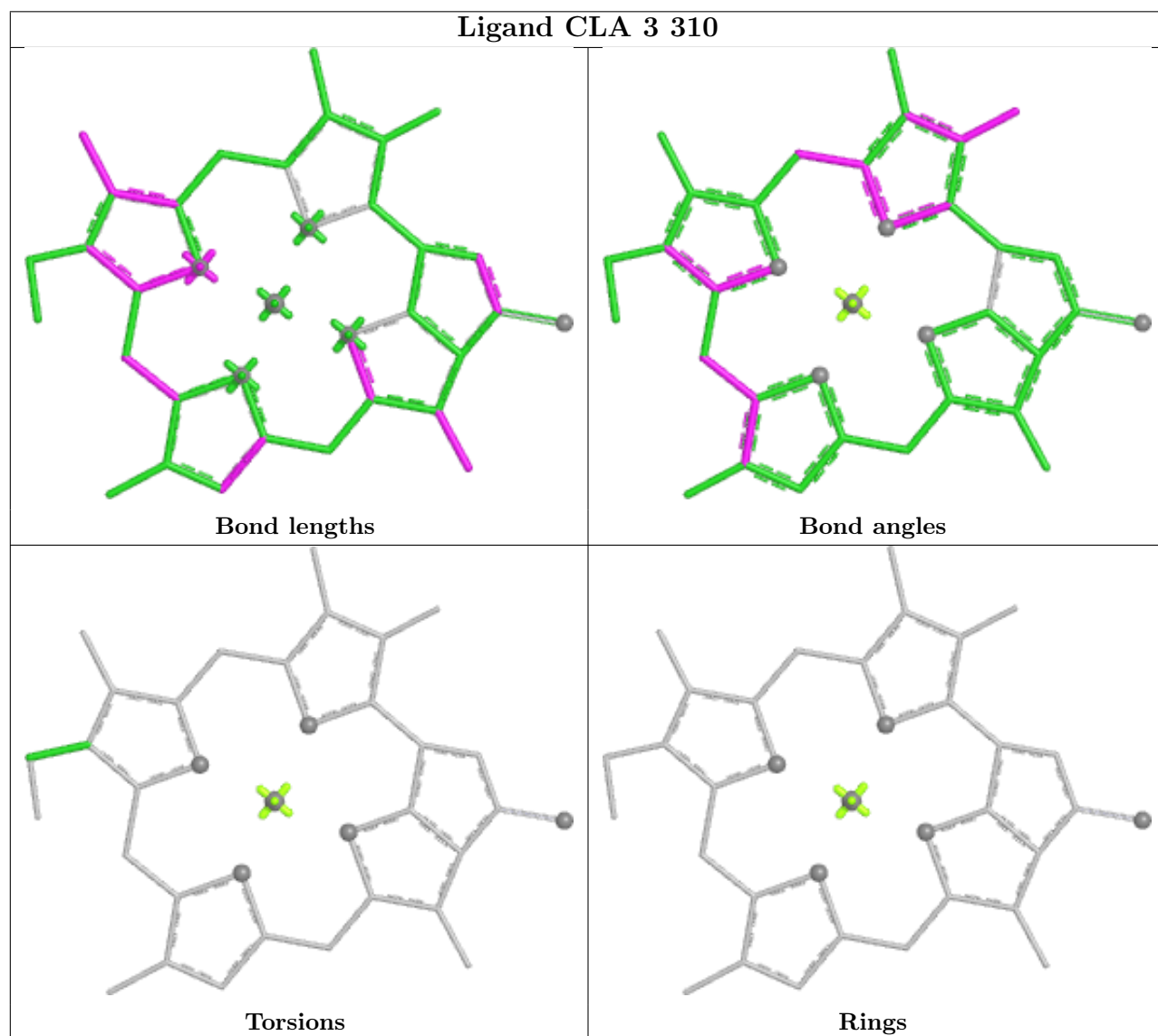
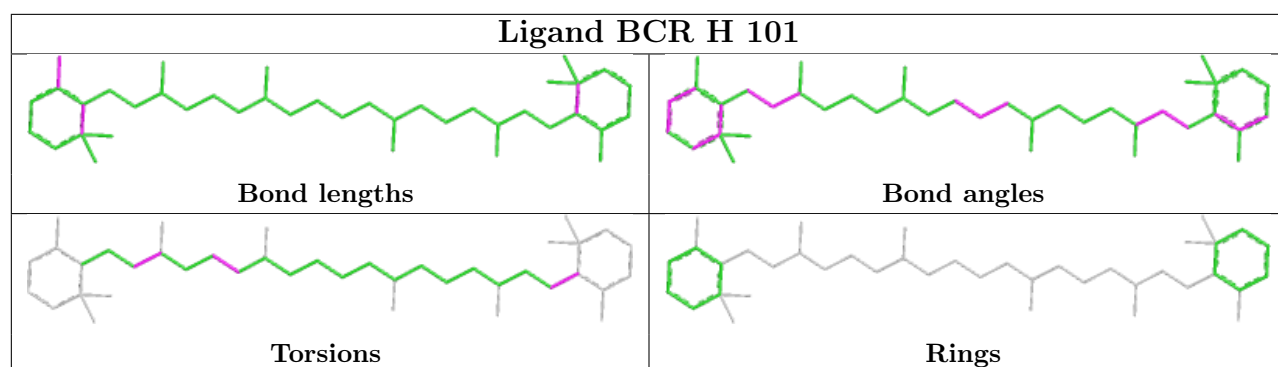
## Ligand CLA 9 209

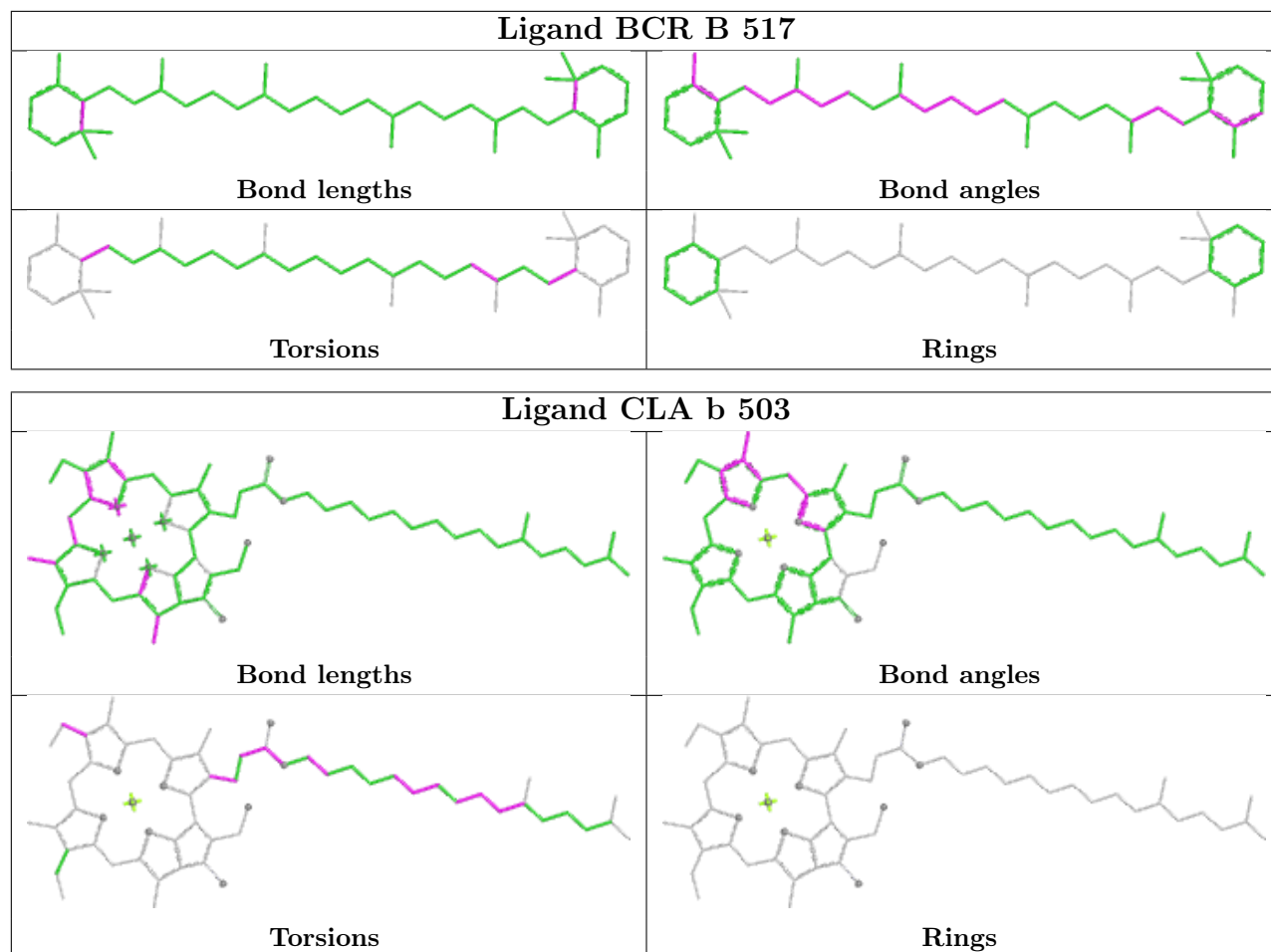


## Ligand PL9 A 410

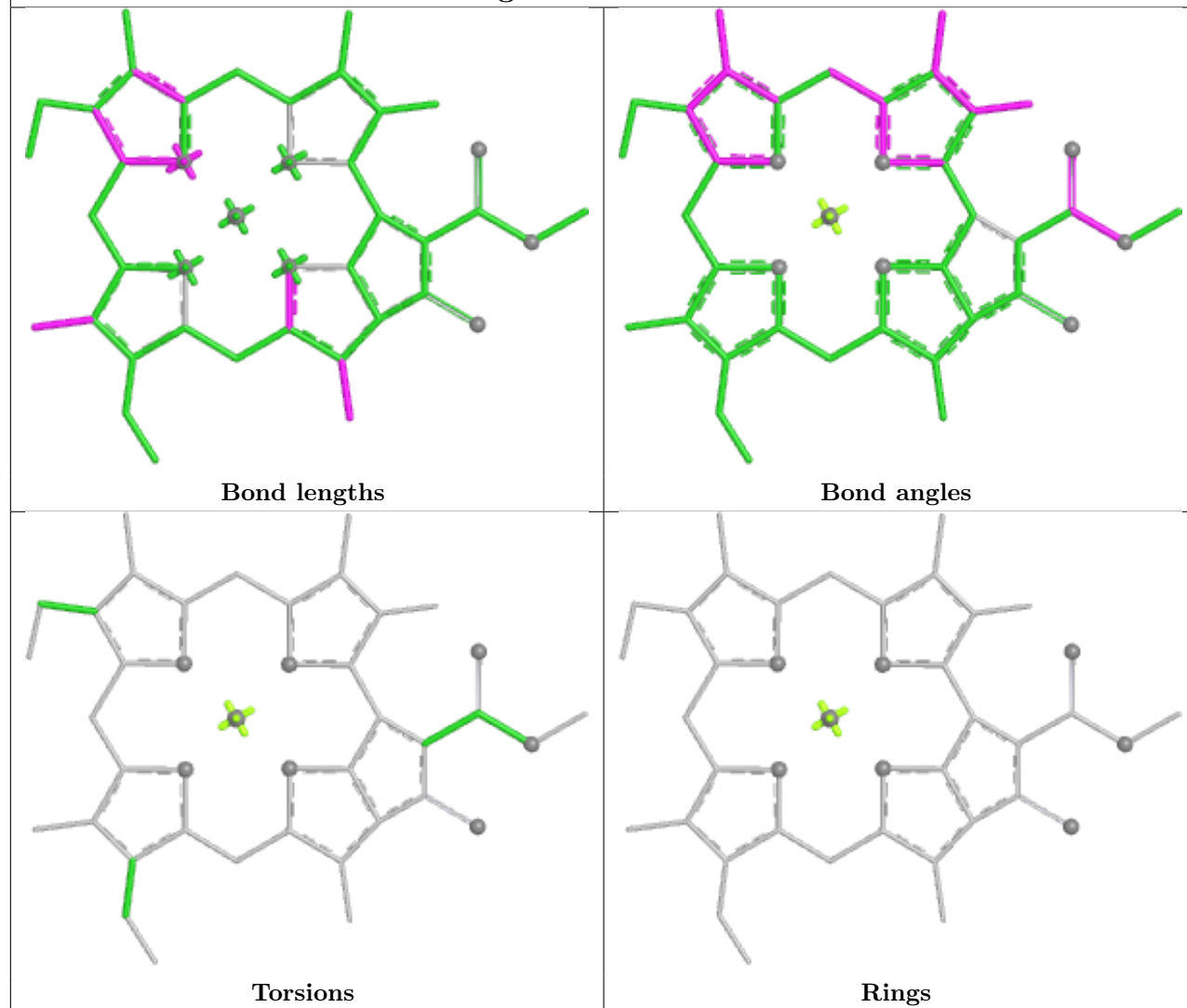




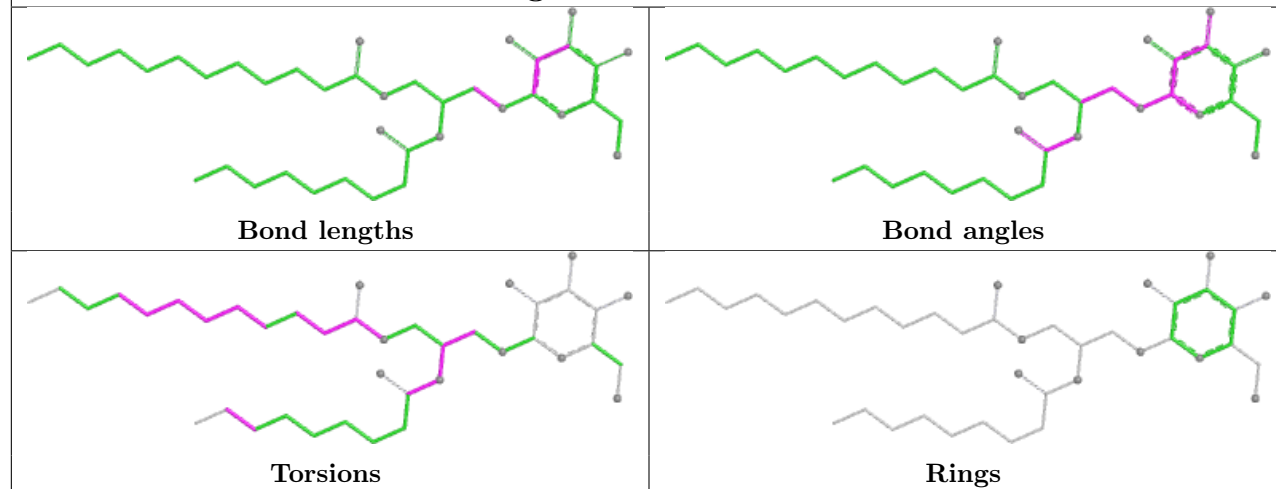




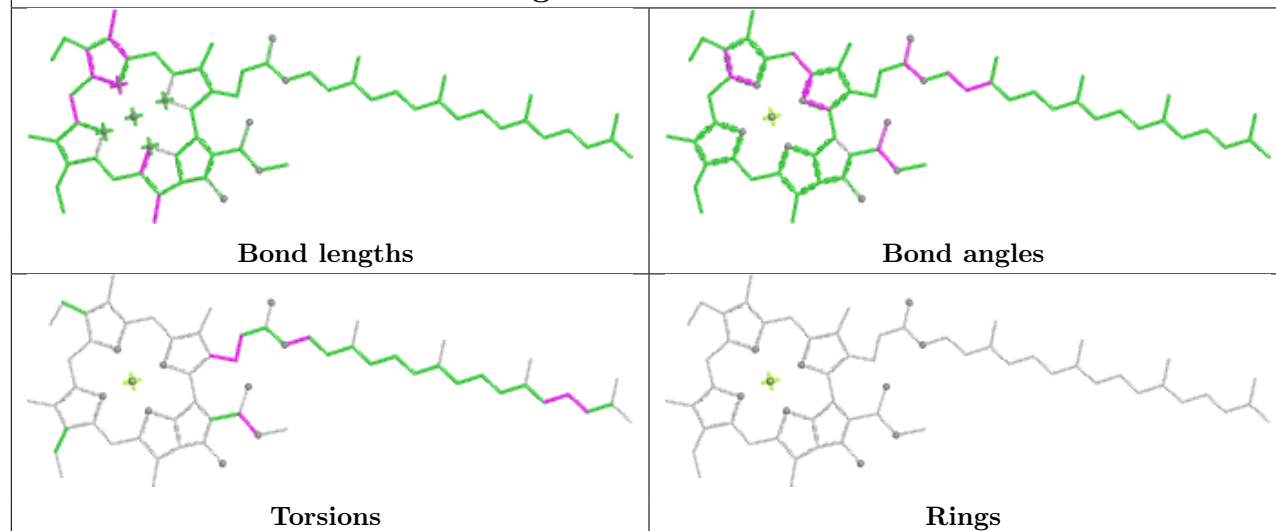
## Ligand CLA b 513



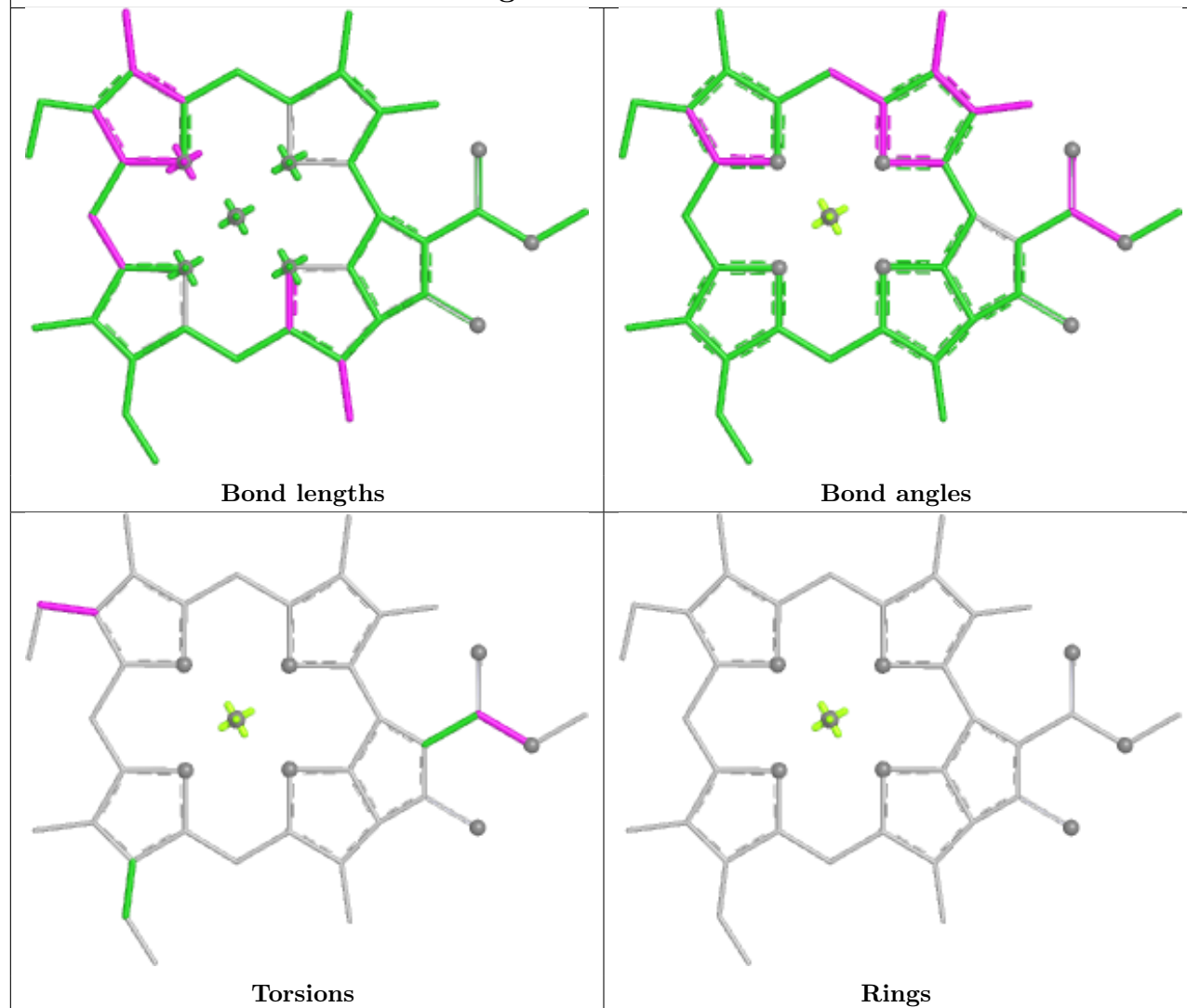
## Ligand LMG D 410

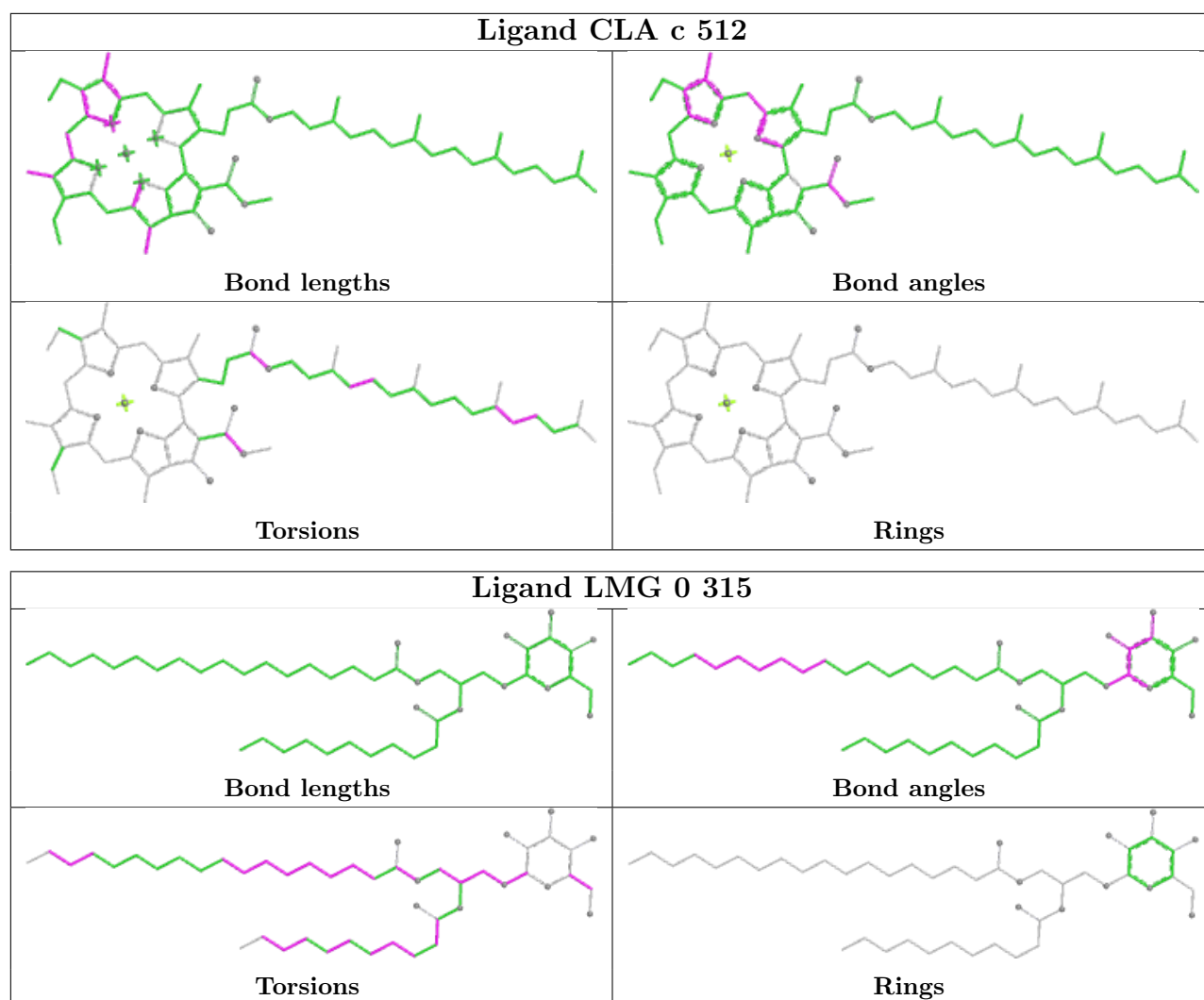


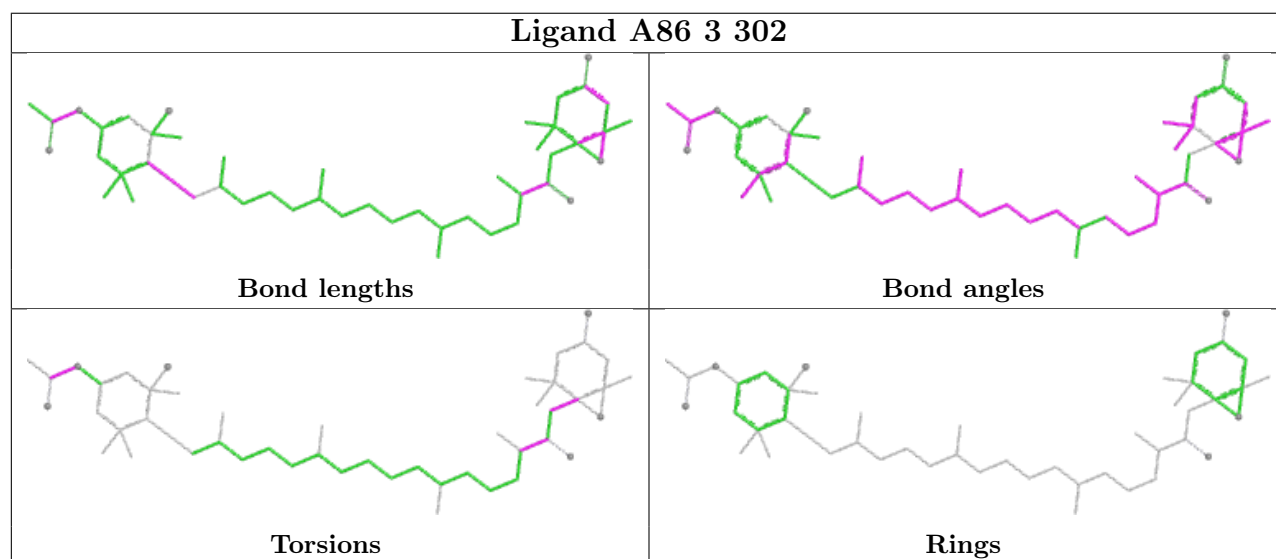
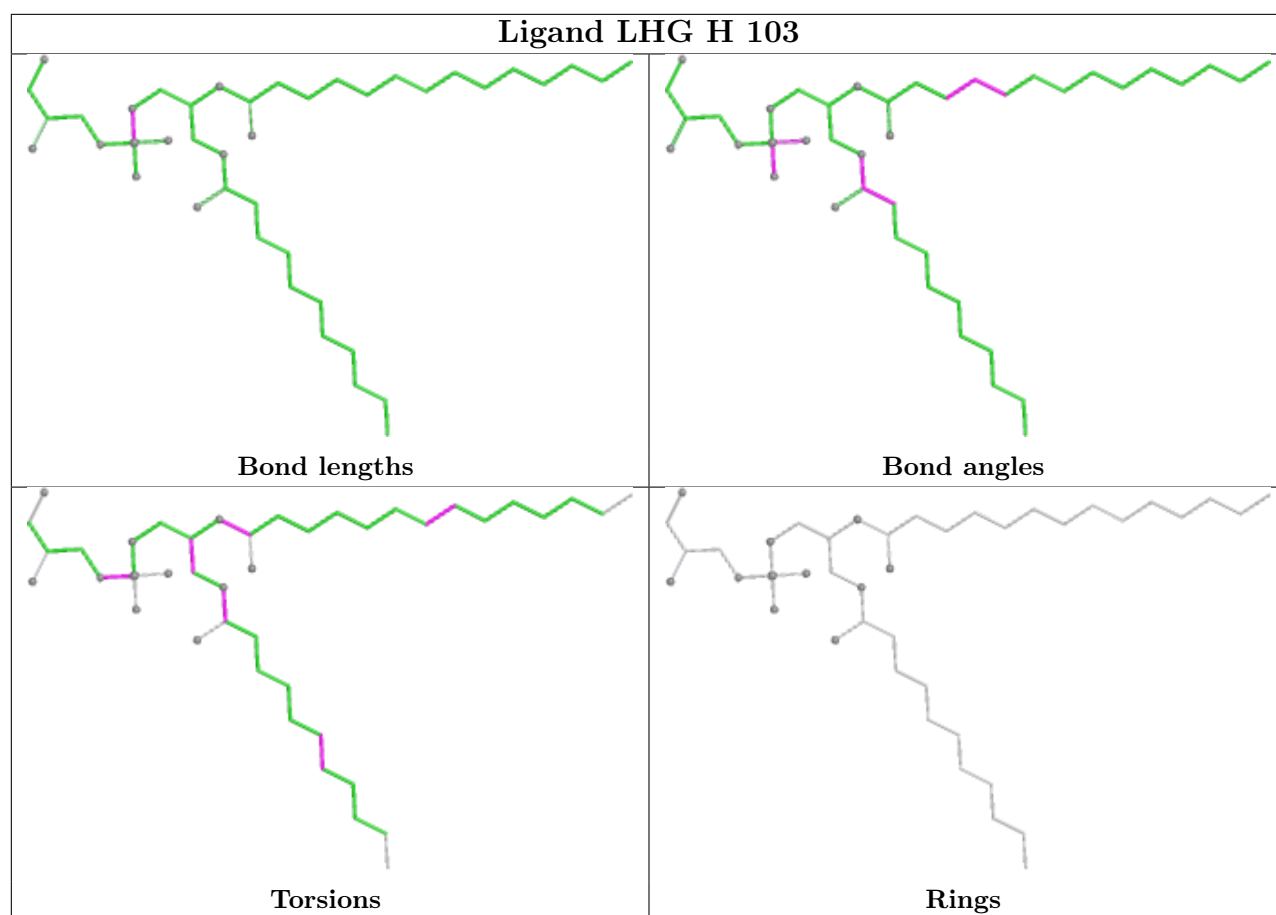
## Ligand CLA B 508

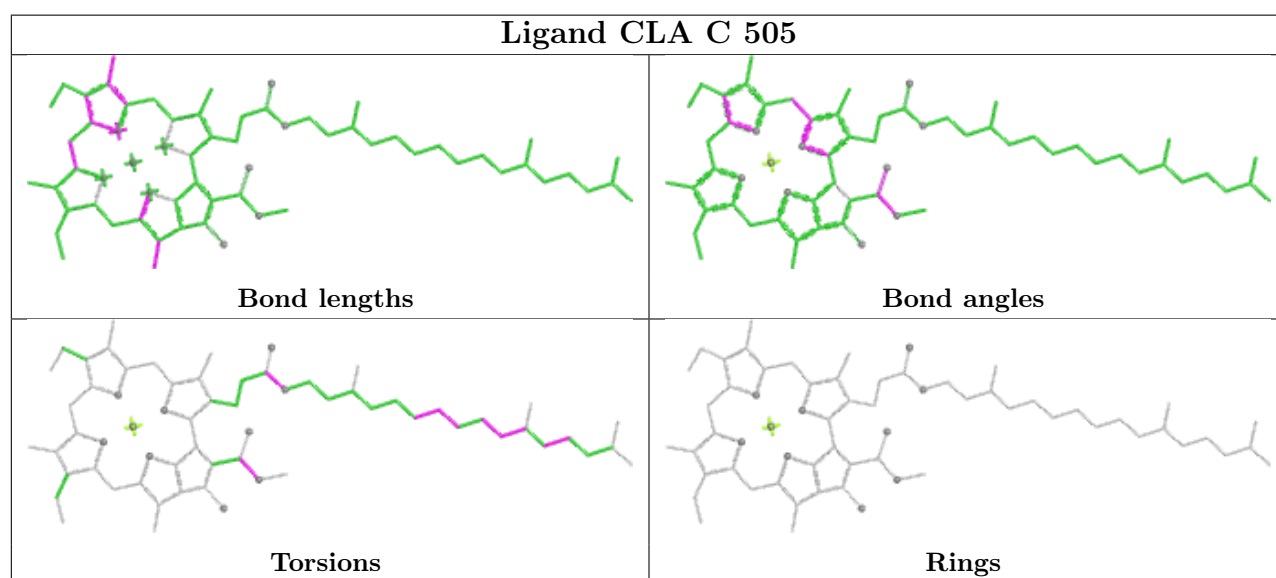
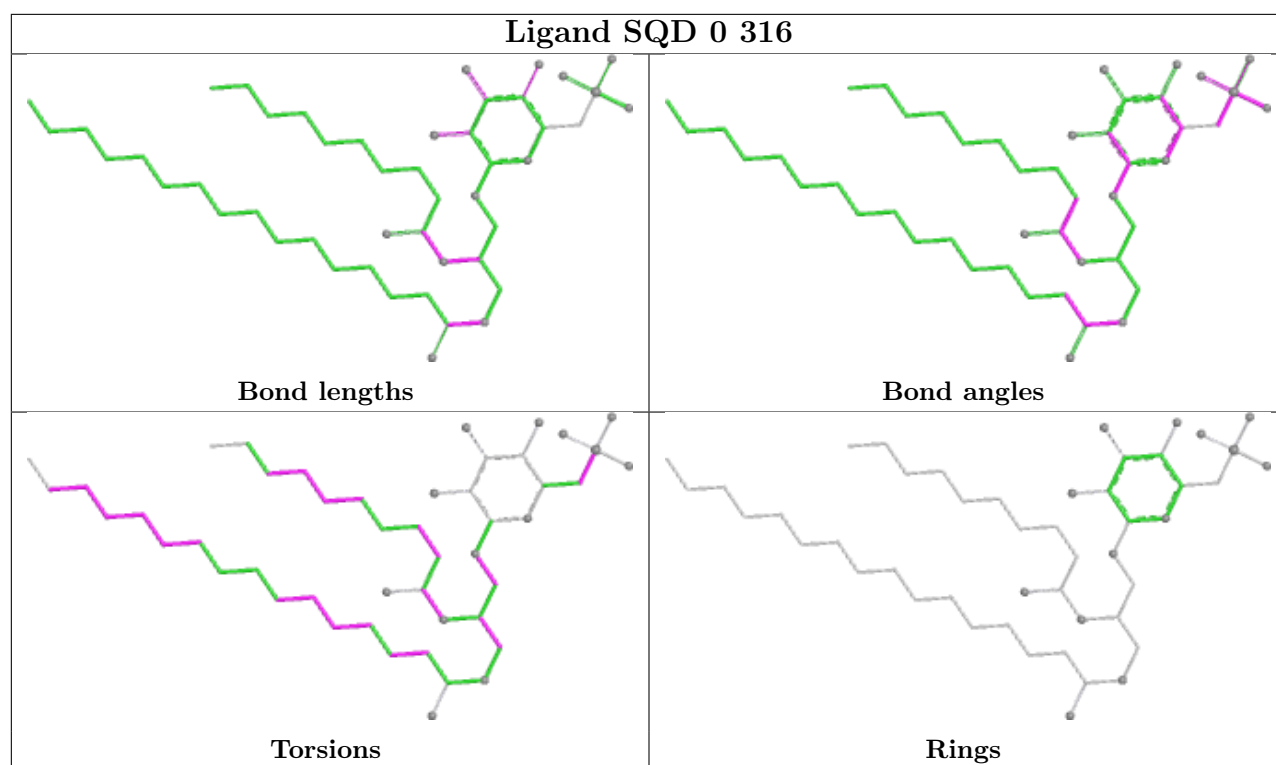


