



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:42 PM UTC

PDB ID : 7RF6 / pdb\_00007rf6  
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 2.01 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                       |   |                                                                  |
|-----------------------|---|------------------------------------------------------------------|
| MolProbity            | : | 4-5-2 with Phenix2.0                                             |
| Mogul                 | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)      | : | 2.0                                                              |
| EDS                   | : | 3.0                                                              |
| Buster-report         | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                  | : | 9.0.010 (Gargrove)                                               |

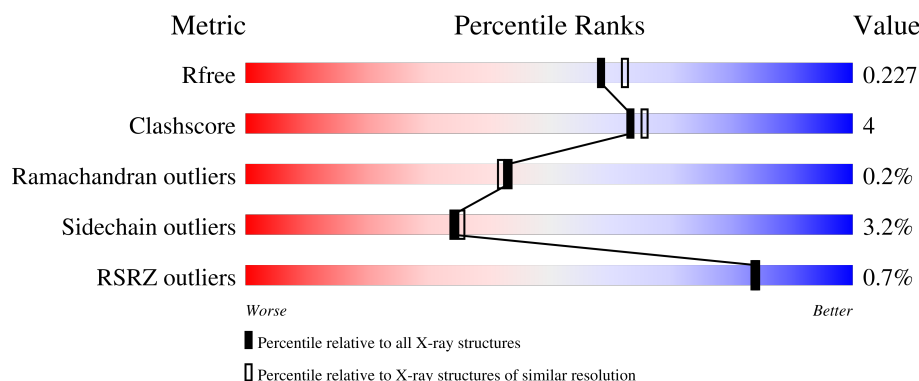
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 10052 (2.00-2.00)                                     |
| Clashscore            | 190562                      | 11152 (2.00-2.00)                                     |
| Ramachandran outliers | 187476                      | 11031 (2.00-2.00)                                     |
| Sidechain outliers    | 187428                      | 11029 (2.00-2.00)                                     |
| RSRZ outliers         | 180081                      | 10067 (2.00-2.00)                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

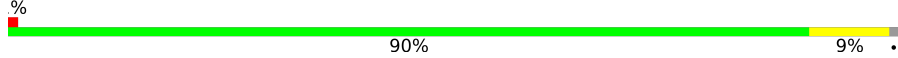
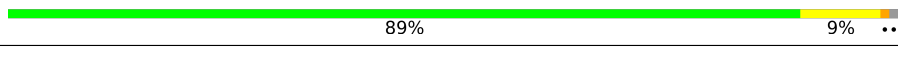
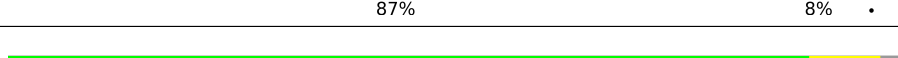
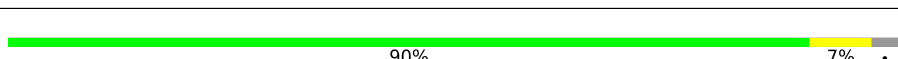
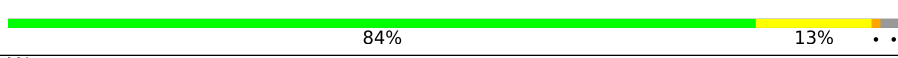
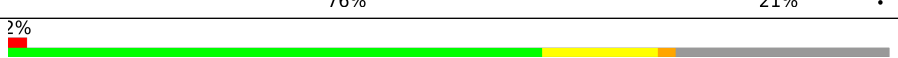
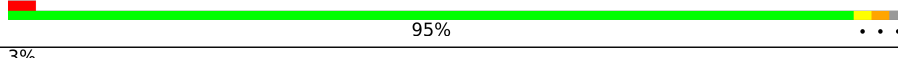
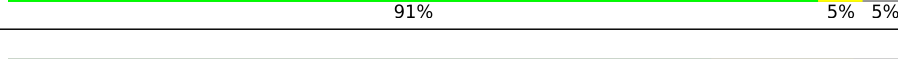
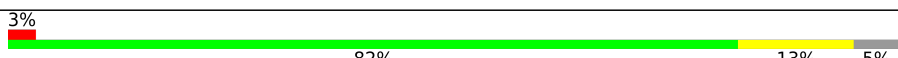
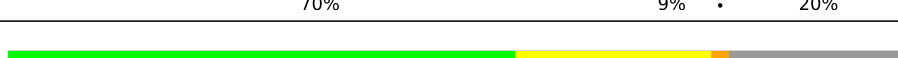
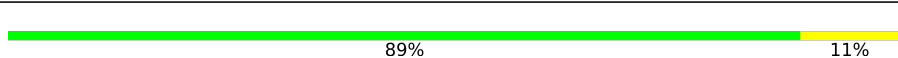
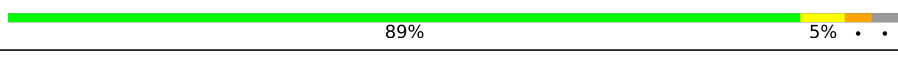
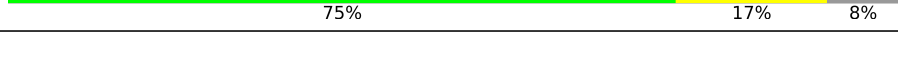
| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 344    |  |
| 1   | a     | 344    |  |

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Density-Fitness : 1.0.12  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49



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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | B     | 510    |    |
| 2   | b     | 510    |    |
| 3   | C     | 461    |    |
| 3   | c     | 461    |    |
| 4   | D     | 352    |    |
| 4   | d     | 352    |    |
| 5   | E     | 84     |    |
| 5   | e     | 84     |    |
| 6   | F     | 45     |    |
| 6   | f     | 45     |   |
| 7   | H     | 66     |  |
| 7   | h     | 66     |  |
| 8   | I     | 38     |  |
| 8   | i     | 38     |  |
| 9   | J     | 40     |  |
| 9   | j     | 40     |  |
| 10  | K     | 46     |  |
| 10  | k     | 46     |  |
| 11  | L     | 37     |  |
| 11  | l     | 37     |  |
| 12  | M     | 36     |  |
| 12  | m     | 36     |  |
| 13  | O     | 272    |  |
| 13  | o     | 272    |  |
| 14  | R     | 41     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | r     | 41     |                  |
| 15  | T     | 32     |                  |
| 15  | t     | 32     |                  |
| 16  | U     | 134    |                  |
| 16  | u     | 134    |                  |
| 17  | V     | 163    |                  |
| 17  | v     | 163    |                  |
| 18  | X     | 41     |                  |
| 18  | x     | 41     |                  |
| 19  | Y     | 46     |                  |
| 19  | y     | 46     |                  |
| 20  | Z     | 62     |                  |
| 20  | z     | 62     |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CLA  | A     | 604 | X         | -        | -       | -                |
| 24  | CLA  | A     | 605 | X         | -        | -       | -                |
| 24  | CLA  | A     | 608 | X         | -        | -       | -                |
| 24  | CLA  | B     | 601 | X         | -        | -       | -                |
| 24  | CLA  | B     | 602 | X         | -        | -       | -                |
| 24  | CLA  | B     | 603 | X         | -        | -       | -                |
| 24  | CLA  | B     | 604 | X         | -        | -       | -                |
| 24  | CLA  | B     | 605 | X         | -        | -       | -                |
| 24  | CLA  | B     | 606 | X         | -        | -       | -                |
| 24  | CLA  | B     | 607 | X         | -        | -       | -                |
| 24  | CLA  | B     | 610 | X         | -        | -       | -                |
| 24  | CLA  | B     | 611 | X         | -        | -       | -                |
| 24  | CLA  | B     | 612 | X         | -        | -       | -                |
| 24  | CLA  | B     | 613 | X         | -        | -       | -                |
| 24  | CLA  | B     | 614 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CLA  | B     | 615 | X         | -        | -       | -                |
| 24  | CLA  | B     | 616 | X         | -        | -       | -                |
| 24  | CLA  | C     | 501 | X         | -        | -       | -                |
| 24  | CLA  | C     | 503 | X         | -        | -       | -                |
| 24  | CLA  | C     | 504 | X         | -        | -       | -                |
| 24  | CLA  | C     | 505 | X         | -        | -       | -                |
| 24  | CLA  | C     | 506 | X         | -        | -       | -                |
| 24  | CLA  | C     | 507 | X         | -        | -       | -                |
| 24  | CLA  | C     | 509 | X         | -        | -       | -                |
| 24  | CLA  | C     | 510 | X         | -        | -       | -                |
| 24  | CLA  | C     | 511 | X         | -        | -       | -                |
| 24  | CLA  | C     | 512 | X         | -        | -       | -                |
| 24  | CLA  | C     | 513 | X         | -        | -       | -                |
| 24  | CLA  | D     | 402 | X         | -        | -       | -                |
| 24  | CLA  | a     | 604 | X         | -        | -       | -                |
| 24  | CLA  | a     | 606 | X         | -        | -       | -                |
| 24  | CLA  | a     | 612 | X         | -        | -       | -                |
| 24  | CLA  | b     | 601 | X         | -        | -       | -                |
| 24  | CLA  | b     | 603 | X         | -        | -       | -                |
| 24  | CLA  | b     | 604 | X         | -        | -       | -                |
| 24  | CLA  | b     | 605 | X         | -        | -       | -                |
| 24  | CLA  | b     | 606 | X         | -        | -       | -                |
| 24  | CLA  | b     | 607 | X         | -        | -       | -                |
| 24  | CLA  | b     | 610 | X         | -        | -       | -                |
| 24  | CLA  | b     | 611 | X         | -        | -       | -                |
| 24  | CLA  | b     | 612 | X         | -        | -       | -                |
| 24  | CLA  | b     | 613 | X         | -        | -       | -                |
| 24  | CLA  | b     | 614 | X         | -        | -       | -                |
| 24  | CLA  | b     | 615 | X         | -        | -       | -                |
| 24  | CLA  | b     | 616 | X         | -        | -       | -                |
| 24  | CLA  | c     | 501 | X         | -        | -       | -                |
| 24  | CLA  | c     | 503 | X         | -        | -       | -                |
| 24  | CLA  | c     | 504 | X         | -        | -       | -                |
| 24  | CLA  | c     | 505 | X         | -        | -       | -                |
| 24  | CLA  | c     | 506 | X         | -        | -       | -                |
| 24  | CLA  | c     | 507 | X         | -        | -       | -                |
| 24  | CLA  | c     | 509 | X         | -        | -       | -                |
| 24  | CLA  | c     | 510 | X         | -        | -       | -                |
| 24  | CLA  | c     | 511 | X         | -        | -       | -                |
| 24  | CLA  | c     | 512 | X         | -        | -       | -                |
| 24  | CLA  | c     | 513 | X         | -        | -       | -                |
| 24  | CLA  | d     | 403 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | CLA  | d     | 404 | X         | -        | -       | -                |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106128 atoms, of which 52762 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 334      | Total | C    | H    | N   | O   | S  | 0       | 66      | 0     |
|     |       |          | 6098  | 2030 | 2985 | 513 | 551 | 19 |         |         |       |
| 1   | a     | 334      | Total | C    | H    | N   | O   | S  | 0       | 66      | 0     |
|     |       |          | 6086  | 2027 | 2976 | 513 | 551 | 19 |         |         |       |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 505      | Total | C    | H    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 7878  | 2631 | 3873 | 666 | 695 | 13 |         |         |       |
| 2   | b     | 505      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 7814  | 2610 | 3836 | 665 | 690 | 13 |         |         |       |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 442      | Total | C    | H    | N   | O   | S  | 0       | 14      | 0     |
|     |       |          | 6941  | 2302 | 3432 | 586 | 607 | 14 |         |         |       |
| 3   | c     | 451      | Total | C    | H    | N   | O   | S  | 0       | 14      | 0     |
|     |       |          | 7086  | 2343 | 3503 | 602 | 624 | 14 |         |         |       |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 341      | Total | C    | H    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 5368  | 1809 | 2637 | 446 | 464 | 12 |         |         |       |
| 4   | d     | 341      | Total | C    | H    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 5380  | 1813 | 2643 | 446 | 466 | 12 |         |         |       |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 5   | E     | 82       | Total | C   | H   | N   | O   | 16      | 1       | 0     |
|     |       |          | 1317  | 436 | 651 | 107 | 123 |         |         |       |
| 5   | e     | 82       | Total | C   | H   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1312  | 434 | 648 | 108 | 122 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 6   | F     | 34       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 557   | 187 | 282 | 45 | 42 |         |         |       |
| 6   | f     | 34       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 557   | 187 | 282 | 45 | 42 |         |         |       |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 7   | H     | 65       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 1042  | 341 | 532 | 82 | 85 |         |         |       |
| 7   | h     | 63       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 1016  | 333 | 518 | 80 | 83 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 8   | I     | 36       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 607   | 200 | 311 | 46 | 49 |         |         |       |
| 8   | i     | 36       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 607   | 200 | 311 | 46 | 49 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 9   | J     | 36       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 525   | 174 | 268 | 40 | 42 |         |         |       |
| 9   | j     | 36       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 525   | 174 | 268 | 40 | 42 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 10  | K     | 37       | Total | C   | H   | N  | 0       | 0       | 0     |
|     |       |          | 598   | 204 | 305 | 43 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 10  | k     | 37       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 598   | 204 | 305 | 43 | 46 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 11  | L     | 37       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 620   | 202 | 316 | 48 | 53 |         |         |       |
| 11  | l     | 36       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 600   | 197 | 304 | 47 | 52 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 12  | M     | 33       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 525   | 171 | 269 | 37 | 47 |         |         |       |
| 12  | m     | 32       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 518   | 168 | 267 | 36 | 46 |         |         |       |

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms |      |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---------|---------|-------|
| 13  | O     | 244      | Total | C    | H    | N   | O   | 0       | 1       | 0     |
|     |       |          | 3700  | 1168 | 1830 | 313 | 385 |         |         |       |
| 13  | o     | 244      | Total | C    | H    | N   | O   | 0       | 0       | 0     |
|     |       |          | 3720  | 1170 | 1846 | 317 | 383 |         |         |       |

- Molecule 14 is a protein called Photosystem II protein Y.

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 14  | R     | 28       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 459   | 151 | 238 | 38 | 32 |         |         |       |
| 14  | r     | 28       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 459   | 151 | 238 | 38 | 32 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 15  | T     | 30       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 519   | 181 | 261 | 36 | 39 |         |         |       |
| 15  | t     | 30       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 512   | 180 | 256 | 36 | 38 |         |         |       |

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms |     |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 16  | U     | 97       | Total | C   | H   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1547  | 491 | 773 | 129 | 154 |         |         |       |
| 16  | u     | 97       | Total | C   | H   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1547  | 491 | 773 | 129 | 154 |         |         |       |

- Molecule 17 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 17  | V     | 137      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2135  | 675 | 1071 | 177 | 208 | 4 |         |         |       |
| 17  | v     | 137      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2135  | 675 | 1071 | 177 | 208 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 18  | X     | 38       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 593   | 188 | 312 | 45 | 48 |         |         |       |
| 18  | x     | 39       | Total | C   | H   | N  | O  | 0       | 0       | 0     |
|     |       |          | 602   | 191 | 316 | 46 | 49 |         |         |       |

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

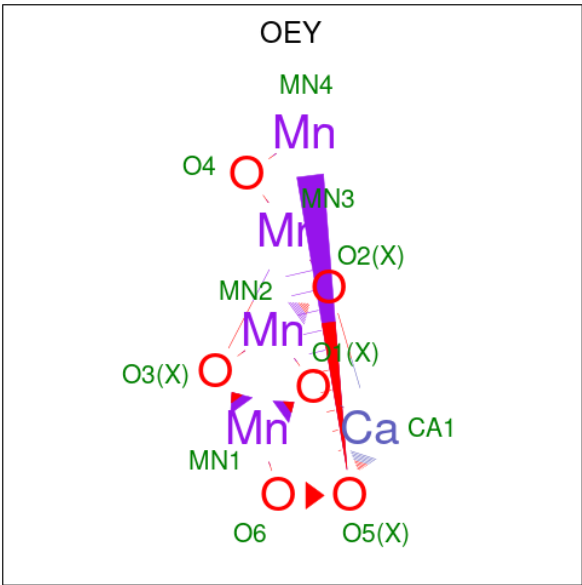
| Mol | Chain | Residues | Atoms |     |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 19  | Y     | 27       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 413   | 128 | 217 | 35 | 30 | 3 |         |         |       |
| 19  | y     | 30       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 144 | 241 | 35 | 36 | 3 |         |         |       |

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms        |          |          |         |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---------|--------|---------|---------|-------|
| 20  | Z     | 62       | Total<br>995 | C<br>328 | H<br>516 | N<br>72 | O<br>77 | S<br>2 | 0       | 0       | 0     |
| 20  | z     | 62       | Total<br>986 | C<br>326 | H<br>509 | N<br>72 | O<br>77 | S<br>2 | 0       | 0       | 0     |

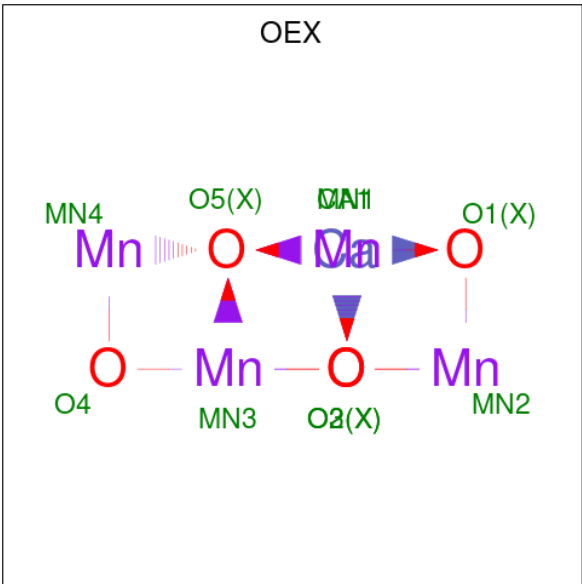
- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 21  | A     | 1        | Total | Ca | Mn | O | 0       | 1       |
|     |       |          | 11    | 1  | 4  | 6 |         |         |
| 21  | a     | 1        | Total | Ca | Mn | O | 0       | 1       |
|     |       |          | 11    | 1  | 4  | 6 |         |         |

- Molecule 22 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 |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22  | A     | 1        | Total | Ca | Mn | O | 0       | 1       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

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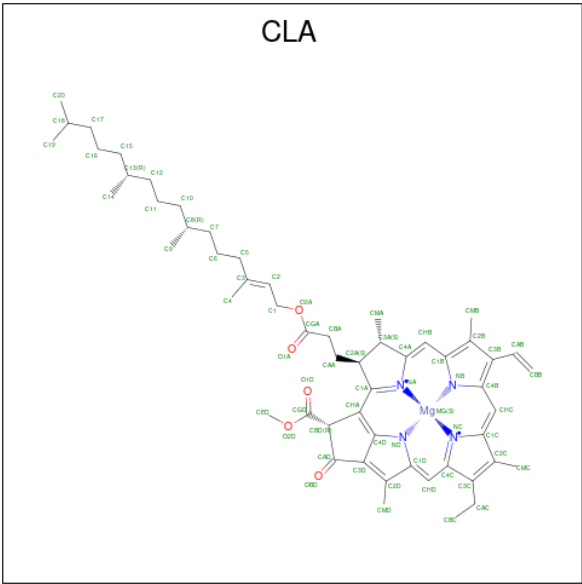
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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22  | a     | 1        | Total | Ca | Mn | O | 0       | 1       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 23  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 23  | a     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 24  | A     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 102   | 44 | 48 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 117   | 49 | 58 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | C     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms        |         |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|---------|--------|--------|---------|---------|
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | D     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | D     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | a     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | a     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | a     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | b     | 1        | Total<br>137 | C<br>55 | H<br>72 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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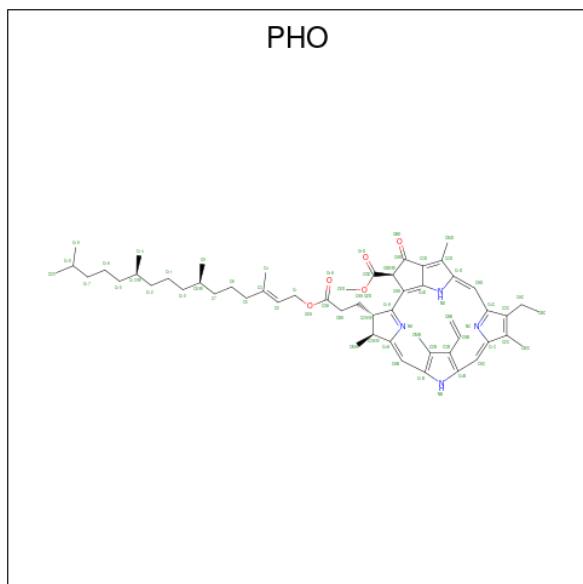
| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 132   | 54 | 68 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | d     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |
| 24  | d     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |

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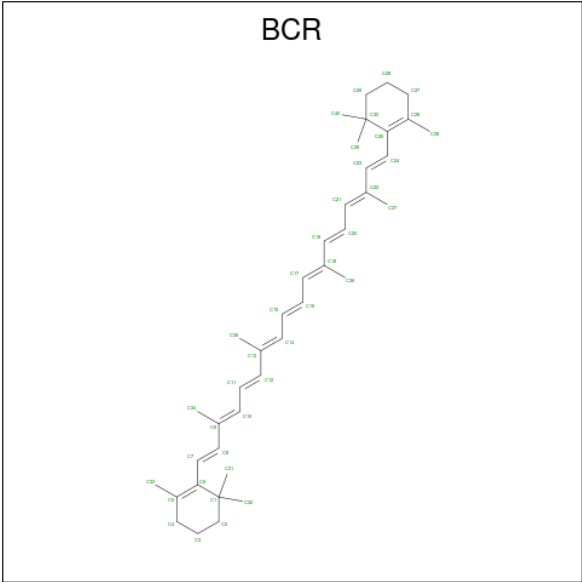
| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 24  | d     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |         |

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|--|---------|---------|
| 25  | A     | 1        | Total | C  | H  | N | O |  | 0       | 0       |
|     |       |          | 138   | 55 | 74 | 4 | 5 |  |         |         |
| 25  | A     | 1        | Total | C  | H  | N | O |  | 0       | 0       |
|     |       |          | 138   | 55 | 74 | 4 | 5 |  |         |         |
| 25  | a     | 1        | Total | C  | H  | N | O |  | 0       | 0       |
|     |       |          | 138   | 55 | 74 | 4 | 5 |  |         |         |
| 25  | d     | 1        | Total | C  | H  | N | O |  | 0       | 0       |
|     |       |          | 138   | 55 | 74 | 4 | 5 |  |         |         |

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 26  | A     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | B     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | B     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | B     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | C     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | C     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | D     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | H     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | K     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | T     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | Y     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | a     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | b     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | b     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |

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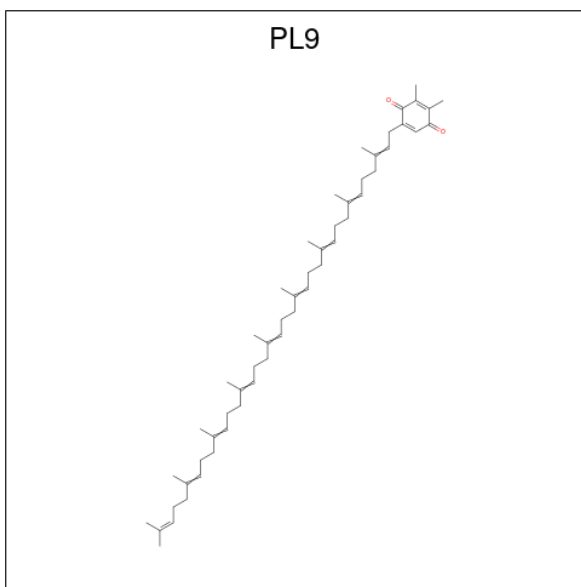
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 26  | b     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | c     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | c     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | d     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | k     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | k     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | t     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |
| 26  | x     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 27  | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 27  | a     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

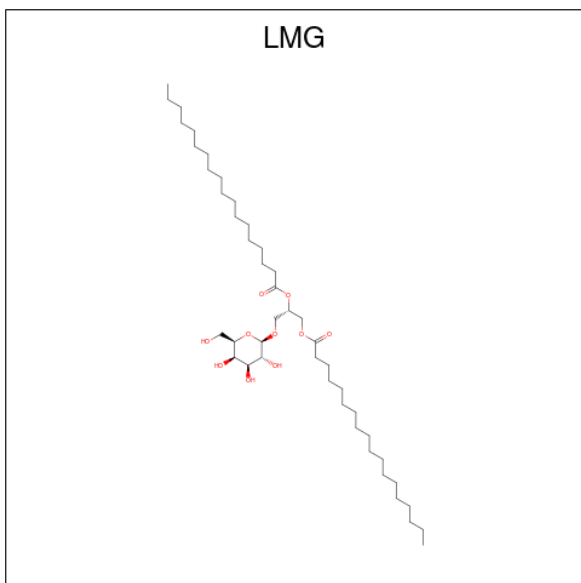
- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





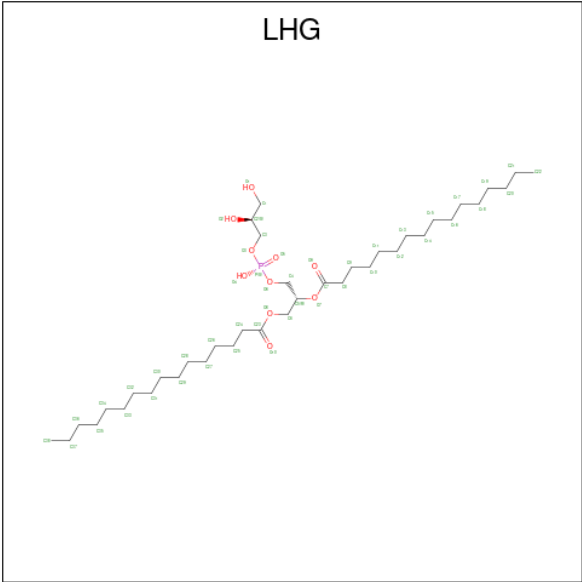
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 28  | A     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 135   | 53 | 80 | 2 |         |         |
| 28  | D     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 135   | 53 | 80 | 2 |         |         |
| 28  | a     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 135   | 53 | 80 | 2 |         |         |
| 28  | d     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 135   | 53 | 80 | 2 |         |         |

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



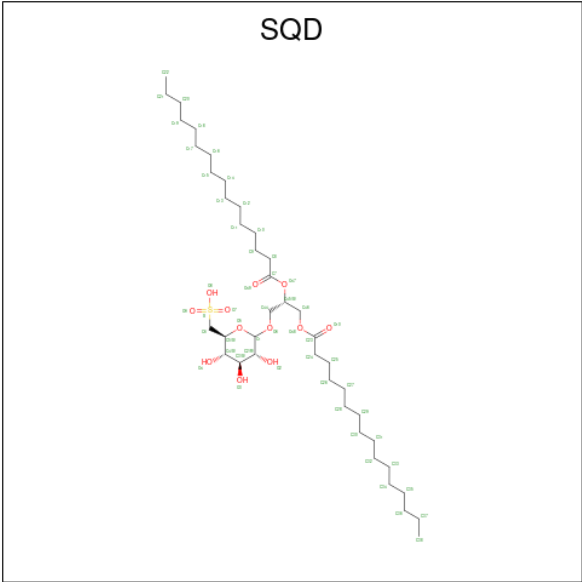
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 29  | A     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 114   | 38 | 66 | 10 |         |         |
| 29  | C     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 114   | 38 | 66 | 10 |         |         |
| 29  | D     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 123   | 41 | 72 | 10 |         |         |
| 29  | D     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 78    | 27 | 45 | 6  |         |         |
| 29  | D     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 68    | 24 | 40 | 4  |         |         |
| 29  | M     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 123   | 41 | 72 | 10 |         |         |
| 29  | a     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 141   | 45 | 86 | 10 |         |         |
| 29  | b     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 123   | 41 | 72 | 10 |         |         |
| 29  | b     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 141   | 45 | 86 | 10 |         |         |
| 29  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 81    | 27 | 44 | 10 |         |         |
| 29  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 117   | 38 | 69 | 10 |         |         |
| 29  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 117   | 39 | 68 | 10 |         |         |
| 29  | d     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 102   | 34 | 58 | 10 |         |         |

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



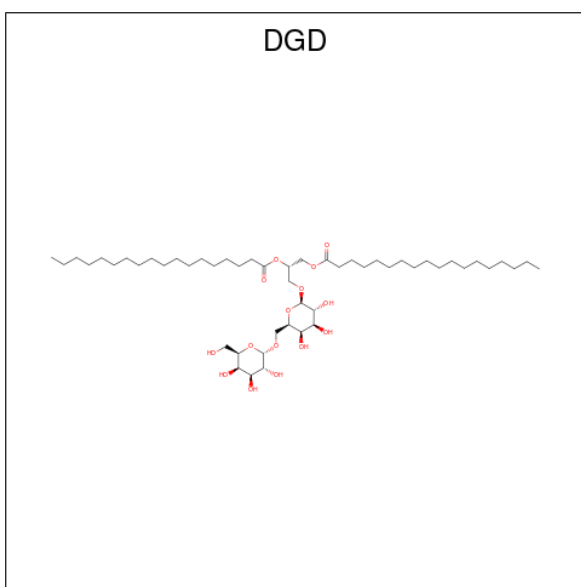
| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 30  | A     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 114   | 36 | 67 | 10 | 1 |         |         |
| 30  | B     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | B     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | D     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | E     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | d     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | d     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |
| 30  | d     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 90    | 28 | 51 | 10 | 1 |         |         |
| 30  | e     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 99    | 31 | 57 | 10 | 1 |         |         |
| 30  | l     | 1        | Total | C  | H  | O  | P | 0       | 0       |
|     |       |          | 123   | 38 | 74 | 10 | 1 |         |         |

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



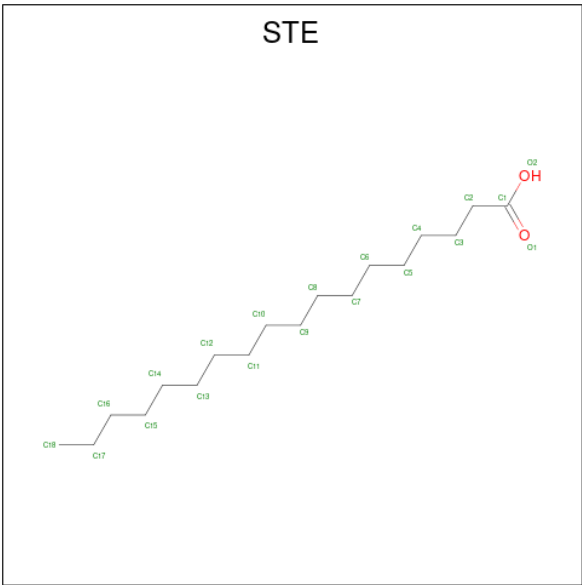
| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 31  | A     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 123   | 39 | 71 | 12 | 1 |         |         |
| 31  | A     | 1        | Total | C  | H  | O  |   | 0       | 0       |
|     |       |          | 104   | 35 | 65 | 4  |   |         |         |
| 31  | B     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 132   | 41 | 78 | 12 | 1 |         |         |
| 31  | D     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 82    | 25 | 46 | 10 | 1 |         |         |
| 31  | a     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 132   | 41 | 78 | 12 | 1 |         |         |
| 31  | a     | 1        | Total | C  | H  | O  |   | 0       | 0       |
|     |       |          | 92    | 31 | 56 | 5  |   |         |         |
| 31  | b     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 114   | 36 | 65 | 12 | 1 |         |         |
| 31  | f     | 1        | Total | C  | H  | O  | S | 0       | 0       |
|     |       |          | 89    | 28 | 48 | 12 | 1 |         |         |

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 32  | A     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 162   | 51 | 96 | 15 |         |         |
| 32  | C     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | C     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | C     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | H     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | c     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |
| 32  | h     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 144   | 47 | 82 | 15 |         |         |

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula:  $C_{18}H_{36}O_2$ ).



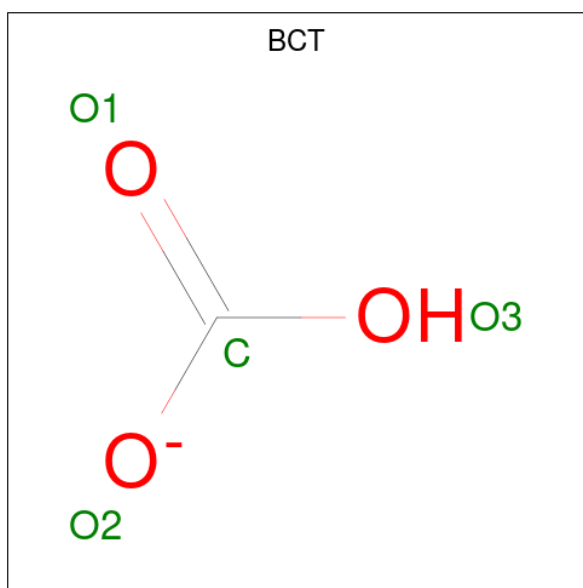
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | B     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 43    | 15 | 26 | 2 |         |         |
| 33  | B     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 34    | 12 | 20 | 2 |         |         |
| 33  | B     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | B     | 1        | Total | C  | H  |   | 0       | 0       |
|     |       |          | 47    | 16 | 31 |   |         |         |
| 33  | B     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | C     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | C     | 1        | Total | C  | H  |   | 0       | 0       |
|     |       |          | 47    | 16 | 31 |   |         |         |
| 33  | C     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | D     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 55    | 18 | 35 | 2 |         |         |
| 33  | E     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | H     | 1        | Total | C  | H  |   | 0       | 0       |
|     |       |          | 53    | 18 | 35 |   |         |         |
| 33  | I     | 1        | Total | C  | H  |   | 0       | 0       |
|     |       |          | 41    | 15 | 26 |   |         |         |
| 33  | J     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 28    | 10 | 16 | 2 |         |         |
| 33  | M     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 37    | 13 | 22 | 2 |         |         |

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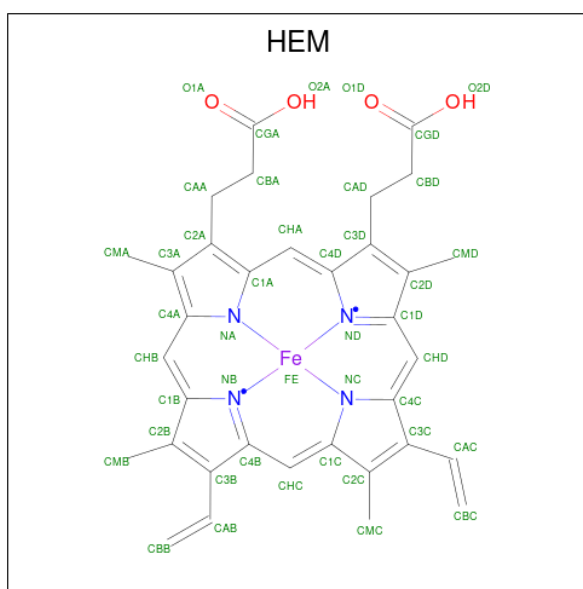
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 33  | M     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 26    | 10 | 16 |         |         |
| 33  | T     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 47    | 16 | 31 |         |         |
| 33  | T     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 44    | 15 | 29 |         |         |
| 33  | Z     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 20    | 8  | 12 |         |         |
| 33  | a     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 26    | 10 | 16 |         |         |
| 33  | a     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 28    | 10 | 16 | 2       | 0       |
| 33  | a     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 41    | 15 | 26 |         |         |
| 33  | b     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 55    | 18 | 35 | 2       | 0       |
| 33  | b     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 40    | 14 | 24 | 2       | 0       |
| 33  | b     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 55    | 18 | 35 | 2       | 0       |
| 33  | b     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 26    | 10 | 16 |         |         |
| 33  | b     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 41    | 14 | 27 |         |         |
| 33  | c     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 55    | 18 | 35 | 2       | 0       |
| 33  | d     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 43    | 15 | 26 | 2       | 0       |
| 33  | d     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 55    | 18 | 35 | 2       | 0       |
| 33  | j     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 28    | 10 | 16 | 2       | 0       |
| 33  | k     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 28    | 10 | 16 | 2       | 0       |
| 33  | l     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 53    | 18 | 35 |         |         |
| 33  | m     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 28    | 10 | 16 | 2       | 0       |
| 33  | t     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 46    | 16 | 28 | 2       | 0       |
| 33  | x     | 1        | Total | C  | H  | O       | 0       |
|     |       |          | 55    | 18 | 35 | 2       | 0       |

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



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 34  | D     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 5     | 1 | 1 | 3 |         |         |
| 34  | a     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 5     | 1 | 1 | 3 |         |         |

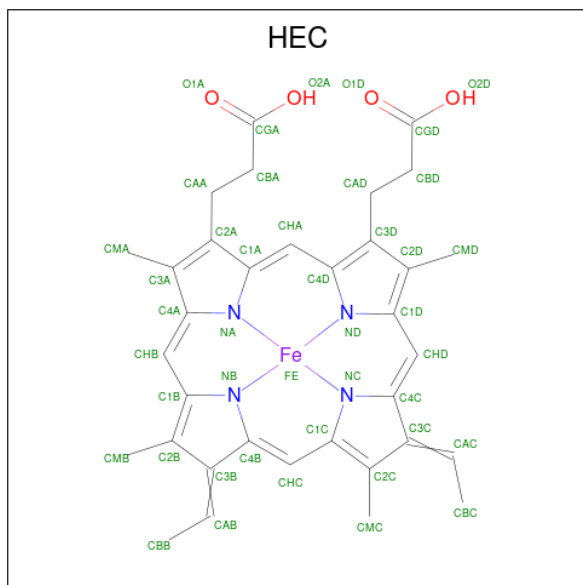
- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 35  | F     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |
| 35  | e     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |

- Molecule 36 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 36  | V     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |
| 36  | v     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 37  | A     | 149      | Total | O   | 0       | 0       |
|     |       |          | 149   | 149 |         |         |
| 37  | B     | 200      | Total | O   | 0       | 0       |
|     |       |          | 200   | 200 |         |         |
| 37  | C     | 166      | Total | O   | 0       | 0       |
|     |       |          | 166   | 166 |         |         |
| 37  | D     | 124      | Total | O   | 0       | 0       |
|     |       |          | 124   | 124 |         |         |
| 37  | E     | 24       | Total | O   | 0       | 0       |
|     |       |          | 24    | 24  |         |         |
| 37  | F     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 37  | H     | 28       | Total O<br>28 28   | 0       | 0       |
| 37  | I     | 6        | Total O<br>6 6     | 0       | 0       |
| 37  | J     | 13       | Total O<br>13 13   | 0       | 0       |
| 37  | K     | 4        | Total O<br>4 4     | 0       | 0       |
| 37  | L     | 12       | Total O<br>12 12   | 0       | 0       |
| 37  | M     | 8        | Total O<br>8 8     | 0       | 0       |
| 37  | O     | 96       | Total O<br>96 96   | 0       | 0       |
| 37  | R     | 5        | Total O<br>5 5     | 0       | 0       |
| 37  | T     | 12       | Total O<br>12 12   | 0       | 0       |
| 37  | U     | 47       | Total O<br>47 47   | 0       | 0       |
| 37  | V     | 78       | Total O<br>78 78   | 0       | 0       |
| 37  | X     | 11       | Total O<br>11 11   | 0       | 0       |
| 37  | Y     | 2        | Total O<br>2 2     | 0       | 0       |
| 37  | Z     | 7        | Total O<br>7 7     | 0       | 0       |
| 37  | a     | 131      | Total O<br>131 131 | 0       | 0       |
| 37  | b     | 207      | Total O<br>207 207 | 0       | 0       |
| 37  | c     | 162      | Total O<br>162 162 | 0       | 0       |
| 37  | d     | 123      | Total O<br>123 123 | 0       | 0       |
| 37  | e     | 29       | Total O<br>29 29   | 0       | 0       |
| 37  | f     | 7        | Total O<br>7 7     | 0       | 0       |
| 37  | h     | 22       | Total O<br>22 22   | 0       | 0       |

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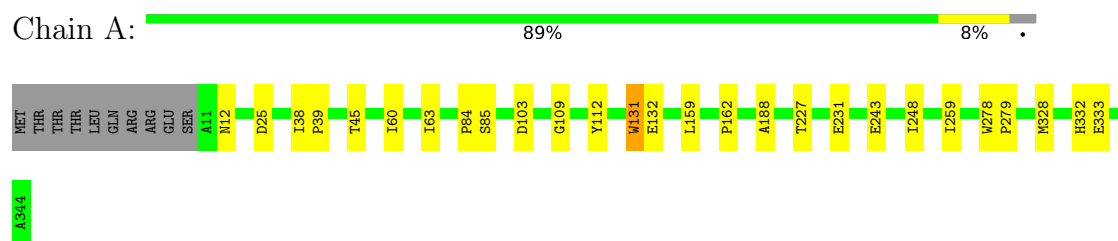
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 37  | i     | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 37  | j     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 37  | k     | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 37  | l     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 37  | m     | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 37  | o     | 104      | Total<br>104 | O<br>104 | 0       | 0       |
| 37  | r     | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 37  | t     | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 37  | u     | 68       | Total<br>68  | O<br>68  | 0       | 0       |
| 37  | v     | 59       | Total<br>59  | O<br>59  | 0       | 0       |
| 37  | x     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 37  | y     | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 37  | z     | 7        | Total<br>7   | O<br>7   | 0       | 0       |

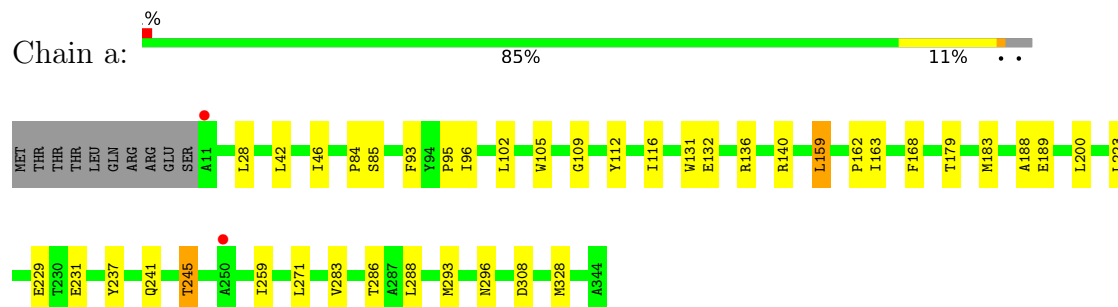
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

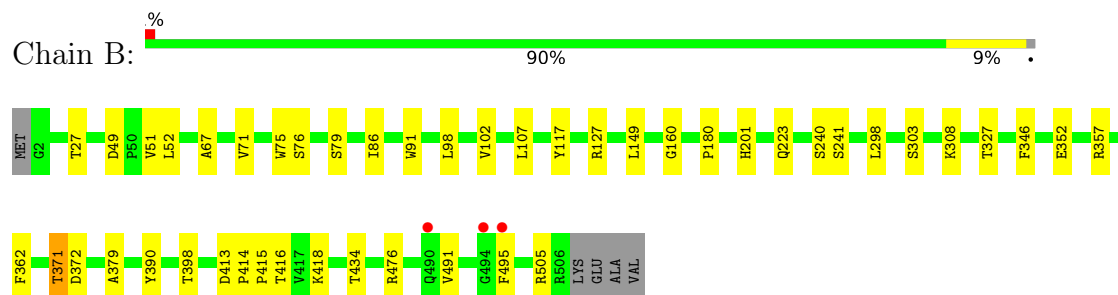
- Molecule 1: Photosystem II protein D1 1



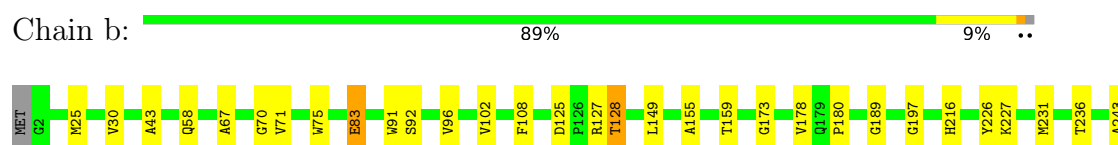
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



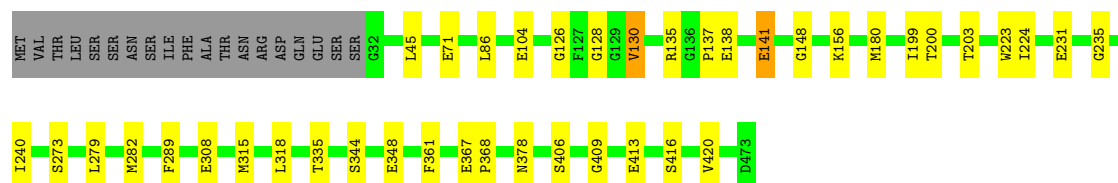
- Molecule 2: Photosystem II CP47 reaction center protein





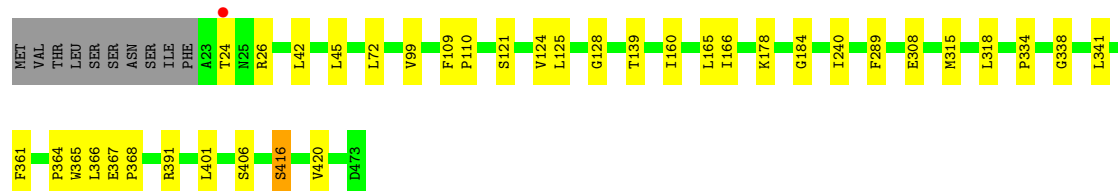
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 8% .



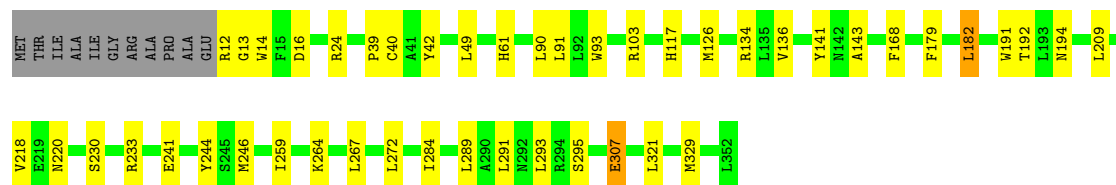
- Molecule 4: Photosystem II D2 protein

Chain D: 90% 7% .



- Molecule 4: Photosystem II D2 protein

Chain d: 84% 13% ..

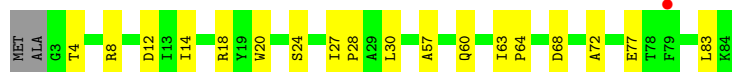
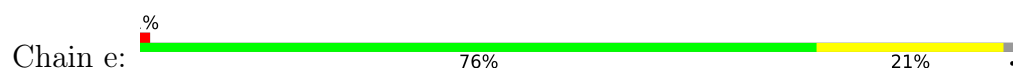


- Molecule 5: Cytochrome b559 subunit alpha

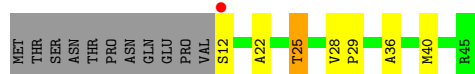
Chain E: 82% 15% .



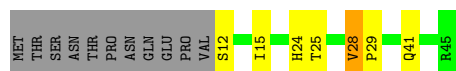
- Molecule 5: Cytochrome b559 subunit alpha



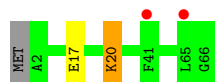
- Molecule 6: Cytochrome b559 subunit beta



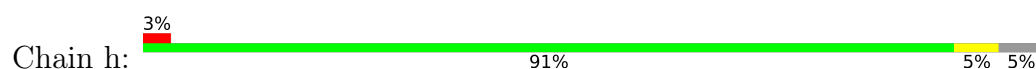
- Molecule 6: Cytochrome b559 subunit beta



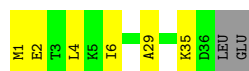
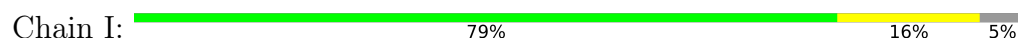
- Molecule 7: Photosystem II reaction center protein H



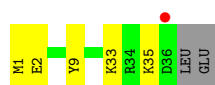
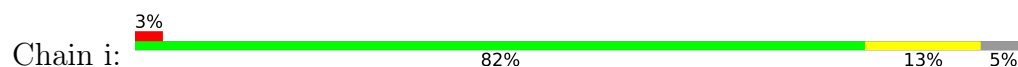
- Molecule 7: Photosystem II reaction center protein H



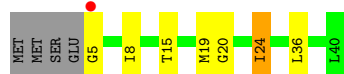
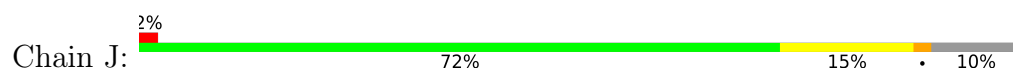
- Molecule 8: Photosystem II reaction center protein I



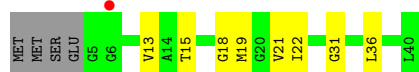
- Molecule 8: Photosystem II reaction center protein I



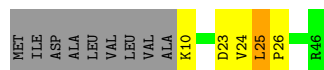
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



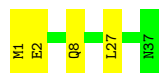
- Molecule 10: Photosystem II reaction center protein K



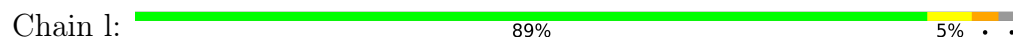
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



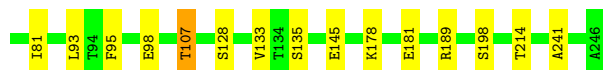
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%



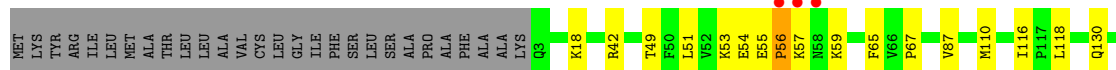
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  78% 10% 10%



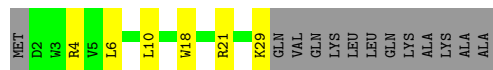
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 8% 10%



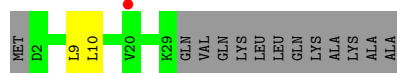
- Molecule 14: Photosystem II protein Y

Chain R:  54% 15% 32%



- Molecule 14: Photosystem II protein Y

Chain r:  63% 5% 32%



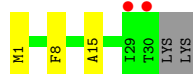
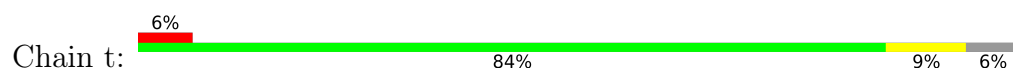
- Molecule 15: Photosystem II reaction center protein T

Chain T:  81% 12% 6%

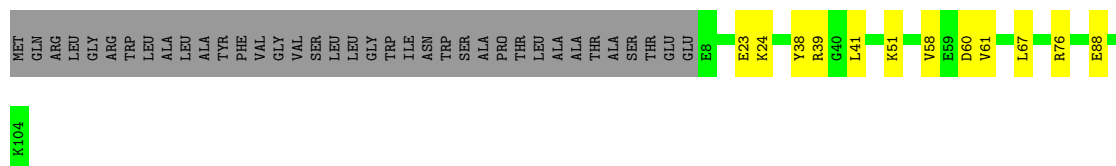


- Molecule 15: Photosystem II reaction center protein T

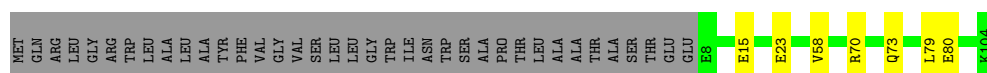




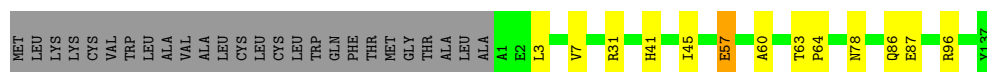
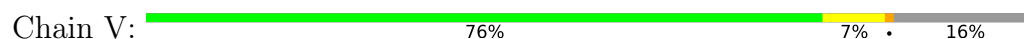
- Molecule 16: Photosystem II 12 kDa extrinsic protein



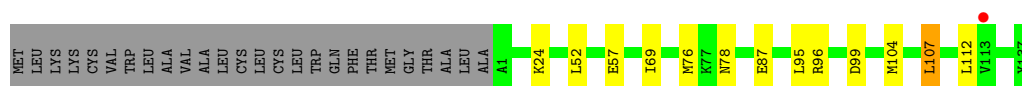
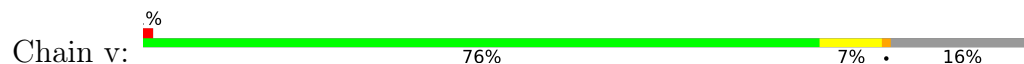
- Molecule 16: Photosystem II 12 kDa extrinsic protein



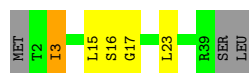
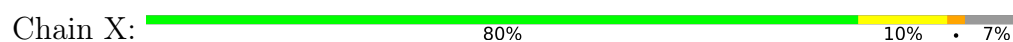
- Molecule 17: Cytochrome c-550



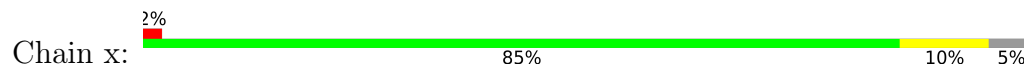
- Molecule 17: Cytochrome c-550

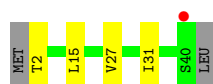


- Molecule 18: Photosystem II reaction center X protein

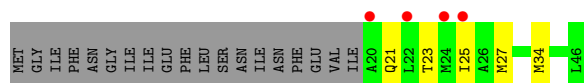


- Molecule 18: Photosystem II reaction center X protein

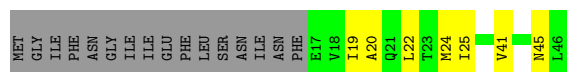




- Molecule 19: Photosystem II reaction center protein Ycf12



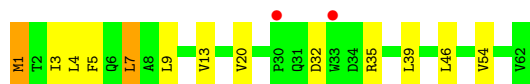
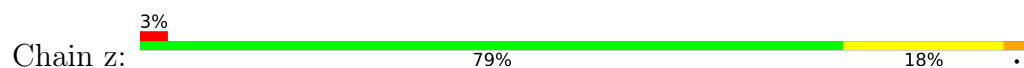
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 117.04Å 221.92Å 308.30Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 33.59 – 2.01<br>33.59 – 2.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (33.59-2.01)<br>86.9 (33.59-2.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.57 (at 2.00Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.19.2_4158                                          | Depositor        |
| R, $R_{free}$                                                           | 0.180 , 0.227<br>0.180 , 0.227                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4767 reflections (0.76%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 26.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.205                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 58.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 106128                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 43.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, DGD, BCT, PL9, CLA, HEM, CL, HEC, PHO, SQD, OEX, LMG, STE, FME, BCR, OEY, 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     | 0.52         | 0/3227      | 0.60        | 1/4397 (0.0%) |
| 1   | a     | 0.48         | 0/3224      | 0.59        | 1/4393 (0.0%) |
| 2   | B     | 0.55         | 0/4161      | 0.62        | 0/5669        |
| 2   | b     | 0.52         | 0/4118      | 0.60        | 0/5611        |
| 3   | C     | 0.53         | 0/3647      | 0.60        | 0/4965        |
| 3   | c     | 0.49         | 0/3719      | 0.59        | 0/5061        |
| 4   | D     | 0.59         | 0/2825      | 0.65        | 0/3847        |
| 4   | d     | 0.54         | 0/2834      | 0.63        | 0/3859        |
| 5   | E     | 0.46         | 0/688       | 0.53        | 0/940         |
| 5   | e     | 0.40         | 0/683       | 0.52        | 0/932         |
| 6   | F     | 0.45         | 0/284       | 0.55        | 0/387         |
| 6   | f     | 0.44         | 0/284       | 0.62        | 0/387         |
| 7   | H     | 0.56         | 0/523       | 0.58        | 0/713         |
| 7   | h     | 0.48         | 0/511       | 0.59        | 0/697         |
| 8   | I     | 0.51         | 0/293       | 0.58        | 0/396         |
| 8   | i     | 0.52         | 0/293       | 0.57        | 0/396         |
| 9   | J     | 0.39         | 0/263       | 0.55        | 0/356         |
| 9   | j     | 0.39         | 0/263       | 0.51        | 0/356         |
| 10  | K     | 0.39         | 0/303       | 0.54        | 0/416         |
| 10  | k     | 0.39         | 0/303       | 0.50        | 0/416         |
| 11  | L     | 0.56         | 0/311       | 0.59        | 0/422         |
| 11  | l     | 0.57         | 0/303       | 0.60        | 0/412         |
| 12  | M     | 0.58         | 0/249       | 0.64        | 0/341         |
| 12  | m     | 0.57         | 0/244       | 0.67        | 0/334         |
| 13  | O     | 0.52         | 0/1904      | 0.61        | 0/2585        |
| 13  | o     | 0.53         | 0/1905      | 0.60        | 0/2583        |
| 14  | R     | 0.33         | 0/227       | 0.42        | 0/313         |
| 14  | r     | 0.28         | 0/227       | 0.38        | 0/313         |
| 15  | T     | 0.59         | 0/257       | 0.64        | 0/349         |
| 15  | t     | 0.61         | 0/255       | 0.55        | 0/346         |
| 16  | U     | 0.46         | 0/785       | 0.56        | 0/1064        |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 16  | u     | 0.49         | 0/785   | 0.59        | 0/1064         |
| 17  | V     | 0.51         | 0/1085  | 0.62        | 0/1473         |
| 17  | v     | 0.48         | 0/1085  | 0.55        | 0/1473         |
| 18  | X     | 0.41         | 0/284   | 0.48        | 0/384          |
| 18  | x     | 0.38         | 0/289   | 0.47        | 0/391          |
| 19  | Y     | 0.38         | 0/197   | 0.45        | 0/264          |
| 19  | y     | 0.35         | 0/219   | 0.47        | 0/294          |
| 20  | Z     | 0.35         | 0/490   | 0.49        | 0/669          |
| 20  | z     | 0.27         | 0/488   | 0.39        | 0/666          |
| All | All   | 0.51         | 0/44035 | 0.59        | 2/59934 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 17  | V     | 0                   | 1                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | a     | 131 | TRP  | CA-CB-CG | -5.19 | 103.73      | 113.60   |
| 1   | A     | 131 | TRP  | CA-CB-CG | -5.02 | 104.06      | 113.60   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 17  | V     | 63  | THR  | Peptide |

## 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     | 3113  | 2985     | 2963     | 15      | 0            |
| 1   | a     | 3110  | 2976     | 2954     | 22      | 0            |
| 2   | B     | 4005  | 3873     | 3867     | 31      | 0            |
| 2   | b     | 3978  | 3836     | 3836     | 32      | 0            |
| 3   | C     | 3509  | 3432     | 3409     | 22      | 0            |
| 3   | c     | 3583  | 3503     | 3492     | 27      | 0            |
| 4   | D     | 2731  | 2637     | 2637     | 17      | 0            |
| 4   | d     | 2737  | 2643     | 2643     | 36      | 0            |
| 5   | E     | 666   | 651      | 651      | 8       | 0            |
| 5   | e     | 664   | 648      | 648      | 10      | 0            |
| 6   | F     | 275   | 282      | 282      | 5       | 0            |
| 6   | f     | 275   | 282      | 282      | 7       | 0            |
| 7   | H     | 510   | 532      | 532      | 1       | 0            |
| 7   | h     | 498   | 518      | 518      | 2       | 0            |
| 8   | I     | 296   | 311      | 311      | 2       | 0            |
| 8   | i     | 296   | 311      | 311      | 2       | 0            |
| 9   | J     | 257   | 268      | 268      | 5       | 0            |
| 9   | j     | 257   | 268      | 268      | 4       | 0            |
| 10  | K     | 293   | 305      | 305      | 3       | 0            |
| 10  | k     | 293   | 305      | 305      | 6       | 0            |
| 11  | L     | 304   | 316      | 316      | 3       | 0            |
| 11  | l     | 296   | 304      | 304      | 1       | 0            |
| 12  | M     | 256   | 269      | 269      | 5       | 0            |
| 12  | m     | 251   | 267      | 267      | 3       | 0            |
| 13  | O     | 1870  | 1830     | 1830     | 22      | 0            |
| 13  | o     | 1874  | 1846     | 1846     | 16      | 0            |
| 14  | R     | 221   | 238      | 238      | 2       | 0            |
| 14  | r     | 221   | 238      | 238      | 0       | 0            |
| 15  | T     | 258   | 261      | 261      | 2       | 0            |
| 15  | t     | 256   | 256      | 256      | 4       | 0            |
| 16  | U     | 774   | 773      | 773      | 8       | 0            |
| 16  | u     | 774   | 773      | 773      | 3       | 0            |
| 17  | V     | 1064  | 1071     | 1073     | 5       | 0            |
| 17  | v     | 1064  | 1071     | 1073     | 8       | 0            |
| 18  | X     | 281   | 312      | 312      | 4       | 0            |
| 18  | x     | 286   | 316      | 314      | 2       | 0            |
| 19  | Y     | 196   | 217      | 217      | 3       | 0            |
| 19  | y     | 218   | 241      | 241      | 2       | 0            |
| 20  | Z     | 479   | 516      | 516      | 8       | 0            |
| 20  | z     | 477   | 509      | 509      | 7       | 0            |
| 21  | A     | 11    | 0        | 0        | 1       | 0            |
| 21  | a     | 11    | 0        | 0        | 1       | 0            |
| 22  | A     | 10    | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | a     | 10    | 0        | 0        | 0       | 0            |
| 23  | A     | 1     | 0        | 0        | 0       | 0            |
| 23  | a     | 1     | 0        | 0        | 0       | 0            |
| 24  | A     | 249   | 264      | 264      | 5       | 0            |
| 24  | B     | 1035  | 1139     | 1139     | 19      | 0            |
| 24  | C     | 839   | 922      | 922      | 6       | 0            |
| 24  | D     | 130   | 144      | 144      | 3       | 0            |
| 24  | a     | 195   | 216      | 216      | 0       | 0            |
| 24  | b     | 1035  | 1139     | 1139     | 13      | 0            |
| 24  | c     | 839   | 919      | 919      | 12      | 0            |
| 24  | d     | 195   | 216      | 216      | 1       | 0            |
| 25  | A     | 128   | 148      | 148      | 1       | 0            |
| 25  | a     | 64    | 74       | 74       | 0       | 0            |
| 25  | d     | 64    | 74       | 74       | 1       | 0            |
| 26  | A     | 40    | 56       | 56       | 0       | 0            |
| 26  | B     | 120   | 168      | 168      | 4       | 0            |
| 26  | C     | 80    | 112      | 112      | 0       | 0            |
| 26  | D     | 40    | 56       | 56       | 1       | 0            |
| 26  | H     | 40    | 56       | 56       | 1       | 0            |
| 26  | K     | 40    | 56       | 56       | 0       | 0            |
| 26  | T     | 40    | 56       | 56       | 1       | 0            |
| 26  | Y     | 40    | 56       | 56       | 1       | 0            |
| 26  | a     | 40    | 56       | 56       | 1       | 0            |
| 26  | b     | 120   | 168      | 168      | 2       | 0            |
| 26  | c     | 80    | 112      | 112      | 1       | 0            |
| 26  | d     | 40    | 56       | 56       | 2       | 0            |
| 26  | k     | 80    | 112      | 112      | 0       | 0            |
| 26  | t     | 40    | 56       | 56       | 3       | 0            |
| 26  | x     | 40    | 56       | 56       | 0       | 0            |
| 27  | A     | 2     | 0        | 0        | 0       | 0            |
| 27  | a     | 2     | 0        | 0        | 0       | 0            |
| 28  | A     | 55    | 80       | 80       | 2       | 0            |
| 28  | D     | 55    | 80       | 80       | 0       | 0            |
| 28  | a     | 55    | 80       | 80       | 2       | 0            |
| 28  | d     | 55    | 80       | 80       | 0       | 0            |
| 29  | A     | 48    | 66       | 66       | 0       | 0            |
| 29  | C     | 48    | 66       | 66       | 0       | 0            |
| 29  | D     | 112   | 157      | 157      | 2       | 0            |
| 29  | M     | 51    | 72       | 72       | 1       | 0            |
| 29  | a     | 55    | 86       | 86       | 5       | 0            |
| 29  | b     | 106   | 158      | 158      | 1       | 0            |
| 29  | c     | 134   | 181      | 181      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | d     | 44    | 58       | 58       | 0       | 0            |
| 30  | A     | 47    | 67       | 67       | 1       | 0            |
| 30  | B     | 98    | 148      | 148      | 1       | 0            |
| 30  | D     | 49    | 74       | 74       | 3       | 0            |
| 30  | E     | 49    | 74       | 74       | 1       | 0            |
| 30  | d     | 137   | 199      | 199      | 5       | 0            |
| 30  | e     | 42    | 57       | 57       | 0       | 0            |
| 30  | l     | 49    | 74       | 74       | 1       | 0            |
| 31  | A     | 91    | 136      | 134      | 2       | 0            |
| 31  | B     | 54    | 78       | 76       | 2       | 0            |
| 31  | D     | 36    | 46       | 45       | 1       | 0            |
| 31  | a     | 90    | 134      | 132      | 0       | 0            |
| 31  | b     | 49    | 65       | 64       | 1       | 0            |
| 31  | f     | 41    | 48       | 47       | 1       | 0            |
| 32  | A     | 66    | 96       | 96       | 3       | 0            |
| 32  | C     | 186   | 246      | 245      | 0       | 0            |
| 32  | H     | 62    | 82       | 81       | 0       | 0            |
| 32  | c     | 186   | 246      | 244      | 2       | 0            |
| 32  | h     | 62    | 82       | 79       | 0       | 0            |
| 33  | B     | 71    | 109      | 109      | 3       | 0            |
| 33  | C     | 40    | 63       | 63       | 0       | 0            |
| 33  | D     | 20    | 35       | 35       | 6       | 0            |
| 33  | E     | 12    | 16       | 16       | 1       | 0            |
| 33  | H     | 18    | 35       | 35       | 1       | 0            |
| 33  | I     | 15    | 26       | 26       | 0       | 0            |
| 33  | J     | 12    | 16       | 16       | 0       | 0            |
| 33  | M     | 25    | 38       | 38       | 1       | 0            |
| 33  | T     | 31    | 60       | 60       | 1       | 0            |
| 33  | Z     | 8     | 12       | 12       | 0       | 0            |
| 33  | a     | 37    | 58       | 58       | 1       | 0            |
| 33  | b     | 80    | 137      | 137      | 4       | 0            |
| 33  | c     | 20    | 35       | 35       | 1       | 0            |
| 33  | d     | 37    | 61       | 61       | 1       | 0            |
| 33  | j     | 12    | 16       | 16       | 0       | 0            |
| 33  | k     | 12    | 16       | 16       | 0       | 0            |
| 33  | l     | 18    | 35       | 35       | 1       | 0            |
| 33  | m     | 12    | 16       | 16       | 1       | 0            |
| 33  | t     | 18    | 28       | 28       | 2       | 0            |
| 33  | x     | 20    | 35       | 35       | 0       | 0            |
| 34  | D     | 4     | 1        | 1        | 1       | 0            |
| 34  | a     | 4     | 1        | 1        | 0       | 0            |
| 35  | F     | 43    | 30       | 30       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | e     | 43    | 30       | 30       | 4       | 0            |
| 36  | V     | 43    | 30       | 30       | 1       | 0            |
| 36  | v     | 43    | 30       | 30       | 1       | 0            |
| 37  | A     | 149   | 0        | 0        | 3       | 0            |
| 37  | B     | 200   | 0        | 0        | 9       | 0            |
| 37  | C     | 166   | 0        | 0        | 4       | 0            |
| 37  | D     | 124   | 0        | 0        | 2       | 0            |
| 37  | E     | 24    | 0        | 0        | 1       | 0            |
| 37  | F     | 10    | 0        | 0        | 1       | 0            |
| 37  | H     | 28    | 0        | 0        | 0       | 0            |
| 37  | I     | 6     | 0        | 0        | 0       | 0            |
| 37  | J     | 13    | 0        | 0        | 2       | 0            |
| 37  | K     | 4     | 0        | 0        | 0       | 0            |
| 37  | L     | 12    | 0        | 0        | 1       | 0            |
| 37  | M     | 8     | 0        | 0        | 3       | 0            |
| 37  | O     | 96    | 0        | 0        | 7       | 0            |
| 37  | R     | 5     | 0        | 0        | 0       | 0            |
| 37  | T     | 12    | 0        | 0        | 1       | 0            |
| 37  | U     | 47    | 0        | 0        | 4       | 0            |
| 37  | V     | 78    | 0        | 0        | 2       | 0            |
| 37  | X     | 11    | 0        | 0        | 0       | 0            |
| 37  | Y     | 2     | 0        | 0        | 0       | 0            |
| 37  | Z     | 7     | 0        | 0        | 0       | 0            |
| 37  | a     | 131   | 0        | 0        | 0       | 0            |
| 37  | b     | 207   | 0        | 0        | 4       | 0            |
| 37  | c     | 162   | 0        | 0        | 6       | 0            |
| 37  | d     | 123   | 0        | 0        | 10      | 0            |
| 37  | e     | 29    | 0        | 0        | 0       | 0            |
| 37  | f     | 7     | 0        | 0        | 1       | 0            |
| 37  | h     | 22    | 0        | 0        | 0       | 0            |
| 37  | i     | 7     | 0        | 0        | 0       | 0            |
| 37  | j     | 8     | 0        | 0        | 1       | 0            |
| 37  | k     | 11    | 0        | 0        | 1       | 0            |
| 37  | l     | 8     | 0        | 0        | 0       | 0            |
| 37  | m     | 9     | 0        | 0        | 1       | 0            |
| 37  | o     | 104   | 0        | 0        | 6       | 0            |
| 37  | r     | 5     | 0        | 0        | 0       | 0            |
| 37  | t     | 9     | 0        | 0        | 0       | 0            |
| 37  | u     | 68    | 0        | 0        | 1       | 0            |
| 37  | v     | 59    | 0        | 0        | 1       | 0            |
| 37  | x     | 8     | 0        | 0        | 0       | 0            |
| 37  | y     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37  | z     | 7     | 0        | 0        | 1       | 0            |
| All | All   | 53366 | 52762    | 52664    | 415     | 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 4.