## Ligand CLA 5 309

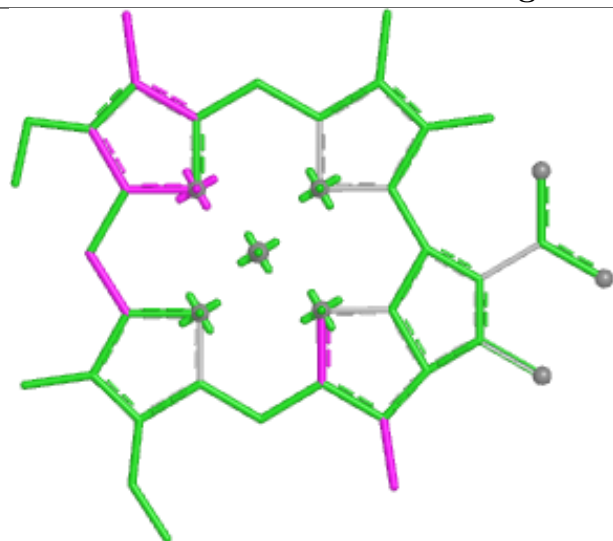




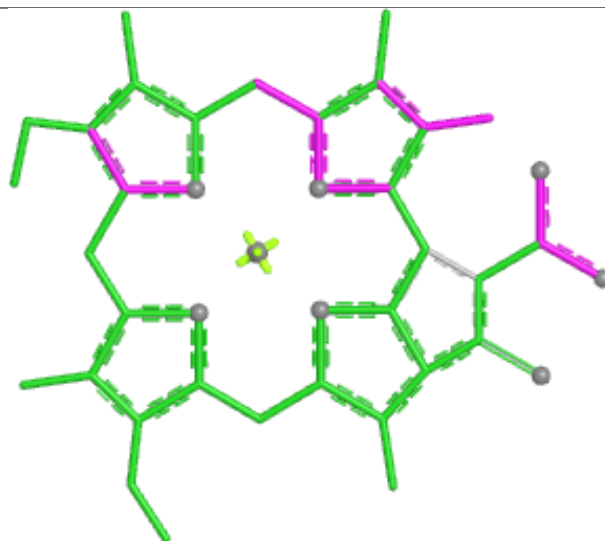




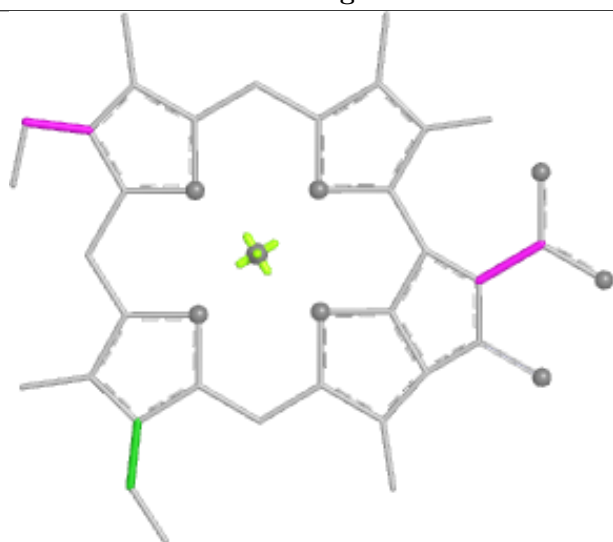
## Ligand CLA 1 213



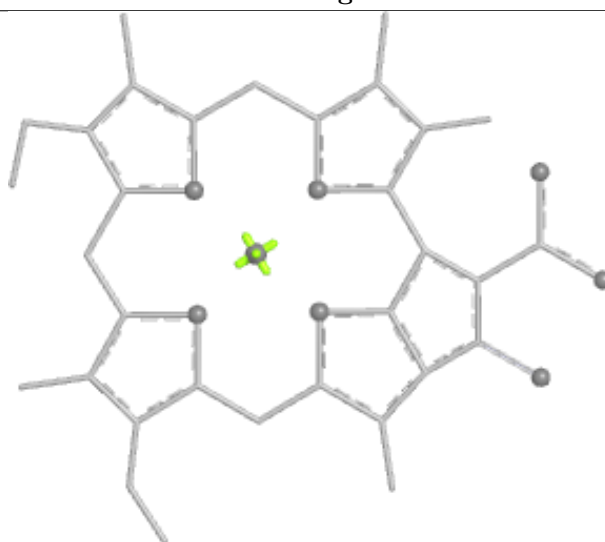
Bond lengths



Bond angles

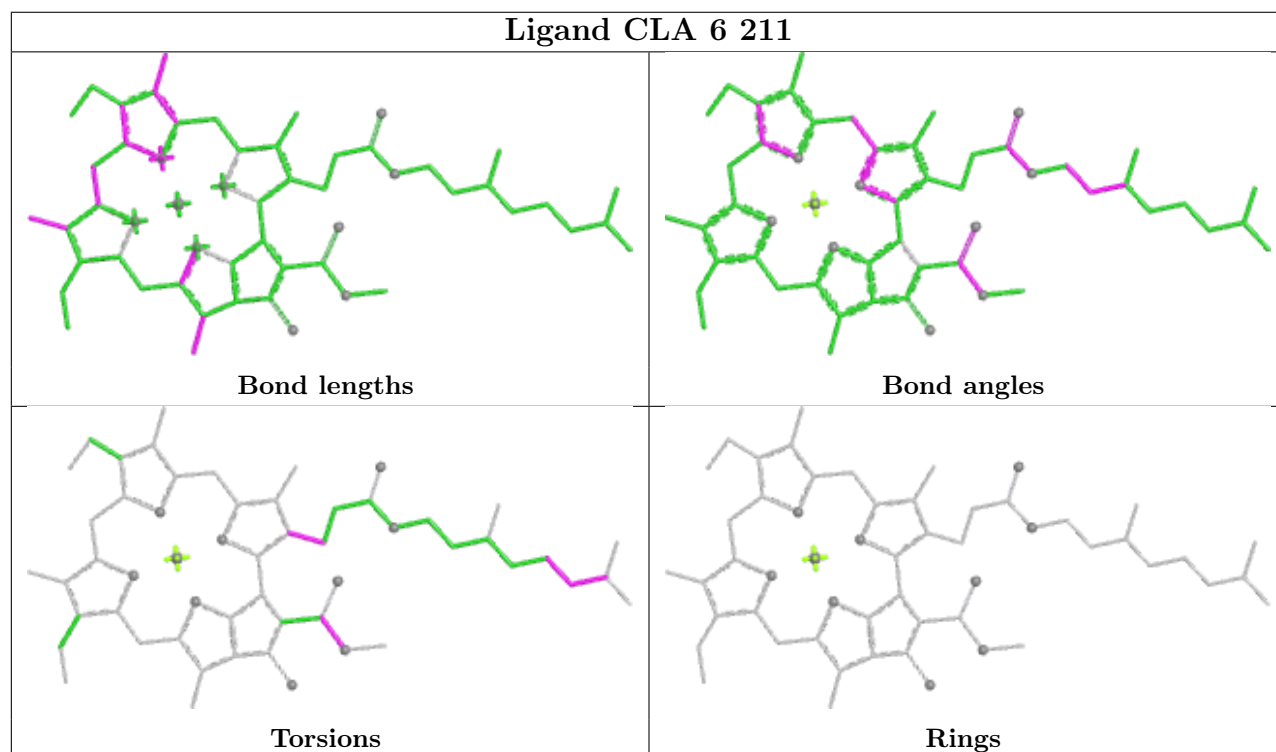
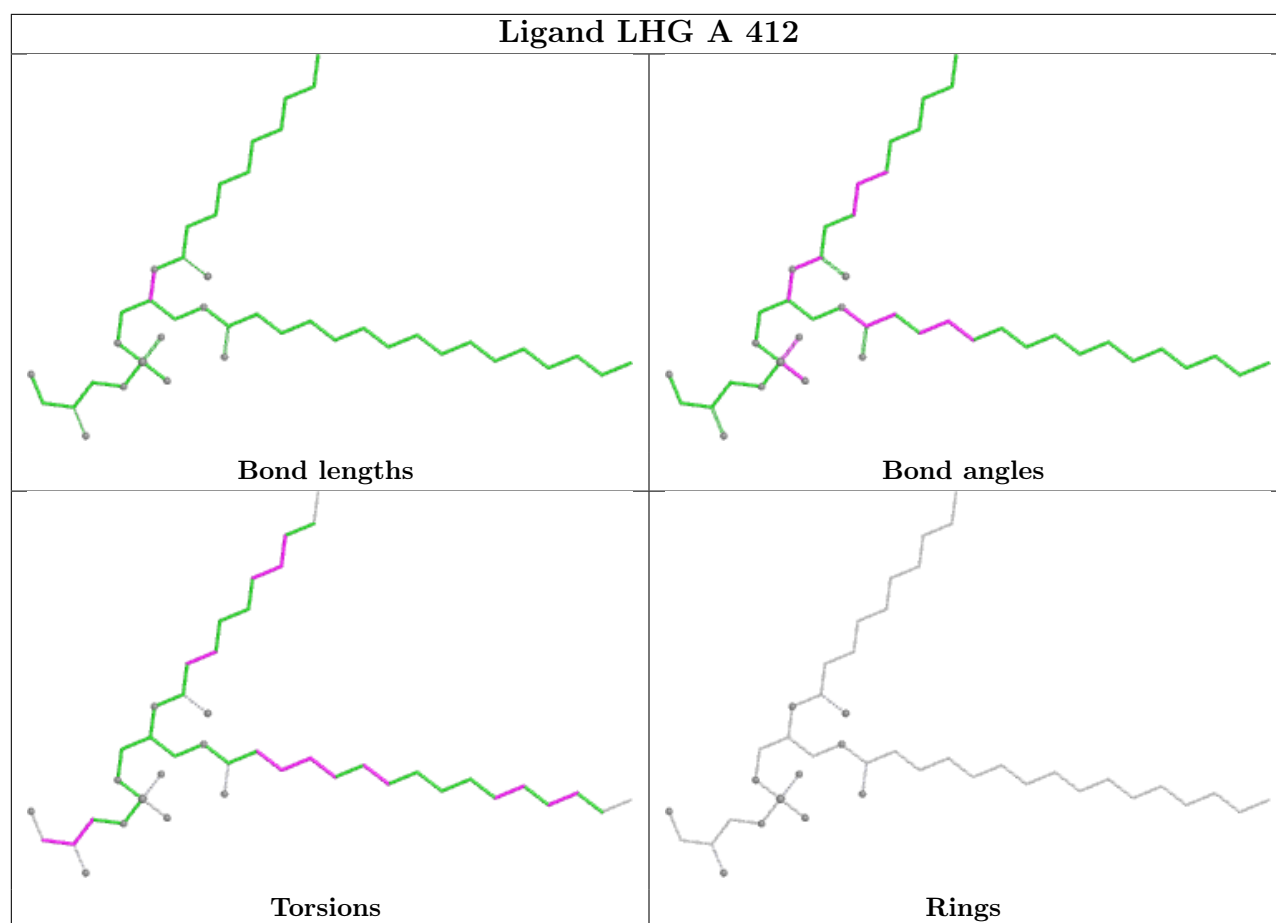


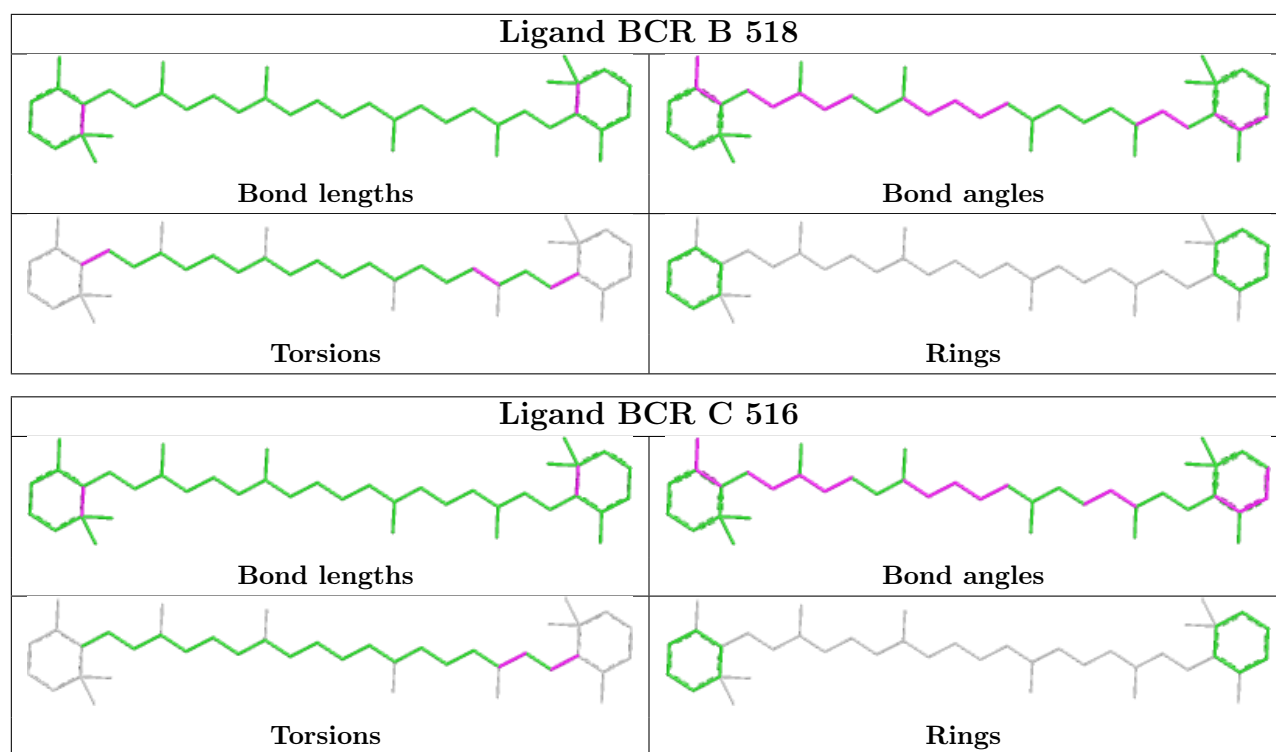
Torsions



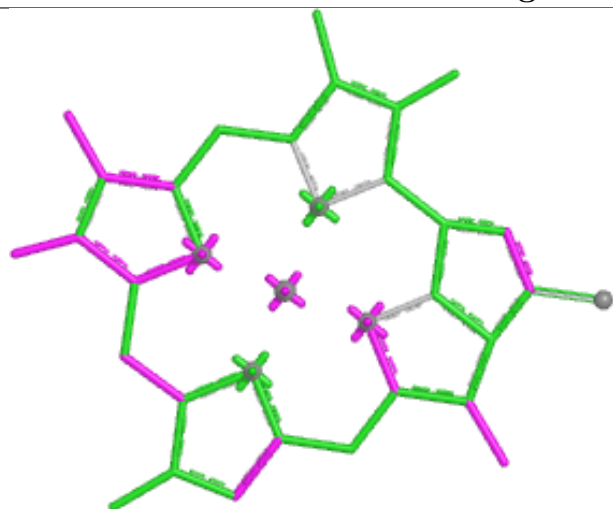
Rings



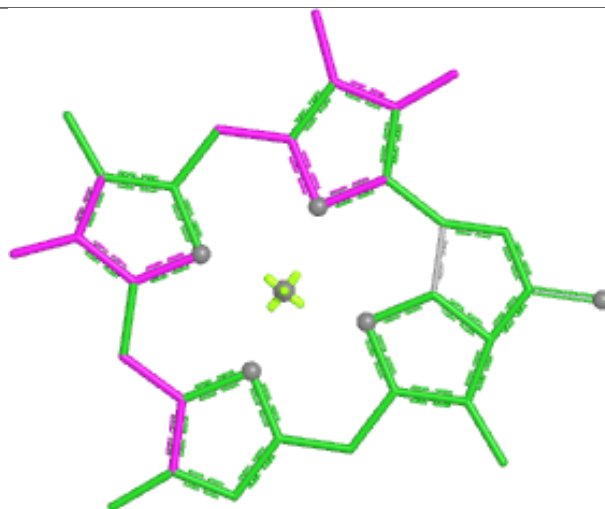




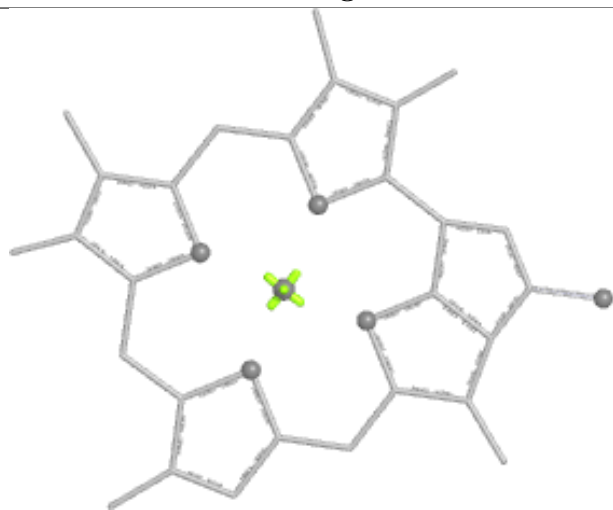
## Ligand CLA 8 304



Bond lengths



Bond angles

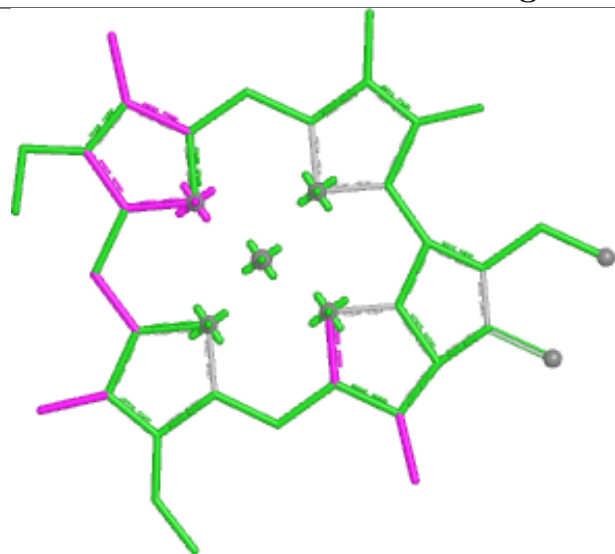


Torsions

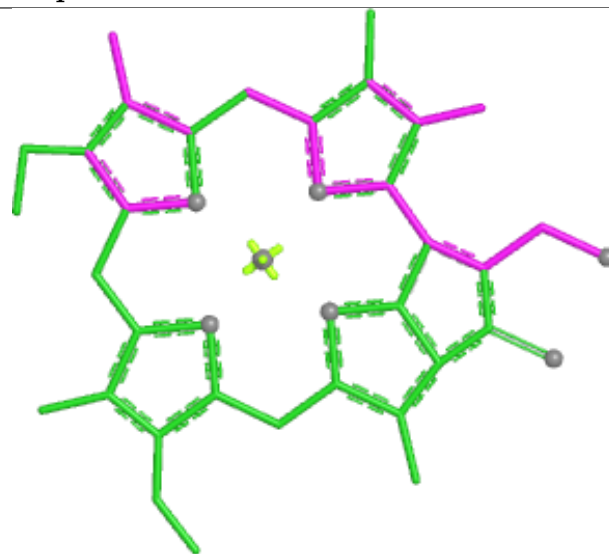


Rings

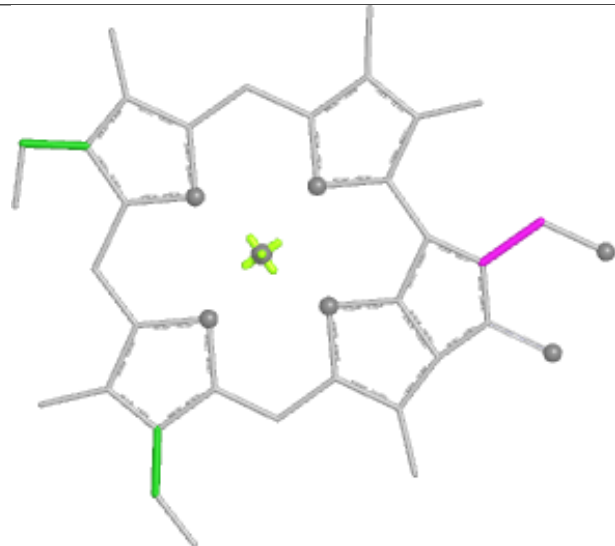
## Ligand CLA p 609



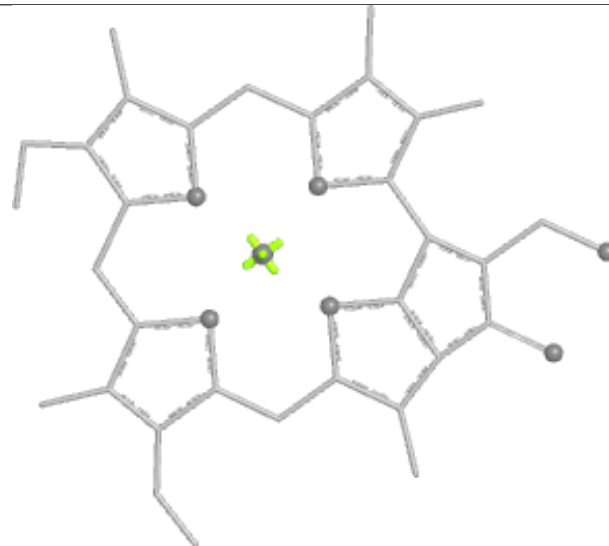
Bond lengths



Bond angles

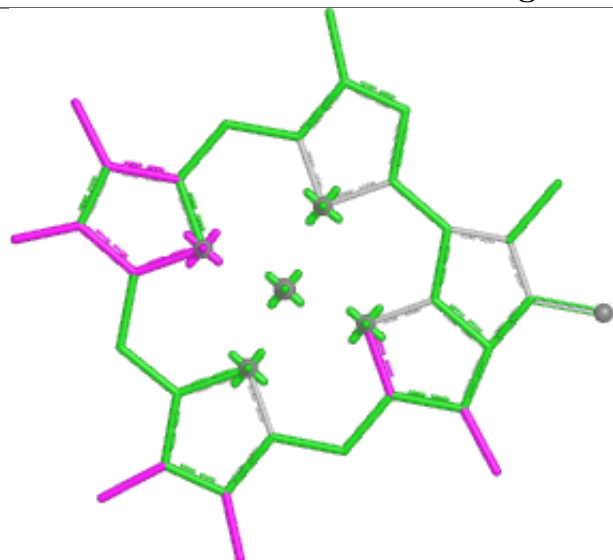


Torsions

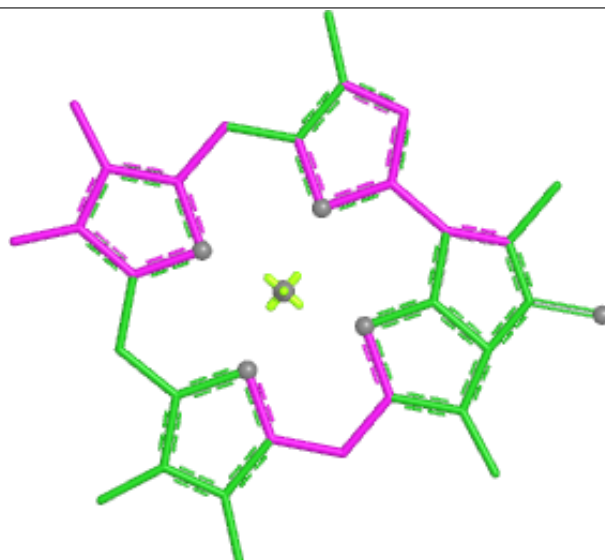


Rings

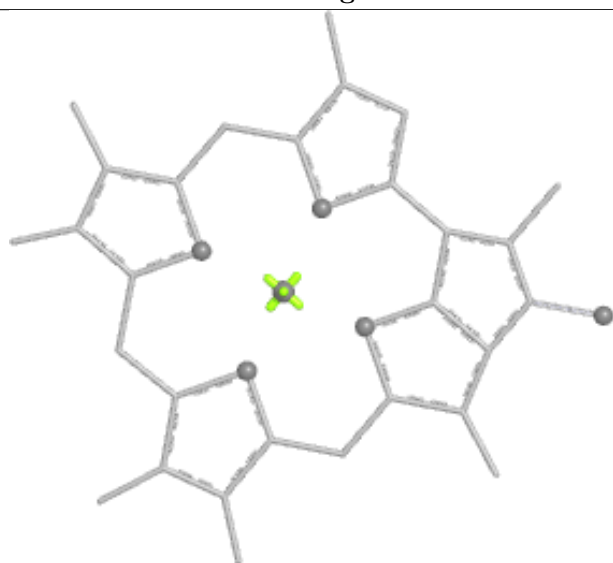
## Ligand CLA 4 213



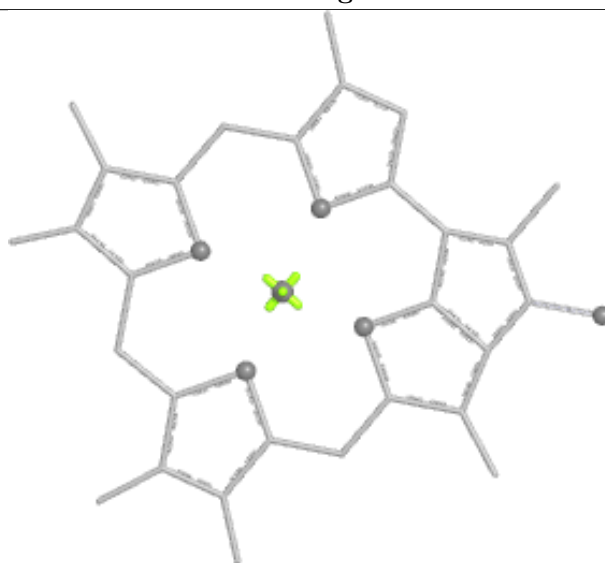
Bond lengths



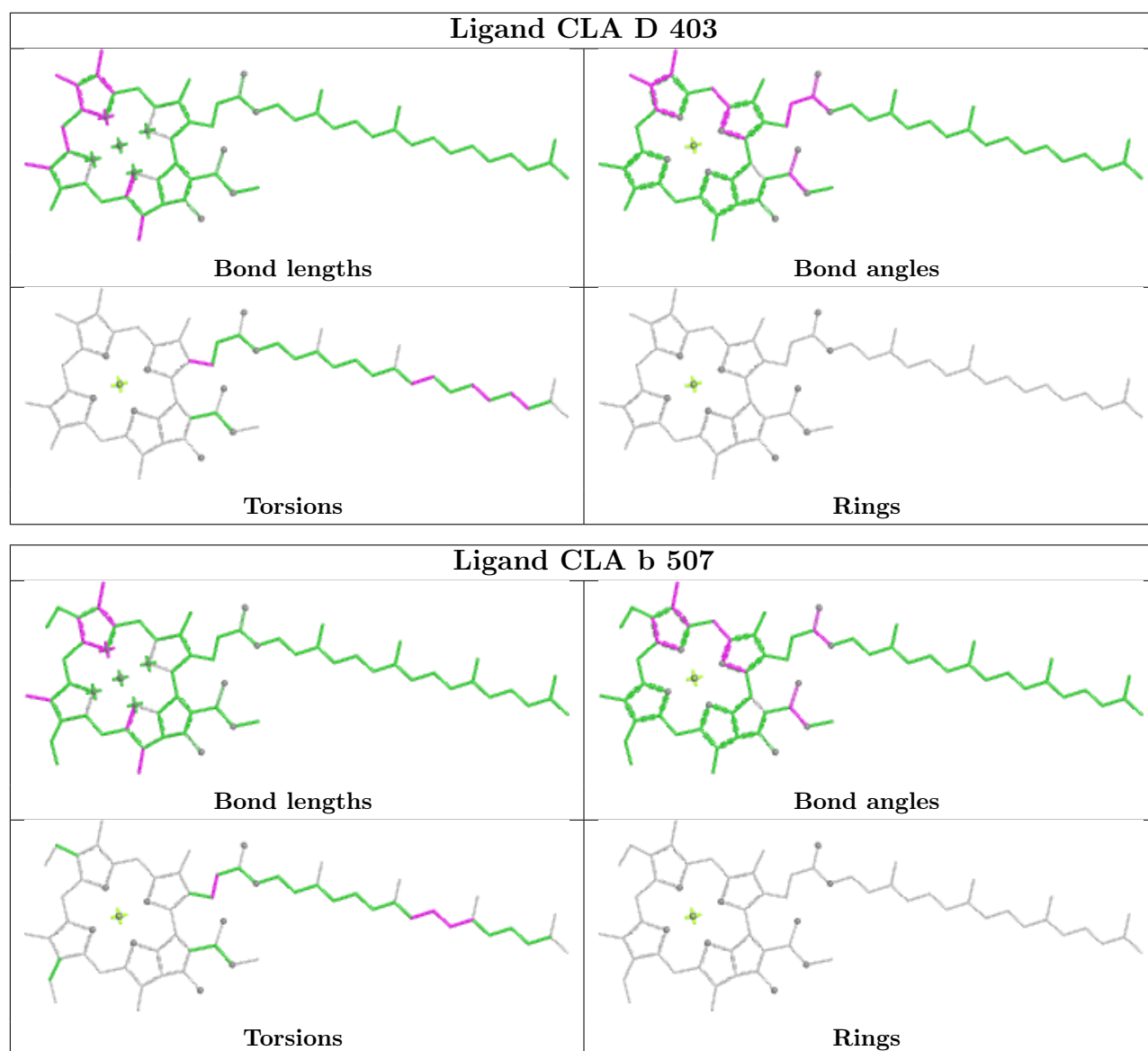
Bond angles



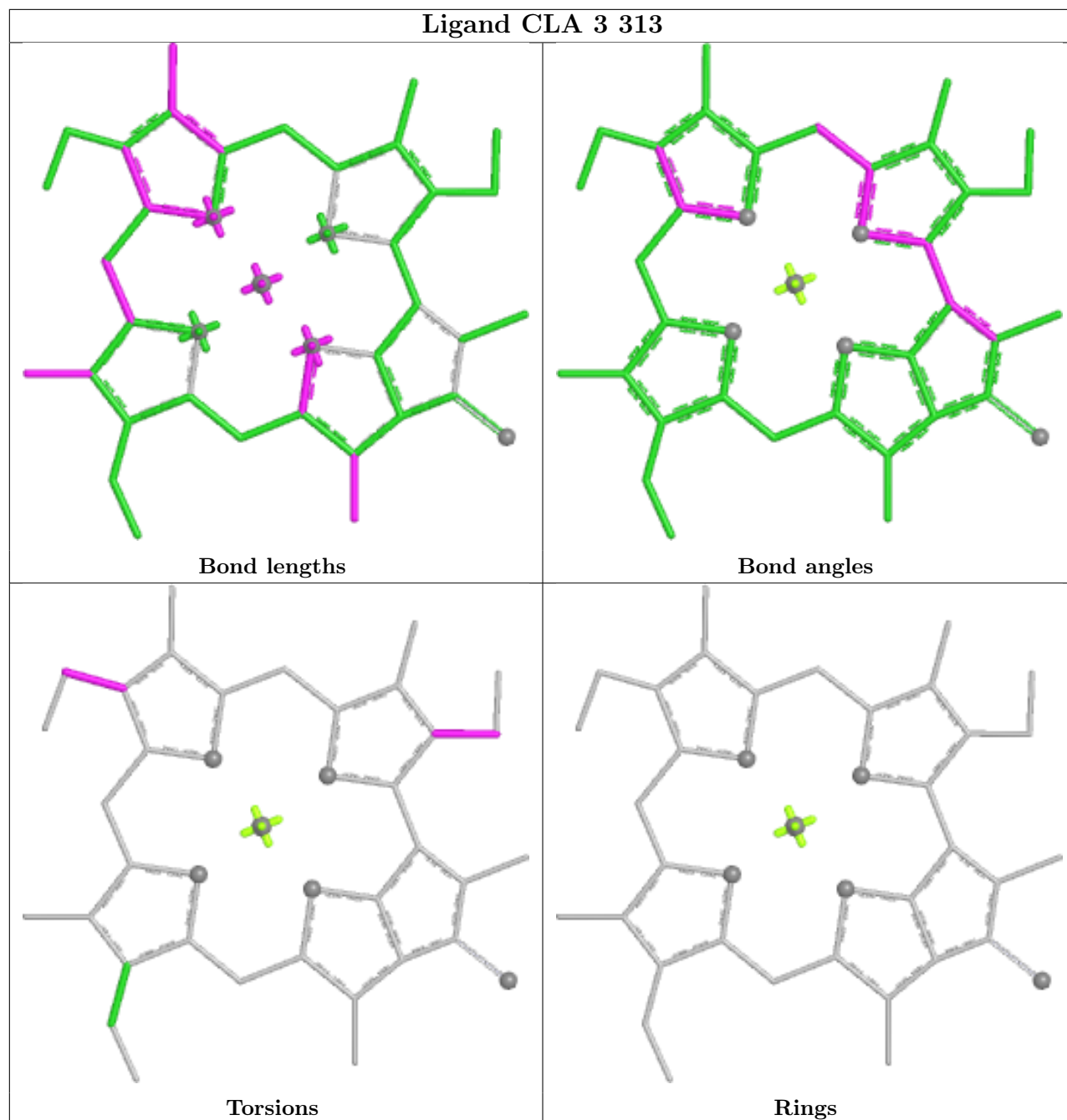
Torsions

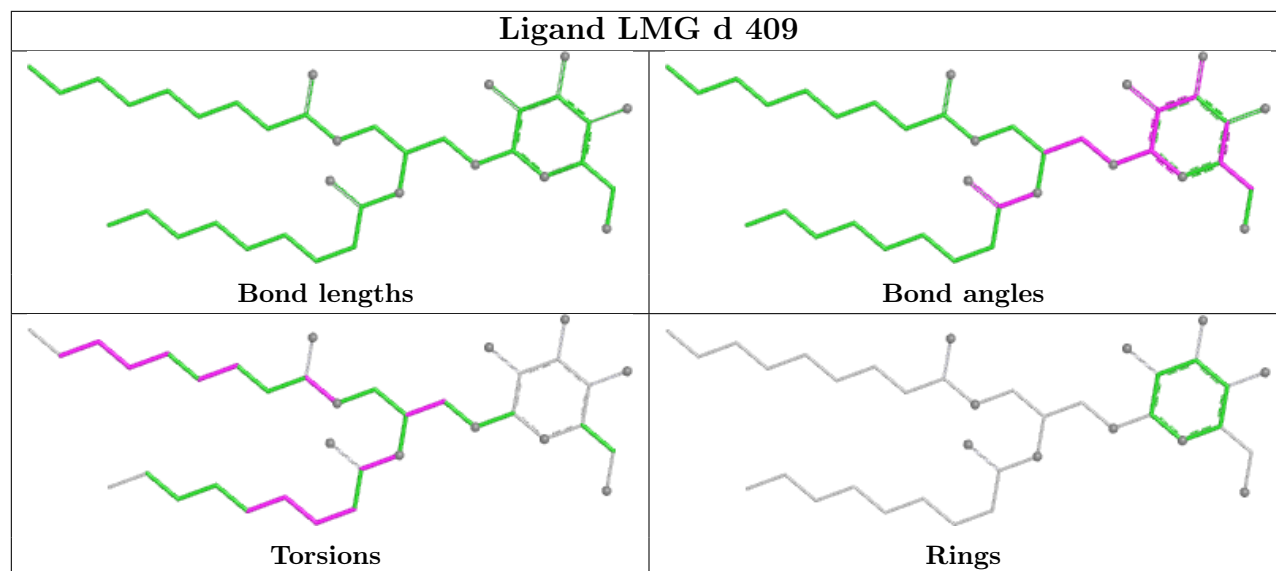
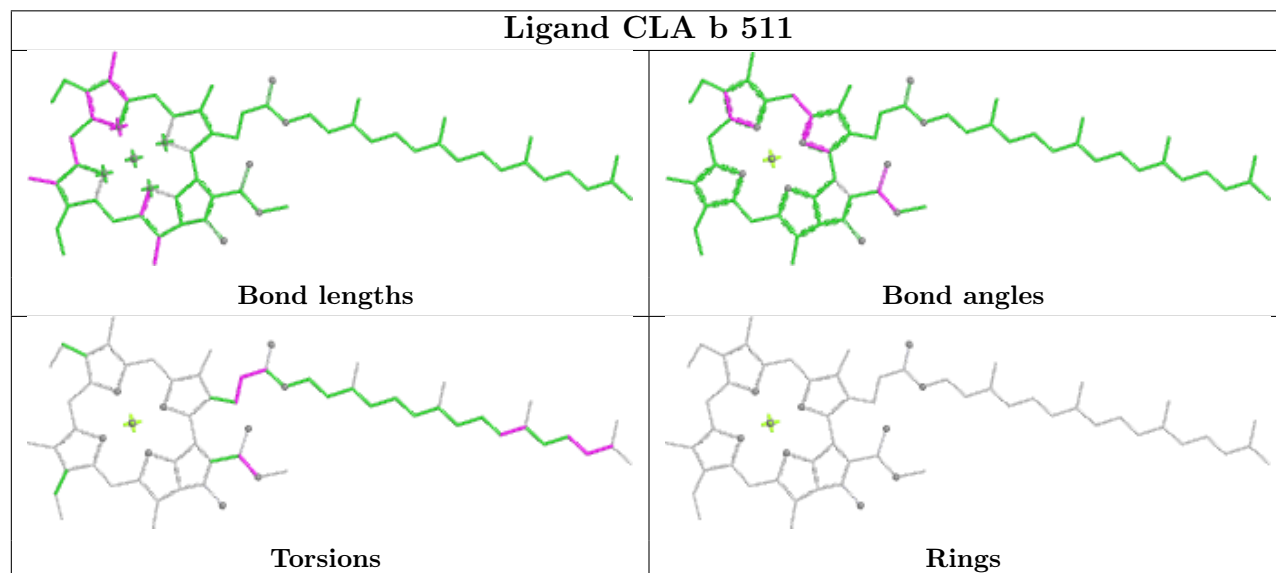
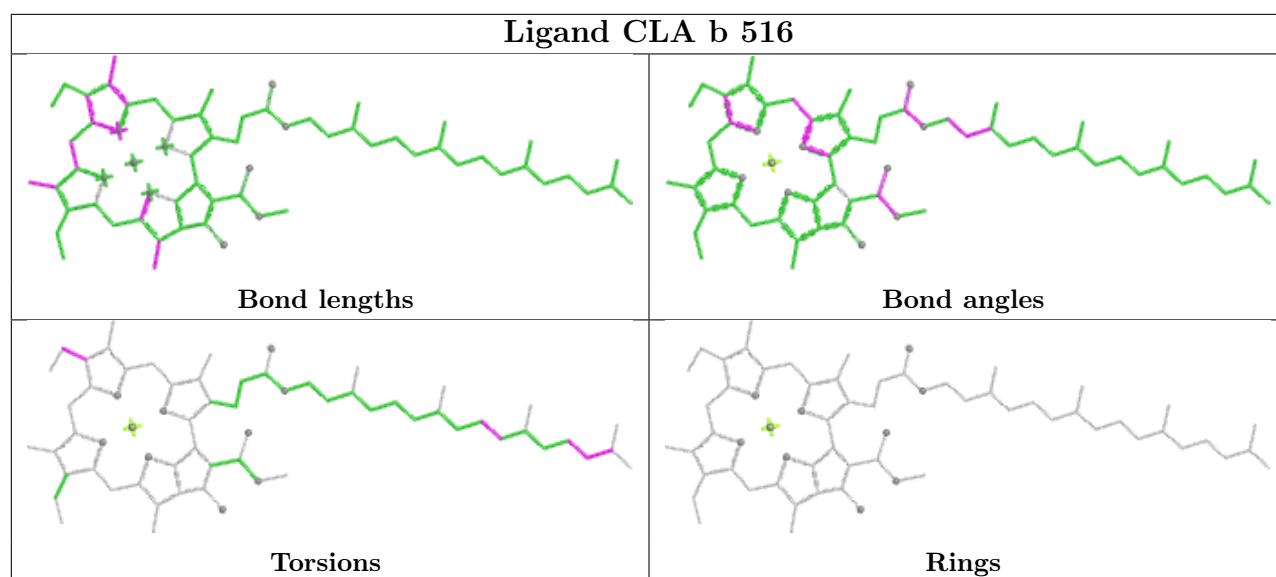


Rings



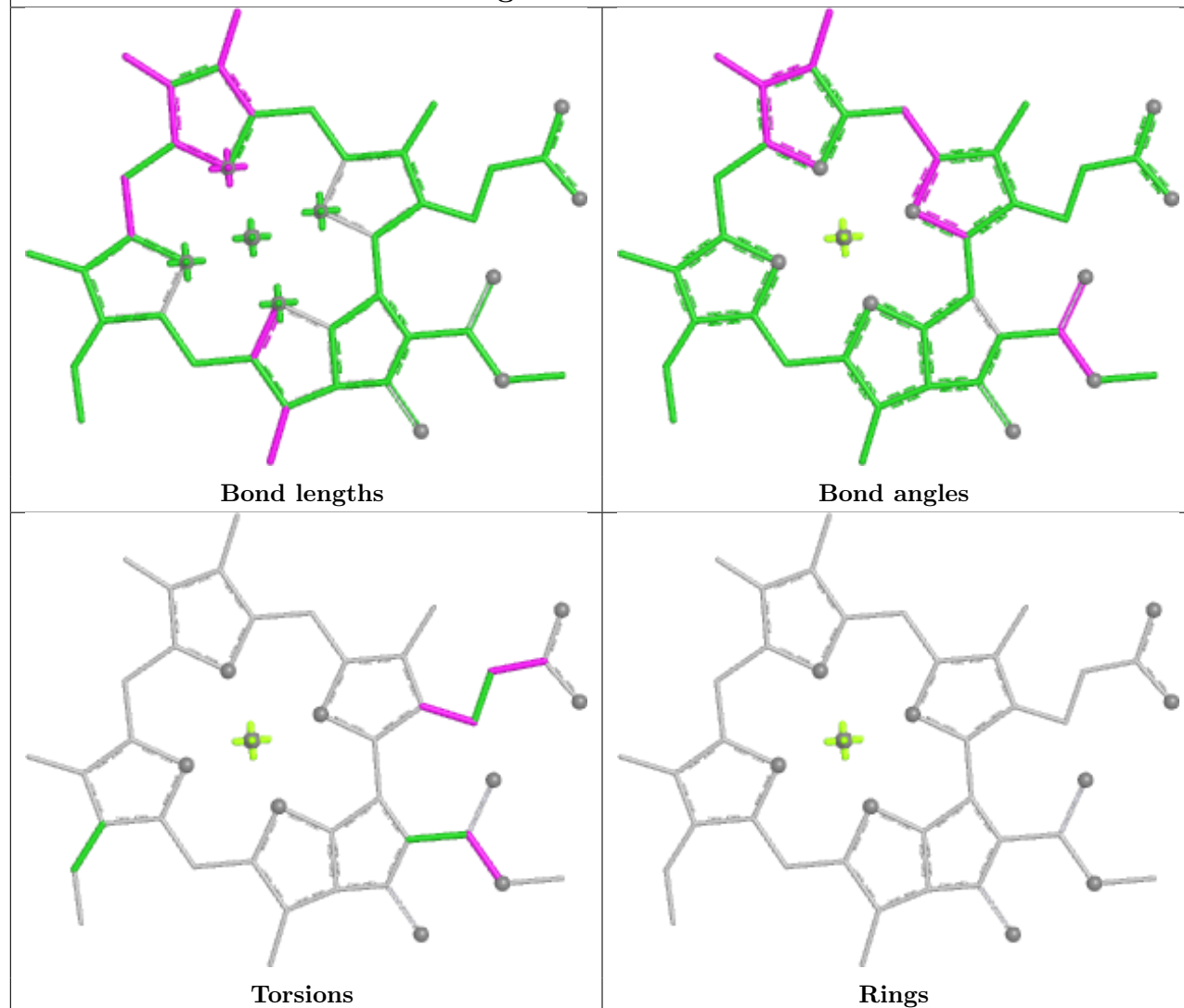
## Ligand CLA 3 313



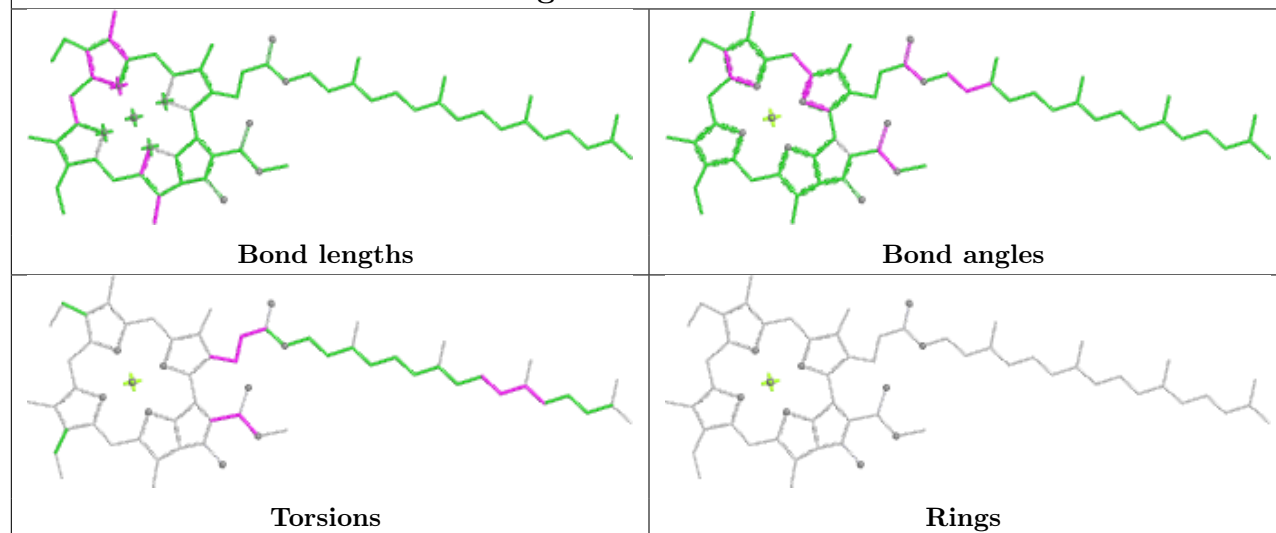


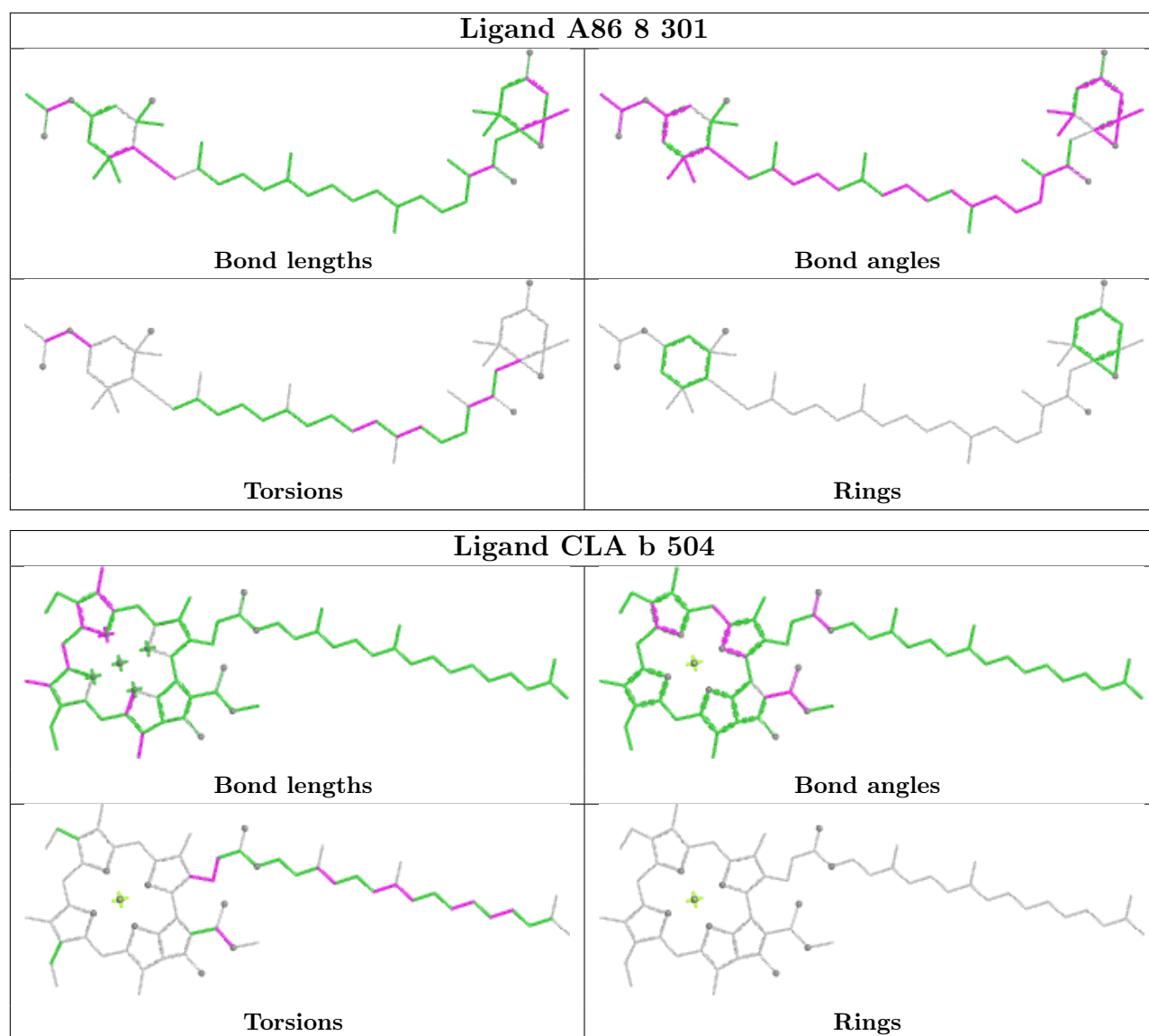


## Ligand CLA 1 209

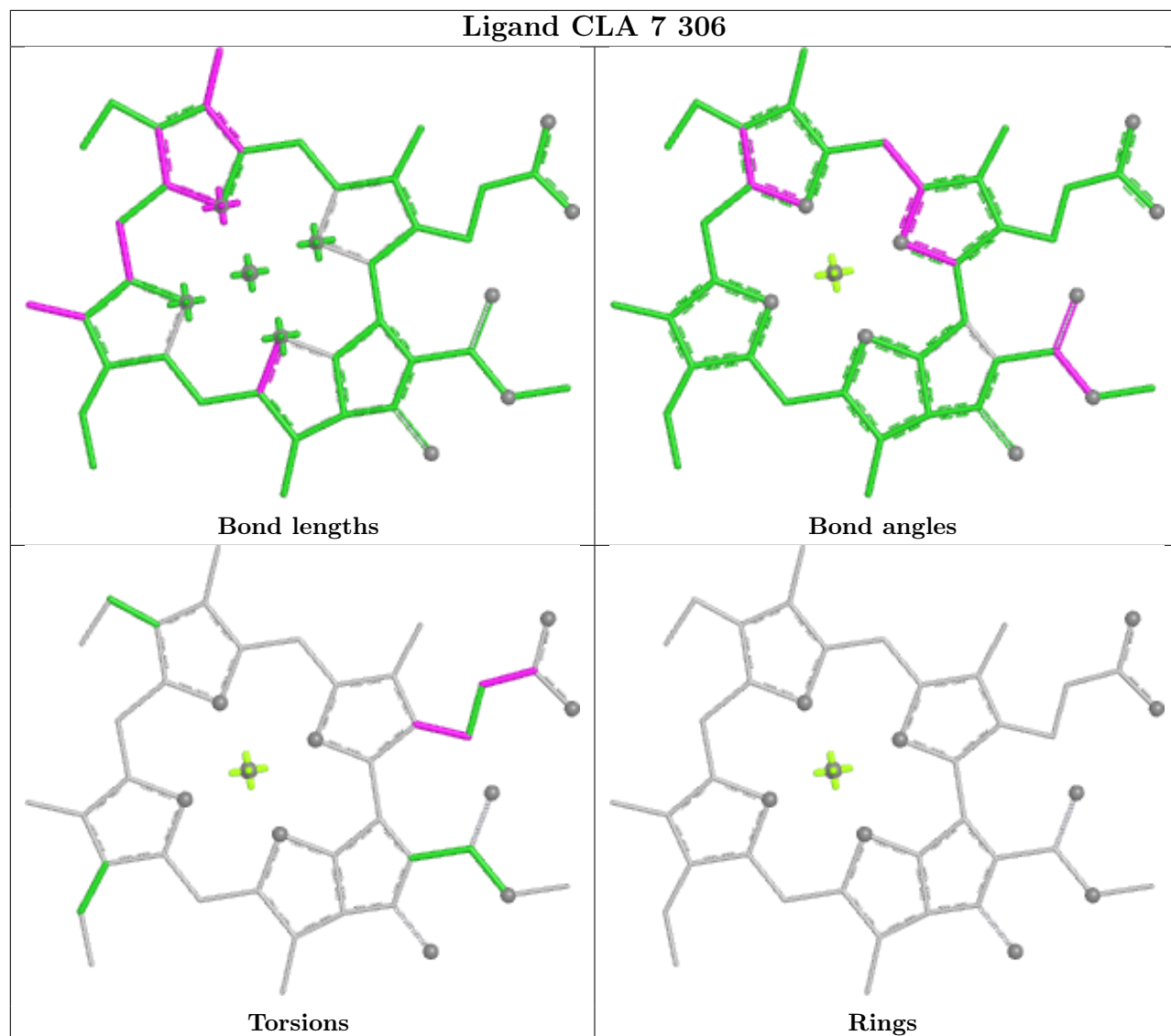


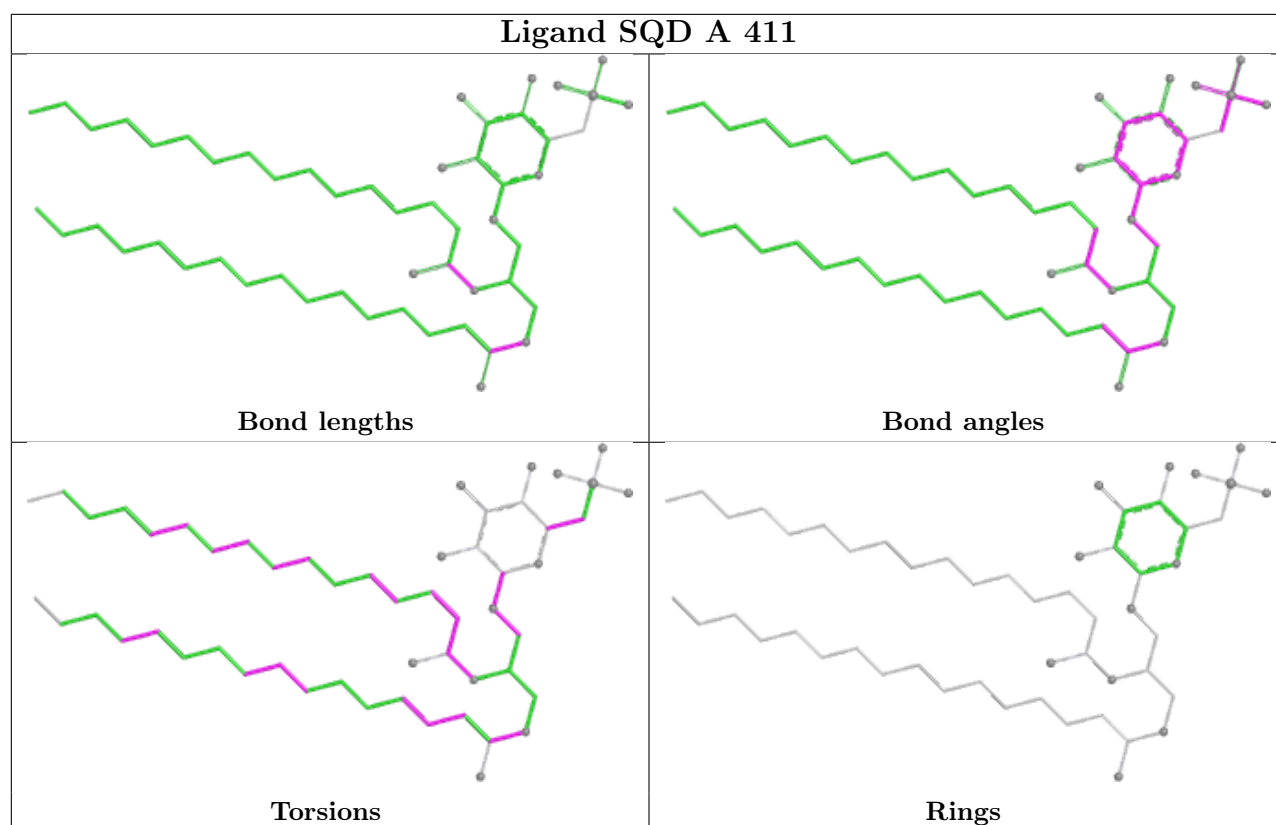
## Ligand CLA c 502



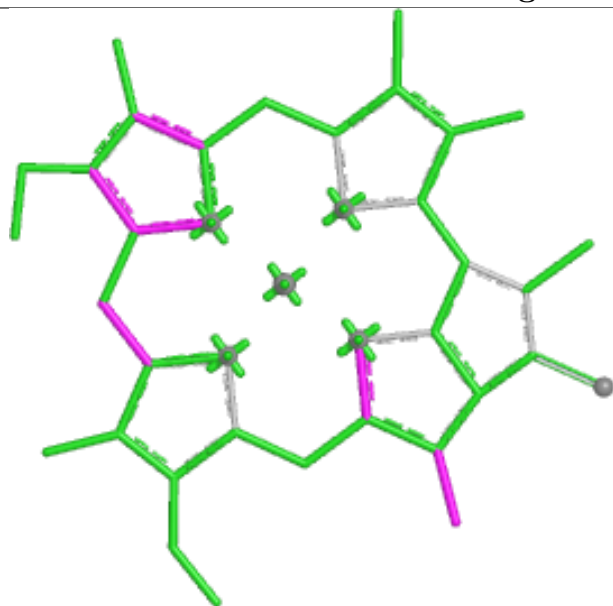


## Ligand CLA 7 306

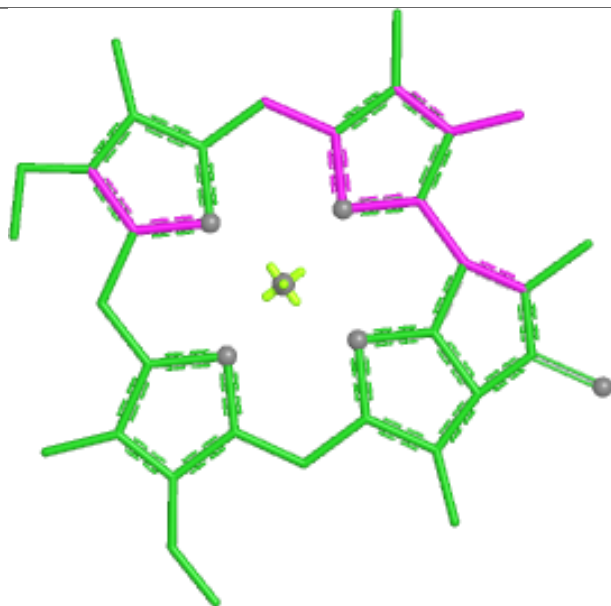




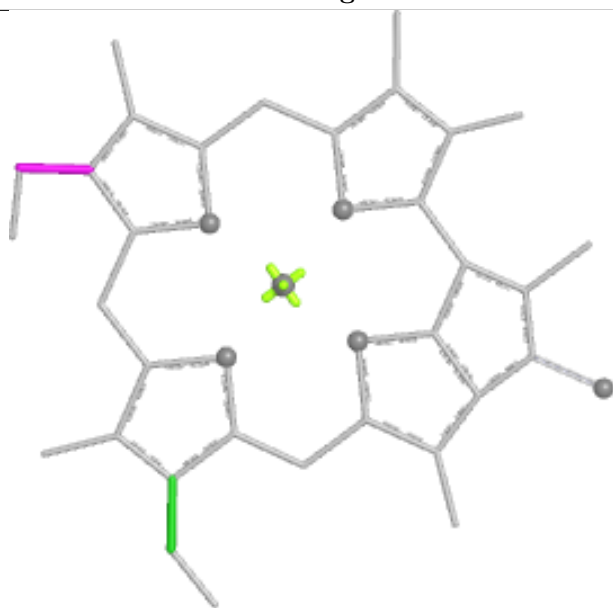
## Ligand CLA 1 216



Bond lengths



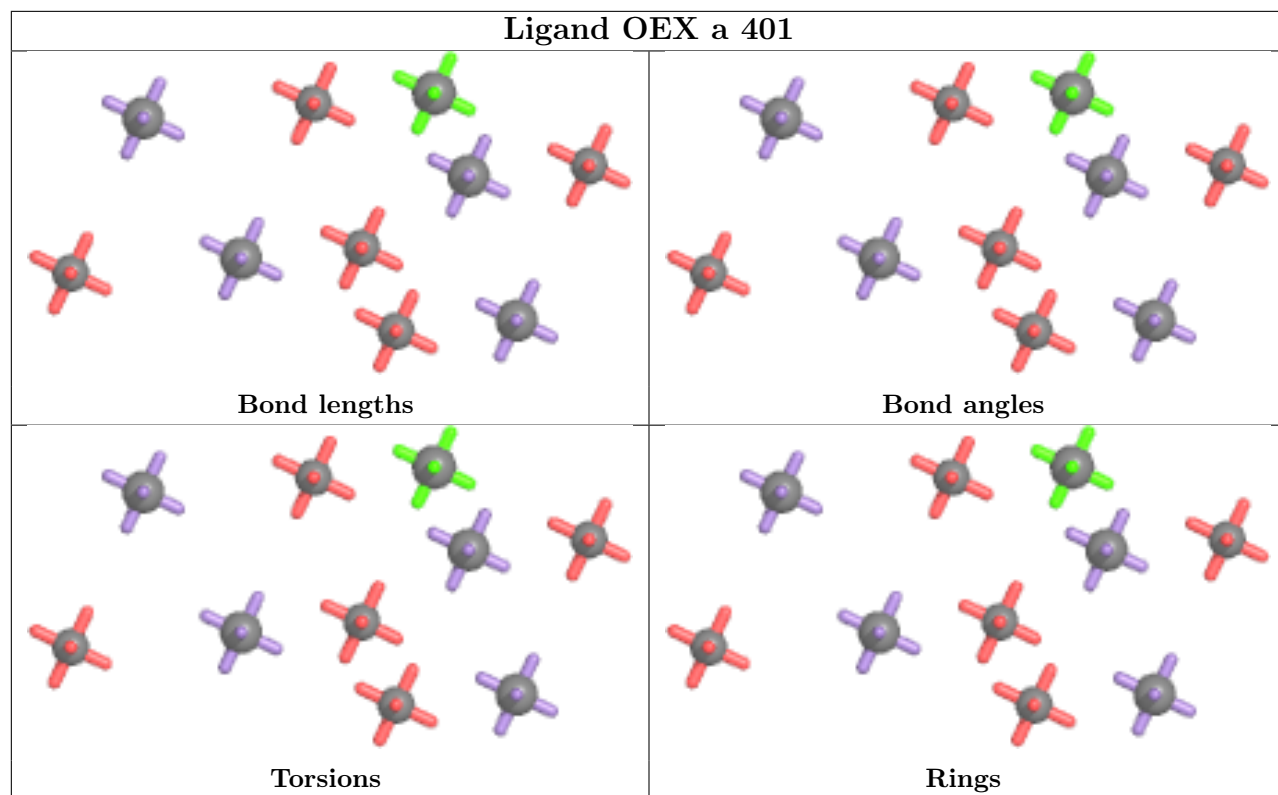
Bond angles



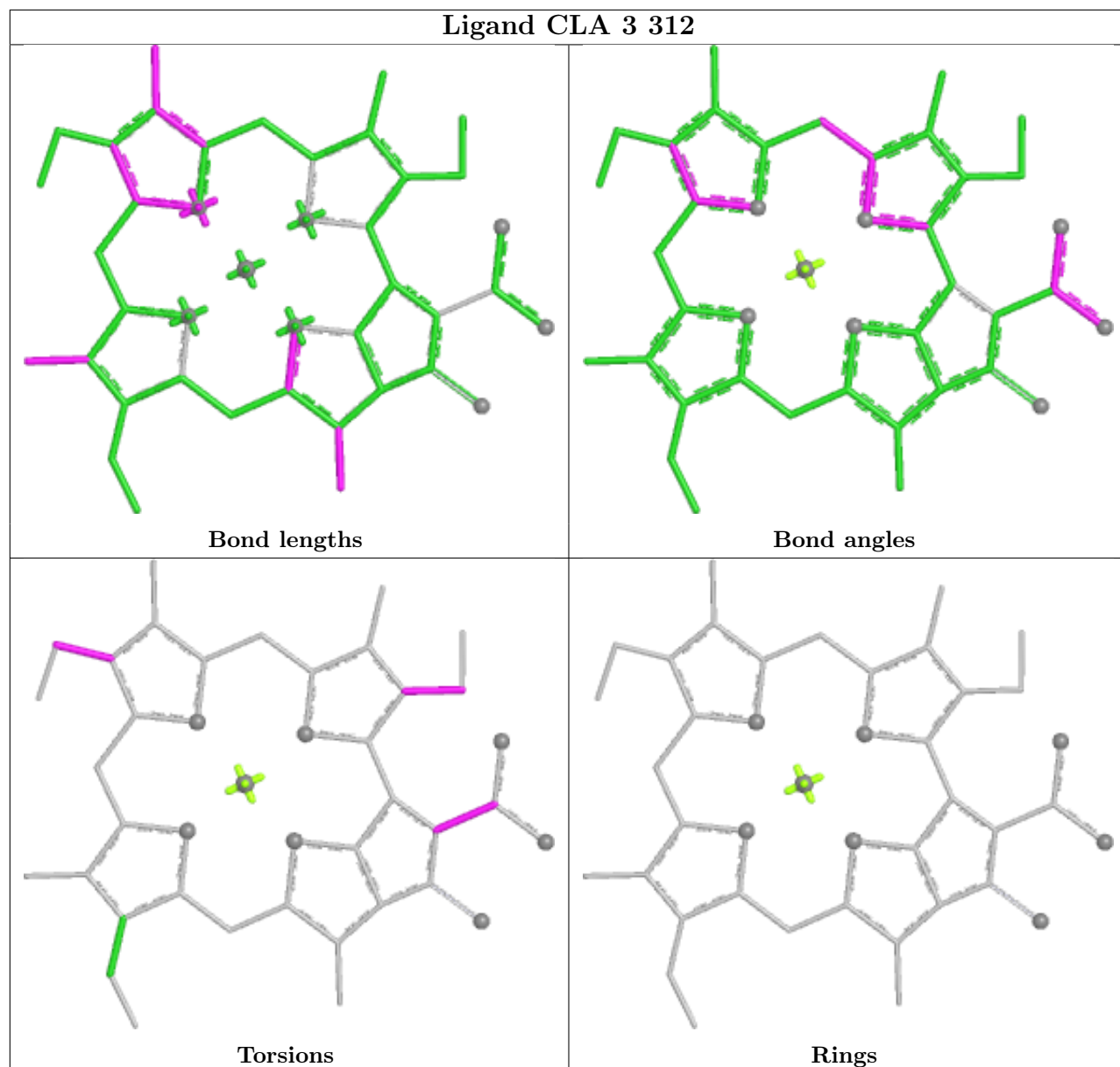
Torsions



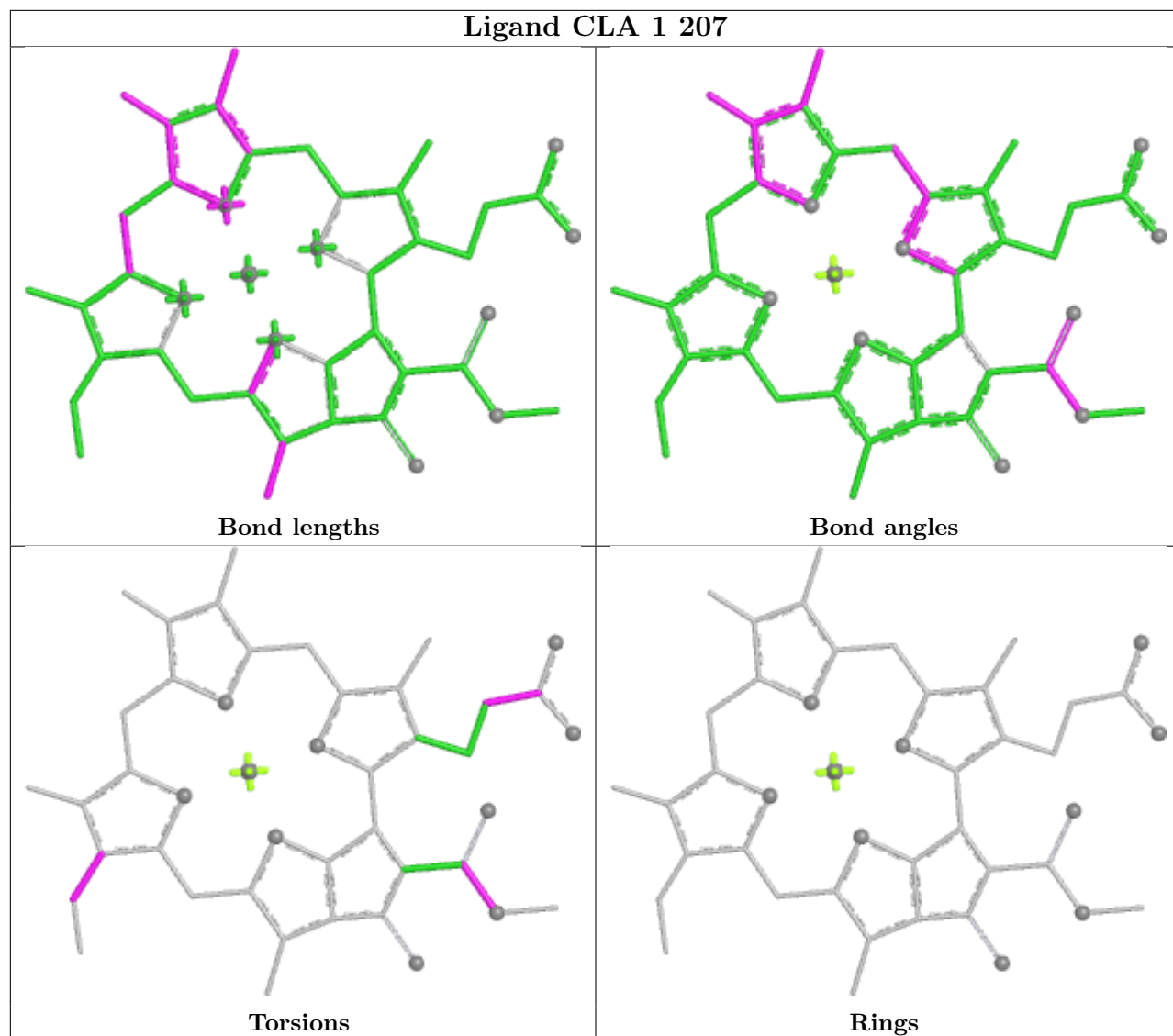
Rings



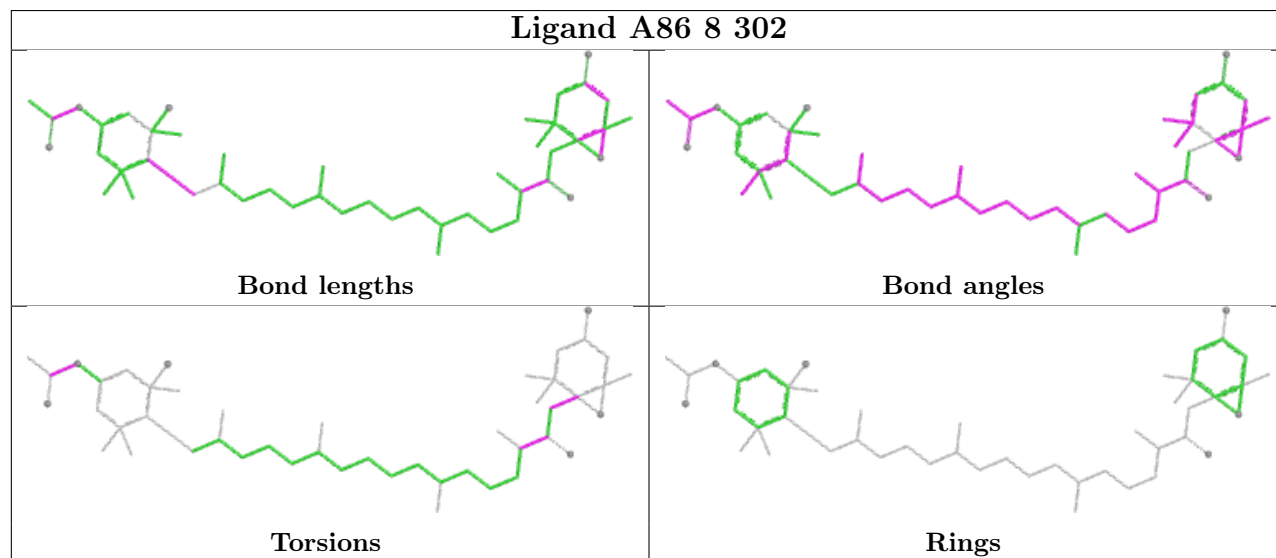
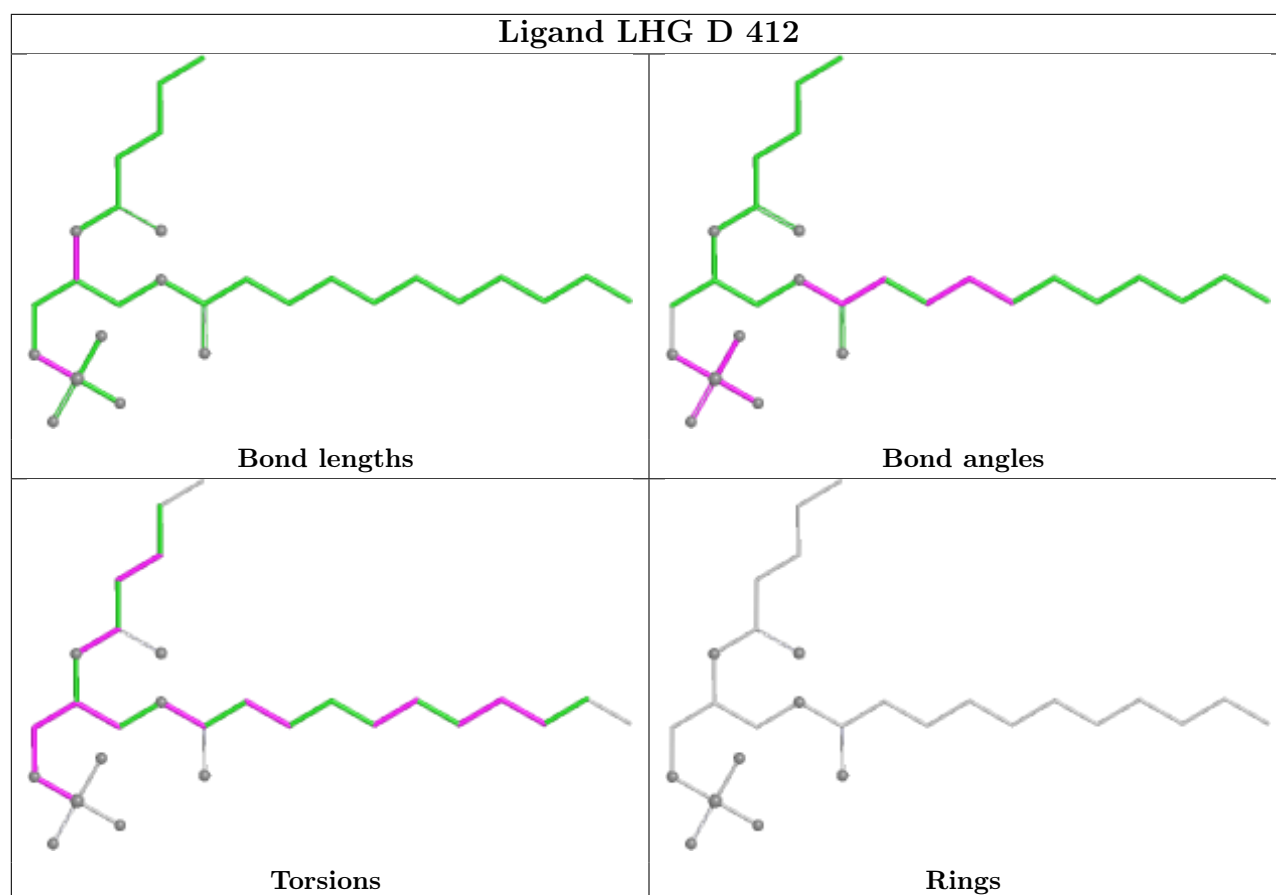
## Ligand CLA 3 312