All (415) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:315:MET:SD     | 37:c:746:HOH:O     | 2.15                     | 1.04              |
| 13:o:54:GLU:HA     | 37:o:302:HOH:O     | 1.61                     | 0.98              |
| 4:d:307:GLU:OE1    | 37:d:501:HOH:O     | 1.83                     | 0.94              |
| 12:M:5:GLN:O       | 37:M:201:HOH:O     | 1.84                     | 0.94              |
| 3:C:231:GLU:OE1    | 37:C:601:HOH:O     | 1.86                     | 0.93              |
| 3:C:378:ASN:OD1    | 37:C:602:HOH:O     | 1.90                     | 0.88              |
| 16:U:88:GLU:OE2    | 37:U:201:HOH:O     | 1.90                     | 0.88              |
| 2:b:372:ASP:OD2    | 37:b:701:HOH:O     | 1.90                     | 0.88              |
| 1:A:25:ASP:OD1     | 37:A:701:HOH:O     | 1.92                     | 0.88              |
| 33:B:624:STE:O2    | 37:B:701:HOH:O     | 1.90                     | 0.88              |
| 10:k:19:ASP:OD1    | 37:k:201:HOH:O     | 1.93                     | 0.87              |
| 4:d:13:GLY:N       | 37:d:502:HOH:O     | 2.02                     | 0.87              |
| 13:o:55:GLU:N      | 37:o:302:HOH:O     | 2.07                     | 0.86              |
| 33:M:102:STE:O1    | 37:M:202:HOH:O     | 1.93                     | 0.85              |
| 13:o:54:GLU:CA     | 37:o:302:HOH:O     | 2.22                     | 0.85              |
| 3:c:391[A]:ARG:NE  | 37:c:601:HOH:O     | 2.14                     | 0.81              |
| 33:B:625:STE:O1    | 37:B:702:HOH:O     | 1.98                     | 0.81              |
| 13:O:98:GLU:OE1    | 37:O:301:HOH:O     | 1.99                     | 0.80              |
| 13:o:54:GLU:C      | 37:o:302:HOH:O     | 2.24                     | 0.79              |
| 2:B:223:GLN:OE1    | 37:B:703:HOH:O     | 2.02                     | 0.77              |
| 9:j:36:LEU:O       | 37:j:201:HOH:O     | 2.02                     | 0.76              |
| 13:O:37:THR:HA     | 37:O:310:HOH:O     | 1.86                     | 0.75              |
| 11:L:8:GLN:OE1     | 37:L:101:HOH:O     | 2.04                     | 0.74              |
| 16:U:76:ARG:NE     | 37:U:202:HOH:O     | 1.96                     | 0.74              |
| 2:B:413:ASP:OD1    | 37:B:705:HOH:O     | 2.06                     | 0.74              |
| 31:b:620:SQD:O9    | 37:b:703:HOH:O     | 2.07                     | 0.73              |
| 21:A:601[B]:OEY:O5 | 21:A:601[B]:OEY:O6 | 2.06                     | 0.73              |
| 3:c:391[A]:ARG:NH1 | 37:c:603:HOH:O     | 2.22                     | 0.72              |
| 17:V:87:GLU:OE2    | 37:V:301:HOH:O     | 2.09                     | 0.71              |
| 9:J:36:LEU:O       | 37:J:201:HOH:O     | 2.09                     | 0.70              |
| 5:e:8:ARG:NH1      | 5:e:12:ASP:OD2     | 2.23                     | 0.70              |
| 12:m:30:GLU:OE2    | 37:m:201:HOH:O     | 2.10                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:T:30:THR:OG1    | 37:T:201:HOH:O     | 2.09                     | 0.69              |
| 3:c:391[B]:ARG:NH1 | 37:c:605:HOH:O     | 2.25                     | 0.69              |
| 5:e:57:ALA:H       | 5:e:60:GLN:HE21    | 1.40                     | 0.69              |
| 2:B:352:GLU:OE1    | 37:B:706:HOH:O     | 2.11                     | 0.69              |
| 17:v:57:GLU:OE2    | 37:v:301:HOH:O     | 2.11                     | 0.67              |
| 2:B:352:GLU:OE1    | 37:B:707:HOH:O     | 2.12                     | 0.67              |
| 3:C:148:GLY:O      | 3:C:156:LYS:NZ     | 2.27                     | 0.67              |
| 4:d:12:ARG:CA      | 37:d:502:HOH:O     | 2.42                     | 0.66              |
| 16:u:80:GLU:OE1    | 37:u:201:HOH:O     | 2.13                     | 0.66              |
| 33:E:102:STE:O1    | 37:E:201:HOH:O     | 2.13                     | 0.66              |
| 28:A:612:PL9:H361  | 6:F:25:THR:HG21    | 1.78                     | 0.66              |
| 9:J:5:GLY:N        | 37:J:202:HOH:O     | 2.29                     | 0.65              |
| 31:B:623:SQD:O2    | 37:B:708:HOH:O     | 2.15                     | 0.64              |
| 4:d:42:TYR:CZ      | 6:f:25:THR:HG22    | 2.32                     | 0.64              |
| 6:f:28:VAL:HG22    | 6:f:29:PRO:HD3     | 1.79                     | 0.63              |
| 1:A:188[A]:ALA:HB2 | 1:A:328[A]:MET:HB2 | 1.81                     | 0.63              |
| 35:F:101:HEM:HBC2  | 35:F:101:HEM:HHD   | 1.80                     | 0.63              |
| 35:e:101:HEM:HHC   | 35:e:101:HEM:HBB2  | 1.80                     | 0.63              |
| 2:B:371:THR:HG23   | 2:B:372:ASP:O      | 2.00                     | 0.62              |
| 5:E:45:ASP:OD2     | 14:R:4:ARG:NH2     | 2.27                     | 0.62              |
| 4:d:12:ARG:HA      | 37:d:502:HOH:O     | 2.00                     | 0.62              |
| 2:b:491:VAL:HG12   | 4:d:136:VAL:HG13   | 1.83                     | 0.61              |
| 26:t:101:BCR:H321  | 26:t:101:BCR:HC8   | 1.84                     | 0.60              |
| 24:c:504:CLA:H91   | 24:c:508:CLA:H172  | 1.84                     | 0.60              |
| 13:o:194:LYS:NZ    | 37:o:301:HOH:O     | 1.96                     | 0.60              |
| 2:B:75:TRP:HB3     | 29:a:618:LMG:HC91  | 1.84                     | 0.59              |
| 3:c:315:MET:HE3    | 3:c:365:TRP:HZ3    | 1.68                     | 0.59              |
| 3:C:141:GLU:OE2    | 37:C:603:HOH:O     | 2.17                     | 0.59              |
| 13:O:27:ARG:O      | 13:O:27:ARG:HG2    | 2.02                     | 0.59              |
| 3:c:391[B]:ARG:NE  | 3:c:391[B]:ARG:HA  | 2.16                     | 0.59              |
| 4:d:126:MET:HE3    | 4:d:143:ALA:O      | 2.01                     | 0.59              |
| 37:A:746:HOH:O     | 13:O:107:THR:HG22  | 2.01                     | 0.59              |
| 3:c:315:MET:HE3    | 3:c:365:TRP:CZ3    | 2.38                     | 0.59              |
| 24:c:508:CLA:H191  | 32:c:517:DGD:HA91  | 1.85                     | 0.58              |
| 29:D:406:LMG:H112  | 37:D:562:HOH:O     | 2.03                     | 0.58              |
| 20:z:1:MET:HB3     | 20:z:4:LEU:HB3     | 1.85                     | 0.58              |
| 13:O:6:THR:HG22    | 13:O:9:ASP:OD2     | 2.03                     | 0.58              |
| 24:b:615:CLA:HHC   | 24:b:615:CLA:HBB1  | 1.85                     | 0.58              |
| 4:d:103:ARG:NH2    | 37:d:509:HOH:O     | 2.37                     | 0.58              |
| 24:B:607:CLA:H193  | 11:L:27:LEU:HD11   | 1.86                     | 0.58              |
| 4:d:230:SER:HB2    | 37:d:561:HOH:O     | 2.04                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:189[B]:GLU:OE1 | 21:a:601[B]:OEY:O6 | 2.23                     | 0.57              |
| 16:U:38:TYR:HB2    | 16:U:41:LEU:HD12   | 1.85                     | 0.57              |
| 24:c:501:CLA:H192  | 24:c:507:CLA:HBB1  | 1.86                     | 0.56              |
| 8:i:33:LYS:O       | 8:i:35:LYS:NZ      | 2.39                     | 0.56              |
| 4:D:264:LYS:NZ     | 34:D:401:BCT:O3    | 2.38                     | 0.56              |
| 2:b:102:VAL:HG11   | 24:b:606:CLA:H142  | 1.88                     | 0.56              |
| 16:U:60:ASP:OD2    | 37:U:203:HOH:O     | 2.18                     | 0.56              |
| 19:Y:23:THR:HG22   | 19:Y:27:MET:HE3    | 1.88                     | 0.56              |
| 1:A:103:ASP:OD1    | 32:A:618:DGD:O2E   | 2.24                     | 0.56              |
| 1:A:63[B]:ILE:HB   | 3:C:335:THR:HG21   | 1.88                     | 0.56              |
| 6:f:12:SER:N       | 37:f:201:HOH:O     | 2.39                     | 0.56              |
| 1:a:188[B]:ALA:HB2 | 1:a:328[B]:MET:HB2 | 1.86                     | 0.55              |
| 1:A:227:THR:HB     | 1:A:231:GLU:HG3    | 1.89                     | 0.55              |
| 20:Z:51:VAL:O      | 20:Z:54:VAL:O      | 2.23                     | 0.55              |
| 16:U:58:VAL:O      | 16:U:61:VAL:HG22   | 2.05                     | 0.55              |
| 30:D:408:LHG:H321  | 15:T:21:ILE:HD11   | 1.89                     | 0.55              |
| 16:U:39:ARG:NH2    | 17:V:60:ALA:O      | 2.39                     | 0.54              |
| 30:A:615:LHG:H151  | 31:A:616:SQD:H272  | 1.88                     | 0.54              |
| 3:c:315:MET:CE     | 3:c:366:LEU:HD13   | 2.38                     | 0.53              |
| 17:V:57:GLU:OE2    | 37:V:302:HOH:O     | 2.19                     | 0.53              |
| 5:e:27:ILE:HB      | 5:e:28:PRO:HD3     | 1.90                     | 0.53              |
| 3:C:406:SER:HA     | 3:C:420:VAL:HG23   | 1.91                     | 0.53              |
| 2:b:127:ARG:NH2    | 7:h:18:TYR:O       | 2.39                     | 0.53              |
| 1:a:179[A]:THR:O   | 1:a:183[A]:MET:HG3 | 2.09                     | 0.53              |
| 36:V:201:HEC:HMC1  | 36:V:201:HEC:HBC3  | 1.90                     | 0.53              |
| 20:Z:55:GLY:HA2    | 20:Z:58:ASN:HB3    | 1.91                     | 0.53              |
| 2:b:476:ARG:HD2    | 37:b:745:HOH:O     | 2.09                     | 0.53              |
| 12:M:6:LEU:HA      | 37:M:201:HOH:O     | 2.08                     | 0.53              |
| 4:D:191:TRP:CE3    | 4:D:289:LEU:HD11   | 2.44                     | 0.52              |
| 30:d:407:LHG:H111  | 30:l:101:LHG:H102  | 1.90                     | 0.52              |
| 6:f:24:HIS:O       | 6:f:28:VAL:HG13    | 2.09                     | 0.52              |
| 2:B:414:PRO:O      | 2:B:418:LYS:HG3    | 2.09                     | 0.52              |
| 10:k:26:PRO:O      | 10:k:29:PRO:HD2    | 2.09                     | 0.52              |
| 29:a:618:LMG:HC92  | 29:a:618:LMG:O9    | 2.09                     | 0.52              |
| 15:t:15:ALA:HB2    | 26:t:101:BCR:H14C  | 1.91                     | 0.52              |
| 2:B:117:TYR:HA     | 11:L:1:MET:HE1     | 1.91                     | 0.52              |
| 4:d:91:LEU:O       | 37:d:503:HOH:O     | 2.19                     | 0.52              |
| 3:c:178:LYS:NZ     | 3:c:184:GLY:O      | 2.42                     | 0.52              |
| 2:B:303:SER:OG     | 37:B:711:HOH:O     | 2.19                     | 0.52              |
| 2:B:491:VAL:HG12   | 4:D:136:VAL:HG13   | 1.92                     | 0.52              |
| 8:I:29:ALA:O       | 8:I:35:LYS:HG2     | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:30:VAL:HG12   | 24:b:605:CLA:HHD  | 1.92                     | 0.51              |
| 4:d:241:GLU:CD    | 4:d:241:GLU:H     | 2.18                     | 0.51              |
| 2:B:27:THR:HG22   | 2:B:107:LEU:HD13  | 1.92                     | 0.51              |
| 1:a:102:LEU:HB2   | 29:a:618:LMG:H111 | 1.92                     | 0.51              |
| 17:v:76:MET:HE2   | 17:v:112:LEU:HD22 | 1.93                     | 0.51              |
| 2:b:348:ASN:HB3   | 2:b:354:LEU:HD11  | 1.92                     | 0.51              |
| 4:d:246:MET:HE3   | 4:d:264:LYS:HG2   | 1.93                     | 0.51              |
| 17:v:104:MET:HA   | 17:v:107:LEU:HD22 | 1.93                     | 0.51              |
| 2:b:492:GLU:OE2   | 2:b:495:PHE:CE1   | 2.64                     | 0.51              |
| 4:d:267:LEU:C     | 4:d:267:LEU:HD23  | 2.36                     | 0.51              |
| 3:c:406:SER:HA    | 3:c:420:VAL:HG23  | 1.91                     | 0.51              |
| 20:z:3:ILE:HG22   | 20:z:7:LEU:HD23   | 1.92                     | 0.50              |
| 4:D:209:LEU:HD23  | 4:D:209:LEU:C     | 2.36                     | 0.50              |
| 3:c:391[B]:ARG:CZ | 37:c:605:HOH:O    | 2.60                     | 0.50              |
| 13:O:145:GLU:HG2  | 37:O:330:HOH:O    | 2.11                     | 0.50              |
| 37:A:807:HOH:O    | 13:O:107:THR:HG21 | 2.10                     | 0.50              |
| 6:F:12:SER:N      | 37:F:202:HOH:O    | 2.44                     | 0.50              |
| 3:C:45:LEU:HD22   | 3:C:138:GLU:HG2   | 1.93                     | 0.50              |
| 2:B:149[B]:LEU:HG | 24:B:604:CLA:H18  | 1.94                     | 0.50              |
| 9:J:15:THR:HG22   | 9:J:19:MET:HE2    | 1.91                     | 0.50              |
| 26:T:101:BCR:H321 | 26:T:101:BCR:HC8  | 1.92                     | 0.50              |
| 2:b:505:ARG:HG3   | 2:b:506:ARG:N     | 2.27                     | 0.50              |
| 12:M:8:LEU:HD11   | 33:T:103:STE:H141 | 1.94                     | 0.50              |
| 2:b:492:GLU:OE2   | 2:b:495:PHE:CD1   | 2.64                     | 0.49              |
| 5:e:14:ILE:O      | 5:e:20:TRP:NE1    | 2.44                     | 0.49              |
| 37:C:683:HOH:O    | 4:D:230:SER:HB2   | 2.12                     | 0.49              |
| 25:A:607:PHO:HBC3 | 4:D:279:LEU:HD22  | 1.94                     | 0.49              |
| 4:d:42:TYR:CE1    | 6:f:25:THR:HG22   | 2.47                     | 0.49              |
| 24:B:610:CLA:HHC  | 24:B:610:CLA:CBB  | 2.43                     | 0.49              |
| 26:b:618:BCR:H331 | 26:b:618:BCR:C8   | 2.42                     | 0.49              |
| 20:Z:29:SER:HB3   | 20:Z:31:GLN:HE21  | 1.77                     | 0.48              |
| 2:b:159:THR:O     | 2:b:180:PRO:HB3   | 2.13                     | 0.48              |
| 33:D:411:STE:H121 | 33:D:411:STE:H92  | 1.67                     | 0.48              |
| 2:b:91:TRP:HE1    | 33:b:622:STE:H111 | 1.77                     | 0.48              |
| 24:b:615:CLA:H2   | 24:b:616:CLA:HBB2 | 1.96                     | 0.48              |
| 35:e:101:HEM:HMC1 | 35:e:101:HEM:HBC2 | 1.94                     | 0.48              |
| 2:B:102:VAL:HA    | 26:B:618:BCR:C40  | 2.44                     | 0.48              |
| 4:D:103:ARG:HH21  | 5:E:77:GLU:HG3    | 1.77                     | 0.48              |
| 24:b:602:CLA:H43  | 7:h:45:ILE:HG22   | 1.94                     | 0.48              |
| 2:b:226:TYR:HA    | 2:b:231:MET:HG3   | 1.94                     | 0.48              |
| 3:c:166:ILE:HG21  | 24:c:512:CLA:H202 | 1.96                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:t:8:PHE:CE2     | 33:t:102:STE:H151 | 2.49                     | 0.48              |
| 26:D:404:BCR:H392  | 26:D:404:BCR:H23C | 1.95                     | 0.48              |
| 13:O:56:PRO:O      | 13:O:58:ASN:N     | 2.44                     | 0.48              |
| 5:e:20:TRP:O       | 5:e:24:SER:OG     | 2.22                     | 0.48              |
| 1:a:84:PRO:HA      | 1:a:112:TYR:CG    | 2.49                     | 0.47              |
| 13:O:78:LEU:HB3    | 13:O:81:ILE:HD11  | 1.95                     | 0.47              |
| 1:a:237:TYR:HB2    | 1:a:245:THR:HG21  | 1.96                     | 0.47              |
| 4:D:85:MET:HE1     | 5:E:72:ALA:HB2    | 1.96                     | 0.47              |
| 4:d:272:LEU:C      | 4:d:272:LEU:HD23  | 2.40                     | 0.47              |
| 3:C:135:ARG:O      | 3:C:135:ARG:HD3   | 2.14                     | 0.47              |
| 9:j:18:GLY:O       | 9:j:22:ILE:HD13   | 2.15                     | 0.47              |
| 10:K:24:VAL:HG13   | 19:Y:25:ILE:HD13  | 1.96                     | 0.47              |
| 4:d:194:ASN:HA     | 4:d:295:SER:OG    | 2.14                     | 0.47              |
| 2:B:51:VAL:HG13    | 2:B:308:LYS:HB2   | 1.96                     | 0.47              |
| 3:C:203:THR:O      | 3:C:235:GLY:HA3   | 2.15                     | 0.47              |
| 2:b:461:LEU:HD21   | 4:d:284:ILE:HD11  | 1.96                     | 0.47              |
| 24:b:613:CLA:H172  | 30:d:407:LHG:H212 | 1.96                     | 0.47              |
| 4:d:61:HIS:CE1     | 4:d:168:PHE:CE1   | 3.03                     | 0.47              |
| 5:e:30:LEU:HD11    | 35:e:101:HEM:CBB  | 2.45                     | 0.47              |
| 4:d:24:ARG:O       | 37:d:504:HOH:O    | 2.20                     | 0.47              |
| 24:D:403:CLA:H141  | 18:X:15:LEU:HD13  | 1.96                     | 0.47              |
| 2:B:160:GLY:HA3    | 2:B:180:PRO:HB3   | 1.97                     | 0.47              |
| 4:d:14:TRP:N       | 37:d:511:HOH:O    | 2.48                     | 0.47              |
| 17:v:99:ASP:N      | 17:v:99:ASP:OD1   | 2.47                     | 0.47              |
| 19:y:20:ALA:O      | 19:y:24:MET:HG2   | 2.14                     | 0.46              |
| 2:B:414:PRO:N      | 2:B:415:PRO:HD2   | 2.29                     | 0.46              |
| 5:E:68:ASP:O       | 5:E:72:ALA:HB2    | 2.15                     | 0.46              |
| 16:u:58:VAL:HG12   | 16:u:79:LEU:HD22  | 1.98                     | 0.46              |
| 4:D:266:TRP:CD1    | 30:D:408:LHG:HC31 | 2.50                     | 0.46              |
| 32:c:517:DGD:HA51  | 32:c:517:DGD:HA81 | 1.77                     | 0.46              |
| 13:O:189:ARG:NH2   | 37:O:303:HOH:O    | 2.35                     | 0.46              |
| 2:b:91:TRP:HE1     | 33:b:622:STE:H141 | 1.79                     | 0.46              |
| 2:b:155:ALA:HB1    | 29:b:623:LMG:H122 | 1.98                     | 0.46              |
| 19:y:22:LEU:HA     | 19:y:25:ILE:HG22  | 1.97                     | 0.46              |
| 1:a:162[A]:PRO:HB3 | 1:a:168[A]:PHE:HA | 1.98                     | 0.46              |
| 2:B:357:ARG:NE     | 37:B:709:HOH:O    | 2.18                     | 0.46              |
| 1:A:131:TRP:CE3    | 1:A:132:GLU:HA    | 2.51                     | 0.46              |
| 2:B:241:SER:HB3    | 24:B:612:CLA:HED3 | 1.98                     | 0.46              |
| 26:Y:101:BCR:H322  | 20:Z:17:PHE:CE2   | 2.51                     | 0.46              |
| 4:d:12:ARG:HH11    | 4:d:16:ASP:HB3    | 1.80                     | 0.46              |
| 24:A:604:CLA:H201  | 30:D:408:LHG:H182 | 1.97                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:B:327:THR:HG21    | 29:M:101:LMG:H291  | 1.96                     | 0.46              |
| 3:C:126:GLY:O       | 3:C:130:VAL:HG13   | 2.16                     | 0.46              |
| 3:C:137:PRO:HD3     | 24:C:513:CLA:HED2  | 1.98                     | 0.46              |
| 2:b:70:GLY:HA2      | 2:b:178:VAL:HG21   | 1.98                     | 0.46              |
| 12:M:20:VAL:HG11    | 12:m:20:VAL:HG22   | 1.98                     | 0.46              |
| 28:a:611:PL9:H371   | 28:a:611:PL9:H351  | 1.81                     | 0.46              |
| 24:b:607:CLA:H191   | 30:d:407:LHG:H141  | 1.97                     | 0.46              |
| 4:d:218:VAL:HG13    | 4:d:244:TYR:CD1    | 2.51                     | 0.46              |
| 2:B:67:ALA:HA       | 2:B:71:VAL:O       | 2.16                     | 0.45              |
| 2:b:58:GLN:C        | 2:b:329:PRO:HB3    | 2.41                     | 0.45              |
| 4:d:93:TRP:O        | 37:d:505:HOH:O     | 2.20                     | 0.45              |
| 35:F:101:HEM:HBB2   | 35:F:101:HEM:HMB1  | 1.98                     | 0.45              |
| 17:v:78:ASN:OD1     | 17:v:96:ARG:NH1    | 2.46                     | 0.45              |
| 24:c:504:CLA:H142   | 24:c:508:CLA:H121  | 1.98                     | 0.45              |
| 13:O:189:ARG:NE     | 37:O:303:HOH:O     | 2.29                     | 0.45              |
| 1:a:241:GLN:NE2     | 1:a:245:THR:HG23   | 2.32                     | 0.45              |
| 3:c:42:LEU:HD21     | 24:c:511:CLA:H2A   | 1.98                     | 0.45              |
| 2:B:379:ALA:HA      | 2:B:390:TYR:HB3    | 1.99                     | 0.45              |
| 13:O:133:VAL:C      | 13:O:135:SER:H     | 2.25                     | 0.45              |
| 20:Z:31:GLN:NE2     | 20:Z:32:ASP:HB2    | 2.32                     | 0.45              |
| 1:a:112:TYR:O       | 1:a:116:ILE:HG12   | 2.17                     | 0.45              |
| 2:b:83:GLU:H        | 2:b:83:GLU:HG2     | 1.63                     | 0.45              |
| 3:c:45:LEU:HA       | 3:c:139:THR:HG22   | 1.98                     | 0.45              |
| 4:d:49:LEU:HD13     | 26:d:405:BCR:C15   | 2.46                     | 0.45              |
| 26:d:405:BCR:C8     | 26:d:405:BCR:H331  | 2.47                     | 0.45              |
| 26:H:101:BCR:H331   | 26:H:101:BCR:C8    | 2.46                     | 0.45              |
| 31:B:623:SQD:H383   | 31:B:623:SQD:H352  | 1.83                     | 0.44              |
| 3:C:308:GLU:HB2     | 3:C:361:PHE:CE1    | 2.52                     | 0.44              |
| 3:C:409:GLY:HA3     | 3:C:413[B]:GLU:HG3 | 1.99                     | 0.44              |
| 9:J:20:GLY:O        | 9:J:24:ILE:HG13    | 2.17                     | 0.44              |
| 10:k:18:PHE:HE2     | 20:z:13:VAL:HG21   | 1.82                     | 0.44              |
| 2:B:413:ASP:OD2     | 2:B:416:THR:OG1    | 2.26                     | 0.44              |
| 3:C:348:GLU:OE2     | 13:O:11:VAL:HA     | 2.17                     | 0.44              |
| 20:Z:34:ASP:O       | 20:Z:37:LYS:HG2    | 2.17                     | 0.44              |
| 1:a:283:VAL:HA      | 1:a:286:THR:HG22   | 2.00                     | 0.44              |
| 2:b:125:ASP:OD2     | 2:b:128:THR:HG23   | 2.17                     | 0.44              |
| 5:e:63:ILE:HG23     | 5:e:64:PRO:HD2     | 1.98                     | 0.44              |
| 2:B:149[A]:LEU:HD21 | 24:B:606:CLA:HBB2  | 1.98                     | 0.44              |
| 16:U:76:ARG:NH2     | 37:U:202:HOH:O     | 2.51                     | 0.44              |
| 29:a:618:LMG:H151   | 29:a:618:LMG:H182  | 1.79                     | 0.44              |
| 2:b:451:PHE:CE2     | 2:b:455:HIS:CE1    | 3.05                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:315:MET:HE1   | 3:c:366:LEU:HD13  | 1.99                     | 0.44              |
| 5:e:18:ARG:HH22   | 6:f:15:ILE:HD11   | 1.82                     | 0.44              |
| 24:D:403:CLA:ND   | 33:D:411:STE:H122 | 2.33                     | 0.44              |
| 13:O:54:GLU:O     | 13:O:63:ALA:HB3   | 2.18                     | 0.44              |
| 16:U:23:GLU:HG3   | 16:U:24:LYS:HG2   | 1.98                     | 0.44              |
| 33:D:411:STE:H142 | 18:X:17:GLY:HA2   | 2.00                     | 0.44              |
| 4:d:246:MET:HE3   | 4:d:264:LYS:CG    | 2.47                     | 0.44              |
| 1:A:279:PRO:HG2   | 4:D:212:ALA:HB2   | 2.00                     | 0.44              |
| 10:K:25:LEU:N     | 10:K:26:PRO:HD2   | 2.33                     | 0.44              |
| 4:D:148:ALA:HB3   | 4:D:149:PRO:CD    | 2.47                     | 0.44              |
| 33:D:411:STE:H52  | 33:D:411:STE:H81  | 1.74                     | 0.44              |
| 33:b:625:STE:H122 | 33:b:625:STE:H151 | 1.84                     | 0.44              |
| 2:B:49:ASP:OD2    | 13:o:57:LYS:HD2   | 2.17                     | 0.44              |
| 24:B:601:CLA:HAB  | 33:H:103:STE:H142 | 1.99                     | 0.44              |
| 1:a:93:PHE:CD2    | 1:a:95:PRO:HD3    | 2.52                     | 0.44              |
| 4:d:134:ARG:HG2   | 33:d:411:STE:O1   | 2.18                     | 0.44              |
| 13:o:53:LYS:HE3   | 13:o:65:PHE:CZ    | 2.52                     | 0.44              |
| 2:b:357:ARG:NE    | 37:b:702:HOH:O    | 1.93                     | 0.43              |
| 4:d:141:TYR:OH    | 30:d:407:LHG:O4   | 2.23                     | 0.43              |
| 31:f:101:SQD:H312 | 18:x:27:VAL:HG11  | 2.00                     | 0.43              |
| 13:O:40:ILE:HD12  | 13:O:95:PHE:CD1   | 2.53                     | 0.43              |
| 24:c:501:CLA:C3D  | 24:c:503:CLA:H2   | 2.48                     | 0.43              |
| 4:d:179:PHE:HA    | 4:d:182:LEU:HD22  | 2.00                     | 0.43              |
| 13:o:216:GLU:OE2  | 13:o:234:LYS:HD2  | 2.17                     | 0.43              |
| 4:D:307:GLU:HG3   | 37:D:529:HOH:O    | 2.18                     | 0.43              |
| 28:a:611:PL9:C49  | 4:d:39:PRO:HG3    | 2.48                     | 0.43              |
| 24:c:508:CLA:H171 | 29:c:519:LMG:H372 | 2.00                     | 0.43              |
| 24:B:601:CLA:HBA1 | 24:B:601:CLA:HBD  | 2.00                     | 0.43              |
| 3:c:334:PRO:HA    | 13:o:153:THR:OG1  | 2.19                     | 0.43              |
| 1:A:38:ILE:HB     | 1:A:39:PRO:HD3    | 2.00                     | 0.43              |
| 2:b:173:GLY:HA3   | 2:b:265:ILE:HD11  | 2.00                     | 0.43              |
| 35:e:101:HEM:HBC2 | 35:e:101:HEM:CMC  | 2.47                     | 0.43              |
| 13:o:54:GLU:O     | 13:o:56:PRO:HD3   | 2.18                     | 0.43              |
| 4:D:32:TRP:CD2    | 29:D:409:LMG:H161 | 2.53                     | 0.43              |
| 24:B:614:CLA:H42  | 33:m:101:STE:H22  | 2.01                     | 0.43              |
| 2:b:189:GLY:O     | 2:b:197:GLY:HA3   | 2.18                     | 0.43              |
| 4:d:12:ARG:NH1    | 4:d:16:ASP:HB3    | 2.33                     | 0.43              |
| 5:E:27:ILE:HB     | 5:E:28:PRO:HD3    | 2.00                     | 0.43              |
| 7:H:17:GLU:OE2    | 7:H:20:LYS:NZ     | 2.45                     | 0.43              |
| 17:V:41:HIS:HA    | 17:V:45:ILE:O     | 2.19                     | 0.43              |
| 2:B:52:LEU:HD12   | 13:o:59:LYS:HE2   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:E:10:PHE:CD2    | 30:E:101:LHG:HC81  | 2.54                     | 0.43              |
| 17:v:95:LEU:HD11  | 17:v:112:LEU:HD11  | 2.00                     | 0.43              |
| 2:B:201:HIS:HB2   | 24:B:602:CLA:CHB   | 2.49                     | 0.43              |
| 24:B:614:CLA:H18  | 24:B:614:CLA:H152  | 1.79                     | 0.43              |
| 24:C:509:CLA:H91  | 24:C:509:CLA:H112  | 1.82                     | 0.43              |
| 13:O:178:LYS:HD2  | 13:O:181:GLU:OE2   | 2.19                     | 0.43              |
| 18:X:3:ILE:O      | 18:X:3:ILE:HG13    | 2.19                     | 0.43              |
| 31:A:617:SQD:H301 | 26:b:619:BCR:H363  | 2.00                     | 0.42              |
| 3:C:180:MET:HG2   | 3:C:199:ILE:O      | 2.20                     | 0.42              |
| 24:D:403:CLA:C1D  | 33:D:411:STE:H122  | 2.49                     | 0.42              |
| 33:D:411:STE:H91  | 18:X:16:SER:HB3    | 2.00                     | 0.42              |
| 17:V:78:ASN:OD1   | 17:V:96:ARG:NH1    | 2.42                     | 0.42              |
| 5:e:68:ASP:O      | 5:e:72:ALA:HB2     | 2.19                     | 0.42              |
| 4:D:61:HIS:HE1    | 4:D:80:THR:O       | 2.02                     | 0.42              |
| 13:O:42:ARG:O     | 13:O:241:ALA:HA    | 2.20                     | 0.42              |
| 24:b:601:CLA:H141 | 24:b:601:CLA:H161  | 1.91                     | 0.42              |
| 24:b:604:CLA:H42  | 24:b:605:CLA:H2    | 2.01                     | 0.42              |
| 24:b:605:CLA:H62  | 24:b:605:CLA:H41   | 1.86                     | 0.42              |
| 3:c:160:ILE:HG21  | 24:c:509:CLA:H203  | 2.01                     | 0.42              |
| 4:d:209:LEU:HD23  | 4:d:209:LEU:C      | 2.44                     | 0.42              |
| 24:B:614:CLA:H41  | 24:B:614:CLA:H61   | 1.80                     | 0.42              |
| 3:C:71:GLU:HB3    | 3:C:86:LEU:HD22    | 2.01                     | 0.42              |
| 3:C:318:LEU:C     | 3:C:318:LEU:HD23   | 2.44                     | 0.42              |
| 3:c:367:GLU:N     | 3:c:368:PRO:CD     | 2.82                     | 0.42              |
| 4:d:103:ARG:NH1   | 5:e:77:GLU:HG3     | 2.34                     | 0.42              |
| 15:t:15:ALA:HA    | 26:t:101:BCR:H12C  | 2.00                     | 0.42              |
| 17:v:76:MET:HE3   | 36:v:201:HEC:HBB3  | 2.00                     | 0.42              |
| 2:B:298:LEU:HD12  | 2:B:298:LEU:HA     | 1.90                     | 0.42              |
| 3:C:279:LEU:HD23  | 3:C:282:MET:HE3    | 2.01                     | 0.42              |
| 32:A:618:DGD:HD5  | 2:b:75:TRP:HB3     | 2.00                     | 0.42              |
| 26:B:618:BCR:C8   | 26:B:618:BCR:H331  | 2.49                     | 0.42              |
| 20:Z:23:VAL:HG22  | 20:Z:40:ILE:HD12   | 2.01                     | 0.42              |
| 1:a:229:GLU:CD    | 1:a:229:GLU:H      | 2.28                     | 0.42              |
| 13:O:37:THR:CA    | 37:O:310:HOH:O     | 2.58                     | 0.42              |
| 4:d:191:TRP:CE3   | 4:d:289:LEU:HD11   | 2.54                     | 0.42              |
| 11:l:7:ARG:HH11   | 33:l:102:STE:C1    | 2.33                     | 0.42              |
| 16:u:70:ARG:NH1   | 16:u:73:GLN:OE1    | 2.53                     | 0.42              |
| 1:A:45:THR:HG23   | 24:A:613:CLA:H191  | 2.01                     | 0.42              |
| 1:A:159[A]:LEU:C  | 1:A:162[A]:PRO:HD2 | 2.45                     | 0.42              |
| 1:a:85:SER:HA     | 1:a:109:GLY:HA3    | 2.02                     | 0.42              |
| 1:a:140:ARG:HB2   | 4:d:220:ASN:HA     | 2.02                     | 0.42              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:c:364:PRO:HG2   | 3:c:391[A]:ARG:HH12 | 1.83                     | 0.42              |
| 10:k:15:TYR:CZ    | 20:z:5:PHE:HZ       | 2.36                     | 0.42              |
| 24:B:606:CLA:H72  | 26:B:619:BCR:H311   | 2.01                     | 0.42              |
| 3:C:344:SER:O     | 13:O:75:THR:HG22    | 2.20                     | 0.42              |
| 2:b:92:SER:O      | 2:b:96:VAL:HG23     | 2.19                     | 0.42              |
| 2:b:227:LYS:HB3   | 2:b:227:LYS:HE2     | 1.94                     | 0.42              |
| 3:c:26:ARG:HA     | 24:c:511:CLA:OBD    | 2.19                     | 0.42              |
| 13:o:42:ARG:O     | 13:o:241:ALA:HA     | 2.20                     | 0.42              |
| 1:A:85:SER:HA     | 1:A:109:GLY:HA3     | 2.02                     | 0.41              |
| 2:B:495:PHE:HD1   | 2:B:505:ARG:NH1     | 2.18                     | 0.41              |
| 24:C:504:CLA:H62  | 24:C:504:CLA:H41    | 1.92                     | 0.41              |
| 24:C:507:CLA:H142 | 24:C:507:CLA:H111   | 1.96                     | 0.41              |
| 4:D:13:GLY:O      | 4:D:17:ILE:HG12     | 2.20                     | 0.41              |
| 3:c:128:GLY:HA3   | 24:c:513:CLA:C3C    | 2.50                     | 0.41              |
| 4:d:192:THR:HG23  | 24:d:403:CLA:HBC2   | 2.00                     | 0.41              |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG      | 2.55                     | 0.41              |
| 2:B:91:TRP:HE1    | 33:B:620:STE:H32    | 1.85                     | 0.41              |
| 24:B:611:CLA:H203 | 24:B:613:CLA:H8     | 2.02                     | 0.41              |
| 5:E:25:ILE:HG13   | 14:R:18:TRP:NE1     | 2.35                     | 0.41              |
| 18:x:27:VAL:O     | 18:x:31:ILE:HG13    | 2.20                     | 0.41              |
| 24:B:615:CLA:H2   | 24:B:616:CLA:HBB2   | 2.02                     | 0.41              |
| 13:O:93:LEU:O     | 13:O:128:SER:HA     | 2.20                     | 0.41              |
| 20:Z:28:ALA:O     | 20:Z:30:PRO:HD3     | 2.20                     | 0.41              |
| 2:b:43:ALA:HA     | 33:b:625:STE:H22    | 2.02                     | 0.41              |
| 24:b:614:CLA:H111 | 24:b:614:CLA:H152   | 1.93                     | 0.41              |
| 13:o:56:PRO:O     | 37:o:303:HOH:O      | 2.21                     | 0.41              |
| 24:B:610:CLA:HHC  | 24:B:610:CLA:HBB1   | 2.03                     | 0.41              |
| 4:D:267:LEU:C     | 4:D:267:LEU:HD23    | 2.46                     | 0.41              |
| 1:a:296:ASN:HB3   | 3:c:401:LEU:HA      | 2.02                     | 0.41              |
| 29:a:618:LMG:O9   | 29:a:618:LMG:C9     | 2.68                     | 0.41              |
| 9:j:15:THR:HG22   | 9:j:19:MET:HE2      | 2.00                     | 0.41              |
| 13:o:110:MET:HE2  | 13:o:116:ILE:HD11   | 2.02                     | 0.41              |
| 24:A:613:CLA:HBA1 | 24:A:613:CLA:C4A    | 2.50                     | 0.41              |
| 12:M:20:VAL:HG11  | 12:m:20:VAL:CG2     | 2.51                     | 0.41              |
| 1:a:159[B]:LEU:O  | 1:a:163[B]:ILE:HG13 | 2.20                     | 0.41              |
| 3:c:109:PHE:N     | 3:c:110:PRO:CD      | 2.83                     | 0.41              |
| 29:c:522:LMG:HC2  | 8:i:9:TYR:OH        | 2.20                     | 0.41              |
| 10:k:25:LEU:N     | 10:k:26:PRO:CD      | 2.83                     | 0.41              |
| 24:C:501:CLA:CAD  | 24:C:503:CLA:H12    | 2.51                     | 0.41              |
| 1:a:96:ILE:HG12   | 1:a:105:TRP:CE2     | 2.55                     | 0.41              |
| 2:B:434:THR:OG1   | 13:O:178:LYS:NZ     | 2.49                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:243:ALA:HA     | 2:b:246:PHE:CE2    | 2.55                     | 0.41              |
| 3:c:318:LEU:C      | 3:c:318:LEU:HD23   | 2.45                     | 0.41              |
| 26:c:515:BCR:H11C  | 26:c:515:BCR:H341  | 1.97                     | 0.41              |
| 17:v:87:GLU:CD     | 17:v:96:ARG:HH12   | 2.28                     | 0.41              |
| 32:A:618:DGD:HB42  | 32:A:618:DGD:HB91  | 2.03                     | 0.41              |
| 24:B:606:CLA:H93   | 24:B:606:CLA:H112  | 1.89                     | 0.41              |
| 1:a:241:GLN:HE22   | 1:a:245:THR:HG23   | 1.85                     | 0.41              |
| 2:b:25:MET:HE1     | 2:b:108:PHE:CD1    | 2.56                     | 0.41              |
| 3:c:121:SER:CB     | 33:c:520:STE:H172  | 2.51                     | 0.41              |
| 30:d:409:LHG:H272  | 30:d:409:LHG:H242  | 1.79                     | 0.41              |
| 1:A:332[B]:HIS:O   | 1:A:333[B]:GLU:C   | 2.64                     | 0.41              |
| 24:B:613:CLA:HBB1  | 24:B:613:CLA:HMB1  | 2.02                     | 0.41              |
| 24:B:613:CLA:H143  | 24:B:613:CLA:H111  | 1.96                     | 0.41              |
| 26:B:618:BCR:H20C  | 26:B:618:BCR:H361  | 1.90                     | 0.41              |
| 6:F:28:VAL:HB      | 6:F:29:PRO:HD3     | 2.02                     | 0.41              |
| 10:K:23:ASP:OD2    | 19:Y:21:GLN:NE2    | 2.53                     | 0.41              |
| 1:a:46:ILE:HD12    | 26:a:607:BCR:H15C  | 2.03                     | 0.41              |
| 1:a:132:GLU:O      | 1:a:136:ARG:HG2    | 2.20                     | 0.41              |
| 2:b:67:ALA:HA      | 2:b:71:VAL:O       | 2.21                     | 0.41              |
| 24:c:504:CLA:H92   | 24:c:504:CLA:H62   | 1.83                     | 0.41              |
| 4:d:40:CYS:HB3     | 4:d:117:HIS:O      | 2.21                     | 0.41              |
| 25:d:402:PHO:HHD   | 25:d:402:PHO:HBC2  | 2.03                     | 0.41              |
| 13:o:216:GLU:CD    | 13:o:234:LYS:HD2   | 2.46                     | 0.41              |
| 3:C:128:GLY:HA3    | 24:C:513:CLA:C3C   | 2.51                     | 0.41              |
| 4:D:24:ARG:NH2     | 31:D:407:SQD:O4    | 2.54                     | 0.41              |
| 8:I:2:GLU:O        | 8:I:6:ILE:HG12     | 2.22                     | 0.41              |
| 13:O:18:LYS:HE2    | 37:O:323:HOH:O     | 2.19                     | 0.41              |
| 3:c:308:GLU:HB2    | 3:c:361:PHE:CE1    | 2.56                     | 0.41              |
| 6:f:41:GLN:OE1     | 9:j:31:GLY:HA3     | 2.20                     | 0.41              |
| 1:A:188[B]:ALA:HB2 | 1:A:328[B]:MET:HB2 | 2.02                     | 0.40              |
| 3:C:223:TRP:CG     | 3:C:224:ILE:H      | 2.37                     | 0.40              |
| 3:C:367:GLU:N      | 3:C:368:PRO:CD     | 2.84                     | 0.40              |
| 29:c:521:LMG:H371  | 29:c:521:LMG:H402  | 1.98                     | 0.40              |
| 2:B:346:PHE:HA     | 2:B:398:THR:O      | 2.22                     | 0.40              |
| 30:B:621:LHG:HC41  | 30:B:622:LHG:O1    | 2.21                     | 0.40              |
| 24:b:615:CLA:H3A   | 24:b:615:CLA:HBA1  | 1.89                     | 0.40              |
| 3:c:338:GLY:HA3    | 3:c:341:LEU:O      | 2.21                     | 0.40              |
| 15:t:8:PHE:CD2     | 33:t:102:STE:H151  | 2.56                     | 0.40              |
| 1:A:278:TRP:HB3    | 1:A:279:PRO:HD3    | 2.02                     | 0.40              |
| 2:b:216:HIS:HE1    | 24:b:609:CLA:C1A   | 2.35                     | 0.40              |
| 24:B:601:CLA:H93   | 24:B:601:CLA:H62   | 1.93                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:308:ASP:OD1   | 1:a:308:ASP:C     | 2.65                     | 0.40              |
| 29:c:521:LMG:H382 | 29:c:521:LMG:H351 | 1.96                     | 0.40              |
| 10:k:18:PHE:CE2   | 20:z:13:VAL:HG21  | 2.56                     | 0.40              |
| 13:o:51:LEU:HD23  | 13:o:67:PRO:HA    | 2.04                     | 0.40              |
| 20:z:9:LEU:HD13   | 20:z:54:VAL:HG11  | 2.02                     | 0.40              |
| 20:z:35:ARG:NH2   | 37:z:101:HOH:O    | 2.54                     | 0.40              |
| 28:A:612:PL9:H351 | 6:F:22:ALA:HA     | 2.04                     | 0.40              |
| 24:A:613:CLA:H161 | 24:A:613:CLA:H141 | 1.83                     | 0.40              |
| 24:A:613:CLA:H162 | 24:A:613:CLA:H193 | 1.87                     | 0.40              |
| 5:E:15:THR:HB     | 9:J:8:ILE:O       | 2.21                     | 0.40              |
| 6:F:36:ALA:O      | 6:F:40:MET:HG3    | 2.21                     | 0.40              |
| 33:a:617:STE:H91  | 33:a:617:STE:H121 | 1.89                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 397/344 (115%) | 392 (99%) | 4 (1%)  | 1 (0%)   | 36          | 35  |
| 1   | a     | 397/344 (115%) | 390 (98%) | 6 (2%)  | 1 (0%)   | 36          | 35  |
| 2   | B     | 508/510 (100%) | 498 (98%) | 10 (2%) | 0        | 100         | 100 |
| 2   | b     | 503/510 (99%)  | 494 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 3   | C     | 454/461 (98%)  | 442 (97%) | 11 (2%) | 1 (0%)   | 43          | 42  |
| 3   | c     | 463/461 (100%) | 448 (97%) | 14 (3%) | 1 (0%)   | 43          | 42  |
| 4   | D     | 340/352 (97%)  | 329 (97%) | 11 (3%) | 0        | 100         | 100 |
| 4   | d     | 341/352 (97%)  | 334 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 5   | E     | 81/84 (96%)    | 81 (100%) | 0       | 0        | 100         | 100 |
| 5   | e     | 80/84 (95%)    | 80 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 6   | F     | 32/45 (71%)     | 32 (100%)  | 0        | 0        | 100         | 100 |
| 6   | f     | 32/45 (71%)     | 31 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 7   | H     | 63/66 (96%)     | 59 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 7   | h     | 61/66 (92%)     | 57 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 8   | I     | 34/38 (90%)     | 33 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 8   | i     | 34/38 (90%)     | 31 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 9   | J     | 34/40 (85%)     | 32 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 9   | j     | 34/40 (85%)     | 34 (100%)  | 0        | 0        | 100         | 100 |
| 10  | K     | 35/46 (76%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | k     | 35/46 (76%)     | 35 (100%)  | 0        | 0        | 100         | 100 |
| 11  | L     | 35/37 (95%)     | 35 (100%)  | 0        | 0        | 100         | 100 |
| 11  | l     | 34/37 (92%)     | 34 (100%)  | 0        | 0        | 100         | 100 |
| 12  | M     | 31/36 (86%)     | 31 (100%)  | 0        | 0        | 100         | 100 |
| 12  | m     | 30/36 (83%)     | 29 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 13  | O     | 243/272 (89%)   | 230 (95%)  | 11 (4%)  | 2 (1%)   | 16          | 11  |
| 13  | o     | 242/272 (89%)   | 234 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 27  |
| 14  | R     | 26/41 (63%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 14  | r     | 26/41 (63%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 15  | T     | 28/32 (88%)     | 28 (100%)  | 0        | 0        | 100         | 100 |
| 15  | t     | 28/32 (88%)     | 28 (100%)  | 0        | 0        | 100         | 100 |
| 16  | U     | 95/134 (71%)    | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 16  | u     | 95/134 (71%)    | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 17  | V     | 135/163 (83%)   | 129 (96%)  | 5 (4%)   | 1 (1%)   | 18          | 14  |
| 17  | v     | 135/163 (83%)   | 130 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 18  | X     | 36/41 (88%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 18  | x     | 37/41 (90%)     | 36 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 19  | Y     | 25/46 (54%)     | 22 (88%)   | 3 (12%)  | 0        | 100         | 100 |
| 19  | y     | 28/46 (61%)     | 26 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 20  | Z     | 60/62 (97%)     | 58 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 20  | z     | 60/62 (97%)     | 56 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| All | All   | 5387/5700 (94%) | 5245 (97%) | 134 (2%) | 8 (0%)   | 43          | 46  |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 416 | SER  |
| 17  | V     | 64  | PRO  |
| 3   | c     | 416 | SER  |
| 13  | O     | 58  | ASN  |
| 13  | O     | 62  | GLU  |
| 1   | A     | 259 | ILE  |
| 1   | a     | 259 | ILE  |
| 13  | o     | 56  | PRO  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 324/280 (116%) | 319 (98%) | 5 (2%)   | 57          | 64 |
| 1   | a     | 323/280 (115%) | 313 (97%) | 10 (3%)  | 35          | 37 |
| 2   | B     | 408/407 (100%) | 399 (98%) | 9 (2%)   | 45          | 50 |
| 2   | b     | 402/407 (99%)  | 394 (98%) | 8 (2%)   | 48          | 54 |
| 3   | C     | 356/362 (98%)  | 348 (98%) | 8 (2%)   | 45          | 50 |
| 3   | c     | 364/362 (101%) | 355 (98%) | 9 (2%)   | 42          | 45 |
| 4   | D     | 277/283 (98%)  | 274 (99%) | 3 (1%)   | 65          | 73 |
| 4   | d     | 278/283 (98%)  | 269 (97%) | 9 (3%)   | 34          | 35 |
| 5   | E     | 72/73 (99%)    | 67 (93%)  | 5 (7%)   | 14          | 11 |
| 5   | e     | 71/73 (97%)    | 69 (97%)  | 2 (3%)   | 38          | 41 |
| 6   | F     | 28/39 (72%)    | 27 (96%)  | 1 (4%)   | 31          | 31 |
| 6   | f     | 28/39 (72%)    | 27 (96%)  | 1 (4%)   | 31          | 31 |
| 7   | H     | 54/55 (98%)    | 53 (98%)  | 1 (2%)   | 50          | 56 |
| 7   | h     | 53/55 (96%)    | 52 (98%)  | 1 (2%)   | 50          | 56 |
| 8   | I     | 32/34 (94%)    | 31 (97%)  | 1 (3%)   | 35          | 37 |
| 8   | i     | 32/34 (94%)    | 31 (97%)  | 1 (3%)   | 35          | 37 |
| 9   | J     | 24/28 (86%)    | 23 (96%)  | 1 (4%)   | 26          | 25 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 9   | j     | 24/28 (86%)     | 22 (92%)   | 2 (8%)   | 10          | 7   |
| 10  | K     | 30/37 (81%)     | 28 (93%)   | 2 (7%)   | 15          | 11  |
| 10  | k     | 30/37 (81%)     | 24 (80%)   | 6 (20%)  | 1           | 0   |
| 11  | L     | 35/35 (100%)    | 34 (97%)   | 1 (3%)   | 37          | 40  |
| 11  | l     | 34/35 (97%)     | 31 (91%)   | 3 (9%)   | 9           | 6   |
| 12  | M     | 28/32 (88%)     | 27 (96%)   | 1 (4%)   | 31          | 31  |
| 12  | m     | 28/32 (88%)     | 26 (93%)   | 2 (7%)   | 13          | 10  |
| 13  | O     | 206/228 (90%)   | 201 (98%)  | 5 (2%)   | 43          | 47  |
| 13  | o     | 207/228 (91%)   | 201 (97%)  | 6 (3%)   | 37          | 40  |
| 14  | R     | 22/33 (67%)     | 18 (82%)   | 4 (18%)  | 2           | 1   |
| 14  | r     | 22/33 (67%)     | 20 (91%)   | 2 (9%)   | 9           | 6   |
| 15  | T     | 26/28 (93%)     | 25 (96%)   | 1 (4%)   | 29          | 29  |
| 15  | t     | 25/28 (89%)     | 25 (100%)  | 0        | 100         | 100 |
| 16  | U     | 84/112 (75%)    | 82 (98%)   | 2 (2%)   | 43          | 47  |
| 16  | u     | 84/112 (75%)    | 82 (98%)   | 2 (2%)   | 43          | 47  |
| 17  | V     | 117/138 (85%)   | 112 (96%)  | 5 (4%)   | 26          | 25  |
| 17  | v     | 117/138 (85%)   | 113 (97%)  | 4 (3%)   | 32          | 33  |
| 18  | X     | 31/34 (91%)     | 29 (94%)   | 2 (6%)   | 15          | 12  |
| 18  | x     | 31/34 (91%)     | 29 (94%)   | 2 (6%)   | 15          | 12  |
| 19  | Y     | 19/37 (51%)     | 18 (95%)   | 1 (5%)   | 20          | 18  |
| 19  | y     | 22/37 (60%)     | 19 (86%)   | 3 (14%)  | 3           | 2   |
| 20  | Z     | 52/52 (100%)    | 46 (88%)   | 6 (12%)  | 5           | 3   |
| 20  | z     | 51/52 (98%)     | 45 (88%)   | 6 (12%)  | 5           | 3   |
| All | All   | 4451/4654 (96%) | 4308 (97%) | 143 (3%) | 34          | 35  |

All (143) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 12    | ASN  |
| 1   | A     | 60[A] | ILE  |
| 1   | A     | 60[B] | ILE  |
| 1   | A     | 243   | GLU  |
| 1   | A     | 248   | ILE  |
| 2   | B     | 76    | SER  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | B     | 79    | SER  |
| 2   | B     | 86    | ILE  |
| 2   | B     | 98    | LEU  |
| 2   | B     | 127   | ARG  |
| 2   | B     | 240   | SER  |
| 2   | B     | 362   | PHE  |
| 2   | B     | 371   | THR  |
| 2   | B     | 476   | ARG  |
| 3   | C     | 104   | GLU  |
| 3   | C     | 130   | VAL  |
| 3   | C     | 141   | GLU  |
| 3   | C     | 200   | THR  |
| 3   | C     | 240   | ILE  |
| 3   | C     | 273   | SER  |
| 3   | C     | 289   | PHE  |
| 3   | C     | 315   | MET  |
| 4   | D     | 43    | LEU  |
| 4   | D     | 154   | VAL  |
| 4   | D     | 259   | ILE  |
| 5   | E     | 11    | SER  |
| 5   | E     | 22[A] | ILE  |
| 5   | E     | 22[B] | ILE  |
| 5   | E     | 61    | ARG  |
| 5   | E     | 81    | GLU  |
| 6   | F     | 25    | THR  |
| 7   | H     | 20    | LYS  |
| 8   | I     | 4     | LEU  |
| 9   | J     | 24    | ILE  |
| 10  | K     | 10    | LYS  |
| 10  | K     | 25    | LEU  |
| 11  | L     | 2     | GLU  |
| 12  | M     | 25    | LEU  |
| 13  | O     | 57    | LYS  |
| 13  | O     | 78    | LEU  |
| 13  | O     | 107   | THR  |
| 13  | O     | 198   | SER  |
| 13  | O     | 214   | THR  |
| 14  | R     | 6     | LEU  |
| 14  | R     | 10    | LEU  |
| 14  | R     | 21    | ARG  |
| 14  | R     | 29    | LYS  |
| 15  | T     | 25    | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 16  | U     | 51     | LYS  |
| 16  | U     | 67     | LEU  |
| 17  | V     | 3      | LEU  |
| 17  | V     | 7      | VAL  |
| 17  | V     | 31     | ARG  |
| 17  | V     | 57     | GLU  |
| 17  | V     | 86     | GLN  |
| 18  | X     | 3      | ILE  |
| 18  | X     | 23     | LEU  |
| 19  | Y     | 34     | MET  |
| 20  | Z     | 2      | THR  |
| 20  | Z     | 15     | LEU  |
| 20  | Z     | 19     | MET  |
| 20  | Z     | 32     | ASP  |
| 20  | Z     | 35     | ARG  |
| 20  | Z     | 50     | LEU  |
| 1   | a     | 28     | LEU  |
| 1   | a     | 42     | LEU  |
| 1   | a     | 159[A] | LEU  |
| 1   | a     | 159[B] | LEU  |
| 1   | a     | 200    | LEU  |
| 1   | a     | 223    | LEU  |
| 1   | a     | 231    | GLU  |
| 1   | a     | 245    | THR  |
| 1   | a     | 271    | LEU  |
| 1   | a     | 288    | LEU  |
| 2   | b     | 83     | GLU  |
| 2   | b     | 128    | THR  |
| 2   | b     | 149    | LEU  |
| 2   | b     | 236    | THR  |
| 2   | b     | 362    | PHE  |
| 2   | b     | 485    | GLU  |
| 2   | b     | 492    | GLU  |
| 2   | b     | 506    | ARG  |
| 3   | c     | 24     | THR  |
| 3   | c     | 72     | LEU  |
| 3   | c     | 99     | VAL  |
| 3   | c     | 124    | VAL  |
| 3   | c     | 125    | LEU  |
| 3   | c     | 165    | LEU  |
| 3   | c     | 240    | ILE  |
| 3   | c     | 289    | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | c     | 416 | SER  |
| 4   | d     | 90  | LEU  |
| 4   | d     | 182 | LEU  |
| 4   | d     | 233 | ARG  |
| 4   | d     | 259 | ILE  |
| 4   | d     | 291 | LEU  |
| 4   | d     | 293 | LEU  |
| 4   | d     | 307 | GLU  |
| 4   | d     | 321 | LEU  |
| 4   | d     | 329 | MET  |
| 5   | e     | 4   | THR  |
| 5   | e     | 83  | LEU  |
| 6   | f     | 28  | VAL  |
| 7   | h     | 7   | LEU  |
| 8   | i     | 2   | GLU  |
| 9   | j     | 13  | VAL  |
| 9   | j     | 21  | VAL  |
| 10  | k     | 10  | LYS  |
| 10  | k     | 13  | GLU  |
| 10  | k     | 25  | LEU  |
| 10  | k     | 27  | VAL  |
| 10  | k     | 30  | VAL  |
| 10  | k     | 35  | LEU  |
| 11  | l     | 7   | ARG  |
| 11  | l     | 21  | LEU  |
| 11  | l     | 30  | LEU  |
| 12  | m     | 13  | LEU  |
| 12  | m     | 16  | LEU  |
| 13  | o     | 18  | LYS  |
| 13  | o     | 49  | THR  |
| 13  | o     | 87  | VAL  |
| 13  | o     | 118 | LEU  |
| 13  | o     | 130 | GLN  |
| 13  | o     | 207 | ARG  |
| 14  | r     | 9   | LEU  |
| 14  | r     | 10  | LEU  |
| 16  | u     | 15  | GLU  |
| 16  | u     | 23  | GLU  |
| 17  | v     | 24  | LYS  |
| 17  | v     | 52  | LEU  |
| 17  | v     | 69  | ILE  |
| 17  | v     | 107 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | x     | 2   | THR  |
| 18  | x     | 15  | LEU  |
| 19  | y     | 19  | ILE  |
| 19  | y     | 41  | VAL  |
| 19  | y     | 45  | ASN  |
| 20  | z     | 1   | MET  |
| 20  | z     | 7   | LEU  |
| 20  | z     | 20  | VAL  |
| 20  | z     | 32  | ASP  |
| 20  | z     | 39  | LEU  |
| 20  | z     | 46  | LEU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 223 | GLN  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 497 | GLN  |
| 3   | C     | 385 | GLN  |
| 3   | C     | 415 | ASN  |
| 4   | D     | 61  | HIS  |
| 4   | D     | 332 | GLN  |
| 5   | E     | 60  | GLN  |
| 12  | M     | 5   | GLN  |
| 13  | O     | 36  | GLN  |
| 13  | O     | 88  | ASN  |
| 13  | O     | 155 | ASN  |
| 14  | R     | 22  | ASN  |
| 16  | U     | 37  | GLN  |
| 16  | U     | 78  | ASN  |
| 17  | V     | 86  | GLN  |
| 18  | X     | 38  | GLN  |
| 20  | Z     | 31  | GLN  |
| 1   | a     | 19  | ASN  |
| 1   | a     | 234 | ASN  |
| 2   | b     | 14  | ASN  |
| 2   | b     | 179 | GLN  |
| 3   | c     | 322 | GLN  |
| 3   | c     | 382 | ASN  |
| 4   | d     | 250 | ASN  |
| 4   | d     | 350 | ASN  |
| 5   | e     | 60  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | e     | 82  | GLN  |
| 7   | h     | 59  | ASN  |
| 13  | o     | 80  | GLN  |
| 13  | o     | 155 | ASN  |
| 18  | x     | 33  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | FME  | m     | 1   | 12   | 8,9,10       | 0.97 | 0        | 8,9,11      | 0.73 | 0        |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 1.07 | 1 (12%)  | 8,9,11      | 0.84 | 0        |
| 12  | FME  | M     | 1   | 12   | 8,9,10       | 1.02 | 1 (12%)  | 8,9,11      | 0.97 | 0        |
| 15  | FME  | t     | 1   | 15   | 8,9,10       | 1.46 | 1 (12%)  | 8,9,11      | 1.03 | 1 (12%)  |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 1.01 | 1 (12%)  | 8,9,11      | 0.94 | 0        |
| 15  | FME  | T     | 1   | 15   | 8,9,10       | 0.97 | 1 (12%)  | 8,9,11      | 1.37 | 1 (12%)  |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 12  | FME  | m     | 1   | 12   | -       | 0/7/9/11 | -     |
| 8   | FME  | i     | 1   | 8    | -       | 0/7/9/11 | -     |
| 12  | FME  | M     | 1   | 12   | -       | 1/7/9/11 | -     |
| 15  | FME  | t     | 1   | 15   | -       | 2/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | FME  | I     | 1   | 8    | -       | 1/7/9/11 | -     |
| 15  | FME  | T     | 1   | 15   | -       | 2/7/9/11 | -     |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | t     | 1   | FME  | CA-N  | -3.55 | 1.41        | 1.46     |
| 8   | i     | 1   | FME  | CA-N  | -2.27 | 1.43        | 1.46     |
| 8   | I     | 1   | FME  | CA-N  | -2.14 | 1.43        | 1.46     |
| 15  | T     | 1   | FME  | CA-N  | -2.05 | 1.43        | 1.46     |
| 12  | M     | 1   | FME  | CA-N  | -2.01 | 1.43        | 1.46     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | T     | 1   | FME  | O1-CN-N | -2.44 | 119.02      | 125.32   |
| 15  | t     | 1   | FME  | CB-CA-N | 2.22  | 114.56      | 110.52   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 12  | M     | 1   | FME  | O-C-CA-CB   |
| 15  | T     | 1   | FME  | O-C-CA-CB   |
| 15  | t     | 1   | FME  | O-C-CA-CB   |
| 15  | t     | 1   | FME  | CB-CG-SD-CE |
| 15  | T     | 1   | FME  | CB-CG-SD-CE |
| 8   | I     | 1   | FME  | CB-CA-N-CN  |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 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$ |
| 24  | CLA  | C     | 501    | -      | 69,73,73     | 1.40 | 8 (11%)     | 82,113,113  | 1.54 | 7 (8%)      |
| 24  | CLA  | C     | 509    | -      | 69,73,73     | 1.23 | 7 (10%)     | 82,113,113  | 1.46 | 8 (9%)      |
| 26  | BCR  | c     | 514    | -      | 41,41,41     | 1.21 | 3 (7%)      | 56,56,56    | 1.26 | 8 (14%)     |
| 33  | STE  | a     | 616    | -      | 11,11,19     | 0.86 | 0           | 11,11,19    | 1.28 | 2 (18%)     |
| 24  | CLA  | B     | 613    | -      | 69,73,73     | 1.24 | 8 (11%)     | 82,113,113  | 1.12 | 7 (8%)      |
| 29  | LMG  | a     | 618    | -      | 55,55,55     | 1.06 | 5 (9%)      | 63,63,63    | 1.45 | 8 (12%)     |
| 24  | CLA  | C     | 504    | 37     | 63,67,73     | 1.17 | 6 (9%)      | 74,105,113  | 1.35 | 7 (9%)      |
| 29  | LMG  | c     | 522    | -      | 49,49,55     | 0.88 | 2 (4%)      | 57,57,63    | 1.30 | 6 (10%)     |
| 25  | PHO  | A     | 606    | -      | 58,69,69     | 1.78 | 14 (24%)    | 55,99,99    | 1.73 | 10 (18%)    |
| 32  | DGD  | c     | 516    | -      | 63,63,67     | 1.17 | 8 (12%)     | 77,77,81    | 1.38 | 11 (14%)    |
| 21  | OEY  | a     | 601[B] | 3,1,37 | 0,16,16      | -    | -           | -           | -    | -           |
| 33  | STE  | B     | 624    | -      | 13,13,19     | 0.70 | 0           | 13,13,19    | 1.12 | 1 (7%)      |
| 24  | CLA  | d     | 404    | -      | 69,73,73     | 1.44 | 10 (14%)    | 82,113,113  | 1.18 | 8 (9%)      |
| 29  | LMG  | c     | 521    | -      | 48,48,55     | 1.09 | 6 (12%)     | 56,56,63    | 1.27 | 3 (5%)      |
| 31  | SQD  | a     | 614    | -      | 35,35,54     | 1.04 | 2 (5%)      | 37,37,65    | 1.52 | 6 (16%)     |
| 26  | BCR  | B     | 618    | -      | 41,41,41     | 1.23 | 4 (9%)      | 56,56,56    | 1.17 | 4 (7%)      |
| 33  | STE  | b     | 625    | -      | 19,19,19     | 0.66 | 0           | 19,19,19    | 1.00 | 1 (5%)      |
| 24  | CLA  | b     | 615    | -      | 69,73,73     | 1.55 | 10 (14%)    | 82,113,113  | 1.60 | 13 (15%)    |
| 26  | BCR  | A     | 609    | -      | 41,41,41     | 1.22 | 5 (12%)     | 56,56,56    | 1.42 | 9 (16%)     |
| 24  | CLA  | B     | 615    | -      | 69,73,73     | 1.33 | 8 (11%)     | 82,113,113  | 1.27 | 7 (8%)      |
| 24  | CLA  | b     | 612    | -      | 69,73,73     | 1.58 | 10 (14%)    | 82,113,113  | 1.27 | 10 (12%)    |
| 33  | STE  | B     | 625    | -      | 11,11,19     | 0.80 | 0           | 11,11,19    | 1.09 | 0           |
| 33  | STE  | a     | 617    | -      | 14,14,19     | 0.43 | 0           | 13,13,19    | 0.80 | 0           |
| 30  | LHG  | d     | 408    | -      | 48,48,48     | 0.86 | 1 (2%)      | 51,54,54    | 1.23 | 4 (7%)      |
| 24  | CLA  | C     | 502    | -      | 69,73,73     | 1.22 | 7 (10%)     | 82,113,113  | 1.36 | 7 (8%)      |
| 24  | CLA  | b     | 605    | -      | 69,73,73     | 1.19 | 8 (11%)     | 82,113,113  | 1.49 | 12 (14%)    |
| 24  | CLA  | B     | 603    | -      | 69,73,73     | 1.33 | 8 (11%)     | 82,113,113  | 1.60 | 11 (13%)    |
| 33  | STE  | b     | 627    | -      | 13,13,19     | 0.49 | 0           | 12,12,19    | 0.54 | 0           |
| 24  | CLA  | b     | 608    | -      | 69,73,73     | 1.28 | 10 (14%)    | 82,113,113  | 1.30 | 12 (14%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | SQD  | b     | 620 | -    | 47,49,54     | 0.99 | 3 (6%)   | 57,60,65    | 1.87 | 14 (24%) |
| 24  | CLA  | b     | 607 | 37   | 69,73,73     | 1.26 | 8 (11%)  | 82,113,113  | 1.23 | 8 (9%)   |
| 33  | STE  | c     | 520 | -    | 19,19,19     | 0.63 | 0        | 19,19,19    | 0.98 | 0        |
| 25  | PHO  | d     | 402 | -    | 58,69,69     | 2.11 | 8 (13%)  | 55,99,99    | 1.53 | 7 (12%)  |
| 33  | STE  | b     | 626 | -    | 9,9,19       | 0.46 | 0        | 8,8,19      | 0.64 | 0        |
| 24  | CLA  | b     | 602 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.56 | 11 (13%) |
| 24  | CLA  | B     | 610 | 37   | 69,73,73     | 1.40 | 10 (14%) | 82,113,113  | 1.43 | 8 (9%)   |
| 24  | CLA  | c     | 508 | -    | 68,72,73     | 1.41 | 7 (10%)  | 80,111,113  | 1.45 | 10 (12%) |
| 25  | PHO  | A     | 607 | -    | 58,69,69     | 2.01 | 9 (15%)  | 55,99,99    | 1.46 | 9 (16%)  |
| 32  | DGD  | h     | 101 | -    | 63,63,67     | 1.16 | 7 (11%)  | 77,77,81    | 1.38 | 12 (15%) |
| 24  | CLA  | c     | 503 | -    | 69,73,73     | 1.25 | 8 (11%)  | 82,113,113  | 1.17 | 5 (6%)   |
| 30  | LHG  | B     | 621 | -    | 48,48,48     | 0.85 | 1 (2%)   | 51,54,54    | 1.19 | 6 (11%)  |
| 24  | CLA  | B     | 614 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.38 | 11 (13%) |
| 24  | CLA  | B     | 604 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.48 | 7 (8%)   |
| 24  | CLA  | c     | 502 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 24  | CLA  | b     | 613 | -    | 69,73,73     | 1.22 | 8 (11%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 33  | STE  | T     | 102 | -    | 15,15,19     | 0.41 | 0        | 14,14,19    | 0.83 | 0        |
| 29  | LMG  | D     | 409 | -    | 31,31,55     | 0.98 | 2 (6%)   | 33,33,63    | 1.11 | 1 (3%)   |
| 29  | LMG  | D     | 410 | -    | 26,26,55     | 0.60 | 0        | 26,26,63    | 1.25 | 1 (3%)   |
| 24  | CLA  | A     | 613 | 37   | 69,73,73     | 1.30 | 11 (15%) | 82,113,113  | 1.40 | 7 (8%)   |
| 24  | CLA  | B     | 605 | -    | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.31 | 9 (10%)  |
| 33  | STE  | C     | 522 | -    | 11,11,19     | 0.70 | 0        | 11,11,19    | 1.36 | 2 (18%)  |
| 31  | SQD  | A     | 617 | -    | 38,38,54     | 0.97 | 3 (7%)   | 40,40,65    | 1.46 | 4 (10%)  |
| 24  | CLA  | b     | 609 | -    | 69,73,73     | 1.47 | 8 (11%)  | 82,113,113  | 1.60 | 12 (14%) |
| 24  | CLA  | C     | 505 | -    | 69,73,73     | 1.33 | 7 (10%)  | 82,113,113  | 1.40 | 8 (9%)   |
| 30  | LHG  | D     | 408 | -    | 48,48,48     | 1.14 | 4 (8%)   | 51,54,54    | 1.27 | 5 (9%)   |
| 30  | LHG  | E     | 101 | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.28 | 5 (9%)   |
| 31  | SQD  | D     | 407 | -    | 34,36,54     | 1.01 | 3 (8%)   | 42,45,65    | 2.09 | 10 (23%) |
| 24  | CLA  | c     | 512 | -    | 69,73,73     | 1.12 | 7 (10%)  | 82,113,113  | 1.34 | 6 (7%)   |
| 24  | CLA  | B     | 601 | 37   | 69,73,73     | 1.27 | 6 (8%)   | 82,113,113  | 1.38 | 9 (10%)  |
| 33  | STE  | b     | 624 | -    | 15,15,19     | 0.83 | 1 (6%)   | 15,15,19    | 0.78 | 0        |
| 33  | STE  | t     | 102 | -    | 17,17,19     | 0.57 | 0        | 17,17,19    | 1.19 | 1 (5%)   |
| 24  | CLA  | d     | 403 | -    | 69,73,73     | 1.33 | 11 (15%) | 82,113,113  | 1.45 | 7 (8%)   |
| 26  | BCR  | T     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 29  | LMG  | b     | 623 | -    | 55,55,55     | 0.87 | 3 (5%)   | 63,63,63    | 1.40 | 8 (12%)  |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | b     | 610    | 37     | 69,73,73     | 1.33 | 7 (10%)  | 82,113,113  | 1.46 | 11 (13%) |
| 24  | CLA  | c     | 501    | -      | 69,73,73     | 1.09 | 3 (4%)   | 82,113,113  | 1.39 | 9 (10%)  |
| 26  | BCR  | Y     | 101    | -      | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.18 | 5 (8%)   |
| 24  | CLA  | b     | 606    | -      | 69,73,73     | 1.73 | 8 (11%)  | 82,113,113  | 1.61 | 9 (10%)  |
| 24  | CLA  | B     | 611    | -      | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.66 | 11 (13%) |
| 28  | PL9  | a     | 611    | -      | 55,55,55     | 1.13 | 6 (10%)  | 68,69,69    | 1.67 | 14 (20%) |
| 26  | BCR  | C     | 514    | -      | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.36 | 8 (14%)  |
| 26  | BCR  | x     | 101    | -      | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 34  | BCT  | a     | 610    | 23     | 3,3,3        | 0.97 | 0        | 2,3,3       | 3.21 | 1 (50%)  |
| 24  | CLA  | C     | 507    | 37     | 69,73,73     | 1.24 | 7 (10%)  | 82,113,113  | 1.50 | 11 (13%) |
| 29  | LMG  | d     | 410    | -      | 44,44,55     | 1.02 | 3 (6%)   | 52,52,63    | 1.26 | 6 (11%)  |
| 29  | LMG  | M     | 101    | -      | 51,51,55     | 1.08 | 4 (7%)   | 59,59,63    | 1.50 | 7 (11%)  |
| 33  | STE  | l     | 102    | -      | 17,17,19     | 0.37 | 0        | 16,16,19    | 0.90 | 0        |
| 24  | CLA  | A     | 605    | 37     | 69,73,73     | 1.29 | 7 (10%)  | 82,113,113  | 1.46 | 11 (13%) |
| 33  | STE  | k     | 103    | -      | 11,11,19     | 0.82 | 0        | 11,11,19    | 0.94 | 0        |
| 26  | BCR  | k     | 102    | -      | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.18 | 4 (7%)   |
| 33  | STE  | d     | 411    | -      | 16,16,19     | 0.60 | 0        | 16,16,19    | 1.43 | 1 (6%)   |
| 29  | LMG  | b     | 621    | -      | 51,51,55     | 0.95 | 3 (5%)   | 59,59,63    | 1.49 | 10 (16%) |
| 33  | STE  | a     | 615    | -      | 9,9,19       | 0.57 | 0        | 8,8,19      | 0.48 | 0        |
| 36  | HEC  | V     | 201    | 17     | 46,50,50     | 1.80 | 5 (10%)  | 58,82,82    | 1.94 | 8 (13%)  |
| 31  | SQD  | A     | 616    | -      | 50,52,54     | 1.12 | 6 (12%)  | 60,63,65    | 2.05 | 11 (18%) |
| 33  | STE  | m     | 101    | -      | 11,11,19     | 0.66 | 0        | 11,11,19    | 1.35 | 1 (9%)   |
| 32  | DGD  | A     | 618    | -      | 67,67,67     | 1.22 | 7 (10%)  | 81,81,81    | 1.38 | 9 (11%)  |
| 24  | CLA  | B     | 607    | 37     | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.34 | 6 (7%)   |
| 24  | CLA  | c     | 509    | -      | 69,73,73     | 1.30 | 5 (7%)   | 82,113,113  | 1.48 | 8 (9%)   |
| 31  | SQD  | a     | 613    | -      | 52,54,54     | 1.05 | 5 (9%)   | 62,65,65    | 1.87 | 11 (17%) |
| 26  | BCR  | C     | 515    | -      | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 26  | BCR  | a     | 607    | -      | 41,41,41     | 1.08 | 4 (9%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 33  | STE  | b     | 622    | -      | 19,19,19     | 0.59 | 0        | 19,19,19    | 1.04 | 1 (5%)   |
| 26  | BCR  | H     | 101    | -      | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 35  | HEM  | F     | 101    | 5,6    | 50,50,50     | 1.35 | 4 (8%)   | 67,82,82    | 1.20 | 6 (8%)   |
| 22  | OEX  | a     | 602[A] | 3,1,37 | 0,15,15      | -    | -        | -           | -    | -        |
| 26  | BCR  | k     | 101    | -      | 41,41,41     | 1.13 | 3 (7%)   | 56,56,56    | 1.05 | 4 (7%)   |
| 24  | CLA  | a     | 606    | -      | 69,73,73     | 1.57 | 11 (15%) | 82,113,113  | 1.30 | 8 (9%)   |
| 30  | LHG  | l     | 101    | -      | 48,48,48     | 0.88 | 1 (2%)   | 51,54,54    | 1.29 | 8 (15%)  |



| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | PL9  | D     | 405    | -      | 55,55,55     | 1.51 | 9 (16%)  | 68,69,69    | 1.66 | 16 (23%) |
| 32  | DGD  | c     | 518    | -      | 63,63,67     | 1.10 | 6 (9%)   | 77,77,81    | 1.42 | 14 (18%) |
| 26  | BCR  | K     | 101    | -      | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.18 | 4 (7%)   |
| 24  | CLA  | c     | 504    | 37     | 64,68,73     | 1.23 | 7 (10%)  | 76,107,113  | 1.24 | 9 (11%)  |
| 29  | LMG  | C     | 519    | -      | 48,48,55     | 0.90 | 3 (6%)   | 56,56,63    | 1.38 | 7 (12%)  |
| 32  | DGD  | C     | 517    | -      | 63,63,67     | 1.19 | 6 (9%)   | 77,77,81    | 1.35 | 8 (10%)  |
| 33  | STE  | T     | 103    | -      | 14,14,19     | 0.45 | 0        | 13,13,19    | 0.79 | 0        |
| 30  | LHG  | d     | 407    | -      | 48,48,48     | 0.88 | 4 (8%)   | 51,54,54    | 1.46 | 7 (13%)  |
| 28  | PL9  | d     | 406    | -      | 55,55,55     | 1.54 | 7 (12%)  | 68,69,69    | 1.75 | 14 (20%) |
| 24  | CLA  | b     | 611    | -      | 69,73,73     | 1.29 | 8 (11%)  | 82,113,113  | 1.40 | 8 (9%)   |
| 31  | SQD  | B     | 623    | -      | 52,54,54     | 0.97 | 3 (5%)   | 62,65,65    | 1.96 | 14 (22%) |
| 24  | CLA  | b     | 614    | -      | 69,73,73     | 1.43 | 9 (13%)  | 82,113,113  | 1.48 | 12 (14%) |
| 26  | BCR  | b     | 619    | -      | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 28  | PL9  | A     | 612    | -      | 55,55,55     | 1.13 | 4 (7%)   | 68,69,69    | 1.57 | 11 (16%) |
| 24  | CLA  | B     | 616    | -      | 64,68,73     | 1.36 | 8 (12%)  | 76,107,113  | 1.56 | 8 (10%)  |
| 24  | CLA  | c     | 507    | 37     | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.39 | 10 (12%) |
| 24  | CLA  | c     | 513    | -      | 69,73,73     | 1.26 | 9 (13%)  | 82,113,113  | 1.23 | 9 (10%)  |
| 26  | BCR  | b     | 617    | -      | 41,41,41     | 1.12 | 3 (7%)   | 56,56,56    | 1.40 | 8 (14%)  |
| 24  | CLA  | B     | 606    | -      | 69,73,73     | 1.31 | 12 (17%) | 82,113,113  | 1.42 | 12 (14%) |
| 24  | CLA  | B     | 608    | -      | 69,73,73     | 1.07 | 5 (7%)   | 82,113,113  | 1.27 | 10 (12%) |
| 24  | CLA  | B     | 602    | -      | 69,73,73     | 1.42 | 9 (13%)  | 82,113,113  | 1.27 | 10 (12%) |
| 33  | STE  | B     | 620    | -      | 16,16,19     | 0.74 | 0        | 16,16,19    | 1.08 | 0        |
| 24  | CLA  | C     | 512    | -      | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.35 | 9 (10%)  |
| 30  | LHG  | d     | 409    | -      | 38,38,48     | 0.93 | 1 (2%)   | 41,44,54    | 1.19 | 2 (4%)   |
| 33  | STE  | x     | 102    | -      | 19,19,19     | 0.77 | 1 (5%)   | 19,19,19    | 1.09 | 1 (5%)   |
| 22  | OEX  | A     | 602[A] | 3,1,37 | 0,15,15      | -    | -        | -           | -    | -        |
| 29  | LMG  | c     | 519    | -      | 37,37,55     | 1.23 | 6 (16%)  | 45,45,63    | 1.35 | 6 (13%)  |
| 24  | CLA  | D     | 402    | -      | 69,73,73     | 1.21 | 10 (14%) | 82,113,113  | 1.34 | 8 (9%)   |
| 33  | STE  | I     | 101    | -      | 14,14,19     | 0.45 | 0        | 13,13,19    | 0.64 | 0        |
| 24  | CLA  | C     | 506    | -      | 69,73,73     | 1.72 | 10 (14%) | 82,113,113  | 1.22 | 7 (8%)   |
| 32  | DGD  | c     | 517    | -      | 63,63,67     | 1.22 | 8 (12%)  | 77,77,81    | 1.40 | 15 (19%) |
| 24  | CLA  | d     | 401    | 37     | 69,73,73     | 1.32 | 12 (17%) | 82,113,113  | 1.37 | 10 (12%) |
| 33  | STE  | D     | 411    | -      | 19,19,19     | 0.57 | 0        | 19,19,19    | 1.24 | 1 (5%)   |
| 26  | BCR  | c     | 515    | -      | 41,41,41     | 1.27 | 4 (9%)   | 56,56,56    | 1.35 | 8 (14%)  |
| 24  | CLA  | a     | 604    | -      | 69,73,73     | 1.25 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | STE  | B     | 627    | -      | 11,11,19     | 0.83 | 0        | 11,11,19    | 1.06 | 1 (9%)   |
| 24  | CLA  | C     | 513    | -      | 69,73,73     | 1.14 | 5 (7%)   | 82,113,113  | 1.43 | 10 (12%) |
| 33  | STE  | M     | 103    | -      | 9,9,19       | 0.41 | 0        | 8,8,19      | 0.88 | 0        |
| 34  | BCT  | D     | 401    | 23     | 3,3,3        | 0.99 | 0        | 2,3,3       | 3.31 | 1 (50%)  |
| 29  | LMG  | D     | 406    | -      | 51,51,55     | 0.96 | 3 (5%)   | 59,59,63    | 1.27 | 3 (5%)   |
| 24  | CLA  | A     | 604    | -      | 69,73,73     | 1.26 | 7 (10%)  | 82,113,113  | 1.24 | 10 (12%) |
| 33  | STE  | E     | 102    | -      | 11,11,19     | 0.88 | 0        | 11,11,19    | 1.18 | 1 (9%)   |
| 24  | CLA  | C     | 511    | 3      | 69,73,73     | 1.54 | 9 (13%)  | 82,113,113  | 1.32 | 7 (8%)   |
| 26  | BCR  | B     | 619    | -      | 41,41,41     | 1.27 | 5 (12%)  | 56,56,56    | 1.28 | 4 (7%)   |
| 30  | LHG  | A     | 615    | -      | 46,46,48     | 1.14 | 4 (8%)   | 49,52,54    | 1.39 | 5 (10%)  |
| 33  | STE  | Z     | 101    | -      | 7,7,19       | 0.48 | 0        | 6,6,19      | 0.46 | 0        |
| 24  | CLA  | C     | 510    | -      | 69,73,73     | 1.23 | 10 (14%) | 82,113,113  | 1.47 | 10 (12%) |
| 26  | BCR  | B     | 617    | -      | 41,41,41     | 1.14 | 3 (7%)   | 56,56,56    | 1.33 | 9 (16%)  |
| 24  | CLA  | A     | 608    | -      | 58,62,73     | 1.37 | 8 (13%)  | 68,99,113   | 1.30 | 6 (8%)   |
| 26  | BCR  | d     | 405    | -      | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 25  | PHO  | a     | 605    | -      | 58,69,69     | 1.90 | 12 (20%) | 55,99,99    | 1.62 | 10 (18%) |
| 32  | DGD  | C     | 518    | -      | 63,63,67     | 1.12 | 5 (7%)   | 77,77,81    | 1.34 | 8 (10%)  |
| 33  | STE  | J     | 101    | -      | 11,11,19     | 0.74 | 0        | 11,11,19    | 1.34 | 1 (9%)   |
| 21  | OEY  | A     | 601[B] | 3,1,37 | 0,16,16      | -    | -        | -           |      |          |
| 24  | CLA  | B     | 609    | -      | 69,73,73     | 1.46 | 9 (13%)  | 82,113,113  | 1.41 | 12 (14%) |
| 26  | BCR  | b     | 618    | -      | 41,41,41     | 1.28 | 4 (9%)   | 56,56,56    | 1.18 | 7 (12%)  |
| 30  | LHG  | B     | 622    | -      | 48,48,48     | 0.92 | 3 (6%)   | 51,54,54    | 1.35 | 8 (15%)  |
| 33  | STE  | C     | 520    | -      | 11,11,19     | 0.92 | 0        | 11,11,19    | 1.03 | 0        |
| 35  | HEM  | e     | 101    | 5,6    | 50,50,50     | 1.39 | 8 (16%)  | 67,82,82    | 1.23 | 6 (8%)   |
| 24  | CLA  | a     | 612    | 37     | 69,73,73     | 1.76 | 11 (15%) | 82,113,113  | 1.48 | 8 (9%)   |
| 24  | CLA  | b     | 616    | -      | 64,68,73     | 1.18 | 9 (14%)  | 76,107,113  | 1.41 | 8 (10%)  |
| 24  | CLA  | D     | 403    | -      | 69,73,73     | 1.56 | 10 (14%) | 82,113,113  | 1.31 | 6 (7%)   |
| 32  | DGD  | H     | 102    | -      | 63,63,67     | 1.35 | 13 (20%) | 77,77,81    | 1.38 | 8 (10%)  |
| 30  | LHG  | e     | 102    | -      | 41,41,48     | 0.89 | 2 (4%)   | 44,47,54    | 1.33 | 5 (11%)  |
| 24  | CLA  | c     | 510    | -      | 69,73,73     | 1.54 | 10 (14%) | 82,113,113  | 1.47 | 11 (13%) |
| 24  | CLA  | C     | 503    | -      | 69,73,73     | 1.31 | 7 (10%)  | 82,113,113  | 1.69 | 11 (13%) |
| 24  | CLA  | c     | 506    | -      | 69,73,73     | 1.43 | 11 (15%) | 82,113,113  | 1.39 | 8 (9%)   |
| 24  | CLA  | b     | 603    | -      | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.43 | 12 (14%) |
| 26  | BCR  | D     | 404    | -      | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.22 | 4 (7%)   |
| 24  | CLA  | b     | 601    | 37     | 69,73,73     | 1.27 | 8 (11%)  | 82,113,113  | 1.40 | 6 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | c     | 505 | -    | 69,73,73     | 1.19 | 10 (14%) | 82,113,113  | 1.31 | 7 (8%)   |
| 33  | STE  | j     | 101 | -    | 11,11,19     | 0.85 | 0        | 11,11,19    | 0.99 | 1 (9%)   |
| 33  | STE  | H     | 103 | -    | 17,17,19     | 0.51 | 0        | 16,16,19    | 0.69 | 0        |
| 33  | STE  | B     | 626 | -    | 15,15,19     | 0.46 | 0        | 14,14,19    | 0.67 | 0        |
| 33  | STE  | d     | 412 | -    | 19,19,19     | 0.55 | 0        | 19,19,19    | 1.14 | 0        |
| 33  | STE  | M     | 102 | -    | 14,14,19     | 0.62 | 0        | 14,14,19    | 1.14 | 1 (7%)   |
| 24  | CLA  | B     | 612 | -    | 69,73,73     | 1.32 | 8 (11%)  | 82,113,113  | 1.49 | 11 (13%) |
| 24  | CLA  | b     | 604 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.48 | 15 (18%) |
| 32  | DGD  | C     | 516 | -    | 63,63,67     | 1.29 | 9 (14%)  | 77,77,81    | 1.39 | 9 (11%)  |
| 24  | CLA  | C     | 508 | -    | 69,73,73     | 1.51 | 10 (14%) | 82,113,113  | 1.47 | 11 (13%) |
| 24  | CLA  | c     | 511 | 3    | 69,73,73     | 1.49 | 9 (13%)  | 82,113,113  | 1.29 | 4 (4%)   |
| 26  | BCR  | t     | 101 | -    | 41,41,41     | 1.15 | 5 (12%)  | 56,56,56    | 1.39 | 8 (14%)  |
| 33  | STE  | C     | 521 | -    | 15,15,19     | 0.37 | 0        | 14,14,19    | 0.86 | 0        |
| 29  | LMG  | A     | 614 | -    | 48,48,55     | 1.04 | 4 (8%)   | 56,56,63    | 1.41 | 6 (10%)  |
| 31  | SQD  | f     | 101 | -    | 39,41,54     | 1.12 | 4 (10%)  | 49,52,65    | 1.94 | 11 (22%) |
| 36  | HEC  | v     | 201 | 17   | 46,50,50     | 1.90 | 5 (10%)  | 58,82,82    | 1.95 | 7 (12%)  |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | CLA  | C     | 501 | -    | 1/1/20/20 | 3/39/115/115  | -       |
| 24  | CLA  | C     | 509 | -    | 1/1/20/20 | 16/39/115/115 | -       |
| 26  | BCR  | c     | 514 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 33  | STE  | a     | 616 | -    | -         | 3/9/9/17      | -       |
| 24  | CLA  | B     | 613 | -    | 1/1/20/20 | 14/39/115/115 | -       |
| 29  | LMG  | a     | 618 | -    | -         | 30/50/70/70   | 0/1/1/1 |
| 24  | CLA  | C     | 504 | 37   | 1/1/18/20 | 7/32/108/115  | -       |
| 29  | LMG  | c     | 522 | -    | -         | 20/44/64/70   | 0/1/1/1 |
| 25  | PHO  | A     | 606 | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 32  | DGD  | c     | 516 | -    | -         | 28/51/91/95   | 0/2/2/2 |
| 33  | STE  | B     | 624 | -    | -         | 3/11/11/17    | -       |
| 24  | CLA  | d     | 404 | -    | 1/1/20/20 | 11/39/115/115 | -       |
| 29  | LMG  | c     | 521 | -    | -         | 23/43/63/70   | 0/1/1/1 |
| 31  | SQD  | a     | 614 | -    | -         | 18/37/37/69   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 26  | BCR  | B     | 618 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 33  | STE  | b     | 625 | -    | -         | 12/17/17/17   | -       |
| 24  | CLA  | b     | 615 | -    | 1/1/20/20 | 8/39/115/115  | -       |
| 26  | BCR  | A     | 609 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 24  | CLA  | B     | 615 | -    | 1/1/20/20 | 12/39/115/115 | -       |
| 24  | CLA  | b     | 612 | -    | 1/1/20/20 | 6/39/115/115  | -       |
| 33  | STE  | B     | 625 | -    | -         | 5/9/9/17      | -       |
| 33  | STE  | a     | 617 | -    | -         | 8/12/12/17    | -       |
| 30  | LHG  | d     | 408 | -    | -         | 18/53/53/53   | -       |
| 24  | CLA  | C     | 502 | -    | -         | 5/39/115/115  | -       |
| 24  | CLA  | b     | 605 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 24  | CLA  | B     | 603 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 33  | STE  | b     | 627 | -    | -         | 6/11/11/17    | -       |
| 24  | CLA  | b     | 608 | -    | -         | 1/39/115/115  | -       |
| 31  | SQD  | b     | 620 | -    | -         | 20/44/64/69   | 0/1/1/1 |
| 24  | CLA  | b     | 607 | 37   | 1/1/20/20 | 12/39/115/115 | -       |
| 33  | STE  | c     | 520 | -    | -         | 10/17/17/17   | -       |
| 25  | PHO  | d     | 402 | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 33  | STE  | b     | 626 | -    | -         | 5/7/7/17      | -       |
| 24  | CLA  | b     | 602 | -    | -         | 4/39/115/115  | -       |
| 24  | CLA  | B     | 610 | 37   | 1/1/20/20 | 5/39/115/115  | -       |
| 24  | CLA  | c     | 508 | -    | -         | 7/38/114/115  | -       |
| 25  | PHO  | A     | 607 | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 32  | DGD  | h     | 101 | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 24  | CLA  | c     | 503 | -    | 1/1/20/20 | 6/39/115/115  | -       |
| 30  | LHG  | B     | 621 | -    | -         | 25/53/53/53   | -       |
| 24  | CLA  | B     | 614 | -    | 1/1/20/20 | 15/39/115/115 | -       |
| 24  | CLA  | B     | 604 | -    | 1/1/20/20 | 8/39/115/115  | -       |
| 24  | CLA  | c     | 502 | -    | -         | 3/39/115/115  | -       |
| 24  | CLA  | b     | 613 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 33  | STE  | T     | 102 | -    | -         | 8/13/13/17    | -       |
| 29  | LMG  | D     | 409 | -    | -         | 16/33/33/70   | -       |
| 29  | LMG  | D     | 410 | -    | -         | 14/22/22/70   | -       |
| 24  | CLA  | A     | 613 | 37   | -         | 4/39/115/115  | -       |
| 24  | CLA  | B     | 605 | -    | 1/1/20/20 | 9/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 33  | STE  | C     | 522 | -    | -         | 3/9/9/17      | -       |
| 31  | SQD  | A     | 617 | -    | -         | 13/39/39/69   | -       |
| 24  | CLA  | b     | 609 | -    | -         | 9/39/115/115  | -       |
| 24  | CLA  | C     | 505 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 30  | LHG  | D     | 408 | -    | -         | 23/53/53/53   | -       |
| 30  | LHG  | E     | 101 | -    | -         | 22/53/53/53   | -       |
| 31  | SQD  | D     | 407 | -    | -         | 14/28/48/69   | 0/1/1/1 |
| 24  | CLA  | c     | 512 | -    | 1/1/20/20 | 20/39/115/115 | -       |
| 24  | CLA  | B     | 601 | 37   | 1/1/20/20 | 15/39/115/115 | -       |
| 33  | STE  | b     | 624 | -    | -         | 10/13/13/17   | -       |
| 33  | STE  | t     | 102 | -    | -         | 9/15/15/17    | -       |
| 24  | CLA  | d     | 403 | -    | 1/1/20/20 | 5/39/115/115  | -       |
| 26  | BCR  | T     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 29  | LMG  | b     | 623 | -    | -         | 25/50/70/70   | 0/1/1/1 |
| 24  | CLA  | b     | 610 | 37   | 1/1/20/20 | 4/39/115/115  | -       |
| 24  | CLA  | c     | 501 | -    | 1/1/20/20 | 1/39/115/115  | -       |
| 26  | BCR  | Y     | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 24  | CLA  | b     | 606 | -    | 1/1/20/20 | 9/39/115/115  | -       |
| 24  | CLA  | B     | 611 | -    | 1/1/20/20 | 6/39/115/115  | -       |
| 28  | PL9  | a     | 611 | -    | -         | 22/53/73/73   | 0/1/1/1 |
| 26  | BCR  | C     | 514 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 26  | BCR  | x     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 24  | CLA  | C     | 507 | 37   | 1/1/20/20 | 11/39/115/115 | -       |
| 29  | LMG  | d     | 410 | -    | -         | 11/39/59/70   | 0/1/1/1 |
| 29  | LMG  | M     | 101 | -    | -         | 24/46/66/70   | 0/1/1/1 |
| 33  | STE  | l     | 102 | -    | -         | 9/15/15/17    | -       |
| 24  | CLA  | A     | 605 | 37   | 1/1/20/20 | 11/39/115/115 | -       |
| 33  | STE  | k     | 103 | -    | -         | 4/9/9/17      | -       |
| 26  | BCR  | k     | 102 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 33  | STE  | d     | 411 | -    | -         | 8/14/14/17    | -       |
| 29  | LMG  | b     | 621 | -    | -         | 24/46/66/70   | 0/1/1/1 |
| 33  | STE  | a     | 615 | -    | -         | 4/7/7/17      | -       |
| 36  | HEC  | V     | 201 | 17   | -         | 6/14/54/54    | -       |
| 31  | SQD  | A     | 616 | -    | -         | 15/47/67/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 33  | STE  | m     | 101 | -    | -         | 3/9/9/17      | -       |
| 32  | DGD  | A     | 618 | -    | -         | 27/55/95/95   | 0/2/2/2 |
| 24  | CLA  | B     | 607 | 37   | 1/1/20/20 | 4/39/115/115  | -       |
| 24  | CLA  | c     | 509 | -    | 1/1/20/20 | 11/39/115/115 | -       |
| 31  | SQD  | a     | 613 | -    | -         | 22/49/69/69   | 0/1/1/1 |
| 26  | BCR  | C     | 515 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 26  | BCR  | a     | 607 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 33  | STE  | b     | 622 | -    | -         | 10/17/17/17   | -       |
| 26  | BCR  | H     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 35  | HEM  | F     | 101 | 5,6  | -         | 2/14/54/54    | -       |
| 26  | BCR  | k     | 101 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 24  | CLA  | a     | 606 | -    | 1/1/20/20 | 8/39/115/115  | -       |
| 30  | LHG  | l     | 101 | -    | -         | 15/53/53/53   | -       |
| 28  | PL9  | D     | 405 | -    | -         | 10/53/73/73   | 0/1/1/1 |
| 32  | DGD  | c     | 518 | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 26  | BCR  | K     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 24  | CLA  | c     | 504 | 37   | 1/1/19/20 | 7/33/109/115  | -       |
| 29  | LMG  | C     | 519 | -    | -         | 17/43/63/70   | 0/1/1/1 |
| 32  | DGD  | C     | 517 | -    | -         | 23/51/91/95   | 0/2/2/2 |
| 33  | STE  | T     | 103 | -    | -         | 11/12/12/17   | -       |
| 30  | LHG  | d     | 407 | -    | -         | 21/53/53/53   | -       |
| 28  | PL9  | d     | 406 | -    | -         | 11/53/73/73   | 0/1/1/1 |
| 24  | CLA  | b     | 611 | -    | 1/1/20/20 | 5/39/115/115  | -       |
| 31  | SQD  | B     | 623 | -    | -         | 22/49/69/69   | 0/1/1/1 |
| 24  | CLA  | b     | 614 | -    | 1/1/20/20 | 12/39/115/115 | -       |
| 26  | BCR  | b     | 619 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 28  | PL9  | A     | 612 | -    | -         | 24/53/73/73   | 0/1/1/1 |
| 24  | CLA  | B     | 616 | -    | 1/1/19/20 | 8/33/109/115  | -       |
| 24  | CLA  | c     | 507 | 37   | 1/1/20/20 | 10/39/115/115 | -       |
| 24  | CLA  | c     | 513 | -    | 1/1/20/20 | 6/39/115/115  | -       |
| 26  | BCR  | b     | 617 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 24  | CLA  | B     | 606 | -    | 1/1/20/20 | 11/39/115/115 | -       |
| 24  | CLA  | B     | 608 | -    | -         | 2/39/115/115  | -       |
| 24  | CLA  | B     | 602 | -    | 1/1/20/20 | 6/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 33  | STE  | B     | 620 | -    | -         | 5/14/14/17    | -       |
| 24  | CLA  | C     | 512 | -    | 1/1/20/20 | 12/39/115/115 | -       |
| 30  | LHG  | d     | 409 | -    | -         | 14/43/43/53   | -       |
| 33  | STE  | x     | 102 | -    | -         | 6/17/17/17    | -       |
| 33  | STE  | I     | 101 | -    | -         | 4/12/12/17    | -       |
| 29  | LMG  | c     | 519 | -    | -         | 11/31/51/70   | 0/1/1/1 |
| 24  | CLA  | D     | 402 | -    | 1/1/20/20 | 5/39/115/115  | -       |
| 24  | CLA  | C     | 506 | -    | 1/1/20/20 | 9/39/115/115  | -       |
| 32  | DGD  | c     | 517 | -    | -         | 18/51/91/95   | 0/2/2/2 |
| 24  | CLA  | d     | 401 | 37   | -         | 12/39/115/115 | -       |
| 33  | STE  | D     | 411 | -    | -         | 11/17/17/17   | -       |
| 26  | BCR  | c     | 515 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 24  | CLA  | a     | 604 | -    | 1/1/20/20 | 4/39/115/115  | -       |
| 33  | STE  | B     | 627 | -    | -         | 5/9/9/17      | -       |
| 24  | CLA  | C     | 513 | -    | 1/1/20/20 | 5/39/115/115  | -       |
| 33  | STE  | M     | 103 | -    | -         | 1/7/7/17      | -       |
| 29  | LMG  | D     | 406 | -    | -         | 14/46/66/70   | 0/1/1/1 |
| 24  | CLA  | A     | 604 | -    | 1/1/20/20 | 4/39/115/115  | -       |
| 33  | STE  | E     | 102 | -    | -         | 4/9/9/17      | -       |
| 24  | CLA  | C     | 511 | 3    | 1/1/20/20 | 3/39/115/115  | -       |
| 26  | BCR  | B     | 619 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 30  | LHG  | A     | 615 | -    | -         | 20/51/51/53   | -       |
| 33  | STE  | Z     | 101 | -    | -         | 2/5/5/17      | -       |
| 24  | CLA  | C     | 510 | -    | 1/1/20/20 | 9/39/115/115  | -       |
| 26  | BCR  | B     | 617 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 24  | CLA  | A     | 608 | -    | 1/1/17/20 | 2/26/102/115  | -       |
| 26  | BCR  | d     | 405 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 25  | PHO  | a     | 605 | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 32  | DGD  | C     | 518 | -    | -         | 18/51/91/95   | 0/2/2/2 |
| 33  | STE  | J     | 101 | -    | -         | 7/9/9/17      | -       |
| 24  | CLA  | B     | 609 | -    | -         | 3/39/115/115  | -       |
| 26  | BCR  | b     | 618 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 30  | LHG  | B     | 622 | -    | -         | 14/53/53/53   | -       |
| 33  | STE  | C     | 520 | -    | -         | 6/9/9/17      | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 35  | HEM  | e     | 101 | 5,6  | -         | 3/14/54/54    | -       |
| 24  | CLA  | a     | 612 | 37   | 1/1/20/20 | 4/39/115/115  | -       |
| 24  | CLA  | b     | 616 | -    | 1/1/19/20 | 10/33/109/115 | -       |
| 24  | CLA  | D     | 403 | -    | -         | 9/39/115/115  | -       |
| 32  | DGD  | H     | 102 | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 30  | LHG  | e     | 102 | -    | -         | 26/46/46/53   | -       |
| 24  | CLA  | c     | 510 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 24  | CLA  | C     | 503 | -    | 1/1/20/20 | 2/39/115/115  | -       |
| 24  | CLA  | c     | 506 | -    | 1/1/20/20 | 13/39/115/115 | -       |
| 24  | CLA  | b     | 603 | -    | 1/1/20/20 | 8/39/115/115  | -       |
| 26  | BCR  | D     | 404 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 24  | CLA  | b     | 601 | 37   | 1/1/20/20 | 16/39/115/115 | -       |
| 24  | CLA  | c     | 505 | -    | 1/1/20/20 | 11/39/115/115 | -       |
| 33  | STE  | j     | 101 | -    | -         | 4/9/9/17      | -       |
| 33  | STE  | H     | 103 | -    | -         | 9/15/15/17    | -       |
| 33  | STE  | B     | 626 | -    | -         | 8/13/13/17    | -       |
| 33  | STE  | d     | 412 | -    | -         | 11/17/17/17   | -       |
| 33  | STE  | M     | 102 | -    | -         | 5/12/12/17    | -       |
| 24  | CLA  | B     | 612 | -    | 1/1/20/20 | 8/39/115/115  | -       |
| 24  | CLA  | b     | 604 | -    | 1/1/20/20 | 7/39/115/115  | -       |
| 32  | DGD  | C     | 516 | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 24  | CLA  | C     | 508 | -    | -         | 7/39/115/115  | -       |
| 24  | CLA  | c     | 511 | 3    | 1/1/20/20 | 11/39/115/115 | -       |
| 26  | BCR  | t     | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 33  | STE  | C     | 521 | -    | -         | 7/13/13/17    | -       |
| 29  | LMG  | A     | 614 | -    | -         | 21/43/63/70   | 0/1/1/1 |
| 31  | SQD  | f     | 101 | -    | -         | 13/36/56/69   | 0/1/1/1 |
| 36  | HEC  | v     | 201 | 17   | -         | 6/14/54/54    | -       |

All (900) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24  | b     | 606 | CLA  | MG-NA   | 9.48 | 2.28        | 2.06     |
| 25  | d     | 402 | PHO  | C1B-C2B | 9.37 | 1.49        | 1.39     |
| 25  | A     | 607 | PHO  | C3B-C4B | 9.23 | 1.50        | 1.41     |
| 25  | d     | 402 | PHO  | C3B-C4B | 9.22 | 1.50        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | a     | 606 | CLA  | MG-ND   | -8.26 | 1.89        | 2.05     |
| 25  | A     | 607 | PHO  | C1B-C2B | 8.11  | 1.48        | 1.39     |
| 25  | a     | 605 | PHO  | C1B-C2B | 8.00  | 1.48        | 1.39     |
| 24  | C     | 506 | CLA  | MG-ND   | -7.96 | 1.90        | 2.05     |
| 24  | a     | 612 | CLA  | MG-NA   | 7.78  | 2.24        | 2.06     |
| 24  | c     | 511 | CLA  | MG-NA   | 7.69  | 2.24        | 2.06     |
| 24  | D     | 403 | CLA  | MG-NB   | -7.43 | 1.91        | 2.05     |
| 24  | c     | 510 | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 25  | A     | 606 | PHO  | C1B-C2B | 7.35  | 1.47        | 1.39     |
| 24  | b     | 612 | CLA  | MG-NC   | -7.19 | 1.89        | 2.06     |
| 24  | B     | 611 | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 24  | B     | 610 | CLA  | MG-ND   | -6.97 | 1.92        | 2.05     |
| 24  | C     | 501 | CLA  | MG-NA   | 6.56  | 2.21        | 2.06     |
| 24  | b     | 614 | CLA  | MG-ND   | -6.47 | 1.93        | 2.05     |
| 36  | v     | 201 | HEC  | CAC-C3C | 6.26  | 1.55        | 1.35     |
| 36  | V     | 201 | HEC  | CAC-C3C | 6.24  | 1.55        | 1.35     |
| 24  | b     | 609 | CLA  | MG-NA   | 6.23  | 2.21        | 2.06     |
| 36  | v     | 201 | HEC  | CAB-C3B | 6.22  | 1.55        | 1.35     |
| 24  | C     | 511 | CLA  | MG-NA   | 6.03  | 2.20        | 2.06     |
| 36  | V     | 201 | HEC  | CAB-C3B | 6.01  | 1.54        | 1.35     |
| 24  | C     | 505 | CLA  | MG-NA   | 5.97  | 2.20        | 2.06     |
| 24  | B     | 616 | CLA  | MG-NA   | 5.94  | 2.20        | 2.06     |
| 24  | C     | 508 | CLA  | MG-NA   | 5.93  | 2.20        | 2.06     |
| 24  | B     | 609 | CLA  | MG-NA   | 5.93  | 2.20        | 2.06     |
| 28  | d     | 406 | PL9  | C6-C1   | -5.92 | 1.38        | 1.48     |
| 24  | a     | 612 | CLA  | MG-NB   | 5.83  | 2.17        | 2.05     |
| 25  | a     | 605 | PHO  | C3B-C4B | 5.83  | 1.47        | 1.41     |
| 24  | b     | 615 | CLA  | MG-NB   | 5.82  | 2.17        | 2.05     |
| 24  | C     | 503 | CLA  | MG-NA   | 5.81  | 2.20        | 2.06     |
| 24  | b     | 611 | CLA  | MG-NB   | 5.45  | 2.16        | 2.05     |
| 24  | d     | 404 | CLA  | MG-NB   | -5.28 | 1.95        | 2.05     |
| 24  | C     | 507 | CLA  | MG-NA   | 5.28  | 2.18        | 2.06     |
| 24  | c     | 506 | CLA  | MG-NB   | 5.25  | 2.16        | 2.05     |
| 36  | v     | 201 | HEC  | C3D-C2D | 5.21  | 1.52        | 1.38     |
| 24  | C     | 506 | CLA  | MG-NB   | 5.09  | 2.15        | 2.05     |
| 24  | d     | 404 | CLA  | MG-NA   | 4.95  | 2.18        | 2.06     |
| 24  | b     | 610 | CLA  | MG-ND   | -4.89 | 1.96        | 2.05     |
| 24  | B     | 609 | CLA  | MG-NB   | -4.87 | 1.96        | 2.05     |
| 24  | B     | 602 | CLA  | C1D-ND  | 4.86  | 1.44        | 1.37     |
| 24  | B     | 612 | CLA  | MG-NC   | 4.84  | 2.17        | 2.06     |
| 24  | c     | 508 | CLA  | MG-NA   | 4.83  | 2.17        | 2.06     |
| 24  | B     | 603 | CLA  | MG-NA   | 4.81  | 2.17        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | D     | 408 | LHG  | O7-C5   | -4.75 | 1.35        | 1.46     |
| 24  | c     | 513 | CLA  | MG-ND   | -4.74 | 1.96        | 2.05     |
| 24  | b     | 615 | CLA  | MG-NA   | 4.73  | 2.17        | 2.06     |
| 24  | b     | 609 | CLA  | MG-ND   | -4.71 | 1.96        | 2.05     |
| 24  | A     | 608 | CLA  | MG-ND   | -4.71 | 1.96        | 2.05     |
| 24  | A     | 608 | CLA  | C1D-ND  | 4.68  | 1.44        | 1.37     |
| 24  | b     | 612 | CLA  | MG-NB   | 4.67  | 2.15        | 2.05     |
| 28  | d     | 406 | PL9  | C53-C6  | -4.62 | 1.41        | 1.50     |
| 24  | c     | 509 | CLA  | MG-NB   | 4.62  | 2.14        | 2.05     |
| 24  | C     | 511 | CLA  | MG-ND   | 4.59  | 2.14        | 2.05     |
| 25  | a     | 605 | PHO  | C1D-C2D | 4.57  | 1.44        | 1.39     |
| 24  | B     | 604 | CLA  | MG-NC   | 4.56  | 2.17        | 2.06     |
| 24  | b     | 603 | CLA  | MG-NA   | 4.55  | 2.17        | 2.06     |
| 24  | c     | 509 | CLA  | C1D-ND  | 4.51  | 1.43        | 1.37     |
| 24  | b     | 606 | CLA  | MG-NB   | -4.48 | 1.96        | 2.05     |
| 24  | B     | 602 | CLA  | MG-NB   | -4.47 | 1.96        | 2.05     |
| 24  | b     | 610 | CLA  | C1D-ND  | 4.44  | 1.43        | 1.37     |
| 36  | V     | 201 | HEC  | C3D-C2D | 4.42  | 1.50        | 1.38     |
| 24  | C     | 502 | CLA  | MG-NA   | 4.39  | 2.16        | 2.06     |
| 26  | c     | 515 | BCR  | C1-C6   | -4.37 | 1.48        | 1.53     |
| 32  | A     | 618 | DGD  | O5D-C6D | -4.35 | 1.36        | 1.43     |
| 24  | B     | 606 | CLA  | MG-NA   | 4.35  | 2.16        | 2.06     |
| 26  | B     | 618 | BCR  | C30-C25 | -4.33 | 1.48        | 1.53     |
| 24  | C     | 506 | CLA  | MG-NA   | 4.32  | 2.16        | 2.06     |
| 26  | Y     | 101 | BCR  | C30-C25 | -4.31 | 1.48        | 1.53     |
| 24  | C     | 511 | CLA  | MG-NB   | -4.31 | 1.97        | 2.05     |
| 24  | d     | 403 | CLA  | C4B-NB  | 4.30  | 1.43        | 1.37     |
| 24  | b     | 602 | CLA  | MG-NB   | 4.26  | 2.14        | 2.05     |
| 24  | c     | 507 | CLA  | MG-ND   | 4.20  | 2.14        | 2.05     |
| 24  | C     | 509 | CLA  | C1D-ND  | 4.19  | 1.43        | 1.37     |
| 26  | C     | 515 | BCR  | C1-C6   | -4.13 | 1.48        | 1.53     |
| 30  | A     | 615 | LHG  | O3-C3   | -4.09 | 1.29        | 1.44     |
| 24  | C     | 508 | CLA  | MG-NC   | -4.09 | 1.96        | 2.06     |
| 25  | A     | 606 | PHO  | C3B-C4B | 4.09  | 1.45        | 1.41     |
| 24  | a     | 612 | CLA  | C1D-ND  | 4.06  | 1.43        | 1.37     |
| 24  | c     | 508 | CLA  | MG-NB   | 4.04  | 2.13        | 2.05     |
| 24  | A     | 605 | CLA  | MG-NB   | -4.01 | 1.97        | 2.05     |
| 24  | b     | 601 | CLA  | MG-NA   | 4.01  | 2.15        | 2.06     |
| 28  | D     | 405 | PL9  | C3-C4   | -4.01 | 1.43        | 1.49     |
| 24  | C     | 508 | CLA  | MG-ND   | 4.01  | 2.13        | 2.05     |
| 32  | C     | 518 | DGD  | O2G-C2G | -4.00 | 1.37        | 1.46     |
| 26  | c     | 514 | BCR  | C1-C6   | -3.98 | 1.48        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | H     | 101 | BCR  | C30-C25 | -3.95 | 1.48        | 1.53     |
| 26  | D     | 404 | BCR  | C30-C25 | -3.94 | 1.48        | 1.53     |
| 24  | b     | 607 | CLA  | C1B-NB  | -3.94 | 1.32        | 1.37     |
| 24  | B     | 615 | CLA  | MG-NA   | 3.93  | 2.15        | 2.06     |
| 29  | a     | 618 | LMG  | C4-C5   | 3.93  | 1.61        | 1.53     |
| 29  | D     | 409 | LMG  | C7-C8   | 3.92  | 1.60        | 1.51     |
| 24  | c     | 504 | CLA  | C4B-NB  | 3.89  | 1.43        | 1.37     |
| 24  | b     | 603 | CLA  | C4B-NB  | 3.86  | 1.42        | 1.37     |
| 26  | C     | 514 | BCR  | C1-C6   | -3.85 | 1.48        | 1.53     |
| 26  | B     | 619 | BCR  | C1-C6   | -3.82 | 1.48        | 1.53     |
| 24  | c     | 504 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 26  | K     | 101 | BCR  | C30-C25 | -3.81 | 1.48        | 1.53     |
| 26  | T     | 101 | BCR  | C30-C25 | -3.79 | 1.48        | 1.53     |
| 26  | d     | 405 | BCR  | C30-C25 | -3.79 | 1.48        | 1.53     |
| 24  | b     | 606 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 24  | c     | 506 | CLA  | C1B-NB  | -3.79 | 1.32        | 1.37     |
| 24  | b     | 615 | CLA  | C1B-C2B | 3.77  | 1.52        | 1.43     |
| 24  | b     | 612 | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 24  | c     | 510 | CLA  | MG-NC   | -3.71 | 1.97        | 2.06     |
| 24  | c     | 506 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 32  | c     | 518 | DGD  | O3G-C3G | -3.70 | 1.37        | 1.43     |
| 31  | b     | 620 | SQD  | O48-C23 | 3.70  | 1.44        | 1.33     |
| 26  | C     | 514 | BCR  | C30-C25 | -3.69 | 1.49        | 1.53     |
| 24  | B     | 605 | CLA  | C1B-C2B | 3.69  | 1.51        | 1.43     |
| 30  | B     | 621 | LHG  | O7-C5   | -3.68 | 1.38        | 1.46     |
| 24  | c     | 501 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 24  | B     | 612 | CLA  | C4B-NB  | 3.64  | 1.42        | 1.37     |
| 24  | b     | 609 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 26  | k     | 101 | BCR  | C30-C25 | -3.62 | 1.49        | 1.53     |
| 24  | D     | 403 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 24  | c     | 508 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 24  | B     | 605 | CLA  | MG-NB   | 3.60  | 2.12        | 2.05     |
| 24  | A     | 604 | CLA  | MG-NC   | 3.59  | 2.14        | 2.06     |
| 32  | C     | 517 | DGD  | O5D-C6D | -3.59 | 1.37        | 1.43     |
| 28  | D     | 405 | PL9  | C7-C3   | -3.58 | 1.46        | 1.51     |
| 28  | d     | 406 | PL9  | C31-C29 | -3.57 | 1.43        | 1.51     |
| 31  | a     | 613 | SQD  | O48-C23 | 3.57  | 1.43        | 1.33     |
| 31  | a     | 614 | SQD  | O48-C23 | 3.55  | 1.43        | 1.33     |
| 29  | A     | 614 | LMG  | O1-C7   | -3.55 | 1.37        | 1.43     |
| 30  | A     | 615 | LHG  | P-O6    | 3.53  | 1.73        | 1.59     |
| 25  | d     | 402 | PHO  | CMC-C2C | -3.53 | 1.45        | 1.50     |
| 24  | b     | 603 | CLA  | MG-NB   | -3.52 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 612 | CLA  | MG-NA   | 3.51  | 2.14        | 2.06     |
| 28  | D     | 405 | PL9  | C6-C1   | -3.51 | 1.42        | 1.48     |
| 24  | a     | 604 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 24  | c     | 502 | CLA  | MG-NB   | -3.49 | 1.98        | 2.05     |
| 26  | k     | 102 | BCR  | C30-C25 | -3.49 | 1.49        | 1.53     |
| 26  | b     | 618 | BCR  | C1-C6   | -3.49 | 1.49        | 1.53     |
| 24  | d     | 401 | CLA  | MG-NB   | 3.48  | 2.12        | 2.05     |
| 29  | c     | 521 | LMG  | O1-C1   | 3.48  | 1.46        | 1.40     |
| 24  | A     | 605 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 26  | c     | 514 | BCR  | C30-C25 | -3.48 | 1.49        | 1.53     |
| 24  | C     | 506 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 28  | D     | 405 | PL9  | C26-C24 | -3.45 | 1.44        | 1.51     |
| 24  | B     | 602 | CLA  | C4B-NB  | 3.45  | 1.42        | 1.37     |
| 29  | c     | 519 | LMG  | C1-C2   | 3.44  | 1.62        | 1.52     |
| 25  | A     | 606 | PHO  | C3D-C4D | 3.44  | 1.45        | 1.41     |
| 24  | B     | 601 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 24  | B     | 609 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 24  | A     | 604 | CLA  | C4B-NB  | 3.42  | 1.42        | 1.37     |
| 24  | B     | 612 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 24  | b     | 613 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 26  | B     | 617 | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 24  | D     | 403 | CLA  | MG-NC   | 3.40  | 2.14        | 2.06     |
| 26  | C     | 515 | BCR  | C30-C25 | -3.40 | 1.49        | 1.53     |
| 25  | a     | 605 | PHO  | C3D-C4D | 3.39  | 1.45        | 1.41     |
| 24  | B     | 601 | CLA  | MG-ND   | -3.39 | 1.99        | 2.05     |
| 24  | b     | 613 | CLA  | MG-ND   | -3.39 | 1.99        | 2.05     |
| 24  | A     | 613 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 32  | C     | 517 | DGD  | C4D-C3D | 3.39  | 1.61        | 1.52     |
| 26  | b     | 618 | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 24  | C     | 501 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 24  | b     | 601 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 24  | A     | 604 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 30  | d     | 407 | LHG  | C24-C23 | 3.36  | 1.60        | 1.50     |
| 25  | A     | 606 | PHO  | C4D-ND  | -3.36 | 1.33        | 1.38     |
| 25  | A     | 606 | PHO  | CMC-C2C | -3.34 | 1.45        | 1.50     |
| 31  | B     | 623 | SQD  | O47-C7  | 3.33  | 1.43        | 1.34     |
| 26  | b     | 617 | BCR  | C30-C25 | -3.33 | 1.49        | 1.53     |
| 24  | b     | 605 | CLA  | C1B-C2B | 3.32  | 1.50        | 1.43     |
| 24  | C     | 513 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 24  | d     | 403 | CLA  | MG-ND   | -3.31 | 1.99        | 2.05     |
| 24  | B     | 614 | CLA  | C4B-NB  | 3.31  | 1.42        | 1.37     |
| 26  | x     | 101 | BCR  | C30-C25 | -3.31 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 614 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 24  | B     | 613 | CLA  | C4B-NB  | 3.30  | 1.42        | 1.37     |
| 26  | c     | 515 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 31  | D     | 407 | SQD  | O48-C23 | 3.30  | 1.43        | 1.33     |
| 28  | d     | 406 | PL9  | C3-C4   | -3.30 | 1.44        | 1.49     |
| 24  | c     | 505 | CLA  | MG-NA   | 3.29  | 2.14        | 2.06     |
| 24  | b     | 601 | CLA  | C1B-C2B | 3.27  | 1.50        | 1.43     |
| 24  | b     | 615 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 24  | B     | 615 | CLA  | C4B-NB  | 3.27  | 1.42        | 1.37     |
| 24  | a     | 604 | CLA  | MG-NC   | 3.26  | 2.14        | 2.06     |
| 32  | c     | 517 | DGD  | C3E-C2E | 3.26  | 1.60        | 1.52     |
| 24  | B     | 602 | CLA  | MG-NA   | 3.25  | 2.14        | 2.06     |
| 29  | d     | 410 | LMG  | C4-C5   | 3.25  | 1.60        | 1.53     |
| 24  | a     | 606 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 24  | b     | 615 | CLA  | C3B-C4B | 3.25  | 1.52        | 1.42     |
| 24  | A     | 613 | CLA  | MG-NB   | 3.24  | 2.12        | 2.05     |
| 24  | d     | 401 | CLA  | MG-NC   | 3.22  | 2.13        | 2.06     |
| 26  | Y     | 101 | BCR  | C1-C6   | -3.22 | 1.49        | 1.53     |
| 24  | c     | 510 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 24  | c     | 503 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 24  | B     | 616 | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 31  | a     | 614 | SQD  | O47-C7  | 3.20  | 1.43        | 1.34     |
| 24  | b     | 613 | CLA  | C1B-NB  | -3.20 | 1.33        | 1.37     |
| 32  | h     | 101 | DGD  | O2D-C2D | -3.20 | 1.35        | 1.43     |
| 24  | B     | 613 | CLA  | CMD-C2D | -3.20 | 1.44        | 1.50     |
| 24  | A     | 613 | CLA  | MG-NA   | 3.20  | 2.13        | 2.06     |
| 24  | B     | 615 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 24  | c     | 507 | CLA  | MG-NB   | -3.18 | 1.99        | 2.05     |
| 24  | B     | 607 | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 32  | C     | 516 | DGD  | C6D-C5D | 3.18  | 1.61        | 1.51     |
| 30  | E     | 101 | LHG  | P-O6    | 3.17  | 1.71        | 1.59     |
| 28  | a     | 611 | PL9  | C3-C4   | -3.17 | 1.44        | 1.49     |
| 32  | H     | 102 | DGD  | O3G-C1D | 3.17  | 1.45        | 1.40     |
| 30  | B     | 622 | LHG  | O7-C5   | -3.17 | 1.39        | 1.46     |
| 31  | B     | 623 | SQD  | O48-C23 | 3.17  | 1.42        | 1.33     |
| 24  | B     | 607 | CLA  | MG-NA   | 3.16  | 2.13        | 2.06     |
| 26  | b     | 619 | BCR  | C30-C25 | -3.16 | 1.49        | 1.53     |
| 32  | A     | 618 | DGD  | C4D-C3D | 3.16  | 1.60        | 1.52     |
| 24  | C     | 509 | CLA  | MG-NB   | -3.15 | 1.99        | 2.05     |
| 24  | c     | 511 | CLA  | MG-NC   | -3.15 | 1.98        | 2.06     |
| 32  | H     | 102 | DGD  | O2D-C2D | -3.15 | 1.35        | 1.43     |
| 24  | B     | 604 | CLA  | MG-NA   | 3.15  | 2.13        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | A     | 609 | BCR  | C33-C5  | -3.15 | 1.45        | 1.50     |
| 26  | d     | 405 | BCR  | C1-C6   | -3.15 | 1.49        | 1.53     |
| 24  | d     | 403 | CLA  | C1B-C2B | 3.14  | 1.50        | 1.43     |
| 31  | A     | 617 | SQD  | O47-C7  | 3.14  | 1.43        | 1.34     |
| 26  | t     | 101 | BCR  | C30-C25 | -3.14 | 1.49        | 1.53     |
| 24  | B     | 603 | CLA  | C1D-ND  | 3.13  | 1.42        | 1.37     |
| 24  | C     | 511 | CLA  | C3B-C4B | 3.13  | 1.51        | 1.42     |
| 25  | a     | 605 | PHO  | C4D-ND  | -3.13 | 1.33        | 1.38     |
| 32  | H     | 102 | DGD  | O5D-C1E | 3.13  | 1.45        | 1.40     |
| 24  | A     | 605 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 32  | A     | 618 | DGD  | C3E-C2E | 3.12  | 1.60        | 1.52     |
| 24  | b     | 616 | CLA  | C1D-ND  | 3.12  | 1.42        | 1.37     |
| 26  | b     | 619 | BCR  | C1-C6   | -3.11 | 1.49        | 1.53     |
| 24  | C     | 507 | CLA  | MG-NB   | -3.10 | 1.99        | 2.05     |
| 24  | b     | 603 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 31  | A     | 616 | SQD  | O48-C23 | 3.08  | 1.42        | 1.33     |
| 24  | a     | 612 | CLA  | MG-ND   | -3.08 | 1.99        | 2.05     |
| 24  | B     | 603 | CLA  | CMB-C2B | -3.07 | 1.44        | 1.50     |
| 24  | C     | 509 | CLA  | C3B-C4B | 3.07  | 1.51        | 1.42     |
| 31  | f     | 101 | SQD  | O48-C23 | 3.07  | 1.42        | 1.33     |
| 24  | B     | 615 | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 32  | c     | 516 | DGD  | O2G-C2G | -3.07 | 1.39        | 1.46     |
| 24  | B     | 601 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |
| 24  | b     | 606 | CLA  | MG-ND   | 3.07  | 2.11        | 2.05     |
| 24  | b     | 604 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 32  | C     | 516 | DGD  | O5D-C1E | 3.06  | 1.45        | 1.40     |
| 24  | b     | 608 | CLA  | MG-ND   | 3.05  | 2.11        | 2.05     |
| 24  | c     | 509 | CLA  | C1B-C2B | 3.05  | 1.50        | 1.43     |
| 24  | C     | 510 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 26  | A     | 609 | BCR  | C1-C6   | -3.05 | 1.49        | 1.53     |
| 26  | B     | 619 | BCR  | C30-C25 | -3.04 | 1.49        | 1.53     |
| 24  | D     | 402 | CLA  | MG-NB   | -3.04 | 1.99        | 2.05     |
| 24  | B     | 613 | CLA  | MG-ND   | -3.04 | 1.99        | 2.05     |
| 35  | F     | 101 | HEM  | FE-NC   | 3.04  | 2.05        | 1.95     |
| 32  | C     | 516 | DGD  | C6E-C5E | 3.04  | 1.62        | 1.51     |
| 24  | a     | 612 | CLA  | MG-NC   | -3.03 | 1.99        | 2.06     |
| 24  | b     | 613 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 25  | A     | 607 | PHO  | CMB-C2B | -3.03 | 1.45        | 1.51     |
| 24  | C     | 506 | CLA  | MG-NC   | -3.03 | 1.99        | 2.06     |
| 24  | C     | 511 | CLA  | C1D-ND  | 3.02  | 1.41        | 1.37     |
| 32  | C     | 517 | DGD  | C6E-C5E | 3.02  | 1.61        | 1.51     |
| 24  | C     | 505 | CLA  | C1B-C2B | 3.01  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 615 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 26  | b     | 617 | BCR  | C1-C6   | -3.01 | 1.49        | 1.53     |
| 26  | k     | 102 | BCR  | C1-C6   | -3.01 | 1.49        | 1.53     |
| 24  | C     | 505 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 24  | a     | 604 | CLA  | C1B-C2B | 3.01  | 1.50        | 1.43     |
| 24  | B     | 612 | CLA  | C1B-C2B | 3.00  | 1.50        | 1.43     |
| 24  | C     | 501 | CLA  | CHC-C1C | 3.00  | 1.44        | 1.38     |
| 28  | a     | 611 | PL9  | C52-C5  | -2.99 | 1.44        | 1.50     |
| 31  | b     | 620 | SQD  | O47-C7  | 2.99  | 1.42        | 1.34     |
| 24  | C     | 504 | CLA  | MG-NB   | 2.99  | 2.11        | 2.05     |
| 31  | a     | 613 | SQD  | O2-C2   | -2.98 | 1.35        | 1.43     |
| 24  | B     | 611 | CLA  | C1B-C2B | 2.98  | 1.50        | 1.43     |
| 29  | a     | 618 | LMG  | C4-C3   | 2.97  | 1.60        | 1.52     |
| 24  | c     | 507 | CLA  | C1B-NB  | -2.97 | 1.34        | 1.37     |
| 24  | c     | 503 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 28  | a     | 611 | PL9  | C53-C6  | -2.97 | 1.44        | 1.50     |
| 24  | a     | 612 | CLA  | C1B-C2B | 2.97  | 1.50        | 1.43     |
| 24  | b     | 602 | CLA  | C1D-ND  | 2.97  | 1.41        | 1.37     |
| 31  | f     | 101 | SQD  | O47-C7  | 2.97  | 1.42        | 1.34     |
| 24  | B     | 609 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 24  | C     | 513 | CLA  | MG-NA   | 2.96  | 2.13        | 2.06     |
| 24  | B     | 615 | CLA  | CMB-C2B | -2.96 | 1.44        | 1.50     |
| 31  | A     | 617 | SQD  | O48-C23 | 2.96  | 1.42        | 1.33     |
| 24  | D     | 403 | CLA  | C1B-C2B | 2.95  | 1.50        | 1.43     |
| 24  | d     | 401 | CLA  | C1D-ND  | 2.95  | 1.41        | 1.37     |
| 32  | C     | 516 | DGD  | O2E-C2E | -2.94 | 1.35        | 1.43     |
| 28  | A     | 612 | PL9  | C3-C4   | -2.94 | 1.45        | 1.49     |
| 32  | c     | 518 | DGD  | O2G-C2G | -2.94 | 1.39        | 1.46     |
| 32  | H     | 102 | DGD  | C4E-C5E | 2.94  | 1.59        | 1.53     |
| 32  | C     | 518 | DGD  | O5D-C1E | 2.94  | 1.45        | 1.40     |
| 32  | H     | 102 | DGD  | C3E-C2E | 2.93  | 1.59        | 1.52     |
| 24  | C     | 508 | CLA  | C1D-ND  | 2.93  | 1.41        | 1.37     |
| 35  | e     | 101 | HEM  | FE-NA   | 2.93  | 2.04        | 1.95     |
| 24  | c     | 502 | CLA  | CMD-C2D | -2.93 | 1.44        | 1.50     |
| 24  | c     | 507 | CLA  | C1D-ND  | 2.92  | 1.41        | 1.37     |
| 24  | a     | 606 | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 24  | C     | 505 | CLA  | CHC-C1C | 2.92  | 1.44        | 1.38     |
| 24  | c     | 508 | CLA  | C1B-C2B | 2.91  | 1.50        | 1.43     |
| 24  | D     | 402 | CLA  | CHC-C1C | 2.91  | 1.44        | 1.38     |
| 26  | D     | 404 | BCR  | C1-C6   | -2.91 | 1.50        | 1.53     |
| 26  | B     | 617 | BCR  | C33-C5  | -2.91 | 1.46        | 1.50     |
| 24  | A     | 605 | CLA  | C1B-C2B | 2.91  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | T     | 101 | BCR  | C1-C6   | -2.91 | 1.50        | 1.53     |
| 24  | C     | 510 | CLA  | C1B-NB  | -2.90 | 1.34        | 1.37     |
| 26  | B     | 617 | BCR  | C30-C25 | -2.90 | 1.50        | 1.53     |
| 32  | h     | 101 | DGD  | C4E-C5E | 2.90  | 1.59        | 1.53     |
| 24  | a     | 606 | CLA  | MG-NB   | -2.90 | 2.00        | 2.05     |
| 24  | D     | 402 | CLA  | C1B-C2B | 2.90  | 1.49        | 1.43     |
| 24  | c     | 505 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 24  | B     | 606 | CLA  | C1D-ND  | 2.90  | 1.41        | 1.37     |
| 24  | C     | 512 | CLA  | MG-NA   | 2.89  | 2.13        | 2.06     |
| 24  | B     | 610 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 24  | c     | 506 | CLA  | C1D-ND  | 2.88  | 1.41        | 1.37     |
| 24  | B     | 614 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 24  | c     | 513 | CLA  | C1D-ND  | 2.87  | 1.41        | 1.37     |
| 24  | A     | 613 | CLA  | CHC-C1C | 2.87  | 1.44        | 1.38     |
| 24  | b     | 614 | CLA  | MG-NA   | 2.87  | 2.13        | 2.06     |
| 24  | B     | 603 | CLA  | MG-ND   | 2.87  | 2.11        | 2.05     |
| 28  | d     | 406 | PL9  | C21-C19 | -2.86 | 1.45        | 1.51     |
| 30  | d     | 409 | LHG  | P-O6    | 2.86  | 1.70        | 1.59     |
| 24  | a     | 606 | CLA  | CMC-C2C | -2.86 | 1.44        | 1.50     |
| 24  | B     | 601 | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 28  | A     | 612 | PL9  | C7-C8   | -2.85 | 1.46        | 1.50     |
| 25  | A     | 606 | PHO  | C3B-C2B | -2.85 | 1.36        | 1.40     |
| 26  | b     | 617 | BCR  | C33-C5  | -2.85 | 1.46        | 1.50     |
| 32  | h     | 101 | DGD  | C4D-C3D | 2.85  | 1.59        | 1.52     |
| 29  | c     | 521 | LMG  | C3-C2   | 2.84  | 1.59        | 1.52     |
| 24  | B     | 607 | CLA  | MG-NB   | -2.84 | 2.00        | 2.05     |
| 24  | b     | 603 | CLA  | CMC-C2C | -2.84 | 1.45        | 1.50     |
| 24  | c     | 511 | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 30  | l     | 101 | LHG  | O7-C5   | -2.84 | 1.39        | 1.46     |
| 24  | C     | 501 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 25  | d     | 402 | PHO  | CMD-C2D | -2.83 | 1.46        | 1.51     |
| 24  | d     | 404 | CLA  | MG-ND   | -2.83 | 2.00        | 2.05     |
| 32  | C     | 516 | DGD  | C4D-C3D | 2.83  | 1.59        | 1.52     |
| 24  | B     | 604 | CLA  | C3B-C4B | 2.83  | 1.51        | 1.42     |
| 24  | C     | 508 | CLA  | CHC-C1C | 2.83  | 1.44        | 1.38     |
| 24  | C     | 511 | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 24  | b     | 607 | CLA  | CMD-C2D | -2.83 | 1.45        | 1.50     |
| 24  | b     | 615 | CLA  | CMB-C2B | -2.83 | 1.45        | 1.50     |
| 24  | b     | 607 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 24  | a     | 606 | CLA  | CMD-C2D | -2.82 | 1.45        | 1.50     |
| 24  | b     | 607 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 24  | B     | 612 | CLA  | C3B-C4B | 2.82  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 615 | CLA  | CMD-C2D | -2.81 | 1.45        | 1.50     |
| 31  | a     | 613 | SQD  | O47-C7  | 2.81  | 1.42        | 1.34     |
| 24  | C     | 512 | CLA  | CMD-C2D | -2.81 | 1.45        | 1.50     |
| 24  | b     | 608 | CLA  | MG-NB   | -2.81 | 2.00        | 2.05     |
| 28  | D     | 405 | PL9  | C30-C29 | -2.81 | 1.43        | 1.50     |
| 24  | b     | 608 | CLA  | CMB-C2B | -2.81 | 1.45        | 1.50     |
| 24  | d     | 404 | CLA  | CMD-C2D | -2.80 | 1.45        | 1.50     |
| 24  | b     | 607 | CLA  | MG-NA   | 2.80  | 2.12        | 2.06     |
| 24  | b     | 612 | CLA  | CMB-C2B | -2.80 | 1.45        | 1.50     |
| 31  | A     | 617 | SQD  | O47-C45 | -2.80 | 1.42        | 1.47     |
| 24  | b     | 610 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 24  | D     | 403 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 25  | d     | 402 | PHO  | CAC-C3C | -2.79 | 1.46        | 1.51     |
| 25  | A     | 607 | PHO  | C1D-C2D | 2.79  | 1.42        | 1.39     |
| 26  | a     | 607 | BCR  | C1-C6   | -2.79 | 1.50        | 1.53     |
| 24  | C     | 511 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 24  | B     | 602 | CLA  | CMB-C2B | -2.78 | 1.45        | 1.50     |
| 26  | a     | 607 | BCR  | C27-C26 | -2.77 | 1.45        | 1.51     |
| 24  | B     | 601 | CLA  | CMB-C2B | -2.77 | 1.45        | 1.50     |
| 24  | d     | 401 | CLA  | C1B-NB  | -2.77 | 1.34        | 1.37     |
| 24  | C     | 503 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 32  | c     | 516 | DGD  | O2E-C2E | -2.76 | 1.36        | 1.43     |
| 25  | A     | 606 | PHO  | C1D-C2D | 2.76  | 1.42        | 1.39     |
| 24  | b     | 614 | CLA  | MG-NB   | 2.76  | 2.11        | 2.05     |
| 36  | V     | 201 | HEC  | CMB-C2B | 2.75  | 1.56        | 1.50     |
| 24  | B     | 616 | CLA  | CMC-C2C | -2.75 | 1.45        | 1.50     |
| 25  | A     | 607 | PHO  | C4D-CHA | 2.75  | 1.43        | 1.39     |
| 24  | B     | 608 | CLA  | C1D-ND  | 2.75  | 1.41        | 1.37     |
| 24  | c     | 510 | CLA  | CMB-C2B | -2.75 | 1.45        | 1.50     |
| 24  | b     | 606 | CLA  | MG-NC   | -2.75 | 1.99        | 2.06     |
| 24  | D     | 403 | CLA  | C1B-NB  | -2.75 | 1.34        | 1.37     |
| 35  | F     | 101 | HEM  | FE-NA   | 2.75  | 2.04        | 1.95     |
| 25  | a     | 605 | PHO  | C3B-C2B | -2.75 | 1.36        | 1.40     |
| 24  | c     | 512 | CLA  | C1D-ND  | 2.74  | 1.41        | 1.37     |
| 24  | B     | 603 | CLA  | CMC-C2C | -2.74 | 1.45        | 1.50     |
| 24  | b     | 601 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 24  | C     | 502 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 32  | C     | 516 | DGD  | O5D-C6D | -2.74 | 1.39        | 1.43     |
| 24  | B     | 605 | CLA  | C3B-C4B | 2.73  | 1.50        | 1.42     |
| 24  | d     | 401 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 30  | D     | 408 | LHG  | P-O3    | 2.72  | 1.70        | 1.59     |
| 24  | c     | 513 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 508 | CLA  | C3B-C4B | 2.72  | 1.50        | 1.42     |
| 29  | M     | 101 | LMG  | C4-C5   | 2.72  | 1.58        | 1.53     |
| 24  | A     | 605 | CLA  | CMD-C2D | -2.72 | 1.45        | 1.50     |
| 24  | C     | 504 | CLA  | C1D-ND  | 2.72  | 1.41        | 1.37     |
| 29  | D     | 406 | LMG  | C4-C5   | 2.71  | 1.58        | 1.53     |
| 24  | b     | 607 | CLA  | C1D-ND  | 2.71  | 1.41        | 1.37     |
| 24  | C     | 513 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 26  | A     | 609 | BCR  | C30-C25 | -2.71 | 1.50        | 1.53     |
| 24  | d     | 403 | CLA  | C1D-ND  | 2.71  | 1.41        | 1.37     |
| 29  | b     | 621 | LMG  | C4-C3   | 2.71  | 1.59        | 1.52     |
| 24  | d     | 404 | CLA  | CMC-C2C | -2.71 | 1.45        | 1.50     |
| 28  | A     | 612 | PL9  | C6-C1   | -2.70 | 1.44        | 1.48     |
| 24  | a     | 612 | CLA  | CMB-C2B | -2.70 | 1.45        | 1.50     |
| 24  | C     | 508 | CLA  | C1D-C2D | 2.70  | 1.50        | 1.45     |
| 24  | b     | 608 | CLA  | MG-NA   | 2.70  | 2.12        | 2.06     |
| 32  | C     | 516 | DGD  | O2G-C1B | 2.70  | 1.41        | 1.34     |
| 24  | C     | 508 | CLA  | C3B-C4B | 2.70  | 1.50        | 1.42     |
| 24  | C     | 501 | CLA  | CMC-C2C | -2.70 | 1.45        | 1.50     |
| 31  | D     | 407 | SQD  | O2-C2   | -2.69 | 1.36        | 1.43     |
| 24  | B     | 608 | CLA  | MG-NA   | 2.69  | 2.12        | 2.06     |
| 24  | D     | 402 | CLA  | CMD-C2D | -2.69 | 1.45        | 1.50     |
| 31  | A     | 616 | SQD  | O2-C2   | -2.69 | 1.36        | 1.43     |
| 26  | k     | 101 | BCR  | C1-C6   | -2.69 | 1.50        | 1.53     |
| 24  | b     | 604 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 28  | D     | 405 | PL9  | C10-C9  | -2.69 | 1.44        | 1.50     |
| 30  | e     | 102 | LHG  | P-O6    | 2.68  | 1.69        | 1.59     |
| 24  | a     | 612 | CLA  | C1B-NB  | -2.68 | 1.34        | 1.37     |
| 24  | D     | 403 | CLA  | CMB-C2B | -2.68 | 1.45        | 1.50     |
| 24  | b     | 610 | CLA  | CMD-C2D | -2.68 | 1.45        | 1.50     |
| 24  | d     | 403 | CLA  | MG-NA   | 2.68  | 2.12        | 2.06     |
| 24  | b     | 616 | CLA  | CMC-C2C | -2.67 | 1.45        | 1.50     |
| 24  | B     | 608 | CLA  | CMD-C2D | -2.67 | 1.45        | 1.50     |
| 24  | d     | 401 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 26  | K     | 101 | BCR  | C1-C6   | -2.66 | 1.50        | 1.53     |
| 25  | a     | 605 | PHO  | O2D-CGD | 2.66  | 1.39        | 1.33     |
| 24  | a     | 604 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 24  | b     | 612 | CLA  | CMC-C2C | -2.65 | 1.45        | 1.50     |
| 24  | B     | 606 | CLA  | C4B-NB  | 2.65  | 1.41        | 1.37     |
| 25  | A     | 607 | PHO  | C4D-ND  | -2.64 | 1.34        | 1.38     |
| 24  | C     | 507 | CLA  | C1D-ND  | 2.64  | 1.41        | 1.37     |
| 24  | a     | 606 | CLA  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 24  | b     | 603 | CLA  | CMB-C2B | -2.64 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | b     | 621 | LMG  | O7-C8   | -2.64 | 1.40        | 1.46     |
| 29  | M     | 101 | LMG  | O7-C8   | -2.64 | 1.40        | 1.46     |
| 28  | a     | 611 | PL9  | C6-C1   | -2.64 | 1.44        | 1.48     |
| 24  | b     | 615 | CLA  | MG-ND   | -2.64 | 2.00        | 2.05     |
| 35  | F     | 101 | HEM  | CAB-C3B | 2.64  | 1.54        | 1.47     |
| 31  | f     | 101 | SQD  | O2-C2   | -2.64 | 1.36        | 1.43     |
| 24  | B     | 613 | CLA  | CMC-C2C | -2.63 | 1.45        | 1.50     |
| 32  | c     | 516 | DGD  | C4D-C5D | 2.63  | 1.58        | 1.53     |
| 32  | c     | 517 | DGD  | O3G-C1D | -2.63 | 1.35        | 1.40     |
| 29  | c     | 522 | LMG  | C4-C5   | 2.63  | 1.58        | 1.53     |
| 32  | c     | 517 | DGD  | O3E-C3E | -2.63 | 1.36        | 1.43     |
| 32  | c     | 516 | DGD  | C6D-C5D | 2.63  | 1.59        | 1.51     |
| 30  | A     | 615 | LHG  | O7-C7   | 2.63  | 1.41        | 1.34     |
| 24  | c     | 506 | CLA  | CHC-C1C | 2.63  | 1.43        | 1.38     |
| 24  | D     | 402 | CLA  | C4B-NB  | 2.62  | 1.41        | 1.37     |
| 24  | B     | 616 | CLA  | C1B-NB  | -2.62 | 1.34        | 1.37     |
| 24  | c     | 510 | CLA  | CMC-C2C | -2.62 | 1.45        | 1.50     |
| 24  | B     | 609 | CLA  | MG-ND   | 2.62  | 2.11        | 2.05     |
| 24  | b     | 609 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 25  | d     | 402 | PHO  | C1D-C2D | 2.62  | 1.42        | 1.39     |
| 32  | H     | 102 | DGD  | C1E-C2E | 2.62  | 1.60        | 1.52     |
| 32  | c     | 517 | DGD  | C4D-C3D | 2.61  | 1.59        | 1.52     |
| 24  | c     | 505 | CLA  | CHC-C1C | 2.61  | 1.43        | 1.38     |
| 31  | B     | 623 | SQD  | O2-C2   | -2.61 | 1.36        | 1.43     |
| 31  | A     | 616 | SQD  | O47-C7  | 2.61  | 1.41        | 1.34     |
| 24  | b     | 610 | CLA  | MG-NB   | -2.60 | 2.00        | 2.05     |
| 25  | A     | 607 | PHO  | CMC-C2C | -2.60 | 1.46        | 1.50     |
| 24  | B     | 614 | CLA  | C1B-NB  | -2.60 | 1.34        | 1.37     |
| 32  | C     | 517 | DGD  | C1E-C2E | 2.60  | 1.60        | 1.52     |
| 24  | B     | 613 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 24  | B     | 610 | CLA  | C1D-ND  | 2.59  | 1.41        | 1.37     |
| 30  | E     | 101 | LHG  | O7-C5   | -2.59 | 1.40        | 1.46     |
| 28  | D     | 405 | PL9  | C5-C4   | -2.59 | 1.38        | 1.47     |
| 24  | A     | 604 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 24  | B     | 609 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 24  | A     | 608 | CLA  | MG-NB   | -2.58 | 2.00        | 2.05     |
| 26  | K     | 101 | BCR  | C33-C5  | -2.58 | 1.46        | 1.50     |
| 24  | d     | 403 | CLA  | CMD-C2D | -2.57 | 1.45        | 1.50     |
| 24  | b     | 604 | CLA  | C1D-ND  | 2.57  | 1.41        | 1.37     |
| 24  | b     | 609 | CLA  | C4B-NB  | 2.57  | 1.41        | 1.37     |
| 24  | c     | 511 | CLA  | CHC-C1C | 2.57  | 1.43        | 1.38     |
| 24  | B     | 614 | CLA  | C1D-ND  | 2.57  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 611 | CLA  | CHC-C1C | 2.57  | 1.43        | 1.38     |
| 30  | A     | 615 | LHG  | C8-C7   | -2.57 | 1.43        | 1.50     |
| 24  | b     | 611 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 29  | c     | 519 | LMG  | C4-C3   | 2.56  | 1.59        | 1.52     |
| 24  | C     | 505 | CLA  | C1B-NB  | -2.56 | 1.34        | 1.37     |
| 24  | c     | 505 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 24  | C     | 507 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 24  | B     | 612 | CLA  | C1B-NB  | -2.56 | 1.34        | 1.37     |
| 24  | A     | 605 | CLA  | C3B-C4B | 2.56  | 1.50        | 1.42     |
| 24  | c     | 503 | CLA  | C5-C3   | -2.55 | 1.46        | 1.51     |
| 24  | A     | 613 | CLA  | C3D-C4D | 2.55  | 1.49        | 1.44     |
| 26  | a     | 607 | BCR  | C30-C25 | -2.55 | 1.50        | 1.53     |
| 24  | c     | 513 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 26  | t     | 101 | BCR  | C33-C5  | -2.55 | 1.46        | 1.50     |
| 24  | C     | 504 | CLA  | C3B-C4B | 2.55  | 1.50        | 1.42     |
| 24  | C     | 509 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 24  | b     | 612 | CLA  | C1D-ND  | 2.54  | 1.41        | 1.37     |
| 24  | c     | 508 | CLA  | CHC-C1C | 2.54  | 1.43        | 1.38     |
| 29  | c     | 521 | LMG  | C4-C3   | 2.54  | 1.58        | 1.52     |
| 24  | b     | 614 | CLA  | CMB-C2B | -2.54 | 1.45        | 1.50     |
| 24  | b     | 602 | CLA  | MG-NA   | -2.54 | 2.00        | 2.06     |
| 24  | b     | 606 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 24  | C     | 505 | CLA  | MG-NC   | -2.54 | 2.00        | 2.06     |
| 24  | b     | 601 | CLA  | CHC-C1C | 2.54  | 1.43        | 1.38     |
| 24  | c     | 502 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 24  | C     | 510 | CLA  | O2A-CGA | 2.53  | 1.40        | 1.33     |
| 24  | b     | 616 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 24  | B     | 606 | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 35  | e     | 101 | HEM  | C3B-C2B | -2.52 | 1.32        | 1.37     |
| 24  | c     | 510 | CLA  | C4B-NB  | 2.52  | 1.41        | 1.37     |
| 30  | B     | 622 | LHG  | C24-C23 | 2.52  | 1.58        | 1.50     |
| 29  | A     | 614 | LMG  | C4-C3   | 2.52  | 1.58        | 1.52     |
| 25  | A     | 606 | PHO  | C4D-CHA | 2.52  | 1.43        | 1.39     |
| 24  | C     | 504 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 24  | b     | 610 | CLA  | CHC-C4B | -2.52 | 1.33        | 1.39     |
| 32  | H     | 102 | DGD  | C6E-C5E | 2.52  | 1.60        | 1.51     |
| 32  | A     | 618 | DGD  | C3G-C2G | 2.52  | 1.58        | 1.50     |
| 29  | M     | 101 | LMG  | O1-C7   | -2.51 | 1.39        | 1.43     |
| 25  | A     | 607 | PHO  | CMD-C2D | -2.51 | 1.46        | 1.51     |
| 24  | d     | 404 | CLA  | C4B-NB  | 2.51  | 1.41        | 1.37     |
| 32  | h     | 101 | DGD  | O2E-C2E | -2.51 | 1.36        | 1.43     |
| 31  | A     | 616 | SQD  | O3-C3   | -2.51 | 1.36        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 510 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 24  | B     | 605 | CLA  | C1B-NB  | -2.51 | 1.34        | 1.37     |
| 24  | b     | 614 | CLA  | CMC-C2C | -2.50 | 1.45        | 1.50     |
| 24  | B     | 612 | CLA  | CHC-C1C | 2.50  | 1.43        | 1.38     |
| 26  | k     | 101 | BCR  | C33-C5  | -2.50 | 1.47        | 1.50     |
| 28  | d     | 406 | PL9  | C45-C44 | -2.50 | 1.44        | 1.50     |
| 24  | C     | 513 | CLA  | C3B-C4B | 2.49  | 1.50        | 1.42     |
| 36  | v     | 201 | HEC  | C3B-C2B | -2.49 | 1.32        | 1.41     |
| 24  | B     | 611 | CLA  | CMC-C2C | -2.49 | 1.45        | 1.50     |
| 29  | b     | 623 | LMG  | C7-C8   | 2.49  | 1.58        | 1.50     |
| 24  | B     | 615 | CLA  | CHC-C4B | -2.49 | 1.33        | 1.39     |
| 24  | B     | 615 | CLA  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 24  | b     | 612 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 31  | A     | 616 | SQD  | O47-C45 | -2.49 | 1.40        | 1.46     |
| 24  | b     | 611 | CLA  | CMC-C2C | -2.48 | 1.45        | 1.50     |
| 24  | c     | 506 | CLA  | CAC-C3C | -2.48 | 1.44        | 1.51     |
| 32  | H     | 102 | DGD  | O2G-C2G | -2.48 | 1.40        | 1.46     |
| 24  | D     | 402 | CLA  | CAA-C2A | -2.48 | 1.49        | 1.54     |
| 30  | d     | 408 | LHG  | O7-C5   | -2.48 | 1.40        | 1.46     |
| 24  | B     | 611 | CLA  | C3B-C4B | 2.48  | 1.49        | 1.42     |
| 24  | b     | 602 | CLA  | CAC-C3C | -2.47 | 1.44        | 1.51     |
| 32  | A     | 618 | DGD  | C4D-C5D | 2.47  | 1.58        | 1.53     |
| 24  | b     | 604 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 24  | b     | 611 | CLA  | CHC-C1C | 2.47  | 1.43        | 1.38     |
| 24  | b     | 612 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 24  | b     | 614 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 24  | D     | 403 | CLA  | CMC-C2C | -2.47 | 1.45        | 1.50     |
| 25  | a     | 605 | PHO  | CMC-C2C | -2.47 | 1.46        | 1.50     |
| 24  | b     | 601 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 24  | C     | 508 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 26  | c     | 515 | BCR  | C33-C5  | -2.47 | 1.47        | 1.50     |
| 24  | b     | 605 | CLA  | MG-NB   | -2.47 | 2.00        | 2.05     |
| 32  | c     | 517 | DGD  | C6E-C5E | 2.47  | 1.60        | 1.51     |
| 32  | c     | 517 | DGD  | C4D-C5D | 2.47  | 1.58        | 1.53     |
| 32  | C     | 518 | DGD  | O3G-C1D | -2.46 | 1.36        | 1.40     |
| 35  | e     | 101 | HEM  | FE-ND   | 2.46  | 2.02        | 1.94     |
| 29  | C     | 519 | LMG  | C4-C5   | 2.46  | 1.58        | 1.53     |
| 24  | B     | 607 | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 24  | b     | 608 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 32  | C     | 517 | DGD  | C6D-C5D | 2.46  | 1.58        | 1.51     |
| 24  | c     | 504 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 24  | B     | 609 | CLA  | O2D-CGD | 2.45  | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 613 | CLA  | CMB-C2B | -2.45 | 1.45        | 1.50     |
| 30  | D     | 408 | LHG  | C8-C7   | -2.45 | 1.43        | 1.50     |
| 31  | a     | 613 | SQD  | O4-C4   | -2.44 | 1.36        | 1.43     |
| 24  | b     | 605 | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 24  | B     | 606 | CLA  | CHC-C4B | -2.44 | 1.33        | 1.39     |
| 24  | B     | 610 | CLA  | CHC-C1C | 2.44  | 1.43        | 1.38     |
| 24  | c     | 508 | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 24  | c     | 509 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 32  | c     | 518 | DGD  | O1G-C1G | -2.43 | 1.39        | 1.45     |
| 31  | b     | 620 | SQD  | O2-C2   | -2.43 | 1.36        | 1.43     |
| 24  | d     | 401 | CLA  | CHC-C1C | 2.43  | 1.43        | 1.38     |
| 24  | C     | 502 | CLA  | CMB-C2B | -2.43 | 1.45        | 1.50     |
| 24  | B     | 613 | CLA  | MG-NC   | 2.42  | 2.12        | 2.06     |
| 24  | d     | 401 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 29  | c     | 519 | LMG  | O1-C1   | 2.42  | 1.44        | 1.40     |
| 29  | M     | 101 | LMG  | C29-C28 | -2.42 | 1.43        | 1.50     |
| 24  | c     | 513 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 24  | B     | 609 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 32  | c     | 518 | DGD  | O5D-C6D | -2.41 | 1.39        | 1.43     |
| 24  | c     | 511 | CLA  | C1D-ND  | 2.41  | 1.41        | 1.37     |
| 25  | d     | 402 | PHO  | CAA-C2A | -2.41 | 1.49        | 1.54     |
| 24  | C     | 510 | CLA  | C4B-NB  | 2.41  | 1.41        | 1.37     |
| 24  | B     | 605 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 24  | B     | 616 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 24  | c     | 510 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 24  | B     | 616 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 24  | B     | 613 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 24  | b     | 610 | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |
| 24  | b     | 602 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 29  | D     | 406 | LMG  | C7-C8   | 2.40  | 1.58        | 1.50     |
| 24  | C     | 510 | CLA  | C3D-C4D | 2.40  | 1.49        | 1.44     |
| 32  | C     | 518 | DGD  | C6D-C5D | 2.40  | 1.58        | 1.51     |
| 24  | C     | 510 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 24  | C     | 512 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 24  | b     | 605 | CLA  | C1B-NB  | -2.40 | 1.34        | 1.37     |
| 24  | b     | 608 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 24  | C     | 507 | CLA  | C1B-NB  | -2.40 | 1.34        | 1.37     |
| 24  | C     | 510 | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 32  | c     | 516 | DGD  | O3G-C3G | -2.39 | 1.39        | 1.43     |
| 24  | c     | 503 | CLA  | C1B-NB  | -2.39 | 1.34        | 1.37     |
| 24  | c     | 503 | CLA  | C4B-NB  | 2.39  | 1.41        | 1.37     |
| 24  | A     | 613 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 606 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.38     |
| 26  | a     | 607 | BCR  | C33-C5  | -2.38 | 1.47        | 1.50     |
| 35  | e     | 101 | HEM  | CHB-C4A | -2.37 | 1.34        | 1.39     |
| 24  | C     | 511 | CLA  | CMB-C2B | -2.37 | 1.45        | 1.50     |
| 24  | b     | 605 | CLA  | MG-NA   | 2.37  | 2.11        | 2.06     |
| 24  | d     | 403 | CLA  | MG-NC   | 2.37  | 2.11        | 2.06     |
| 24  | c     | 502 | CLA  | C1D-ND  | 2.37  | 1.41        | 1.37     |
| 24  | b     | 611 | CLA  | MG-ND   | -2.37 | 2.01        | 2.05     |
| 24  | B     | 603 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 31  | f     | 101 | SQD  | O3-C3   | -2.36 | 1.37        | 1.43     |
| 28  | A     | 612 | PL9  | C37-C38 | 2.36  | 1.57        | 1.50     |
| 24  | d     | 404 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 24  | C     | 506 | CLA  | C4B-NB  | 2.36  | 1.41        | 1.37     |
| 24  | C     | 509 | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 24  | A     | 613 | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 24  | A     | 608 | CLA  | C4B-NB  | 2.35  | 1.41        | 1.37     |
| 24  | c     | 511 | CLA  | C4B-NB  | 2.35  | 1.41        | 1.37     |
| 24  | c     | 512 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 29  | A     | 614 | LMG  | C4-C5   | 2.35  | 1.58        | 1.53     |
| 24  | c     | 504 | CLA  | CMD-C2D | -2.35 | 1.46        | 1.50     |
| 26  | x     | 101 | BCR  | C1-C6   | -2.35 | 1.50        | 1.53     |
| 24  | d     | 403 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 24  | A     | 604 | CLA  | MG-NB   | -2.34 | 2.01        | 2.05     |
| 24  | b     | 605 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 24  | a     | 604 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 24  | b     | 614 | CLA  | C4B-NB  | 2.33  | 1.40        | 1.37     |
| 24  | c     | 506 | CLA  | CMC-C2C | -2.33 | 1.46        | 1.50     |
| 24  | b     | 608 | CLA  | C1B-NB  | -2.33 | 1.34        | 1.37     |
| 24  | B     | 606 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 24  | c     | 501 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 30  | d     | 407 | LHG  | O7-C5   | -2.32 | 1.41        | 1.46     |
| 24  | b     | 609 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 24  | c     | 503 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 24  | c     | 512 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 24  | B     | 607 | CLA  | CMB-C2B | -2.32 | 1.46        | 1.50     |
| 26  | t     | 101 | BCR  | C27-C26 | -2.32 | 1.46        | 1.51     |
| 35  | e     | 101 | HEM  | CAB-C3B | 2.31  | 1.53        | 1.47     |
| 28  | D     | 405 | PL9  | C7-C8   | -2.31 | 1.46        | 1.50     |
| 29  | b     | 623 | LMG  | C3-C2   | 2.31  | 1.58        | 1.52     |
| 24  | B     | 610 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 26  | A     | 609 | BCR  | C38-C26 | -2.31 | 1.47        | 1.50     |
| 24  | B     | 602 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | b     | 621 | LMG  | C1-C2   | 2.31  | 1.59        | 1.52     |
| 24  | C     | 512 | CLA  | CMC-C2C | -2.31 | 1.46        | 1.50     |
| 24  | c     | 512 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 24  | A     | 604 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.50     |
| 24  | c     | 511 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 24  | c     | 502 | CLA  | C4B-NB  | 2.30  | 1.40        | 1.37     |
| 24  | b     | 616 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 24  | d     | 403 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.50     |
| 24  | B     | 602 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 24  | a     | 606 | CLA  | CHC-C4B | -2.30 | 1.34        | 1.39     |
| 24  | C     | 503 | CLA  | C4B-NB  | 2.29  | 1.40        | 1.37     |
| 29  | d     | 410 | LMG  | O1-C1   | 2.29  | 1.44        | 1.40     |
| 32  | c     | 516 | DGD  | O3D-C3D | -2.29 | 1.37        | 1.43     |
| 24  | b     | 616 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 28  | a     | 611 | PL9  | C46-C44 | -2.29 | 1.46        | 1.51     |
| 24  | B     | 610 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 24  | C     | 501 | CLA  | C1B-NB  | -2.29 | 1.34        | 1.37     |
| 24  | b     | 616 | CLA  | MG-NA   | 2.29  | 2.11        | 2.06     |
| 24  | c     | 504 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 24  | c     | 506 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 32  | H     | 102 | DGD  | C6D-C5D | 2.28  | 1.58        | 1.51     |
| 32  | c     | 518 | DGD  | O3D-C3D | -2.28 | 1.37        | 1.43     |
| 24  | b     | 604 | CLA  | C3D-C4D | 2.28  | 1.49        | 1.44     |
| 24  | b     | 613 | CLA  | CMC-C2C | -2.28 | 1.46        | 1.50     |
| 32  | A     | 618 | DGD  | O3D-C3D | -2.28 | 1.37        | 1.43     |
| 25  | d     | 402 | PHO  | C4D-ND  | -2.28 | 1.35        | 1.38     |
| 24  | B     | 608 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 24  | c     | 501 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 24  | B     | 615 | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 29  | c     | 521 | LMG  | O7-C8   | -2.28 | 1.41        | 1.46     |
| 24  | b     | 601 | CLA  | O2A-CGA | 2.27  | 1.40        | 1.33     |
| 30  | D     | 408 | LHG  | O8-C6   | -2.27 | 1.40        | 1.45     |
| 24  | c     | 512 | CLA  | MG-NB   | 2.27  | 2.10        | 2.05     |
| 24  | B     | 606 | CLA  | CAB-C3B | -2.27 | 1.41        | 1.47     |
| 24  | b     | 604 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 35  | e     | 101 | HEM  | CMC-C2C | 2.27  | 1.55        | 1.50     |
| 24  | C     | 510 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 24  | b     | 606 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 32  | H     | 102 | DGD  | C4D-C5D | 2.27  | 1.57        | 1.53     |
| 24  | B     | 613 | CLA  | C1B-NB  | -2.27 | 1.34        | 1.37     |
| 26  | B     | 619 | BCR  | C31-C1  | -2.27 | 1.49        | 1.53     |
| 25  | a     | 605 | PHO  | CMB-C2B | -2.27 | 1.47        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 502 | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 26  | B     | 618 | BCR  | C27-C26 | -2.26 | 1.46        | 1.51     |
| 24  | a     | 612 | CLA  | CHB-C1B | 2.26  | 1.44        | 1.39     |
| 26  | C     | 515 | BCR  | C33-C5  | -2.26 | 1.47        | 1.50     |
| 24  | A     | 613 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 24  | d     | 403 | CLA  | CHC-C4B | -2.26 | 1.34        | 1.39     |
| 29  | c     | 519 | LMG  | O2-C2   | -2.26 | 1.37        | 1.43     |
| 24  | C     | 512 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 24  | b     | 611 | CLA  | O2D-CGD | 2.25  | 1.38        | 1.33     |
| 24  | c     | 505 | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 24  | C     | 502 | CLA  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 24  | b     | 605 | CLA  | CHC-C4B | -2.25 | 1.34        | 1.39     |
| 24  | c     | 513 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 24  | B     | 610 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 24  | b     | 602 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 24  | B     | 604 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 24  | B     | 608 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 24  | D     | 403 | CLA  | CHC-C4B | -2.24 | 1.34        | 1.39     |
| 33  | b     | 624 | STE  | O1-C1   | 2.24  | 1.29        | 1.22     |
| 24  | B     | 604 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 24  | a     | 612 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 24  | c     | 505 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 24  | C     | 508 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 24  | C     | 501 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 30  | B     | 622 | LHG  | P-O4    | -2.23 | 1.45        | 1.55     |
| 24  | d     | 401 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 26  | b     | 618 | BCR  | C27-C26 | -2.23 | 1.46        | 1.51     |
| 24  | c     | 503 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 24  | B     | 603 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 24  | B     | 610 | CLA  | MG-NA   | 2.23  | 2.11        | 2.06     |
| 24  | b     | 612 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 24  | B     | 607 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 24  | C     | 507 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 24  | C     | 511 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 32  | C     | 517 | DGD  | O1G-C1G | -2.22 | 1.40        | 1.45     |
| 24  | b     | 603 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 29  | D     | 406 | LMG  | O7-C10  | 2.22  | 1.40        | 1.34     |
| 24  | c     | 507 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 24  | A     | 613 | CLA  | C1B-NB  | -2.22 | 1.34        | 1.37     |
| 24  | A     | 613 | CLA  | C4B-NB  | 2.22  | 1.40        | 1.37     |
| 24  | c     | 502 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 24  | A     | 608 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | C     | 510 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 32  | C     | 516 | DGD  | C3G-C2G | 2.21  | 1.57        | 1.50     |
| 25  | A     | 606 | PHO  | CAC-C3C | -2.21 | 1.47        | 1.51     |
| 24  | b     | 613 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 24  | a     | 606 | CLA  | CMA-C3A | -2.20 | 1.48        | 1.53     |
| 24  | C     | 507 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 26  | B     | 618 | BCR  | C1-C6   | -2.20 | 1.51        | 1.53     |
| 24  | c     | 504 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 32  | c     | 516 | DGD  | O3E-C3E | -2.20 | 1.37        | 1.43     |
| 24  | c     | 506 | CLA  | O2D-CGD | 2.20  | 1.38        | 1.33     |
| 25  | a     | 605 | PHO  | CAC-C3C | -2.20 | 1.47        | 1.51     |
| 29  | a     | 618 | LMG  | C7-C8   | 2.19  | 1.57        | 1.50     |
| 24  | c     | 513 | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 24  | C     | 510 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 24  | D     | 403 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 26  | t     | 101 | BCR  | C31-C1  | -2.19 | 1.49        | 1.53     |
| 24  | C     | 502 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 25  | A     | 606 | PHO  | CHA-CBD | -2.18 | 1.49        | 1.51     |
| 24  | c     | 505 | CLA  | MG-ND   | 2.18  | 2.10        | 2.05     |
| 29  | b     | 623 | LMG  | O6-C1   | 2.18  | 1.47        | 1.41     |
| 24  | b     | 613 | CLA  | C1B-C2B | 2.18  | 1.48        | 1.43     |
| 29  | A     | 614 | LMG  | O7-C8   | -2.18 | 1.41        | 1.46     |
| 24  | C     | 503 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 24  | B     | 607 | CLA  | CAC-C3C | -2.18 | 1.45        | 1.51     |
| 24  | c     | 511 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 28  | D     | 405 | PL9  | C52-C5  | -2.17 | 1.46        | 1.50     |
| 24  | b     | 602 | CLA  | C1B-C2B | 2.17  | 1.48        | 1.43     |
| 29  | a     | 618 | LMG  | C1-C2   | 2.17  | 1.58        | 1.52     |
| 26  | d     | 405 | BCR  | C33-C5  | -2.17 | 1.47        | 1.50     |
| 32  | H     | 102 | DGD  | O1G-C1G | -2.17 | 1.40        | 1.45     |
| 24  | B     | 611 | CLA  | C4B-NB  | 2.17  | 1.40        | 1.37     |
| 24  | B     | 606 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 24  | C     | 502 | CLA  | MG-ND   | 2.17  | 2.10        | 2.05     |
| 24  | C     | 506 | CLA  | C3D-C4D | 2.16  | 1.49        | 1.44     |
| 24  | b     | 616 | CLA  | O2D-CED | -2.16 | 1.40        | 1.45     |
| 28  | a     | 611 | PL9  | C30-C29 | -2.16 | 1.45        | 1.50     |
| 24  | b     | 609 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 24  | B     | 610 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 31  | A     | 616 | SQD  | O4-C4   | -2.16 | 1.37        | 1.43     |
| 26  | t     | 101 | BCR  | C1-C6   | -2.16 | 1.51        | 1.53     |
| 24  | B     | 602 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 24  | d     | 404 | CLA  | CHC-C4B | -2.16 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | C     | 505 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 24  | d     | 401 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 24  | c     | 502 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 32  | h     | 101 | DGD  | C1E-C2E | 2.15  | 1.58        | 1.52     |
| 29  | C     | 519 | LMG  | O7-C8   | -2.15 | 1.41        | 1.46     |
| 31  | D     | 407 | SQD  | O3-C3   | -2.15 | 1.37        | 1.43     |
| 24  | b     | 608 | CLA  | C1D-ND  | 2.15  | 1.40        | 1.37     |
| 24  | a     | 612 | CLA  | C4B-NB  | 2.15  | 1.40        | 1.37     |
| 32  | H     | 102 | DGD  | C4E-C3E | 2.15  | 1.57        | 1.52     |
| 24  | B     | 614 | CLA  | MG-NA   | 2.14  | 2.11        | 2.06     |
| 26  | b     | 618 | BCR  | C33-C5  | -2.14 | 1.47        | 1.50     |
| 24  | c     | 505 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 24  | d     | 404 | CLA  | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 24  | c     | 504 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 24  | C     | 504 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 25  | a     | 605 | PHO  | C4D-CHA | 2.14  | 1.42        | 1.39     |
| 24  | C     | 506 | CLA  | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 24  | c     | 511 | CLA  | C3D-C4D | 2.14  | 1.49        | 1.44     |
| 24  | B     | 604 | CLA  | C3C-C2C | 2.14  | 1.41        | 1.36     |
| 35  | e     | 101 | HEM  | CAC-C3C | 2.13  | 1.53        | 1.47     |
| 24  | c     | 503 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 36  | v     | 201 | HEC  | CMA-C3A | 2.13  | 1.55        | 1.50     |
| 29  | c     | 519 | LMG  | C7-C8   | 2.13  | 1.57        | 1.50     |
| 29  | c     | 521 | LMG  | C7-C8   | 2.13  | 1.57        | 1.50     |
| 24  | c     | 505 | CLA  | MG-NC   | 2.13  | 2.11        | 2.06     |
| 24  | c     | 505 | CLA  | C1D-ND  | 2.13  | 1.40        | 1.37     |
| 24  | b     | 611 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 26  | B     | 619 | BCR  | C27-C26 | -2.13 | 1.47        | 1.51     |
| 24  | b     | 611 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 30  | d     | 407 | LHG  | P-O6    | 2.12  | 1.67        | 1.59     |
| 24  | C     | 501 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 24  | b     | 601 | CLA  | C1D-C2D | 2.12  | 1.49        | 1.45     |
| 24  | B     | 601 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 29  | d     | 410 | LMG  | O7-C8   | -2.12 | 1.41        | 1.46     |
| 24  | B     | 614 | CLA  | CAA-C2A | -2.12 | 1.50        | 1.54     |
| 32  | A     | 618 | DGD  | O6E-C5E | -2.12 | 1.39        | 1.44     |
| 26  | A     | 609 | BCR  | C37-C22 | -2.11 | 1.46        | 1.50     |
| 32  | H     | 102 | DGD  | O6E-C1E | 2.11  | 1.47        | 1.41     |
| 24  | b     | 614 | CLA  | CAC-C3C | -2.11 | 1.45        | 1.51     |
| 35  | F     | 101 | HEM  | CMA-C3A | 2.11  | 1.55        | 1.50     |
| 32  | c     | 517 | DGD  | O3D-C3D | -2.11 | 1.37        | 1.43     |
| 24  | C     | 508 | CLA  | C3D-C4D | 2.11  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | A     | 606 | PHO  | C1D-ND  | 2.11  | 1.42        | 1.38     |
| 24  | D     | 402 | CLA  | MG-ND   | 2.11  | 2.10        | 2.05     |
| 30  | e     | 102 | LHG  | O8-C23  | 2.11  | 1.39        | 1.33     |
| 24  | B     | 606 | CLA  | C3B-C2B | -2.11 | 1.34        | 1.41     |
| 36  | V     | 201 | HEC  | C3B-C2B | -2.11 | 1.34        | 1.41     |
| 24  | C     | 506 | CLA  | C1B-NB  | -2.11 | 1.35        | 1.37     |
| 24  | c     | 513 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 24  | C     | 503 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 24  | b     | 616 | CLA  | CAC-C3C | -2.10 | 1.45        | 1.51     |
| 24  | D     | 402 | CLA  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 29  | a     | 618 | LMG  | C3-C2   | 2.10  | 1.57        | 1.52     |
| 24  | A     | 604 | CLA  | C1D-C2D | 2.10  | 1.49        | 1.45     |
| 29  | C     | 519 | LMG  | C4-C3   | 2.10  | 1.57        | 1.52     |
| 24  | C     | 503 | CLA  | O2D-CED | -2.10 | 1.40        | 1.45     |
| 32  | h     | 101 | DGD  | O4D-C4D | -2.09 | 1.37        | 1.43     |
| 24  | c     | 509 | CLA  | C1B-NB  | -2.09 | 1.35        | 1.37     |
| 24  | d     | 401 | CLA  | CHC-C4B | -2.09 | 1.34        | 1.39     |
| 25  | A     | 607 | PHO  | C1C-NC  | -2.09 | 1.31        | 1.37     |
| 24  | b     | 616 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 24  | b     | 604 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 24  | B     | 602 | CLA  | MG-ND   | -2.09 | 2.01        | 2.05     |
| 24  | A     | 608 | CLA  | CHC-C4B | -2.09 | 1.34        | 1.39     |
| 26  | c     | 514 | BCR  | C33-C5  | -2.09 | 1.47        | 1.50     |
| 24  | a     | 606 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 24  | b     | 608 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 31  | a     | 613 | SQD  | O3-C3   | -2.08 | 1.37        | 1.43     |
| 29  | c     | 519 | LMG  | C3-C2   | 2.08  | 1.57        | 1.52     |
| 25  | A     | 606 | PHO  | CBD-CGD | -2.08 | 1.49        | 1.52     |
| 24  | C     | 512 | CLA  | C3D-C4D | 2.08  | 1.48        | 1.44     |
| 26  | c     | 515 | BCR  | C27-C26 | -2.08 | 1.47        | 1.51     |
| 24  | d     | 403 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 24  | B     | 607 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 26  | k     | 102 | BCR  | C27-C26 | -2.08 | 1.47        | 1.51     |
| 24  | B     | 609 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 24  | c     | 513 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 24  | A     | 605 | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 24  | c     | 512 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 24  | c     | 510 | CLA  | CHC-C4B | -2.07 | 1.34        | 1.39     |
| 24  | C     | 509 | CLA  | C4B-NB  | 2.07  | 1.40        | 1.37     |
| 24  | c     | 502 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 24  | C     | 502 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 24  | d     | 404 | CLA  | CAC-C3C | -2.07 | 1.45        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 607 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 24  | B     | 606 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 24  | A     | 608 | CLA  | C1B-C2B | 2.06  | 1.48        | 1.43     |
| 32  | C     | 516 | DGD  | O1G-C1A | 2.06  | 1.39        | 1.33     |
| 26  | H     | 101 | BCR  | C33-C5  | -2.06 | 1.47        | 1.50     |
| 25  | A     | 606 | PHO  | CMB-C2B | -2.06 | 1.47        | 1.51     |
| 24  | C     | 506 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 24  | B     | 610 | CLA  | C1A-CHA | -2.06 | 1.34        | 1.43     |
| 24  | c     | 506 | CLA  | C1B-C2B | 2.06  | 1.48        | 1.43     |
| 24  | A     | 613 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 24  | b     | 607 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 24  | b     | 609 | CLA  | MG-NB   | 2.05  | 2.09        | 2.05     |
| 24  | B     | 616 | CLA  | CAB-C3B | -2.05 | 1.41        | 1.47     |
| 24  | b     | 606 | CLA  | C3D-C4D | 2.05  | 1.48        | 1.44     |
| 35  | e     | 101 | HEM  | CMA-C3A | 2.05  | 1.55        | 1.50     |
| 29  | c     | 522 | LMG  | O1-C7   | -2.04 | 1.40        | 1.43     |
| 32  | c     | 516 | DGD  | O4D-C4D | -2.04 | 1.37        | 1.43     |
| 32  | h     | 101 | DGD  | O2G-C2G | -2.04 | 1.41        | 1.46     |
| 24  | d     | 401 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 24  | a     | 604 | CLA  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 26  | B     | 618 | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 24  | C     | 509 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 25  | a     | 605 | PHO  | C4C-NC  | 2.04  | 1.44        | 1.37     |
| 26  | C     | 514 | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 24  | C     | 504 | CLA  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 24  | D     | 402 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 24  | a     | 604 | CLA  | MG-NB   | 2.04  | 2.09        | 2.05     |
| 24  | c     | 512 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 25  | A     | 606 | PHO  | CMA-C3A | -2.04 | 1.49        | 1.53     |
| 24  | A     | 608 | CLA  | C3D-C4D | 2.04  | 1.48        | 1.44     |
| 24  | a     | 606 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 24  | B     | 606 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 24  | B     | 611 | CLA  | C1D-ND  | 2.03  | 1.40        | 1.37     |
| 24  | B     | 604 | CLA  | C1B-C2B | 2.03  | 1.47        | 1.43     |
| 24  | B     | 616 | CLA  | C4B-NB  | 2.03  | 1.40        | 1.37     |
| 24  | B     | 603 | CLA  | C3D-C4D | 2.03  | 1.48        | 1.44     |
| 24  | C     | 503 | CLA  | CAC-C3C | -2.02 | 1.45        | 1.51     |
| 24  | C     | 513 | CLA  | CHC-C4B | -2.02 | 1.34        | 1.39     |
| 26  | B     | 619 | BCR  | C33-C5  | -2.02 | 1.47        | 1.50     |
| 32  | c     | 517 | DGD  | C4E-C5E | 2.02  | 1.57        | 1.53     |
| 24  | b     | 608 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 32  | c     | 518 | DGD  | O3E-C3E | -2.02 | 1.38        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 602 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 24  | b     | 605 | CLA  | C1A-CHA | -2.02 | 1.34        | 1.43     |
| 24  | b     | 615 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 24  | D     | 402 | CLA  | C1C-NC  | -2.01 | 1.34        | 1.37     |
| 29  | D     | 409 | LMG  | O8-C28  | 2.01  | 1.39        | 1.33     |
| 24  | a     | 604 | CLA  | O2D-CED | -2.01 | 1.40        | 1.45     |
| 30  | d     | 407 | LHG  | P-O4    | -2.01 | 1.46        | 1.55     |
| 24  | c     | 510 | CLA  | O2D-CED | -2.01 | 1.40        | 1.45     |
| 28  | d     | 406 | PL9  | C27-C28 | -2.01 | 1.44        | 1.50     |
| 33  | x     | 102 | STE  | C2-C1   | 2.01  | 1.55        | 1.50     |
| 29  | c     | 521 | LMG  | O2-C2   | 2.01  | 1.47        | 1.43     |
| 32  | C     | 518 | DGD  | C1D-C2D | 2.00  | 1.58        | 1.52     |
| 24  | c     | 506 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 24  | B     | 612 | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |