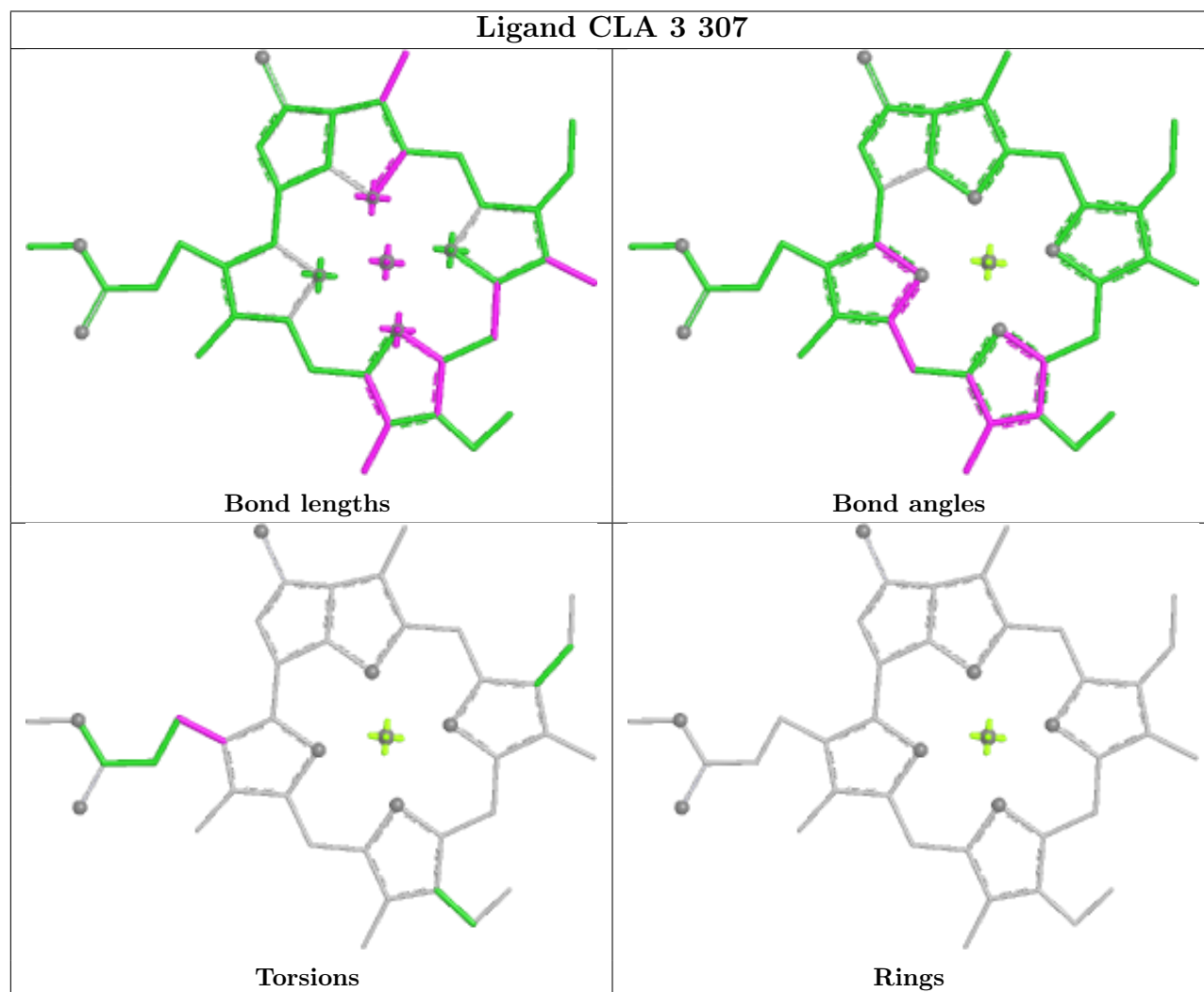
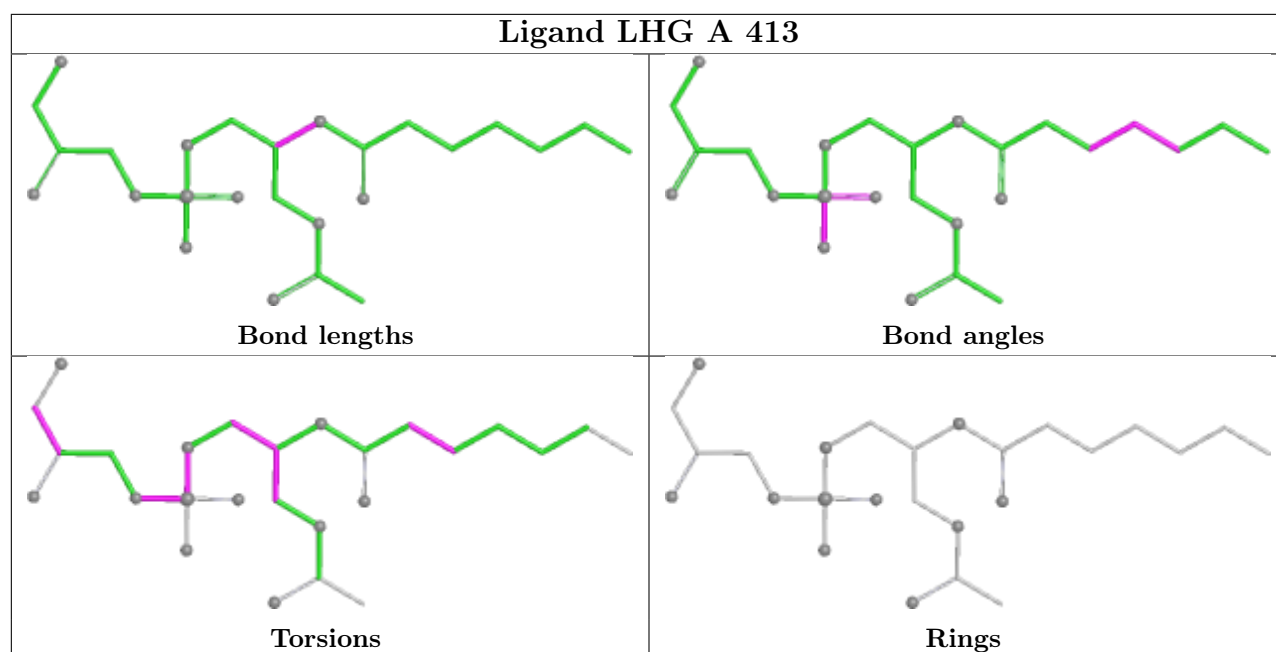


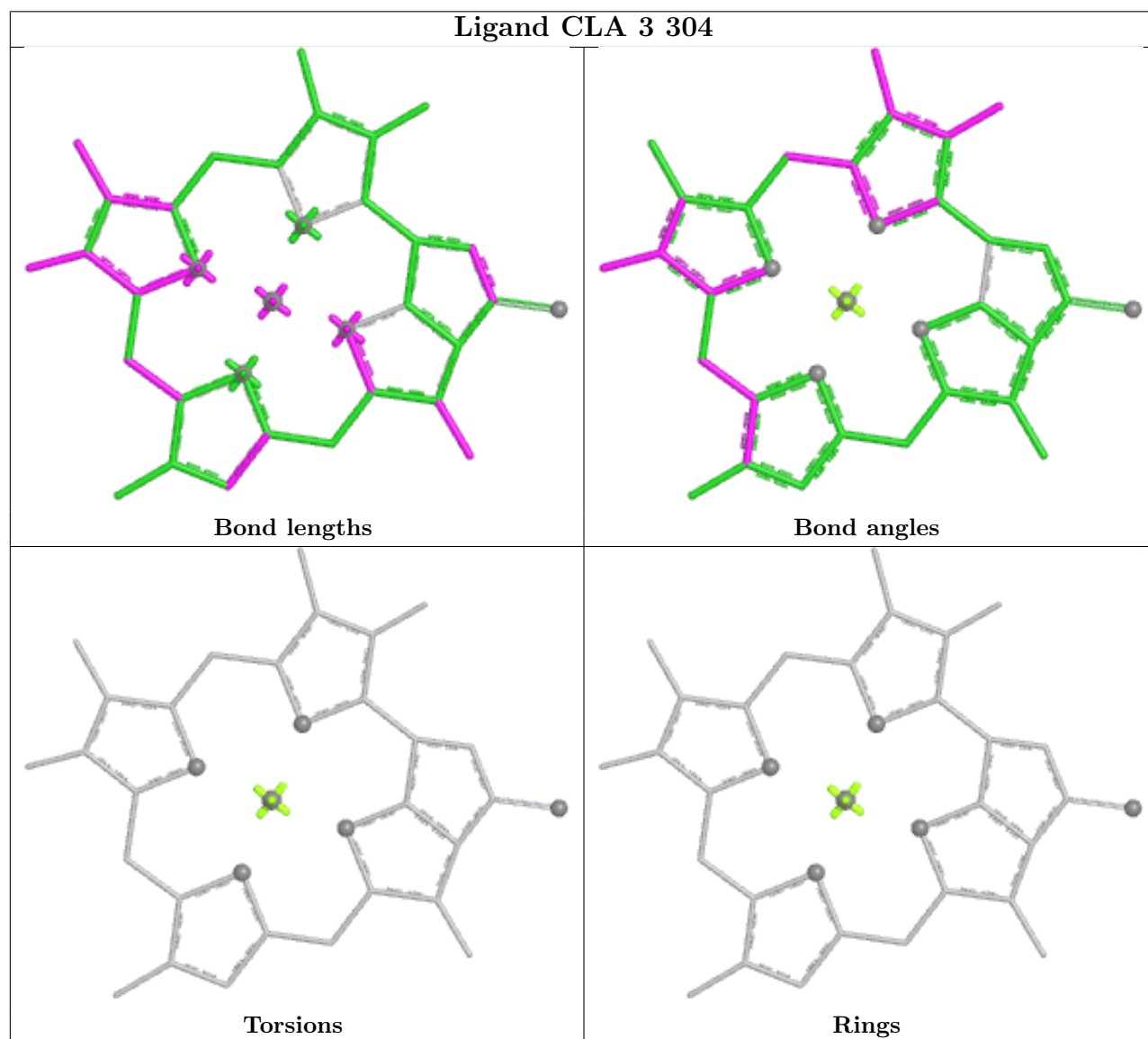
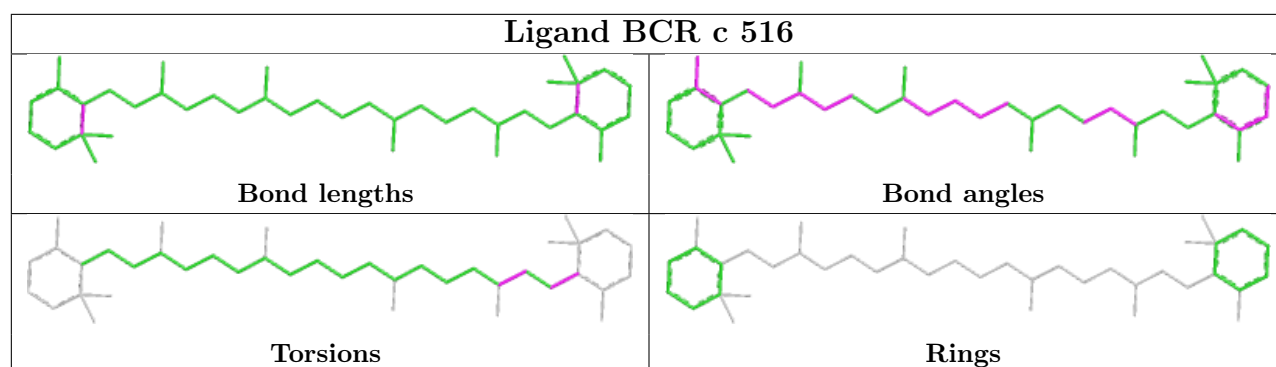
## Ligand CLA 1 207

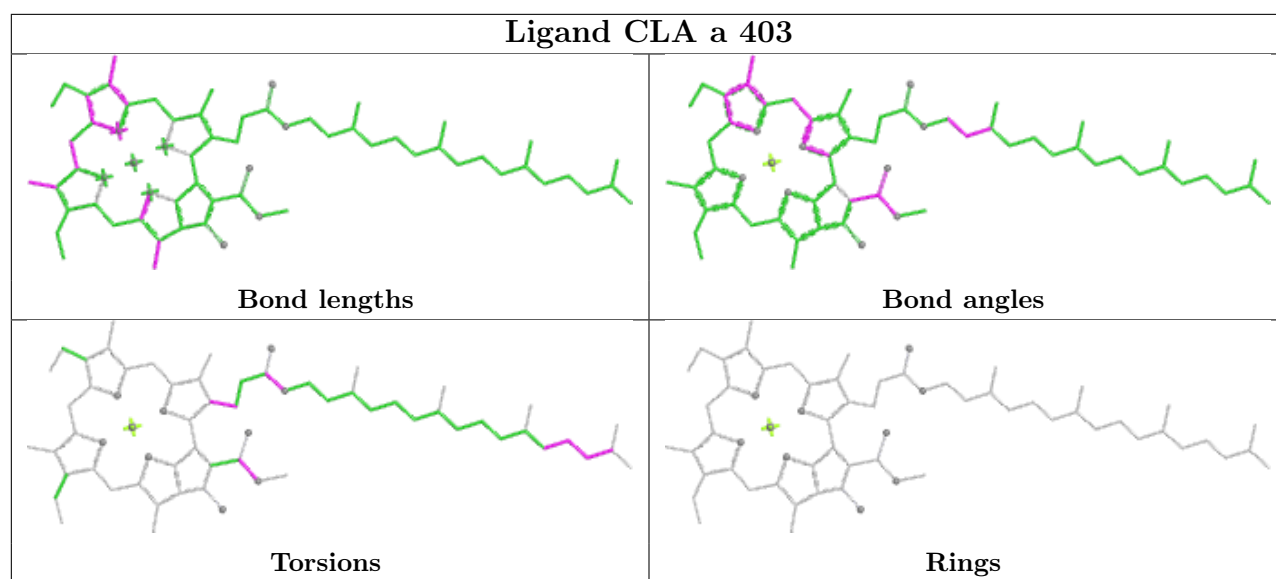




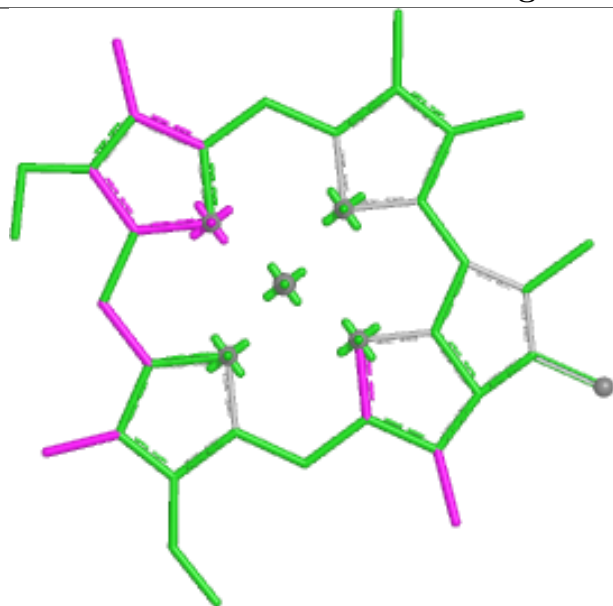




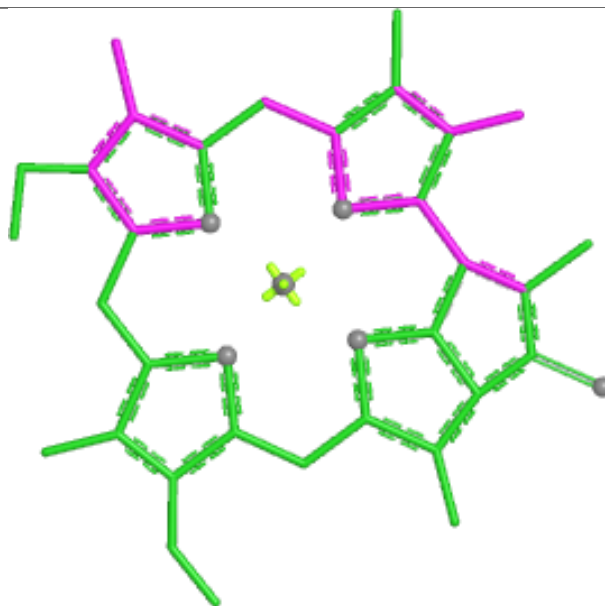




## Ligand CLA 9 210



Bond lengths



Bond angles

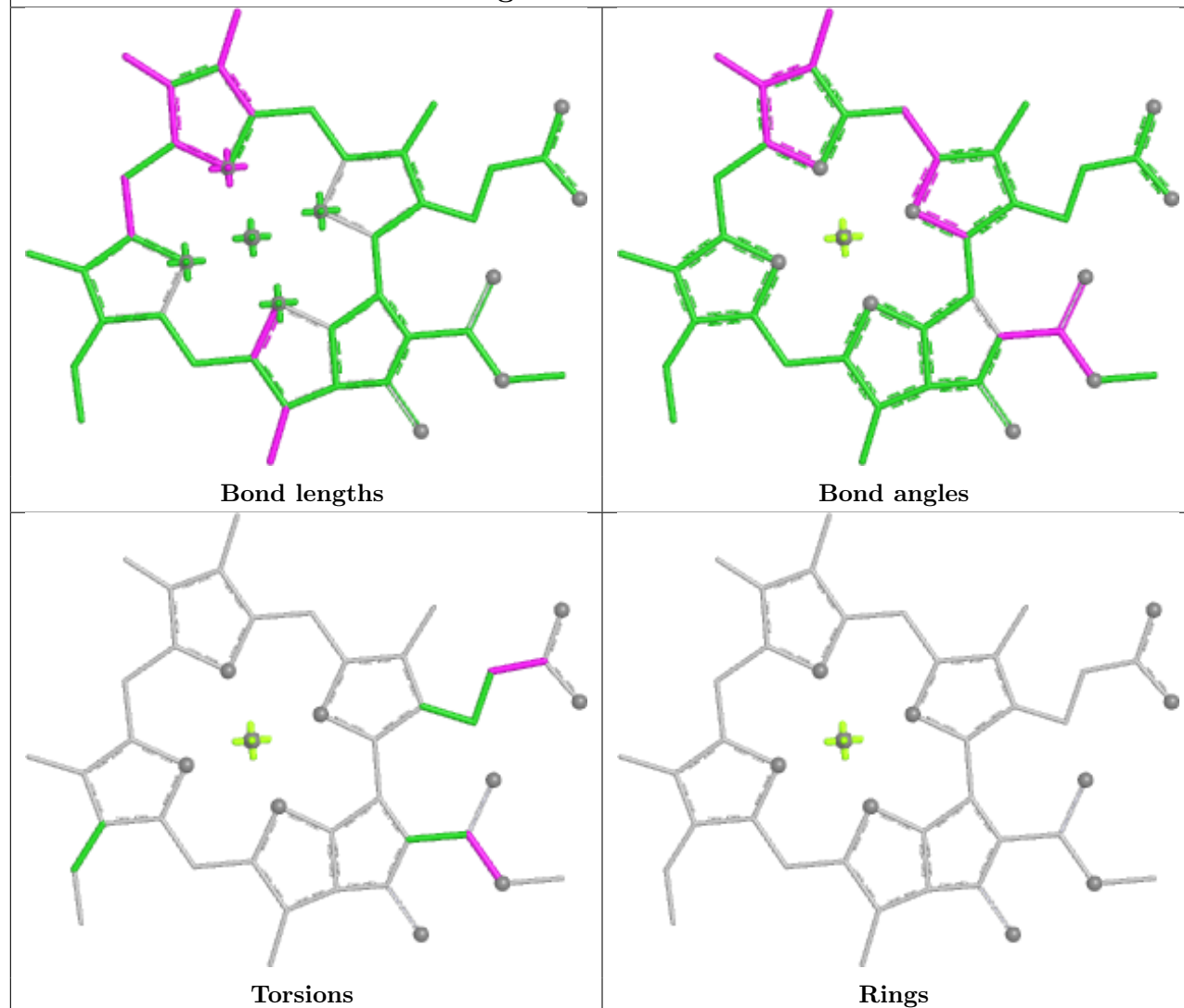


Torsions

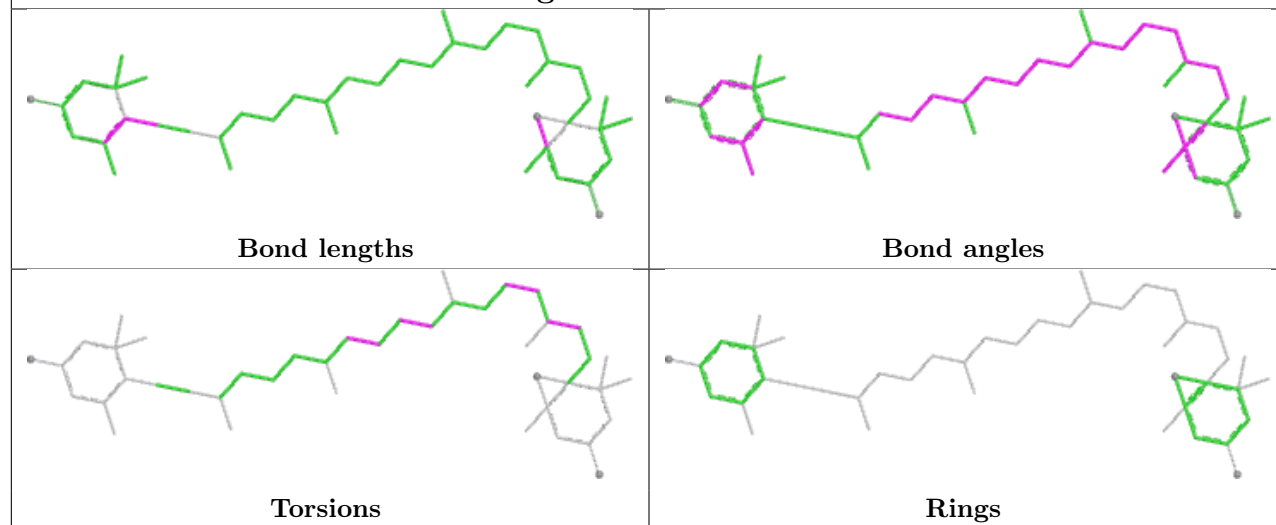


Rings

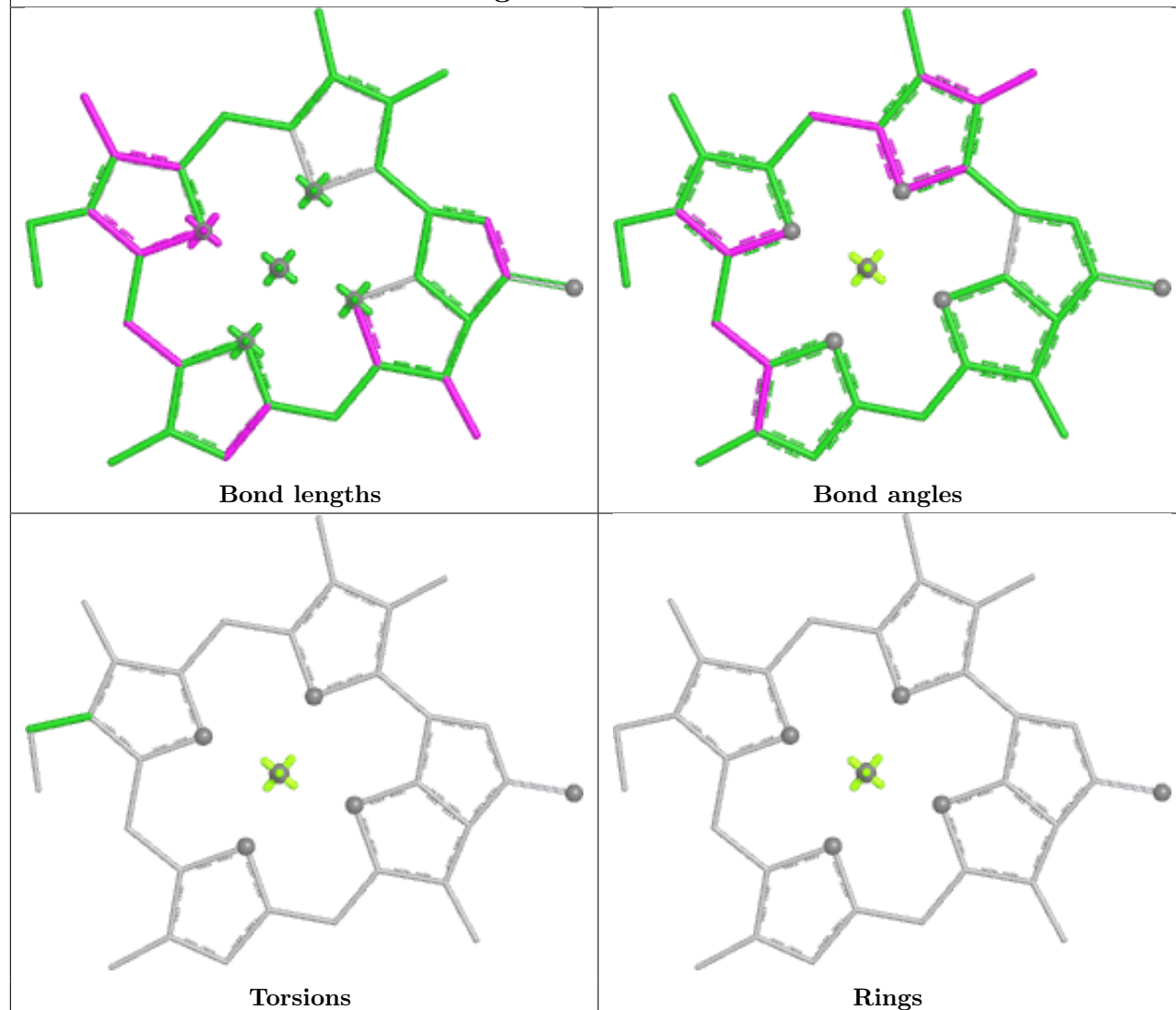
## Ligand CLA 1 201



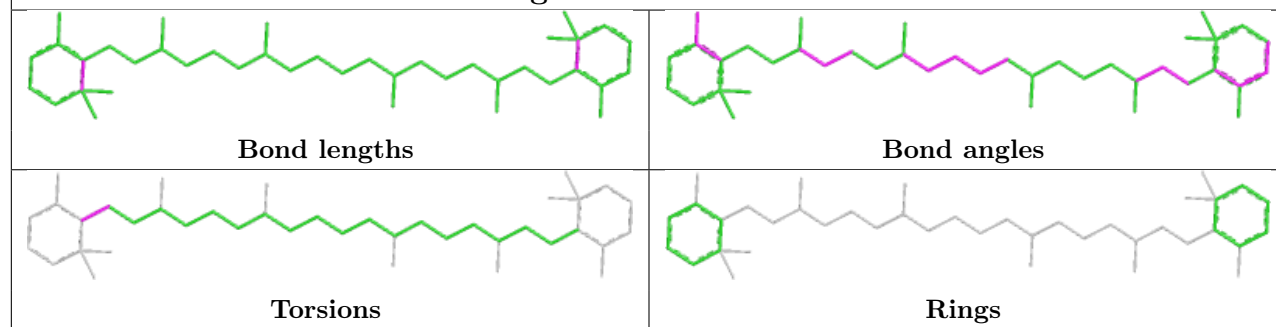
## Ligand DD6 6 204

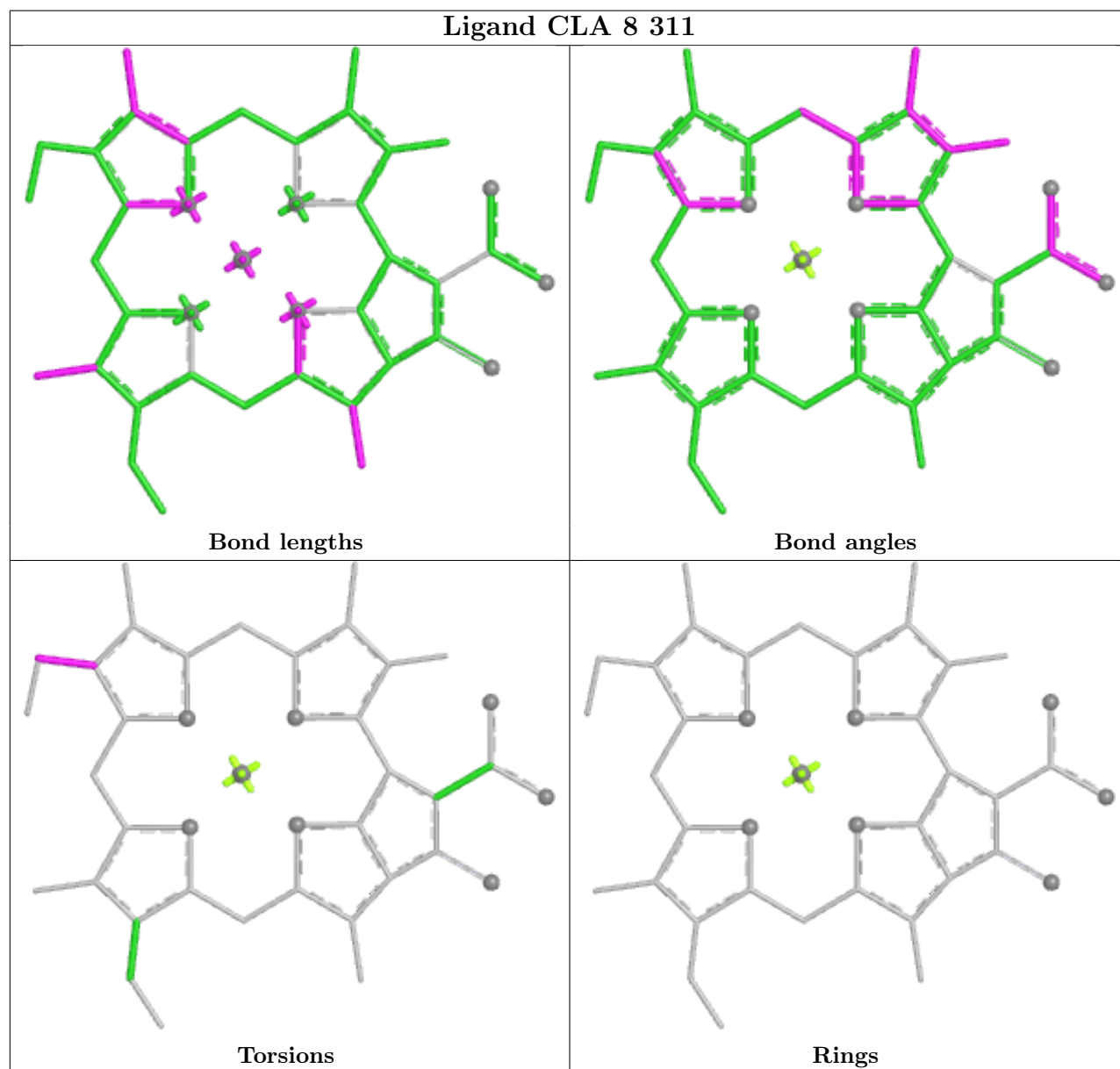
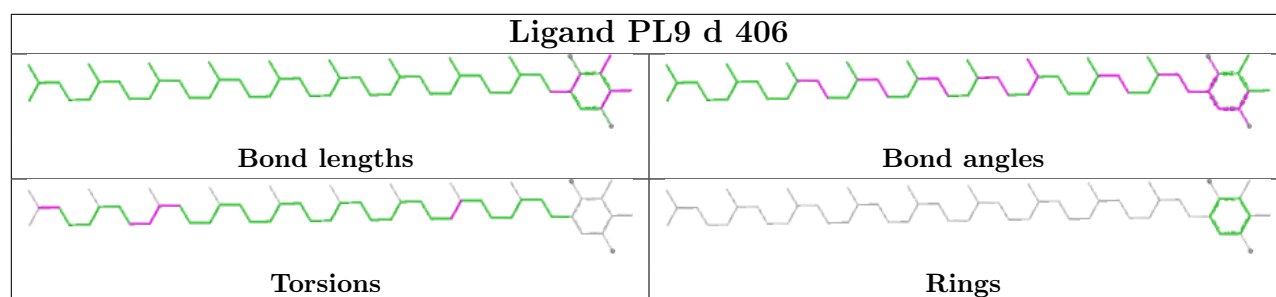