All (1203) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 503 | CLA  | C4A-NA-C1A  | 9.98  | 111.23      | 106.68   |
| 24  | b     | 615 | CLA  | C4A-NA-C1A  | 9.30  | 110.92      | 106.68   |
| 31  | a     | 613 | SQD  | O6-C1-C2    | 9.24  | 122.30      | 108.27   |
| 24  | B     | 611 | CLA  | C4A-NA-C1A  | 9.16  | 110.86      | 106.68   |
| 36  | V     | 201 | HEC  | CBB-CAB-C3B | -8.93 | 109.58      | 127.43   |
| 36  | v     | 201 | HEC  | CBB-CAB-C3B | -8.89 | 109.66      | 127.43   |
| 24  | B     | 603 | CLA  | C4A-NA-C1A  | 8.54  | 110.57      | 106.68   |
| 24  | b     | 606 | CLA  | C4A-NA-C1A  | 8.41  | 110.52      | 106.68   |
| 24  | B     | 616 | CLA  | C4A-NA-C1A  | 8.40  | 110.51      | 106.68   |
| 31  | D     | 407 | SQD  | O6-C1-C2    | 8.37  | 120.98      | 108.27   |
| 24  | B     | 604 | CLA  | C4A-NA-C1A  | 8.29  | 110.46      | 106.68   |
| 31  | B     | 623 | SQD  | O6-C1-C2    | 8.13  | 120.61      | 108.27   |
| 24  | C     | 507 | CLA  | C4A-NA-C1A  | 8.02  | 110.34      | 106.68   |
| 24  | b     | 601 | CLA  | C4A-NA-C1A  | 7.97  | 110.32      | 106.68   |
| 36  | v     | 201 | HEC  | CBC-CAC-C3C | -7.93 | 111.58      | 127.43   |
| 24  | d     | 403 | CLA  | C4A-NA-C1A  | 7.93  | 110.30      | 106.68   |
| 24  | B     | 612 | CLA  | C4A-NA-C1A  | 7.82  | 110.25      | 106.68   |
| 24  | b     | 609 | CLA  | C4A-NA-C1A  | 7.79  | 110.23      | 106.68   |
| 24  | A     | 613 | CLA  | C4A-NA-C1A  | 7.76  | 110.22      | 106.68   |
| 24  | c     | 510 | CLA  | C4A-NA-C1A  | 7.61  | 110.15      | 106.68   |
| 24  | C     | 501 | CLA  | C4A-NA-C1A  | 7.51  | 110.11      | 106.68   |
| 36  | V     | 201 | HEC  | CBC-CAC-C3C | -7.42 | 112.61      | 127.43   |
| 24  | C     | 511 | CLA  | C4A-NA-C1A  | 7.37  | 110.04      | 106.68   |
| 24  | A     | 605 | CLA  | C4A-NA-C1A  | 7.35  | 110.03      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | c     | 509 | CLA  | C4A-NA-C1A  | 7.29  | 110.00      | 106.68   |
| 24  | c     | 511 | CLA  | C4A-NA-C1A  | 7.29  | 110.00      | 106.68   |
| 31  | A     | 616 | SQD  | O7-S-C6     | 7.21  | 117.53      | 106.76   |
| 24  | B     | 601 | CLA  | C4A-NA-C1A  | 7.15  | 109.94      | 106.68   |
| 24  | C     | 509 | CLA  | C4A-NA-C1A  | 7.09  | 109.91      | 106.68   |
| 24  | b     | 614 | CLA  | C4A-NA-C1A  | 7.05  | 109.90      | 106.68   |
| 31  | b     | 620 | SQD  | O6-C1-C2    | 6.97  | 118.86      | 108.27   |
| 25  | A     | 606 | PHO  | C4D-CHA-CBD | -6.91 | 105.14      | 108.45   |
| 24  | b     | 616 | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 24  | c     | 508 | CLA  | C4A-NA-C1A  | 6.84  | 109.80      | 106.68   |
| 31  | f     | 101 | SQD  | O6-C1-C2    | 6.80  | 118.60      | 108.27   |
| 24  | a     | 612 | CLA  | C4A-NA-C1A  | 6.71  | 109.74      | 106.68   |
| 24  | C     | 513 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 31  | A     | 616 | SQD  | O6-C1-C2    | 6.57  | 118.26      | 108.27   |
| 24  | D     | 403 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 24  | C     | 502 | CLA  | C4A-NA-C1A  | 6.39  | 109.60      | 106.68   |
| 24  | B     | 606 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 24  | c     | 502 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 24  | c     | 506 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 24  | B     | 609 | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 25  | a     | 605 | PHO  | C4D-CHA-CBD | -6.13 | 105.52      | 108.45   |
| 24  | b     | 602 | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 24  | C     | 510 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 24  | C     | 508 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 24  | C     | 505 | CLA  | C4A-NA-C1A  | 5.97  | 109.40      | 106.68   |
| 24  | B     | 607 | CLA  | C4A-NA-C1A  | 5.86  | 109.35      | 106.68   |
| 28  | d     | 406 | PL9  | C7-C3-C4    | 5.67  | 121.58      | 116.91   |
| 24  | d     | 401 | CLA  | C4A-NA-C1A  | 5.64  | 109.25      | 106.68   |
| 24  | a     | 604 | CLA  | C4A-NA-C1A  | 5.60  | 109.23      | 106.68   |
| 28  | a     | 611 | PL9  | C7-C3-C4    | 5.58  | 121.51      | 116.91   |
| 24  | B     | 615 | CLA  | C4A-NA-C1A  | 5.54  | 109.21      | 106.68   |
| 24  | C     | 512 | CLA  | C4A-NA-C1A  | 5.54  | 109.21      | 106.68   |
| 31  | A     | 616 | SQD  | O9-S-O7     | -5.54 | 95.80       | 113.82   |
| 31  | A     | 617 | SQD  | C45-O47-C7  | 5.39  | 125.55      | 117.78   |
| 24  | c     | 501 | CLA  | O2D-CGD-O1D | -5.30 | 113.53      | 123.85   |
| 24  | b     | 606 | CLA  | O2D-CGD-O1D | -5.25 | 113.62      | 123.85   |
| 24  | c     | 512 | CLA  | C4A-NA-C1A  | 5.24  | 109.07      | 106.68   |
| 24  | B     | 610 | CLA  | O2D-CGD-O1D | -5.22 | 113.68      | 123.85   |
| 31  | f     | 101 | SQD  | O7-S-C6     | 5.21  | 114.54      | 106.76   |
| 24  | b     | 610 | CLA  | C4A-NA-C1A  | 5.19  | 109.05      | 106.68   |
| 24  | C     | 501 | CLA  | O2D-CGD-O1D | -5.15 | 113.82      | 123.85   |
| 24  | B     | 605 | CLA  | C4A-NA-C1A  | 5.07  | 108.99      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 614 | SQD  | O47-C7-C8   | 5.06  | 122.44      | 111.48   |
| 31  | A     | 616 | SQD  | C1-C2-C3    | -5.01 | 99.47       | 110.01   |
| 24  | C     | 510 | CLA  | O2D-CGD-O1D | -5.01 | 114.10      | 123.85   |
| 28  | d     | 406 | PL9  | C40-C39-C41 | 5.01  | 123.92      | 115.23   |
| 24  | c     | 501 | CLA  | C4A-NA-C1A  | 4.98  | 108.95      | 106.68   |
| 24  | b     | 607 | CLA  | C4A-NA-C1A  | 4.96  | 108.94      | 106.68   |
| 24  | b     | 604 | CLA  | C4A-NA-C1A  | 4.94  | 108.93      | 106.68   |
| 24  | B     | 611 | CLA  | O2D-CGD-O1D | -4.94 | 114.24      | 123.85   |
| 24  | c     | 504 | CLA  | C4A-NA-C1A  | 4.91  | 108.92      | 106.68   |
| 24  | A     | 613 | CLA  | C3B-C4B-NB  | -4.89 | 106.17      | 110.53   |
| 25  | d     | 402 | PHO  | C4D-CHA-CBD | -4.87 | 106.12      | 108.45   |
| 24  | c     | 505 | CLA  | C4A-NA-C1A  | 4.86  | 108.90      | 106.68   |
| 24  | D     | 402 | CLA  | C4A-NA-C1A  | 4.80  | 108.87      | 106.68   |
| 29  | a     | 618 | LMG  | C1-C2-C3    | -4.78 | 99.95       | 110.01   |
| 24  | c     | 507 | CLA  | C4A-NA-C1A  | 4.76  | 108.85      | 106.68   |
| 24  | b     | 602 | CLA  | O2D-CGD-O1D | -4.74 | 114.62      | 123.85   |
| 24  | C     | 501 | CLA  | O2D-CGD-CBD | 4.68  | 119.42      | 111.23   |
| 30  | A     | 615 | LHG  | O4-P-O5     | 4.65  | 134.08      | 112.44   |
| 24  | B     | 614 | CLA  | C3B-C4B-NB  | -4.64 | 106.39      | 110.53   |
| 24  | b     | 605 | CLA  | O2D-CGD-O1D | -4.59 | 114.90      | 123.85   |
| 30  | E     | 101 | LHG  | O4-P-O5     | 4.55  | 133.62      | 112.44   |
| 24  | b     | 611 | CLA  | O2D-CGD-CBD | 4.55  | 119.19      | 111.23   |
| 24  | C     | 508 | CLA  | CHD-C1D-ND  | -4.49 | 118.48      | 124.80   |
| 24  | D     | 402 | CLA  | C3B-C4B-NB  | -4.47 | 106.54      | 110.53   |
| 31  | A     | 616 | SQD  | C1-O5-C5    | -4.40 | 105.12      | 113.72   |
| 24  | c     | 513 | CLA  | C4A-NA-C1A  | 4.39  | 108.68      | 106.68   |
| 24  | C     | 506 | CLA  | C4A-NA-C1A  | 4.37  | 108.67      | 106.68   |
| 31  | f     | 101 | SQD  | O9-S-O7     | -4.37 | 99.62       | 113.82   |
| 30  | d     | 409 | LHG  | O4-P-O5     | 4.34  | 132.65      | 112.44   |
| 34  | D     | 401 | BCT  | O2-C-O1     | 4.34  | 130.78      | 119.68   |
| 25  | d     | 402 | PHO  | O1D-CGD-CBD | 4.30  | 131.24      | 124.72   |
| 30  | e     | 102 | LHG  | O4-P-O5     | 4.30  | 132.43      | 112.44   |
| 30  | B     | 622 | LHG  | O4-P-O5     | 4.29  | 132.41      | 112.44   |
| 28  | a     | 611 | PL9  | C35-C34-C36 | 4.28  | 122.67      | 115.23   |
| 35  | e     | 101 | HEM  | CBD-CAD-C3D | -4.28 | 100.69      | 112.53   |
| 24  | B     | 610 | CLA  | C4A-NA-C1A  | 4.26  | 108.62      | 106.68   |
| 24  | c     | 509 | CLA  | CHB-C4A-NA  | 4.26  | 130.55      | 124.40   |
| 24  | b     | 610 | CLA  | O2D-CGD-O1D | -4.25 | 115.57      | 123.85   |
| 30  | d     | 408 | LHG  | O4-P-O5     | 4.24  | 132.19      | 112.44   |
| 28  | a     | 611 | PL9  | C7-C3-C2    | -4.23 | 118.40      | 123.39   |
| 24  | a     | 606 | CLA  | C4A-NA-C1A  | 4.23  | 108.61      | 106.68   |
| 29  | b     | 621 | LMG  | O7-C10-O9   | -4.22 | 113.83      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 513 | CLA  | O2D-CGD-O1D | -4.20 | 115.67      | 123.85   |
| 24  | C     | 510 | CLA  | O2D-CGD-CBD | 4.20  | 118.57      | 111.23   |
| 30  | d     | 407 | LHG  | O4-P-O5     | 4.19  | 131.92      | 112.44   |
| 24  | b     | 605 | CLA  | O1D-CGD-CBD | 4.16  | 132.73      | 124.52   |
| 30  | D     | 408 | LHG  | O4-P-O5     | 4.16  | 131.80      | 112.44   |
| 34  | a     | 610 | BCT  | O2-C-O1     | 4.14  | 130.27      | 119.68   |
| 24  | b     | 603 | CLA  | C4A-NA-C1A  | 4.12  | 108.56      | 106.68   |
| 26  | b     | 617 | BCR  | C2-C1-C6    | 4.11  | 116.41      | 110.44   |
| 31  | b     | 620 | SQD  | O7-S-C6     | 4.11  | 112.89      | 106.76   |
| 24  | a     | 612 | CLA  | CMB-C2B-C1B | -4.08 | 119.21      | 125.42   |
| 24  | b     | 602 | CLA  | O2D-CGD-CBD | 4.08  | 118.36      | 111.23   |
| 24  | C     | 505 | CLA  | CMB-C2B-C1B | -4.06 | 119.24      | 125.42   |
| 24  | B     | 608 | CLA  | O2D-CGD-O1D | -4.05 | 115.96      | 123.85   |
| 25  | A     | 606 | PHO  | C2B-C1B-NB  | -4.03 | 106.51      | 109.43   |
| 31  | D     | 407 | SQD  | O8-S-C6     | 4.03  | 113.76      | 105.97   |
| 24  | B     | 614 | CLA  | O2D-CGD-O1D | -4.03 | 116.01      | 123.85   |
| 32  | C     | 518 | DGD  | O6D-C1D-O3G | -4.02 | 100.54      | 110.04   |
| 24  | b     | 609 | CLA  | CMB-C2B-C1B | -4.01 | 119.31      | 125.42   |
| 29  | b     | 623 | LMG  | C1-O6-C5    | -4.01 | 105.90      | 113.72   |
| 32  | H     | 102 | DGD  | O3G-C3G-C2G | -4.01 | 101.08      | 110.82   |
| 26  | B     | 619 | BCR  | C2-C1-C6    | 3.99  | 116.23      | 110.44   |
| 31  | D     | 407 | SQD  | O9-S-C6     | 3.99  | 112.71      | 106.76   |
| 24  | B     | 602 | CLA  | O2D-CGD-CBD | 3.98  | 118.19      | 111.23   |
| 24  | b     | 603 | CLA  | O2D-CGD-O1D | -3.98 | 116.10      | 123.85   |
| 24  | C     | 509 | CLA  | CMB-C2B-C1B | -3.98 | 119.36      | 125.42   |
| 25  | d     | 402 | PHO  | C1-C2-C3    | -3.97 | 119.69      | 126.20   |
| 35  | F     | 101 | HEM  | CBD-CAD-C3D | -3.95 | 101.61      | 112.53   |
| 24  | A     | 608 | CLA  | O2D-CGD-O1D | -3.94 | 116.19      | 123.85   |
| 25  | A     | 607 | PHO  | O1D-CGD-CBD | 3.93  | 130.69      | 124.72   |
| 30  | l     | 101 | LHG  | O4-P-O5     | 3.92  | 130.66      | 112.44   |
| 28  | d     | 406 | PL9  | C7-C3-C2    | -3.89 | 118.80      | 123.39   |
| 28  | A     | 612 | PL9  | C40-C39-C41 | 3.88  | 121.97      | 115.23   |
| 24  | b     | 611 | CLA  | C4A-NA-C1A  | 3.88  | 108.45      | 106.68   |
| 24  | b     | 602 | CLA  | CHB-C4A-NA  | 3.87  | 129.99      | 124.40   |
| 24  | C     | 504 | CLA  | C4A-NA-C1A  | 3.87  | 108.44      | 106.68   |
| 24  | B     | 607 | CLA  | C3B-C4B-NB  | -3.86 | 107.08      | 110.53   |
| 30  | d     | 407 | LHG  | O8-C23-O10  | -3.86 | 113.98      | 123.63   |
| 26  | C     | 515 | BCR  | C15-C16-C17 | -3.86 | 115.63      | 123.52   |
| 32  | C     | 518 | DGD  | O3G-C3G-C2G | -3.85 | 101.44      | 110.82   |
| 31  | A     | 616 | SQD  | O47-C7-C8   | 3.85  | 119.81      | 111.48   |
| 24  | B     | 606 | CLA  | C3B-C4B-NB  | -3.84 | 107.11      | 110.53   |
| 24  | A     | 605 | CLA  | CED-O2D-CGD | -3.83 | 107.22      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | a     | 611 | PL9  | C25-C24-C26 | 3.81  | 121.84      | 115.23   |
| 30  | B     | 621 | LHG  | O4-P-O5     | 3.79  | 130.08      | 112.44   |
| 24  | C     | 501 | CLA  | C3B-C4B-NB  | -3.78 | 107.15      | 110.53   |
| 32  | C     | 516 | DGD  | O3G-C3G-C2G | -3.78 | 101.62      | 110.82   |
| 24  | b     | 608 | CLA  | C3B-C4B-NB  | -3.77 | 107.17      | 110.53   |
| 26  | A     | 609 | BCR  | C27-C26-C25 | 3.75  | 127.77      | 122.70   |
| 24  | B     | 604 | CLA  | C3B-C4B-NB  | -3.74 | 107.19      | 110.53   |
| 24  | C     | 506 | CLA  | O2D-CGD-O1D | -3.74 | 116.56      | 123.85   |
| 32  | c     | 518 | DGD  | O3G-C3G-C2G | -3.71 | 101.79      | 110.82   |
| 26  | c     | 515 | BCR  | C27-C26-C25 | 3.70  | 127.70      | 122.70   |
| 24  | d     | 403 | CLA  | O2D-CGD-CBD | 3.70  | 117.69      | 111.23   |
| 32  | c     | 516 | DGD  | O3G-C3G-C2G | -3.69 | 101.85      | 110.82   |
| 24  | a     | 612 | CLA  | O2D-CGD-CBD | 3.67  | 117.65      | 111.23   |
| 24  | d     | 403 | CLA  | O2D-CGD-O1D | -3.67 | 116.70      | 123.85   |
| 24  | b     | 614 | CLA  | CMB-C2B-C1B | -3.67 | 119.83      | 125.42   |
| 28  | D     | 405 | PL9  | C27-C28-C29 | -3.66 | 119.24      | 127.62   |
| 24  | B     | 601 | CLA  | O2D-CGD-O1D | -3.66 | 116.72      | 123.85   |
| 24  | c     | 513 | CLA  | O2D-CGD-O1D | -3.66 | 116.72      | 123.85   |
| 24  | b     | 605 | CLA  | C4-C3-C5    | 3.66  | 121.58      | 115.23   |
| 24  | C     | 504 | CLA  | C3B-C4B-NB  | -3.65 | 107.27      | 110.53   |
| 31  | a     | 614 | SQD  | O48-C23-C24 | 3.64  | 122.94      | 111.83   |
| 29  | M     | 101 | LMG  | C1-O6-C5    | -3.64 | 106.61      | 113.72   |
| 24  | c     | 506 | CLA  | C3B-C4B-NB  | -3.63 | 107.29      | 110.53   |
| 31  | B     | 623 | SQD  | C1-O5-C5    | -3.63 | 106.64      | 113.72   |
| 24  | C     | 512 | CLA  | C1-C2-C3    | -3.62 | 120.27      | 126.20   |
| 31  | B     | 623 | SQD  | O5-C5-C4    | 3.61  | 116.21      | 109.70   |
| 24  | B     | 613 | CLA  | C1-C2-C3    | -3.59 | 120.31      | 126.20   |
| 24  | d     | 401 | CLA  | CHB-C4A-NA  | 3.58  | 129.57      | 124.40   |
| 24  | C     | 508 | CLA  | O2D-CGD-O1D | -3.58 | 116.88      | 123.85   |
| 26  | C     | 514 | BCR  | C2-C1-C6    | 3.58  | 115.64      | 110.44   |
| 28  | D     | 405 | PL9  | C30-C29-C31 | -3.57 | 109.03      | 115.23   |
| 31  | B     | 623 | SQD  | O47-C7-C8   | 3.57  | 119.19      | 111.48   |
| 25  | A     | 606 | PHO  | O2D-CGD-CBD | 3.57  | 114.86      | 110.95   |
| 24  | c     | 512 | CLA  | C3B-C4B-NB  | -3.56 | 107.35      | 110.53   |
| 24  | b     | 611 | CLA  | C3B-C4B-NB  | -3.55 | 107.36      | 110.53   |
| 24  | c     | 509 | CLA  | O2A-CGA-O1A | -3.55 | 114.76      | 123.63   |
| 31  | B     | 623 | SQD  | O7-S-C6     | 3.54  | 112.04      | 106.76   |
| 28  | A     | 612 | PL9  | C7-C3-C4    | 3.54  | 119.82      | 116.91   |
| 31  | a     | 613 | SQD  | O9-S-O7     | -3.53 | 102.33      | 113.82   |
| 25  | A     | 607 | PHO  | O2D-CGD-O1D | -3.53 | 116.97      | 123.85   |
| 30  | e     | 102 | LHG  | O8-C23-C24  | 3.53  | 122.59      | 111.83   |
| 26  | B     | 617 | BCR  | C2-C1-C6    | 3.52  | 115.56      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | f     | 101 | SQD  | C1-C2-C3    | -3.52 | 102.61      | 110.01   |
| 28  | D     | 405 | PL9  | C7-C3-C4    | 3.52  | 119.81      | 116.91   |
| 28  | A     | 612 | PL9  | O1-C4-C3    | -3.51 | 117.02      | 120.73   |
| 24  | B     | 603 | CLA  | O2D-CGD-O1D | -3.51 | 117.01      | 123.85   |
| 24  | C     | 509 | CLA  | CMB-C2B-C3B | 3.51  | 134.81      | 126.55   |
| 24  | B     | 616 | CLA  | CMB-C2B-C1B | -3.51 | 120.08      | 125.42   |
| 24  | b     | 613 | CLA  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 28  | A     | 612 | PL9  | C20-C19-C21 | 3.50  | 121.31      | 115.23   |
| 30  | d     | 407 | LHG  | O8-C23-C24  | 3.50  | 122.51      | 111.83   |
| 24  | c     | 512 | CLA  | O2D-CGD-O1D | -3.50 | 117.03      | 123.85   |
| 24  | c     | 501 | CLA  | CED-O2D-CGD | -3.49 | 108.00      | 115.92   |
| 31  | B     | 623 | SQD  | O48-C23-C24 | 3.49  | 122.47      | 111.83   |
| 28  | d     | 406 | PL9  | C37-C38-C39 | -3.48 | 119.66      | 127.62   |
| 24  | a     | 604 | CLA  | C3B-C4B-NB  | -3.48 | 107.43      | 110.53   |
| 24  | c     | 505 | CLA  | C3B-C4B-NB  | -3.48 | 107.43      | 110.53   |
| 24  | B     | 612 | CLA  | C3B-C4B-NB  | -3.47 | 107.43      | 110.53   |
| 25  | A     | 607 | PHO  | C2B-C1B-NB  | -3.47 | 106.92      | 109.43   |
| 24  | b     | 608 | CLA  | CMB-C2B-C1B | -3.46 | 120.15      | 125.42   |
| 24  | c     | 512 | CLA  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |
| 35  | e     | 101 | HEM  | CHB-C1B-NB  | 3.46  | 128.65      | 124.37   |
| 28  | D     | 405 | PL9  | C36-C34-C33 | -3.45 | 113.43      | 121.17   |
| 24  | A     | 608 | CLA  | O2D-CGD-CBD | 3.45  | 117.25      | 111.23   |
| 24  | B     | 602 | CLA  | C4A-NA-C1A  | 3.44  | 108.25      | 106.68   |
| 28  | A     | 612 | PL9  | C22-C23-C24 | -3.44 | 119.76      | 127.62   |
| 24  | b     | 601 | CLA  | O2D-CGD-O1D | -3.43 | 117.17      | 123.85   |
| 32  | h     | 101 | DGD  | O2D-C2D-C1D | -3.42 | 101.91      | 110.08   |
| 24  | A     | 604 | CLA  | C4A-NA-C1A  | 3.42  | 108.24      | 106.68   |
| 24  | D     | 403 | CLA  | O2D-CGD-O1D | -3.42 | 117.20      | 123.85   |
| 24  | b     | 604 | CLA  | O2D-CGD-O1D | -3.42 | 117.20      | 123.85   |
| 31  | B     | 623 | SQD  | O48-C23-O10 | -3.39 | 115.14      | 123.63   |
| 29  | c     | 522 | LMG  | O6-C1-O1    | -3.39 | 102.04      | 110.04   |
| 24  | B     | 614 | CLA  | O1D-CGD-CBD | 3.38  | 131.18      | 124.52   |
| 24  | b     | 613 | CLA  | CHB-C4A-NA  | 3.37  | 129.27      | 124.40   |
| 26  | d     | 405 | BCR  | C27-C26-C25 | 3.37  | 127.25      | 122.70   |
| 26  | A     | 609 | BCR  | C37-C22-C21 | -3.36 | 117.37      | 122.82   |
| 24  | C     | 503 | CLA  | O1D-CGD-CBD | 3.36  | 131.15      | 124.52   |
| 24  | c     | 510 | CLA  | O2D-CGD-O1D | -3.36 | 117.30      | 123.85   |
| 26  | H     | 101 | BCR  | C2-C1-C6    | 3.35  | 115.31      | 110.44   |
| 29  | M     | 101 | LMG  | O1-C1-C2    | -3.33 | 103.22      | 108.27   |
| 26  | b     | 619 | BCR  | C29-C30-C25 | 3.32  | 115.27      | 110.44   |
| 24  | B     | 611 | CLA  | O2D-CGD-CBD | 3.32  | 117.03      | 111.23   |
| 28  | D     | 405 | PL9  | C42-C43-C44 | -3.31 | 120.04      | 127.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 613 | SQD  | C1-C2-C3    | -3.31 | 103.04      | 110.01   |
| 24  | C     | 503 | CLA  | C7-C6-C5    | -3.31 | 104.43      | 113.26   |
| 24  | c     | 502 | CLA  | O2D-CGD-O1D | -3.31 | 117.41      | 123.85   |
| 24  | B     | 603 | CLA  | C3B-C4B-NB  | -3.31 | 107.58      | 110.53   |
| 24  | C     | 510 | CLA  | C3B-C4B-NB  | -3.30 | 107.58      | 110.53   |
| 24  | A     | 604 | CLA  | CHB-C4A-NA  | 3.30  | 129.16      | 124.40   |
| 29  | A     | 614 | LMG  | O6-C1-O1    | -3.30 | 102.25      | 110.04   |
| 24  | c     | 501 | CLA  | O2D-CGD-CBD | 3.28  | 116.97      | 111.23   |
| 24  | b     | 606 | CLA  | O2D-CGD-CBD | 3.28  | 116.97      | 111.23   |
| 24  | b     | 610 | CLA  | O1D-CGD-CBD | 3.28  | 130.99      | 124.52   |
| 29  | D     | 406 | LMG  | O6-C1-O1    | -3.28 | 102.30      | 110.04   |
| 24  | b     | 614 | CLA  | O2A-CGA-O1A | -3.27 | 115.44      | 123.63   |
| 24  | c     | 508 | CLA  | CHB-C4A-NA  | 3.27  | 129.12      | 124.40   |
| 25  | A     | 607 | PHO  | C4D-CHA-CBD | -3.27 | 106.89      | 108.45   |
| 32  | h     | 101 | DGD  | O3G-C3G-C2G | -3.27 | 102.86      | 110.82   |
| 28  | D     | 405 | PL9  | C35-C34-C36 | 3.27  | 120.90      | 115.23   |
| 24  | C     | 504 | CLA  | C4-C3-C5    | 3.26  | 120.89      | 115.23   |
| 24  | B     | 605 | CLA  | O2D-CGD-O1D | -3.26 | 117.51      | 123.85   |
| 25  | a     | 605 | PHO  | C2B-C1B-NB  | -3.25 | 107.08      | 109.43   |
| 24  | d     | 401 | CLA  | C2D-C1D-ND  | -3.25 | 106.91      | 110.13   |
| 24  | b     | 612 | CLA  | CHB-C4A-NA  | 3.25  | 129.09      | 124.40   |
| 32  | C     | 517 | DGD  | O3G-C3G-C2G | -3.24 | 102.94      | 110.82   |
| 24  | c     | 503 | CLA  | C3B-C4B-NB  | -3.24 | 107.64      | 110.53   |
| 24  | C     | 506 | CLA  | O1D-CGD-CBD | 3.24  | 130.90      | 124.52   |
| 24  | b     | 601 | CLA  | CHB-C4A-NA  | 3.23  | 129.06      | 124.40   |
| 32  | C     | 516 | DGD  | C3D-C4D-C5D | -3.23 | 104.38      | 110.23   |
| 24  | B     | 610 | CLA  | O2A-CGA-O1A | -3.22 | 115.57      | 123.63   |
| 30  | d     | 409 | LHG  | C26-C25-C24 | 3.21  | 124.93      | 113.13   |
| 25  | a     | 605 | PHO  | CMB-C2B-C3B | 3.21  | 131.10      | 124.68   |
| 24  | d     | 404 | CLA  | CMB-C2B-C1B | -3.21 | 120.53      | 125.42   |
| 24  | C     | 502 | CLA  | C4D-CHA-C1A | 3.21  | 125.07      | 121.24   |
| 31  | B     | 623 | SQD  | C3-C4-C5    | 3.20  | 116.04      | 110.23   |
| 24  | B     | 603 | CLA  | C4-C3-C5    | 3.20  | 120.79      | 115.23   |
| 24  | a     | 612 | CLA  | CHB-C4A-NA  | 3.20  | 129.02      | 124.40   |
| 31  | a     | 613 | SQD  | C1-O5-C5    | -3.19 | 107.49      | 113.72   |
| 24  | B     | 604 | CLA  | CHB-C4A-NA  | 3.18  | 129.00      | 124.40   |
| 24  | C     | 502 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 24  | b     | 615 | CLA  | CHB-C4A-NA  | 3.18  | 128.99      | 124.40   |
| 32  | C     | 516 | DGD  | O6D-C1D-O3G | -3.18 | 102.54      | 110.04   |
| 25  | d     | 402 | PHO  | C2B-C1B-NB  | -3.18 | 107.14      | 109.43   |
| 25  | A     | 607 | PHO  | CMB-C2B-C3B | 3.18  | 131.03      | 124.68   |
| 24  | b     | 602 | CLA  | CMB-C2B-C1B | -3.17 | 120.59      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 616 | CLA  | CMB-C2B-C3B | 3.17  | 134.01      | 126.55   |
| 26  | T     | 101 | BCR  | C27-C26-C25 | 3.16  | 126.98      | 122.70   |
| 24  | B     | 602 | CLA  | CMB-C2B-C1B | -3.16 | 120.60      | 125.42   |
| 31  | b     | 620 | SQD  | O5-C5-C4    | 3.16  | 115.40      | 109.70   |
| 24  | c     | 507 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 26  | t     | 101 | BCR  | C1-C6-C5    | -3.16 | 118.31      | 122.64   |
| 31  | b     | 620 | SQD  | O48-C23-C24 | 3.16  | 121.47      | 111.83   |
| 24  | B     | 616 | CLA  | O2A-CGA-O1A | -3.16 | 115.72      | 123.63   |
| 24  | b     | 614 | CLA  | C4-C3-C5    | 3.16  | 120.71      | 115.23   |
| 26  | b     | 617 | BCR  | C27-C26-C25 | 3.15  | 126.95      | 122.70   |
| 24  | B     | 602 | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 24  | D     | 402 | CLA  | CED-O2D-CGD | 3.14  | 123.04      | 115.92   |
| 24  | b     | 616 | CLA  | CHB-C4A-NA  | 3.13  | 128.92      | 124.40   |
| 36  | V     | 201 | HEC  | C4D-ND-C1D  | 3.13  | 110.93      | 105.82   |
| 31  | B     | 623 | SQD  | O8-S-C6     | 3.13  | 112.01      | 105.97   |
| 31  | A     | 617 | SQD  | O48-C23-C24 | 3.12  | 121.36      | 111.83   |
| 24  | c     | 502 | CLA  | C3B-C4B-NB  | -3.12 | 107.74      | 110.53   |
| 24  | a     | 604 | CLA  | CMB-C2B-C1B | -3.12 | 120.66      | 125.42   |
| 28  | d     | 406 | PL9  | C7-C8-C9    | -3.12 | 121.45      | 126.83   |
| 24  | c     | 507 | CLA  | CHB-C4A-NA  | 3.12  | 128.90      | 124.40   |
| 29  | a     | 618 | LMG  | C9-C8-C7    | -3.12 | 104.52      | 111.78   |
| 24  | C     | 504 | CLA  | O2A-CGA-O1A | -3.12 | 115.83      | 123.63   |
| 24  | c     | 512 | CLA  | CHB-C4A-NA  | 3.11  | 128.90      | 124.40   |
| 24  | c     | 503 | CLA  | C7-C6-C5    | -3.11 | 104.96      | 113.26   |
| 28  | D     | 405 | PL9  | C22-C23-C24 | -3.11 | 120.50      | 127.62   |
| 24  | b     | 612 | CLA  | C1-C2-C3    | -3.11 | 121.10      | 126.20   |
| 33  | D     | 411 | STE  | C3-C2-C1    | -3.10 | 106.41      | 114.51   |
| 24  | b     | 603 | CLA  | CHB-C1B-NB  | 3.10  | 128.71      | 124.05   |
| 24  | b     | 611 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 31  | D     | 407 | SQD  | C1-C2-C3    | -3.10 | 103.49      | 110.01   |
| 24  | B     | 615 | CLA  | CHC-C4B-NB  | 3.10  | 128.69      | 124.05   |
| 24  | C     | 505 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 26  | T     | 101 | BCR  | C35-C13-C14 | -3.09 | 117.80      | 122.82   |
| 24  | a     | 606 | CLA  | CHB-C4A-NA  | 3.09  | 128.87      | 124.40   |
| 31  | b     | 620 | SQD  | C1-C2-C3    | -3.09 | 103.50      | 110.01   |
| 24  | C     | 513 | CLA  | C1-O2A-CGA  | -3.09 | 109.18      | 116.65   |
| 29  | b     | 623 | LMG  | O1-C1-C2    | -3.09 | 103.59      | 108.27   |
| 24  | C     | 512 | CLA  | CMB-C2B-C1B | -3.07 | 120.74      | 125.42   |
| 24  | C     | 507 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 24  | b     | 603 | CLA  | CMB-C2B-C1B | -3.07 | 120.74      | 125.42   |
| 28  | A     | 612 | PL9  | C36-C34-C33 | -3.07 | 114.28      | 121.17   |
| 32  | c     | 517 | DGD  | O3G-C3G-C2G | -3.06 | 103.37      | 110.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 512 | CLA  | CHB-C4A-NA  | 3.06  | 128.82      | 124.40   |
| 26  | Y     | 101 | BCR  | C27-C26-C25 | 3.06  | 126.84      | 122.70   |
| 26  | D     | 404 | BCR  | C27-C26-C25 | 3.06  | 126.84      | 122.70   |
| 24  | b     | 605 | CLA  | C4A-NA-C1A  | 3.06  | 108.08      | 106.68   |
| 28  | d     | 406 | PL9  | C42-C43-C44 | -3.06 | 120.62      | 127.62   |
| 26  | T     | 101 | BCR  | C7-C8-C9    | -3.06 | 121.72      | 126.23   |
| 25  | A     | 607 | PHO  | C3B-C4B-NB  | -3.05 | 105.47      | 107.46   |
| 24  | b     | 610 | CLA  | CAC-C3C-C4C | 3.05  | 128.76      | 124.79   |
| 24  | B     | 610 | CLA  | O2D-CGD-CBD | 3.05  | 116.56      | 111.23   |
| 32  | c     | 518 | DGD  | C3D-C4D-C5D | -3.05 | 104.71      | 110.23   |
| 24  | b     | 602 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 24  | b     | 614 | CLA  | C1-C2-C3    | -3.04 | 121.22      | 126.20   |
| 31  | b     | 620 | SQD  | O9-S-C6     | 3.04  | 111.29      | 106.76   |
| 24  | c     | 511 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 26  | C     | 514 | BCR  | C27-C26-C25 | 3.04  | 126.81      | 122.70   |
| 32  | C     | 517 | DGD  | O6D-C1D-O3G | -3.04 | 102.87      | 110.04   |
| 31  | a     | 613 | SQD  | O47-C7-C8   | 3.03  | 118.04      | 111.48   |
| 24  | c     | 508 | CLA  | O2D-CGD-O1D | -3.03 | 117.96      | 123.85   |
| 29  | d     | 410 | LMG  | O2-C2-C1    | -3.02 | 102.88      | 110.08   |
| 24  | B     | 612 | CLA  | CMB-C2B-C1B | -3.02 | 120.82      | 125.42   |
| 24  | d     | 401 | CLA  | C1D-ND-C4D  | 3.02  | 108.43      | 106.31   |
| 31  | a     | 613 | SQD  | O7-S-C6     | 3.02  | 111.26      | 106.76   |
| 31  | a     | 614 | SQD  | O48-C23-O10 | -3.01 | 116.09      | 123.63   |
| 24  | b     | 608 | CLA  | CMB-C2B-C3B | 3.01  | 133.64      | 126.55   |
| 24  | c     | 505 | CLA  | C1-C2-C3    | -3.01 | 121.26      | 126.20   |
| 24  | b     | 609 | CLA  | O1D-CGD-CBD | 3.01  | 130.46      | 124.52   |
| 24  | b     | 605 | CLA  | CHB-C1B-NB  | 3.01  | 128.56      | 124.05   |
| 24  | B     | 614 | CLA  | C4A-NA-C1A  | 3.01  | 108.05      | 106.68   |
| 24  | a     | 612 | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 30  | d     | 407 | LHG  | C11-C10-C9  | -3.00 | 99.19       | 114.37   |
| 24  | a     | 606 | CLA  | O2D-CGD-CBD | 3.00  | 116.48      | 111.23   |
| 24  | c     | 503 | CLA  | C4A-NA-C1A  | 3.00  | 108.05      | 106.68   |
| 29  | b     | 621 | LMG  | C9-C8-C7    | -3.00 | 104.79      | 111.78   |
| 24  | C     | 507 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 31  | a     | 613 | SQD  | O9-S-C6     | 3.00  | 111.23      | 106.76   |
| 31  | A     | 616 | SQD  | O5-C1-O6    | 2.99  | 117.12      | 110.04   |
| 24  | D     | 402 | CLA  | CMD-C2D-C1D | -2.99 | 119.46      | 124.73   |
| 24  | C     | 507 | CLA  | O2D-CGD-CBD | 2.98  | 116.45      | 111.23   |
| 32  | C     | 517 | DGD  | C6D-O5D-C1E | 2.98  | 120.19      | 113.80   |
| 26  | A     | 609 | BCR  | C2-C1-C6    | 2.98  | 114.77      | 110.44   |
| 24  | B     | 607 | CLA  | CHB-C1B-NB  | 2.98  | 128.52      | 124.05   |
| 25  | a     | 605 | PHO  | OBD-CAD-CBD | -2.98 | 121.45      | 125.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 602 | CLA  | CMB-C2B-C3B | 2.98  | 133.55      | 126.55   |
| 32  | A     | 618 | DGD  | C3G-C2G-C1G | -2.98 | 104.84      | 111.78   |
| 30  | B     | 622 | LHG  | O8-C23-C24  | 2.98  | 120.91      | 111.83   |
| 24  | B     | 602 | CLA  | C1-C2-C3    | -2.98 | 121.32      | 126.20   |
| 31  | b     | 620 | SQD  | O9-S-O7     | -2.97 | 104.16      | 113.82   |
| 24  | c     | 510 | CLA  | O2A-CGA-O1A | -2.97 | 116.20      | 123.63   |
| 29  | c     | 521 | LMG  | O3-C3-C2    | -2.97 | 103.38      | 110.38   |
| 25  | A     | 606 | PHO  | OBD-CAD-CBD | -2.96 | 121.48      | 125.82   |
| 26  | c     | 514 | BCR  | C27-C26-C25 | 2.96  | 126.70      | 122.70   |
| 33  | C     | 522 | STE  | C3-C2-C1    | -2.96 | 106.79      | 114.51   |
| 24  | b     | 604 | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 28  | A     | 612 | PL9  | C27-C28-C29 | -2.95 | 120.88      | 127.62   |
| 25  | d     | 402 | PHO  | CMB-C2B-C3B | 2.95  | 130.57      | 124.68   |
| 24  | b     | 613 | CLA  | C4A-NA-C1A  | 2.95  | 108.02      | 106.68   |
| 31  | D     | 407 | SQD  | O48-C23-C24 | 2.94  | 120.80      | 111.83   |
| 36  | V     | 201 | HEC  | CHD-C4C-NC  | 2.94  | 127.66      | 124.45   |
| 24  | c     | 506 | CLA  | CHB-C4A-NA  | 2.94  | 128.64      | 124.40   |
| 24  | A     | 605 | CLA  | CMB-C2B-C1B | -2.94 | 120.95      | 125.42   |
| 26  | d     | 405 | BCR  | C38-C26-C25 | -2.94 | 121.28      | 124.48   |
| 32  | A     | 618 | DGD  | O3G-C3G-C2G | -2.93 | 103.69      | 110.82   |
| 24  | c     | 513 | CLA  | CMB-C2B-C1B | -2.92 | 120.97      | 125.42   |
| 31  | a     | 613 | SQD  | O48-C23-C24 | 2.92  | 120.73      | 111.83   |
| 24  | C     | 508 | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 24  | C     | 510 | CLA  | CMB-C2B-C1B | -2.92 | 120.98      | 125.42   |
| 24  | C     | 509 | CLA  | CHB-C4A-NA  | 2.92  | 128.61      | 124.40   |
| 30  | E     | 101 | LHG  | O8-C23-C24  | 2.91  | 120.72      | 111.83   |
| 33  | d     | 411 | STE  | O2-C1-C2    | 2.91  | 123.20      | 114.00   |
| 36  | V     | 201 | HEC  | CBD-CAD-C3D | -2.91 | 104.49      | 112.53   |
| 24  | d     | 404 | CLA  | CMB-C2B-C3B | 2.91  | 133.39      | 126.55   |
| 24  | c     | 509 | CLA  | CHC-C1C-NC  | 2.90  | 128.69      | 124.31   |
| 28  | D     | 405 | PL9  | C20-C19-C21 | 2.90  | 120.26      | 115.23   |
| 24  | c     | 506 | CLA  | CBC-CAC-C3C | -2.90 | 104.56      | 112.42   |
| 31  | b     | 620 | SQD  | C3-C4-C5    | 2.90  | 115.48      | 110.23   |
| 29  | d     | 410 | LMG  | O1-C1-C2    | -2.90 | 103.88      | 108.27   |
| 24  | c     | 505 | CLA  | CMB-C2B-C1B | -2.89 | 121.02      | 125.42   |
| 29  | b     | 621 | LMG  | C38-C37-C36 | -2.89 | 99.76       | 114.37   |
| 24  | c     | 504 | CLA  | CHB-C4A-NA  | 2.89  | 128.57      | 124.40   |
| 24  | B     | 611 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 25  | a     | 605 | PHO  | C3D-C4D-ND  | 2.88  | 111.41      | 107.71   |
| 31  | D     | 407 | SQD  | C1-O5-C5    | -2.88 | 108.09      | 113.72   |
| 26  | t     | 101 | BCR  | C7-C8-C9    | -2.88 | 121.97      | 126.23   |
| 32  | C     | 518 | DGD  | O3D-C3D-C4D | -2.88 | 103.59      | 110.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 609 | CLA  | CMB-C2B-C3B | 2.88  | 133.31      | 126.55   |
| 24  | B     | 609 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 26  | x     | 101 | BCR  | C38-C26-C25 | -2.87 | 121.35      | 124.48   |
| 24  | c     | 507 | CLA  | C4-C3-C5    | 2.87  | 120.21      | 115.23   |
| 24  | C     | 503 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 29  | A     | 614 | LMG  | C9-C8-C7    | -2.87 | 105.09      | 111.78   |
| 31  | A     | 616 | SQD  | O47-C7-O49  | -2.87 | 117.00      | 123.70   |
| 24  | b     | 610 | CLA  | O2A-CGA-O1A | -2.87 | 116.46      | 123.63   |
| 24  | B     | 614 | CLA  | C4-C3-C5    | 2.86  | 120.20      | 115.23   |
| 29  | C     | 519 | LMG  | O6-C1-O1    | -2.86 | 103.28      | 110.04   |
| 24  | d     | 401 | CLA  | CAC-C3C-C4C | 2.86  | 128.51      | 124.79   |
| 24  | b     | 613 | CLA  | CMB-C2B-C1B | -2.85 | 121.07      | 125.42   |
| 24  | A     | 605 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 24  | c     | 505 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 26  | d     | 405 | BCR  | C2-C1-C6    | 2.85  | 114.58      | 110.44   |
| 29  | b     | 623 | LMG  | C3-C4-C5    | -2.85 | 105.06      | 110.23   |
| 24  | C     | 505 | CLA  | CMB-C2B-C3B | 2.85  | 133.25      | 126.55   |
| 32  | c     | 516 | DGD  | O2D-C2D-C3D | -2.84 | 103.68      | 110.38   |
| 24  | b     | 615 | CLA  | O2D-CGD-CBD | 2.84  | 116.19      | 111.23   |
| 24  | C     | 513 | CLA  | O2A-CGA-O1A | -2.84 | 116.53      | 123.63   |
| 24  | b     | 615 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 24  | c     | 511 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 24  | C     | 506 | CLA  | CHB-C4A-NA  | 2.83  | 128.48      | 124.40   |
| 24  | B     | 606 | CLA  | CHA-C1A-NA  | -2.82 | 119.99      | 126.39   |
| 36  | V     | 201 | HEC  | CMC-C2C-C1C | -2.82 | 121.13      | 125.42   |
| 32  | C     | 518 | DGD  | CDB-CCB-CBB | -2.82 | 100.14      | 114.37   |
| 24  | b     | 610 | CLA  | CHB-C4A-NA  | 2.81  | 128.46      | 124.40   |
| 24  | b     | 611 | CLA  | CHD-C1D-ND  | -2.81 | 120.84      | 124.80   |
| 32  | c     | 518 | DGD  | O6D-C1D-O3G | -2.81 | 103.40      | 110.04   |
| 31  | D     | 407 | SQD  | O5-C1-C2    | -2.81 | 104.60      | 110.37   |
| 30  | D     | 408 | LHG  | O8-C23-C24  | 2.81  | 120.39      | 111.83   |
| 29  | b     | 621 | LMG  | O3-C3-C2    | -2.80 | 103.78      | 110.38   |
| 33  | a     | 616 | STE  | C3-C2-C1    | -2.79 | 107.22      | 114.51   |
| 24  | c     | 513 | CLA  | CHB-C4A-NA  | 2.79  | 128.42      | 124.40   |
| 24  | b     | 610 | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 24  | C     | 503 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 26  | c     | 515 | BCR  | C2-C1-C6    | 2.79  | 114.48      | 110.44   |
| 26  | c     | 515 | BCR  | C7-C8-C9    | -2.78 | 122.12      | 126.23   |
| 31  | f     | 101 | SQD  | O5-C1-C2    | -2.78 | 104.65      | 110.37   |
| 24  | A     | 604 | CLA  | O1D-CGD-CBD | 2.78  | 130.00      | 124.52   |
| 24  | b     | 606 | CLA  | CMB-C2B-C1B | -2.78 | 121.18      | 125.42   |
| 26  | k     | 102 | BCR  | C29-C30-C25 | 2.78  | 114.48      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | b     | 620 | SQD  | C45-O47-C7  | 2.78  | 124.44      | 117.80   |
| 24  | b     | 604 | CLA  | C6-C5-C3    | -2.78 | 106.71      | 113.47   |
| 24  | B     | 610 | CLA  | CHB-C4A-NA  | 2.78  | 128.41      | 124.40   |
| 24  | a     | 604 | CLA  | CAC-C3C-C4C | 2.77  | 128.40      | 124.79   |
| 24  | b     | 615 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 29  | b     | 623 | LMG  | O6-C5-C6    | 2.77  | 113.30      | 106.44   |
| 24  | b     | 615 | CLA  | C11-C10-C8  | -2.77 | 106.77      | 115.97   |
| 29  | b     | 623 | LMG  | O2-C2-C1    | -2.77 | 103.49      | 110.08   |
| 26  | C     | 515 | BCR  | C36-C18-C17 | -2.76 | 118.34      | 122.82   |
| 29  | b     | 621 | LMG  | C1-O6-C5    | -2.76 | 108.33      | 113.72   |
| 33  | m     | 101 | STE  | O2-C1-C2    | 2.76  | 122.72      | 114.00   |
| 28  | D     | 405 | PL9  | C40-C39-C38 | -2.76 | 116.54      | 123.63   |
| 24  | b     | 604 | CLA  | C1-C2-C3    | -2.76 | 121.68      | 126.20   |
| 26  | b     | 617 | BCR  | C15-C16-C17 | -2.76 | 117.88      | 123.52   |
| 26  | t     | 101 | BCR  | C36-C18-C19 | 2.76  | 122.30      | 118.09   |
| 29  | M     | 101 | LMG  | O3-C3-C2    | -2.75 | 103.89      | 110.38   |
| 24  | B     | 606 | CLA  | C1-C2-C3    | -2.75 | 121.69      | 126.20   |
| 24  | a     | 606 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 24  | B     | 605 | CLA  | C16-C15-C13 | -2.75 | 106.83      | 115.97   |
| 32  | C     | 516 | DGD  | O2D-C2D-C1D | -2.75 | 103.53      | 110.08   |
| 24  | C     | 505 | CLA  | CHB-C1B-NB  | 2.74  | 128.16      | 124.05   |
| 26  | B     | 619 | BCR  | C29-C30-C25 | 2.74  | 114.41      | 110.44   |
| 24  | C     | 502 | CLA  | C1D-ND-C4D  | 2.74  | 108.23      | 106.31   |
| 32  | A     | 618 | DGD  | C4E-C3E-C2E | -2.73 | 106.03      | 110.83   |
| 24  | B     | 613 | CLA  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 24  | C     | 508 | CLA  | CHD-C1D-C2D | 2.73  | 131.17      | 125.49   |
| 32  | C     | 517 | DGD  | O5D-C6D-C5D | -2.73 | 103.27      | 109.42   |
| 26  | k     | 101 | BCR  | C38-C26-C25 | -2.73 | 121.51      | 124.48   |
| 24  | b     | 603 | CLA  | CHC-C4B-NB  | 2.73  | 128.14      | 124.05   |
| 25  | d     | 402 | PHO  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 31  | b     | 620 | SQD  | O2-C2-C1    | 2.72  | 116.56      | 110.08   |
| 32  | H     | 102 | DGD  | O2D-C2D-C1D | -2.72 | 103.59      | 110.08   |
| 24  | b     | 602 | CLA  | CHC-C1C-NC  | 2.72  | 128.41      | 124.31   |
| 25  | a     | 605 | PHO  | OBD-CAD-C3D | 2.72  | 132.13      | 127.89   |
| 24  | C     | 511 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 35  | e     | 101 | HEM  | C3B-C2B-C1B | 2.71  | 108.45      | 106.41   |
| 30  | d     | 408 | LHG  | O8-C23-C24  | 2.71  | 120.10      | 111.83   |
| 26  | C     | 514 | BCR  | C11-C10-C9  | -2.71 | 123.48      | 127.28   |
| 24  | D     | 402 | CLA  | CMD-C2D-C3D | 2.71  | 133.90      | 127.69   |
| 26  | A     | 609 | BCR  | C36-C18-C17 | -2.71 | 118.43      | 122.82   |
| 24  | C     | 512 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 24  | B     | 615 | CLA  | CAC-C3C-C4C | 2.70  | 128.30      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 613 | SQD  | C3-C4-C5    | 2.70  | 115.12      | 110.23   |
| 26  | A     | 609 | BCR  | C38-C26-C25 | -2.70 | 121.54      | 124.48   |
| 32  | H     | 102 | DGD  | C3D-C4D-C5D | -2.69 | 105.35      | 110.23   |
| 24  | C     | 508 | CLA  | C1-C2-C3    | -2.69 | 121.79      | 126.20   |
| 26  | b     | 617 | BCR  | C38-C26-C25 | -2.69 | 121.55      | 124.48   |
| 31  | a     | 614 | SQD  | O49-C7-C8   | -2.69 | 113.26      | 123.78   |
| 24  | b     | 608 | CLA  | C4A-NA-C1A  | 2.69  | 107.91      | 106.68   |
| 28  | d     | 406 | PL9  | C20-C19-C21 | 2.69  | 119.89      | 115.23   |
| 24  | b     | 612 | CLA  | CMB-C2B-C1B | -2.69 | 121.33      | 125.42   |
| 24  | C     | 509 | CLA  | CED-O2D-CGD | 2.68  | 122.00      | 115.92   |
| 26  | B     | 617 | BCR  | C29-C30-C25 | 2.68  | 114.34      | 110.44   |
| 24  | B     | 611 | CLA  | C1-C2-C3    | -2.68 | 121.80      | 126.20   |
| 24  | a     | 606 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 26  | C     | 514 | BCR  | C38-C26-C25 | -2.68 | 121.56      | 124.48   |
| 24  | A     | 604 | CLA  | CMB-C2B-C3B | 2.68  | 132.85      | 126.55   |
| 30  | l     | 101 | LHG  | C20-C19-C18 | -2.68 | 100.83      | 114.37   |
| 24  | b     | 609 | CLA  | O2A-CGA-O1A | -2.68 | 116.93      | 123.63   |
| 32  | A     | 618 | DGD  | CDB-CCB-CBB | -2.68 | 100.83      | 114.37   |
| 24  | b     | 603 | CLA  | O2D-CGD-CBD | 2.68  | 115.91      | 111.23   |
| 26  | Y     | 101 | BCR  | C39-C30-C25 | -2.68 | 106.05      | 110.24   |
| 32  | A     | 618 | DGD  | C1D-C2D-C3D | -2.67 | 104.38      | 110.01   |
| 24  | c     | 510 | CLA  | CMB-C2B-C1B | -2.67 | 121.35      | 125.42   |
| 32  | C     | 516 | DGD  | O5D-C6D-C5D | -2.67 | 103.40      | 109.42   |
| 32  | c     | 517 | DGD  | O6D-C1D-O3G | -2.67 | 103.74      | 110.04   |
| 24  | B     | 601 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 32  | H     | 102 | DGD  | O3E-C3E-C2E | -2.66 | 104.09      | 110.38   |
| 24  | b     | 616 | CLA  | CMB-C2B-C3B | 2.66  | 132.81      | 126.55   |
| 24  | B     | 614 | CLA  | CHC-C4B-NB  | 2.66  | 128.04      | 124.05   |
| 24  | B     | 612 | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 26  | D     | 404 | BCR  | C2-C1-C6    | 2.66  | 114.30      | 110.44   |
| 24  | B     | 605 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 29  | b     | 621 | LMG  | O1-C1-C2    | -2.66 | 104.23      | 108.27   |
| 26  | a     | 607 | BCR  | C37-C22-C23 | 2.66  | 122.15      | 118.09   |
| 25  | A     | 606 | PHO  | CMB-C2B-C3B | 2.66  | 129.99      | 124.68   |
| 24  | B     | 610 | CLA  | O1D-CGD-CBD | 2.66  | 129.76      | 124.52   |
| 29  | b     | 621 | LMG  | O1-C7-C8    | -2.66 | 104.36      | 110.82   |
| 24  | a     | 612 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 24  | A     | 613 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 28  | D     | 405 | PL9  | C8-C7-C3    | 2.65  | 118.88      | 112.03   |
| 29  | c     | 519 | LMG  | O6-C1-O1    | -2.65 | 103.79      | 110.04   |
| 32  | c     | 518 | DGD  | O3D-C3D-C4D | -2.65 | 104.14      | 110.38   |
| 24  | b     | 616 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 507 | CLA  | CHC-C4B-NB  | 2.65  | 128.02      | 124.05   |
| 24  | b     | 614 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 24  | B     | 616 | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 24  | C     | 512 | CLA  | CMB-C2B-C3B | 2.64  | 132.75      | 126.55   |
| 24  | b     | 613 | CLA  | C7-C6-C5    | -2.64 | 106.23      | 113.26   |
| 24  | C     | 501 | CLA  | CHB-C1B-NB  | 2.64  | 128.00      | 124.05   |
| 24  | D     | 403 | CLA  | CMB-C2B-C1B | -2.63 | 121.41      | 125.42   |
| 26  | t     | 101 | BCR  | C15-C16-C17 | -2.63 | 118.13      | 123.52   |
| 26  | b     | 618 | BCR  | C37-C22-C21 | -2.63 | 118.56      | 122.82   |
| 24  | C     | 509 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 33  | x     | 102 | STE  | O2-C1-O1    | -2.62 | 116.59      | 123.33   |
| 24  | B     | 616 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 24  | b     | 612 | CLA  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 26  | H     | 101 | BCR  | C37-C22-C21 | -2.62 | 118.57      | 122.82   |
| 26  | C     | 515 | BCR  | C27-C26-C25 | 2.62  | 126.24      | 122.70   |
| 24  | b     | 601 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 24  | b     | 607 | CLA  | C1-O2A-CGA  | 2.62  | 122.99      | 116.65   |
| 24  | A     | 605 | CLA  | CMB-C2B-C3B | 2.61  | 132.70      | 126.55   |
| 24  | B     | 606 | CLA  | CGD-CBD-CAD | -2.61 | 102.39      | 110.85   |
| 32  | c     | 516 | DGD  | O6E-C5E-C4E | 2.61  | 114.41      | 109.70   |
| 32  | C     | 517 | DGD  | C1D-C2D-C3D | -2.61 | 104.51      | 110.01   |
| 31  | B     | 623 | SQD  | O5-C1-C2    | -2.61 | 105.01      | 110.37   |
| 24  | B     | 601 | CLA  | O2D-CGD-CBD | 2.61  | 115.79      | 111.23   |
| 26  | H     | 101 | BCR  | C16-C15-C14 | -2.61 | 118.18      | 123.52   |
| 24  | c     | 508 | CLA  | CHD-C1D-ND  | -2.61 | 121.13      | 124.80   |
| 26  | H     | 101 | BCR  | C27-C26-C25 | 2.61  | 126.23      | 122.70   |
| 26  | c     | 514 | BCR  | C15-C16-C17 | -2.61 | 118.19      | 123.52   |
| 30  | l     | 101 | LHG  | C11-C10-C9  | -2.61 | 101.19      | 114.37   |
| 29  | A     | 614 | LMG  | O3-C3-C2    | -2.60 | 104.24      | 110.38   |
| 24  | c     | 507 | CLA  | O2A-CGA-O1A | -2.60 | 117.11      | 123.63   |
| 24  | C     | 513 | CLA  | O2D-CGD-CBD | 2.60  | 115.78      | 111.23   |
| 32  | C     | 517 | DGD  | C3E-C4E-C5E | -2.60 | 105.52      | 110.23   |
| 24  | B     | 611 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 31  | D     | 407 | SQD  | O5-C5-C4    | 2.60  | 114.38      | 109.70   |
| 24  | B     | 604 | CLA  | O2A-CGA-O1A | -2.60 | 117.13      | 123.63   |
| 26  | B     | 618 | BCR  | C7-C8-C9    | -2.60 | 122.39      | 126.23   |
| 24  | a     | 612 | CLA  | CMB-C2B-C3B | 2.60  | 132.66      | 126.55   |
| 26  | H     | 101 | BCR  | C1-C6-C5    | -2.60 | 119.09      | 122.64   |
| 31  | f     | 101 | SQD  | C3-C4-C5    | 2.59  | 114.94      | 110.23   |
| 30  | l     | 101 | LHG  | C18-C17-C16 | -2.59 | 101.25      | 114.37   |
| 24  | b     | 612 | CLA  | C11-C12-C13 | -2.59 | 107.36      | 115.97   |
| 24  | C     | 504 | CLA  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 610 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 24  | B     | 609 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 28  | D     | 405 | PL9  | C37-C38-C39 | -2.59 | 121.70      | 127.62   |
| 26  | D     | 404 | BCR  | C38-C26-C25 | -2.59 | 121.66      | 124.48   |
| 24  | b     | 612 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.79   |
| 30  | D     | 408 | LHG  | C11-C10-C9  | -2.58 | 101.31      | 114.37   |
| 24  | c     | 501 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 24  | A     | 608 | CLA  | C4-C3-C5    | 2.58  | 119.71      | 115.23   |
| 26  | c     | 514 | BCR  | C2-C1-C6    | 2.58  | 114.18      | 110.44   |
| 24  | c     | 508 | CLA  | CHD-C4C-NC  | 2.58  | 128.23      | 124.23   |
| 24  | A     | 605 | CLA  | O2D-CGD-CBD | 2.58  | 115.73      | 111.23   |
| 24  | d     | 403 | CLA  | O2A-CGA-O1A | -2.58 | 117.19      | 123.63   |
| 24  | C     | 511 | CLA  | O2A-CGA-O1A | -2.57 | 117.19      | 123.63   |
| 24  | B     | 609 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 24  | B     | 606 | CLA  | C4-C3-C5    | 2.57  | 119.69      | 115.23   |
| 24  | D     | 402 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 24  | b     | 615 | CLA  | CHC-C1C-NC  | 2.57  | 128.19      | 124.31   |
| 32  | C     | 516 | DGD  | CDB-CCB-CBB | -2.57 | 101.36      | 114.37   |
| 29  | c     | 519 | LMG  | C9-C8-C7    | -2.57 | 105.79      | 111.78   |
| 24  | c     | 502 | CLA  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |
| 24  | B     | 612 | CLA  | C11-C12-C13 | -2.57 | 107.43      | 115.97   |
| 31  | A     | 616 | SQD  | O48-C23-C24 | 2.57  | 119.66      | 111.83   |
| 30  | D     | 408 | LHG  | C20-C19-C18 | -2.57 | 101.39      | 114.37   |
| 24  | a     | 606 | CLA  | O2A-CGA-O1A | -2.57 | 117.21      | 123.63   |
| 26  | k     | 102 | BCR  | C27-C26-C25 | 2.56  | 126.17      | 122.70   |
| 26  | b     | 619 | BCR  | C27-C26-C25 | 2.56  | 126.17      | 122.70   |
| 24  | B     | 613 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 26  | b     | 617 | BCR  | C36-C18-C19 | 2.56  | 122.00      | 118.09   |
| 26  | x     | 101 | BCR  | C27-C26-C25 | 2.56  | 126.16      | 122.70   |
| 24  | b     | 616 | CLA  | CMB-C2B-C1B | -2.56 | 121.53      | 125.42   |
| 24  | B     | 612 | CLA  | CMB-C2B-C3B | 2.55  | 132.56      | 126.55   |
| 24  | B     | 605 | CLA  | C7-C6-C5    | -2.55 | 106.46      | 113.26   |
| 35  | e     | 101 | HEM  | C4C-C3C-C2C | 2.55  | 109.03      | 106.81   |
| 29  | d     | 410 | LMG  | O6-C1-O1    | -2.55 | 104.01      | 110.04   |
| 24  | C     | 506 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 24  | b     | 605 | CLA  | CHD-C1D-ND  | -2.55 | 121.21      | 124.80   |
| 24  | b     | 605 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 24  | C     | 510 | CLA  | CMB-C2B-C3B | 2.55  | 132.54      | 126.55   |
| 24  | b     | 611 | CLA  | CHD-C1D-C2D | 2.55  | 130.78      | 125.49   |
| 24  | B     | 613 | CLA  | CHA-C1A-NA  | -2.55 | 120.63      | 126.39   |
| 26  | a     | 607 | BCR  | C29-C30-C25 | 2.54  | 114.13      | 110.44   |
| 26  | k     | 101 | BCR  | C27-C26-C25 | 2.54  | 126.14      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | c     | 510 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 32  | c     | 516 | DGD  | CDB-CCB-CBB | -2.54 | 101.53      | 114.37   |
| 30  | B     | 622 | LHG  | C11-C10-C9  | -2.53 | 101.55      | 114.37   |
| 24  | b     | 602 | CLA  | C1-C2-C3    | -2.53 | 122.04      | 126.20   |
| 24  | c     | 510 | CLA  | C7-C6-C5    | -2.53 | 106.51      | 113.26   |
| 24  | c     | 513 | CLA  | CMB-C2B-C3B | 2.53  | 132.51      | 126.55   |
| 32  | c     | 518 | DGD  | O5D-C1E-C2E | 2.53  | 112.12      | 108.27   |
| 24  | b     | 610 | CLA  | CHA-C1A-NA  | -2.53 | 120.66      | 126.39   |
| 24  | c     | 502 | CLA  | CMB-C2B-C1B | -2.53 | 121.57      | 125.42   |
| 24  | c     | 511 | CLA  | O2D-CGD-CBD | 2.53  | 115.65      | 111.23   |
| 25  | A     | 606 | PHO  | C2D-C1D-ND  | 2.53  | 111.25      | 109.43   |
| 24  | a     | 604 | CLA  | CMB-C2B-C3B | 2.52  | 132.49      | 126.55   |
| 35  | F     | 101 | HEM  | CHB-C1B-NB  | 2.52  | 127.49      | 124.37   |
| 24  | b     | 612 | CLA  | CHD-C1D-ND  | -2.52 | 121.25      | 124.80   |
| 24  | C     | 509 | CLA  | C1-C2-C3    | -2.52 | 122.07      | 126.20   |
| 24  | B     | 603 | CLA  | O2A-CGA-O1A | -2.52 | 117.32      | 123.63   |
| 24  | B     | 605 | CLA  | CHD-C1D-ND  | -2.52 | 121.26      | 124.80   |
| 32  | H     | 102 | DGD  | C3E-C4E-C5E | -2.52 | 105.67      | 110.23   |
| 31  | D     | 407 | SQD  | O9-S-O7     | -2.52 | 105.64      | 113.82   |
| 24  | c     | 507 | CLA  | CHD-C1D-ND  | -2.52 | 121.26      | 124.80   |
| 24  | c     | 508 | CLA  | O2D-CGD-CBD | 2.52  | 115.63      | 111.23   |
| 32  | H     | 102 | DGD  | O5D-C1E-C2E | 2.51  | 112.09      | 108.27   |
| 26  | B     | 617 | BCR  | C27-C26-C25 | 2.51  | 126.10      | 122.70   |
| 24  | b     | 606 | CLA  | CHB-C1B-NB  | 2.51  | 127.82      | 124.05   |
| 31  | b     | 620 | SQD  | O47-C45-C46 | 2.51  | 117.36      | 108.34   |
| 26  | B     | 618 | BCR  | C29-C30-C25 | 2.51  | 114.08      | 110.44   |
| 24  | b     | 616 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 26  | c     | 514 | BCR  | C37-C22-C23 | 2.51  | 121.92      | 118.09   |
| 32  | h     | 101 | DGD  | C4E-C3E-C2E | -2.51 | 106.43      | 110.83   |
| 24  | b     | 614 | CLA  | CMB-C2B-C3B | 2.51  | 132.45      | 126.55   |
| 24  | b     | 613 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 26  | K     | 101 | BCR  | C27-C26-C25 | 2.51  | 126.09      | 122.70   |
| 24  | b     | 615 | CLA  | CMB-C2B-C1B | -2.50 | 121.61      | 125.42   |
| 24  | b     | 610 | CLA  | C2A-C1A-CHA | 2.50  | 128.21      | 123.87   |
| 24  | B     | 602 | CLA  | O2A-CGA-O1A | -2.50 | 117.37      | 123.63   |
| 31  | b     | 620 | SQD  | O8-S-C6     | 2.50  | 110.80      | 105.97   |
| 33  | J     | 101 | STE  | C3-C2-C1    | -2.50 | 107.99      | 114.51   |
| 24  | b     | 604 | CLA  | CMA-C3A-C4A | 2.50  | 118.49      | 111.77   |
| 24  | C     | 508 | CLA  | CMB-C2B-C1B | -2.50 | 121.62      | 125.42   |
| 32  | A     | 618 | DGD  | O5D-C6D-C5D | -2.49 | 103.80      | 109.42   |
| 28  | a     | 611 | PL9  | C27-C28-C29 | -2.49 | 121.92      | 127.62   |
| 24  | C     | 513 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | d     | 404 | CLA  | CHA-C1A-NA  | -2.49 | 120.75      | 126.39   |
| 24  | d     | 401 | CLA  | CHD-C1D-C2D | 2.49  | 130.66      | 125.49   |
| 32  | h     | 101 | DGD  | C3D-C4D-C5D | -2.49 | 105.72      | 110.23   |
| 24  | C     | 507 | CLA  | C2A-C1A-CHA | 2.48  | 128.18      | 123.87   |
| 29  | b     | 623 | LMG  | O1-C7-C8    | -2.48 | 104.78      | 110.82   |
| 24  | c     | 501 | CLA  | O1D-CGD-CBD | 2.48  | 129.41      | 124.52   |
| 24  | b     | 605 | CLA  | CMB-C2B-C1B | -2.48 | 121.65      | 125.42   |
| 24  | C     | 513 | CLA  | CMB-C2B-C3B | 2.48  | 132.37      | 126.55   |
| 26  | c     | 515 | BCR  | C1-C6-C5    | -2.47 | 119.26      | 122.64   |
| 26  | a     | 607 | BCR  | C27-C26-C25 | 2.47  | 126.04      | 122.70   |
| 35  | e     | 101 | HEM  | CHD-C4C-NC  | 2.47  | 127.14      | 124.45   |
| 24  | b     | 604 | CLA  | O1D-CGD-CBD | 2.47  | 129.38      | 124.52   |
| 26  | C     | 514 | BCR  | C33-C5-C6   | -2.47 | 121.79      | 124.48   |
| 30  | d     | 407 | LHG  | C18-C17-C16 | -2.46 | 101.91      | 114.37   |
| 24  | C     | 501 | CLA  | O2A-CGA-O1A | -2.46 | 117.47      | 123.63   |
| 24  | a     | 604 | CLA  | O2A-CGA-O1A | -2.46 | 117.47      | 123.63   |
| 32  | h     | 101 | DGD  | O3E-C3E-C2E | -2.46 | 104.58      | 110.38   |
| 24  | b     | 601 | CLA  | CHD-C1D-ND  | -2.46 | 121.34      | 124.80   |
| 24  | b     | 614 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 24  | B     | 603 | CLA  | CHD-C4C-NC  | 2.46  | 128.04      | 124.23   |
| 24  | C     | 507 | CLA  | C1-C2-C3    | -2.46 | 122.17      | 126.20   |
| 24  | B     | 604 | CLA  | CGD-CBD-CAD | -2.46 | 102.90      | 110.85   |
| 24  | d     | 401 | CLA  | CHC-C1C-NC  | 2.45  | 128.01      | 124.31   |
| 26  | b     | 619 | BCR  | C2-C1-C6    | 2.45  | 114.00      | 110.44   |
| 36  | V     | 201 | HEC  | CMD-C2D-C1D | 2.45  | 129.15      | 125.42   |
| 24  | B     | 606 | CLA  | OBD-CAD-C3D | 2.45  | 134.14      | 128.42   |
| 26  | B     | 617 | BCR  | C3-C4-C5    | -2.45 | 109.69      | 114.06   |
| 30  | A     | 615 | LHG  | O8-C6-C5    | -2.44 | 101.35      | 108.40   |
| 24  | B     | 608 | CLA  | CMB-C2B-C3B | 2.44  | 132.30      | 126.55   |
| 24  | C     | 508 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 24  | A     | 613 | CLA  | O2D-CGD-O1D | -2.44 | 119.09      | 123.85   |
| 29  | c     | 519 | LMG  | O2-C2-C1    | -2.44 | 104.26      | 110.08   |
| 29  | A     | 614 | LMG  | O8-C28-O10  | -2.44 | 117.52      | 123.63   |
| 24  | b     | 607 | CLA  | C4D-CHA-C1A | 2.44  | 124.15      | 121.24   |
| 30  | d     | 408 | LHG  | C20-C19-C18 | -2.44 | 102.04      | 114.37   |
| 32  | C     | 518 | DGD  | C1D-C2D-C3D | -2.44 | 104.88      | 110.01   |
| 26  | t     | 101 | BCR  | C2-C1-C6    | 2.44  | 113.98      | 110.44   |
| 24  | c     | 509 | CLA  | CMB-C2B-C3B | 2.44  | 132.28      | 126.55   |
| 24  | c     | 501 | CLA  | C3B-C4B-NB  | -2.44 | 108.36      | 110.53   |
| 32  | c     | 518 | DGD  | O6E-C1E-O5D | -2.43 | 104.29      | 110.04   |
| 26  | c     | 514 | BCR  | C7-C8-C9    | -2.43 | 122.63      | 126.23   |
| 29  | c     | 522 | LMG  | C38-C37-C36 | -2.43 | 102.07      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | c     | 513 | CLA  | O2D-CGD-CBD | 2.43  | 115.48      | 111.23   |
| 24  | C     | 507 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 33  | B     | 624 | STE  | C3-C2-C1    | -2.43 | 108.16      | 114.51   |
| 24  | B     | 603 | CLA  | O1D-CGD-CBD | 2.43  | 129.31      | 124.52   |
| 29  | c     | 519 | LMG  | C3-C4-C5    | -2.43 | 105.83      | 110.23   |
| 31  | A     | 617 | SQD  | O47-C7-C8   | 2.43  | 116.73      | 111.48   |
| 28  | a     | 611 | PL9  | O2-C1-C6    | 2.43  | 124.34      | 120.48   |
| 24  | c     | 506 | CLA  | OBD-CAD-C3D | 2.43  | 134.09      | 128.42   |
| 31  | D     | 407 | SQD  | C44-O6-C1   | 2.42  | 117.82      | 113.68   |
| 24  | C     | 506 | CLA  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 24  | B     | 608 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 24  | d     | 403 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 25  | A     | 607 | PHO  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 24  | c     | 509 | CLA  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 24  | B     | 612 | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 29  | A     | 614 | LMG  | C12-C11-C10 | -2.42 | 104.83      | 113.69   |
| 24  | A     | 604 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 24  | A     | 608 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 24  | B     | 604 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 24  | C     | 504 | CLA  | CHD-C1D-ND  | -2.42 | 121.40      | 124.80   |
| 24  | B     | 605 | CLA  | O1D-CGD-CBD | 2.41  | 129.28      | 124.52   |
| 28  | d     | 406 | PL9  | C22-C23-C24 | -2.41 | 122.10      | 127.62   |
| 26  | b     | 619 | BCR  | C7-C8-C9    | -2.41 | 122.67      | 126.23   |
| 29  | C     | 519 | LMG  | O7-C10-O9   | -2.41 | 118.07      | 123.70   |
| 24  | c     | 501 | CLA  | CMB-C2B-C3B | 2.41  | 132.22      | 126.55   |
| 24  | C     | 513 | CLA  | CMB-C2B-C1B | -2.41 | 121.75      | 125.42   |
| 26  | Y     | 101 | BCR  | C38-C26-C25 | -2.41 | 121.86      | 124.48   |
| 24  | A     | 604 | CLA  | O2D-CGD-CBD | -2.41 | 107.02      | 111.23   |
| 24  | c     | 508 | CLA  | C7-C6-C5    | -2.41 | 106.84      | 113.26   |
| 29  | a     | 618 | LMG  | C40-C39-C38 | -2.41 | 102.20      | 114.37   |
| 24  | c     | 506 | CLA  | C4-C3-C2    | -2.40 | 117.45      | 123.63   |
| 26  | c     | 515 | BCR  | C8-C9-C10   | 2.40  | 122.79      | 119.01   |
| 26  | C     | 515 | BCR  | C2-C1-C6    | 2.40  | 113.93      | 110.44   |
| 26  | T     | 101 | BCR  | C1-C6-C5    | -2.40 | 119.36      | 122.64   |
| 24  | c     | 502 | CLA  | O1D-CGD-CBD | 2.40  | 129.25      | 124.52   |
| 36  | v     | 201 | HEC  | C4D-ND-C1D  | 2.40  | 109.73      | 105.82   |
| 24  | C     | 508 | CLA  | O2D-CGD-CBD | 2.40  | 115.42      | 111.23   |
| 29  | C     | 519 | LMG  | O2-C2-C1    | -2.39 | 104.37      | 110.08   |
| 24  | b     | 610 | CLA  | CAA-CBA-CGA | -2.39 | 106.41      | 113.21   |
| 32  | c     | 517 | DGD  | C3E-C4E-C5E | -2.39 | 105.90      | 110.23   |
| 25  | a     | 605 | PHO  | C3B-C4B-NB  | -2.39 | 105.91      | 107.46   |
| 24  | c     | 507 | CLA  | C1D-ND-C4D  | 2.39  | 107.99      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | c     | 517 | DGD  | O3G-C1D-C2D | -2.39 | 104.64      | 108.27   |
| 24  | b     | 605 | CLA  | C4D-CHA-C1A | 2.39  | 124.09      | 121.24   |
| 26  | T     | 101 | BCR  | C38-C26-C27 | -2.39 | 108.51      | 113.60   |
| 28  | a     | 611 | PL9  | C12-C13-C14 | -2.39 | 122.16      | 127.62   |
| 25  | a     | 605 | PHO  | O2A-CGA-O1A | -2.39 | 117.66      | 123.63   |
| 24  | B     | 610 | CLA  | C1-C2-C3    | -2.39 | 122.29      | 126.20   |
| 28  | a     | 611 | PL9  | C22-C23-C24 | -2.39 | 122.16      | 127.62   |
| 29  | c     | 521 | LMG  | O2-C2-C1    | -2.39 | 104.39      | 110.08   |
| 32  | H     | 102 | DGD  | CDB-CCB-CBB | -2.38 | 102.32      | 114.37   |
| 24  | b     | 604 | CLA  | O2A-CGA-O1A | -2.38 | 117.67      | 123.63   |
| 24  | b     | 613 | CLA  | CHA-C1A-NA  | -2.38 | 121.00      | 126.39   |
| 26  | b     | 617 | BCR  | C29-C30-C25 | 2.38  | 113.90      | 110.44   |
| 24  | d     | 401 | CLA  | O2A-CGA-O1A | -2.38 | 117.67      | 123.63   |
| 24  | C     | 502 | CLA  | CHA-C1A-NA  | -2.38 | 121.00      | 126.39   |
| 24  | C     | 508 | CLA  | CMB-C2B-C3B | 2.38  | 132.15      | 126.55   |
| 33  | E     | 102 | STE  | O2-C1-C2    | 2.38  | 121.52      | 114.00   |
| 24  | b     | 612 | CLA  | CMD-C2D-C3D | 2.38  | 133.14      | 127.69   |
| 31  | a     | 614 | SQD  | O48-C46-C45 | 2.38  | 115.25      | 108.40   |
| 29  | b     | 621 | LMG  | O6-C1-O1    | -2.38 | 104.43      | 110.04   |
| 29  | c     | 521 | LMG  | O6-C1-O1    | -2.38 | 104.43      | 110.04   |
| 32  | A     | 618 | DGD  | CBB-CAB-C9B | -2.38 | 102.36      | 114.37   |
| 24  | b     | 615 | CLA  | C1-O2A-CGA  | 2.38  | 122.40      | 116.65   |
| 28  | A     | 612 | PL9  | C26-C24-C23 | -2.37 | 115.84      | 121.17   |
| 32  | c     | 518 | DGD  | O6E-C5E-C4E | 2.37  | 113.97      | 109.70   |
| 24  | B     | 615 | CLA  | CHD-C1D-ND  | -2.37 | 121.46      | 124.80   |
| 24  | B     | 604 | CLA  | O2D-CGD-CBD | 2.37  | 115.38      | 111.23   |
| 32  | C     | 516 | DGD  | O1G-C1A-C2A | -2.37 | 104.61      | 111.83   |
| 24  | b     | 604 | CLA  | C11-C12-C13 | -2.37 | 108.09      | 115.97   |
| 24  | d     | 404 | CLA  | CHB-C1B-NB  | 2.37  | 127.60      | 124.05   |
| 24  | b     | 603 | CLA  | O2A-CGA-O1A | -2.37 | 117.70      | 123.63   |
| 24  | b     | 602 | CLA  | C4-C3-C5    | 2.37  | 119.34      | 115.23   |
| 26  | B     | 617 | BCR  | C15-C16-C17 | -2.37 | 118.68      | 123.52   |
| 24  | b     | 609 | CLA  | CHA-C1A-NA  | -2.37 | 121.03      | 126.39   |
| 24  | C     | 513 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 26  | H     | 101 | BCR  | C37-C22-C23 | 2.36  | 121.70      | 118.09   |
| 32  | c     | 518 | DGD  | CDB-CCB-CBB | -2.36 | 102.42      | 114.37   |
| 24  | C     | 504 | CLA  | CHC-C1C-NC  | 2.36  | 127.87      | 124.31   |
| 26  | x     | 101 | BCR  | C37-C22-C21 | -2.36 | 118.99      | 122.82   |
| 33  | B     | 627 | STE  | O2-C1-C2    | 2.36  | 121.46      | 114.00   |
| 30  | B     | 622 | LHG  | C20-C19-C18 | -2.36 | 102.44      | 114.37   |
| 24  | c     | 510 | CLA  | C3B-C4B-NB  | -2.36 | 108.43      | 110.53   |
| 30  | B     | 622 | LHG  | O8-C23-O10  | -2.36 | 117.73      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | E     | 101 | LHG  | C18-C17-C16 | -2.35 | 102.47      | 114.37   |
| 26  | t     | 101 | BCR  | C4-C5-C6    | 2.35  | 125.88      | 122.70   |
| 32  | h     | 101 | DGD  | O5E-C6E-C5E | -2.35 | 103.33      | 111.33   |
| 29  | D     | 406 | LMG  | O3-C3-C2    | -2.35 | 104.83      | 110.38   |
| 24  | B     | 601 | CLA  | CHC-C4B-NB  | 2.35  | 127.57      | 124.05   |
| 29  | M     | 101 | LMG  | O1-C7-C8    | -2.35 | 105.11      | 110.82   |
| 26  | A     | 609 | BCR  | C15-C16-C17 | -2.35 | 118.72      | 123.52   |
| 24  | C     | 502 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 30  | e     | 102 | LHG  | C11-C10-C9  | -2.35 | 102.51      | 114.37   |
| 24  | b     | 608 | CLA  | CHB-C1B-NB  | 2.34  | 127.56      | 124.05   |
| 24  | C     | 510 | CLA  | C11-C10-C8  | -2.34 | 108.17      | 115.97   |
| 24  | c     | 502 | CLA  | CMB-C2B-C3B | 2.34  | 132.06      | 126.55   |
| 26  | C     | 514 | BCR  | C15-C16-C17 | -2.34 | 118.72      | 123.52   |
| 24  | B     | 606 | CLA  | C2A-C1A-CHA | 2.34  | 127.93      | 123.87   |
| 24  | c     | 508 | CLA  | CHD-C1D-C2D | 2.34  | 130.36      | 125.49   |
| 24  | B     | 608 | CLA  | C4A-NA-C1A  | 2.34  | 107.75      | 106.68   |
| 26  | a     | 607 | BCR  | C37-C22-C21 | -2.34 | 119.03      | 122.82   |
| 32  | c     | 517 | DGD  | C3D-C4D-C5D | -2.34 | 105.99      | 110.23   |
| 24  | C     | 503 | CLA  | CHC-C4B-NB  | 2.34  | 127.56      | 124.05   |
| 29  | D     | 409 | LMG  | O1-C7-C8    | -2.34 | 105.76      | 111.77   |
| 24  | b     | 608 | CLA  | O2A-CGA-O1A | -2.34 | 117.78      | 123.63   |
| 25  | d     | 402 | PHO  | C3D-C4D-ND  | 2.33  | 110.70      | 107.71   |
| 24  | B     | 605 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 32  | c     | 516 | DGD  | O3E-C3E-C2E | -2.33 | 104.89      | 110.38   |
| 26  | d     | 405 | BCR  | C3-C4-C5    | -2.33 | 109.90      | 114.06   |
| 29  | a     | 618 | LMG  | O6-C5-C4    | 2.33  | 113.89      | 109.70   |
| 24  | A     | 613 | CLA  | O2D-CGD-CBD | 2.33  | 115.30      | 111.23   |
| 28  | d     | 406 | PL9  | C8-C7-C3    | 2.32  | 118.04      | 112.03   |
| 24  | b     | 603 | CLA  | CHD-C1D-ND  | -2.32 | 121.53      | 124.80   |
| 24  | B     | 609 | CLA  | C6-C5-C3    | 2.32  | 119.12      | 113.47   |
| 24  | B     | 602 | CLA  | C3B-C4B-NB  | -2.32 | 108.46      | 110.53   |
| 24  | c     | 505 | CLA  | CAC-C3C-C4C | 2.32  | 127.81      | 124.79   |
| 28  | a     | 611 | PL9  | C36-C34-C33 | -2.32 | 115.96      | 121.17   |
| 26  | x     | 101 | BCR  | C2-C1-C6    | 2.32  | 113.80      | 110.44   |
| 28  | a     | 611 | PL9  | C20-C19-C21 | 2.31  | 119.25      | 115.23   |
| 25  | A     | 606 | PHO  | O2D-CGD-O1D | -2.31 | 119.34      | 123.85   |
| 24  | B     | 609 | CLA  | CHA-C1A-NA  | -2.31 | 121.15      | 126.39   |
| 24  | A     | 605 | CLA  | C1-O2A-CGA  | 2.31  | 122.25      | 116.65   |
| 24  | b     | 606 | CLA  | O1D-CGD-CBD | 2.31  | 129.08      | 124.52   |
| 24  | c     | 512 | CLA  | O1D-CGD-CBD | 2.31  | 129.08      | 124.52   |
| 26  | d     | 405 | BCR  | C24-C23-C22 | -2.31 | 122.82      | 126.23   |
| 31  | b     | 620 | SQD  | O10-C23-C24 | -2.31 | 114.75      | 123.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | F     | 101 | HEM  | C4C-C3C-C2C | 2.31  | 108.81      | 106.81   |
| 24  | b     | 603 | CLA  | C4-C3-C5    | 2.31  | 119.23      | 115.23   |
| 24  | b     | 614 | CLA  | CAC-C3C-C4C | 2.31  | 127.79      | 124.79   |
| 24  | d     | 404 | CLA  | CHB-C1B-C2B | -2.31 | 120.73      | 127.43   |
| 29  | A     | 614 | LMG  | C1-O6-C5    | -2.31 | 109.22      | 113.72   |
| 24  | D     | 402 | CLA  | C6-C5-C3    | 2.30  | 119.08      | 113.47   |
| 33  | C     | 522 | STE  | C4-C3-C2    | -2.30 | 104.66      | 113.13   |
| 24  | C     | 511 | CLA  | C1-C2-C3    | -2.30 | 122.43      | 126.20   |
| 24  | B     | 612 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 30  | A     | 615 | LHG  | C27-C26-C25 | -2.30 | 102.75      | 114.37   |
| 24  | B     | 605 | CLA  | CHD-C1D-C2D | 2.30  | 130.27      | 125.49   |
| 24  | b     | 603 | CLA  | CMB-C2B-C3B | 2.30  | 131.95      | 126.55   |
| 26  | Y     | 101 | BCR  | C30-C25-C26 | -2.30 | 119.50      | 122.64   |
| 31  | f     | 101 | SQD  | O5-C5-C4    | 2.30  | 113.83      | 109.70   |
| 32  | C     | 517 | DGD  | CDB-CCB-CBB | -2.29 | 102.78      | 114.37   |
| 32  | c     | 516 | DGD  | CBB-CAB-C9B | -2.29 | 102.78      | 114.37   |
| 24  | B     | 607 | CLA  | CHD-C4C-NC  | 2.29  | 127.78      | 124.23   |
| 32  | c     | 517 | DGD  | C4E-C3E-C2E | -2.29 | 106.81      | 110.83   |
| 32  | c     | 518 | DGD  | O2D-C2D-C1D | -2.29 | 104.63      | 110.08   |
| 24  | B     | 608 | CLA  | O1D-CGD-CBD | 2.28  | 129.02      | 124.52   |
| 30  | A     | 615 | LHG  | C3-C2-C1    | -2.28 | 104.08      | 111.77   |
| 29  | M     | 101 | LMG  | C1-C2-C3    | -2.28 | 105.21      | 110.01   |
| 24  | b     | 607 | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 24  | B     | 601 | CLA  | O2A-CGA-O1A | -2.28 | 117.92      | 123.63   |
| 24  | A     | 608 | CLA  | C1-C2-C3    | -2.28 | 122.46      | 126.20   |
| 26  | b     | 618 | BCR  | C15-C16-C17 | -2.28 | 118.85      | 123.52   |
| 32  | h     | 101 | DGD  | O6E-C5E-C4E | 2.28  | 113.81      | 109.70   |
| 24  | b     | 612 | CLA  | CMB-C2B-C3B | 2.28  | 131.91      | 126.55   |
| 28  | D     | 405 | PL9  | C32-C33-C34 | -2.28 | 122.41      | 127.62   |
| 32  | c     | 517 | DGD  | C8B-C7B-C6B | -2.28 | 102.85      | 114.37   |
| 24  | b     | 609 | CLA  | C11-C10-C8  | -2.28 | 108.40      | 115.97   |
| 36  | v     | 201 | HEC  | CHB-C1B-NB  | 2.28  | 127.99      | 123.86   |
| 24  | b     | 605 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 30  | A     | 615 | LHG  | O8-C23-C24  | 2.27  | 118.77      | 111.83   |
| 24  | C     | 509 | CLA  | C2A-C3A-C4A | 2.27  | 105.54      | 101.87   |
| 28  | a     | 611 | PL9  | C7-C8-C9    | -2.27 | 122.92      | 126.83   |
| 24  | b     | 607 | CLA  | C2A-C1A-CHA | 2.27  | 127.81      | 123.87   |
| 26  | b     | 618 | BCR  | C36-C18-C17 | -2.27 | 119.14      | 122.82   |
| 30  | E     | 101 | LHG  | C11-C10-C9  | -2.27 | 102.90      | 114.37   |
| 24  | B     | 612 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 26  | b     | 619 | BCR  | C38-C26-C25 | -2.26 | 122.01      | 124.48   |
| 24  | B     | 614 | CLA  | CAC-C3C-C4C | 2.26  | 127.74      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | B     | 617 | BCR  | C36-C18-C17 | -2.26 | 119.15      | 122.82   |
| 33  | b     | 625 | STE  | C4-C3-C2    | -2.26 | 104.82      | 113.13   |
| 26  | B     | 618 | BCR  | C15-C16-C17 | -2.26 | 118.89      | 123.52   |
| 24  | B     | 602 | CLA  | CHA-C4D-ND  | 2.26  | 137.21      | 132.55   |
| 24  | C     | 502 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 24  | d     | 403 | CLA  | C2A-C1A-CHA | 2.26  | 127.79      | 123.87   |
| 28  | a     | 611 | PL9  | O2-C1-C2    | -2.26 | 116.69      | 121.83   |
| 25  | A     | 606 | PHO  | CBC-CAC-C3C | 2.26  | 116.10      | 112.87   |
| 35  | e     | 101 | HEM  | CAB-C3B-C2B | -2.26 | 121.10      | 128.43   |
| 32  | C     | 516 | DGD  | C5B-C4B-C3B | -2.26 | 102.97      | 114.37   |
| 32  | c     | 518 | DGD  | CBB-CAB-C9B | -2.25 | 102.99      | 114.37   |
| 26  | b     | 618 | BCR  | C15-C14-C13 | -2.25 | 124.12      | 127.28   |
| 24  | b     | 608 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 30  | D     | 408 | LHG  | C27-C26-C25 | -2.25 | 103.00      | 114.37   |
| 26  | b     | 617 | BCR  | C36-C18-C17 | -2.25 | 119.17      | 122.82   |
| 30  | d     | 408 | LHG  | C18-C17-C16 | -2.25 | 103.00      | 114.37   |
| 24  | B     | 611 | CLA  | C9-C8-C10   | -2.25 | 103.27      | 111.27   |
| 30  | l     | 101 | LHG  | O8-C23-C24  | 2.25  | 118.68      | 111.83   |
| 31  | f     | 101 | SQD  | C46-C45-C44 | -2.25 | 106.55      | 111.78   |
| 32  | h     | 101 | DGD  | CDB-CCB-CBB | -2.24 | 103.03      | 114.37   |
| 32  | c     | 517 | DGD  | O2E-C2E-C1E | -2.24 | 104.73      | 110.08   |
| 25  | A     | 607 | PHO  | C3D-C4D-ND  | 2.24  | 110.58      | 107.71   |
| 24  | b     | 607 | CLA  | CMB-C2B-C1B | -2.24 | 122.01      | 125.42   |
| 24  | d     | 401 | CLA  | C3B-C4B-NB  | -2.24 | 108.53      | 110.53   |
| 28  | A     | 612 | PL9  | O2-C1-C2    | -2.24 | 116.74      | 121.83   |
| 29  | D     | 406 | LMG  | C38-C37-C36 | -2.24 | 103.06      | 114.37   |
| 24  | c     | 504 | CLA  | O1A-CGA-CBA | 2.23  | 132.52      | 123.78   |
| 32  | h     | 101 | DGD  | C6D-C5D-C4D | 2.23  | 116.75      | 112.07   |
| 24  | b     | 606 | CLA  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 24  | A     | 613 | CLA  | CHC-C4B-NB  | 2.23  | 127.40      | 124.05   |
| 24  | c     | 507 | CLA  | C2C-C1C-NC  | 2.23  | 112.33      | 109.98   |
| 32  | c     | 516 | DGD  | C5B-C4B-C3B | -2.23 | 103.10      | 114.37   |
| 32  | c     | 516 | DGD  | O1G-C1A-C2A | -2.23 | 105.04      | 111.83   |
| 32  | C     | 518 | DGD  | O3E-C3E-C2E | -2.23 | 105.13      | 110.38   |
| 24  | b     | 616 | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 24  | c     | 504 | CLA  | O2D-CGD-CBD | 2.23  | 115.12      | 111.23   |
| 24  | c     | 507 | CLA  | CMB-C2B-C3B | 2.23  | 131.79      | 126.55   |
| 29  | c     | 519 | LMG  | C1-O6-C5    | -2.22 | 109.38      | 113.72   |
| 24  | B     | 615 | CLA  | C6-C7-C8    | -2.22 | 108.58      | 115.97   |
| 24  | b     | 605 | CLA  | O1A-CGA-CBA | 2.22  | 132.46      | 123.78   |
| 24  | c     | 509 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 26  | B     | 619 | BCR  | C36-C18-C17 | -2.22 | 119.22      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 603 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 24  | A     | 605 | CLA  | C2D-C1D-ND  | -2.22 | 107.93      | 110.13   |
| 30  | l     | 101 | LHG  | C27-C26-C25 | -2.22 | 103.16      | 114.37   |
| 24  | b     | 604 | CLA  | C6-C7-C8    | -2.22 | 108.59      | 115.97   |
| 26  | C     | 514 | BCR  | C24-C23-C22 | -2.22 | 122.95      | 126.23   |
| 30  | d     | 407 | LHG  | C20-C19-C18 | -2.22 | 103.17      | 114.37   |
| 29  | a     | 618 | LMG  | C42-C41-C40 | -2.21 | 103.17      | 114.37   |
| 24  | C     | 511 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 26  | T     | 101 | BCR  | C4-C5-C6    | 2.21  | 125.69      | 122.70   |
| 28  | a     | 611 | PL9  | C37-C38-C39 | -2.21 | 122.56      | 127.62   |
| 28  | D     | 405 | PL9  | C50-C49-C48 | -2.21 | 116.03      | 122.66   |
| 29  | M     | 101 | LMG  | C31-C30-C29 | -2.21 | 105.02      | 113.13   |
| 32  | c     | 518 | DGD  | O5E-C6E-C5E | -2.21 | 103.82      | 111.33   |
| 24  | c     | 506 | CLA  | C4-C3-C5    | 2.20  | 119.05      | 115.23   |
| 24  | B     | 608 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 24  | C     | 512 | CLA  | C6-C5-C3    | -2.20 | 108.10      | 113.47   |
| 24  | b     | 604 | CLA  | CHB-C1B-NB  | 2.20  | 127.35      | 124.05   |
| 30  | E     | 101 | LHG  | C20-C19-C18 | -2.20 | 103.24      | 114.37   |
| 24  | B     | 601 | CLA  | C2A-C1A-CHA | 2.20  | 127.69      | 123.87   |
| 24  | b     | 604 | CLA  | CAC-C3C-C4C | 2.20  | 127.65      | 124.79   |
| 24  | b     | 604 | CLA  | C3A-C2A-C1A | 2.20  | 104.63      | 101.34   |
| 24  | a     | 612 | CLA  | C2B-C1B-NB  | -2.20 | 108.05      | 110.33   |
| 24  | c     | 502 | CLA  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 24  | C     | 512 | CLA  | O2A-CGA-O1A | -2.20 | 118.14      | 123.63   |
| 24  | B     | 609 | CLA  | CHC-C4B-NB  | 2.20  | 127.34      | 124.05   |
| 26  | x     | 101 | BCR  | C16-C15-C14 | -2.19 | 119.03      | 123.52   |
| 26  | d     | 405 | BCR  | C30-C25-C26 | -2.19 | 119.64      | 122.64   |
| 24  | b     | 611 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 24  | A     | 604 | CLA  | CHC-C4B-NB  | 2.19  | 127.34      | 124.05   |
| 24  | A     | 604 | CLA  | CAA-CBA-CGA | -2.19 | 106.98      | 113.21   |
| 24  | B     | 606 | CLA  | CHC-C4B-NB  | 2.19  | 127.33      | 124.05   |
| 29  | c     | 522 | LMG  | C8-O7-C10   | 2.19  | 123.04      | 117.80   |
| 24  | b     | 610 | CLA  | C2C-C1C-NC  | 2.19  | 112.28      | 109.98   |
| 35  | F     | 101 | HEM  | C3B-C4B-NB  | 2.19  | 111.04      | 109.47   |
| 29  | b     | 623 | LMG  | C40-C39-C38 | -2.19 | 103.31      | 114.37   |
| 30  | B     | 621 | LHG  | C20-C19-C18 | -2.19 | 103.31      | 114.37   |
| 32  | c     | 517 | DGD  | O4E-C4E-C3E | -2.19 | 105.22      | 110.38   |
| 24  | B     | 601 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 24  | B     | 612 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 24  | a     | 606 | CLA  | CHA-C1A-NA  | -2.18 | 121.44      | 126.39   |
| 24  | b     | 615 | CLA  | C6-C5-C3    | -2.18 | 108.15      | 113.47   |
| 24  | b     | 604 | CLA  | CGD-CBD-CAD | -2.18 | 103.78      | 110.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 608 | CLA  | C6-C7-C8    | -2.18 | 108.71      | 115.97   |
| 26  | B     | 618 | BCR  | C2-C1-C6    | 2.18  | 113.61      | 110.44   |
| 24  | A     | 605 | CLA  | CHB-C4A-NA  | 2.18  | 127.55      | 124.40   |
| 28  | A     | 612 | PL9  | C7-C3-C2    | -2.18 | 120.82      | 123.39   |
| 26  | H     | 101 | BCR  | C29-C30-C25 | 2.18  | 113.60      | 110.44   |
| 26  | c     | 514 | BCR  | C33-C5-C6   | -2.18 | 122.11      | 124.48   |
| 24  | b     | 606 | CLA  | CMB-C2B-C3B | 2.18  | 131.67      | 126.55   |
| 24  | b     | 601 | CLA  | O2D-CGD-CBD | 2.17  | 115.03      | 111.23   |
| 24  | c     | 509 | CLA  | CHD-C1D-ND  | -2.17 | 121.74      | 124.80   |
| 24  | A     | 613 | CLA  | C7-C6-C5    | -2.17 | 107.47      | 113.26   |
| 28  | D     | 405 | PL9  | C12-C13-C14 | -2.17 | 122.65      | 127.62   |
| 26  | K     | 101 | BCR  | C37-C22-C21 | -2.17 | 119.30      | 122.82   |
| 26  | c     | 515 | BCR  | C15-C16-C17 | -2.17 | 119.08      | 123.52   |
| 32  | H     | 102 | DGD  | C1E-O6E-C5E | 2.17  | 117.96      | 113.72   |
| 24  | d     | 404 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 33  | M     | 102 | STE  | C3-C2-C1    | -2.17 | 108.85      | 114.51   |
| 36  | v     | 201 | HEC  | CHA-C4D-ND  | 2.17  | 127.79      | 123.86   |
| 24  | B     | 614 | CLA  | CHB-C1B-NB  | 2.17  | 127.30      | 124.05   |
| 24  | B     | 609 | CLA  | C2C-C1C-NC  | 2.17  | 112.26      | 109.98   |
| 26  | c     | 515 | BCR  | C36-C18-C17 | -2.16 | 119.31      | 122.82   |
| 24  | B     | 608 | CLA  | O2D-CGD-CBD | 2.16  | 115.01      | 111.23   |
| 24  | b     | 608 | CLA  | C11-C10-C8  | -2.16 | 108.78      | 115.97   |
| 29  | C     | 519 | LMG  | O8-C28-O10  | -2.16 | 118.23      | 123.63   |
| 24  | A     | 605 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 26  | C     | 515 | BCR  | C1-C6-C5    | -2.16 | 119.69      | 122.64   |
| 28  | D     | 405 | PL9  | C7-C3-C2    | -2.16 | 120.85      | 123.39   |
| 24  | c     | 506 | CLA  | CHD-C1D-ND  | -2.16 | 121.77      | 124.80   |
| 33  | t     | 102 | STE  | C3-C2-C1    | -2.16 | 108.88      | 114.51   |
| 24  | c     | 501 | CLA  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 24  | C     | 507 | CLA  | CHA-C1A-NA  | -2.15 | 121.51      | 126.39   |
| 32  | c     | 517 | DGD  | O3E-C3E-C4E | -2.15 | 105.30      | 110.38   |
| 26  | D     | 404 | BCR  | C7-C8-C9    | -2.15 | 123.05      | 126.23   |
| 24  | B     | 608 | CLA  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 32  | c     | 518 | DGD  | C3G-C2G-C1G | -2.15 | 106.77      | 111.78   |
| 31  | B     | 623 | SQD  | C25-C24-C23 | -2.15 | 105.81      | 113.69   |
| 24  | C     | 503 | CLA  | C3A-C2A-C1A | 2.15  | 104.56      | 101.34   |
| 24  | B     | 611 | CLA  | C14-C13-C15 | -2.15 | 103.61      | 111.27   |
| 26  | b     | 617 | BCR  | C3-C4-C5    | -2.15 | 110.22      | 114.06   |
| 25  | a     | 605 | PHO  | O2D-CGD-O1D | -2.15 | 119.66      | 123.85   |
| 35  | F     | 101 | HEM  | CHC-C1C-NC  | 2.15  | 126.79      | 124.45   |
| 24  | A     | 608 | CLA  | CAA-CBA-CGA | -2.15 | 107.11      | 113.21   |
| 32  | h     | 101 | DGD  | C4D-C3D-C2D | -2.15 | 107.06      | 110.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 603 | CLA  | C3B-C4B-NB  | -2.15 | 108.61      | 110.53   |
| 24  | B     | 603 | CLA  | C5-C3-C2    | -2.15 | 116.35      | 121.17   |
| 24  | D     | 403 | CLA  | O2D-CGD-CBD | 2.15  | 114.98      | 111.23   |
| 24  | b     | 612 | CLA  | C4D-C3D-CAD | -2.15 | 105.78      | 108.11   |
| 24  | b     | 614 | CLA  | O1A-CGA-CBA | 2.15  | 132.17      | 123.78   |
| 29  | d     | 410 | LMG  | O3-C3-C2    | -2.14 | 105.32      | 110.38   |
| 24  | B     | 612 | CLA  | C16-C15-C13 | -2.14 | 108.84      | 115.97   |
| 24  | c     | 507 | CLA  | CHD-C1D-C2D | 2.14  | 129.94      | 125.49   |
| 24  | c     | 508 | CLA  | C3B-C4B-NB  | -2.14 | 108.62      | 110.53   |
| 24  | d     | 404 | CLA  | O2D-CGD-O1D | -2.14 | 119.68      | 123.85   |
| 24  | A     | 604 | CLA  | CMB-C2B-C1B | -2.14 | 122.16      | 125.42   |
| 32  | c     | 517 | DGD  | C1D-C2D-C3D | -2.14 | 105.51      | 110.01   |
| 26  | k     | 101 | BCR  | C1-C6-C5    | -2.14 | 119.71      | 122.64   |
| 24  | b     | 603 | CLA  | CHB-C1B-C2B | -2.14 | 121.22      | 127.43   |
| 24  | B     | 613 | CLA  | CMB-C2B-C1B | -2.13 | 122.17      | 125.42   |
| 24  | c     | 510 | CLA  | O1A-CGA-CBA | 2.13  | 132.13      | 123.78   |
| 29  | c     | 522 | LMG  | C40-C39-C38 | -2.13 | 103.59      | 114.37   |
| 26  | c     | 514 | BCR  | C38-C26-C25 | -2.13 | 122.16      | 124.48   |
| 24  | C     | 503 | CLA  | O2A-C1-C2   | -2.13 | 99.90       | 108.11   |
| 24  | B     | 603 | CLA  | CHC-C1C-NC  | 2.13  | 127.52      | 124.31   |
| 24  | c     | 510 | CLA  | CHB-C1B-NB  | 2.13  | 127.25      | 124.05   |
| 36  | V     | 201 | HEC  | O1D-CGD-CBD | -2.13 | 116.34      | 123.09   |
| 24  | c     | 505 | CLA  | CMD-C2D-C3D | 2.13  | 132.57      | 127.69   |
| 24  | c     | 504 | CLA  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 24  | B     | 609 | CLA  | C1D-ND-C4D  | -2.13 | 104.82      | 106.31   |
| 24  | b     | 608 | CLA  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 26  | B     | 617 | BCR  | C11-C10-C9  | -2.13 | 124.30      | 127.28   |
| 31  | f     | 101 | SQD  | O5-C1-O6    | 2.13  | 115.07      | 110.04   |
| 26  | Y     | 101 | BCR  | C1-C6-C5    | -2.12 | 119.73      | 122.64   |
| 24  | b     | 615 | CLA  | CHA-C4D-ND  | 2.12  | 136.93      | 132.55   |
| 25  | a     | 605 | PHO  | O2D-CGD-CBD | 2.12  | 113.28      | 110.95   |
| 24  | C     | 510 | CLA  | CHD-C1D-ND  | -2.12 | 121.81      | 124.80   |
| 26  | b     | 618 | BCR  | C7-C8-C9    | -2.12 | 123.09      | 126.23   |
| 24  | B     | 614 | CLA  | CHB-C4A-NA  | 2.12  | 127.46      | 124.40   |
| 24  | B     | 611 | CLA  | C11-C12-C13 | -2.12 | 108.92      | 115.97   |
| 24  | C     | 510 | CLA  | C16-C15-C13 | -2.12 | 108.92      | 115.97   |
| 24  | C     | 508 | CLA  | C4D-C3D-CAD | -2.12 | 105.81      | 108.11   |
| 30  | B     | 622 | LHG  | C13-C12-C11 | -2.12 | 103.67      | 114.37   |
| 31  | f     | 101 | SQD  | O9-S-C6     | 2.12  | 109.92      | 106.76   |
| 30  | B     | 622 | LHG  | O3-P-O5     | -2.12 | 100.55      | 108.94   |
| 24  | c     | 504 | CLA  | CHD-C1D-ND  | -2.12 | 121.83      | 124.80   |
| 24  | b     | 608 | CLA  | O2D-CGD-CBD | 2.11  | 114.93      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 623 | SQD  | C27-C26-C25 | -2.11 | 103.69      | 114.37   |
| 26  | b     | 618 | BCR  | C27-C26-C25 | 2.11  | 125.56      | 122.70   |
| 26  | A     | 609 | BCR  | C40-C30-C39 | -2.11 | 102.58      | 108.63   |
| 29  | d     | 410 | LMG  | C40-C39-C38 | -2.11 | 103.69      | 114.37   |
| 24  | b     | 614 | CLA  | CHB-C1B-NB  | 2.11  | 127.22      | 124.05   |
| 24  | C     | 501 | CLA  | C3A-C2A-C1A | 2.11  | 104.50      | 101.34   |
| 31  | B     | 623 | SQD  | O9-S-O7     | -2.11 | 106.96      | 113.82   |
| 30  | l     | 101 | LHG  | C5-O7-C7    | -2.11 | 112.75      | 117.80   |
| 24  | B     | 613 | CLA  | O1D-CGD-CBD | 2.11  | 128.67      | 124.52   |
| 24  | C     | 505 | CLA  | C3B-C4B-NB  | -2.11 | 108.65      | 110.53   |
| 24  | b     | 604 | CLA  | CHC-C1C-C2C | -2.11 | 120.96      | 126.95   |
| 24  | b     | 611 | CLA  | C11-C12-C13 | -2.11 | 108.97      | 115.97   |
| 31  | f     | 101 | SQD  | O48-C23-C24 | 2.11  | 118.25      | 111.83   |
| 26  | t     | 101 | BCR  | C15-C14-C13 | -2.10 | 124.33      | 127.28   |
| 28  | d     | 406 | PL9  | C36-C34-C33 | -2.10 | 116.44      | 121.17   |
| 24  | d     | 401 | CLA  | CMA-C3A-C4A | -2.10 | 106.12      | 111.77   |
| 24  | B     | 611 | CLA  | O1D-CGD-CBD | 2.10  | 128.66      | 124.52   |
| 32  | A     | 618 | DGD  | O5E-C6E-C5E | -2.10 | 104.17      | 111.33   |
| 28  | d     | 406 | PL9  | C32-C33-C34 | -2.10 | 122.81      | 127.62   |
| 24  | C     | 511 | CLA  | C4-C3-C5    | 2.10  | 118.88      | 115.23   |
| 32  | c     | 516 | DGD  | CAB-C9B-C8B | -2.10 | 103.74      | 114.37   |
| 24  | c     | 503 | CLA  | C4D-C3D-CAD | -2.10 | 105.83      | 108.11   |
| 28  | d     | 406 | PL9  | C12-C13-C14 | -2.10 | 122.82      | 127.62   |
| 26  | k     | 102 | BCR  | C1-C6-C5    | -2.10 | 119.77      | 122.64   |
| 29  | C     | 519 | LMG  | O1-C7-C8    | -2.10 | 105.72      | 110.82   |
| 28  | D     | 405 | PL9  | C31-C29-C28 | 2.10  | 125.87      | 121.17   |
| 31  | a     | 614 | SQD  | C9-C8-C7    | -2.10 | 106.02      | 113.69   |
| 24  | b     | 614 | CLA  | C4-C3-C2    | -2.09 | 118.25      | 123.63   |
| 30  | B     | 622 | LHG  | C18-C17-C16 | -2.09 | 103.79      | 114.37   |
| 24  | B     | 602 | CLA  | CMB-C2B-C3B | 2.09  | 131.47      | 126.55   |
| 30  | e     | 102 | LHG  | O8-C23-O10  | -2.09 | 118.40      | 123.63   |
| 29  | c     | 522 | LMG  | O2-C2-C3    | -2.09 | 105.45      | 110.38   |
| 24  | D     | 402 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 24  | B     | 616 | CLA  | C4D-CHA-C1A | 2.09  | 123.74      | 121.24   |
| 36  | v     | 201 | HEC  | CBA-CAA-C2A | -2.09 | 106.76      | 112.53   |
| 32  | c     | 517 | DGD  | O2D-C2D-C1D | -2.09 | 105.10      | 110.08   |
| 32  | c     | 516 | DGD  | C8B-C7B-C6B | -2.09 | 103.81      | 114.37   |
| 26  | H     | 101 | BCR  | C38-C26-C25 | -2.09 | 122.21      | 124.48   |
| 30  | B     | 621 | LHG  | O7-C7-O9    | -2.09 | 118.83      | 123.70   |
| 31  | a     | 613 | SQD  | O8-S-C6     | 2.08  | 110.00      | 105.97   |
| 24  | B     | 608 | CLA  | C3B-C4B-NB  | -2.08 | 108.67      | 110.53   |
| 24  | b     | 616 | CLA  | C2A-C3A-C4A | 2.08  | 105.23      | 101.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 614 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 24  | A     | 605 | CLA  | CAC-C3C-C4C | 2.08  | 127.50      | 124.79   |
| 24  | b     | 608 | CLA  | CHD-C1D-C2D | 2.08  | 129.82      | 125.49   |
| 24  | c     | 513 | CLA  | C3B-C4B-NB  | -2.08 | 108.67      | 110.53   |
| 24  | c     | 513 | CLA  | CHD-C1D-ND  | -2.08 | 121.88      | 124.80   |
| 30  | d     | 407 | LHG  | O3-P-O5     | -2.08 | 100.69      | 108.94   |
| 26  | t     | 101 | BCR  | C27-C26-C25 | 2.08  | 125.51      | 122.70   |
| 29  | d     | 410 | LMG  | C38-C37-C36 | -2.08 | 103.86      | 114.37   |
| 30  | e     | 102 | LHG  | C20-C19-C18 | -2.08 | 103.86      | 114.37   |
| 24  | B     | 609 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 26  | b     | 619 | BCR  | C36-C18-C17 | -2.08 | 119.45      | 122.82   |
| 25  | A     | 606 | PHO  | OBD-CAD-C3D | 2.08  | 131.13      | 127.89   |
| 24  | B     | 614 | CLA  | C1-C2-C3    | -2.08 | 122.80      | 126.20   |
| 24  | D     | 403 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 32  | C     | 518 | DGD  | O5E-C6E-C5E | -2.07 | 104.27      | 111.33   |
| 24  | b     | 615 | CLA  | CHC-C1C-C2C | -2.07 | 121.05      | 126.95   |
| 24  | B     | 606 | CLA  | O1A-CGA-CBA | 2.07  | 131.89      | 123.78   |
| 24  | B     | 615 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 24  | b     | 609 | CLA  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 29  | D     | 410 | LMG  | O7-C10-O9   | -2.07 | 118.00      | 123.33   |
| 24  | B     | 602 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 24  | b     | 615 | CLA  | CHB-C1B-NB  | 2.07  | 127.16      | 124.05   |
| 28  | d     | 406 | PL9  | C40-C39-C38 | -2.07 | 118.31      | 123.63   |
| 30  | B     | 621 | LHG  | O8-C23-C24  | 2.07  | 118.15      | 111.83   |
| 24  | b     | 609 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 24  | C     | 503 | CLA  | CMB-C2B-C3B | 2.07  | 131.41      | 126.55   |
| 26  | B     | 619 | BCR  | C38-C26-C25 | -2.07 | 122.23      | 124.48   |
| 29  | C     | 519 | LMG  | C40-C39-C38 | -2.07 | 103.93      | 114.37   |
| 24  | B     | 606 | CLA  | C4D-CHA-C1A | 2.06  | 123.71      | 121.24   |
| 24  | b     | 607 | CLA  | CMB-C2B-C3B | 2.06  | 131.41      | 126.55   |
| 24  | a     | 606 | CLA  | CHC-C4B-NB  | 2.06  | 127.15      | 124.05   |
| 24  | b     | 606 | CLA  | C2C-C1C-NC  | 2.06  | 112.15      | 109.98   |
| 28  | A     | 612 | PL9  | O2-C1-C6    | 2.06  | 123.76      | 120.48   |
| 32  | C     | 517 | DGD  | O2D-C2D-C1D | -2.06 | 105.16      | 110.08   |
| 24  | b     | 609 | CLA  | C1D-ND-C4D  | 2.06  | 107.76      | 106.31   |
| 24  | b     | 605 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 32  | c     | 517 | DGD  | CBB-CAB-C9B | -2.06 | 103.97      | 114.37   |
| 30  | B     | 621 | LHG  | C18-C17-C16 | -2.06 | 103.97      | 114.37   |
| 31  | A     | 617 | SQD  | O48-C23-O10 | -2.06 | 118.48      | 123.63   |
| 33  | b     | 622 | STE  | C3-C2-C1    | -2.06 | 109.14      | 114.51   |
| 29  | b     | 623 | LMG  | C38-C37-C36 | -2.06 | 103.98      | 114.37   |
| 24  | C     | 505 | CLA  | C11-C10-C8  | -2.06 | 109.13      | 115.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 511 | CLA  | C3B-C4B-NB  | -2.05 | 108.70      | 110.53   |
| 24  | c     | 504 | CLA  | CMB-C2B-C1B | -2.05 | 122.29      | 125.42   |
| 24  | B     | 601 | CLA  | C4-C3-C5    | 2.05  | 118.79      | 115.23   |
| 26  | a     | 607 | BCR  | C8-C7-C6    | -2.05 | 121.51      | 127.00   |
| 24  | c     | 504 | CLA  | O2D-CGD-O1D | -2.05 | 119.85      | 123.85   |
| 36  | v     | 201 | HEC  | CBD-CAD-C3D | -2.05 | 106.86      | 112.53   |
| 24  | B     | 606 | CLA  | CHB-C1B-NB  | 2.05  | 127.13      | 124.05   |
| 26  | k     | 102 | BCR  | C2-C1-C6    | 2.05  | 113.42      | 110.44   |
| 24  | b     | 602 | CLA  | CHC-C1C-C2C | -2.05 | 121.12      | 126.95   |
| 33  | a     | 616 | STE  | O2-C1-C2    | 2.05  | 120.47      | 114.00   |
| 24  | c     | 503 | CLA  | CMB-C2B-C1B | -2.05 | 122.30      | 125.42   |
| 24  | b     | 607 | CLA  | O2D-CGD-O1D | -2.05 | 119.86      | 123.85   |
| 24  | B     | 609 | CLA  | CHD-C1D-ND  | -2.05 | 121.92      | 124.80   |
| 32  | h     | 101 | DGD  | O3G-C1D-C2D | -2.05 | 105.17      | 108.27   |
| 24  | B     | 611 | CLA  | C7-C6-C5    | -2.04 | 107.81      | 113.26   |
| 24  | C     | 507 | CLA  | CHD-C1D-ND  | -2.04 | 121.92      | 124.80   |
| 24  | B     | 603 | CLA  | C2A-C1A-CHA | 2.04  | 127.42      | 123.87   |
| 26  | B     | 617 | BCR  | C8-C7-C6    | -2.04 | 121.54      | 127.00   |
| 29  | c     | 519 | LMG  | C40-C39-C38 | -2.04 | 104.04      | 114.37   |
| 31  | A     | 616 | SQD  | O8-S-O9     | 2.04  | 116.51      | 111.40   |
| 31  | b     | 620 | SQD  | O48-C23-O10 | -2.04 | 118.52      | 123.63   |
| 24  | B     | 607 | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 24  | D     | 403 | CLA  | C11-C10-C8  | -2.04 | 109.18      | 115.97   |
| 26  | A     | 609 | BCR  | C16-C15-C14 | -2.04 | 119.34      | 123.52   |
| 24  | d     | 403 | CLA  | C4-C3-C5    | 2.04  | 118.77      | 115.23   |
| 24  | c     | 513 | CLA  | C1-C2-C3    | -2.04 | 122.85      | 126.20   |
| 30  | l     | 101 | LHG  | C29-C28-C27 | -2.04 | 104.05      | 114.37   |
| 24  | C     | 505 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 24  | d     | 404 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 29  | b     | 621 | LMG  | O8-C28-O10  | -2.04 | 118.53      | 123.63   |
| 32  | c     | 518 | DGD  | CAB-C9B-C8B | -2.04 | 104.06      | 114.37   |
| 28  | d     | 406 | PL9  | C35-C34-C36 | 2.04  | 118.77      | 115.23   |
| 24  | b     | 609 | CLA  | CHB-C1B-NB  | 2.04  | 127.11      | 124.05   |
| 24  | B     | 616 | CLA  | C1-O2A-CGA  | -2.04 | 111.72      | 116.65   |
| 24  | C     | 507 | CLA  | CBC-CAC-C3C | -2.04 | 106.90      | 112.42   |
| 24  | C     | 503 | CLA  | C2C-C1C-NC  | 2.04  | 112.12      | 109.98   |
| 29  | a     | 618 | LMG  | O6-C1-C2    | -2.04 | 106.19      | 110.37   |
| 32  | C     | 516 | DGD  | C6B-C5B-C4B | -2.03 | 104.08      | 114.37   |
| 31  | B     | 623 | SQD  | C1-C2-C3    | -2.03 | 105.73      | 110.01   |
| 24  | c     | 508 | CLA  | CMB-C2B-C3B | 2.03  | 131.33      | 126.55   |
| 24  | C     | 513 | CLA  | O1D-CGD-CBD | 2.03  | 128.53      | 124.52   |
| 24  | B     | 609 | CLA  | CHD-C4C-NC  | 2.03  | 127.38      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | c     | 518 | DGD  | C5B-C4B-C3B | -2.03 | 104.10      | 114.37   |
| 26  | b     | 618 | BCR  | C29-C30-C25 | 2.03  | 113.39      | 110.44   |
| 24  | c     | 510 | CLA  | O1D-CGD-CBD | 2.03  | 128.52      | 124.52   |
| 25  | A     | 607 | PHO  | CAC-C3C-C2C | 2.03  | 131.29      | 127.56   |
| 31  | a     | 613 | SQD  | O4-C4-C3    | -2.03 | 105.59      | 110.38   |
| 24  | c     | 504 | CLA  | C3B-C4B-NB  | -2.03 | 108.72      | 110.53   |
| 26  | K     | 101 | BCR  | C29-C30-C25 | 2.03  | 113.38      | 110.44   |
| 31  | A     | 616 | SQD  | O9-S-C6     | 2.03  | 109.78      | 106.76   |
| 24  | C     | 503 | CLA  | CHD-C1D-ND  | -2.03 | 121.95      | 124.80   |
| 24  | B     | 615 | CLA  | C2C-C1C-NC  | 2.03  | 112.11      | 109.98   |
| 24  | B     | 607 | CLA  | CHD-C1D-ND  | -2.02 | 121.95      | 124.80   |
| 26  | a     | 607 | BCR  | C7-C8-C9    | -2.02 | 123.24      | 126.23   |
| 29  | M     | 101 | LMG  | C6-C5-C4    | -2.02 | 108.05      | 113.02   |
| 26  | A     | 609 | BCR  | C4-C5-C6    | 2.02  | 125.44      | 122.70   |
| 32  | c     | 517 | DGD  | CDB-CCB-CBB | -2.02 | 104.14      | 114.37   |
| 29  | a     | 618 | LMG  | O7-C10-O9   | -2.02 | 118.98      | 123.70   |
| 32  | c     | 517 | DGD  | O6E-C1E-O5D | -2.02 | 105.27      | 110.04   |
| 32  | c     | 516 | DGD  | O6D-C1D-O3G | -2.02 | 105.27      | 110.04   |
| 24  | C     | 506 | CLA  | CHD-C1D-ND  | -2.02 | 121.96      | 124.80   |
| 24  | b     | 613 | CLA  | CMB-C2B-C3B | 2.02  | 131.30      | 126.55   |
| 26  | C     | 514 | BCR  | C36-C18-C17 | -2.02 | 119.55      | 122.82   |
| 29  | C     | 519 | LMG  | C38-C37-C36 | -2.02 | 104.18      | 114.37   |
| 25  | A     | 606 | PHO  | C1A-C2A-C3A | -2.01 | 100.92      | 102.84   |
| 26  | B     | 617 | BCR  | C37-C22-C23 | 2.01  | 121.16      | 118.09   |
| 28  | a     | 611 | PL9  | O1-C4-C3    | -2.01 | 118.61      | 120.73   |
| 24  | C     | 510 | CLA  | CHB-C4A-NA  | 2.01  | 127.31      | 124.40   |
| 35  | F     | 101 | HEM  | O2D-CGD-CBD | 2.01  | 120.36      | 114.00   |
| 24  | b     | 609 | CLA  | C7-C6-C5    | -2.01 | 107.90      | 113.26   |
| 30  | B     | 621 | LHG  | C27-C26-C25 | -2.01 | 104.20      | 114.37   |
| 26  | c     | 514 | BCR  | C37-C22-C21 | -2.01 | 119.56      | 122.82   |
| 24  | C     | 512 | CLA  | CMA-C3A-C2A | -2.01 | 106.21      | 113.98   |
| 24  | B     | 608 | CLA  | CED-O2D-CGD | -2.01 | 111.36      | 115.92   |
| 24  | A     | 604 | CLA  | C7-C6-C5    | -2.01 | 107.91      | 113.26   |
| 29  | c     | 522 | LMG  | C30-C29-C28 | -2.01 | 106.34      | 113.69   |
| 24  | c     | 510 | CLA  | C9-C8-C7    | -2.01 | 104.12      | 111.27   |
| 26  | K     | 101 | BCR  | C8-C7-C6    | -2.01 | 121.64      | 127.00   |
| 29  | b     | 621 | LMG  | C22-C21-C20 | -2.01 | 104.23      | 114.37   |
| 33  | j     | 101 | STE  | O2-C1-O1    | -2.01 | 118.17      | 123.33   |
| 32  | h     | 101 | DGD  | O6D-C1D-O3G | -2.01 | 105.31      | 110.04   |
| 32  | C     | 518 | DGD  | O6D-C5D-C4D | -2.00 | 106.09      | 109.70   |
| 32  | A     | 618 | DGD  | C8B-C7B-C6B | -2.00 | 104.25      | 114.37   |
| 29  | a     | 618 | LMG  | O6-C1-O1    | -2.00 | 105.31      | 110.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | c     | 515 | BCR  | C21-C20-C19 | -2.00 | 117.40      | 123.20   |
| 26  | k     | 101 | BCR  | C4-C5-C6    | 2.00  | 125.41      | 122.70   |
| 24  | B     | 613 | CLA  | CAC-C3C-C4C | 2.00  | 127.39      | 124.79   |

All (58) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | A     | 604 | CLA  | ND   |
| 24  | A     | 605 | CLA  | ND   |
| 24  | A     | 608 | CLA  | ND   |
| 24  | B     | 601 | CLA  | ND   |
| 24  | B     | 602 | CLA  | ND   |
| 24  | B     | 603 | CLA  | ND   |
| 24  | B     | 604 | CLA  | ND   |
| 24  | B     | 605 | CLA  | ND   |
| 24  | B     | 606 | CLA  | ND   |
| 24  | B     | 607 | CLA  | ND   |
| 24  | B     | 610 | CLA  | ND   |
| 24  | B     | 611 | CLA  | ND   |
| 24  | B     | 612 | CLA  | ND   |
| 24  | B     | 613 | CLA  | ND   |
| 24  | B     | 614 | CLA  | ND   |
| 24  | B     | 615 | CLA  | ND   |
| 24  | B     | 616 | CLA  | ND   |
| 24  | C     | 501 | CLA  | ND   |
| 24  | C     | 503 | CLA  | ND   |
| 24  | C     | 504 | CLA  | ND   |
| 24  | C     | 505 | CLA  | ND   |
| 24  | C     | 506 | CLA  | ND   |
| 24  | C     | 507 | CLA  | ND   |
| 24  | C     | 509 | CLA  | ND   |
| 24  | C     | 510 | CLA  | ND   |
| 24  | C     | 511 | CLA  | ND   |
| 24  | C     | 512 | CLA  | ND   |
| 24  | C     | 513 | CLA  | ND   |
| 24  | D     | 402 | CLA  | ND   |
| 24  | a     | 604 | CLA  | ND   |
| 24  | a     | 606 | CLA  | ND   |
| 24  | a     | 612 | CLA  | ND   |
| 24  | b     | 601 | CLA  | ND   |
| 24  | b     | 603 | CLA  | ND   |
| 24  | b     | 604 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24  | b     | 605 | CLA  | ND   |
| 24  | b     | 606 | CLA  | ND   |
| 24  | b     | 607 | CLA  | ND   |
| 24  | b     | 610 | CLA  | ND   |
| 24  | b     | 611 | CLA  | ND   |
| 24  | b     | 612 | CLA  | ND   |
| 24  | b     | 613 | CLA  | ND   |
| 24  | b     | 614 | CLA  | ND   |
| 24  | b     | 615 | CLA  | ND   |
| 24  | b     | 616 | CLA  | ND   |
| 24  | c     | 501 | CLA  | ND   |
| 24  | c     | 503 | CLA  | ND   |
| 24  | c     | 504 | CLA  | ND   |
| 24  | c     | 505 | CLA  | ND   |
| 24  | c     | 506 | CLA  | ND   |
| 24  | c     | 507 | CLA  | ND   |
| 24  | c     | 509 | CLA  | ND   |
| 24  | c     | 510 | CLA  | ND   |
| 24  | c     | 511 | CLA  | ND   |
| 24  | c     | 512 | CLA  | ND   |
| 24  | c     | 513 | CLA  | ND   |
| 24  | d     | 403 | CLA  | ND   |
| 24  | d     | 404 | CLA  | ND   |