## Ligand CLA 8 310

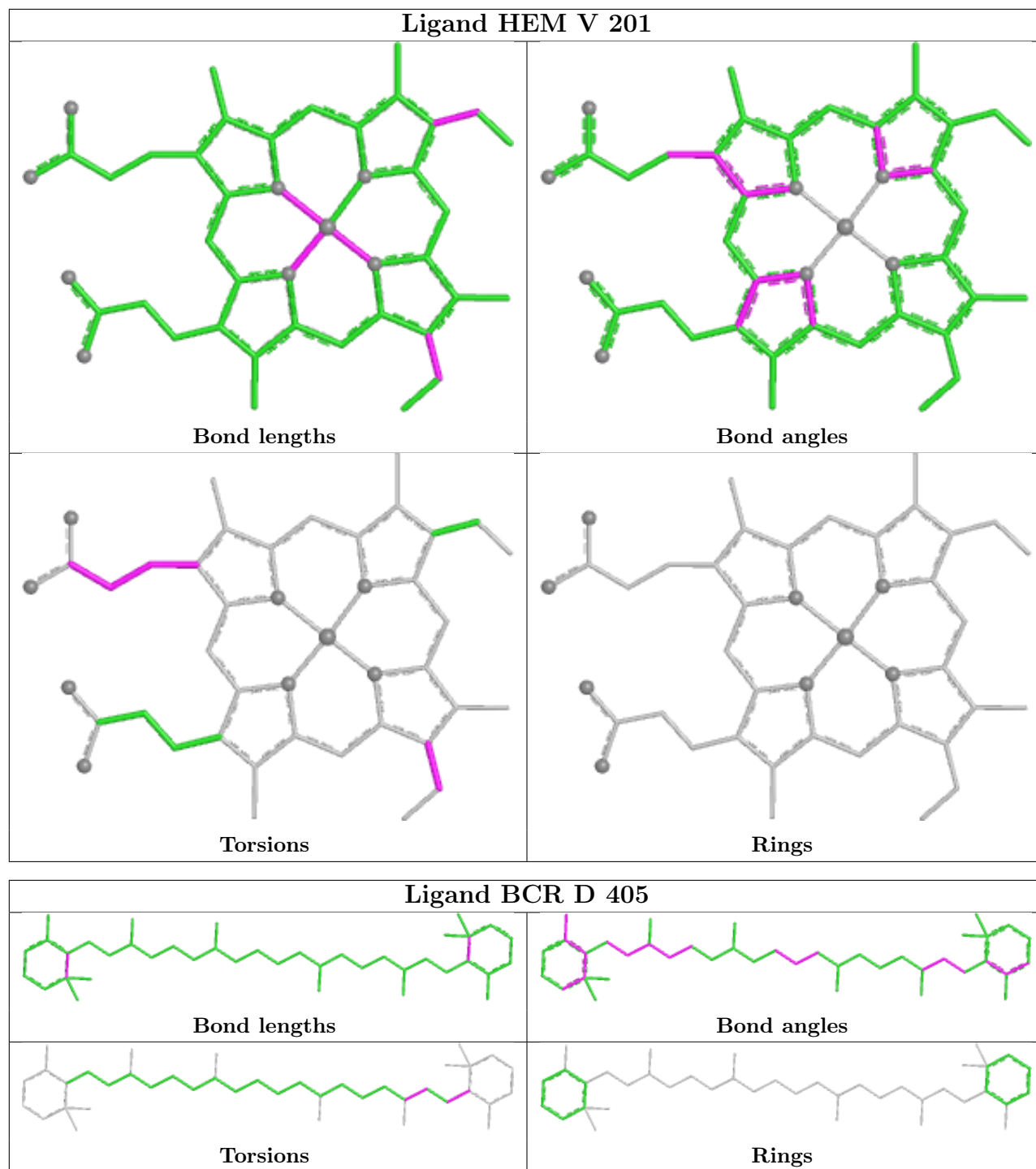


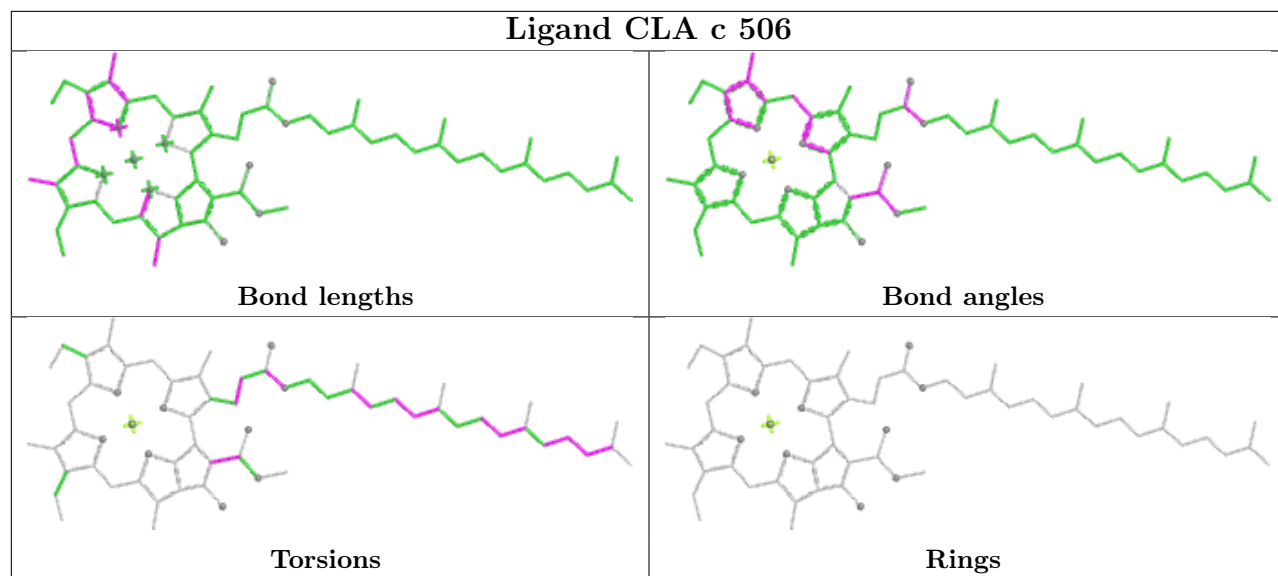
## Ligand BCR C 517



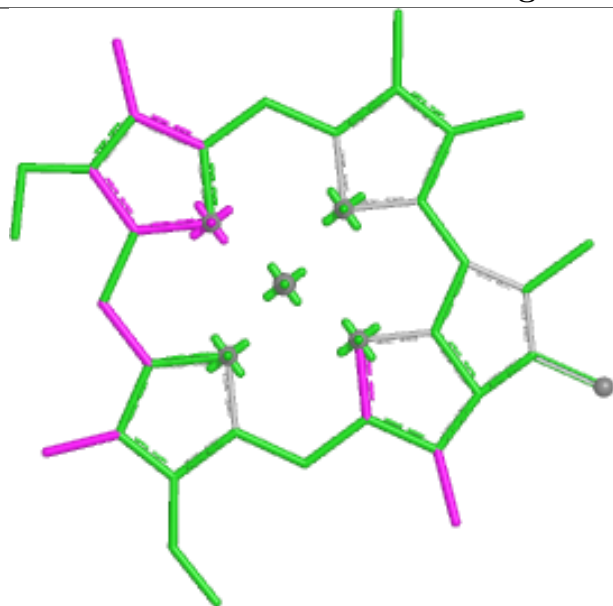




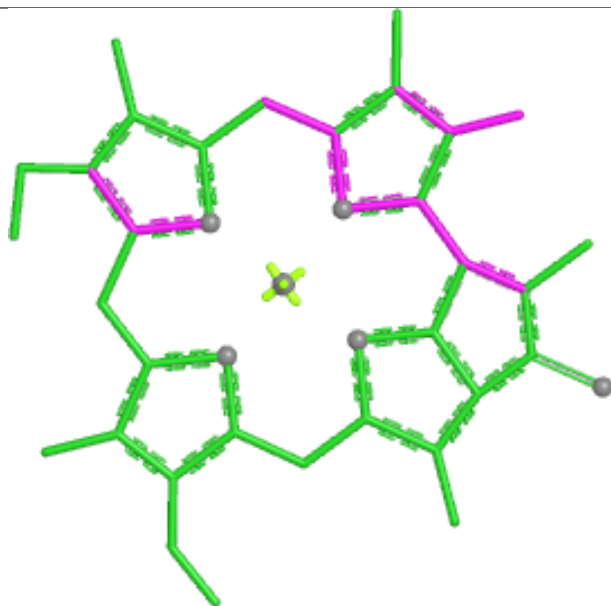




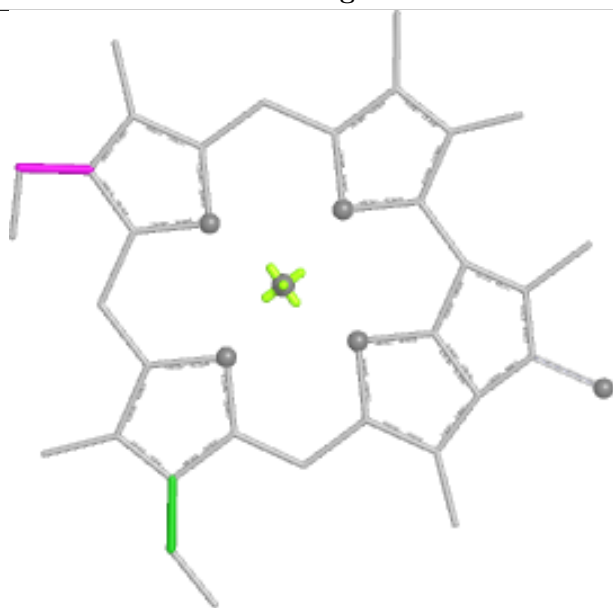
## Ligand CLA 4 204



Bond lengths



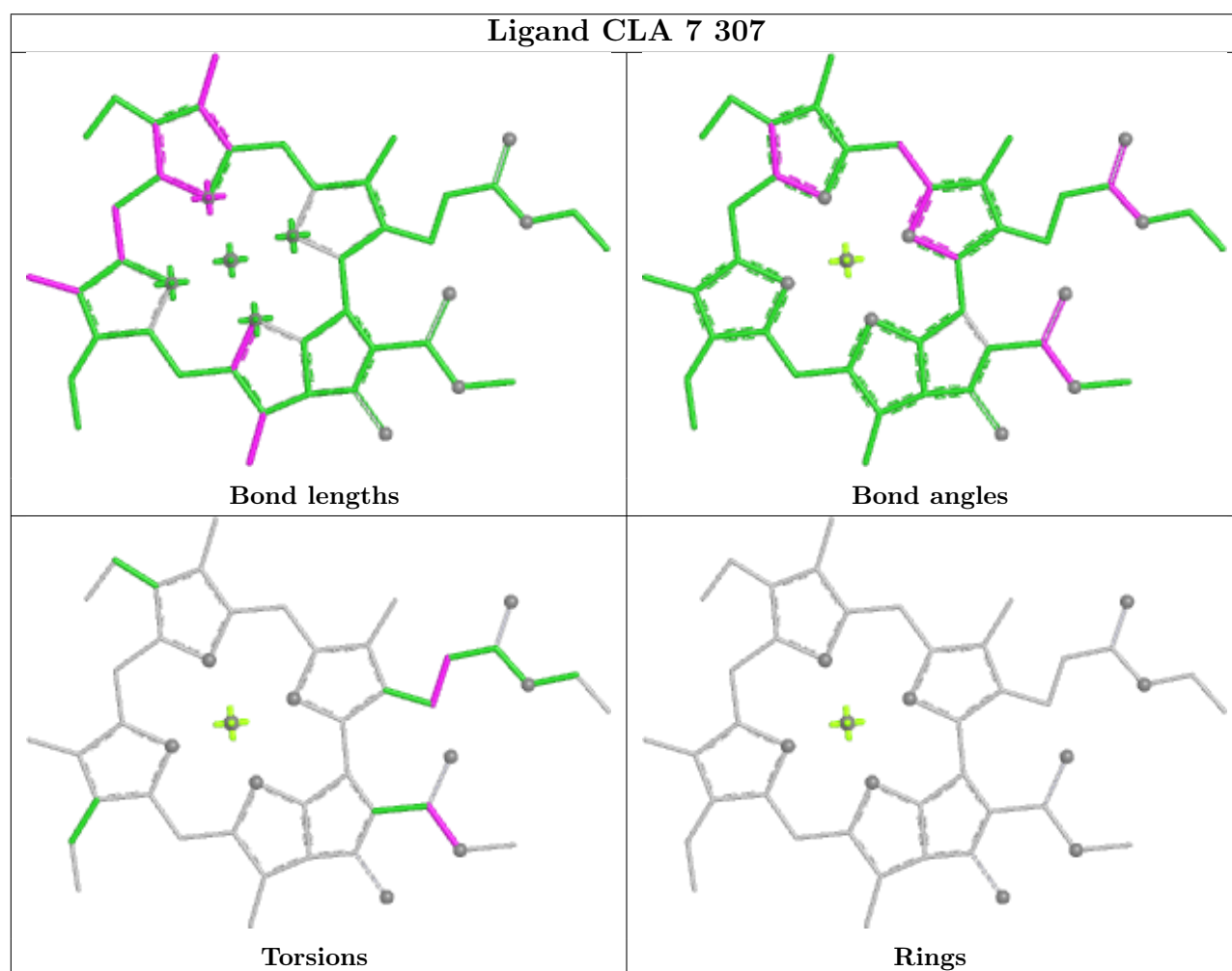
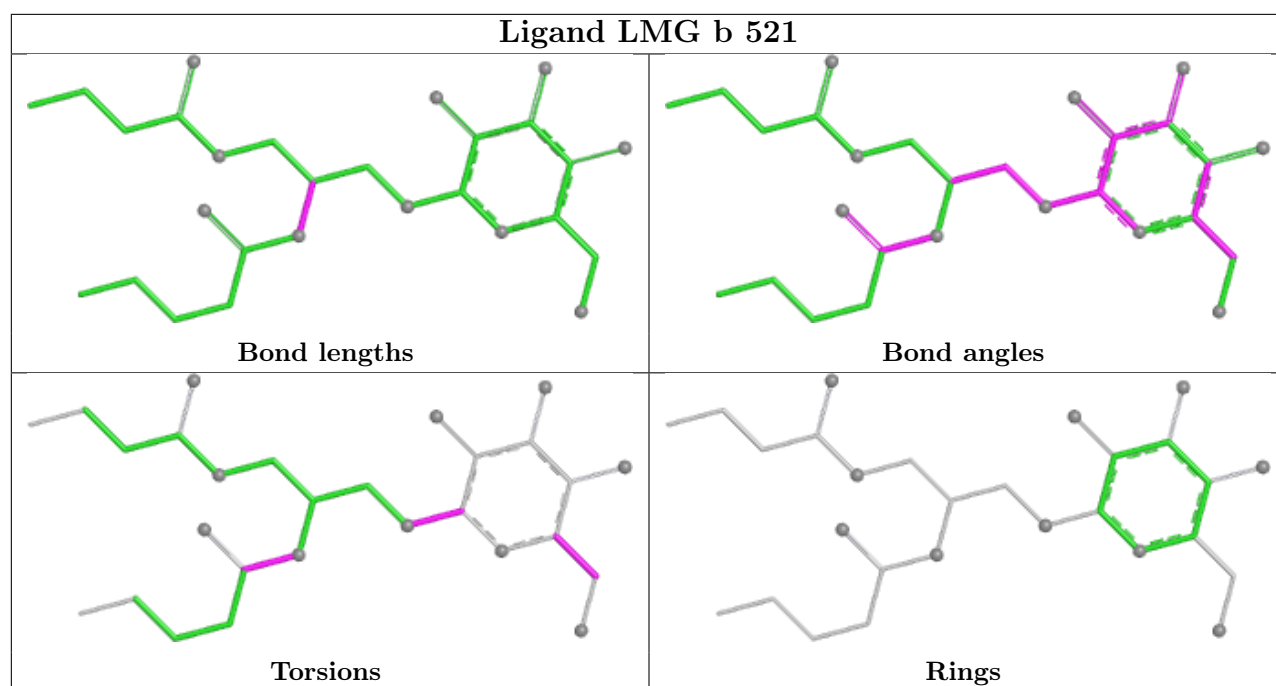
Bond angles