All (1751) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | B     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 24  | B     | 601 | CLA  | CAD-CBD-CGD-O1D |
| 24  | B     | 601 | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 603 | CLA  | C4-C3-C5-C6     |
| 24  | B     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 24  | B     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 24  | B     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 507 | CLA  | CHA-CBD-CGD-O2D |
| 24  | C     | 507 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 24  | b     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 507 | CLA  | CHA-CBD-CGD-O1D |
| 24  | c     | 507 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | c     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 24  | c     | 512 | CLA  | C2B-C3B-CAB-CBB |
| 26  | B     | 617 | BCR  | C35-C13-C14-C15 |
| 26  | C     | 514 | BCR  | C11-C12-C13-C35 |
| 26  | C     | 515 | BCR  | C11-C12-C13-C14 |
| 26  | D     | 404 | BCR  | C21-C22-C23-C24 |
| 26  | D     | 404 | BCR  | C23-C24-C25-C26 |
| 26  | D     | 404 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 101 | BCR  | C37-C22-C23-C24 |
| 26  | T     | 101 | BCR  | C11-C12-C13-C35 |
| 26  | Y     | 101 | BCR  | C5-C6-C7-C8     |
| 26  | b     | 617 | BCR  | C21-C22-C23-C24 |
| 26  | c     | 514 | BCR  | C20-C21-C22-C37 |
| 26  | d     | 405 | BCR  | C37-C22-C23-C24 |
| 26  | k     | 101 | BCR  | C5-C6-C7-C8     |
| 28  | A     | 612 | PL9  | C12-C13-C14-C15 |
| 28  | A     | 612 | PL9  | C12-C13-C14-C16 |
| 28  | A     | 612 | PL9  | C22-C23-C24-C26 |
| 28  | A     | 612 | PL9  | C37-C38-C39-C40 |
| 28  | A     | 612 | PL9  | C37-C38-C39-C41 |
| 28  | A     | 612 | PL9  | C40-C39-C41-C42 |
| 28  | D     | 405 | PL9  | C32-C33-C34-C36 |
| 28  | D     | 405 | PL9  | C37-C38-C39-C40 |
| 28  | a     | 611 | PL9  | C12-C13-C14-C15 |
| 28  | a     | 611 | PL9  | C17-C18-C19-C21 |
| 28  | a     | 611 | PL9  | C20-C19-C21-C22 |
| 28  | a     | 611 | PL9  | C22-C23-C24-C25 |
| 28  | a     | 611 | PL9  | C22-C23-C24-C26 |
| 28  | a     | 611 | PL9  | C25-C24-C26-C27 |
| 28  | d     | 406 | PL9  | C32-C33-C34-C36 |
| 28  | d     | 406 | PL9  | C38-C39-C41-C42 |
| 28  | d     | 406 | PL9  | C42-C43-C44-C45 |
| 29  | A     | 614 | LMG  | O9-C10-O7-C8    |
| 29  | D     | 409 | LMG  | O1-C7-C8-C9     |
| 29  | D     | 409 | LMG  | O1-C7-C8-O7     |
| 29  | b     | 623 | LMG  | C11-C10-O7-C8   |
| 29  | c     | 522 | LMG  | O6-C1-O1-C7     |
| 30  | A     | 615 | LHG  | C3-O3-P-O6      |
| 30  | B     | 621 | LHG  | C4-O6-P-O3      |
| 30  | B     | 621 | LHG  | C4-O6-P-O5      |
| 30  | D     | 408 | LHG  | O1-C1-C2-C3     |
| 30  | D     | 408 | LHG  | C1-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | D     | 408 | LHG  | O2-C2-C3-O3     |
| 30  | D     | 408 | LHG  | C3-O3-P-O5      |
| 30  | D     | 408 | LHG  | C3-O3-P-O6      |
| 30  | D     | 408 | LHG  | C4-O6-P-O3      |
| 30  | D     | 408 | LHG  | C4-O6-P-O4      |
| 30  | E     | 101 | LHG  | O1-C1-C2-C3     |
| 30  | E     | 101 | LHG  | O10-C23-O8-C6   |
| 30  | E     | 101 | LHG  | C24-C23-O8-C6   |
| 30  | d     | 407 | LHG  | C3-O3-P-O4      |
| 30  | d     | 407 | LHG  | C3-O3-P-O6      |
| 30  | d     | 408 | LHG  | O1-C1-C2-C3     |
| 30  | d     | 408 | LHG  | C3-O3-P-O4      |
| 30  | d     | 408 | LHG  | C3-O3-P-O6      |
| 30  | d     | 408 | LHG  | C4-O6-P-O3      |
| 30  | d     | 408 | LHG  | C4-O6-P-O4      |
| 30  | d     | 409 | LHG  | C4-O6-P-O4      |
| 30  | e     | 102 | LHG  | C1-C2-C3-O3     |
| 30  | e     | 102 | LHG  | C3-O3-P-O5      |
| 30  | e     | 102 | LHG  | C3-O3-P-O6      |
| 30  | e     | 102 | LHG  | C4-O6-P-O5      |
| 30  | e     | 102 | LHG  | O6-C4-C5-O7     |
| 30  | e     | 102 | LHG  | O10-C23-O8-C6   |
| 30  | e     | 102 | LHG  | C24-C23-O8-C6   |
| 30  | l     | 101 | LHG  | C4-O6-P-O3      |
| 31  | A     | 617 | SQD  | C46-C45-O47-C7  |
| 31  | B     | 623 | SQD  | O5-C1-O6-C44    |
| 31  | B     | 623 | SQD  | O6-C44-C45-O47  |
| 31  | B     | 623 | SQD  | O49-C7-O47-C45  |
| 31  | D     | 407 | SQD  | O5-C1-O6-C44    |
| 31  | D     | 407 | SQD  | O10-C23-O48-C46 |
| 31  | a     | 613 | SQD  | O6-C44-C45-O47  |
| 31  | a     | 614 | SQD  | O6-C44-C45-C46  |
| 31  | a     | 614 | SQD  | O6-C44-C45-O47  |
| 31  | a     | 614 | SQD  | C8-C7-O47-C45   |
| 31  | a     | 614 | SQD  | O10-C23-O48-C46 |
| 31  | a     | 614 | SQD  | C24-C23-O48-C46 |
| 31  | f     | 101 | SQD  | C2-C1-O6-C44    |
| 31  | f     | 101 | SQD  | O5-C1-O6-C44    |
| 32  | A     | 618 | DGD  | C2B-C1B-O2G-C2G |
| 32  | A     | 618 | DGD  | O1B-C1B-O2G-C2G |
| 36  | V     | 201 | HEC  | C2B-C3B-CAB-CBB |
| 36  | V     | 201 | HEC  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | V     | 201 | HEC  | C2C-C3C-CAC-CBC |
| 36  | V     | 201 | HEC  | C4C-C3C-CAC-CBC |
| 36  | v     | 201 | HEC  | C2B-C3B-CAB-CBB |
| 36  | v     | 201 | HEC  | C2C-C3C-CAC-CBC |
| 36  | v     | 201 | HEC  | C4C-C3C-CAC-CBC |
| 24  | c     | 513 | CLA  | CBD-CGD-O2D-CED |
| 29  | c     | 522 | LMG  | O10-C28-O8-C9   |
| 24  | B     | 614 | CLA  | C15-C16-C17-C18 |
| 31  | D     | 407 | SQD  | C24-C23-O48-C46 |
| 31  | f     | 101 | SQD  | C24-C23-O48-C46 |
| 29  | M     | 101 | LMG  | O10-C28-O8-C9   |
| 29  | c     | 521 | LMG  | O10-C28-O8-C9   |
| 31  | f     | 101 | SQD  | O10-C23-O48-C46 |
| 29  | D     | 409 | LMG  | O9-C10-O7-C8    |
| 29  | b     | 623 | LMG  | O9-C10-O7-C8    |
| 31  | a     | 614 | SQD  | O49-C7-O47-C45  |
| 24  | B     | 614 | CLA  | C3-C5-C6-C7     |
| 29  | c     | 522 | LMG  | C29-C28-O8-C9   |
| 31  | b     | 620 | SQD  | C24-C23-O48-C46 |
| 24  | C     | 509 | CLA  | CBD-CGD-O2D-CED |
| 29  | A     | 614 | LMG  | C11-C10-O7-C8   |
| 29  | a     | 618 | LMG  | C11-C10-O7-C8   |
| 31  | B     | 623 | SQD  | C8-C7-O47-C45   |
| 31  | b     | 620 | SQD  | O10-C23-O48-C46 |
| 24  | A     | 608 | CLA  | C4-C3-C5-C6     |
| 24  | B     | 614 | CLA  | C4-C3-C5-C6     |
| 24  | C     | 504 | CLA  | C4-C3-C5-C6     |
| 24  | b     | 603 | CLA  | C4-C3-C5-C6     |
| 24  | b     | 605 | CLA  | C4-C3-C5-C6     |
| 24  | c     | 507 | CLA  | C4-C3-C5-C6     |
| 28  | a     | 611 | PL9  | C35-C34-C36-C37 |
| 28  | d     | 406 | PL9  | C40-C39-C41-C42 |
| 24  | A     | 608 | CLA  | C2-C3-C5-C6     |
| 24  | B     | 603 | CLA  | C2-C3-C5-C6     |
| 24  | B     | 614 | CLA  | C2-C3-C5-C6     |
| 24  | C     | 504 | CLA  | C2-C3-C5-C6     |
| 24  | C     | 507 | CLA  | C2-C3-C5-C6     |
| 24  | b     | 603 | CLA  | C2-C3-C5-C6     |
| 28  | A     | 612 | PL9  | C43-C44-C46-C47 |
| 28  | D     | 405 | PL9  | C33-C34-C36-C37 |
| 28  | a     | 611 | PL9  | C23-C24-C26-C27 |
| 24  | b     | 601 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 602 | CLA  | C3-C5-C6-C7     |
| 24  | d     | 404 | CLA  | C3-C5-C6-C7     |
| 24  | B     | 616 | CLA  | CBA-CGA-O2A-C1  |
| 29  | c     | 521 | LMG  | C29-C28-O8-C9   |
| 28  | A     | 612 | PL9  | C22-C23-C24-C25 |
| 28  | d     | 406 | PL9  | C32-C33-C34-C35 |
| 28  | a     | 611 | PL9  | C42-C43-C44-C46 |
| 31  | B     | 623 | SQD  | O10-C23-O48-C46 |
| 28  | A     | 612 | PL9  | C47-C48-C49-C51 |
| 30  | e     | 102 | LHG  | O2-C2-C3-O3     |
| 24  | c     | 513 | CLA  | O1D-CGD-O2D-CED |
| 24  | B     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 24  | C     | 511 | CLA  | CBD-CGD-O2D-CED |
| 29  | C     | 519 | LMG  | C11-C10-O7-C8   |
| 29  | D     | 409 | LMG  | C11-C10-O7-C8   |
| 32  | A     | 618 | DGD  | O6E-C5E-C6E-O5E |
| 29  | A     | 614 | LMG  | O6-C5-C6-O5     |
| 29  | M     | 101 | LMG  | C29-C28-O8-C9   |
| 24  | C     | 507 | CLA  | C4-C3-C5-C6     |
| 24  | b     | 605 | CLA  | C2-C3-C5-C6     |
| 24  | b     | 614 | CLA  | C2-C3-C5-C6     |
| 24  | c     | 507 | CLA  | C2-C3-C5-C6     |
| 28  | A     | 612 | PL9  | C23-C24-C26-C27 |
| 33  | T     | 102 | STE  | C5-C6-C7-C8     |
| 28  | A     | 612 | PL9  | C9-C11-C12-C13  |
| 28  | A     | 612 | PL9  | C34-C36-C37-C38 |
| 28  | a     | 611 | PL9  | C19-C21-C22-C23 |
| 28  | a     | 611 | PL9  | C24-C26-C27-C28 |
| 28  | a     | 611 | PL9  | C34-C36-C37-C38 |
| 32  | A     | 618 | DGD  | C4E-C5E-C6E-O5E |
| 24  | C     | 501 | CLA  | CBD-CGD-O2D-CED |
| 24  | B     | 616 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 623 | SQD  | C24-C23-O48-C46 |
| 29  | a     | 618 | LMG  | O6-C5-C6-O5     |
| 28  | D     | 405 | PL9  | C27-C28-C29-C30 |
| 24  | B     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 24  | c     | 508 | CLA  | CBD-CGD-O2D-CED |
| 28  | d     | 406 | PL9  | C47-C48-C49-C51 |
| 30  | d     | 409 | LHG  | C30-C31-C32-C33 |
| 24  | c     | 506 | CLA  | CBA-CGA-O2A-C1  |
| 24  | B     | 612 | CLA  | CBD-CGD-O2D-CED |
| 30  | d     | 409 | LHG  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 614 | CLA  | C4-C3-C5-C6     |
| 28  | a     | 611 | PL9  | C33-C34-C36-C37 |
| 24  | A     | 605 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 610 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 613 | CLA  | C11-C12-C13-C14 |
| 24  | B     | 614 | CLA  | C6-C7-C8-C9     |
| 24  | B     | 614 | CLA  | C14-C13-C15-C16 |
| 24  | C     | 509 | CLA  | C11-C10-C8-C9   |
| 24  | C     | 512 | CLA  | C11-C10-C8-C9   |
| 24  | D     | 403 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 601 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 602 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 613 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 616 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 509 | CLA  | C6-C7-C8-C9     |
| 24  | c     | 509 | CLA  | C11-C12-C13-C14 |
| 24  | c     | 512 | CLA  | C6-C7-C8-C9     |
| 24  | d     | 404 | CLA  | C6-C7-C8-C9     |
| 29  | A     | 614 | LMG  | C4-C5-C6-O5     |
| 29  | a     | 618 | LMG  | C4-C5-C6-O5     |
| 26  | C     | 515 | BCR  | C36-C18-C19-C20 |
| 26  | H     | 101 | BCR  | C11-C12-C13-C35 |
| 26  | K     | 101 | BCR  | C36-C18-C19-C20 |
| 26  | T     | 101 | BCR  | C7-C8-C9-C34    |
| 26  | Y     | 101 | BCR  | C37-C22-C23-C24 |
| 26  | b     | 619 | BCR  | C11-C12-C13-C35 |
| 26  | b     | 619 | BCR  | C37-C22-C23-C24 |
| 26  | k     | 101 | BCR  | C7-C8-C9-C34    |
| 26  | k     | 102 | BCR  | C37-C22-C23-C24 |
| 26  | t     | 101 | BCR  | C7-C8-C9-C34    |
| 26  | t     | 101 | BCR  | C11-C12-C13-C35 |
| 26  | x     | 101 | BCR  | C7-C8-C9-C34    |
| 28  | A     | 612 | PL9  | C47-C48-C49-C50 |
| 24  | C     | 509 | CLA  | O1D-CGD-O2D-CED |
| 33  | B     | 627 | STE  | C1-C2-C3-C4     |
| 33  | C     | 522 | STE  | C4-C5-C6-C7     |
| 24  | B     | 611 | CLA  | C13-C15-C16-C17 |
| 24  | C     | 513 | CLA  | C15-C16-C17-C18 |
| 28  | A     | 612 | PL9  | C32-C33-C34-C36 |
| 24  | B     | 611 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 613 | CLA  | C11-C10-C8-C7   |
| 24  | C     | 510 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | A     | 612 | PL9  | C44-C46-C47-C48 |
| 33  | D     | 411 | STE  | C11-C12-C13-C14 |
| 24  | c     | 503 | CLA  | C8-C10-C11-C12  |
| 32  | C     | 518 | DGD  | C8A-C9A-CAA-CBA |
| 31  | B     | 623 | SQD  | C45-C46-O48-C23 |
| 29  | b     | 623 | LMG  | C28-C29-C30-C31 |
| 29  | d     | 410 | LMG  | C10-C11-C12-C13 |
| 30  | E     | 101 | LHG  | C23-C24-C25-C26 |
| 30  | d     | 407 | LHG  | C23-C24-C25-C26 |
| 30  | d     | 409 | LHG  | C23-C24-C25-C26 |
| 32  | c     | 518 | DGD  | C1A-C2A-C3A-C4A |
| 33  | C     | 520 | STE  | C1-C2-C3-C4     |
| 33  | E     | 102 | STE  | C1-C2-C3-C4     |
| 29  | c     | 521 | LMG  | C11-C10-O7-C8   |
| 24  | B     | 605 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 613 | CLA  | C8-C10-C11-C12  |
| 24  | D     | 402 | CLA  | C15-C16-C17-C18 |
| 24  | c     | 512 | CLA  | C13-C15-C16-C17 |
| 24  | b     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 26  | c     | 514 | BCR  | C18-C19-C20-C21 |
| 24  | B     | 609 | CLA  | C13-C15-C16-C17 |
| 24  | B     | 614 | CLA  | C13-C15-C16-C17 |
| 24  | a     | 606 | CLA  | C10-C11-C12-C13 |
| 24  | a     | 606 | CLA  | C15-C16-C17-C18 |
| 29  | D     | 406 | LMG  | C10-C11-C12-C13 |
| 29  | D     | 409 | LMG  | C28-C29-C30-C31 |
| 30  | B     | 622 | LHG  | C23-C24-C25-C26 |
| 30  | d     | 407 | LHG  | C7-C8-C9-C10    |
| 33  | d     | 412 | STE  | C7-C8-C9-C10    |
| 24  | A     | 604 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 601 | CLA  | C5-C6-C7-C8     |
| 24  | B     | 602 | CLA  | C13-C15-C16-C17 |
| 24  | B     | 606 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 616 | CLA  | C5-C6-C7-C8     |
| 24  | C     | 503 | CLA  | C5-C6-C7-C8     |
| 24  | C     | 506 | CLA  | C8-C10-C11-C12  |
| 24  | C     | 510 | CLA  | C10-C11-C12-C13 |
| 24  | b     | 611 | CLA  | C15-C16-C17-C18 |
| 24  | b     | 614 | CLA  | C5-C6-C7-C8     |
| 24  | c     | 505 | CLA  | C5-C6-C7-C8     |
| 24  | c     | 509 | CLA  | C13-C15-C16-C17 |
| 24  | c     | 511 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | d     | 407 | LHG  | O2-C2-C3-O3     |
| 24  | c     | 506 | CLA  | O1A-CGA-O2A-C1  |
| 29  | c     | 519 | LMG  | C28-C29-C30-C31 |
| 33  | b     | 624 | STE  | C1-C2-C3-C4     |
| 24  | B     | 612 | CLA  | C13-C15-C16-C17 |
| 24  | C     | 508 | CLA  | C15-C16-C17-C18 |
| 24  | b     | 615 | CLA  | C10-C11-C12-C13 |
| 24  | C     | 506 | CLA  | C15-C16-C17-C18 |
| 24  | b     | 607 | CLA  | C10-C11-C12-C13 |
| 24  | c     | 511 | CLA  | CBD-CGD-O2D-CED |
| 29  | c     | 521 | LMG  | C10-C11-C12-C13 |
| 24  | C     | 512 | CLA  | C13-C15-C16-C17 |
| 24  | b     | 611 | CLA  | C13-C15-C16-C17 |
| 24  | c     | 509 | CLA  | C10-C11-C12-C13 |
| 24  | c     | 511 | CLA  | C13-C15-C16-C17 |
| 24  | c     | 512 | CLA  | C8-C10-C11-C12  |
| 29  | a     | 618 | LMG  | C29-C28-O8-C9   |
| 29  | b     | 621 | LMG  | C10-C11-C12-C13 |
| 24  | c     | 506 | CLA  | C13-C15-C16-C17 |
| 26  | c     | 514 | BCR  | C13-C14-C15-C16 |
| 32  | c     | 518 | DGD  | O1A-C1A-O1G-C1G |
| 31  | B     | 623 | SQD  | C29-C30-C31-C32 |
| 29  | M     | 101 | LMG  | O9-C10-O7-C8    |
| 30  | e     | 102 | LHG  | O9-C7-O7-C5     |
| 30  | d     | 407 | LHG  | C1-C2-C3-O3     |
| 31  | D     | 407 | SQD  | C44-C45-C46-O48 |
| 24  | C     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 24  | C     | 509 | CLA  | C10-C11-C12-C13 |
| 24  | C     | 512 | CLA  | C10-C11-C12-C13 |
| 24  | D     | 403 | CLA  | C10-C11-C12-C13 |
| 24  | b     | 611 | CLA  | C8-C10-C11-C12  |
| 24  | b     | 615 | CLA  | C15-C16-C17-C18 |
| 24  | c     | 506 | CLA  | C15-C16-C17-C18 |
| 29  | d     | 410 | LMG  | C28-C29-C30-C31 |
| 30  | e     | 102 | LHG  | C7-C8-C9-C10    |
| 24  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 24  | b     | 601 | CLA  | C8-C10-C11-C12  |
| 24  | c     | 503 | CLA  | C5-C6-C7-C8     |
| 24  | b     | 607 | CLA  | C8-C10-C11-C12  |
| 31  | b     | 620 | SQD  | C8-C7-O47-C45   |
| 29  | c     | 522 | LMG  | C2-C1-O1-C7     |
| 31  | B     | 623 | SQD  | C2-C1-O6-C44    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | C     | 517 | DGD  | C2E-C1E-O5D-C6D |
| 32  | c     | 517 | DGD  | C2E-C1E-O5D-C6D |
| 24  | a     | 606 | CLA  | C5-C6-C7-C8     |
| 24  | B     | 606 | CLA  | C16-C17-C18-C19 |
| 26  | A     | 609 | BCR  | C11-C10-C9-C34  |
| 26  | A     | 609 | BCR  | C35-C13-C14-C15 |
| 26  | A     | 609 | BCR  | C20-C21-C22-C37 |
| 26  | B     | 617 | BCR  | C11-C10-C9-C34  |
| 26  | D     | 404 | BCR  | C20-C21-C22-C37 |
| 26  | K     | 101 | BCR  | C11-C10-C9-C34  |
| 26  | b     | 617 | BCR  | C20-C21-C22-C37 |
| 26  | b     | 618 | BCR  | C16-C17-C18-C36 |
| 26  | c     | 514 | BCR  | C16-C17-C18-C36 |
| 26  | k     | 101 | BCR  | C35-C13-C14-C15 |
| 26  | t     | 101 | BCR  | C35-C13-C14-C15 |
| 26  | t     | 101 | BCR  | C20-C21-C22-C37 |
| 32  | c     | 516 | DGD  | C1A-C2A-C3A-C4A |
| 26  | A     | 609 | BCR  | C36-C18-C19-C20 |
| 26  | A     | 609 | BCR  | C37-C22-C23-C24 |
| 26  | B     | 619 | BCR  | C11-C12-C13-C35 |
| 26  | B     | 619 | BCR  | C37-C22-C23-C24 |
| 26  | C     | 515 | BCR  | C11-C12-C13-C35 |
| 26  | b     | 618 | BCR  | C37-C22-C23-C24 |
| 26  | C     | 514 | BCR  | C11-C12-C13-C14 |
| 26  | T     | 101 | BCR  | C7-C8-C9-C10    |
| 26  | Y     | 101 | BCR  | C21-C22-C23-C24 |
| 24  | B     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 24  | c     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 24  | b     | 614 | CLA  | C8-C10-C11-C12  |
| 30  | d     | 407 | LHG  | O1-C1-C2-C3     |
| 30  | d     | 409 | LHG  | O1-C1-C2-C3     |
| 24  | B     | 614 | CLA  | C16-C17-C18-C20 |
| 24  | D     | 403 | CLA  | C16-C17-C18-C19 |
| 24  | a     | 604 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 504 | CLA  | C11-C12-C13-C14 |
| 24  | c     | 511 | CLA  | C16-C17-C18-C19 |
| 24  | d     | 403 | CLA  | C16-C17-C18-C19 |
| 24  | d     | 403 | CLA  | C16-C17-C18-C20 |
| 24  | b     | 603 | CLA  | C13-C15-C16-C17 |
| 26  | B     | 618 | BCR  | C20-C21-C22-C23 |
| 26  | B     | 619 | BCR  | C11-C10-C9-C8   |
| 26  | B     | 619 | BCR  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | C     | 514 | BCR  | C11-C10-C9-C8   |
| 26  | K     | 101 | BCR  | C11-C10-C9-C8   |
| 26  | K     | 101 | BCR  | C20-C21-C22-C23 |
| 26  | T     | 101 | BCR  | C12-C13-C14-C15 |
| 26  | b     | 617 | BCR  | C20-C21-C22-C23 |
| 26  | b     | 618 | BCR  | C20-C21-C22-C23 |
| 26  | c     | 514 | BCR  | C20-C21-C22-C23 |
| 26  | k     | 101 | BCR  | C11-C10-C9-C8   |
| 26  | k     | 102 | BCR  | C11-C10-C9-C8   |
| 26  | x     | 101 | BCR  | C11-C10-C9-C8   |
| 26  | x     | 101 | BCR  | C12-C13-C14-C15 |
| 26  | x     | 101 | BCR  | C16-C17-C18-C19 |
| 32  | C     | 517 | DGD  | O6E-C1E-O5D-C6D |
| 32  | c     | 517 | DGD  | O6E-C1E-O5D-C6D |
| 29  | c     | 522 | LMG  | C11-C10-O7-C8   |
| 29  | b     | 621 | LMG  | C29-C28-O8-C9   |
| 24  | B     | 611 | CLA  | C8-C10-C11-C12  |
| 24  | C     | 511 | CLA  | O1D-CGD-O2D-CED |
| 24  | B     | 615 | CLA  | C16-C17-C18-C20 |
| 24  | c     | 510 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 511 | CLA  | C16-C17-C18-C20 |
| 24  | C     | 505 | CLA  | C10-C11-C12-C13 |
| 29  | c     | 521 | LMG  | C33-C34-C35-C36 |
| 30  | E     | 101 | LHG  | C9-C10-C11-C12  |
| 33  | C     | 520 | STE  | C6-C7-C8-C9     |
| 26  | C     | 514 | BCR  | C14-C15-C16-C17 |
| 30  | A     | 615 | LHG  | C11-C12-C13-C14 |
| 30  | D     | 408 | LHG  | C30-C31-C32-C33 |
| 32  | c     | 516 | DGD  | C7A-C8A-C9A-CAA |
| 32  | h     | 101 | DGD  | C5B-C6B-C7B-C8B |
| 33  | B     | 620 | STE  | C4-C5-C6-C7     |
| 33  | T     | 102 | STE  | C7-C8-C9-C10    |
| 33  | t     | 102 | STE  | C2-C3-C4-C5     |
| 29  | a     | 618 | LMG  | C12-C13-C14-C15 |
| 29  | c     | 519 | LMG  | C33-C34-C35-C36 |
| 33  | b     | 627 | STE  | C11-C12-C13-C14 |
| 33  | l     | 102 | STE  | C14-C15-C16-C17 |
| 29  | a     | 618 | LMG  | O10-C28-O8-C9   |
| 29  | A     | 614 | LMG  | C14-C15-C16-C17 |
| 29  | D     | 410 | LMG  | C14-C15-C16-C17 |
| 29  | M     | 101 | LMG  | C36-C37-C38-C39 |
| 29  | c     | 521 | LMG  | C40-C41-C42-C43 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | c     | 522 | LMG  | C12-C13-C14-C15 |
| 29  | d     | 410 | LMG  | C36-C37-C38-C39 |
| 30  | A     | 615 | LHG  | C12-C13-C14-C15 |
| 30  | B     | 621 | LHG  | C31-C32-C33-C34 |
| 30  | E     | 101 | LHG  | C27-C28-C29-C30 |
| 30  | d     | 407 | LHG  | C10-C11-C12-C13 |
| 31  | a     | 614 | SQD  | C12-C13-C14-C15 |
| 32  | C     | 518 | DGD  | C9A-CAA-CBA-CCA |
| 32  | c     | 517 | DGD  | CAB-CBB-CCB-CDB |
| 33  | B     | 626 | STE  | C4-C5-C6-C7     |
| 33  | T     | 103 | STE  | C13-C14-C15-C16 |
| 33  | x     | 102 | STE  | C11-C12-C13-C14 |
| 29  | c     | 521 | LMG  | O9-C10-O7-C8    |
| 30  | D     | 408 | LHG  | O1-C1-C2-O2     |
| 30  | E     | 101 | LHG  | O1-C1-C2-O2     |
| 30  | d     | 407 | LHG  | O1-C1-C2-O2     |
| 30  | d     | 408 | LHG  | O1-C1-C2-O2     |
| 29  | A     | 614 | LMG  | C13-C14-C15-C16 |
| 29  | b     | 621 | LMG  | C32-C33-C34-C35 |
| 29  | d     | 410 | LMG  | C33-C34-C35-C36 |
| 30  | B     | 621 | LHG  | C17-C18-C19-C20 |
| 30  | E     | 101 | LHG  | C28-C29-C30-C31 |
| 32  | h     | 101 | DGD  | C9A-CAA-CBA-CCA |
| 33  | d     | 412 | STE  | C14-C15-C16-C17 |
| 24  | C     | 501 | CLA  | O1D-CGD-O2D-CED |
| 24  | B     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 24  | c     | 512 | CLA  | C4B-C3B-CAB-CBB |
| 32  | c     | 516 | DGD  | C1B-C2B-C3B-C4B |
| 33  | m     | 101 | STE  | C1-C2-C3-C4     |
| 33  | x     | 102 | STE  | C1-C2-C3-C4     |
| 32  | c     | 517 | DGD  | CCA-CDA-CEA-CFA |
| 24  | a     | 604 | CLA  | C16-C17-C18-C20 |
| 24  | b     | 601 | CLA  | C16-C17-C18-C20 |
| 24  | b     | 607 | CLA  | C16-C17-C18-C20 |
| 29  | c     | 521 | LMG  | C30-C31-C32-C33 |
| 30  | d     | 408 | LHG  | C32-C33-C34-C35 |
| 31  | a     | 614 | SQD  | C10-C11-C12-C13 |
| 32  | c     | 517 | DGD  | CBB-CCB-CDB-CEB |
| 33  | b     | 627 | STE  | C9-C10-C11-C12  |
| 33  | t     | 102 | STE  | C5-C6-C7-C8     |
| 24  | b     | 607 | CLA  | C5-C6-C7-C8     |
| 24  | c     | 506 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | E     | 101 | LHG  | C24-C25-C26-C27 |
| 33  | T     | 102 | STE  | C6-C7-C8-C9     |
| 30  | A     | 615 | LHG  | C32-C33-C34-C35 |
| 29  | A     | 614 | LMG  | C28-C29-C30-C31 |
| 24  | C     | 505 | CLA  | C5-C6-C7-C8     |
| 29  | d     | 410 | LMG  | O6-C5-C6-O5     |
| 29  | b     | 621 | LMG  | C14-C15-C16-C17 |
| 29  | c     | 519 | LMG  | C39-C40-C41-C42 |
| 31  | a     | 613 | SQD  | C25-C26-C27-C28 |
| 33  | b     | 624 | STE  | C10-C11-C12-C13 |
| 33  | b     | 625 | STE  | C4-C5-C6-C7     |
| 24  | c     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 29  | a     | 618 | LMG  | C36-C37-C38-C39 |
| 29  | c     | 521 | LMG  | C39-C40-C41-C42 |
| 32  | H     | 102 | DGD  | CCB-CDB-CEB-CFB |
| 33  | B     | 624 | STE  | C6-C7-C8-C9     |
| 33  | b     | 622 | STE  | C14-C15-C16-C17 |
| 33  | k     | 103 | STE  | C6-C7-C8-C9     |
| 33  | H     | 103 | STE  | C11-C12-C13-C14 |
| 33  | M     | 102 | STE  | C11-C10-C9-C8   |
| 24  | b     | 613 | CLA  | C13-C15-C16-C17 |
| 24  | d     | 401 | CLA  | C8-C10-C11-C12  |
| 29  | b     | 623 | LMG  | C10-C11-C12-C13 |
| 24  | B     | 606 | CLA  | C16-C17-C18-C20 |
| 24  | B     | 607 | CLA  | C16-C17-C18-C20 |
| 24  | B     | 614 | CLA  | C16-C17-C18-C19 |
| 29  | A     | 614 | LMG  | C38-C39-C40-C41 |
| 29  | M     | 101 | LMG  | C29-C30-C31-C32 |
| 31  | B     | 623 | SQD  | C33-C34-C35-C36 |
| 31  | a     | 613 | SQD  | C24-C25-C26-C27 |
| 29  | b     | 623 | LMG  | C11-C12-C13-C14 |
| 30  | E     | 101 | LHG  | C33-C34-C35-C36 |
| 31  | B     | 623 | SQD  | C11-C12-C13-C14 |
| 31  | f     | 101 | SQD  | C29-C30-C31-C32 |
| 24  | B     | 612 | CLA  | O1D-CGD-O2D-CED |
| 29  | d     | 410 | LMG  | C32-C33-C34-C35 |
| 31  | A     | 617 | SQD  | C12-C13-C14-C15 |
| 31  | a     | 613 | SQD  | C34-C35-C36-C37 |
| 32  | C     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 32  | H     | 102 | DGD  | C8B-C9B-CAB-CBB |
| 32  | c     | 516 | DGD  | C4B-C5B-C6B-C7B |
| 33  | D     | 411 | STE  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | b     | 627 | STE  | C7-C8-C9-C10    |
| 29  | M     | 101 | LMG  | C28-C29-C30-C31 |
| 29  | A     | 614 | LMG  | C11-C12-C13-C14 |
| 29  | A     | 614 | LMG  | C35-C36-C37-C38 |
| 29  | c     | 521 | LMG  | C41-C42-C43-C44 |
| 30  | B     | 621 | LHG  | C12-C13-C14-C15 |
| 32  | H     | 102 | DGD  | C6B-C7B-C8B-C9B |
| 32  | c     | 516 | DGD  | C3A-C4A-C5A-C6A |
| 32  | c     | 517 | DGD  | C7B-C8B-C9B-CAB |
| 33  | T     | 103 | STE  | C5-C6-C7-C8     |
| 33  | k     | 103 | STE  | C2-C3-C4-C5     |
| 24  | C     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 29  | D     | 410 | LMG  | C29-C30-C31-C32 |
| 31  | A     | 616 | SQD  | C30-C31-C32-C33 |
| 32  | h     | 101 | DGD  | C6B-C7B-C8B-C9B |
| 33  | H     | 103 | STE  | C13-C14-C15-C16 |
| 29  | b     | 621 | LMG  | C33-C34-C35-C36 |
| 29  | b     | 623 | LMG  | C13-C14-C15-C16 |
| 30  | A     | 615 | LHG  | C29-C30-C31-C32 |
| 32  | h     | 101 | DGD  | O6E-C5E-C6E-O5E |
| 29  | A     | 614 | LMG  | C17-C18-C19-C20 |
| 29  | c     | 519 | LMG  | C38-C39-C40-C41 |
| 30  | l     | 101 | LHG  | C29-C30-C31-C32 |
| 32  | A     | 618 | DGD  | C5B-C6B-C7B-C8B |
| 32  | C     | 516 | DGD  | C5B-C6B-C7B-C8B |
| 33  | C     | 521 | STE  | C7-C8-C9-C10    |
| 33  | d     | 411 | STE  | C4-C5-C6-C7     |
| 24  | C     | 509 | CLA  | C16-C17-C18-C19 |
| 30  | B     | 622 | LHG  | C7-C8-C9-C10    |
| 24  | B     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 26  | Y     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | k     | 101 | BCR  | C1-C6-C7-C8     |
| 29  | b     | 621 | LMG  | C18-C19-C20-C21 |
| 30  | d     | 409 | LHG  | C26-C27-C28-C29 |
| 29  | M     | 101 | LMG  | C11-C10-O7-C8   |
| 30  | e     | 102 | LHG  | C8-C7-O7-C5     |
| 24  | C     | 512 | CLA  | C3-C5-C6-C7     |
| 29  | c     | 521 | LMG  | C16-C17-C18-C19 |
| 32  | C     | 517 | DGD  | C7B-C8B-C9B-CAB |
| 32  | c     | 517 | DGD  | C6A-C7A-C8A-C9A |
| 33  | c     | 520 | STE  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | c     | 508 | CLA  | O1D-CGD-O2D-CED |
| 29  | D     | 410 | LMG  | C30-C31-C32-C33 |
| 29  | c     | 521 | LMG  | C31-C32-C33-C34 |
| 31  | A     | 617 | SQD  | C10-C11-C12-C13 |
| 32  | C     | 516 | DGD  | C8A-C9A-CAA-CBA |
| 29  | D     | 410 | LMG  | C28-C29-C30-C31 |
| 32  | c     | 517 | DGD  | C1B-C2B-C3B-C4B |
| 29  | b     | 623 | LMG  | C37-C38-C39-C40 |
| 30  | d     | 409 | LHG  | C32-C33-C34-C35 |
| 31  | A     | 616 | SQD  | C9-C10-C11-C12  |
| 31  | B     | 623 | SQD  | C34-C35-C36-C37 |
| 33  | a     | 617 | STE  | C10-C11-C12-C13 |
| 30  | B     | 622 | LHG  | C29-C30-C31-C32 |
| 30  | e     | 102 | LHG  | C26-C27-C28-C29 |
| 32  | C     | 516 | DGD  | CCB-CDB-CEB-CFB |
| 33  | a     | 617 | STE  | C5-C6-C7-C8     |
| 29  | D     | 410 | LMG  | C16-C17-C18-C19 |
| 31  | a     | 613 | SQD  | C29-C30-C31-C32 |
| 32  | C     | 517 | DGD  | C5A-C6A-C7A-C8A |
| 26  | B     | 619 | BCR  | C10-C11-C12-C13 |
| 24  | B     | 612 | CLA  | C10-C11-C12-C13 |
| 28  | A     | 612 | PL9  | C18-C19-C21-C22 |
| 29  | a     | 618 | LMG  | C13-C14-C15-C16 |
| 29  | b     | 621 | LMG  | C17-C18-C19-C20 |
| 31  | b     | 620 | SQD  | C25-C26-C27-C28 |
| 33  | H     | 103 | STE  | C2-C3-C4-C5     |
| 33  | j     | 101 | STE  | C4-C5-C6-C7     |
| 33  | x     | 102 | STE  | C6-C7-C8-C9     |
| 31  | a     | 613 | SQD  | C24-C23-O48-C46 |
| 24  | B     | 606 | CLA  | C11-C12-C13-C14 |
| 24  | C     | 503 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 607 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 511 | CLA  | C14-C13-C15-C16 |
| 25  | A     | 607 | PHO  | C6-C7-C8-C9     |
| 29  | M     | 101 | LMG  | C17-C18-C19-C20 |
| 30  | d     | 407 | LHG  | C30-C31-C32-C33 |
| 32  | c     | 516 | DGD  | C5B-C6B-C7B-C8B |
| 33  | B     | 620 | STE  | C11-C12-C13-C14 |
| 24  | B     | 603 | CLA  | C8-C10-C11-C12  |
| 30  | A     | 615 | LHG  | C27-C28-C29-C30 |
| 30  | l     | 101 | LHG  | C14-C15-C16-C17 |
| 26  | b     | 617 | BCR  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | b     | 623 | LMG  | C21-C22-C23-C24 |
| 29  | d     | 410 | LMG  | C30-C31-C32-C33 |
| 30  | D     | 408 | LHG  | C11-C12-C13-C14 |
| 33  | J     | 101 | STE  | C5-C6-C7-C8     |
| 33  | c     | 520 | STE  | C9-C10-C11-C12  |
| 31  | D     | 407 | SQD  | C2-C1-O6-C44    |
| 24  | C     | 510 | CLA  | CBD-CGD-O2D-CED |
| 29  | A     | 614 | LMG  | C31-C32-C33-C34 |
| 30  | D     | 408 | LHG  | C34-C35-C36-C37 |
| 30  | d     | 408 | LHG  | C33-C34-C35-C36 |
| 32  | C     | 517 | DGD  | CAB-CBB-CCB-CDB |
| 33  | B     | 626 | STE  | C14-C15-C16-C17 |
| 33  | b     | 625 | STE  | C5-C6-C7-C8     |
| 33  | d     | 412 | STE  | C9-C10-C11-C12  |
| 29  | D     | 406 | LMG  | C17-C18-C19-C20 |
| 30  | B     | 622 | LHG  | C27-C28-C29-C30 |
| 32  | c     | 516 | DGD  | C2A-C3A-C4A-C5A |
| 32  | c     | 518 | DGD  | C3A-C4A-C5A-C6A |
| 33  | x     | 102 | STE  | C3-C4-C5-C6     |
| 29  | C     | 519 | LMG  | C32-C33-C34-C35 |
| 29  | b     | 623 | LMG  | C41-C42-C43-C44 |
| 32  | A     | 618 | DGD  | C4B-C5B-C6B-C7B |
| 32  | C     | 517 | DGD  | C9A-CAA-CBA-CCA |
| 32  | H     | 102 | DGD  | C5B-C6B-C7B-C8B |
| 33  | B     | 626 | STE  | C5-C6-C7-C8     |
| 24  | D     | 403 | CLA  | C16-C17-C18-C20 |
| 32  | A     | 618 | DGD  | C2A-C3A-C4A-C5A |
| 33  | H     | 103 | STE  | C10-C11-C12-C13 |
| 30  | B     | 621 | LHG  | C14-C15-C16-C17 |
| 30  | e     | 102 | LHG  | C13-C14-C15-C16 |
| 24  | b     | 602 | CLA  | C8-C10-C11-C12  |
| 31  | f     | 101 | SQD  | O49-C7-O47-C45  |
| 29  | D     | 406 | LMG  | C32-C33-C34-C35 |
| 29  | c     | 519 | LMG  | C36-C37-C38-C39 |
| 30  | B     | 622 | LHG  | C14-C15-C16-C17 |
| 30  | d     | 407 | LHG  | C25-C26-C27-C28 |
| 33  | T     | 103 | STE  | C14-C15-C16-C17 |
| 29  | C     | 519 | LMG  | C15-C16-C17-C18 |
| 30  | A     | 615 | LHG  | C9-C10-C11-C12  |
| 31  | D     | 407 | SQD  | C31-C32-C33-C34 |
| 26  | k     | 101 | BCR  | C37-C22-C23-C24 |
| 30  | d     | 408 | LHG  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | a     | 618 | LMG  | C8-C7-O1-C1     |
| 30  | D     | 408 | LHG  | C25-C26-C27-C28 |
| 32  | h     | 101 | DGD  | CCA-CDA-CEA-CFA |
| 33  | d     | 411 | STE  | C10-C11-C12-C13 |
| 24  | b     | 616 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 616 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 510 | CLA  | C16-C17-C18-C20 |
| 24  | c     | 512 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 512 | CLA  | C16-C17-C18-C20 |
| 29  | A     | 614 | LMG  | C16-C17-C18-C19 |
| 29  | A     | 614 | LMG  | C36-C37-C38-C39 |
| 29  | b     | 623 | LMG  | C23-C24-C25-C26 |
| 29  | c     | 522 | LMG  | C15-C16-C17-C18 |
| 30  | e     | 102 | LHG  | C16-C17-C18-C19 |
| 33  | a     | 617 | STE  | C12-C13-C14-C15 |
| 29  | M     | 101 | LMG  | C11-C12-C13-C14 |
| 31  | D     | 407 | SQD  | C32-C33-C34-C35 |
| 31  | a     | 613 | SQD  | C17-C18-C19-C20 |
| 33  | B     | 620 | STE  | C9-C10-C11-C12  |
| 33  | C     | 522 | STE  | C6-C7-C8-C9     |
| 33  | b     | 625 | STE  | C7-C8-C9-C10    |
| 32  | h     | 101 | DGD  | C2B-C3B-C4B-C5B |
| 30  | B     | 621 | LHG  | C29-C30-C31-C32 |
| 24  | A     | 613 | CLA  | C13-C15-C16-C17 |
| 29  | b     | 621 | LMG  | C12-C13-C14-C15 |
| 31  | a     | 614 | SQD  | C11-C12-C13-C14 |
| 33  | d     | 411 | STE  | C11-C12-C13-C14 |
| 29  | b     | 621 | LMG  | O9-C10-O7-C8    |
| 29  | b     | 623 | LMG  | O6-C5-C6-O5     |
| 29  | c     | 521 | LMG  | C14-C15-C16-C17 |
| 29  | c     | 522 | LMG  | C33-C34-C35-C36 |
| 32  | H     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 24  | b     | 609 | CLA  | CBD-CGD-O2D-CED |
| 24  | A     | 613 | CLA  | C15-C16-C17-C18 |
| 24  | C     | 509 | CLA  | C16-C17-C18-C20 |
| 30  | e     | 102 | LHG  | C11-C10-C9-C8   |
| 33  | B     | 627 | STE  | C5-C6-C7-C8     |
| 29  | A     | 614 | LMG  | C33-C34-C35-C36 |
| 32  | c     | 518 | DGD  | C8B-C9B-CAB-CBB |
| 24  | C     | 513 | CLA  | C5-C6-C7-C8     |
| 24  | b     | 604 | CLA  | C5-C6-C7-C8     |
| 29  | M     | 101 | LMG  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | c     | 522 | LMG  | C30-C31-C32-C33 |
| 31  | B     | 623 | SQD  | C28-C29-C30-C31 |
| 33  | E     | 102 | STE  | C3-C4-C5-C6     |
| 29  | D     | 406 | LMG  | O6-C5-C6-O5     |
| 31  | A     | 616 | SQD  | O6-C44-C45-O47  |
| 32  | A     | 618 | DGD  | O2G-C2G-C3G-O3G |
| 29  | c     | 522 | LMG  | C37-C38-C39-C40 |
| 33  | t     | 102 | STE  | C7-C8-C9-C10    |
| 33  | t     | 102 | STE  | C11-C12-C13-C14 |
| 29  | D     | 409 | LMG  | C31-C32-C33-C34 |
| 30  | A     | 615 | LHG  | C30-C31-C32-C33 |
| 33  | t     | 102 | STE  | C4-C5-C6-C7     |
| 24  | b     | 607 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 507 | CLA  | C5-C6-C7-C8     |
| 29  | D     | 409 | LMG  | C14-C15-C16-C17 |
| 30  | e     | 102 | LHG  | C27-C28-C29-C30 |
| 33  | T     | 103 | STE  | C11-C10-C9-C8   |
| 33  | B     | 624 | STE  | C11-C10-C9-C8   |
| 24  | B     | 605 | CLA  | C3-C5-C6-C7     |
| 24  | B     | 616 | CLA  | C3-C5-C6-C7     |
| 29  | b     | 623 | LMG  | C16-C17-C18-C19 |
| 29  | c     | 522 | LMG  | C17-C18-C19-C20 |
| 30  | e     | 102 | LHG  | C18-C19-C20-C21 |
| 32  | C     | 517 | DGD  | C4A-C5A-C6A-C7A |
| 32  | h     | 101 | DGD  | C3B-C4B-C5B-C6B |
| 33  | T     | 103 | STE  | C6-C7-C8-C9     |
| 28  | a     | 611 | PL9  | C42-C43-C44-C45 |
| 30  | d     | 408 | LHG  | C28-C29-C30-C31 |
| 32  | A     | 618 | DGD  | C5A-C6A-C7A-C8A |
| 33  | b     | 622 | STE  | C7-C8-C9-C10    |
| 32  | H     | 102 | DGD  | C7B-C8B-C9B-CAB |
| 32  | A     | 618 | DGD  | CAA-CBA-CCA-CDA |
| 29  | C     | 519 | LMG  | C16-C17-C18-C19 |
| 30  | l     | 101 | LHG  | C27-C28-C29-C30 |
| 29  | b     | 623 | LMG  | O10-C28-O8-C9   |
| 29  | a     | 618 | LMG  | C35-C36-C37-C38 |
| 24  | c     | 513 | CLA  | C1A-C2A-CAA-CBA |
| 32  | C     | 517 | DGD  | CBA-CCA-CDA-CEA |
| 32  | h     | 101 | DGD  | C7A-C8A-C9A-CAA |
| 33  | D     | 411 | STE  | C5-C6-C7-C8     |
| 29  | b     | 621 | LMG  | C16-C17-C18-C19 |
| 29  | b     | 621 | LMG  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | B     | 622 | LHG  | C28-C29-C30-C31 |
| 33  | b     | 622 | STE  | C5-C6-C7-C8     |
| 30  | B     | 621 | LHG  | O6-C4-C5-C6     |
| 32  | C     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 29  | C     | 519 | LMG  | O9-C10-O7-C8    |
| 29  | c     | 522 | LMG  | O9-C10-O7-C8    |
| 30  | B     | 621 | LHG  | C27-C28-C29-C30 |
| 32  | A     | 618 | DGD  | CEB-CFB-CGB-CHB |
| 32  | C     | 518 | DGD  | CBA-CCA-CDA-CEA |
| 32  | c     | 517 | DGD  | C7A-C8A-C9A-CAA |
| 33  | b     | 627 | STE  | C10-C11-C12-C13 |
| 24  | A     | 605 | CLA  | C11-C12-C13-C15 |
| 24  | B     | 603 | CLA  | C12-C13-C15-C16 |
| 24  | C     | 507 | CLA  | C11-C10-C8-C7   |
| 24  | C     | 510 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 607 | CLA  | C6-C7-C8-C10    |
| 24  | c     | 505 | CLA  | C12-C13-C15-C16 |
| 24  | c     | 513 | CLA  | C11-C12-C13-C15 |
| 24  | d     | 401 | CLA  | C11-C10-C8-C7   |
| 24  | d     | 404 | CLA  | C11-C12-C13-C15 |
| 24  | d     | 404 | CLA  | C12-C13-C15-C16 |
| 30  | E     | 101 | LHG  | C11-C12-C13-C14 |
| 24  | B     | 616 | CLA  | C11-C12-C13-C15 |
| 24  | b     | 615 | CLA  | C16-C17-C18-C19 |
| 24  | B     | 608 | CLA  | C15-C16-C17-C18 |
| 24  | C     | 509 | CLA  | C5-C6-C7-C8     |
| 32  | c     | 517 | DGD  | C1A-C2A-C3A-C4A |
| 28  | D     | 405 | PL9  | C45-C44-C46-C47 |
| 24  | c     | 505 | CLA  | C2-C3-C5-C6     |
| 24  | A     | 605 | CLA  | C11-C12-C13-C14 |
| 24  | B     | 604 | CLA  | C11-C12-C13-C14 |
| 24  | C     | 510 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 604 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 607 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 609 | CLA  | C14-C13-C15-C16 |
| 24  | c     | 506 | CLA  | C6-C7-C8-C9     |
| 24  | c     | 506 | CLA  | C11-C12-C13-C14 |
| 24  | d     | 404 | CLA  | C14-C13-C15-C16 |
| 29  | D     | 409 | LMG  | C15-C16-C17-C18 |
| 29  | D     | 409 | LMG  | C16-C17-C18-C19 |
| 30  | B     | 621 | LHG  | C34-C35-C36-C37 |
| 29  | D     | 406 | LMG  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | B     | 625 | STE  | C3-C4-C5-C6     |
| 24  | c     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 28  | a     | 611 | PL9  | C17-C18-C19-C20 |
| 33  | E     | 102 | STE  | C4-C5-C6-C7     |
| 29  | a     | 618 | LMG  | O9-C10-O7-C8    |
| 24  | B     | 605 | CLA  | C8-C10-C11-C12  |
| 24  | b     | 615 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 617 | SQD  | C9-C10-C11-C12  |
| 29  | M     | 101 | LMG  | C7-C8-C9-O8     |
| 29  | c     | 521 | LMG  | O1-C7-C8-C9     |
| 29  | c     | 522 | LMG  | O1-C7-C8-C9     |
| 31  | A     | 616 | SQD  | O6-C44-C45-C46  |
| 31  | B     | 623 | SQD  | O6-C44-C45-C46  |
| 31  | b     | 620 | SQD  | C44-C45-C46-O48 |
| 32  | A     | 618 | DGD  | C1G-C2G-C3G-O3G |
| 29  | C     | 519 | LMG  | C17-C18-C19-C20 |
| 30  | E     | 101 | LHG  | C16-C17-C18-C19 |
| 30  | E     | 101 | LHG  | C32-C33-C34-C35 |
| 32  | C     | 517 | DGD  | C6A-C7A-C8A-C9A |
| 32  | c     | 516 | DGD  | CBB-CCB-CDB-CEB |
| 29  | c     | 521 | LMG  | C11-C12-C13-C14 |
| 24  | b     | 609 | CLA  | C15-C16-C17-C18 |
| 30  | D     | 408 | LHG  | C28-C29-C30-C31 |
| 32  | C     | 518 | DGD  | CAB-CBB-CCB-CDB |
| 32  | c     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 24  | B     | 607 | CLA  | C16-C17-C18-C19 |
| 24  | B     | 613 | CLA  | C16-C17-C18-C20 |
| 31  | b     | 620 | SQD  | C27-C28-C29-C30 |
| 33  | d     | 412 | STE  | C12-C13-C14-C15 |
| 30  | D     | 408 | LHG  | C17-C18-C19-C20 |
| 32  | c     | 517 | DGD  | C8B-C9B-CAB-CBB |
| 33  | T     | 102 | STE  | C9-C10-C11-C12  |
| 29  | D     | 406 | LMG  | C34-C35-C36-C37 |
| 32  | C     | 518 | DGD  | C5A-C6A-C7A-C8A |
| 26  | D     | 404 | BCR  | C11-C10-C9-C34  |
| 24  | b     | 601 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 623 | SQD  | C35-C36-C37-C38 |
| 33  | B     | 620 | STE  | C2-C3-C4-C5     |
| 33  | b     | 622 | STE  | C10-C11-C12-C13 |
| 30  | d     | 407 | LHG  | C14-C15-C16-C17 |
| 24  | C     | 505 | CLA  | C4-C3-C5-C6     |
| 24  | c     | 505 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | C     | 505 | CLA  | C2-C3-C5-C6     |
| 28  | a     | 611 | PL9  | C38-C39-C41-C42 |
| 24  | D     | 402 | CLA  | C10-C11-C12-C13 |
| 24  | b     | 614 | CLA  | C15-C16-C17-C18 |
| 26  | k     | 101 | BCR  | C36-C18-C19-C20 |
| 33  | T     | 103 | STE  | C11-C12-C13-C14 |
| 33  | a     | 617 | STE  | C11-C12-C13-C14 |
| 24  | b     | 601 | CLA  | C10-C11-C12-C13 |
| 29  | b     | 623 | LMG  | C32-C33-C34-C35 |
| 30  | A     | 615 | LHG  | C25-C26-C27-C28 |
| 32  | C     | 516 | DGD  | C3A-C4A-C5A-C6A |
| 33  | d     | 412 | STE  | C2-C3-C4-C5     |
| 29  | C     | 519 | LMG  | C30-C31-C32-C33 |
| 31  | B     | 623 | SQD  | C9-C10-C11-C12  |
| 30  | B     | 621 | LHG  | C7-C8-C9-C10    |
| 31  | a     | 613 | SQD  | C23-C24-C25-C26 |
| 29  | a     | 618 | LMG  | C30-C31-C32-C33 |
| 32  | c     | 516 | DGD  | C6B-C7B-C8B-C9B |
| 24  | C     | 513 | CLA  | O2A-C1-C2-C3    |
| 29  | a     | 618 | LMG  | C9-C8-O7-C10    |
| 29  | M     | 101 | LMG  | C31-C32-C33-C34 |
| 32  | C     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 24  | C     | 506 | CLA  | C13-C15-C16-C17 |
| 24  | C     | 509 | CLA  | C8-C10-C11-C12  |
| 31  | a     | 613 | SQD  | C18-C19-C20-C21 |
| 32  | A     | 618 | DGD  | C9B-CAB-CBB-CCB |
| 32  | C     | 517 | DGD  | C9B-CAB-CBB-CCB |
| 33  | B     | 627 | STE  | C2-C3-C4-C5     |
| 26  | T     | 101 | BCR  | C13-C14-C15-C16 |
| 24  | C     | 507 | CLA  | C16-C17-C18-C20 |
| 32  | C     | 516 | DGD  | C8B-C9B-CAB-CBB |
| 33  | M     | 102 | STE  | C9-C10-C11-C12  |
| 26  | a     | 607 | BCR  | C12-C13-C14-C15 |
| 26  | c     | 514 | BCR  | C16-C17-C18-C19 |
| 24  | d     | 404 | CLA  | C13-C15-C16-C17 |
| 29  | b     | 621 | LMG  | C37-C38-C39-C40 |
| 33  | C     | 522 | STE  | C5-C6-C7-C8     |
| 31  | D     | 407 | SQD  | C30-C31-C32-C33 |
| 33  | b     | 622 | STE  | C13-C14-C15-C16 |
| 31  | a     | 614 | SQD  | C31-C32-C33-C34 |
| 29  | b     | 621 | LMG  | C39-C40-C41-C42 |
| 31  | A     | 616 | SQD  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | C     | 521 | STE  | C4-C5-C6-C7     |
| 24  | B     | 610 | CLA  | C15-C16-C17-C18 |
| 30  | B     | 622 | LHG  | C19-C20-C21-C22 |
| 32  | C     | 518 | DGD  | CDA-CEA-CFA-CGA |
| 29  | b     | 621 | LMG  | C11-C12-C13-C14 |
| 31  | A     | 617 | SQD  | C16-C17-C18-C19 |
| 32  | A     | 618 | DGD  | C2B-C3B-C4B-C5B |
| 33  | B     | 626 | STE  | C6-C7-C8-C9     |
| 29  | A     | 614 | LMG  | C34-C35-C36-C37 |
| 29  | c     | 521 | LMG  | C34-C35-C36-C37 |
| 29  | c     | 521 | LMG  | C38-C39-C40-C41 |
| 33  | d     | 411 | STE  | C5-C6-C7-C8     |
| 29  | a     | 618 | LMG  | C33-C34-C35-C36 |
| 29  | c     | 522 | LMG  | C31-C32-C33-C34 |
| 30  | d     | 408 | LHG  | C12-C13-C14-C15 |
| 33  | J     | 101 | STE  | C6-C7-C8-C9     |
| 33  | Z     | 101 | STE  | C12-C13-C14-C15 |
| 33  | a     | 615 | STE  | C5-C6-C7-C8     |
| 31  | a     | 613 | SQD  | O47-C45-C46-O48 |
| 30  | E     | 101 | LHG  | O2-C2-C3-O3     |
| 30  | B     | 621 | LHG  | C30-C31-C32-C33 |
| 30  | B     | 622 | LHG  | C18-C19-C20-C21 |
| 33  | b     | 626 | STE  | C4-C5-C6-C7     |
| 29  | b     | 621 | LMG  | C22-C23-C24-C25 |
| 30  | l     | 101 | LHG  | C13-C14-C15-C16 |
| 32  | c     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 33  | m     | 101 | STE  | C7-C8-C9-C10    |
| 31  | B     | 623 | SQD  | C13-C14-C15-C16 |
| 32  | C     | 518 | DGD  | CCA-CDA-CEA-CFA |
| 33  | a     | 615 | STE  | C2-C3-C4-C5     |
| 31  | A     | 616 | SQD  | C17-C18-C19-C20 |
| 32  | c     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 24  | C     | 507 | CLA  | C10-C11-C12-C13 |
| 33  | b     | 625 | STE  | C3-C4-C5-C6     |
| 24  | b     | 601 | CLA  | C16-C17-C18-C19 |
| 32  | C     | 517 | DGD  | CDB-CEB-CFB-CGB |
| 33  | B     | 625 | STE  | C7-C8-C9-C10    |
| 24  | b     | 609 | CLA  | O1D-CGD-O2D-CED |
| 24  | c     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 30  | E     | 101 | LHG  | C19-C20-C21-C22 |
| 33  | C     | 521 | STE  | C3-C4-C5-C6     |
| 31  | D     | 407 | SQD  | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | a     | 613 | SQD  | C27-C28-C29-C30 |
| 32  | C     | 516 | DGD  | C2A-C3A-C4A-C5A |
| 33  | d     | 412 | STE  | C6-C7-C8-C9     |
| 29  | C     | 519 | LMG  | C29-C28-O8-C9   |
| 29  | a     | 618 | LMG  | C16-C17-C18-C19 |
| 29  | c     | 519 | LMG  | C31-C32-C33-C34 |
| 32  | c     | 518 | DGD  | C4B-C5B-C6B-C7B |
| 32  | c     | 518 | DGD  | C5B-C6B-C7B-C8B |
| 32  | H     | 102 | DGD  | CDB-CEB-CFB-CGB |
| 31  | b     | 620 | SQD  | C11-C12-C13-C14 |
| 32  | h     | 101 | DGD  | CBA-CCA-CDA-CEA |
| 24  | C     | 512 | CLA  | C8-C10-C11-C12  |
| 32  | c     | 516 | DGD  | O1A-C1A-O1G-C1G |
| 29  | b     | 621 | LMG  | C38-C39-C40-C41 |
| 30  | d     | 407 | LHG  | C28-C29-C30-C31 |
| 24  | B     | 604 | CLA  | C2C-C3C-CAC-CBC |
| 32  | C     | 517 | DGD  | C6B-C7B-C8B-C9B |
| 24  | c     | 510 | CLA  | C8-C10-C11-C12  |
| 24  | B     | 616 | CLA  | C11-C12-C13-C14 |
| 28  | d     | 406 | PL9  | C45-C44-C46-C47 |
| 29  | A     | 614 | LMG  | C40-C41-C42-C43 |
| 29  | c     | 522 | LMG  | C8-C9-O8-C28    |
| 29  | C     | 519 | LMG  | C31-C32-C33-C34 |
| 29  | D     | 406 | LMG  | C21-C22-C23-C24 |
| 29  | D     | 409 | LMG  | C34-C35-C36-C37 |
| 29  | b     | 623 | LMG  | C42-C43-C44-C45 |
| 30  | e     | 102 | LHG  | C28-C29-C30-C31 |
| 33  | T     | 102 | STE  | C15-C16-C17-C18 |
| 30  | d     | 407 | LHG  | C15-C16-C17-C18 |
| 32  | C     | 518 | DGD  | C8B-C9B-CAB-CBB |
| 33  | d     | 412 | STE  | C5-C6-C7-C8     |
| 29  | a     | 618 | LMG  | C34-C35-C36-C37 |
| 30  | D     | 408 | LHG  | C33-C34-C35-C36 |
| 32  | C     | 516 | DGD  | C9B-CAB-CBB-CCB |
| 33  | b     | 624 | STE  | C6-C7-C8-C9     |
| 30  | d     | 409 | LHG  | O1-C1-C2-O2     |
| 31  | D     | 407 | SQD  | C45-C44-O6-C1   |
| 24  | A     | 613 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 603 | CLA  | C14-C13-C15-C16 |
| 24  | C     | 509 | CLA  | C11-C12-C13-C14 |
| 24  | D     | 402 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 606 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 607 | CLA  | C6-C7-C8-C9     |
| 24  | b     | 607 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 615 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 510 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 513 | CLA  | C11-C12-C13-C14 |
| 24  | d     | 401 | CLA  | C11-C10-C8-C9   |
| 24  | d     | 401 | CLA  | C14-C13-C15-C16 |
| 24  | d     | 404 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 612 | CLA  | C10-C11-C12-C13 |
| 24  | c     | 504 | CLA  | C5-C6-C7-C8     |
| 24  | B     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 24  | d     | 401 | CLA  | C4B-C3B-CAB-CBB |
| 29  | b     | 623 | LMG  | C22-C23-C24-C25 |
| 33  | b     | 625 | STE  | C11-C10-C9-C8   |
| 24  | C     | 510 | CLA  | O1D-CGD-O2D-CED |
| 29  | c     | 519 | LMG  | O6-C5-C6-O5     |
| 24  | C     | 507 | CLA  | C16-C17-C18-C19 |
| 24  | b     | 615 | CLA  | C16-C17-C18-C20 |
| 29  | a     | 618 | LMG  | C17-C18-C19-C20 |
| 29  | D     | 406 | LMG  | C38-C39-C40-C41 |
| 31  | A     | 617 | SQD  | C14-C15-C16-C17 |
| 33  | C     | 520 | STE  | C2-C3-C4-C5     |
| 33  | I     | 101 | STE  | C4-C5-C6-C7     |
| 33  | Z     | 101 | STE  | C13-C14-C15-C16 |
| 24  | C     | 509 | CLA  | C3-C5-C6-C7     |
| 31  | a     | 614 | SQD  | C19-C20-C21-C22 |
| 31  | b     | 620 | SQD  | C19-C20-C21-C22 |
| 30  | e     | 102 | LHG  | O6-C4-C5-C6     |
| 29  | b     | 623 | LMG  | C18-C19-C20-C21 |
| 30  | B     | 622 | LHG  | C25-C26-C27-C28 |
| 32  | H     | 102 | DGD  | CCA-CDA-CEA-CFA |
| 29  | D     | 406 | LMG  | C14-C15-C16-C17 |
| 24  | B     | 604 | CLA  | C11-C12-C13-C15 |
| 24  | B     | 613 | CLA  | C12-C13-C15-C16 |
| 24  | C     | 509 | CLA  | C11-C12-C13-C15 |
| 24  | C     | 512 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 601 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 604 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 607 | CLA  | C11-C12-C13-C15 |
| 24  | b     | 614 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 615 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 505 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | c     | 506 | CLA  | C6-C7-C8-C10    |
| 24  | c     | 506 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 509 | CLA  | C6-C7-C8-C10    |
| 24  | c     | 512 | CLA  | C12-C13-C15-C16 |
| 24  | d     | 401 | CLA  | C12-C13-C15-C16 |
| 24  | C     | 512 | CLA  | C15-C16-C17-C18 |
| 24  | b     | 604 | CLA  | C13-C15-C16-C17 |
| 31  | D     | 407 | SQD  | O6-C44-C45-C46  |
| 29  | A     | 614 | LMG  | C30-C31-C32-C33 |
| 32  | h     | 101 | DGD  | C5A-C6A-C7A-C8A |
| 30  | d     | 408 | LHG  | O9-C7-O7-C5     |
| 32  | c     | 517 | DGD  | C5B-C6B-C7B-C8B |
| 32  | h     | 101 | DGD  | CAB-CBB-CCB-CDB |
| 30  | E     | 101 | LHG  | C29-C30-C31-C32 |
| 31  | a     | 613 | SQD  | C28-C29-C30-C31 |
| 28  | a     | 611 | PL9  | C45-C44-C46-C47 |
| 29  | c     | 519 | LMG  | C4-C5-C6-O5     |
| 24  | D     | 403 | CLA  | C5-C6-C7-C8     |
| 32  | C     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 30  | e     | 102 | LHG  | C10-C11-C12-C13 |
| 33  | M     | 102 | STE  | C4-C5-C6-C7     |
| 24  | a     | 606 | CLA  | CBA-CGA-O2A-C1  |
| 26  | T     | 101 | BCR  | C9-C10-C11-C12  |
| 32  | C     | 516 | DGD  | CDA-CEA-CFA-CGA |
| 33  | T     | 102 | STE  | C3-C4-C5-C6     |
| 29  | M     | 101 | LMG  | C39-C40-C41-C42 |
| 29  | a     | 618 | LMG  | C23-C24-C25-C26 |
| 33  | l     | 102 | STE  | C2-C3-C4-C5     |
| 26  | k     | 101 | BCR  | C17-C18-C19-C20 |
| 29  | b     | 621 | LMG  | C20-C21-C22-C23 |
| 32  | C     | 516 | DGD  | CBA-CCA-CDA-CEA |
| 30  | E     | 101 | LHG  | C4-C5-C6-O8     |
| 31  | a     | 613 | SQD  | O6-C44-C45-C46  |
| 31  | a     | 613 | SQD  | C44-C45-C46-O48 |
| 32  | A     | 618 | DGD  | O1G-C1G-C2G-C3G |
| 32  | c     | 516 | DGD  | O1G-C1G-C2G-C3G |
| 29  | M     | 101 | LMG  | C38-C39-C40-C41 |
| 30  | D     | 408 | LHG  | C11-C10-C9-C8   |
| 33  | E     | 102 | STE  | C6-C7-C8-C9     |
| 30  | e     | 102 | LHG  | C14-C15-C16-C17 |
| 32  | c     | 517 | DGD  | C9B-CAB-CBB-CCB |
| 32  | C     | 517 | DGD  | CDA-CEA-CFA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | A     | 605 | CLA  | C16-C17-C18-C19 |
| 29  | C     | 519 | LMG  | C12-C13-C14-C15 |
| 32  | C     | 517 | DGD  | C3A-C4A-C5A-C6A |
| 33  | b     | 622 | STE  | C4-C5-C6-C7     |
| 33  | b     | 624 | STE  | C11-C10-C9-C8   |
| 33  | T     | 103 | STE  | C7-C8-C9-C10    |
| 28  | a     | 611 | PL9  | C40-C39-C41-C42 |
| 33  | j     | 101 | STE  | C1-C2-C3-C4     |
| 33  | j     | 101 | STE  | C2-C3-C4-C5     |
| 24  | c     | 511 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 617 | SQD  | C31-C32-C33-C34 |
| 31  | a     | 614 | SQD  | C17-C18-C19-C20 |
| 24  | B     | 604 | CLA  | C16-C17-C18-C20 |
| 30  | B     | 621 | LHG  | O9-C7-O7-C5     |
| 24  | d     | 401 | CLA  | C2B-C3B-CAB-CBB |
| 26  | B     | 617 | BCR  | C1-C6-C7-C8     |
| 26  | k     | 102 | BCR  | C1-C6-C7-C8     |
| 32  | c     | 517 | DGD  | C5A-C6A-C7A-C8A |
| 31  | a     | 613 | SQD  | C11-C10-C9-C8   |
| 33  | b     | 625 | STE  | C6-C7-C8-C9     |
| 24  | B     | 613 | CLA  | C10-C11-C12-C13 |
| 33  | l     | 102 | STE  | C1-C2-C3-C4     |
| 30  | d     | 407 | LHG  | C32-C33-C34-C35 |
| 32  | C     | 518 | DGD  | C3A-C4A-C5A-C6A |
| 31  | A     | 616 | SQD  | C24-C25-C26-C27 |
| 33  | d     | 412 | STE  | C4-C5-C6-C7     |
| 24  | c     | 504 | CLA  | C11-C12-C13-C15 |
| 29  | c     | 521 | LMG  | O1-C7-C8-O7     |
| 29  | c     | 521 | LMG  | O7-C8-C9-O8     |
| 29  | c     | 522 | LMG  | O1-C7-C8-O7     |
| 31  | b     | 620 | SQD  | O6-C44-C45-O47  |
| 29  | b     | 623 | LMG  | C24-C25-C26-C27 |
| 28  | a     | 611 | PL9  | C4-C3-C7-C8     |
| 30  | l     | 101 | LHG  | C32-C33-C34-C35 |
| 29  | M     | 101 | LMG  | C40-C41-C42-C43 |
| 30  | A     | 615 | LHG  | C11-C10-C9-C8   |
| 33  | D     | 411 | STE  | C12-C13-C14-C15 |
| 26  | c     | 514 | BCR  | C10-C11-C12-C13 |
| 24  | B     | 602 | CLA  | C8-C10-C11-C12  |
| 30  | B     | 621 | LHG  | C10-C11-C12-C13 |
| 32  | C     | 518 | DGD  | C3B-C4B-C5B-C6B |
| 29  | D     | 406 | LMG  | C39-C40-C41-C42 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | A     | 615 | LHG  | C33-C34-C35-C36 |
| 24  | b     | 616 | CLA  | O1D-CGD-O2D-CED |
| 24  | B     | 604 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 613 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 615 | CLA  | C11-C12-C13-C14 |
| 24  | C     | 506 | CLA  | C14-C13-C15-C16 |
| 24  | C     | 508 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 512 | CLA  | C14-C13-C15-C16 |
| 30  | B     | 621 | LHG  | C11-C12-C13-C14 |
| 26  | A     | 609 | BCR  | C14-C15-C16-C17 |
| 29  | d     | 410 | LMG  | C38-C39-C40-C41 |
| 33  | H     | 103 | STE  | C9-C10-C11-C12  |
| 30  | D     | 408 | LHG  | C29-C30-C31-C32 |
| 33  | l     | 102 | STE  | C7-C8-C9-C10    |
| 24  | c     | 513 | CLA  | C13-C15-C16-C17 |
| 29  | D     | 409 | LMG  | C11-C12-C13-C14 |
| 30  | A     | 615 | LHG  | C34-C35-C36-C37 |
| 30  | D     | 408 | LHG  | C10-C11-C12-C13 |
| 31  | A     | 616 | SQD  | C11-C12-C13-C14 |
| 29  | c     | 519 | LMG  | C30-C31-C32-C33 |
| 32  | C     | 518 | DGD  | O1A-C1A-O1G-C1G |
| 33  | d     | 412 | STE  | C1-C2-C3-C4     |
| 32  | A     | 618 | DGD  | CCB-CDB-CEB-CFB |
| 26  | c     | 514 | BCR  | C15-C16-C17-C18 |
| 24  | B     | 615 | CLA  | C16-C17-C18-C19 |
| 32  | A     | 618 | DGD  | CDB-CEB-CFB-CGB |
| 30  | d     | 407 | LHG  | C16-C17-C18-C19 |
| 30  | d     | 408 | LHG  | C26-C27-C28-C29 |
| 33  | x     | 102 | STE  | C2-C3-C4-C5     |
| 33  | b     | 625 | STE  | C10-C11-C12-C13 |
| 24  | b     | 616 | CLA  | C8-C10-C11-C12  |
| 29  | a     | 618 | LMG  | C29-C30-C31-C32 |
| 26  | C     | 514 | BCR  | C16-C17-C18-C36 |
| 26  | k     | 101 | BCR  | C11-C10-C9-C34  |
| 26  | x     | 101 | BCR  | C16-C17-C18-C36 |
| 33  | H     | 103 | STE  | C1-C2-C3-C4     |
| 24  | c     | 509 | CLA  | CAA-CBA-CGA-O2A |
| 29  | D     | 409 | LMG  | C33-C34-C35-C36 |
| 32  | A     | 618 | DGD  | CFA-CGA-CHA-CIA |
| 24  | B     | 610 | CLA  | C16-C17-C18-C19 |
| 29  | a     | 618 | LMG  | C32-C33-C34-C35 |
| 33  | T     | 103 | STE  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | d     | 412 | STE  | C11-C10-C9-C8   |
| 33  | t     | 102 | STE  | C10-C11-C12-C13 |
| 24  | B     | 604 | CLA  | C12-C13-C15-C16 |
| 24  | B     | 605 | CLA  | C11-C10-C8-C7   |
| 24  | B     | 613 | CLA  | C11-C12-C13-C15 |
| 24  | B     | 614 | CLA  | C12-C13-C15-C16 |
| 24  | B     | 615 | CLA  | C11-C12-C13-C15 |
| 24  | C     | 505 | CLA  | C6-C7-C8-C10    |
| 24  | C     | 508 | CLA  | C11-C10-C8-C7   |
| 24  | C     | 510 | CLA  | C11-C10-C8-C7   |
| 24  | C     | 512 | CLA  | C11-C10-C8-C7   |
| 24  | b     | 602 | CLA  | C11-C10-C8-C7   |
| 24  | b     | 609 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 616 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 512 | CLA  | C11-C12-C13-C15 |
| 33  | J     | 101 | STE  | C1-C2-C3-C4     |
| 33  | c     | 520 | STE  | C4-C5-C6-C7     |
| 29  | a     | 618 | LMG  | C19-C20-C21-C22 |
| 29  | a     | 618 | LMG  | C21-C22-C23-C24 |
| 29  | d     | 410 | LMG  | C14-C15-C16-C17 |
| 32  | C     | 517 | DGD  | C8B-C9B-CAB-CBB |
| 33  | d     | 411 | STE  | C7-C8-C9-C10    |
| 24  | b     | 616 | CLA  | CBD-CGD-O2D-CED |
| 33  | M     | 103 | STE  | C1-C2-C3-C4     |
| 26  | K     | 101 | BCR  | C17-C18-C19-C20 |
| 26  | k     | 101 | BCR  | C21-C22-C23-C24 |
| 32  | C     | 517 | DGD  | C2G-C3G-O3G-C1D |
| 32  | C     | 517 | DGD  | C5D-C6D-O5D-C1E |
| 32  | c     | 517 | DGD  | C5D-C6D-O5D-C1E |
| 29  | b     | 623 | LMG  | C34-C35-C36-C37 |
| 31  | A     | 617 | SQD  | C11-C12-C13-C14 |
| 33  | H     | 103 | STE  | C12-C13-C14-C15 |
| 30  | B     | 621 | LHG  | C18-C19-C20-C21 |
| 33  | D     | 411 | STE  | C6-C7-C8-C9     |
| 29  | D     | 410 | LMG  | C34-C35-C36-C37 |
| 24  | c     | 512 | CLA  | C4-C3-C5-C6     |
| 28  | A     | 612 | PL9  | C25-C24-C26-C27 |
| 29  | D     | 410 | LMG  | C37-C38-C39-C40 |
| 30  | d     | 408 | LHG  | C11-C12-C13-C14 |
| 30  | d     | 409 | LHG  | C35-C36-C37-C38 |
| 33  | d     | 411 | STE  | C12-C13-C14-C15 |
| 33  | b     | 627 | STE  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | b     | 623 | LMG  | C19-C20-C21-C22 |
| 24  | b     | 606 | CLA  | C8-C10-C11-C12  |
| 29  | c     | 522 | LMG  | C9-C8-O7-C10    |
| 32  | C     | 517 | DGD  | O1A-C1A-O1G-C1G |
| 30  | E     | 101 | LHG  | C31-C32-C33-C34 |
| 31  | b     | 620 | SQD  | C12-C13-C14-C15 |
| 30  | l     | 101 | LHG  | C19-C20-C21-C22 |
| 30  | D     | 408 | LHG  | C32-C33-C34-C35 |
| 33  | D     | 411 | STE  | C9-C10-C11-C12  |
| 24  | b     | 604 | CLA  | C3-C5-C6-C7     |
| 33  | a     | 616 | STE  | C5-C6-C7-C8     |
| 33  | C     | 520 | STE  | C3-C4-C5-C6     |
| 28  | D     | 405 | PL9  | C47-C48-C49-C51 |
| 30  | l     | 101 | LHG  | O6-C4-C5-O7     |
| 29  | D     | 406 | LMG  | C15-C16-C17-C18 |
| 30  | A     | 615 | LHG  | C17-C18-C19-C20 |
| 28  | d     | 406 | PL9  | C34-C36-C37-C38 |
| 29  | c     | 521 | LMG  | C7-C8-C9-O8     |
| 35  | e     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 24  | B     | 611 | CLA  | C16-C17-C18-C20 |
| 24  | B     | 613 | CLA  | C16-C17-C18-C19 |
| 33  | C     | 521 | STE  | C10-C11-C12-C13 |
| 33  | I     | 101 | STE  | C11-C10-C9-C8   |
| 33  | a     | 617 | STE  | C7-C8-C9-C10    |
| 33  | T     | 102 | STE  | C10-C11-C12-C13 |
| 24  | C     | 506 | CLA  | C4-C3-C5-C6     |
| 28  | D     | 405 | PL9  | C43-C44-C46-C47 |
| 29  | M     | 101 | LMG  | C12-C13-C14-C15 |
| 33  | C     | 521 | STE  | C11-C10-C9-C8   |
| 32  | C     | 517 | DGD  | CBB-CCB-CDB-CEB |
| 33  | B     | 626 | STE  | C9-C10-C11-C12  |
| 24  | B     | 606 | CLA  | C8-C10-C11-C12  |
| 31  | a     | 614 | SQD  | C24-C25-C26-C27 |
| 31  | a     | 614 | SQD  | O47-C45-C46-O48 |
| 32  | A     | 618 | DGD  | O1G-C1G-C2G-O2G |
| 32  | c     | 516 | DGD  | O1G-C1G-C2G-O2G |
| 32  | c     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 24  | B     | 605 | CLA  | C11-C10-C8-C9   |
| 24  | C     | 505 | CLA  | C6-C7-C8-C9     |
| 24  | b     | 609 | CLA  | C6-C7-C8-C9     |
| 24  | c     | 512 | CLA  | C11-C12-C13-C14 |
| 24  | d     | 401 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | B     | 610 | CLA  | C16-C17-C18-C20 |
| 32  | C     | 516 | DGD  | C7A-C8A-C9A-CAA |
| 33  | b     | 622 | STE  | C3-C4-C5-C6     |
| 32  | c     | 516 | DGD  | O1G-C1A-C2A-C3A |
| 29  | b     | 621 | LMG  | C31-C32-C33-C34 |
| 30  | B     | 622 | LHG  | C9-C10-C11-C12  |
| 30  | B     | 622 | LHG  | C32-C33-C34-C35 |
| 31  | f     | 101 | SQD  | C33-C34-C35-C36 |
| 24  | a     | 604 | CLA  | C15-C16-C17-C18 |
| 29  | a     | 618 | LMG  | C22-C23-C24-C25 |
| 29  | b     | 623 | LMG  | C12-C13-C14-C15 |
| 24  | c     | 509 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 609 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 506 | CLA  | C16-C17-C18-C20 |
| 24  | B     | 612 | CLA  | C15-C16-C17-C18 |
| 29  | b     | 623 | LMG  | C20-C21-C22-C23 |
| 33  | l     | 102 | STE  | C4-C5-C6-C7     |
| 28  | D     | 405 | PL9  | C35-C34-C36-C37 |
| 24  | d     | 403 | CLA  | C3-C5-C6-C7     |
| 24  | C     | 506 | CLA  | C2-C3-C5-C6     |
| 33  | a     | 617 | STE  | C13-C14-C15-C16 |
| 32  | A     | 618 | DGD  | CBA-CCA-CDA-CEA |
| 33  | I     | 101 | STE  | C7-C8-C9-C10    |
| 24  | c     | 505 | CLA  | C15-C16-C17-C18 |
| 33  | l     | 102 | STE  | C10-C11-C12-C13 |
| 31  | D     | 407 | SQD  | C29-C30-C31-C32 |
| 33  | D     | 411 | STE  | C11-C10-C9-C8   |
| 28  | A     | 612 | PL9  | C39-C41-C42-C43 |
| 29  | D     | 406 | LMG  | C37-C38-C39-C40 |
| 32  | H     | 102 | DGD  | C5A-C6A-C7A-C8A |
| 32  | c     | 516 | DGD  | CBA-CCA-CDA-CEA |
| 24  | C     | 504 | CLA  | C4B-C3B-CAB-CBB |
| 24  | C     | 508 | CLA  | C1A-C2A-CAA-CBA |
| 24  | b     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 24  | c     | 511 | CLA  | C1A-C2A-CAA-CBA |
| 26  | C     | 514 | BCR  | C9-C10-C11-C12  |
| 33  | I     | 101 | STE  | C2-C3-C4-C5     |
| 30  | d     | 409 | LHG  | C29-C30-C31-C32 |
| 33  | H     | 103 | STE  | C14-C15-C16-C17 |
| 30  | l     | 101 | LHG  | O6-C4-C5-C6     |
| 31  | D     | 407 | SQD  | C33-C34-C35-C36 |
| 31  | A     | 617 | SQD  | O49-C7-O47-C45  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 616 | SQD  | C14-C15-C16-C17 |
| 33  | T     | 103 | STE  | C9-C10-C11-C12  |
| 33  | b     | 624 | STE  | C11-C12-C13-C14 |
| 33  | a     | 615 | STE  | C4-C5-C6-C7     |
| 24  | A     | 605 | CLA  | C11-C10-C8-C7   |
| 24  | A     | 605 | CLA  | C12-C13-C15-C16 |
| 24  | B     | 615 | CLA  | C6-C7-C8-C10    |
| 24  | B     | 616 | CLA  | C6-C7-C8-C10    |
| 24  | C     | 506 | CLA  | C12-C13-C15-C16 |
| 24  | C     | 509 | CLA  | C11-C10-C8-C7   |
| 24  | D     | 403 | CLA  | C11-C10-C8-C7   |
| 24  | D     | 403 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 507 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 512 | CLA  | C6-C7-C8-C10    |
| 24  | d     | 404 | CLA  | C6-C7-C8-C10    |
| 24  | B     | 604 | CLA  | C16-C17-C18-C19 |
| 24  | d     | 404 | CLA  | C16-C17-C18-C19 |
| 32  | H     | 102 | DGD  | CBA-CCA-CDA-CEA |
| 32  | c     | 516 | DGD  | C6A-C7A-C8A-C9A |
| 33  | a     | 617 | STE  | C3-C4-C5-C6     |
| 32  | A     | 618 | DGD  | CEA-CFA-CGA-CHA |
| 24  | c     | 503 | CLA  | CBA-CGA-O2A-C1  |
| 29  | C     | 519 | LMG  | C37-C38-C39-C40 |
| 30  | d     | 407 | LHG  | C29-C30-C31-C32 |
| 33  | C     | 521 | STE  | C12-C13-C14-C15 |
| 31  | B     | 623 | SQD  | C18-C19-C20-C21 |
| 31  | a     | 614 | SQD  | C13-C14-C15-C16 |
| 30  | d     | 409 | LHG  | C27-C28-C29-C30 |
| 36  | v     | 201 | HEC  | C4B-C3B-CAB-CBB |
| 32  | H     | 102 | DGD  | C2B-C3B-C4B-C5B |
| 24  | B     | 615 | CLA  | C5-C6-C7-C8     |
| 24  | b     | 616 | CLA  | C10-C11-C12-C13 |
| 29  | M     | 101 | LMG  | C13-C14-C15-C16 |
| 33  | b     | 625 | STE  | C14-C15-C16-C17 |
| 32  | C     | 518 | DGD  | O6D-C5D-C6D-O5D |
| 24  | C     | 510 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 508 | CLA  | C11-C12-C13-C14 |
| 29  | a     | 618 | LMG  | C37-C38-C39-C40 |
| 29  | a     | 618 | LMG  | C41-C42-C43-C44 |
| 29  | c     | 519 | LMG  | C35-C36-C37-C38 |
| 29  | M     | 101 | LMG  | C35-C36-C37-C38 |
| 30  | d     | 408 | LHG  | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | A     | 605 | CLA  | C15-C16-C17-C18 |
| 24  | c     | 510 | CLA  | C15-C16-C17-C18 |
| 30  | E     | 101 | LHG  | O7-C5-C6-O8     |
| 33  | t     | 102 | STE  | C13-C14-C15-C16 |
| 32  | c     | 518 | DGD  | C5A-C6A-C7A-C8A |
| 29  | a     | 618 | LMG  | O1-C7-C8-C9     |
| 31  | a     | 614 | SQD  | C44-C45-C46-O48 |
| 24  | B     | 607 | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 502 | CLA  | CAD-CBD-CGD-O2D |
| 29  | b     | 621 | LMG  | C4-C5-C6-O5     |
| 24  | a     | 606 | CLA  | O1A-CGA-O2A-C1  |
| 33  | J     | 101 | STE  | C3-C4-C5-C6     |
| 24  | d     | 404 | CLA  | C16-C17-C18-C20 |
| 24  | b     | 604 | CLA  | C8-C10-C11-C12  |
| 33  | b     | 625 | STE  | C11-C12-C13-C14 |
| 30  | A     | 615 | LHG  | C14-C15-C16-C17 |
| 24  | B     | 607 | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 504 | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 507 | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 509 | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 509 | CLA  | CHA-CBD-CGD-O2D |
| 24  | b     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 24  | b     | 616 | CLA  | CHA-CBD-CGD-O2D |
| 24  | c     | 502 | CLA  | CAD-CBD-CGD-O1D |
| 24  | c     | 504 | CLA  | CAD-CBD-CGD-O1D |
| 26  | C     | 514 | BCR  | C13-C14-C15-C16 |
| 26  | d     | 405 | BCR  | C20-C21-C22-C37 |
| 30  | A     | 615 | LHG  | C3-O3-P-O5      |
| 30  | B     | 622 | LHG  | C3-O3-P-O4      |
| 30  | D     | 408 | LHG  | C3-O3-P-O4      |
| 30  | D     | 408 | LHG  | C4-O6-P-O5      |
| 30  | d     | 407 | LHG  | C3-O3-P-O5      |
| 30  | d     | 408 | LHG  | C4-O6-P-O5      |
| 30  | e     | 102 | LHG  | C4-O6-P-O3      |
| 30  | l     | 101 | LHG  | C4-O6-P-O5      |
| 29  | b     | 623 | LMG  | C17-C18-C19-C20 |
| 24  | b     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 26  | d     | 405 | BCR  | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | C     | 518 | DGD  | C4B-C5B-C6B-C7B |
| 28  | A     | 612 | PL9  | C38-C39-C41-C42 |
| 26  | B     | 617 | BCR  | C11-C12-C13-C35 |
| 29  | b     | 621 | LMG  | O6-C5-C6-O5     |
| 30  | d     | 409 | LHG  | C9-C10-C11-C12  |
| 33  | b     | 624 | STE  | C3-C4-C5-C6     |
| 33  | c     | 520 | STE  | C3-C4-C5-C6     |
| 33  | D     | 411 | STE  | C1-C2-C3-C4     |
| 28  | A     | 612 | PL9  | C4-C3-C7-C8     |
| 24  | A     | 605 | CLA  | C16-C17-C18-C20 |
| 29  | b     | 621 | LMG  | C28-C29-C30-C31 |
| 30  | d     | 409 | LHG  | C25-C26-C27-C28 |
| 24  | c     | 503 | CLA  | O1A-CGA-O2A-C1  |
| 24  | C     | 507 | CLA  | C5-C6-C7-C8     |
| 33  | b     | 625 | STE  | C12-C13-C14-C15 |
| 29  | D     | 409 | LMG  | C9-C8-O7-C10    |
| 31  | B     | 623 | SQD  | C46-C45-O47-C7  |
| 31  | b     | 620 | SQD  | C46-C45-O47-C7  |
| 32  | C     | 518 | DGD  | C9B-CAB-CBB-CCB |
| 32  | C     | 516 | DGD  | O1G-C1A-C2A-C3A |
| 24  | C     | 511 | CLA  | C8-C10-C11-C12  |
| 24  | c     | 511 | CLA  | C8-C10-C11-C12  |
| 24  | c     | 512 | CLA  | C2-C3-C5-C6     |
| 30  | D     | 408 | LHG  | C23-C24-C25-C26 |
| 29  | D     | 410 | LMG  | C13-C14-C15-C16 |
| 31  | A     | 616 | SQD  | C29-C30-C31-C32 |
| 33  | l     | 102 | STE  | C15-C16-C17-C18 |
| 24  | B     | 605 | CLA  | C6-C7-C8-C9     |
| 24  | C     | 512 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 614 | CLA  | C14-C13-C15-C16 |
| 24  | c     | 504 | CLA  | C11-C10-C8-C9   |
| 30  | B     | 621 | LHG  | C13-C14-C15-C16 |
| 33  | C     | 521 | STE  | C11-C12-C13-C14 |
| 24  | B     | 615 | CLA  | C12-C13-C15-C16 |
| 24  | D     | 402 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 612 | CLA  | C11-C10-C8-C7   |
| 24  | b     | 615 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 504 | CLA  | C11-C10-C8-C7   |
| 24  | d     | 401 | CLA  | C6-C7-C8-C10    |
| 33  | b     | 624 | STE  | C5-C6-C7-C8     |
| 26  | B     | 617 | BCR  | C12-C13-C14-C15 |
| 26  | C     | 514 | BCR  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | H     | 101 | BCR  | C12-C13-C14-C15 |
| 29  | C     | 519 | LMG  | C13-C14-C15-C16 |
| 30  | B     | 621 | LHG  | O6-C4-C5-O7     |
| 24  | b     | 611 | CLA  | C16-C17-C18-C19 |
| 32  | h     | 101 | DGD  | O2G-C1B-C2B-C3B |
| 29  | b     | 621 | LMG  | C19-C20-C21-C22 |
| 24  | b     | 606 | CLA  | C15-C16-C17-C18 |
| 30  | e     | 102 | LHG  | C12-C13-C14-C15 |
| 32  | c     | 518 | DGD  | C2A-C1A-O1G-C1G |
| 24  | c     | 505 | CLA  | C16-C17-C18-C20 |
| 32  | C     | 518 | DGD  | C2A-C3A-C4A-C5A |
| 33  | x     | 102 | STE  | C10-C11-C12-C13 |
| 29  | M     | 101 | LMG  | O7-C8-C9-O8     |
| 29  | a     | 618 | LMG  | O1-C7-C8-O7     |
| 31  | b     | 620 | SQD  | O47-C45-C46-O48 |
| 32  | H     | 102 | DGD  | O2G-C1B-C2B-C3B |
| 30  | e     | 102 | LHG  | C11-C12-C13-C14 |
| 30  | l     | 101 | LHG  | C23-C24-C25-C26 |
| 24  | B     | 609 | CLA  | C16-C17-C18-C20 |
| 24  | c     | 506 | CLA  | C16-C17-C18-C19 |
| 31  | a     | 613 | SQD  | C8-C7-O47-C45   |
| 33  | d     | 412 | STE  | C13-C14-C15-C16 |
| 24  | c     | 506 | CLA  | C2-C1-O2A-CGA   |
| 29  | C     | 519 | LMG  | O1-C7-C8-C9     |
| 32  | A     | 618 | DGD  | CBB-CCB-CDB-CEB |
| 30  | A     | 615 | LHG  | C24-C25-C26-C27 |
| 26  | c     | 515 | BCR  | C21-C22-C23-C24 |
| 28  | a     | 611 | PL9  | C21-C22-C23-C24 |
| 32  | c     | 516 | DGD  | C5D-C6D-O5D-C1E |
| 31  | f     | 101 | SQD  | C32-C33-C34-C35 |
| 30  | e     | 102 | LHG  | C24-C25-C26-C27 |
| 33  | c     | 520 | STE  | C1-C2-C3-C4     |
| 29  | c     | 522 | LMG  | C36-C37-C38-C39 |
| 30  | B     | 621 | LHG  | C32-C33-C34-C35 |
| 33  | B     | 626 | STE  | C7-C8-C9-C10    |
| 24  | B     | 616 | CLA  | C6-C7-C8-C9     |
| 24  | b     | 601 | CLA  | C11-C12-C13-C14 |
| 24  | c     | 505 | CLA  | C6-C7-C8-C9     |
| 24  | c     | 505 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 507 | CLA  | C11-C10-C8-C9   |
| 32  | c     | 518 | DGD  | C8A-C9A-CAA-CBA |
| 24  | C     | 505 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | d     | 410 | LMG  | C15-C16-C17-C18 |
| 30  | l     | 101 | LHG  | C12-C13-C14-C15 |
| 24  | b     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 33  | k     | 103 | STE  | C1-C2-C3-C4     |
| 30  | d     | 408 | LHG  | C19-C20-C21-C22 |
| 24  | d     | 401 | CLA  | C16-C17-C18-C20 |
| 33  | T     | 102 | STE  | C12-C13-C14-C15 |
| 29  | D     | 409 | LMG  | C29-C28-O8-C9   |
| 24  | a     | 612 | CLA  | C2C-C3C-CAC-CBC |
| 24  | a     | 612 | CLA  | C4C-C3C-CAC-CBC |
| 29  | c     | 522 | LMG  | C34-C35-C36-C37 |
| 31  | A     | 616 | SQD  | C26-C27-C28-C29 |
| 29  | C     | 519 | LMG  | C18-C19-C20-C21 |
| 29  | b     | 623 | LMG  | C31-C32-C33-C34 |
| 24  | C     | 508 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 603 | CLA  | C6-C7-C8-C10    |
| 24  | b     | 614 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 505 | CLA  | C11-C10-C8-C7   |
| 32  | C     | 516 | DGD  | O1A-C1A-O1G-C1G |
| 32  | H     | 102 | DGD  | C9A-CAA-CBA-CCA |
| 33  | D     | 411 | STE  | C4-C5-C6-C7     |
| 24  | B     | 611 | CLA  | C16-C17-C18-C19 |
| 31  | a     | 613 | SQD  | C10-C11-C12-C13 |
| 24  | B     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 30  | B     | 621 | LHG  | C24-C25-C26-C27 |
| 29  | a     | 618 | LMG  | O8-C28-C29-C30  |
| 29  | c     | 521 | LMG  | C42-C43-C44-C45 |
| 31  | b     | 620 | SQD  | C30-C31-C32-C33 |
| 24  | B     | 613 | CLA  | C2-C1-O2A-CGA   |
| 24  | d     | 403 | CLA  | C2-C1-O2A-CGA   |
| 30  | l     | 101 | LHG  | C17-C18-C19-C20 |
| 33  | b     | 624 | STE  | C9-C10-C11-C12  |
| 30  | A     | 615 | LHG  | C2-C3-O3-P      |
| 33  | b     | 626 | STE  | C7-C8-C9-C10    |
| 31  | a     | 613 | SQD  | C19-C20-C21-C22 |
| 31  | a     | 614 | SQD  | C30-C31-C32-C33 |
| 28  | d     | 406 | PL9  | C43-C44-C46-C47 |
| 32  | h     | 101 | DGD  | CDB-CEB-CFB-CGB |
| 32  | H     | 102 | DGD  | C4E-C5E-C6E-O5E |
| 30  | E     | 101 | LHG  | C1-C2-C3-O3     |
| 30  | l     | 101 | LHG  | C4-C5-C6-O8     |
| 32  | A     | 618 | DGD  | C6A-C7A-C8A-C9A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | c     | 516 | DGD  | CDB-CEB-CFB-CGB |
| 24  | A     | 604 | CLA  | C14-C13-C15-C16 |
| 24  | A     | 605 | CLA  | C6-C7-C8-C9     |
| 24  | A     | 605 | CLA  | C11-C10-C8-C9   |
| 24  | B     | 606 | CLA  | C11-C10-C8-C9   |
| 24  | C     | 507 | CLA  | C14-C13-C15-C16 |
| 24  | C     | 512 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 605 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 507 | CLA  | C14-C13-C15-C16 |
| 24  | c     | 511 | CLA  | C11-C10-C8-C9   |
| 29  | M     | 101 | LMG  | C20-C21-C22-C23 |
| 24  | c     | 505 | CLA  | C10-C11-C12-C13 |
| 33  | b     | 626 | STE  | C1-C2-C3-C4     |
| 31  | b     | 620 | SQD  | C11-C10-C9-C8   |
| 33  | B     | 620 | STE  | C7-C8-C9-C10    |
| 25  | a     | 605 | PHO  | O2A-C1-C2-C3    |
| 31  | A     | 617 | SQD  | C17-C18-C19-C20 |
| 32  | A     | 618 | DGD  | O6D-C5D-C6D-O5D |
| 24  | c     | 508 | CLA  | C4-C3-C5-C6     |
| 28  | D     | 405 | PL9  | C40-C39-C41-C42 |
| 31  | D     | 407 | SQD  | C23-C24-C25-C26 |
| 24  | B     | 601 | CLA  | C16-C17-C18-C19 |
| 24  | c     | 507 | CLA  | C15-C16-C17-C18 |
| 33  | l     | 102 | STE  | C12-C13-C14-C15 |
| 36  | v     | 201 | HEC  | CAD-CBD-CGD-O1D |
| 29  | M     | 101 | LMG  | C19-C20-C21-C22 |
| 24  | c     | 508 | CLA  | C1A-C2A-CAA-CBA |
| 26  | B     | 617 | BCR  | C11-C10-C9-C8   |
| 33  | M     | 102 | STE  | O1-C1-C2-C3     |
| 29  | C     | 519 | LMG  | C28-C29-C30-C31 |
| 32  | c     | 516 | DGD  | C5A-C6A-C7A-C8A |
| 24  | B     | 614 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 623 | SQD  | C10-C11-C12-C13 |
| 33  | k     | 103 | STE  | C4-C5-C6-C7     |
| 24  | B     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 615 | CLA  | C2B-C3B-CAB-CBB |
| 24  | C     | 504 | CLA  | C2B-C3B-CAB-CBB |
| 24  | d     | 403 | CLA  | C2B-C3B-CAB-CBB |
| 26  | B     | 617 | BCR  | C5-C6-C7-C8     |
| 26  | H     | 101 | BCR  | C23-C24-C25-C26 |
| 26  | H     | 101 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 101 | BCR  | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | T     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | b     | 617 | BCR  | C1-C6-C7-C8     |
| 26  | b     | 617 | BCR  | C5-C6-C7-C8     |
| 26  | k     | 102 | BCR  | C5-C6-C7-C8     |
| 26  | k     | 102 | BCR  | C23-C24-C25-C30 |
| 26  | t     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | x     | 101 | BCR  | C23-C24-C25-C30 |
| 33  | b     | 622 | STE  | C1-C2-C3-C4     |
| 33  | B     | 626 | STE  | C11-C12-C13-C14 |
| 24  | a     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 33  | C     | 520 | STE  | C4-C5-C6-C7     |
| 35  | F     | 101 | HEM  | CAD-CBD-CGD-O1D |
| 36  | v     | 201 | HEC  | CAD-CBD-CGD-O2D |
| 24  | b     | 609 | CLA  | C4-C3-C5-C6     |
| 33  | a     | 616 | STE  | C4-C5-C6-C7     |
| 24  | b     | 605 | CLA  | C15-C16-C17-C18 |
| 29  | D     | 410 | LMG  | O9-C10-C11-C12  |
| 33  | b     | 624 | STE  | O1-C1-C2-C3     |
| 24  | c     | 510 | CLA  | C10-C11-C12-C13 |
| 24  | A     | 604 | CLA  | C12-C13-C15-C16 |
| 24  | B     | 614 | CLA  | C6-C7-C8-C10    |
| 24  | C     | 502 | CLA  | C12-C13-C15-C16 |
| 24  | b     | 606 | CLA  | C11-C10-C8-C7   |
| 24  | b     | 606 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 507 | CLA  | C11-C12-C13-C15 |
| 24  | b     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 33  | b     | 627 | STE  | C6-C7-C8-C9     |
| 33  | B     | 627 | STE  | C3-C4-C5-C6     |
| 33  | H     | 103 | STE  | C7-C8-C9-C10    |
| 33  | b     | 625 | STE  | O1-C1-C2-C3     |
| 29  | D     | 406 | LMG  | C20-C21-C22-C23 |
| 24  | b     | 606 | CLA  | C10-C11-C12-C13 |
| 32  | H     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 33  | j     | 101 | STE  | C5-C6-C7-C8     |
| 35  | e     | 101 | HEM  | CAD-CBD-CGD-O1D |
| 24  | C     | 510 | CLA  | C4-C3-C5-C6     |
| 24  | a     | 606 | CLA  | C4-C3-C5-C6     |
| 28  | A     | 612 | PL9  | C30-C29-C31-C32 |
| 28  | A     | 612 | PL9  | C33-C34-C36-C37 |
| 30  | e     | 102 | LHG  | C25-C26-C27-C28 |
| 26  | k     | 101 | BCR  | C7-C8-C9-C10    |
| 30  | B     | 621 | LHG  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | A     | 614 | LMG  | C19-C20-C21-C22 |
| 31  | a     | 614 | SQD  | C15-C16-C17-C18 |
| 24  | B     | 602 | CLA  | C11-C12-C13-C14 |
| 33  | c     | 520 | STE  | C10-C11-C12-C13 |
| 33  | J     | 101 | STE  | C7-C8-C9-C10    |
| 31  | b     | 620 | SQD  | C10-C11-C12-C13 |
| 32  | C     | 518 | DGD  | C4A-C5A-C6A-C7A |
| 31  | a     | 613 | SQD  | C35-C36-C37-C38 |
| 33  | D     | 411 | STE  | C15-C16-C17-C18 |
| 24  | D     | 403 | CLA  | C13-C15-C16-C17 |
| 30  | d     | 409 | LHG  | C2-C3-O3-P      |
| 25  | d     | 402 | PHO  | C2C-C3C-CAC-CBC |
| 24  | B     | 605 | CLA  | C2-C3-C5-C6     |
| 24  | d     | 401 | CLA  | C16-C17-C18-C19 |
| 36  | V     | 201 | HEC  | CAD-CBD-CGD-O2D |
| 32  | C     | 517 | DGD  | C5B-C6B-C7B-C8B |
| 24  | c     | 508 | CLA  | C10-C11-C12-C13 |
| 33  | C     | 520 | STE  | C5-C6-C7-C8     |
| 32  | C     | 516 | DGD  | O1G-C1G-C2G-C3G |
| 32  | C     | 518 | DGD  | C2B-C3B-C4B-C5B |
| 29  | a     | 618 | LMG  | C24-C25-C26-C27 |
| 24  | B     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 24  | b     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 24  | c     | 501 | CLA  | C2A-CAA-CBA-CGA |
| 33  | b     | 626 | STE  | C5-C6-C7-C8     |
| 33  | M     | 102 | STE  | O2-C1-C2-C3     |
| 30  | d     | 408 | LHG  | C14-C15-C16-C17 |
| 24  | B     | 615 | CLA  | C4-C3-C5-C6     |
| 36  | V     | 201 | HEC  | CAD-CBD-CGD-O1D |
| 24  | b     | 611 | CLA  | C16-C17-C18-C20 |
| 30  | E     | 101 | LHG  | C10-C11-C12-C13 |
| 33  | b     | 625 | STE  | O2-C1-C2-C3     |
| 35  | e     | 101 | HEM  | CAD-CBD-CGD-O2D |
| 31  | A     | 616 | SQD  | C31-C32-C33-C34 |
| 30  | B     | 622 | LHG  | C31-C32-C33-C34 |
| 26  | Y     | 101 | BCR  | C16-C17-C18-C36 |
| 24  | B     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 35  | F     | 101 | HEM  | CAD-CBD-CGD-O2D |
| 33  | B     | 625 | STE  | C6-C7-C8-C9     |
| 30  | D     | 408 | LHG  | O6-C4-C5-C6     |
| 24  | C     | 508 | CLA  | C16-C17-C18-C19 |
| 24  | b     | 608 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | d     | 404 | CLA  | C10-C11-C12-C13 |
| 33  | b     | 624 | STE  | O2-C1-C2-C3     |
| 28  | d     | 406 | PL9  | C13-C14-C16-C17 |
| 24  | d     | 401 | CLA  | C15-C16-C17-C18 |
| 26  | c     | 515 | BCR  | C7-C8-C9-C34    |
| 24  | A     | 605 | CLA  | C6-C7-C8-C10    |
| 24  | c     | 509 | CLA  | C11-C12-C13-C15 |
| 32  | c     | 518 | DGD  | O6D-C5D-C6D-O5D |
| 33  | T     | 103 | STE  | C15-C16-C17-C18 |
| 33  | t     | 102 | STE  | O2-C1-C2-C3     |
| 29  | D     | 406 | LMG  | C18-C19-C20-C21 |
| 33  | D     | 411 | STE  | C13-C14-C15-C16 |
| 33  | J     | 101 | STE  | O2-C1-C2-C3     |
| 24  | B     | 615 | CLA  | C6-C7-C8-C9     |
| 24  | C     | 506 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 603 | CLA  | C6-C7-C8-C9     |
| 24  | b     | 612 | CLA  | C11-C10-C8-C9   |
| 24  | c     | 502 | CLA  | C6-C7-C8-C9     |
| 24  | a     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 29  | M     | 101 | LMG  | C8-C7-O1-C1     |
| 29  | b     | 621 | LMG  | C8-C7-O1-C1     |
| 31  | a     | 613 | SQD  | C5-C6-S-O8      |
| 24  | B     | 601 | CLA  | C13-C15-C16-C17 |
| 24  | b     | 614 | CLA  | C13-C15-C16-C17 |
| 24  | D     | 402 | CLA  | C2-C1-O2A-CGA   |
| 24  | B     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 29  | D     | 410 | LMG  | C17-C18-C19-C20 |
| 31  | b     | 620 | SQD  | C13-C14-C15-C16 |
| 28  | A     | 612 | PL9  | C13-C14-C16-C17 |
| 32  | C     | 517 | DGD  | C1B-C2B-C3B-C4B |
| 33  | B     | 625 | STE  | O2-C1-C2-C3     |
| 33  | c     | 520 | STE  | O2-C1-C2-C3     |
| 24  | b     | 612 | CLA  | C8-C10-C11-C12  |
| 30  | B     | 621 | LHG  | C23-C24-C25-C26 |
| 26  | d     | 405 | BCR  | C18-C19-C20-C21 |
| 32  | h     | 101 | DGD  | CDA-CEA-CFA-CGA |
| 32  | c     | 518 | DGD  | C7B-C8B-C9B-CAB |
| 30  | A     | 615 | LHG  | C35-C36-C37-C38 |
| 30  | B     | 621 | LHG  | C35-C36-C37-C38 |
| 33  | c     | 520 | STE  | O1-C1-C2-C3     |
| 28  | a     | 611 | PL9  | C47-C48-C49-C50 |
| 24  | b     | 605 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | C     | 518 | DGD  | C1B-C2B-C3B-C4B |
| 29  | A     | 614 | LMG  | C7-C8-C9-O8     |
| 31  | b     | 620 | SQD  | O6-C44-C45-C46  |
| 24  | C     | 508 | CLA  | O1A-CGA-O2A-C1  |
| 24  | b     | 601 | CLA  | O1A-CGA-O2A-C1  |
| 31  | f     | 101 | SQD  | C24-C25-C26-C27 |
| 33  | B     | 627 | STE  | C4-C5-C6-C7     |
| 33  | l     | 102 | STE  | C9-C10-C11-C12  |
| 26  | k     | 101 | BCR  | C19-C20-C21-C22 |
| 24  | B     | 613 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 616 | SQD  | C25-C26-C27-C28 |
| 33  | B     | 625 | STE  | O1-C1-C2-C3     |
| 33  | t     | 102 | STE  | O1-C1-C2-C3     |
| 29  | D     | 409 | LMG  | C37-C38-C39-C40 |
| 30  | d     | 407 | LHG  | C17-C18-C19-C20 |
| 29  | C     | 519 | LMG  | O1-C7-C8-O7     |
| 24  | C     | 502 | CLA  | C14-C13-C15-C16 |
| 24  | a     | 606 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 604 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 606 | CLA  | C11-C12-C13-C14 |
| 24  | c     | 503 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 617 | SQD  | C32-C33-C34-C35 |
| 30  | B     | 621 | LHG  | O7-C7-C8-C9     |
| 30  | E     | 101 | LHG  | C26-C27-C28-C29 |
| 33  | J     | 101 | STE  | O1-C1-C2-C3     |
| 24  | B     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 602 | CLA  | C11-C12-C13-C15 |
| 24  | B     | 613 | CLA  | C11-C10-C8-C7   |
| 24  | C     | 512 | CLA  | C11-C12-C13-C15 |
| 24  | a     | 606 | CLA  | C11-C10-C8-C7   |
| 24  | b     | 601 | CLA  | C11-C12-C13-C15 |
| 24  | b     | 603 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 511 | CLA  | C12-C13-C15-C16 |
| 29  | D     | 410 | LMG  | C33-C34-C35-C36 |
| 24  | C     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 26  | A     | 609 | BCR  | C23-C24-C25-C26 |
| 26  | A     | 609 | BCR  | C23-C24-C25-C30 |
| 26  | B     | 618 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 101 | BCR  | C23-C24-C25-C26 |
| 26  | T     | 101 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | c     | 514 | BCR  | C1-C6-C7-C8     |
| 26  | c     | 514 | BCR  | C5-C6-C7-C8     |
| 26  | d     | 405 | BCR  | C23-C24-C25-C26 |
| 26  | k     | 102 | BCR  | C23-C24-C25-C26 |
| 26  | t     | 101 | BCR  | C5-C6-C7-C8     |
| 26  | x     | 101 | BCR  | C23-C24-C25-C26 |
| 29  | C     | 519 | LMG  | C39-C40-C41-C42 |
| 30  | d     | 407 | LHG  | C33-C34-C35-C36 |
| 32  | c     | 518 | DGD  | CAA-CBA-CCA-CDA |
| 32  | c     | 517 | DGD  | C3B-C4B-C5B-C6B |
| 32  | c     | 517 | DGD  | C6B-C7B-C8B-C9B |
| 33  | a     | 616 | STE  | C6-C7-C8-C9     |
| 32  | A     | 618 | DGD  | O6D-C1D-O3G-C3G |
| 33  | B     | 624 | STE  | C3-C4-C5-C6     |
| 24  | B     | 601 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 617 | SQD  | O48-C23-C24-C25 |
| 24  | b     | 609 | CLA  | C2-C3-C5-C6     |
| 28  | D     | 405 | PL9  | C13-C14-C16-C17 |
| 32  | C     | 517 | DGD  | O1B-C1B-O2G-C2G |
| 29  | c     | 522 | LMG  | C18-C19-C20-C21 |
| 24  | C     | 501 | CLA  | C2A-CAA-CBA-CGA |
| 30  | d     | 407 | LHG  | C18-C19-C20-C21 |
| 29  | D     | 410 | LMG  | O7-C10-C11-C12  |
| 31  | B     | 623 | SQD  | C31-C32-C33-C34 |
| 24  | c     | 509 | CLA  | CAA-CBA-CGA-O1A |
| 33  | T     | 103 | STE  | C4-C5-C6-C7     |
| 24  | B     | 601 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 613 | SQD  | O47-C7-C8-C9    |
| 32  | H     | 102 | DGD  | CBB-CCB-CDB-CEB |
| 33  | a     | 615 | STE  | C3-C4-C5-C6     |
| 31  | b     | 620 | SQD  | C26-C27-C28-C29 |
| 24  | B     | 615 | CLA  | C2-C3-C5-C6     |
| 28  | d     | 406 | PL9  | C18-C19-C21-C22 |
| 24  | c     | 509 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 601 | CLA  | CBD-CGD-O2D-CED |
| 33  | b     | 622 | STE  | C9-C10-C11-C12  |
| 32  | A     | 618 | DGD  | CCA-CDA-CEA-CFA |
| 32  | H     | 102 | DGD  | CDA-CEA-CFA-CGA |
| 28  | a     | 611 | PL9  | C39-C41-C42-C43 |
| 29  | c     | 519 | LMG  | O1-C7-C8-C9     |
| 31  | f     | 101 | SQD  | O6-C44-C45-C46  |
| 32  | c     | 516 | DGD  | C1G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | B     | 612 | CLA  | C8-C10-C11-C12  |
| 24  | b     | 610 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 24  | C     | 502 | CLA  | C1A-C2A-CAA-CBA |
| 33  | c     | 520 | STE  | C11-C10-C9-C8   |
| 26  | b     | 618 | BCR  | C22-C23-C24-C25 |
| 32  | C     | 517 | DGD  | O6D-C1D-O3G-C3G |
| 32  | c     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 31  | A     | 616 | SQD  | O47-C7-C8-C9    |
| 32  | c     | 516 | DGD  | O2G-C1B-C2B-C3B |
| 29  | A     | 614 | LMG  | O1-C7-C8-O7     |
| 30  | l     | 101 | LHG  | O7-C5-C6-O8     |
| 31  | f     | 101 | SQD  | O6-C44-C45-O47  |
| 26  | c     | 515 | BCR  | C13-C14-C15-C16 |
| 26  | k     | 102 | BCR  | C19-C20-C21-C22 |
| 29  | M     | 101 | LMG  | C33-C34-C35-C36 |
| 31  | b     | 620 | SQD  | O47-C7-C8-C9    |
| 31  | A     | 616 | SQD  | C5-C6-S-O7      |
| 31  | a     | 613 | SQD  | C5-C6-S-O7      |
| 24  | c     | 506 | CLA  | C4-C3-C5-C6     |
| 24  | B     | 606 | CLA  | C11-C12-C13-C15 |
| 24  | B     | 608 | CLA  | C6-C7-C8-C10    |
| 24  | B     | 613 | CLA  | C6-C7-C8-C10    |
| 24  | b     | 614 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 503 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 508 | CLA  | C11-C10-C8-C7   |
| 24  | c     | 510 | CLA  | C11-C10-C8-C7   |
| 29  | c     | 521 | LMG  | C35-C36-C37-C38 |
| 24  | C     | 512 | CLA  | O2A-C1-C2-C3    |
| 24  | b     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 32  | c     | 516 | DGD  | C2B-C3B-C4B-C5B |
| 33  | a     | 617 | STE  | C4-C5-C6-C7     |
| 30  | A     | 615 | LHG  | C10-C11-C12-C13 |
| 24  | A     | 613 | CLA  | C16-C17-C18-C19 |
| 29  | D     | 410 | LMG  | O8-C28-C29-C30  |
| 32  | H     | 102 | DGD  | CAA-CBA-CCA-CDA |
| 33  | b     | 626 | STE  | C3-C4-C5-C6     |
| 29  | M     | 101 | LMG  | C10-C11-C12-C13 |
| 24  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 24  | b     | 601 | CLA  | C4-C3-C5-C6     |
| 31  | f     | 101 | SQD  | C25-C26-C27-C28 |
| 30  | A     | 615 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | C     | 515 | BCR  | C11-C10-C9-C8   |
| 33  | b     | 622 | STE  | O1-C1-C2-C3     |
| 24  | b     | 613 | CLA  | C15-C16-C17-C18 |
| 24  | b     | 601 | CLA  | CBA-CGA-O2A-C1  |
| 32  | h     | 101 | DGD  | O1B-C1B-C2B-C3B |
| 24  | c     | 512 | CLA  | C5-C6-C7-C8     |
| 24  | B     | 611 | CLA  | C6-C7-C8-C9     |
| 24  | B     | 613 | CLA  | C6-C7-C8-C9     |
| 24  | B     | 615 | CLA  | C14-C13-C15-C16 |
| 24  | D     | 403 | CLA  | C11-C10-C8-C9   |
| 24  | a     | 604 | CLA  | C14-C13-C15-C16 |
| 24  | b     | 603 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 603 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 613 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 617 | SQD  | O10-C23-C24-C25 |
| 29  | D     | 409 | LMG  | C36-C37-C38-C39 |
| 30  | B     | 622 | LHG  | C16-C17-C18-C19 |
| 32  | c     | 516 | DGD  | CAA-CBA-CCA-CDA |
| 24  | b     | 606 | CLA  | C5-C6-C7-C8     |
| 24  | b     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 29  | b     | 621 | LMG  | O8-C28-C29-C30  |
| 24  | B     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 29  | a     | 618 | LMG  | O7-C10-C11-C12  |
| 33  | d     | 411 | STE  | O2-C1-C2-C3     |
| 24  | c     | 509 | CLA  | C8-C10-C11-C12  |
| 24  | A     | 604 | CLA  | C4C-C3C-CAC-CBC |
| 33  | c     | 520 | STE  | C11-C12-C13-C14 |
| 31  | b     | 620 | SQD  | C45-C44-O6-C1   |
| 32  | c     | 517 | DGD  | C2G-C3G-O3G-C1D |
| 32  | C     | 516 | DGD  | O1G-C1G-C2G-O2G |
| 32  | c     | 516 | DGD  | O1B-C1B-C2B-C3B |
| 24  | C     | 504 | CLA  | C10-C11-C12-C13 |
| 28  | A     | 612 | PL9  | C20-C19-C21-C22 |
| 32  | H     | 102 | DGD  | C3A-C4A-C5A-C6A |
| 24  | B     | 603 | CLA  | C10-C11-C12-C13 |
| 24  | B     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 30  | B     | 621 | LHG  | C16-C17-C18-C19 |
| 24  | b     | 607 | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 601 | CLA  | CAA-CBA-CGA-O2A |
| 33  | m     | 101 | STE  | C6-C7-C8-C9     |
| 24  | B     | 606 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 25  | A     | 606 | PHO  | C8-C10-C11-C12  |
| 32  | A     | 618 | DGD  | C4D-C5D-C6D-O5D |
| 29  | c     | 521 | LMG  | C15-C16-C17-C18 |
| 29  | d     | 410 | LMG  | C37-C38-C39-C40 |
| 32  | C     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 24  | B     | 604 | CLA  | C13-C15-C16-C17 |
| 24  | C     | 506 | CLA  | C2-C1-O2A-CGA   |
| 29  | D     | 410 | LMG  | O10-C28-C29-C30 |
| 29  | b     | 623 | LMG  | O10-C28-C29-C30 |
| 33  | B     | 626 | STE  | C3-C4-C5-C6     |
| 31  | f     | 101 | SQD  | C30-C31-C32-C33 |
| 33  | d     | 411 | STE  | O1-C1-C2-C3     |
| 31  | B     | 623 | SQD  | O10-C23-C24-C25 |

There are no ring outliers.

105 monomers are involved in 141 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | C     | 501    | CLA  | 1       | 0            |
| 24  | C     | 509    | CLA  | 1       | 0            |
| 24  | B     | 613    | CLA  | 3       | 0            |
| 29  | a     | 618    | LMG  | 5       | 0            |
| 24  | C     | 504    | CLA  | 1       | 0            |
| 29  | c     | 522    | LMG  | 1       | 0            |
| 21  | a     | 601[B] | OEY  | 1       | 0            |
| 33  | B     | 624    | STE  | 1       | 0            |
| 29  | c     | 521    | LMG  | 2       | 0            |
| 26  | B     | 618    | BCR  | 3       | 0            |
| 33  | b     | 625    | STE  | 2       | 0            |
| 24  | b     | 615    | CLA  | 3       | 0            |
| 24  | B     | 615    | CLA  | 1       | 0            |
| 33  | B     | 625    | STE  | 1       | 0            |
| 33  | a     | 617    | STE  | 1       | 0            |
| 24  | b     | 605    | CLA  | 3       | 0            |
| 31  | b     | 620    | SQD  | 1       | 0            |
| 24  | b     | 607    | CLA  | 1       | 0            |
| 33  | c     | 520    | STE  | 1       | 0            |
| 25  | d     | 402    | PHO  | 1       | 0            |
| 24  | b     | 602    | CLA  | 1       | 0            |
| 24  | B     | 610    | CLA  | 2       | 0            |
| 24  | c     | 508    | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | A     | 607 | PHO  | 1       | 0            |
| 24  | c     | 503 | CLA  | 1       | 0            |
| 30  | B     | 621 | LHG  | 1       | 0            |
| 24  | B     | 614 | CLA  | 3       | 0            |
| 24  | B     | 604 | CLA  | 1       | 0            |
| 24  | b     | 613 | CLA  | 1       | 0            |
| 29  | D     | 409 | LMG  | 1       | 0            |
| 24  | A     | 613 | CLA  | 4       | 0            |
| 31  | A     | 617 | SQD  | 1       | 0            |
| 24  | b     | 609 | CLA  | 1       | 0            |
| 30  | D     | 408 | LHG  | 3       | 0            |
| 30  | E     | 101 | LHG  | 1       | 0            |
| 31  | D     | 407 | SQD  | 1       | 0            |
| 24  | c     | 512 | CLA  | 1       | 0            |
| 24  | B     | 601 | CLA  | 3       | 0            |
| 33  | t     | 102 | STE  | 2       | 0            |
| 24  | d     | 403 | CLA  | 1       | 0            |
| 26  | T     | 101 | BCR  | 1       | 0            |
| 29  | b     | 623 | LMG  | 1       | 0            |
| 24  | c     | 501 | CLA  | 2       | 0            |
| 26  | Y     | 101 | BCR  | 1       | 0            |
| 24  | b     | 606 | CLA  | 1       | 0            |
| 24  | B     | 611 | CLA  | 1       | 0            |
| 28  | a     | 611 | PL9  | 2       | 0            |
| 24  | C     | 507 | CLA  | 1       | 0            |
| 29  | M     | 101 | LMG  | 1       | 0            |
| 33  | l     | 102 | STE  | 1       | 0            |
| 33  | d     | 411 | STE  | 1       | 0            |
| 36  | V     | 201 | HEC  | 1       | 0            |
| 31  | A     | 616 | SQD  | 1       | 0            |
| 33  | m     | 101 | STE  | 1       | 0            |
| 32  | A     | 618 | DGD  | 3       | 0            |
| 24  | B     | 607 | CLA  | 1       | 0            |
| 24  | c     | 509 | CLA  | 1       | 0            |
| 26  | a     | 607 | BCR  | 1       | 0            |
| 33  | b     | 622 | STE  | 2       | 0            |
| 26  | H     | 101 | BCR  | 1       | 0            |
| 35  | F     | 101 | HEM  | 2       | 0            |
| 30  | l     | 101 | LHG  | 1       | 0            |
| 24  | c     | 504 | CLA  | 3       | 0            |
| 33  | T     | 103 | STE  | 1       | 0            |
| 30  | d     | 407 | LHG  | 4       | 0            |

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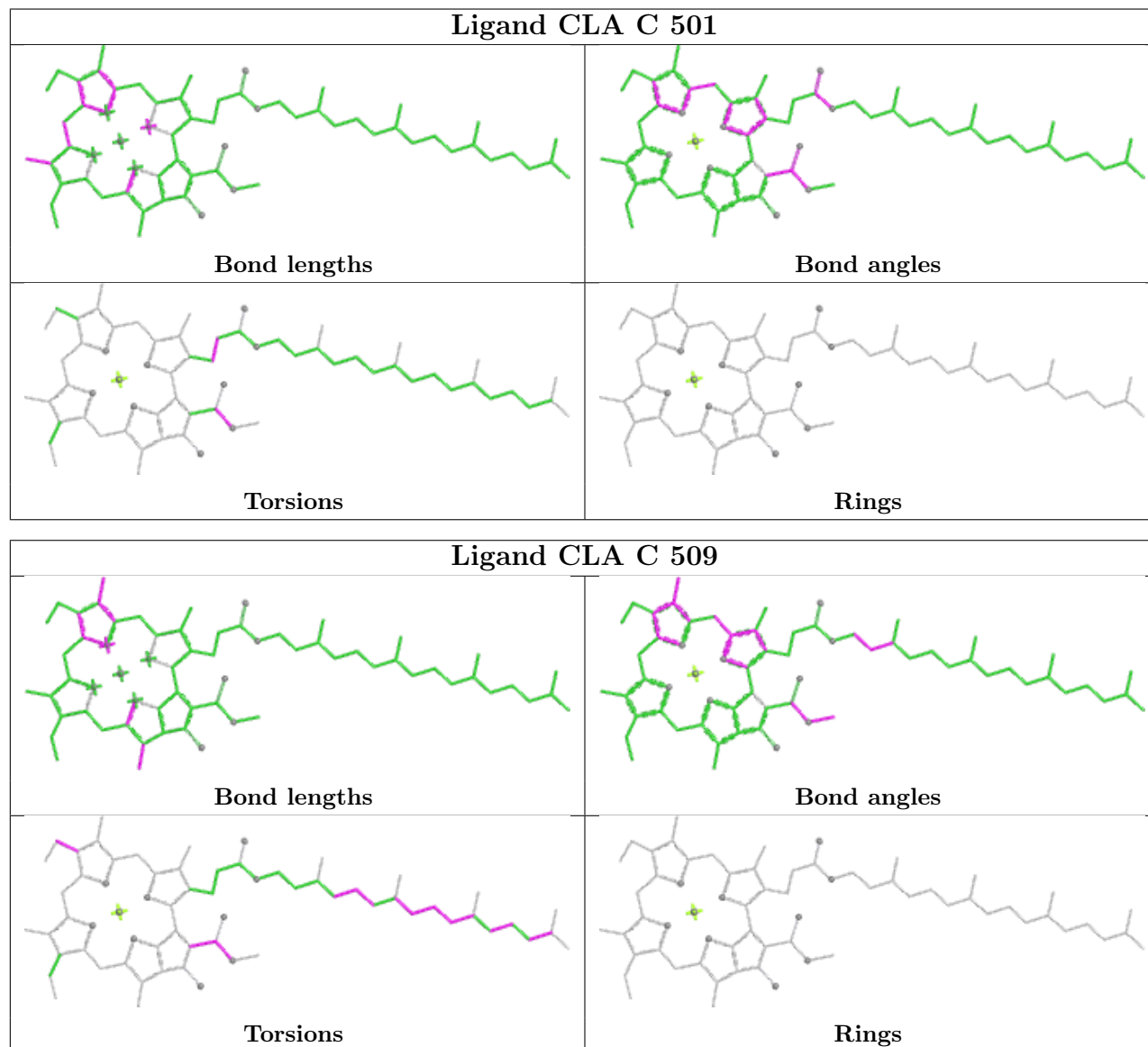
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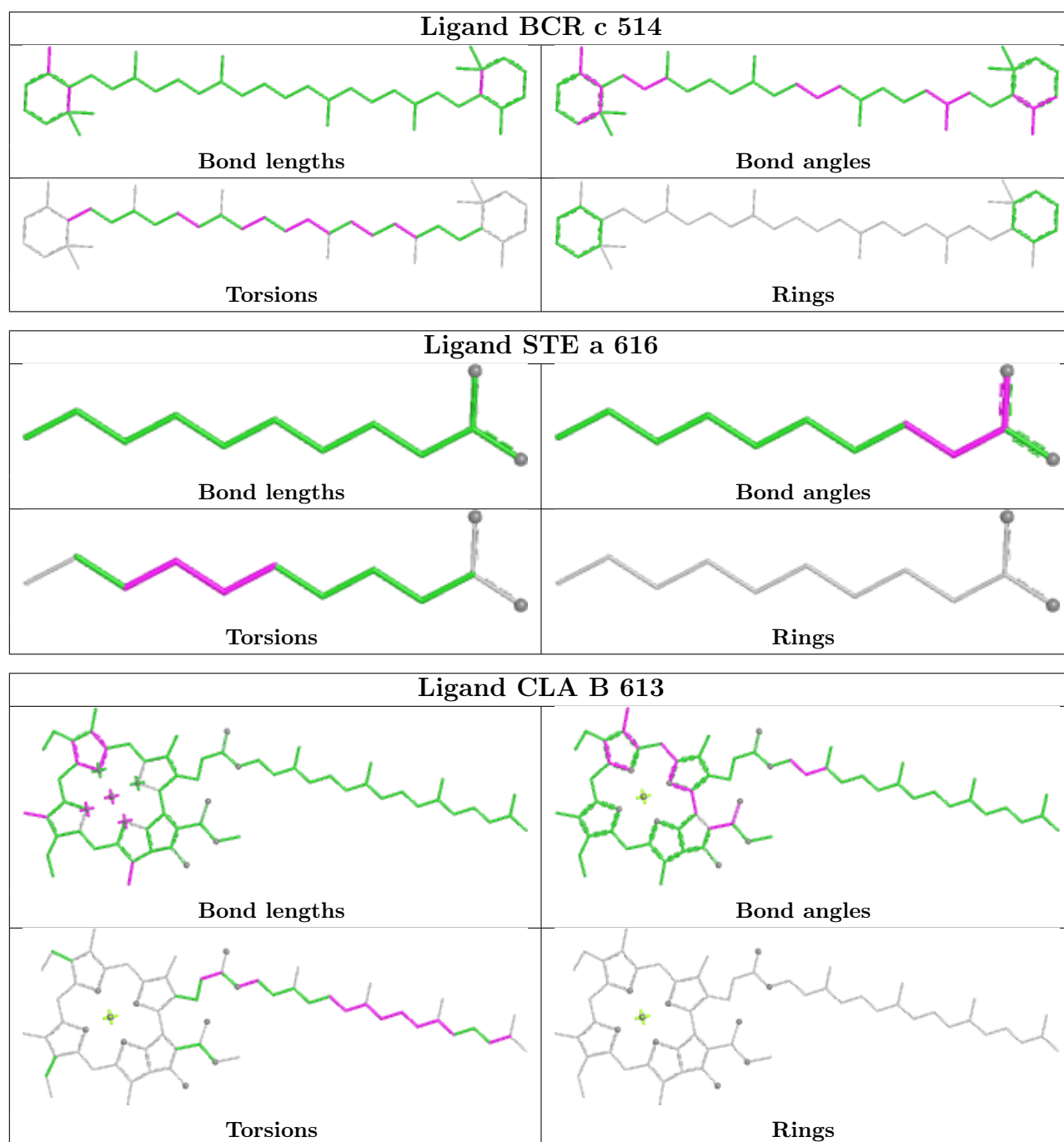
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 31  | B     | 623    | SQD  | 2       | 0            |
| 24  | b     | 614    | CLA  | 1       | 0            |
| 26  | b     | 619    | BCR  | 1       | 0            |
| 28  | A     | 612    | PL9  | 2       | 0            |
| 24  | B     | 616    | CLA  | 1       | 0            |
| 24  | c     | 507    | CLA  | 1       | 0            |
| 24  | c     | 513    | CLA  | 1       | 0            |
| 24  | B     | 606    | CLA  | 3       | 0            |
| 24  | B     | 602    | CLA  | 1       | 0            |
| 33  | B     | 620    | STE  | 1       | 0            |
| 30  | d     | 409    | LHG  | 1       | 0            |
| 29  | c     | 519    | LMG  | 1       | 0            |
| 32  | c     | 517    | DGD  | 2       | 0            |
| 33  | D     | 411    | STE  | 6       | 0            |
| 26  | c     | 515    | BCR  | 1       | 0            |
| 24  | C     | 513    | CLA  | 2       | 0            |
| 34  | D     | 401    | BCT  | 1       | 0            |
| 29  | D     | 406    | LMG  | 1       | 0            |
| 24  | A     | 604    | CLA  | 1       | 0            |
| 33  | E     | 102    | STE  | 1       | 0            |
| 26  | B     | 619    | BCR  | 1       | 0            |
| 30  | A     | 615    | LHG  | 1       | 0            |
| 26  | d     | 405    | BCR  | 2       | 0            |
| 21  | A     | 601[B] | OEY  | 1       | 0            |
| 26  | b     | 618    | BCR  | 1       | 0            |
| 30  | B     | 622    | LHG  | 1       | 0            |
| 35  | e     | 101    | HEM  | 4       | 0            |
| 24  | b     | 616    | CLA  | 1       | 0            |
| 24  | D     | 403    | CLA  | 3       | 0            |
| 24  | C     | 503    | CLA  | 1       | 0            |
| 26  | D     | 404    | BCR  | 1       | 0            |
| 24  | b     | 601    | CLA  | 1       | 0            |
| 33  | H     | 103    | STE  | 1       | 0            |
| 33  | M     | 102    | STE  | 1       | 0            |
| 24  | B     | 612    | CLA  | 1       | 0            |
| 24  | b     | 604    | CLA  | 1       | 0            |
| 24  | c     | 511    | CLA  | 2       | 0            |
| 26  | t     | 101    | BCR  | 3       | 0            |
| 31  | f     | 101    | SQD  | 1       | 0            |
| 36  | v     | 201    | HEC  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