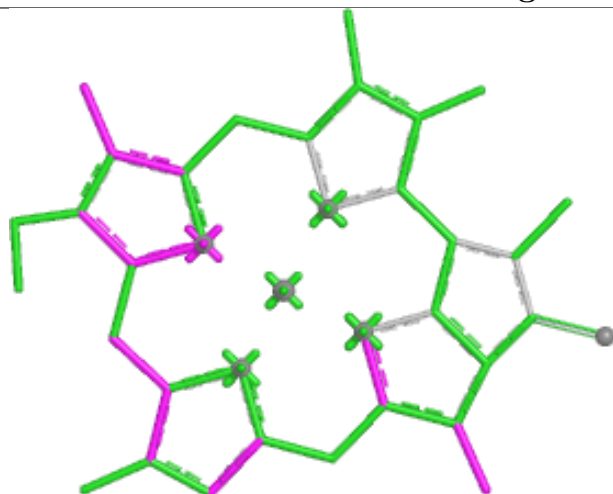
Torsions



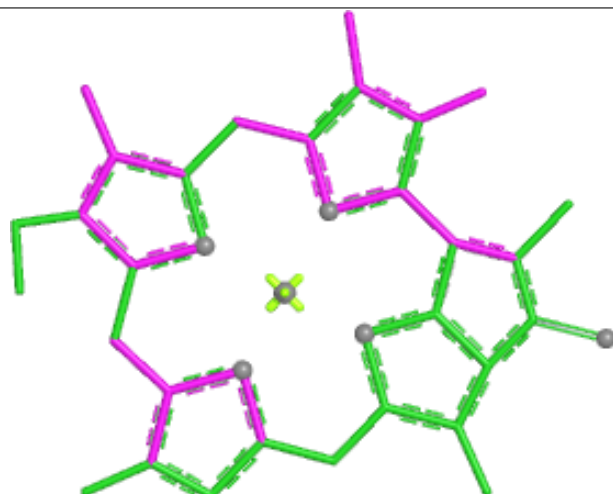
Rings



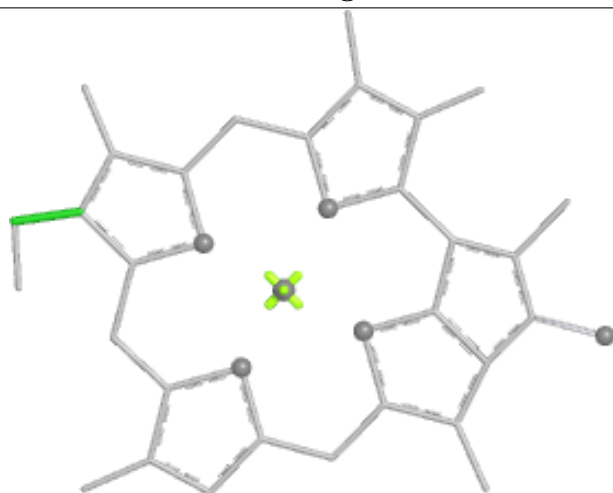
## Ligand CLA 7 312



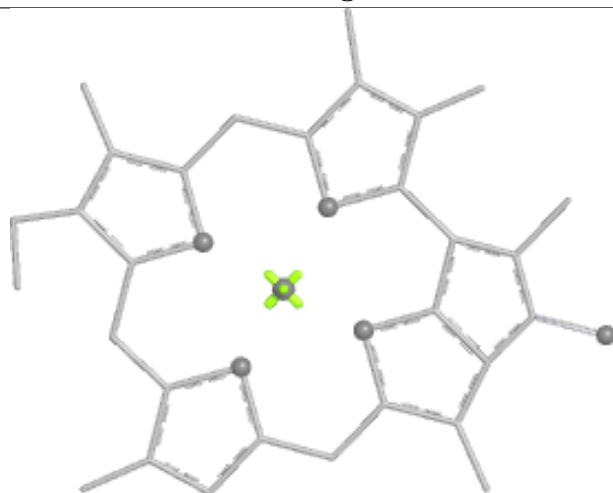
Bond lengths



Bond angles

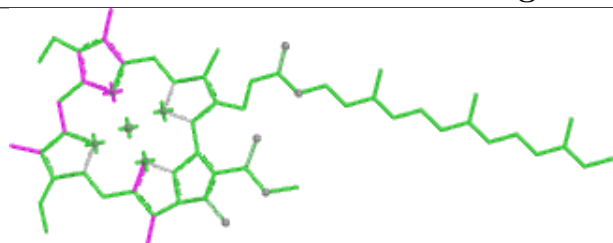


Torsions

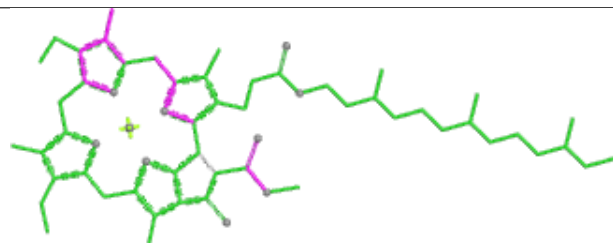


Rings

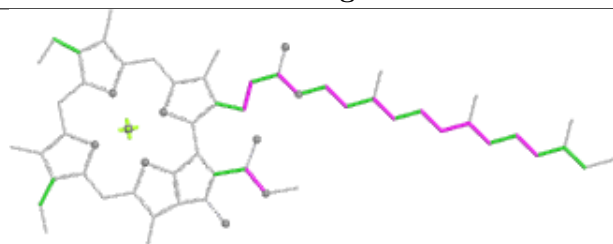
## Ligand CLA 0 305



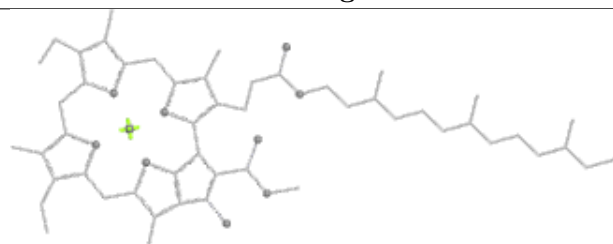
Bond lengths



Bond angles

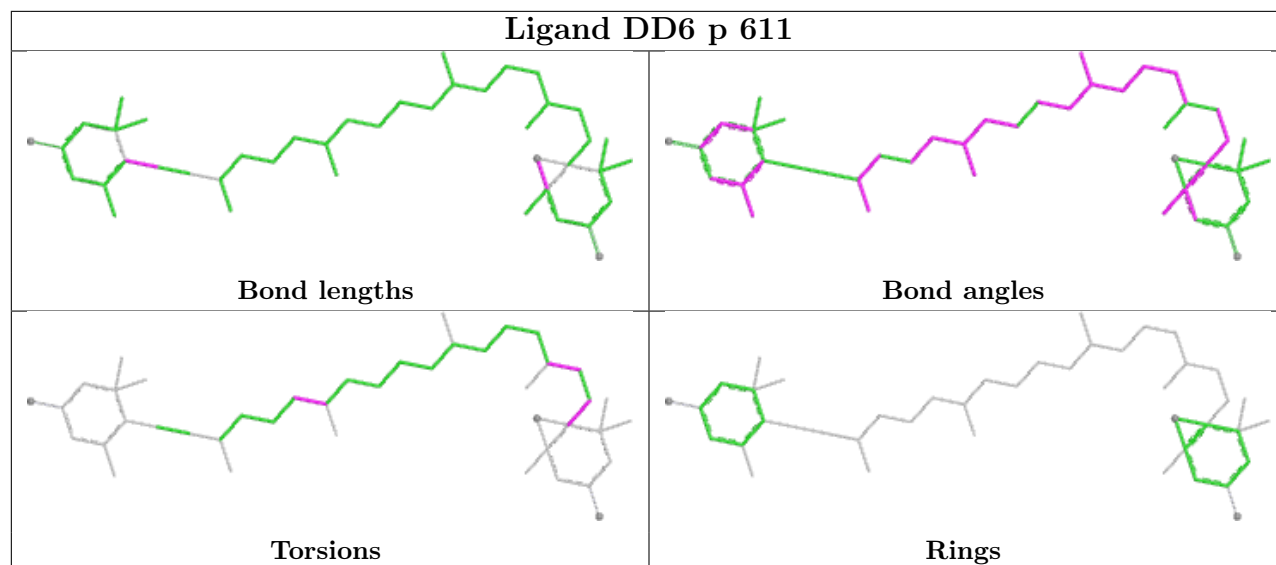


Torsions

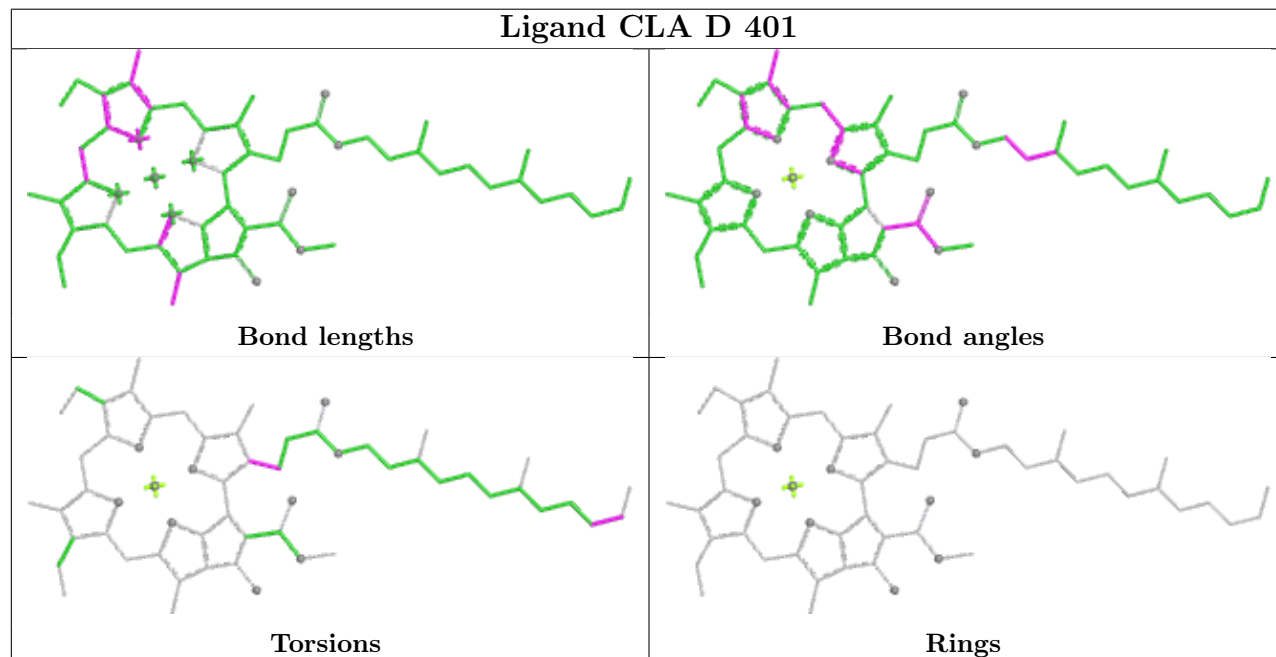


Rings

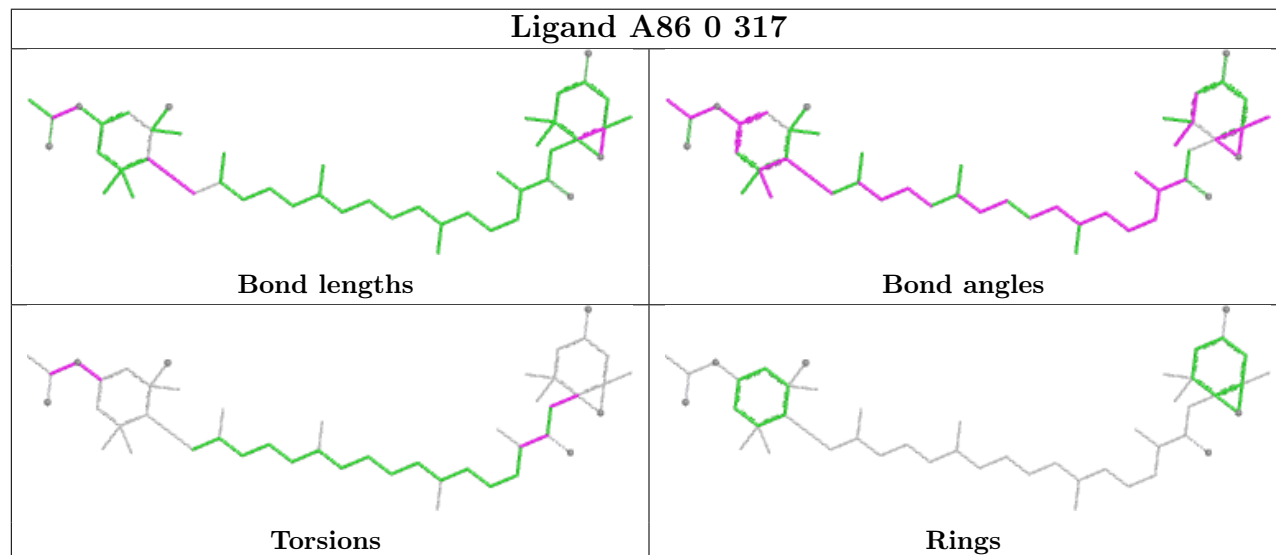
## Ligand DD6 p 611



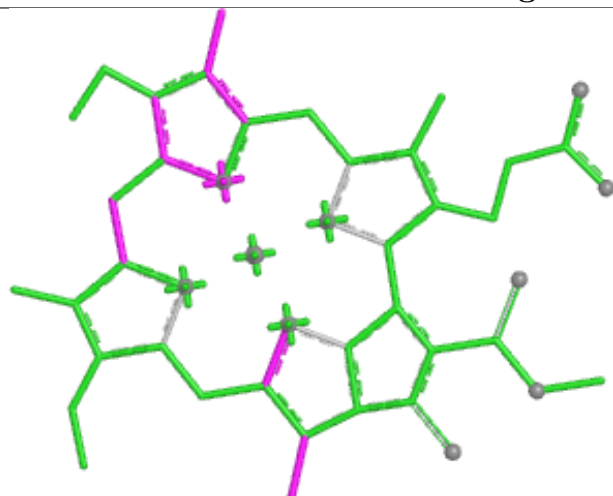
## Ligand CLA D 401



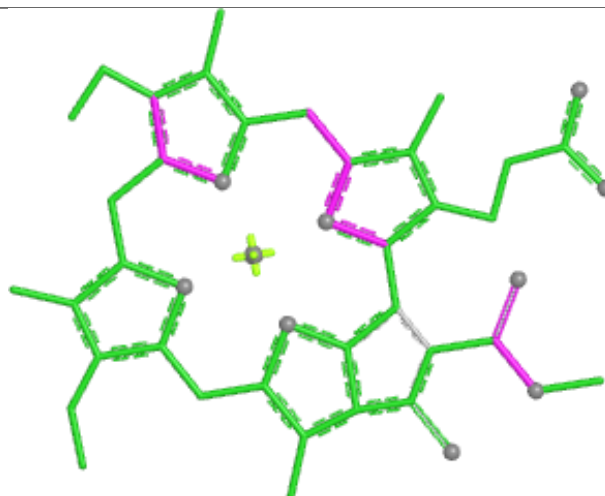
## Ligand A86 0 317



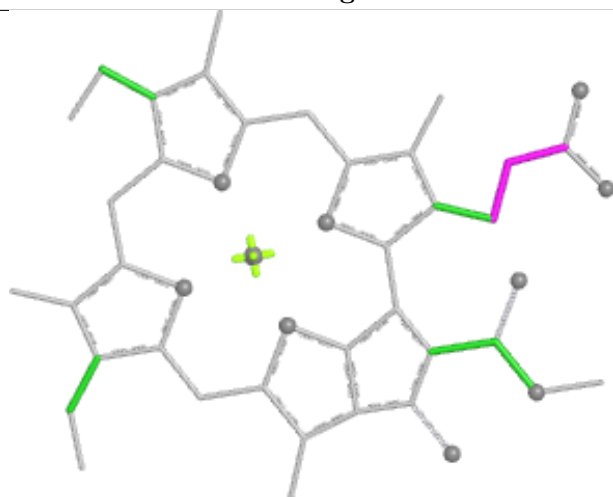
## Ligand CLA 0 306



Bond lengths



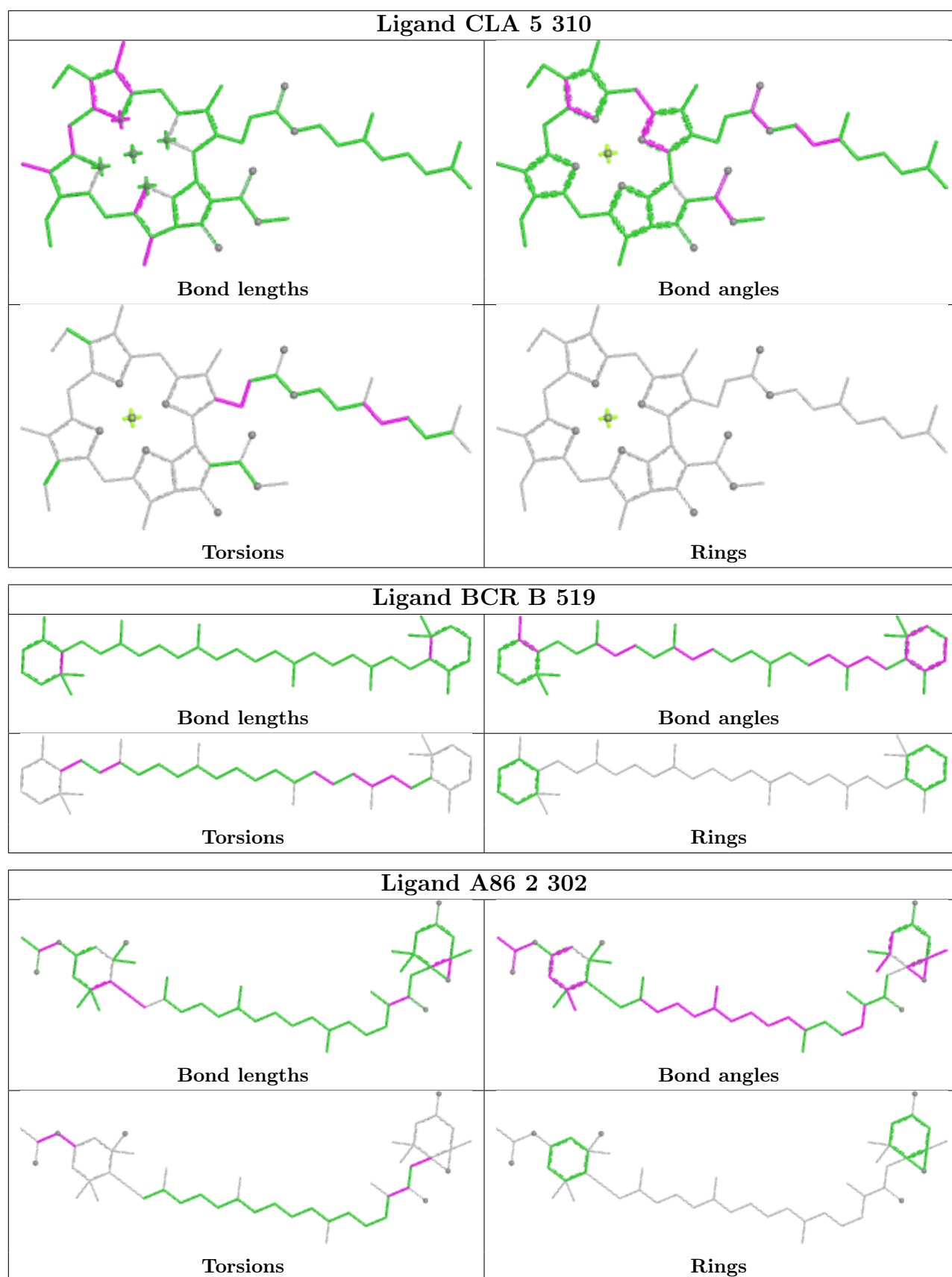
Bond angles



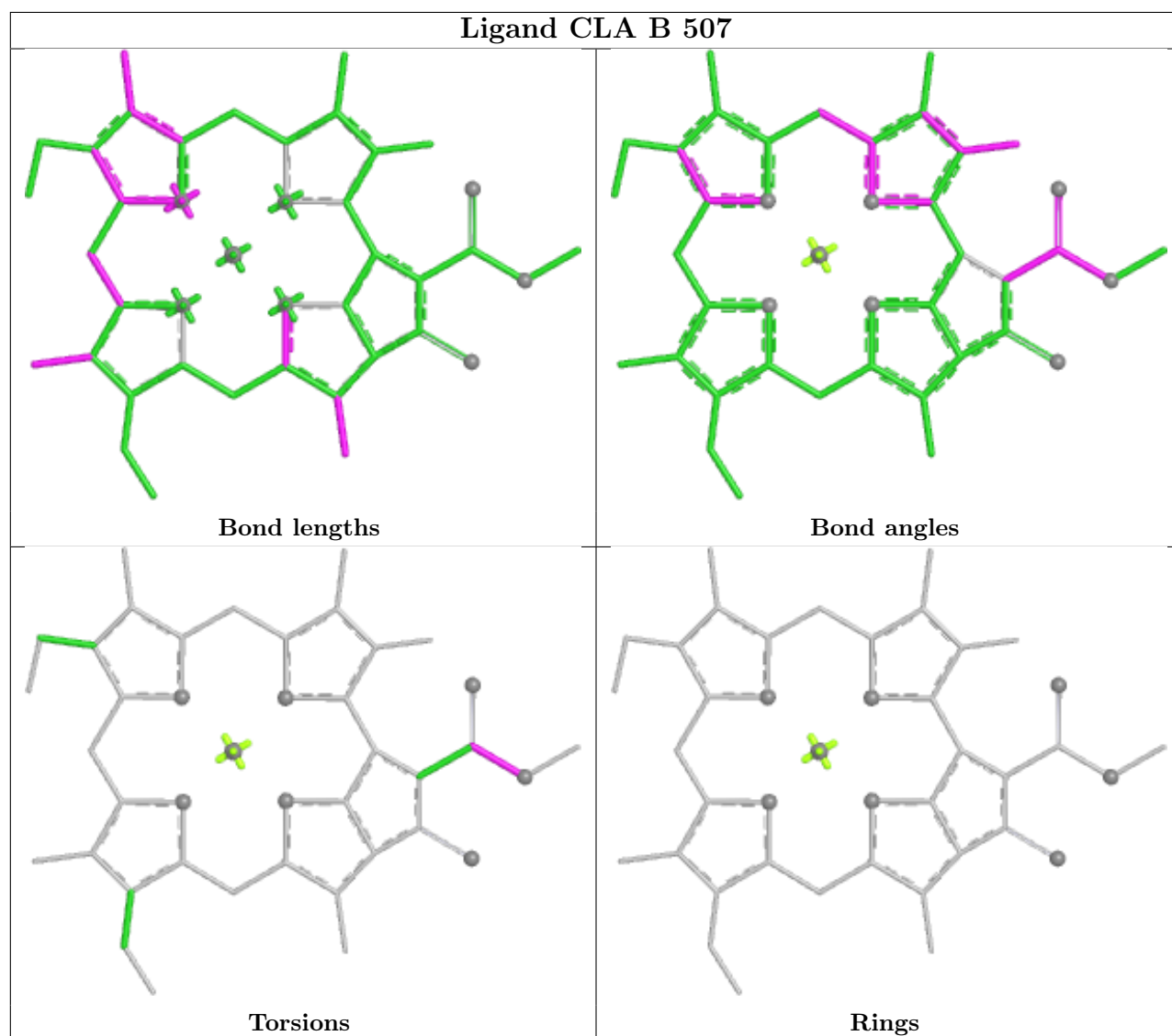
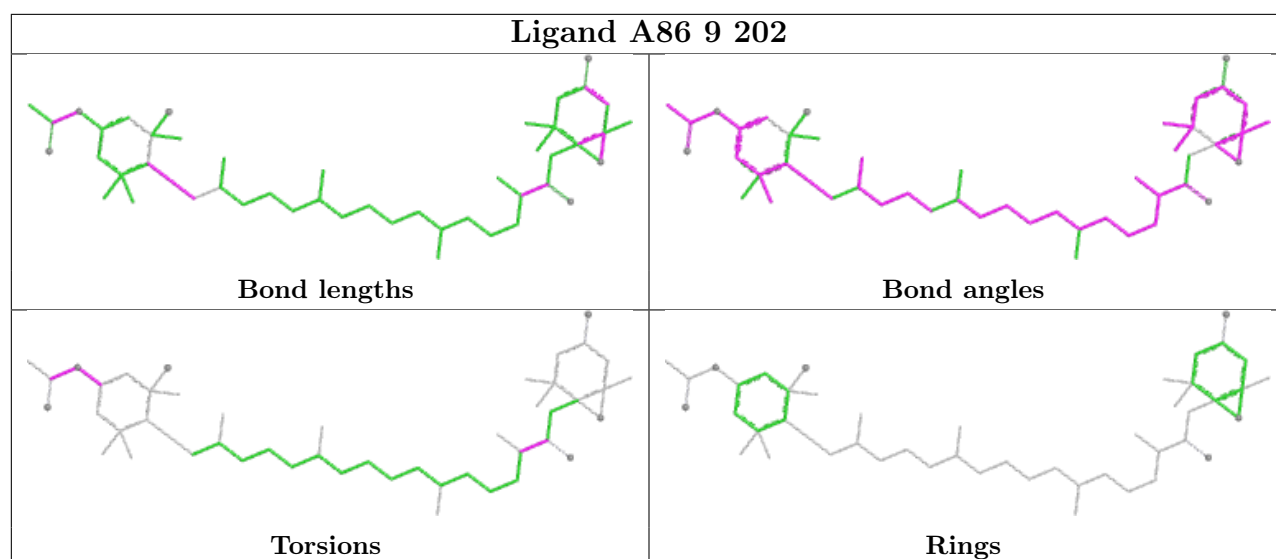
Torsions

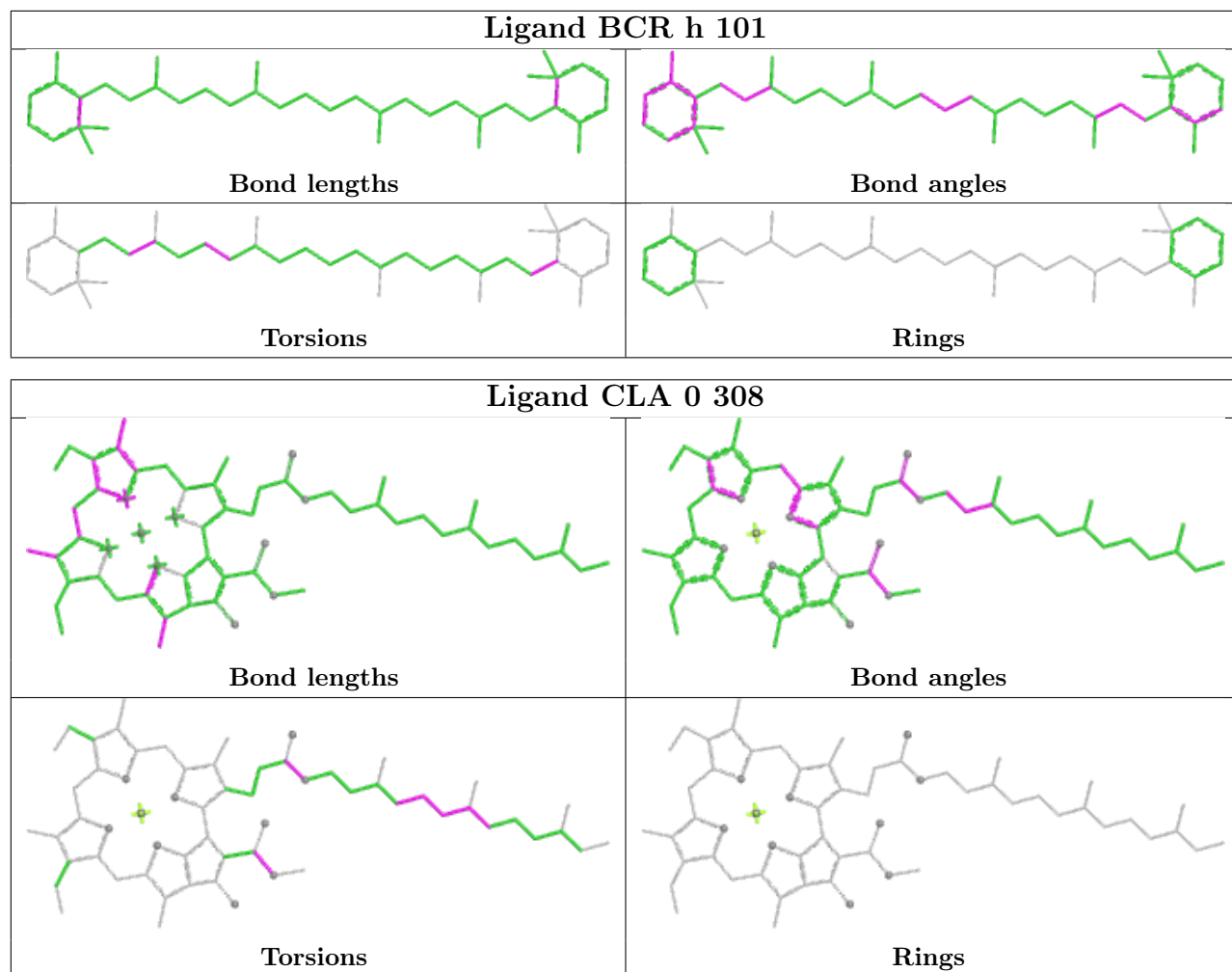


Rings

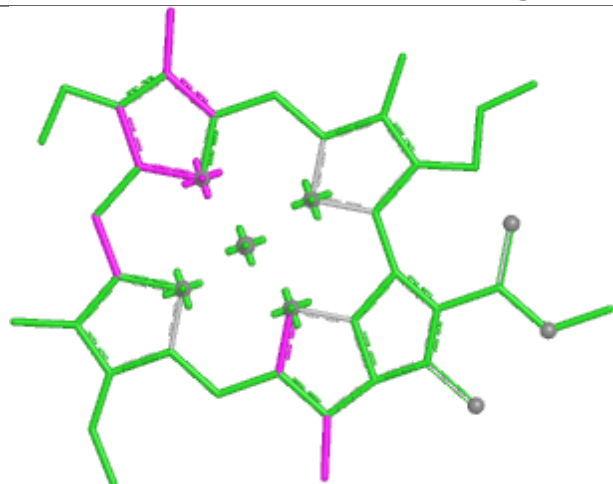




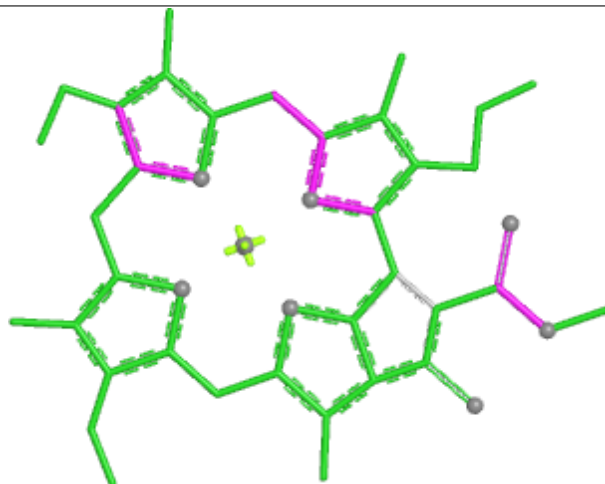




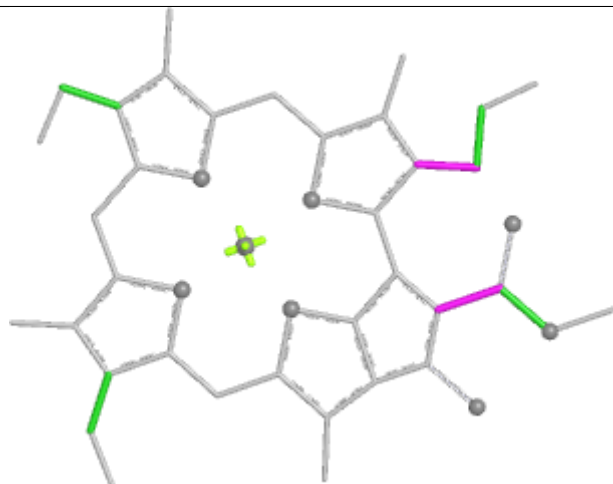
## Ligand CLA B 501



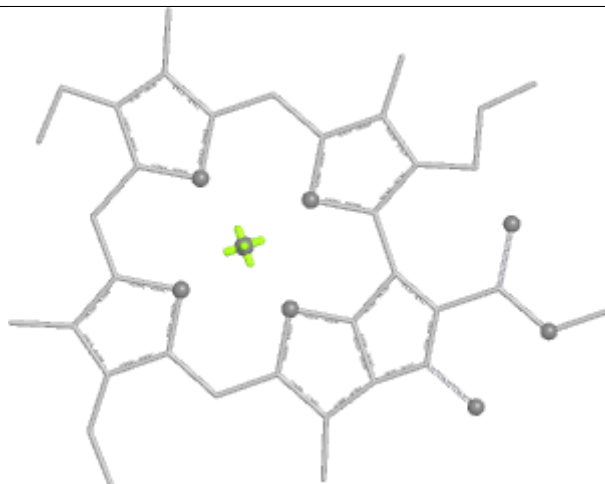
Bond lengths



Bond angles

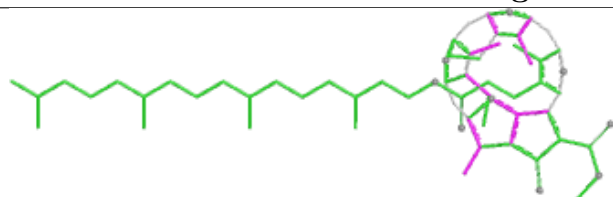


Torsions

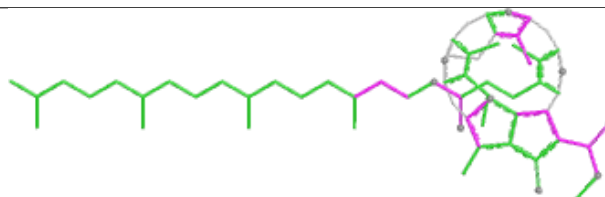


Rings

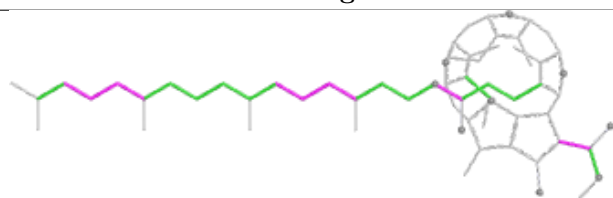
## Ligand PHO A 405



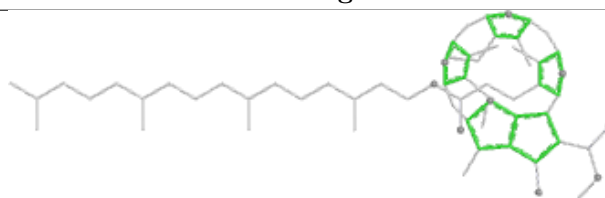
Bond lengths



Bond angles

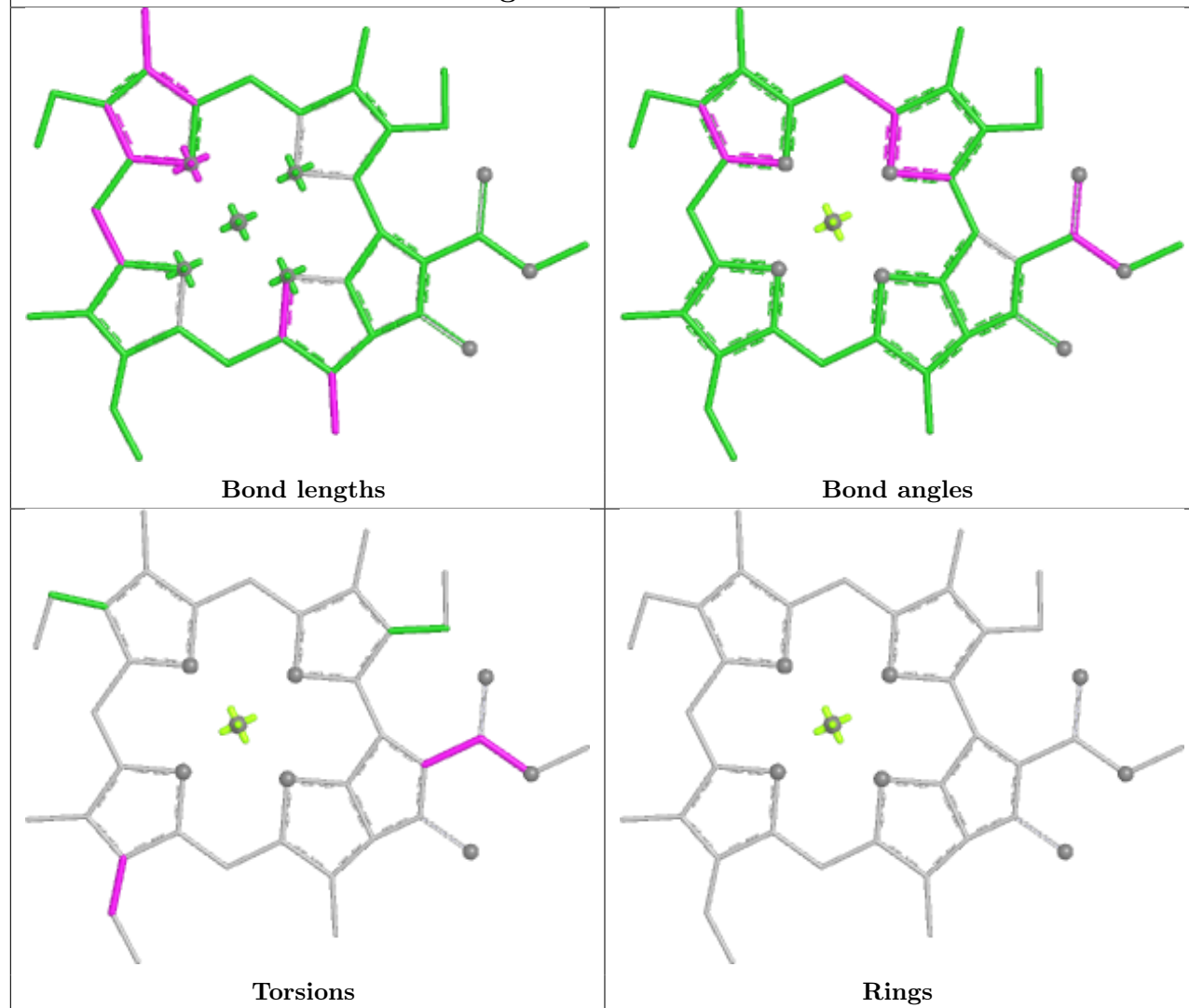


Torsions

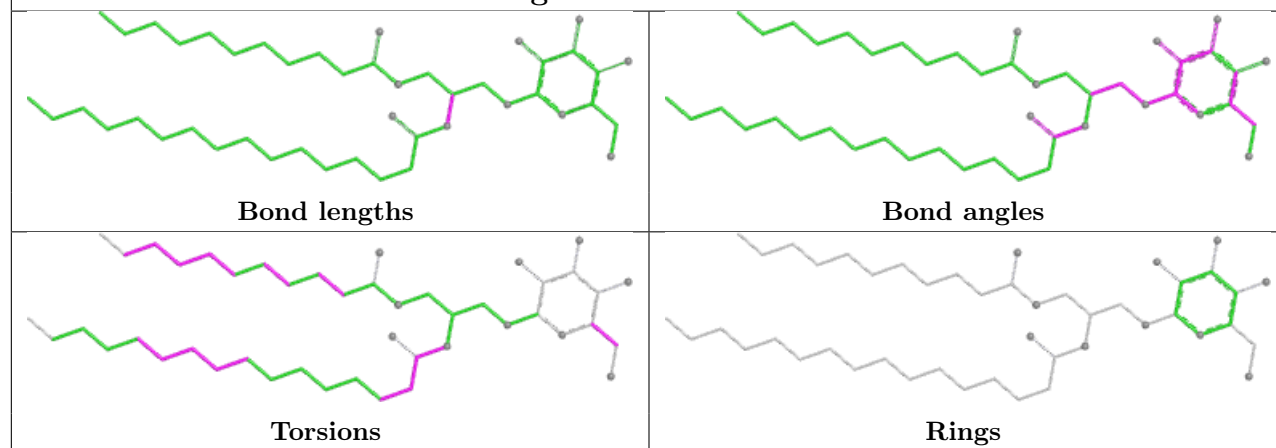


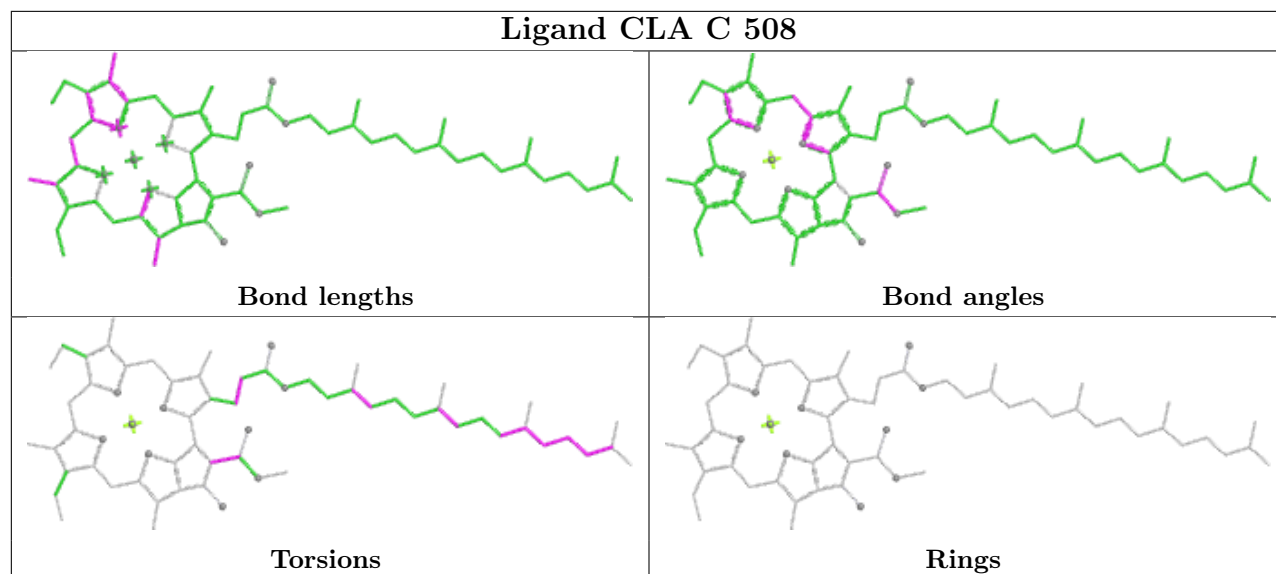
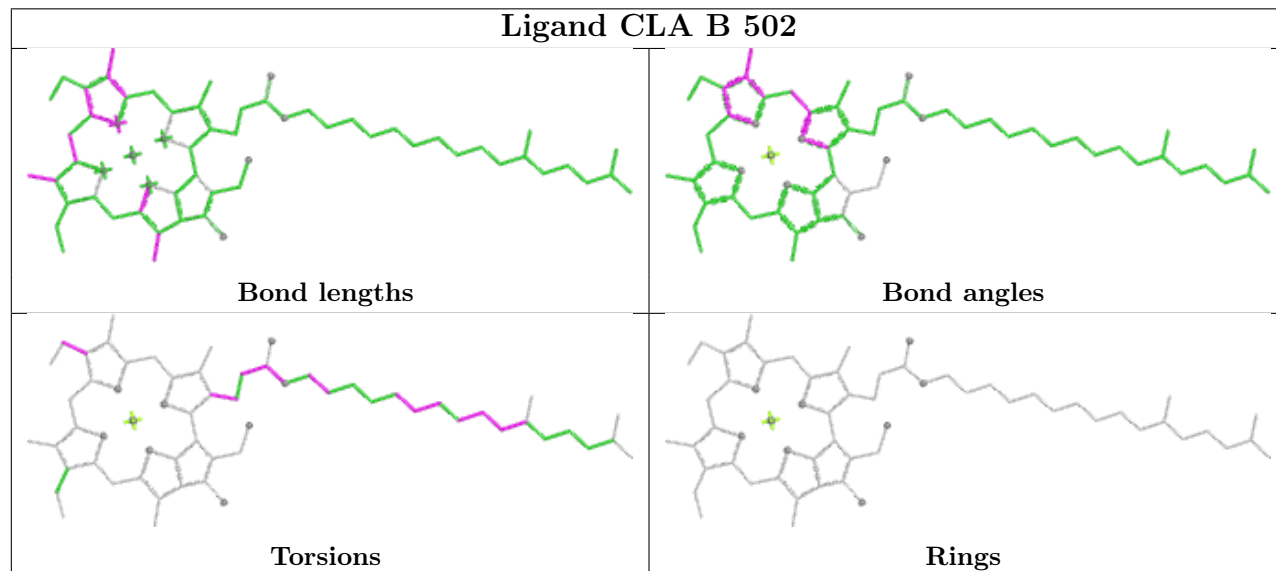
Rings

## Ligand CLA 5 312

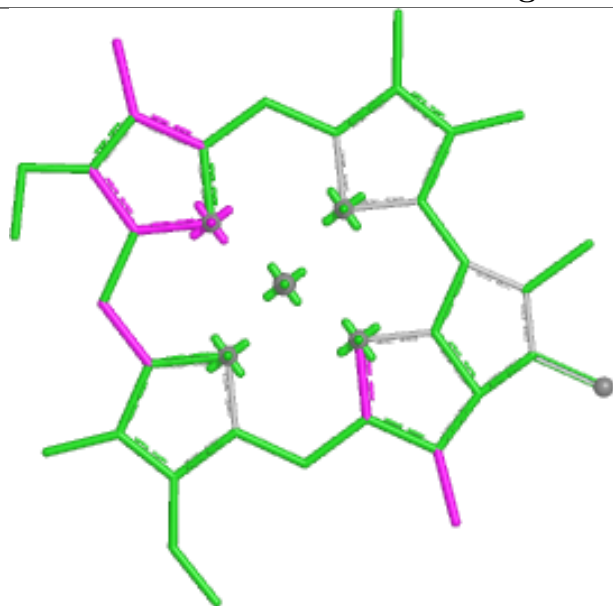


## Ligand LMG d 408

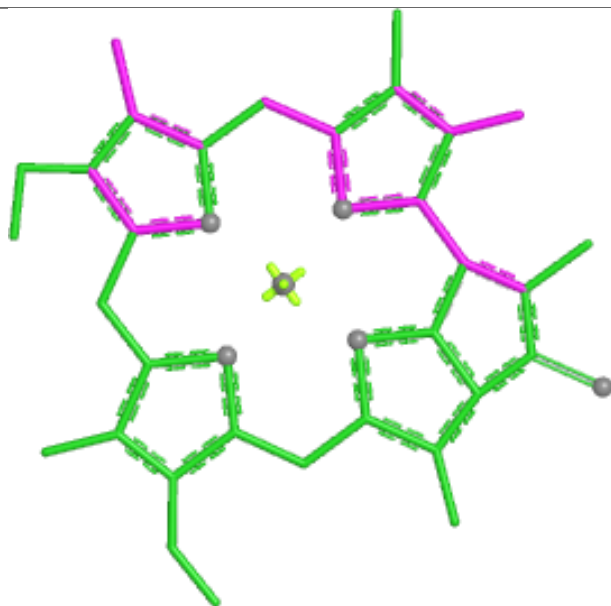


**Ligand CLA C 508****Ligand CLA B 502**

## Ligand CLA 7 314



Bond lengths



Bond angles

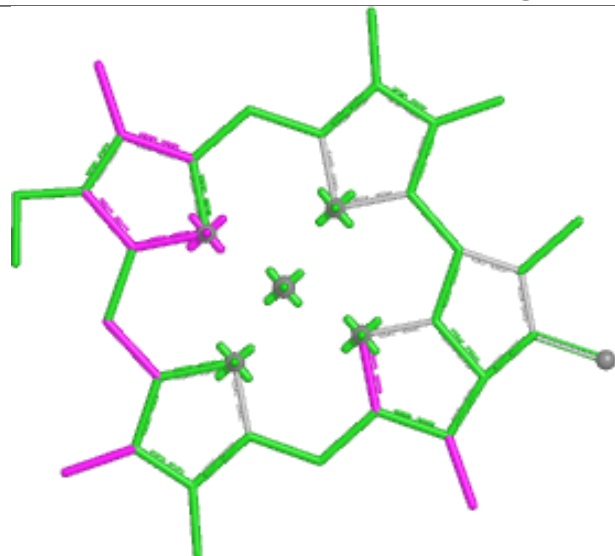


Torsions

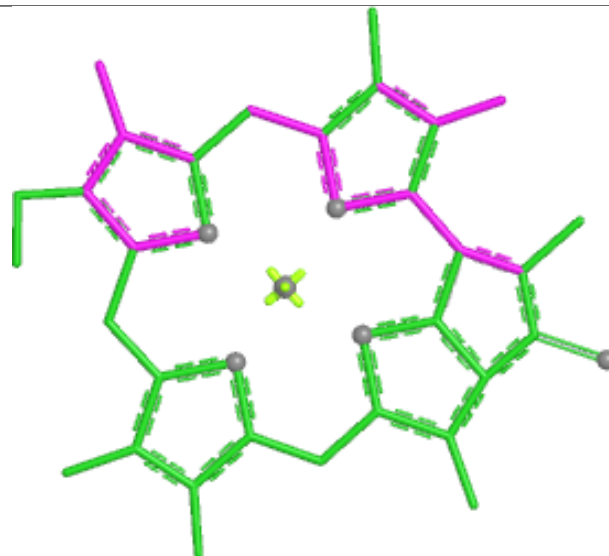


Rings

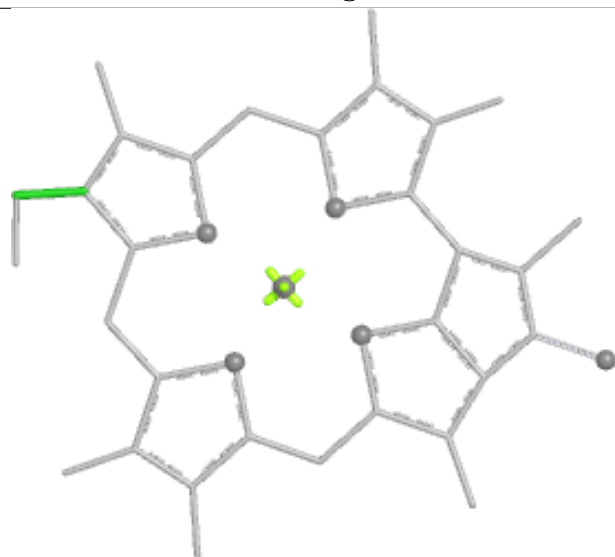
## Ligand CLA P 603



Bond lengths



Bond angles

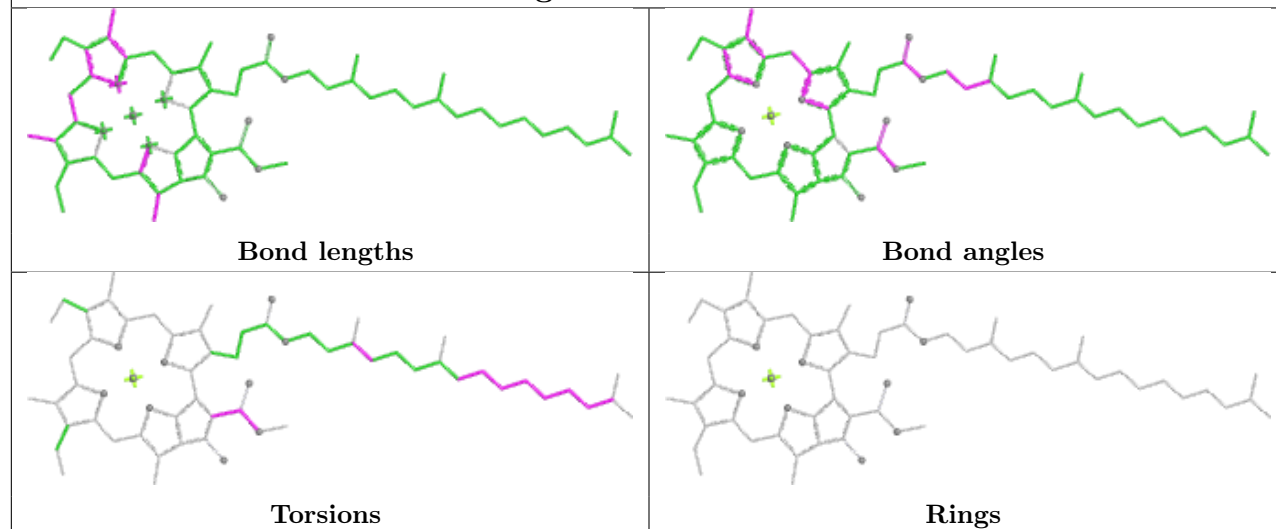


Torsions

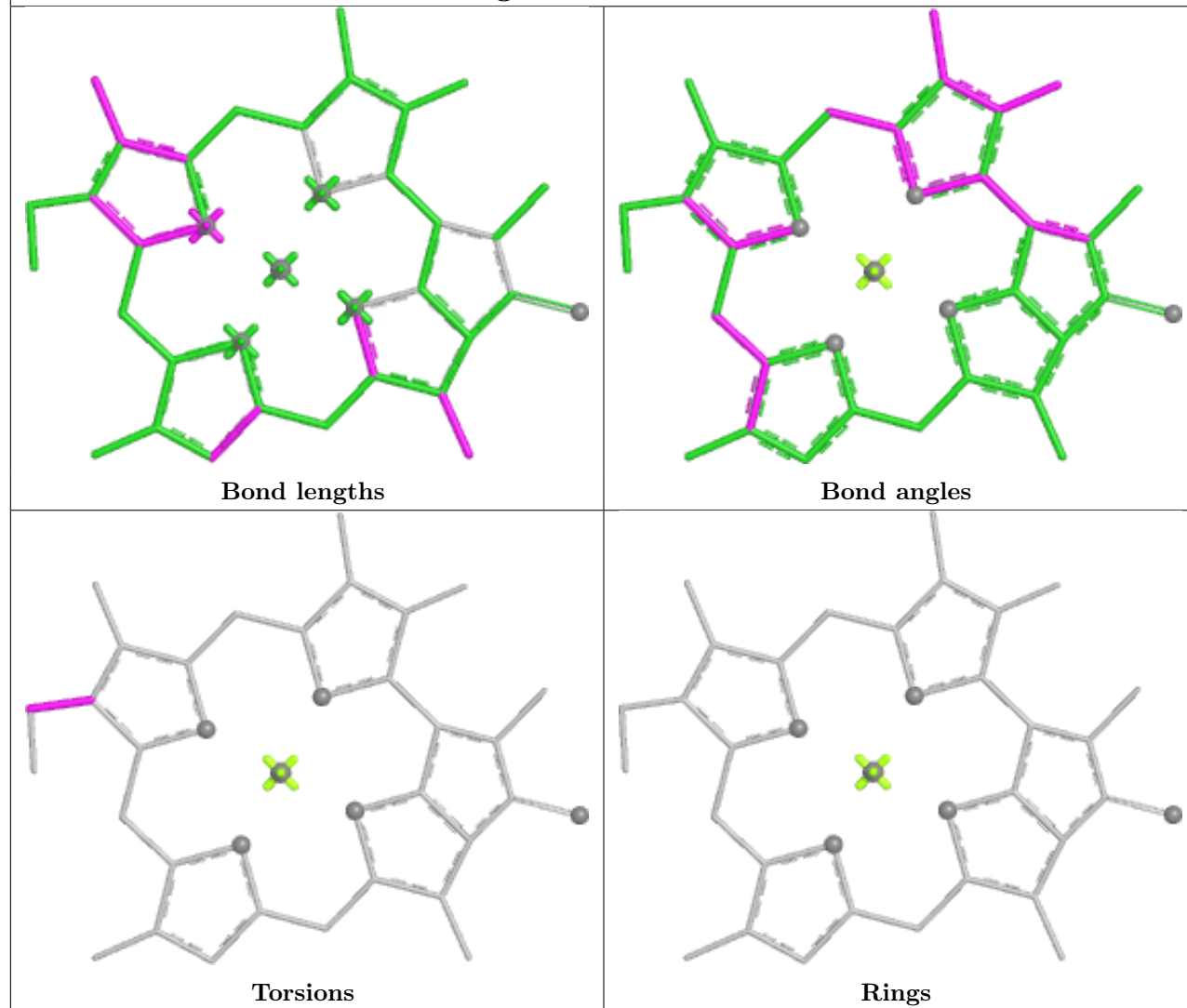


Rings

## Ligand CLA b 512

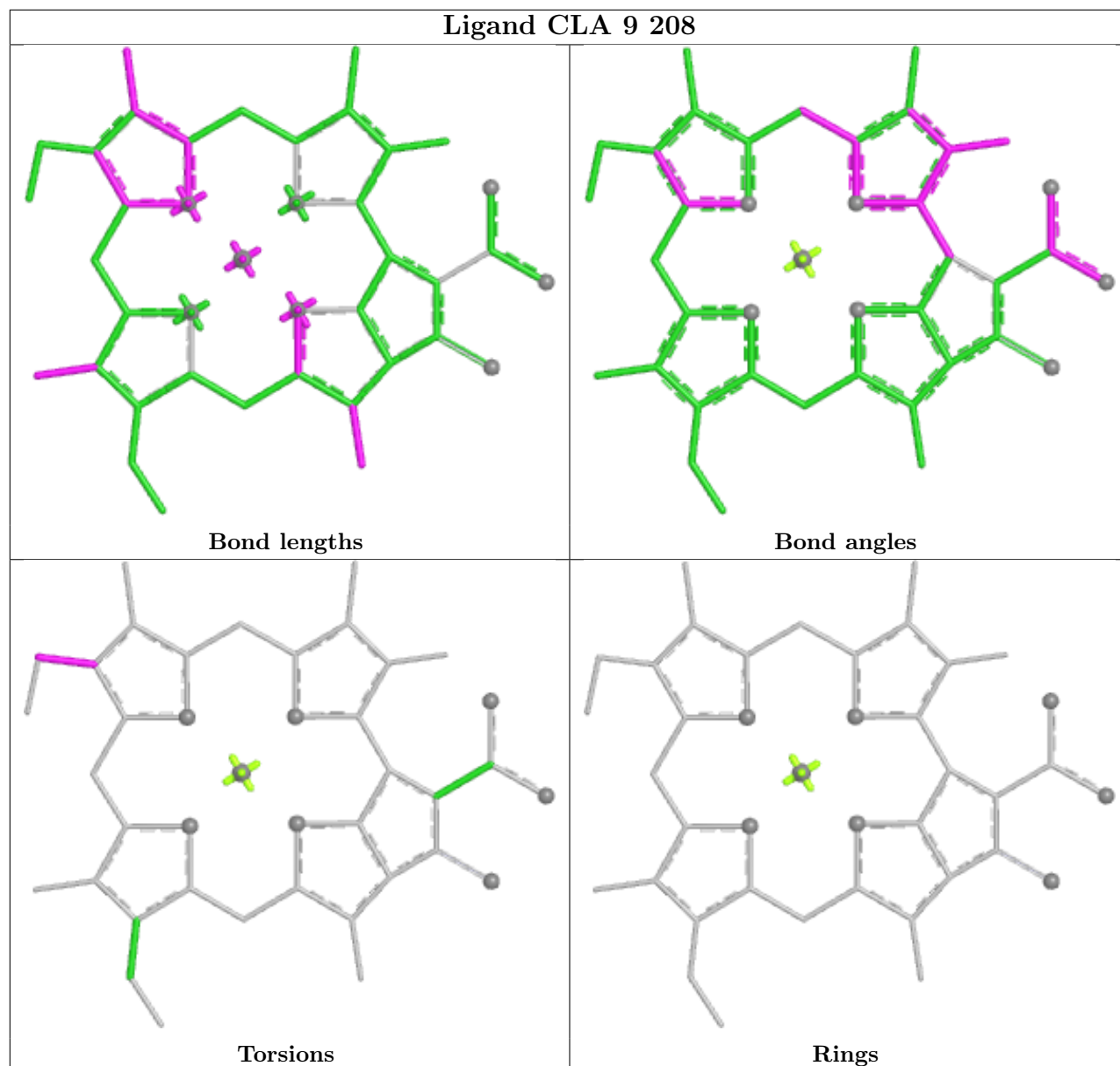


## Ligand CLA P 601

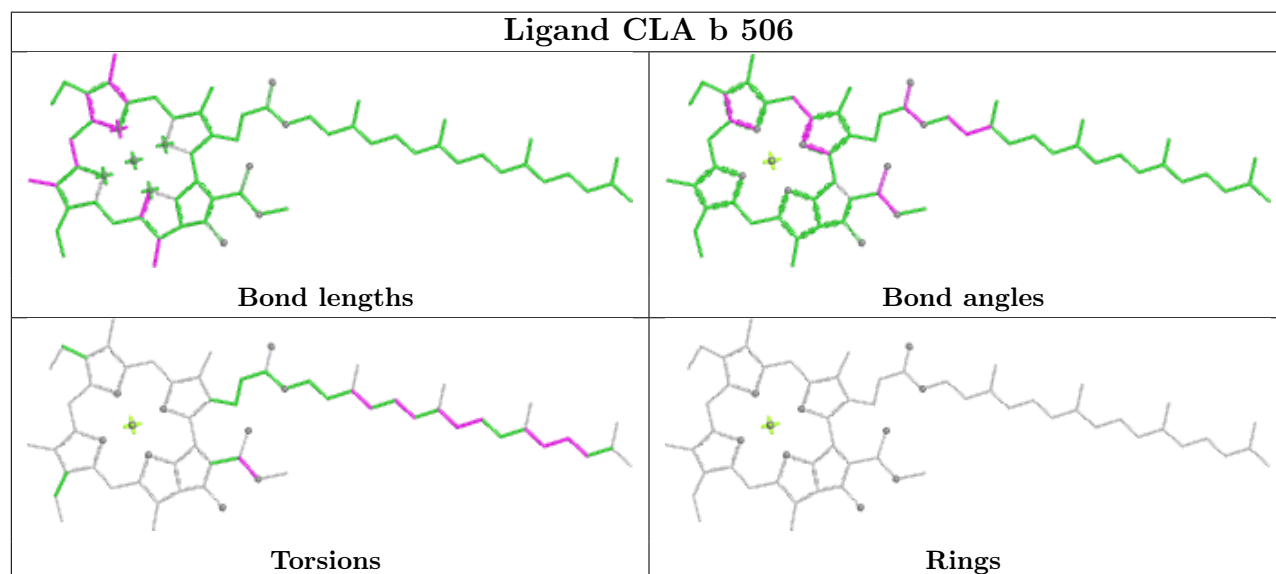




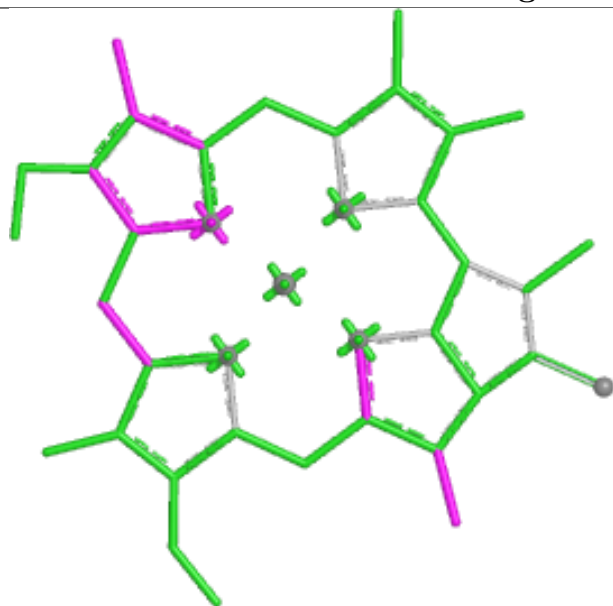
## Ligand CLA 9 208



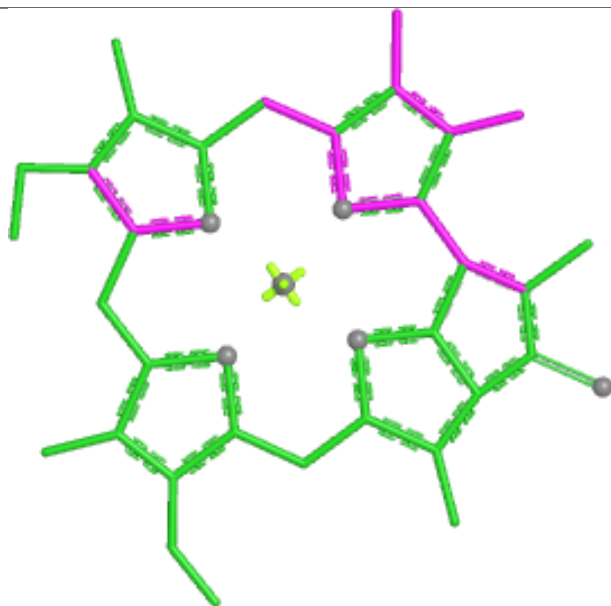
## Ligand CLA b 506



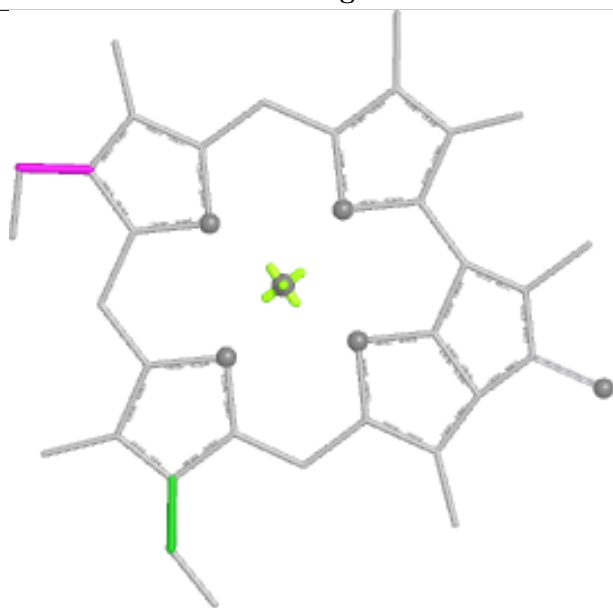
## Ligand CLA 7 315



Bond lengths



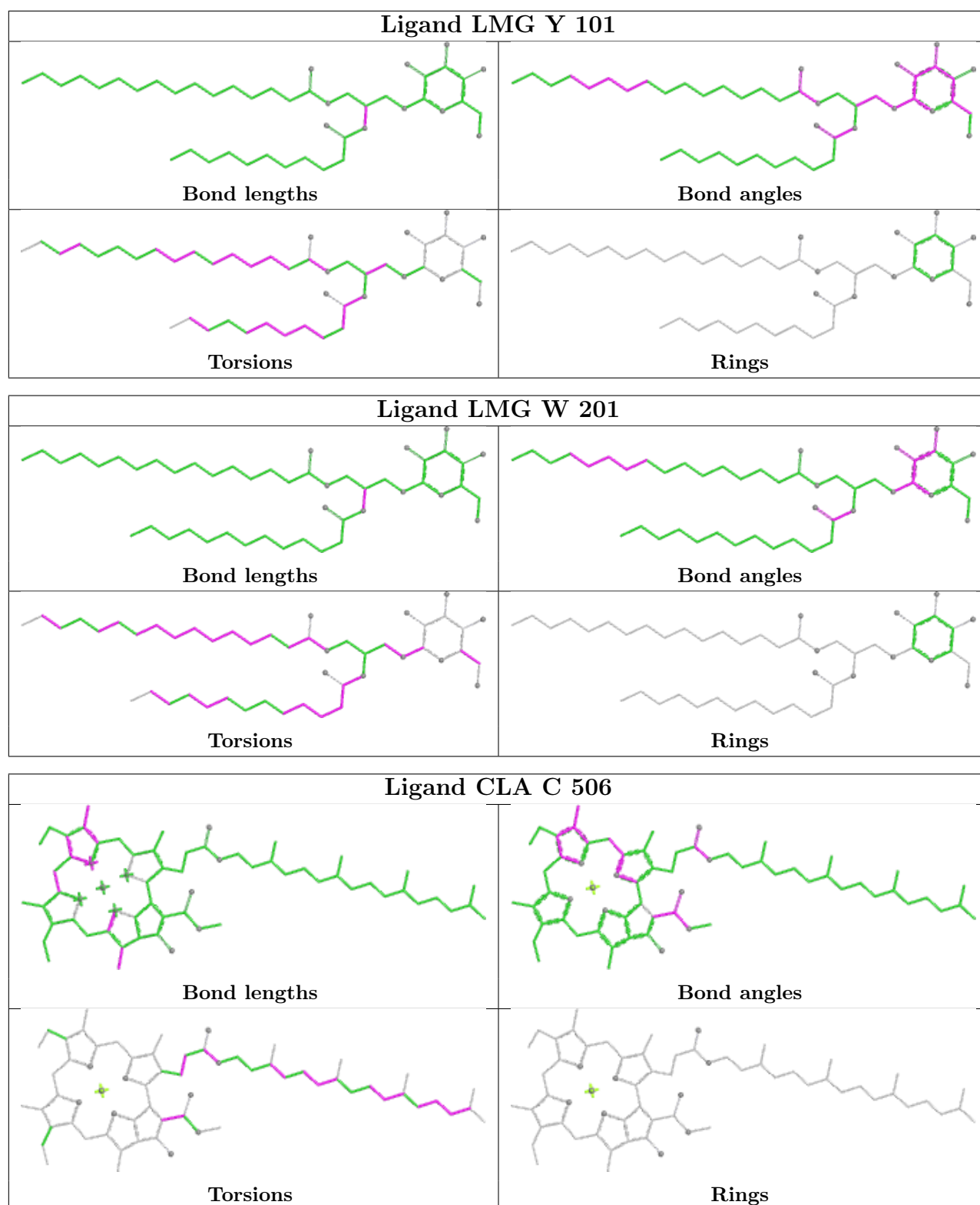
Bond angles



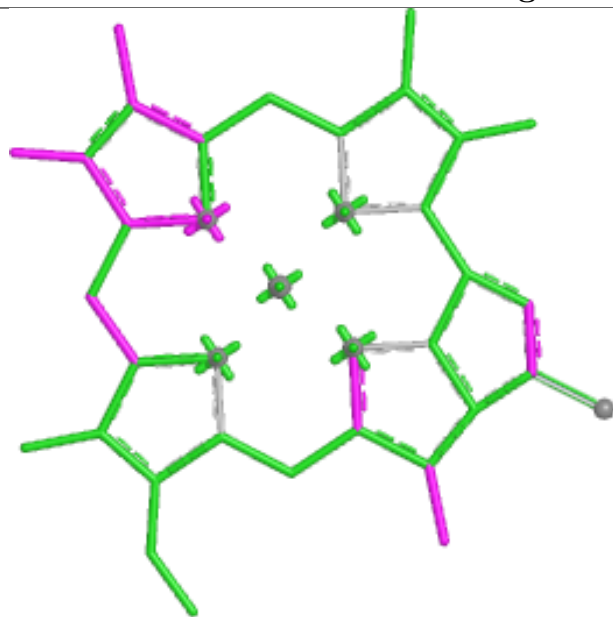
Torsions



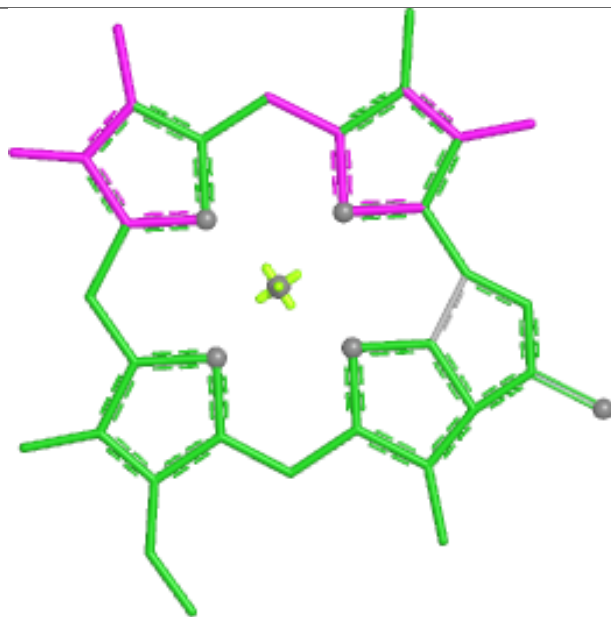
Rings



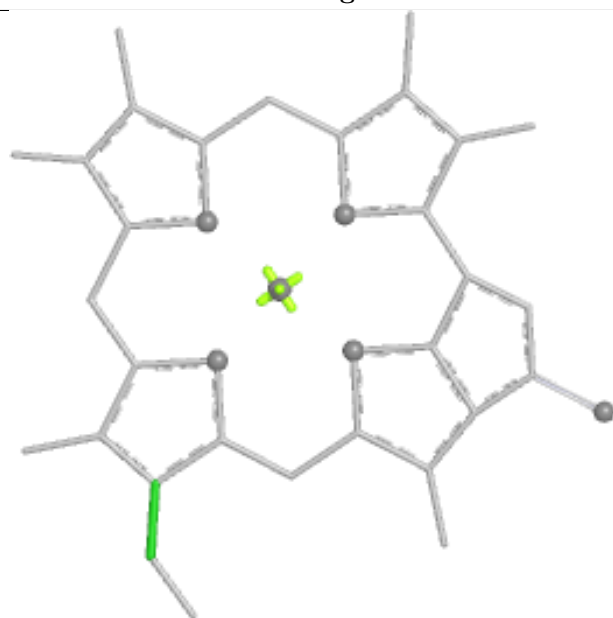
## Ligand CLA 4 212



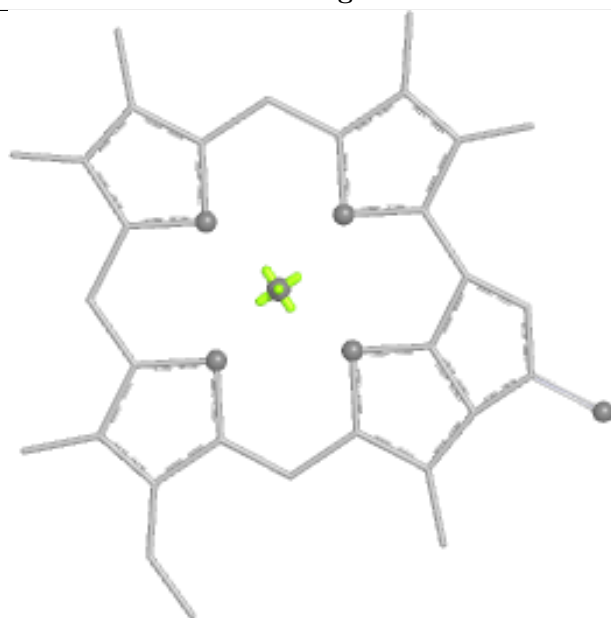
Bond lengths



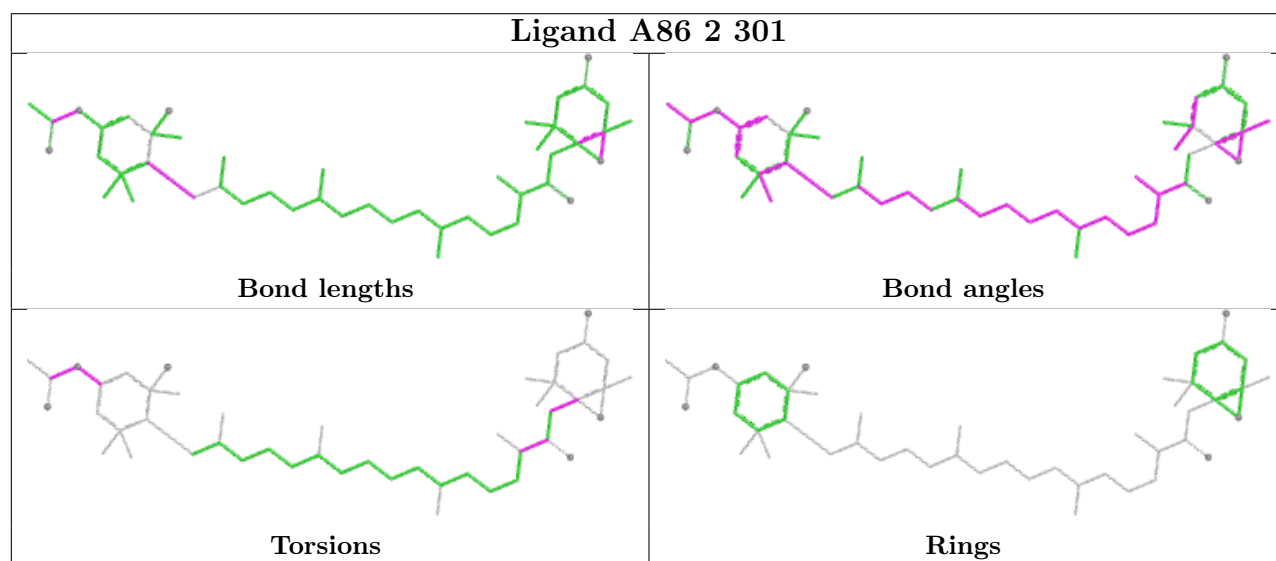
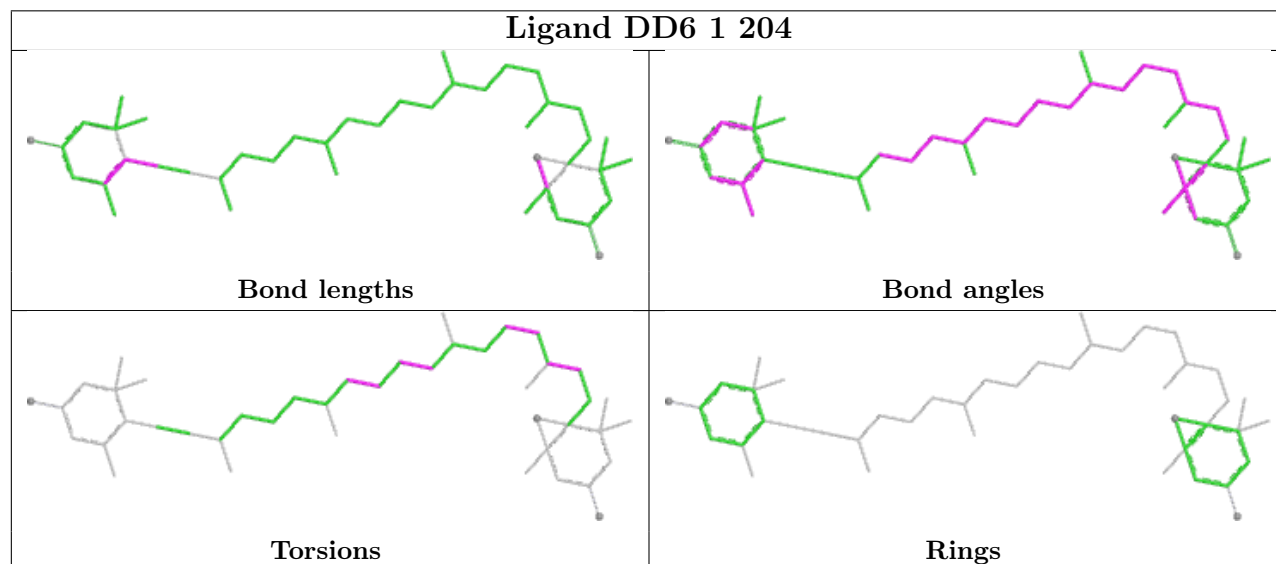
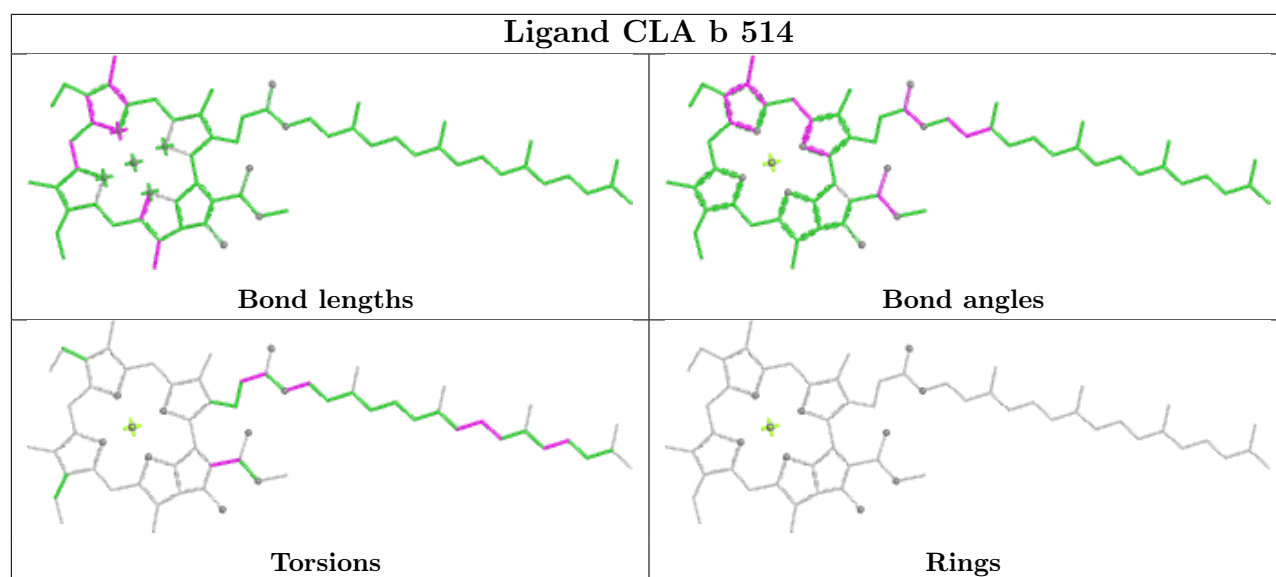
Bond angles



Torsions



Rings



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

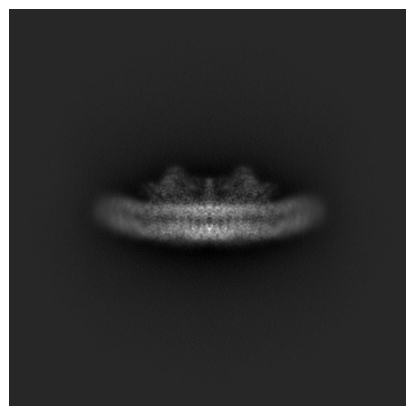
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35987. These allow visual inspection of the internal detail of the map and identification of artifacts.

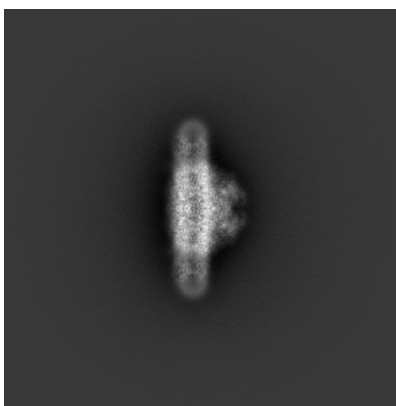
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

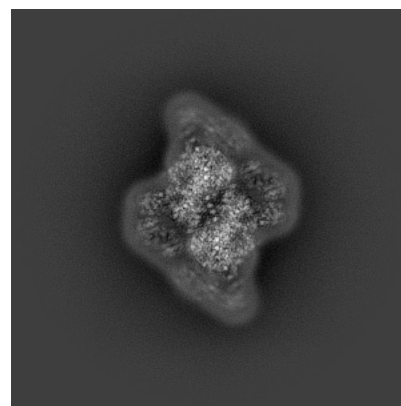
#### 6.1.1 Primary map



X

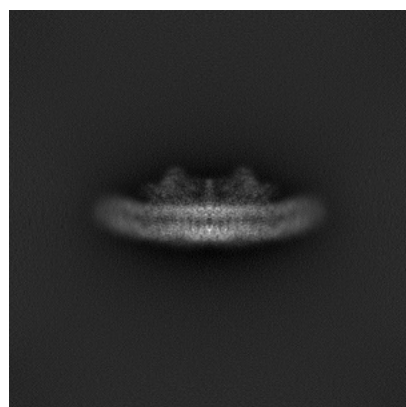


Y

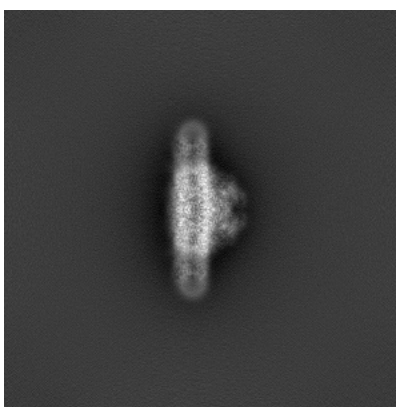


Z

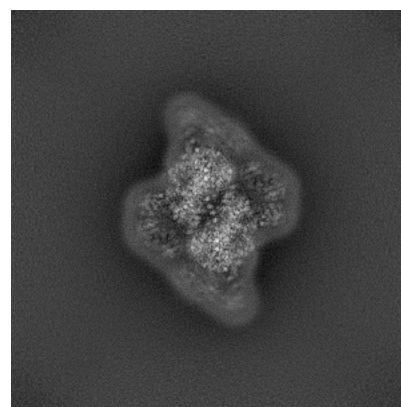
#### 6.1.2 Raw map



X



Y

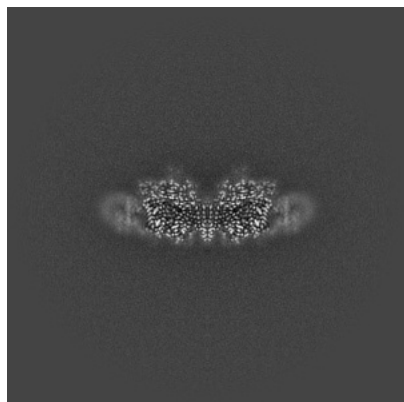


Z

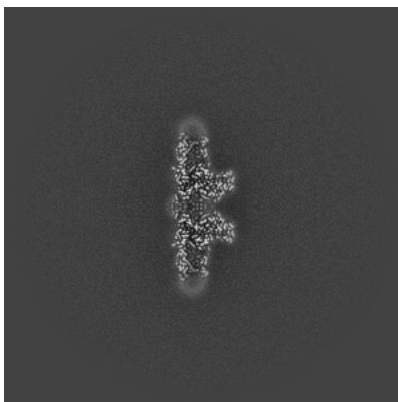
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

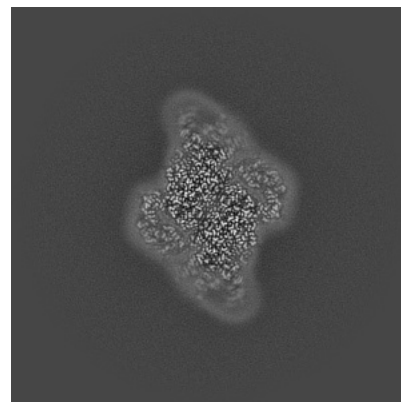
### 6.2.1 Primary map



X Index: 256

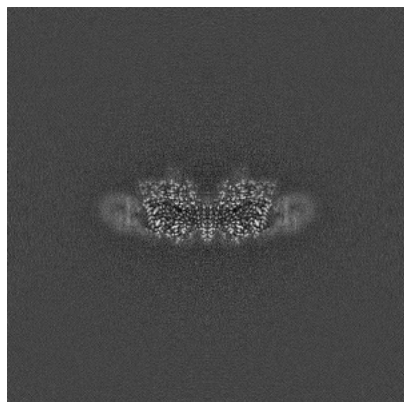


Y Index: 256

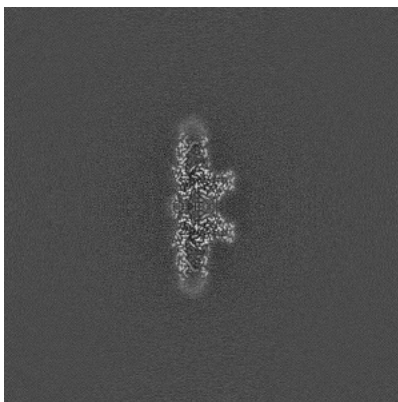


Z Index: 256

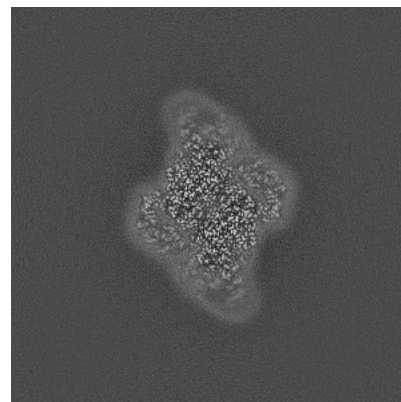
### 6.2.2 Raw map



X Index: 256



Y Index: 256



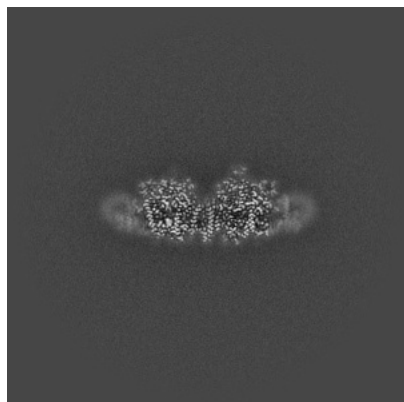
Z Index: 256

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

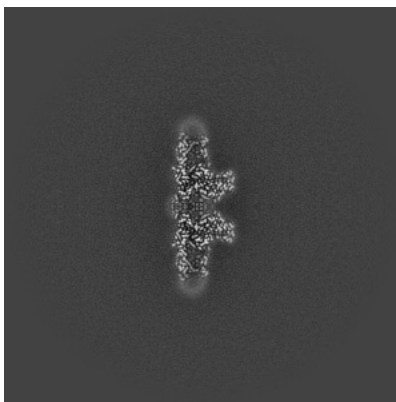


## 6.3 Largest variance slices [i](#)

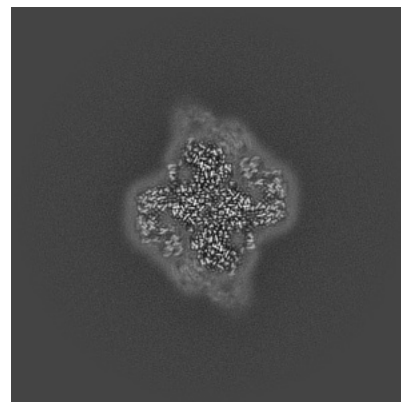
### 6.3.1 Primary map



X Index: 254

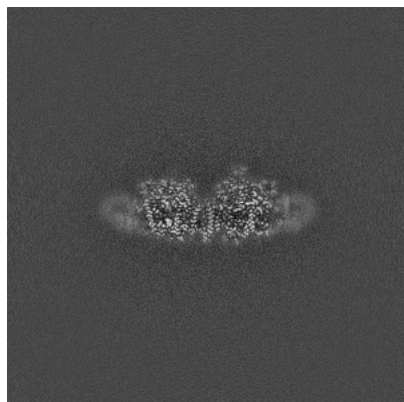


Y Index: 256

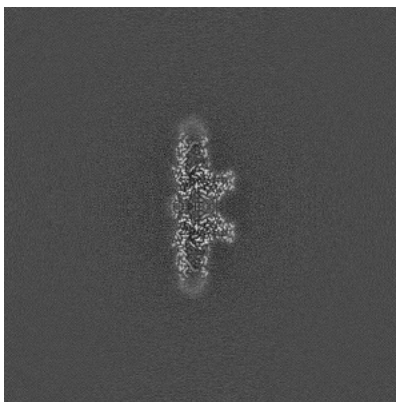


Z Index: 230

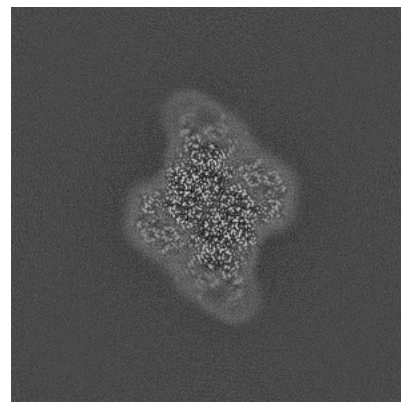
### 6.3.2 Raw map



X Index: 254



Y Index: 256

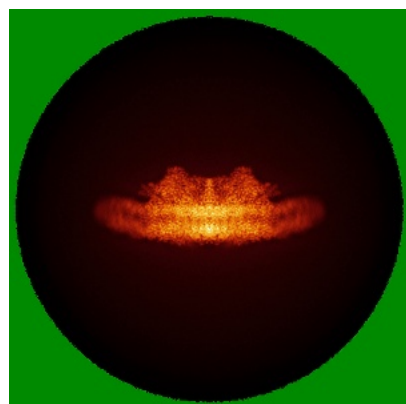


Z Index: 255

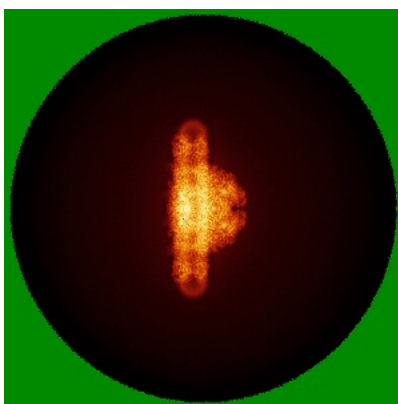
The images above show the largest variance slices of the map in three orthogonal directions.

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

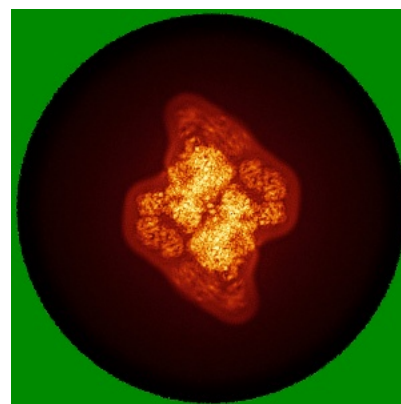
### 6.4.1 Primary map



X

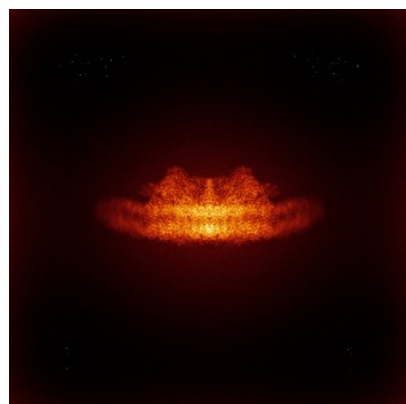


Y

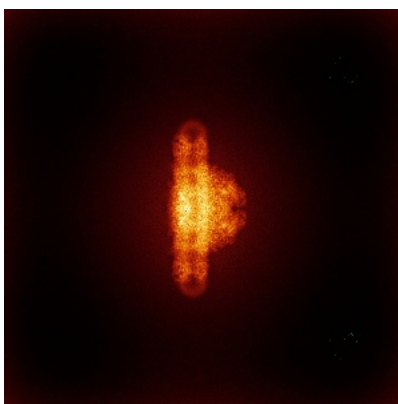


Z

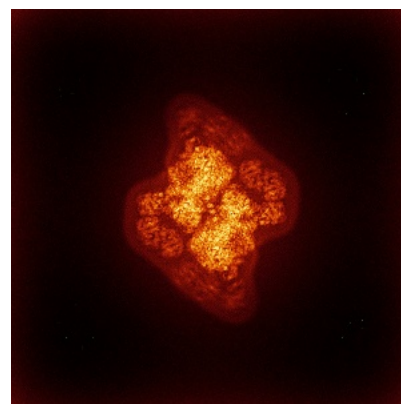
### 6.4.2 Raw map



X



Y

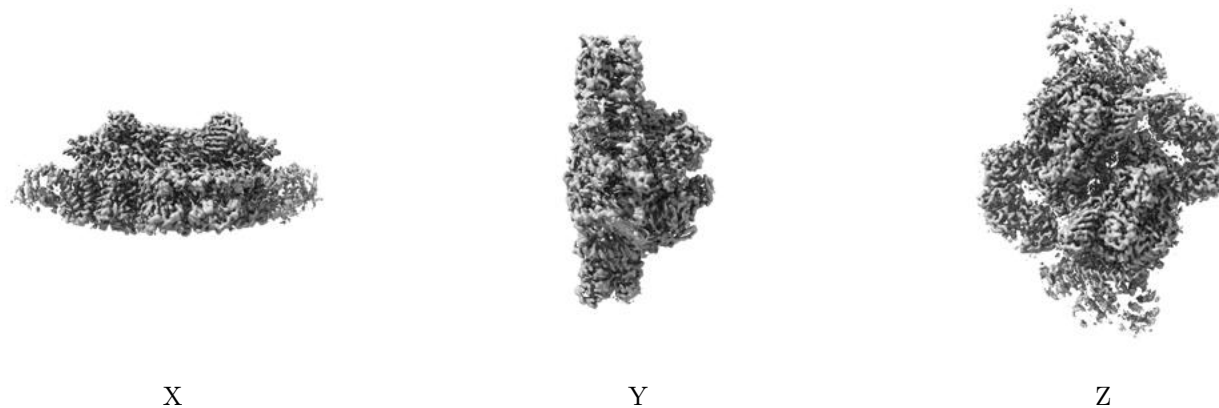


Z

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

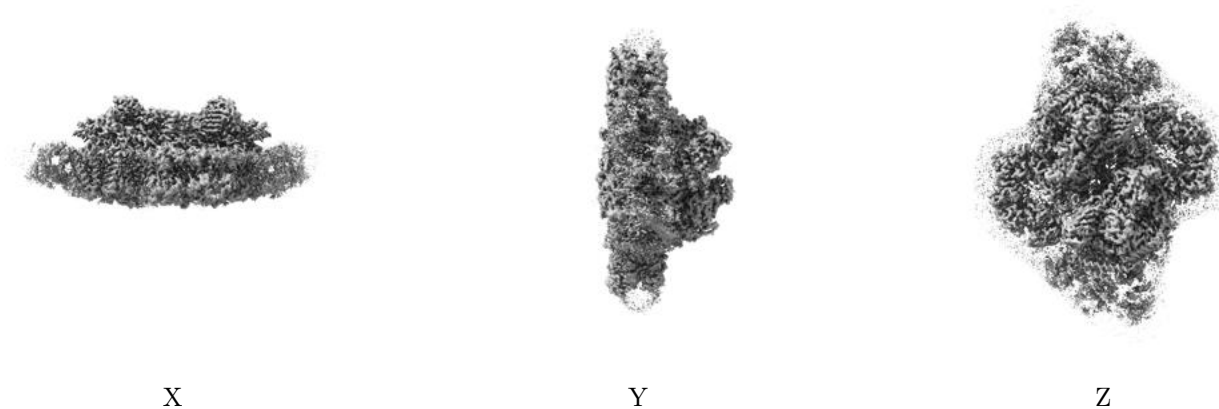
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.158. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

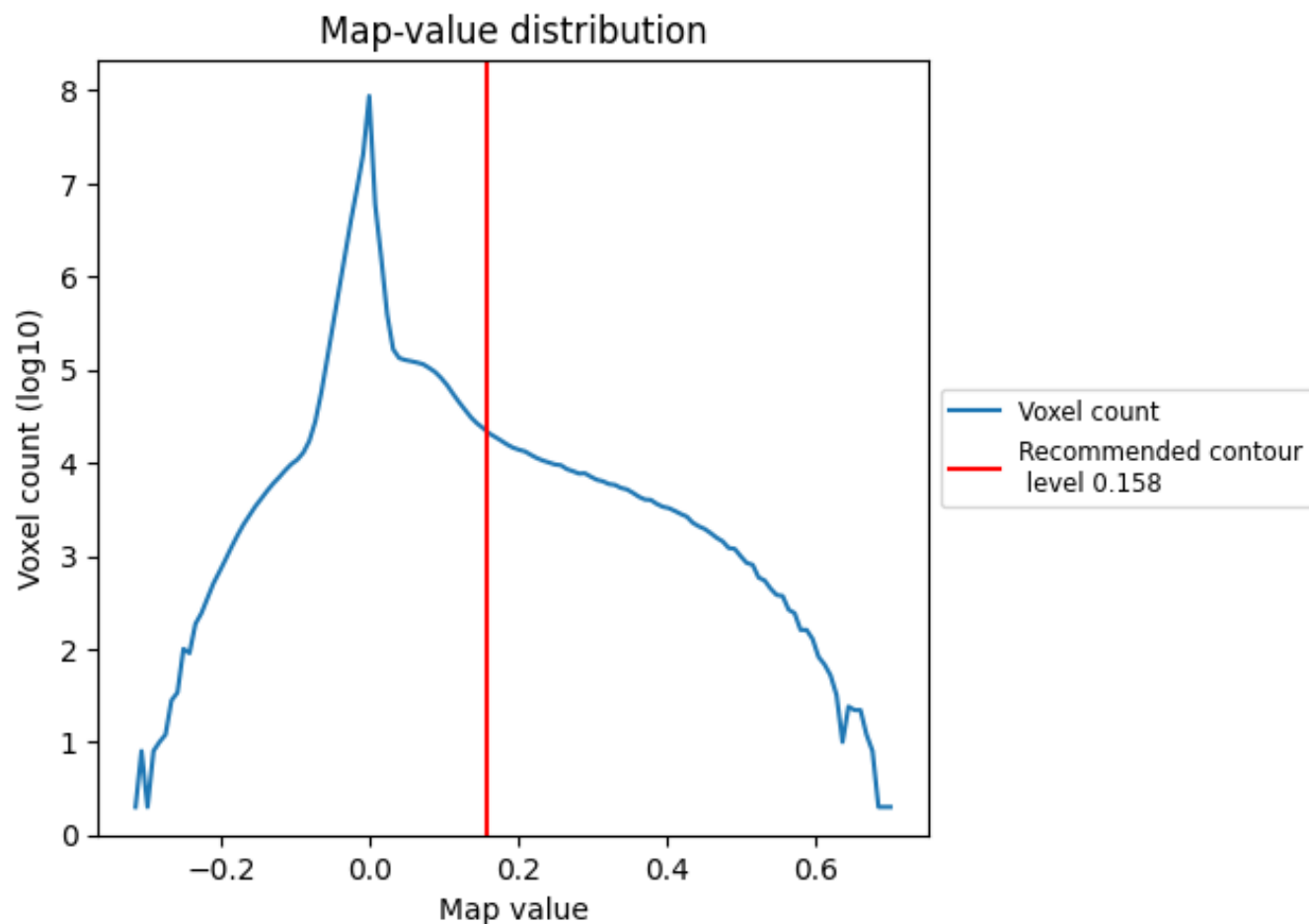
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

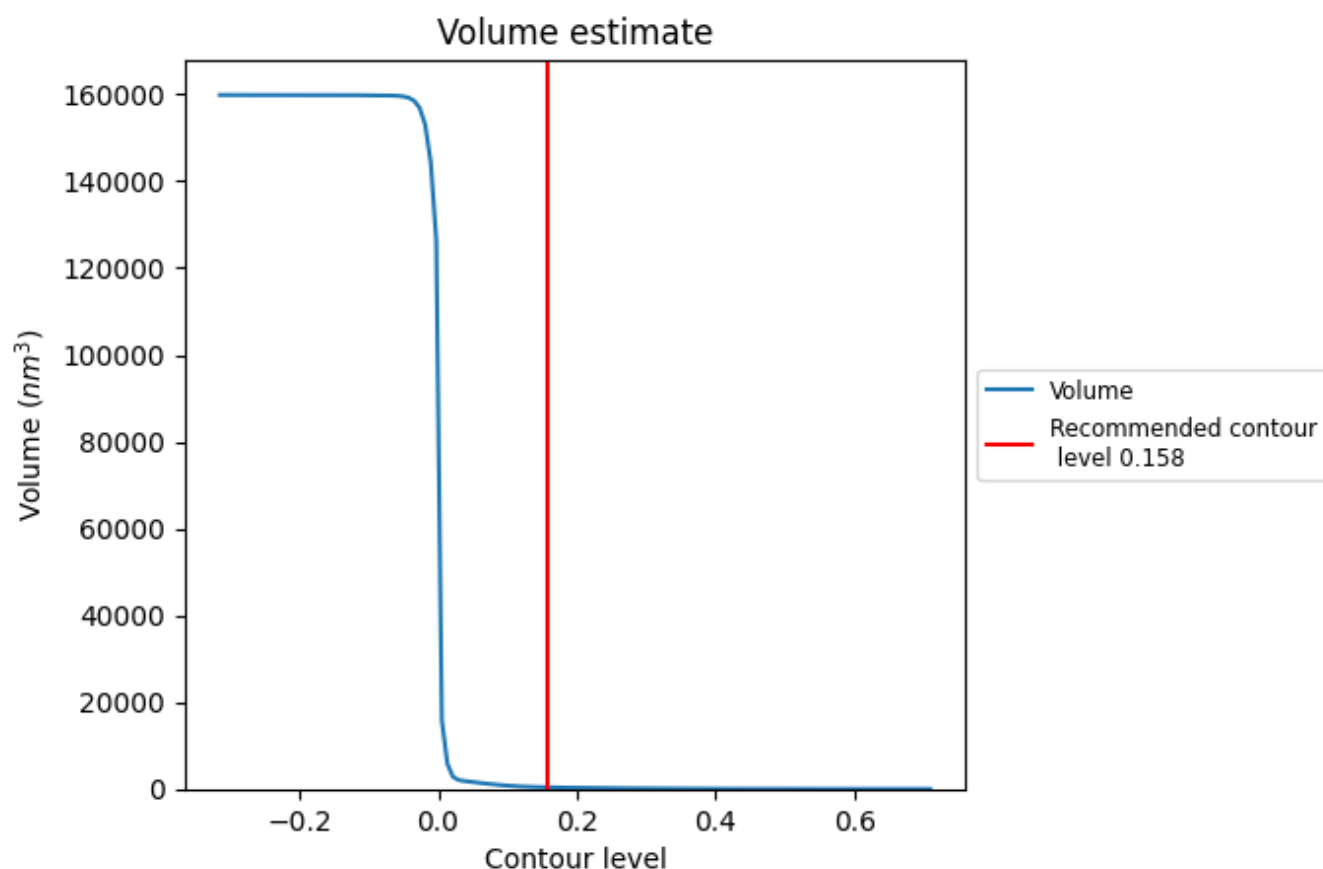
This section contains the results of statistical analysis of the map.

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



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

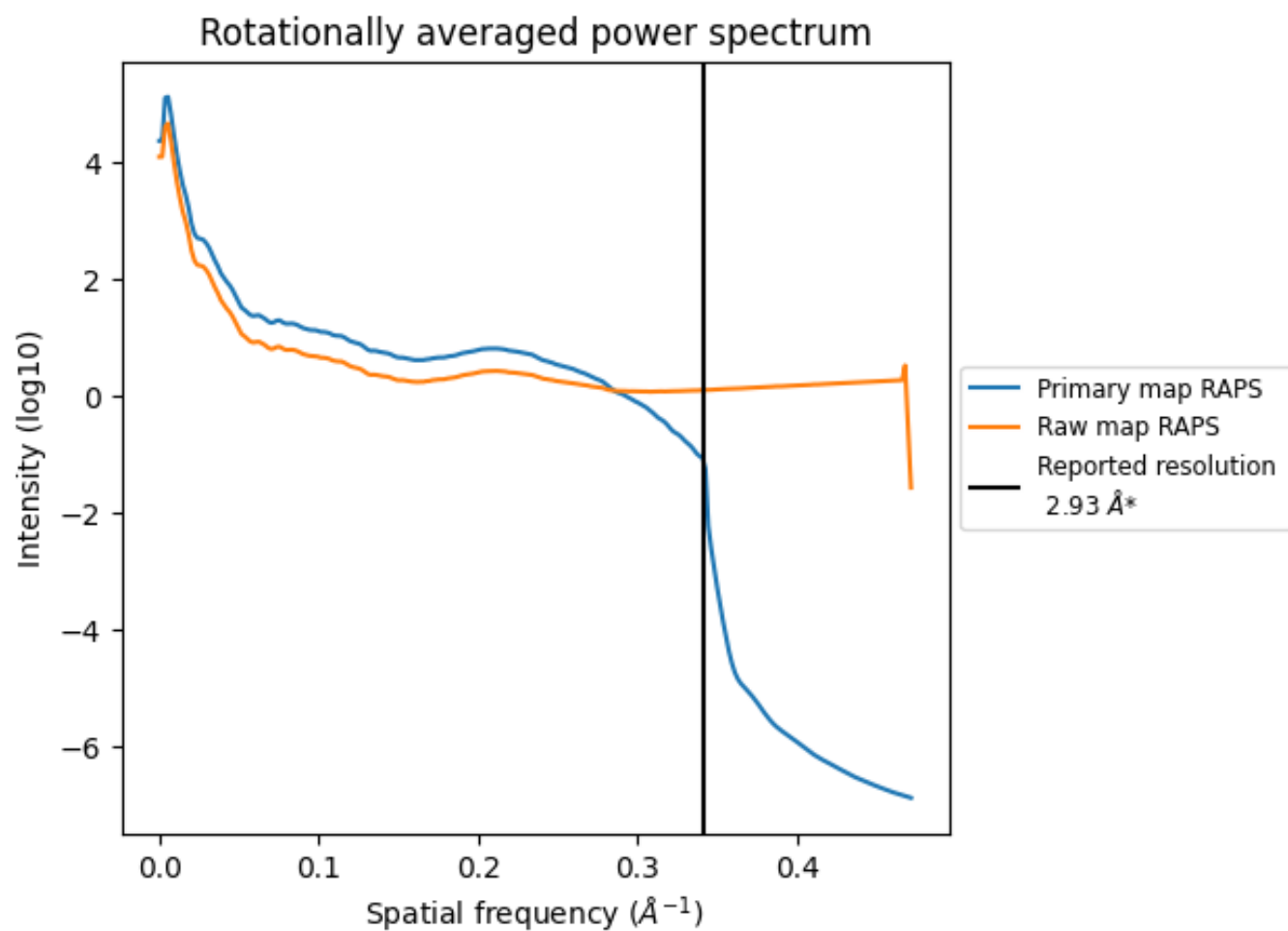
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm<sup>3</sup>; this corresponds to an approximate mass of 339 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 ⓘ

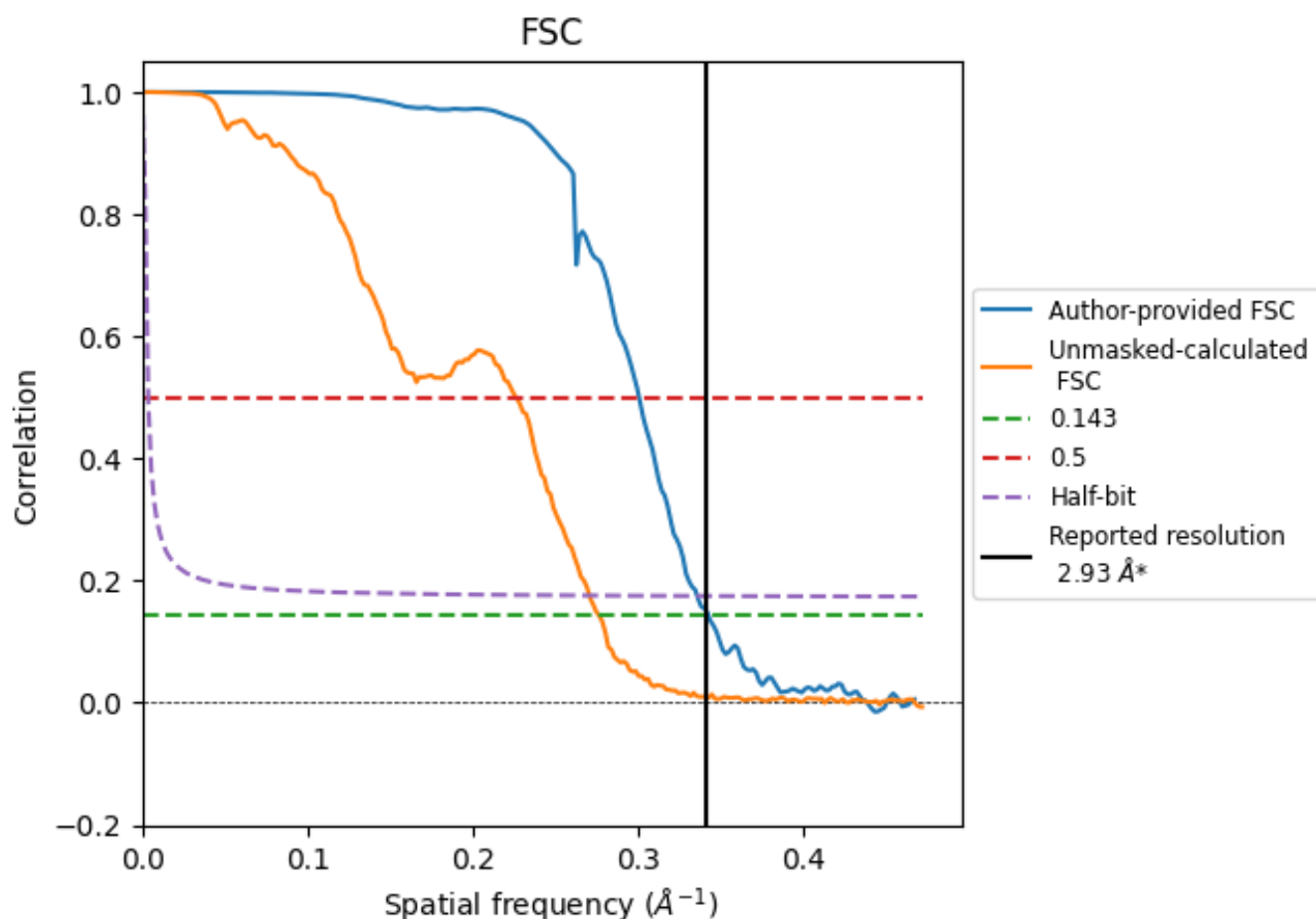


\*Reported resolution corresponds to spatial frequency of 0.341 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.341  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.93                               | -    | -        |
| Author-provided FSC curve | 2.92                               | 3.33 | 2.98     |
| Unmasked-calculated*      | 3.62                               | 4.42 | 3.70     |

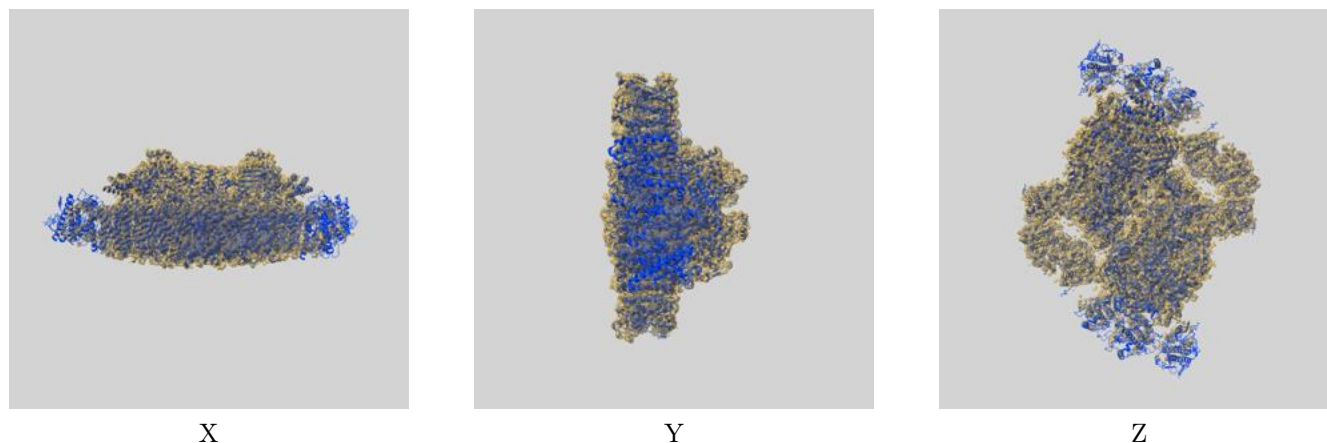
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 2.93 by more than 10 %



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

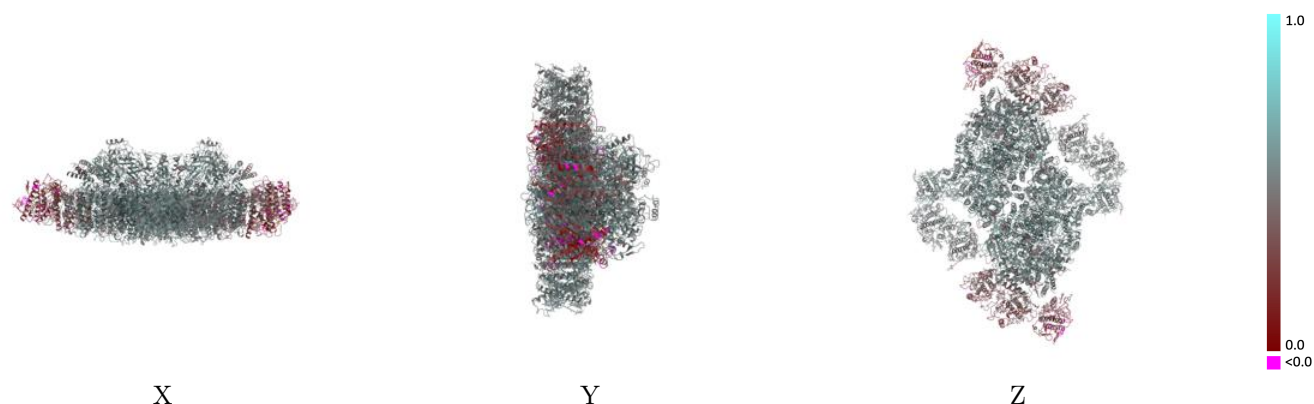
This section contains information regarding the fit between EMDB map EMD-35987 and PDB model 8J5K. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

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



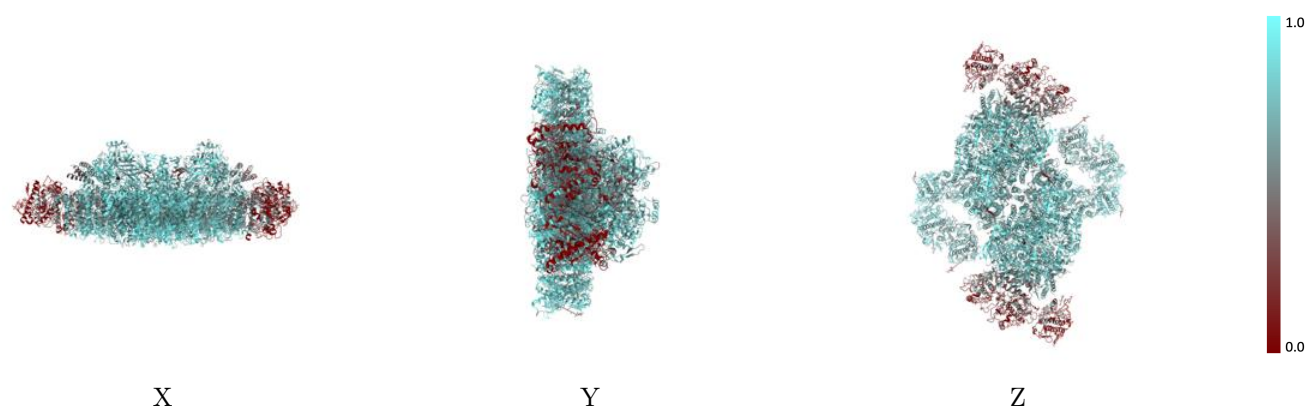
The images above show the 3D surface view of the map at the recommended contour level 0.158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



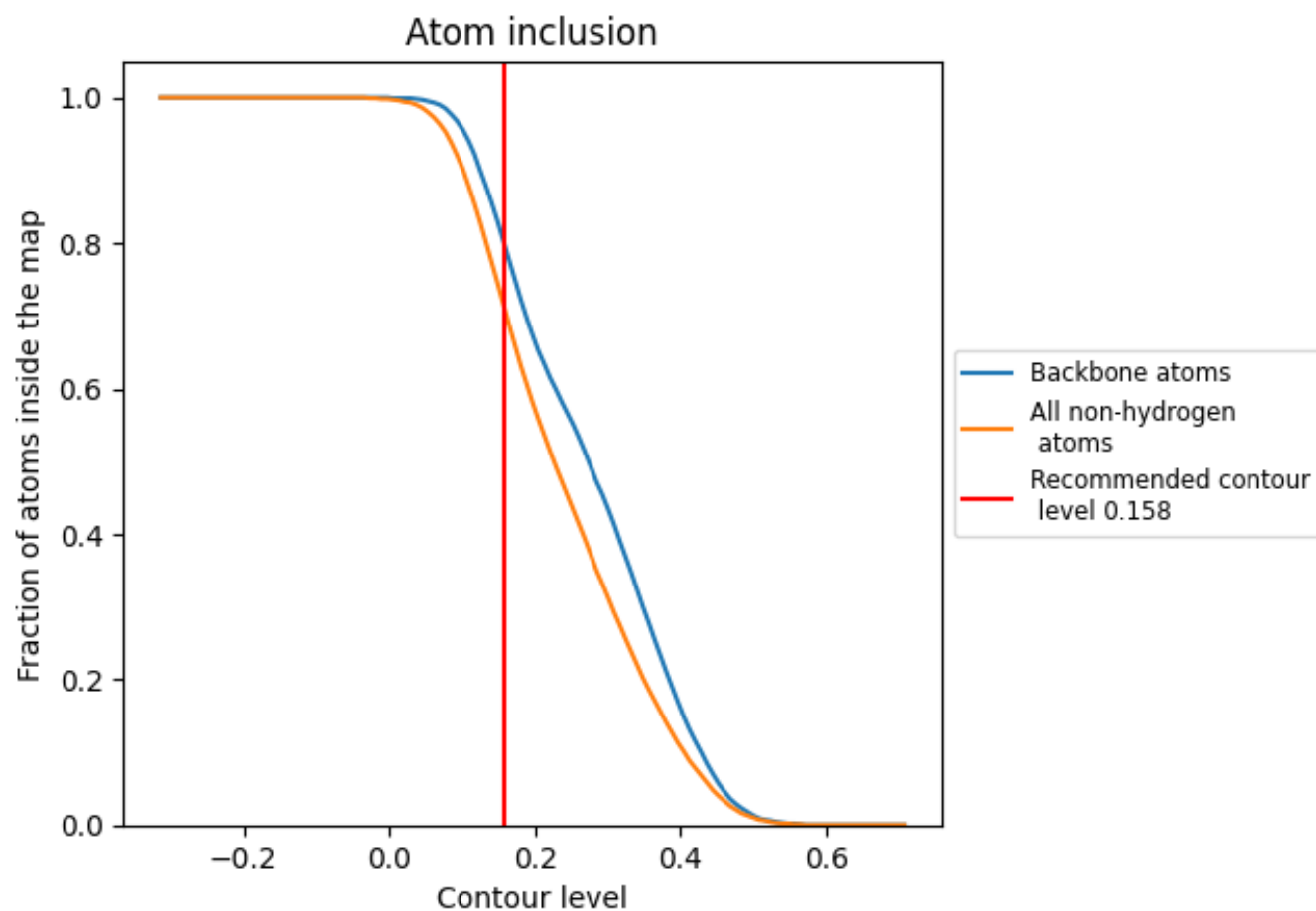
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.158).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.158) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7130   |  0.5040   |
| 0     |  0.7910   |  0.5330   |
| 1     |  0.7530   |  0.5000   |
| 2     |  0.6890   |  0.4730   |
| 3     |  0.2070   |  0.2790   |
| 4     |  0.1270   |  0.1640   |
| 5     |  0.7910   |  0.5340   |
| 6     |  0.7530   |  0.5000   |
| 7     |  0.6880   |  0.4740   |
| 8     |  0.2140   |  0.2820   |
| 9     |  0.1320   |  0.1850   |
| A     |  0.8080   |  0.5670   |
| B     |  0.8430   |  0.5670   |
| C     |  0.8320   |  0.5600   |
| D     |  0.8480  |  0.5720  |
| E     |  0.7890 |  0.5110 |
| F     |  0.8080 |  0.5150 |
| H     |  0.8140 |  0.5580 |
| I     |  0.8520 |  0.5500 |
| J     |  0.6470 |  0.5260 |
| K     |  0.7820 |  0.5170 |
| L     |  0.8580 |  0.5820 |
| M     |  0.7210 |  0.5590 |
| N     |  0.7000 |  0.4400 |
| O     |  0.7150 |  0.5260 |
| P     |  0.2690 |  0.2840 |
| Q     |  0.5210 |  0.4800 |
| T     |  0.7490 |  0.5580 |
| U     |  0.7670 |  0.5160 |
| V     |  0.7710 |  0.5320 |
| W     |  0.7160 |  0.4810 |
| X     |  0.7790 |  0.5410 |
| Y     |  0.6610 |  0.4860 |
| Z     |  0.7290 |  0.4790 |
| a     |  0.8200 |  0.5700 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| b     |  0.8480   |  0.5690   |
| c     |  0.8310   |  0.5600   |
| d     |  0.8460   |  0.5730   |
| e     |  0.7840   |  0.5110   |
| f     |  0.8080   |  0.5160   |
| h     |  0.8090   |  0.5590   |
| i     |  0.8440   |  0.5450   |
| j     |  0.6400   |  0.5240   |
| k     |  0.7820   |  0.5120   |
| l     |  0.8510   |  0.5740   |
| m     |  0.7260   |  0.5600   |
| n     |  0.7130   |  0.4310   |
| o     |  0.7190   |  0.5250   |
| p     |  0.2710   |  0.2870   |
| q     |  0.5150   |  0.4750   |
| t     |  0.7530   |  0.5600   |
| u     |  0.7590   |  0.5170   |
| v     |  0.7800  |  0.5300  |
| w     |  0.7180 |  0.4830 |
| x     |  0.7880 |  0.5390 |
| y     |  0.6580 |  0.4930 |
| z     |  0.7310 |  0.4820 |