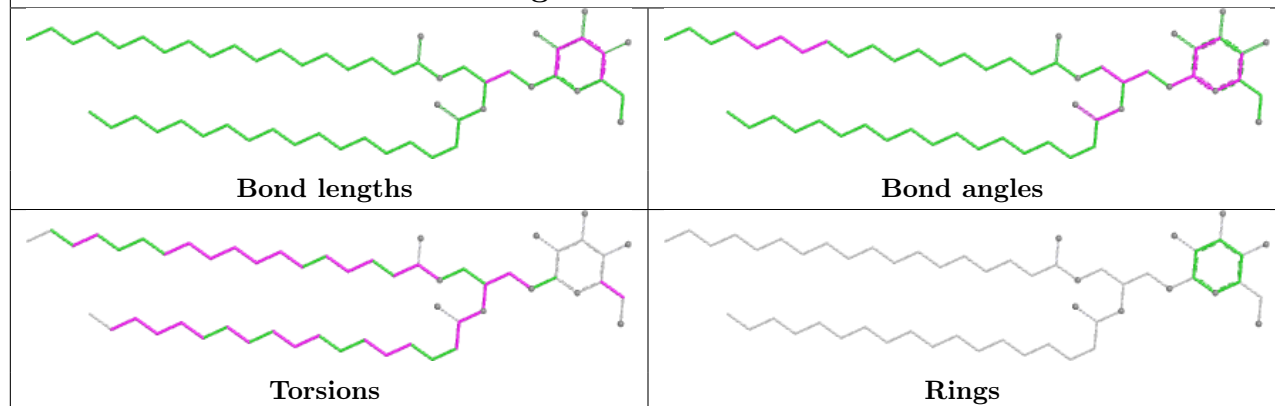


addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

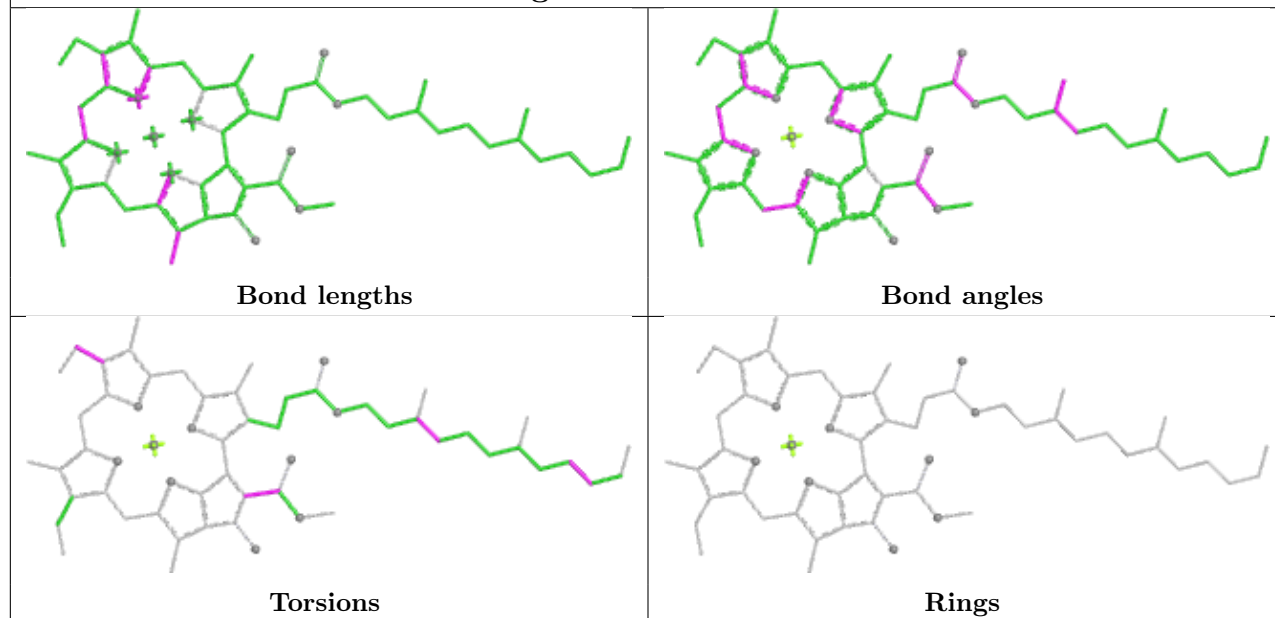




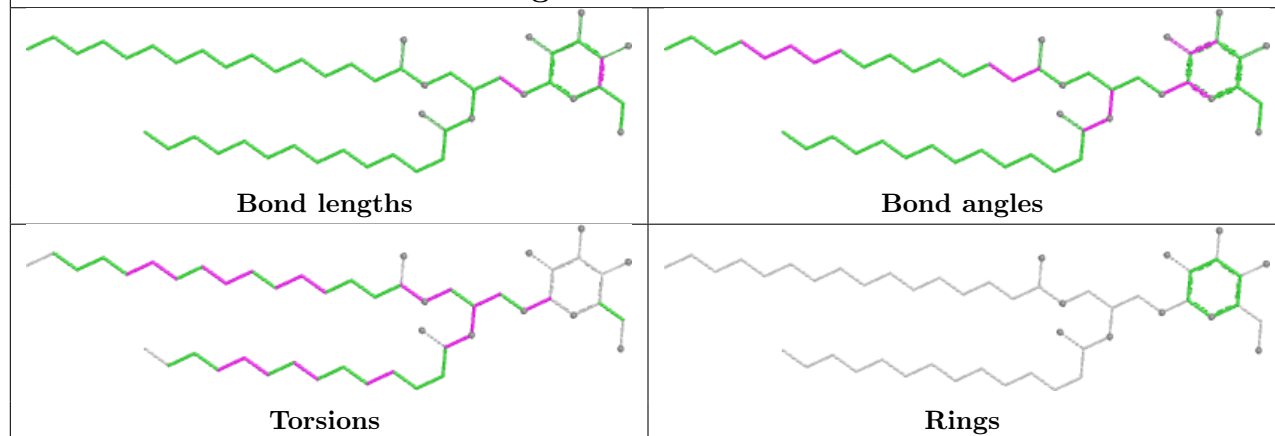
## Ligand LMG a 618

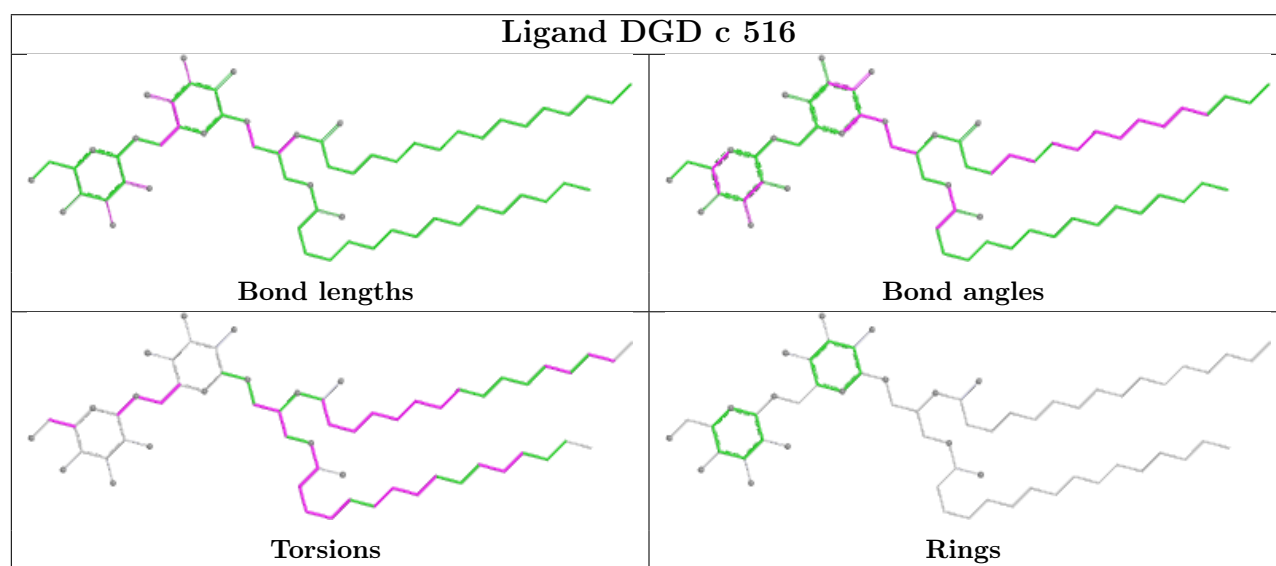
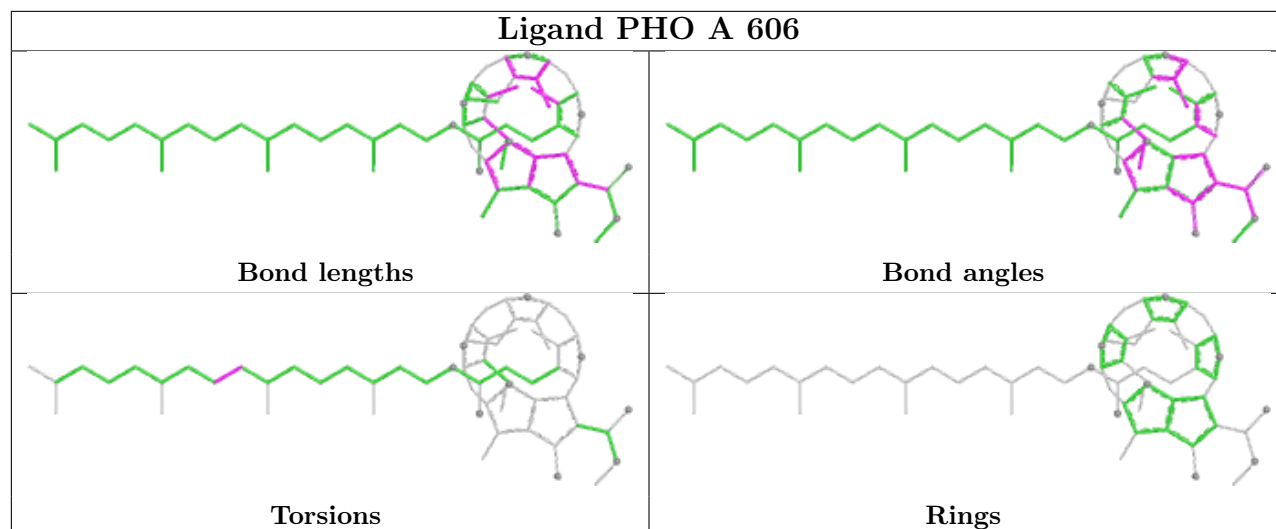


## Ligand CLA C 504

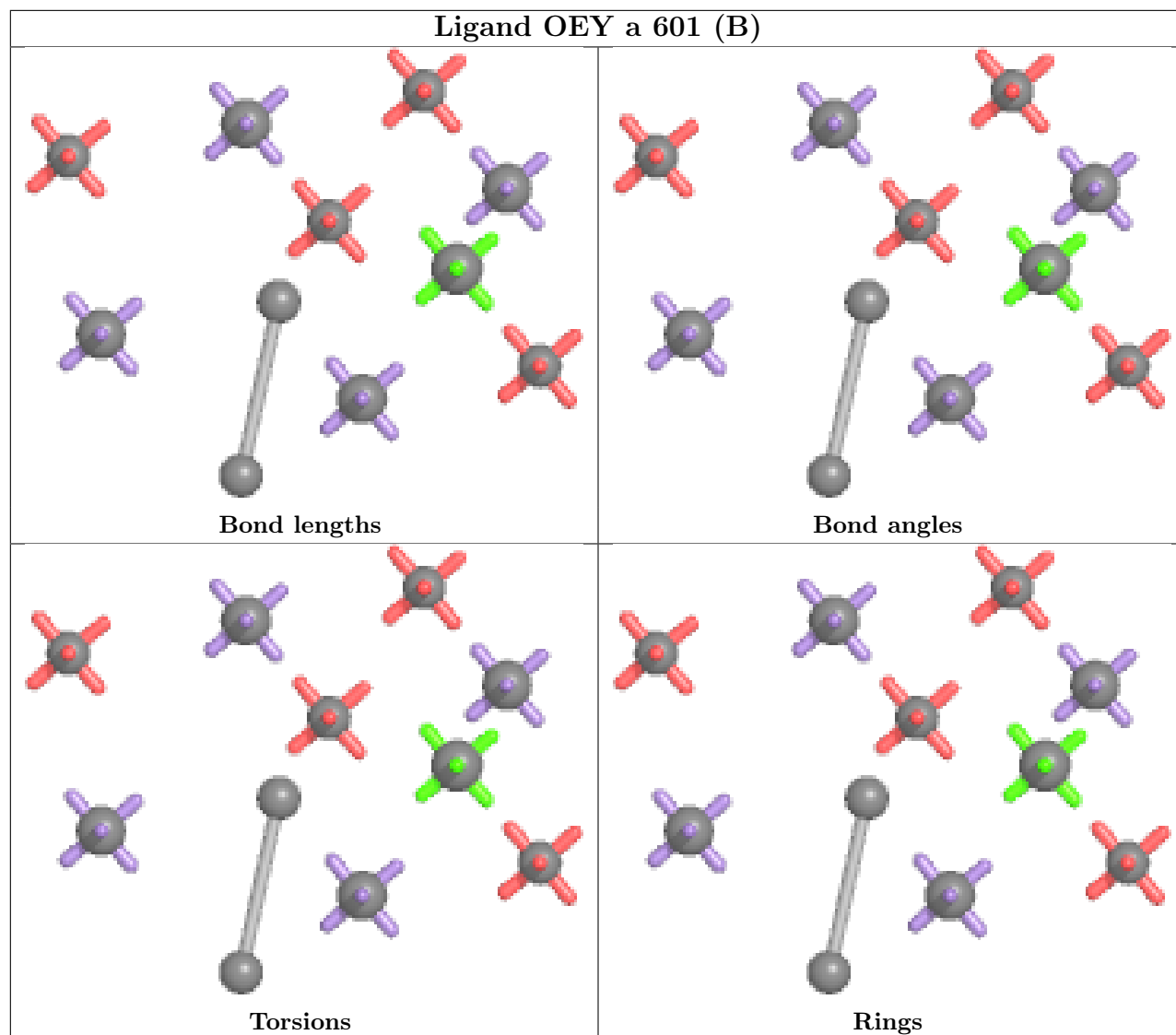


## Ligand LMG c 522

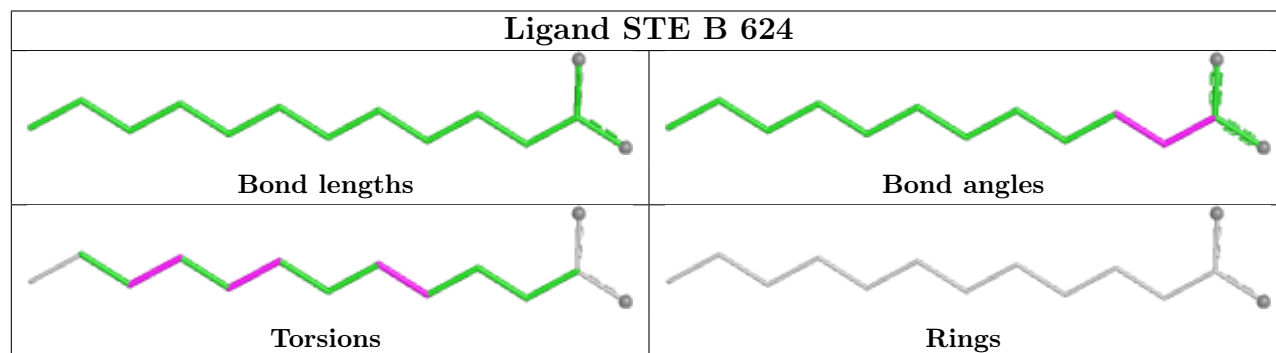


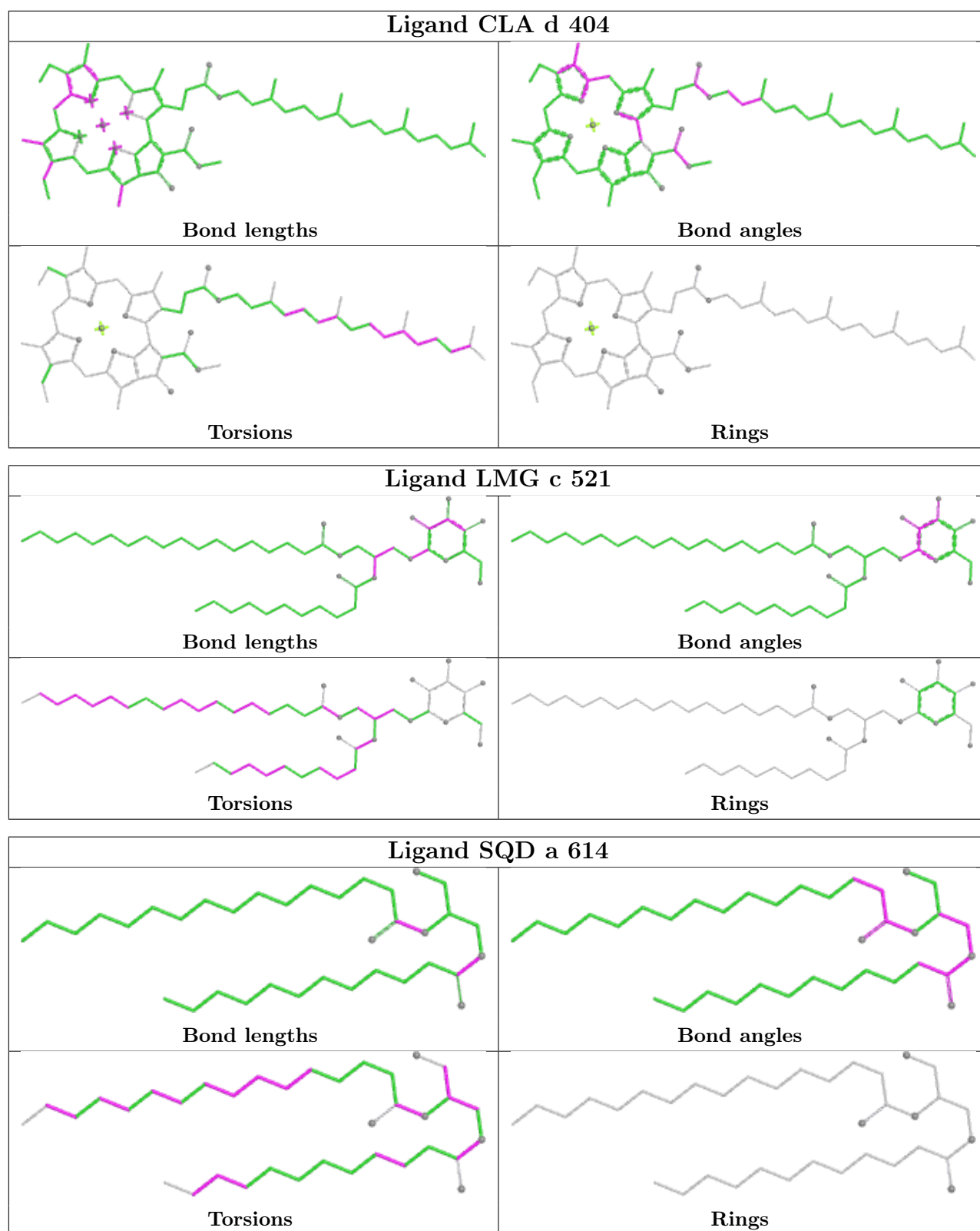


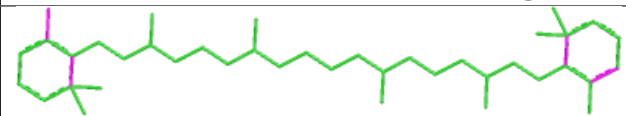
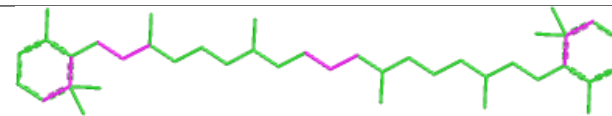
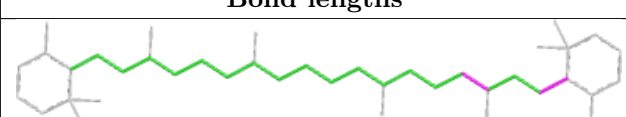
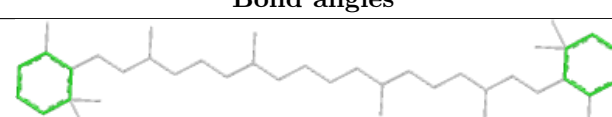
## Ligand OEY a 601 (B)

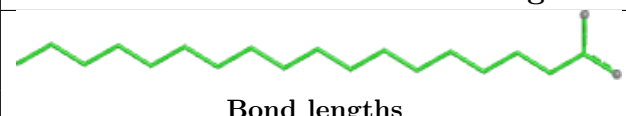
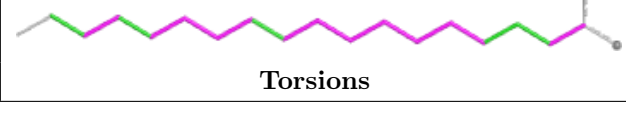
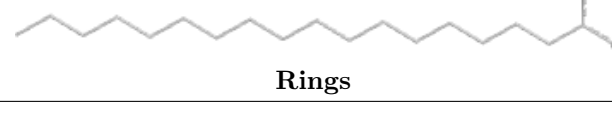


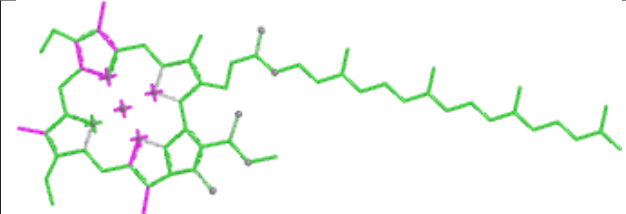
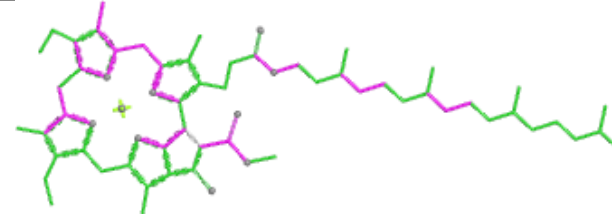
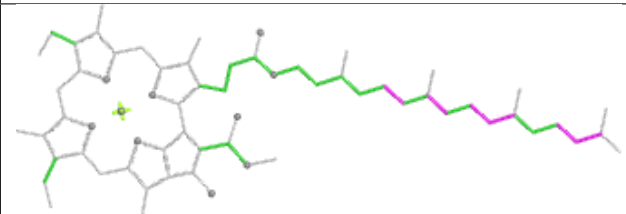
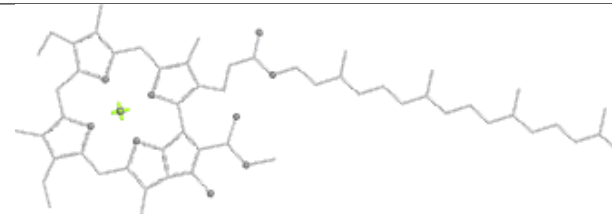
## Ligand STE B 624

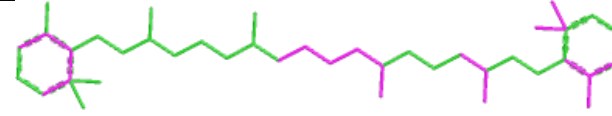
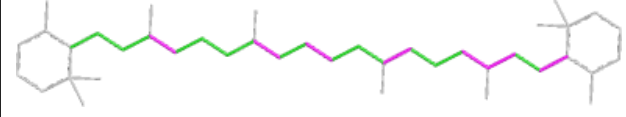
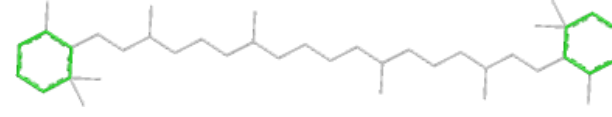


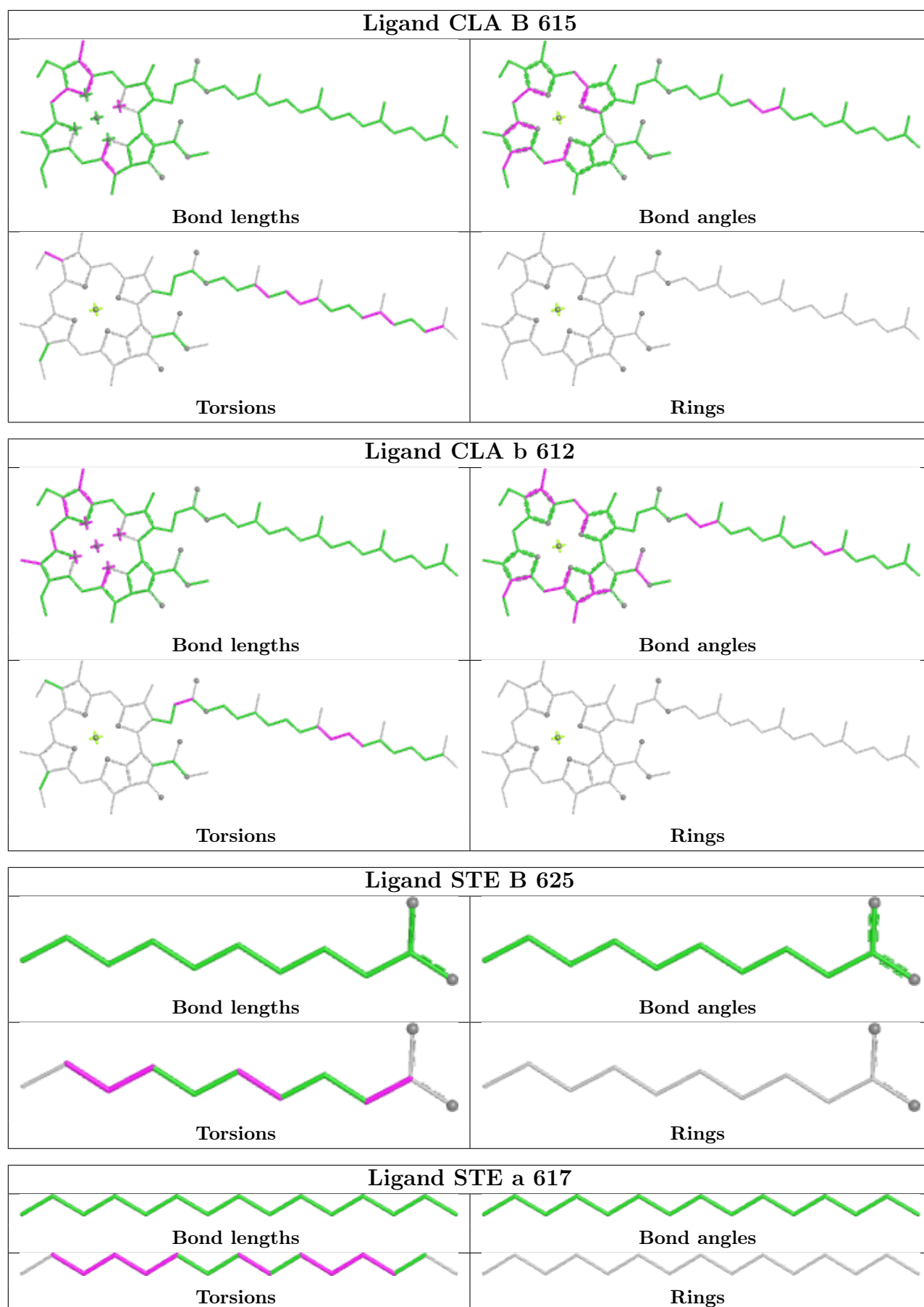


| Ligand BCR B 618                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand STE b 625                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

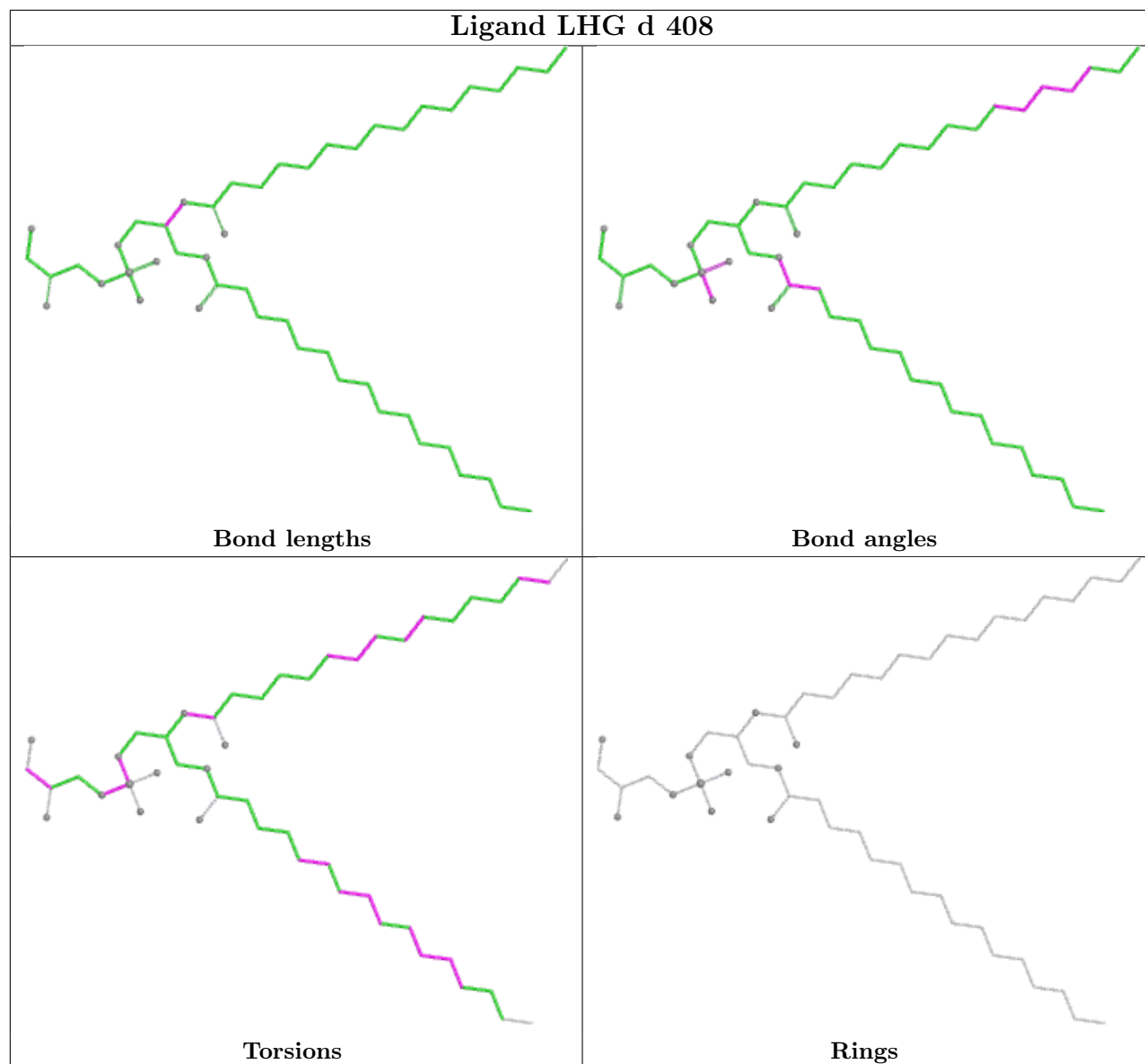
| Ligand CLA b 615                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR A 609                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

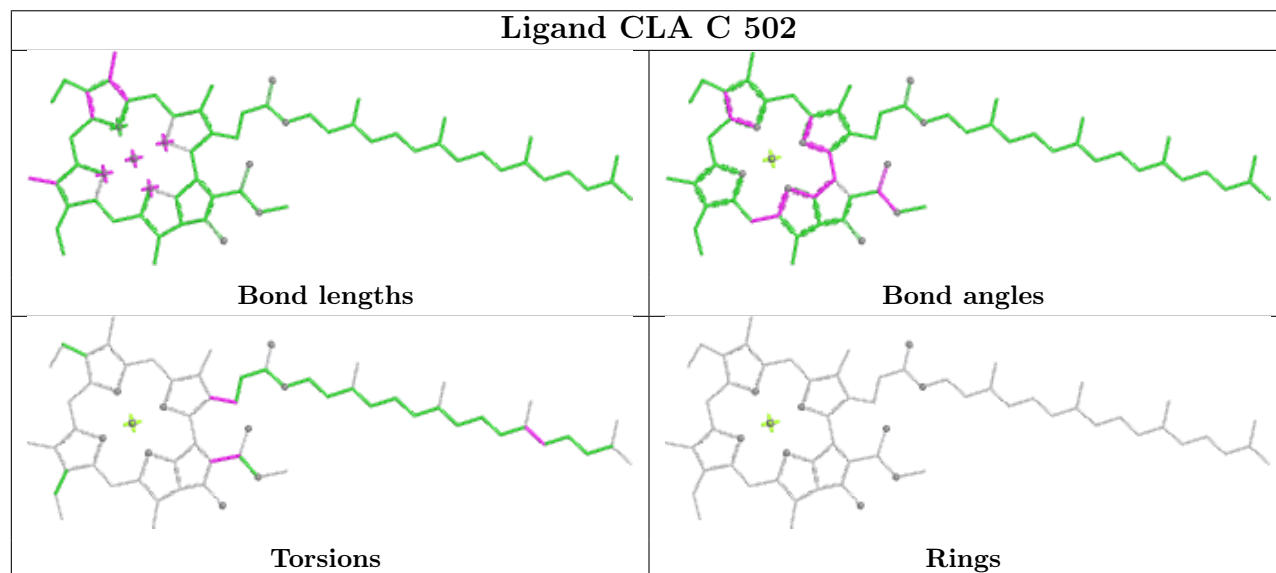


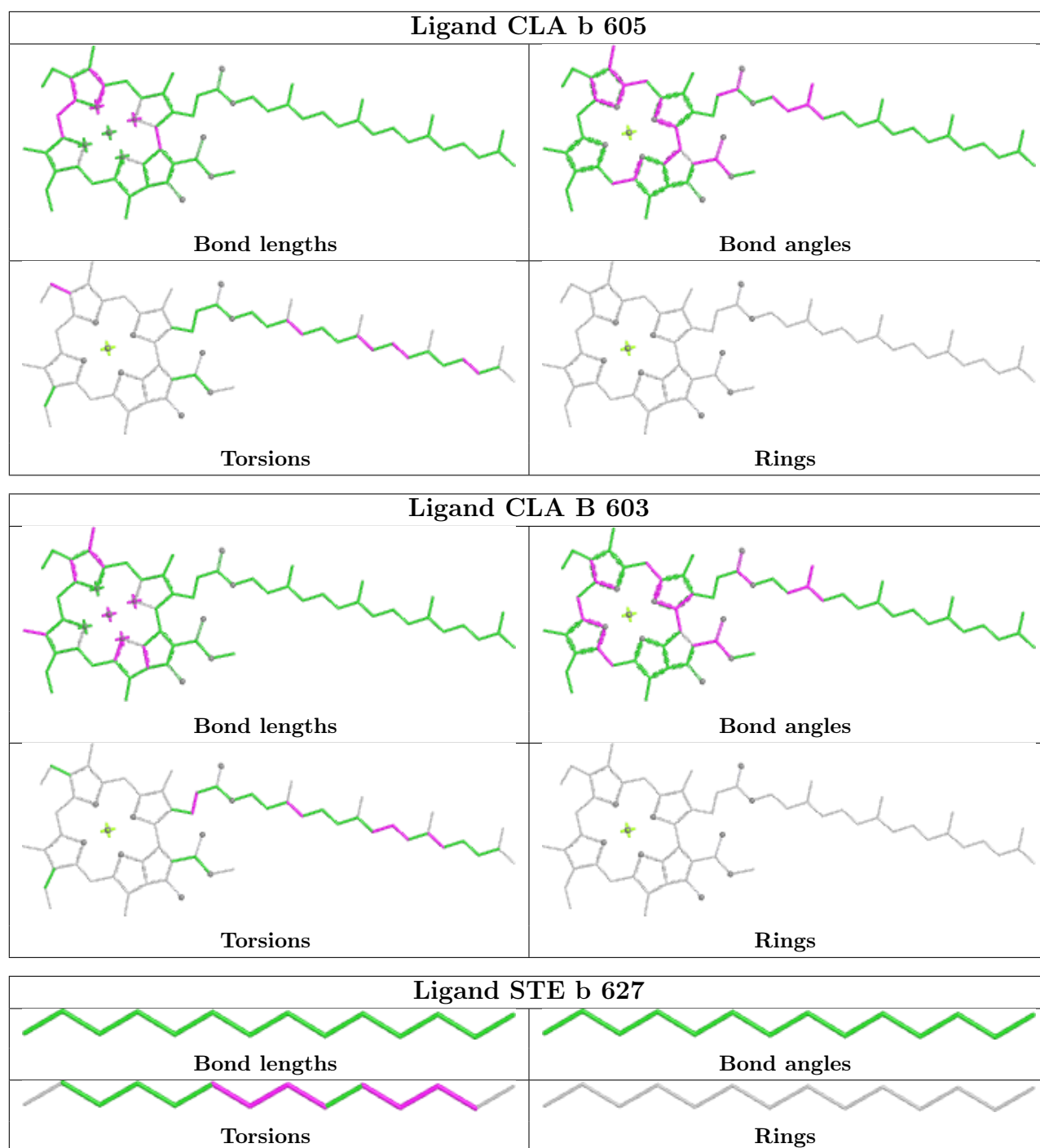


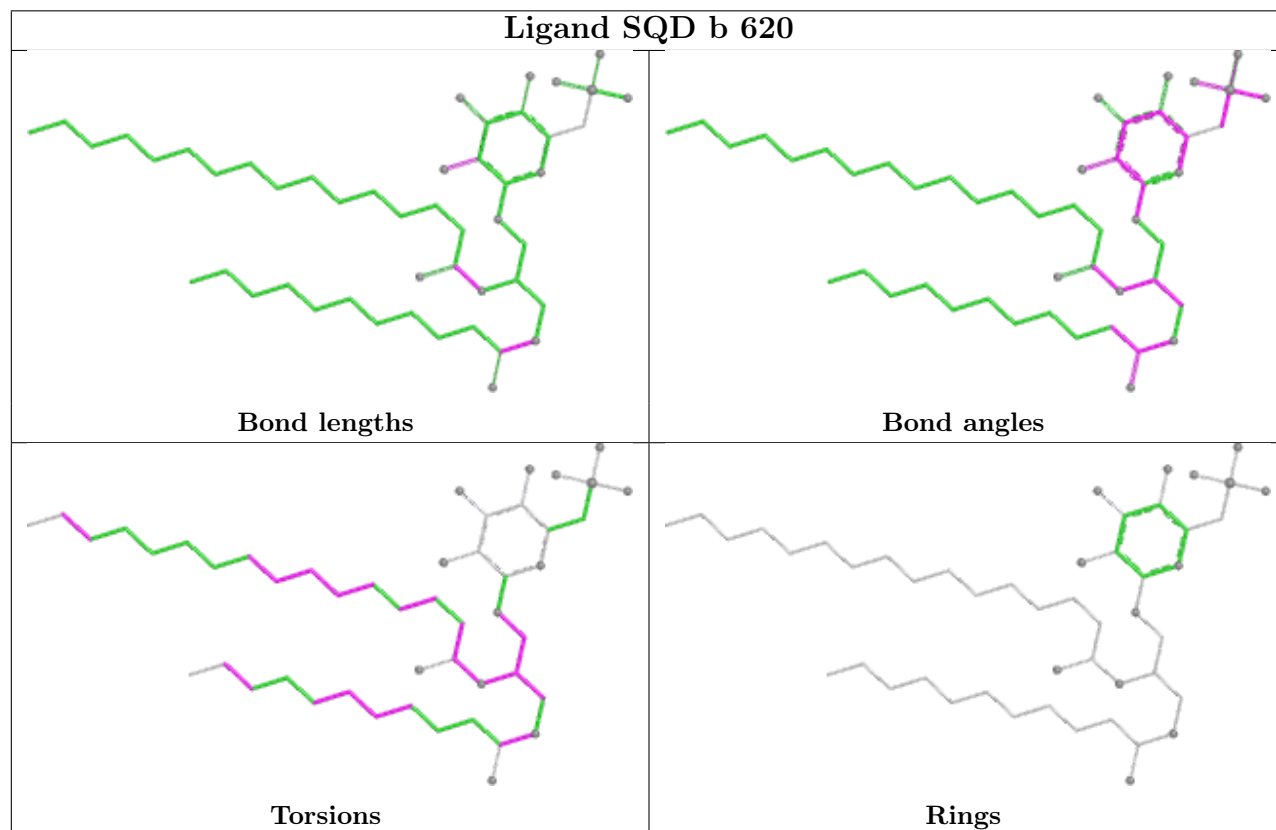
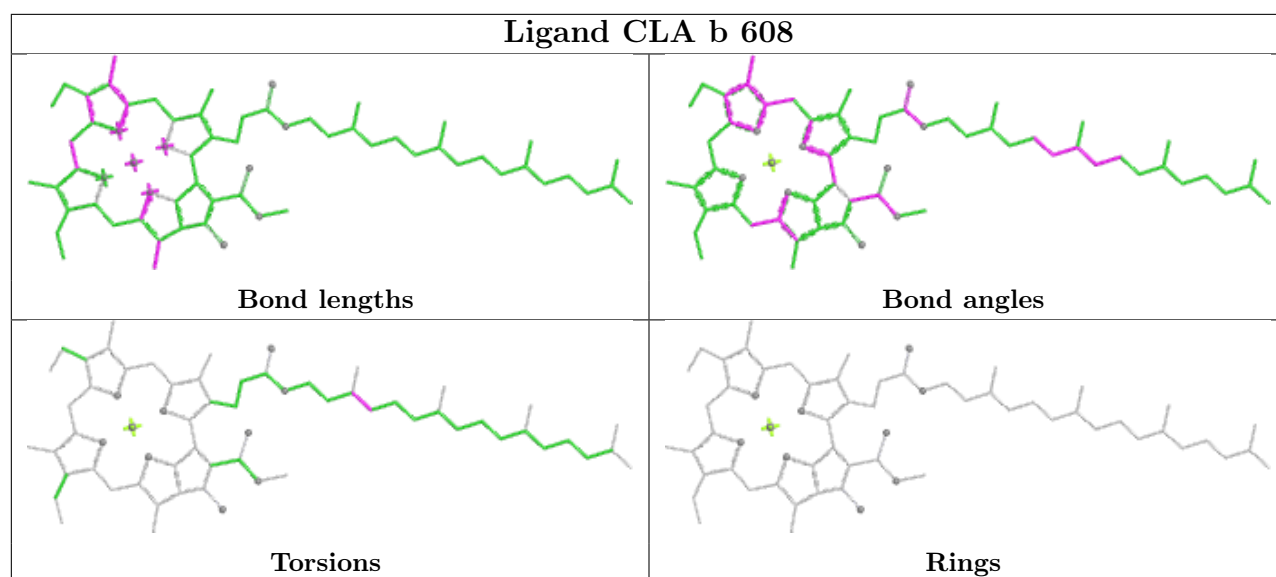
## Ligand LHG d 408

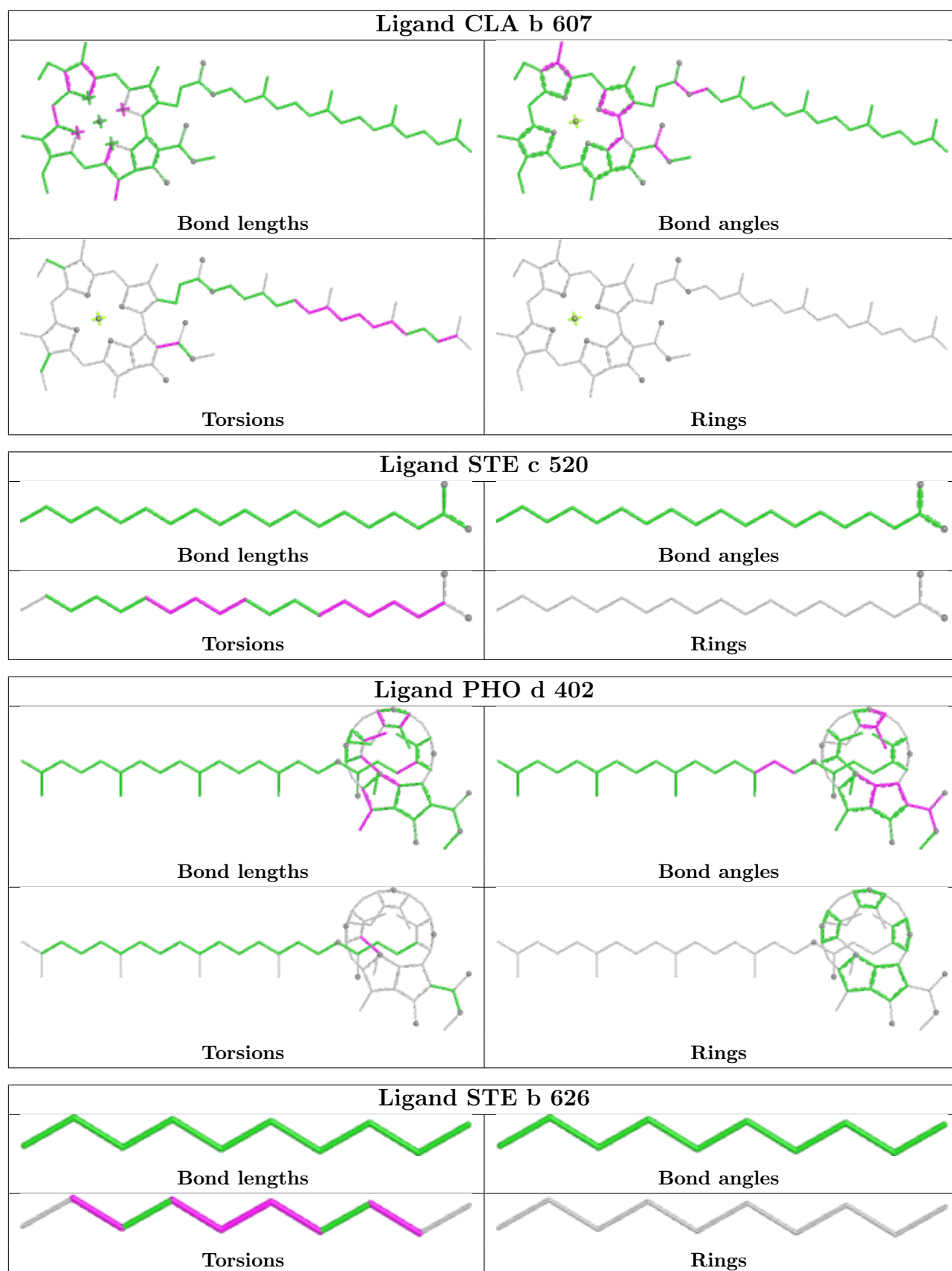


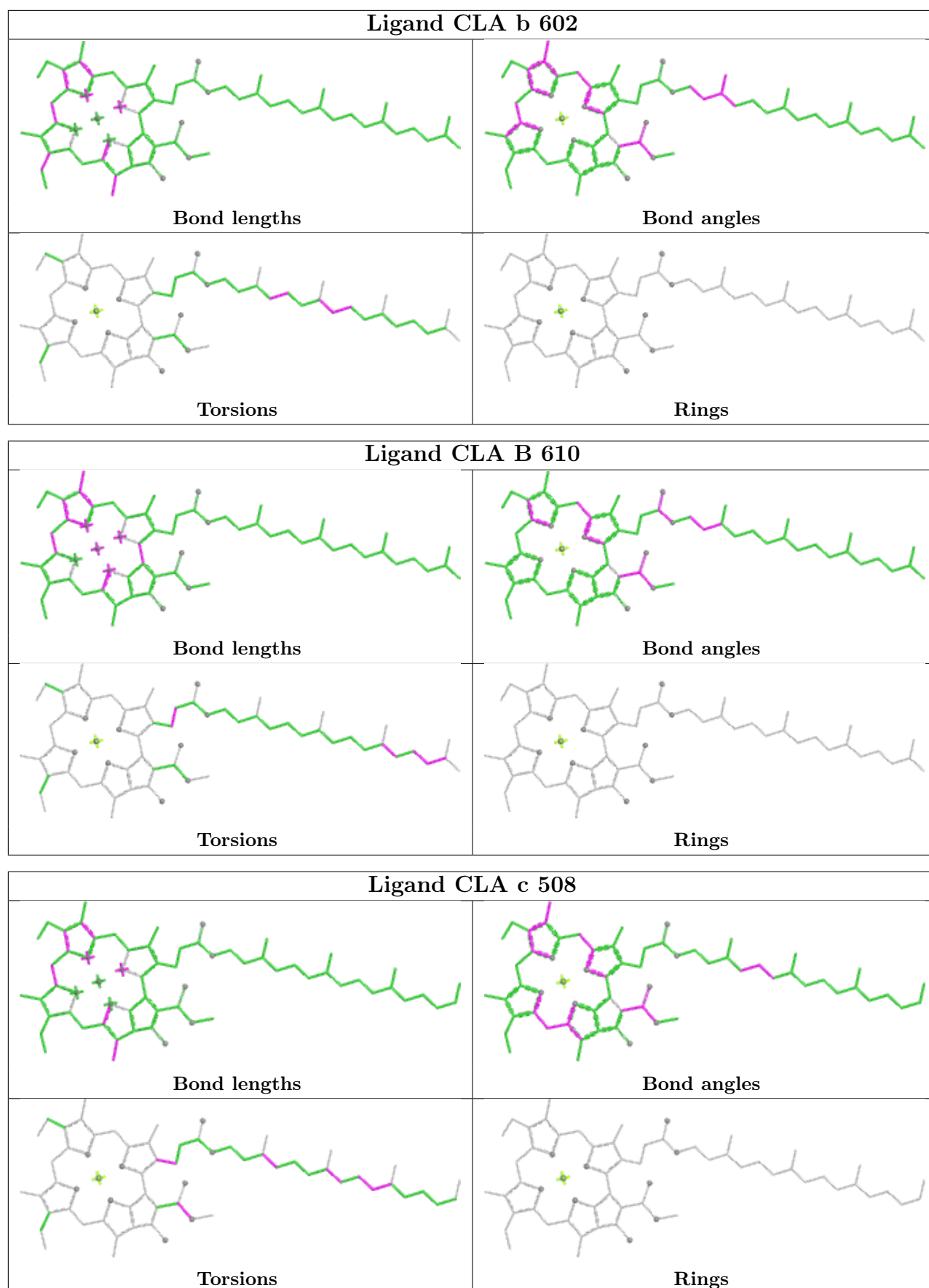
## Ligand CLA C 502

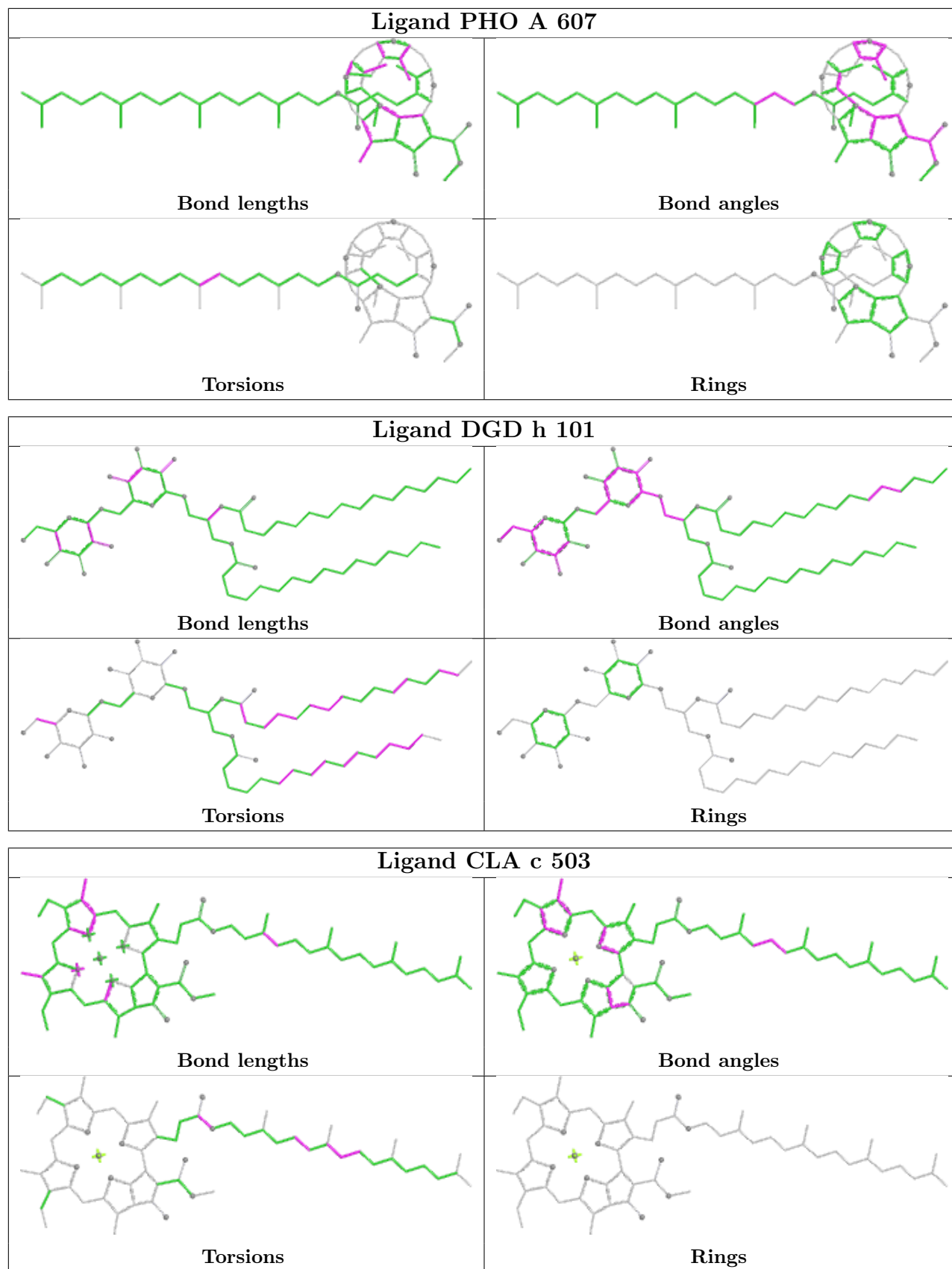


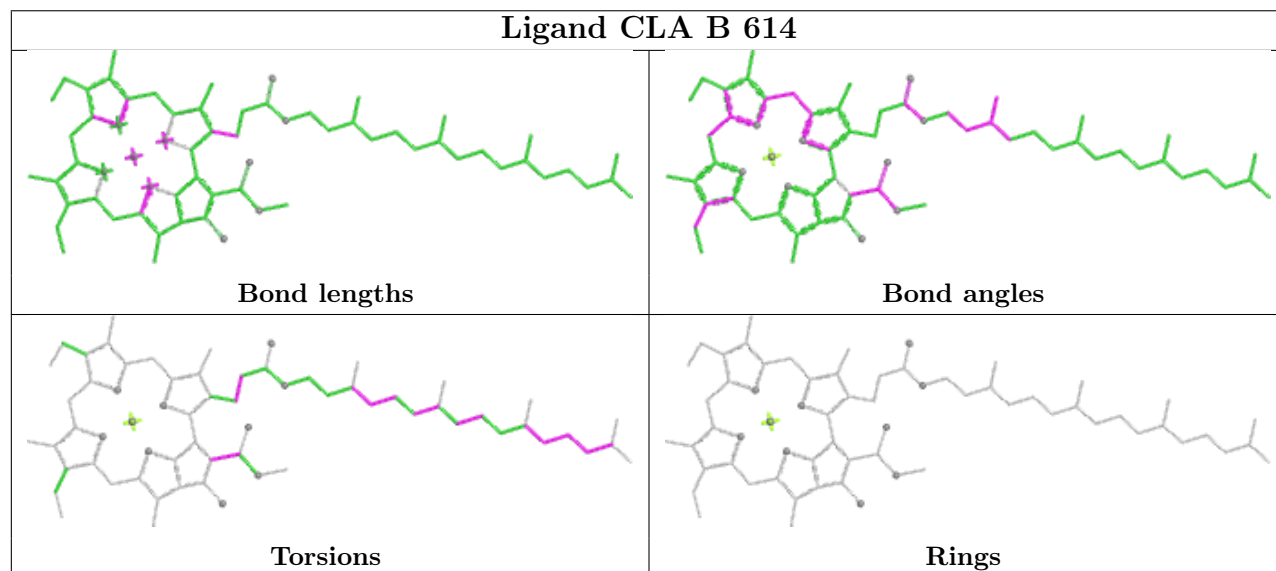
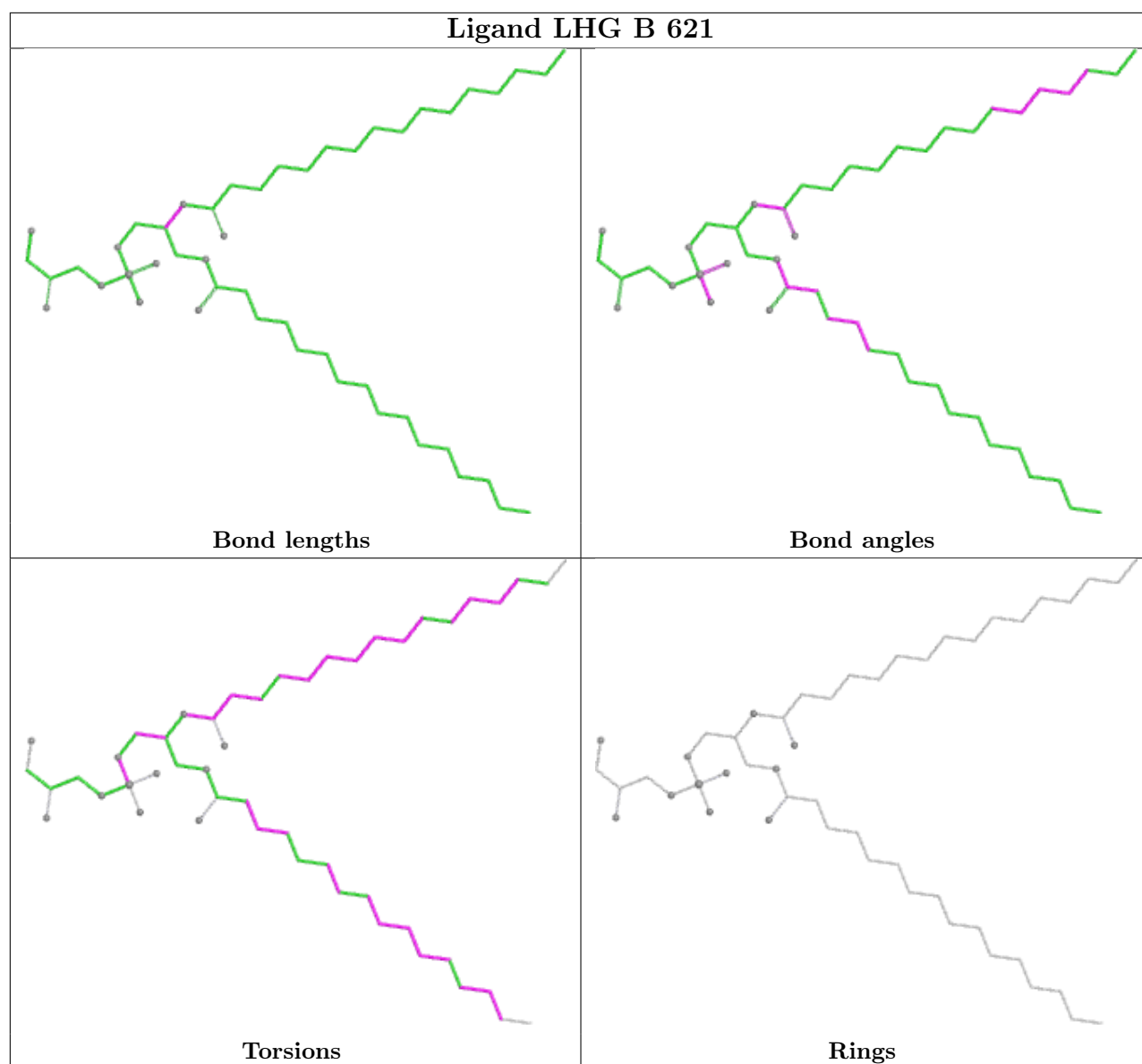




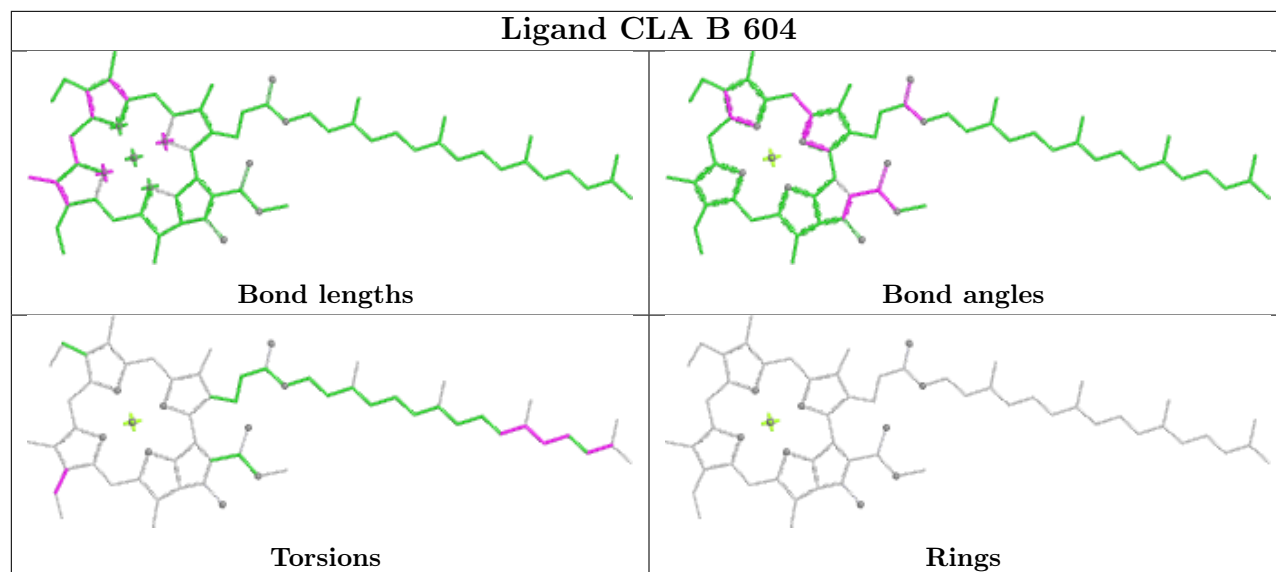




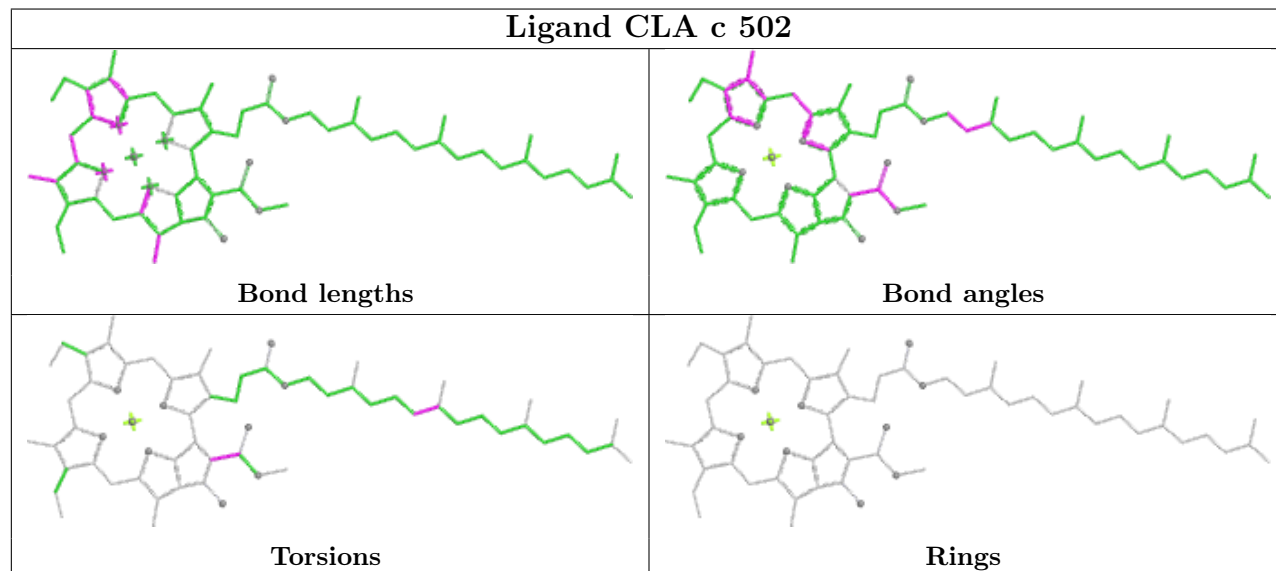




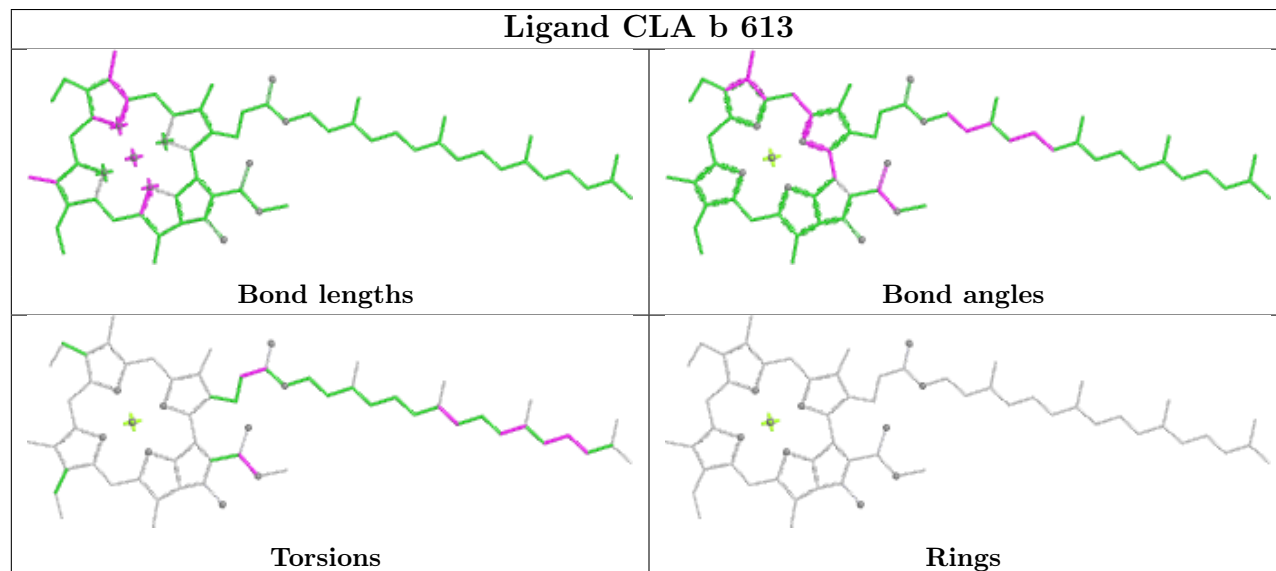
## Ligand CLA B 604



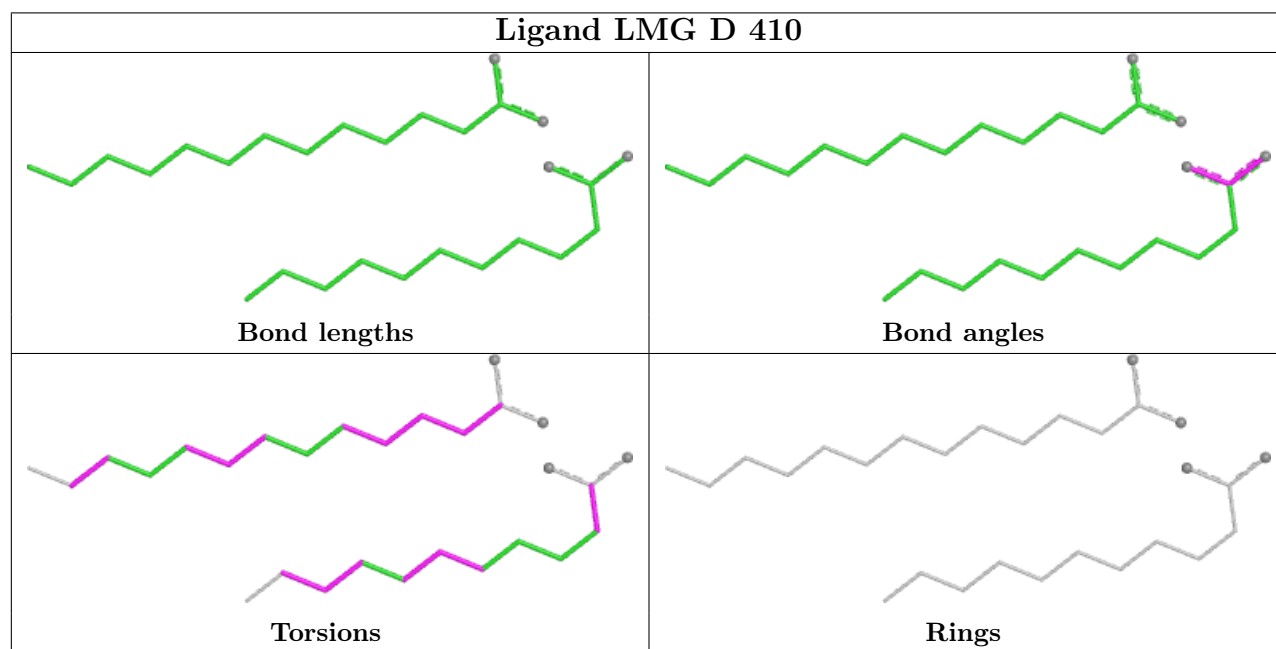
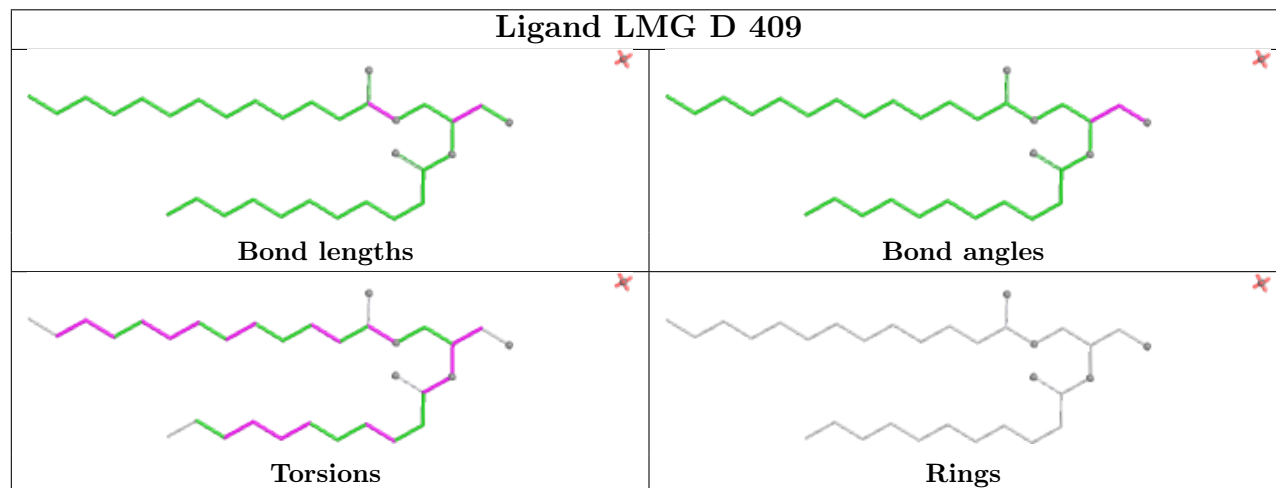
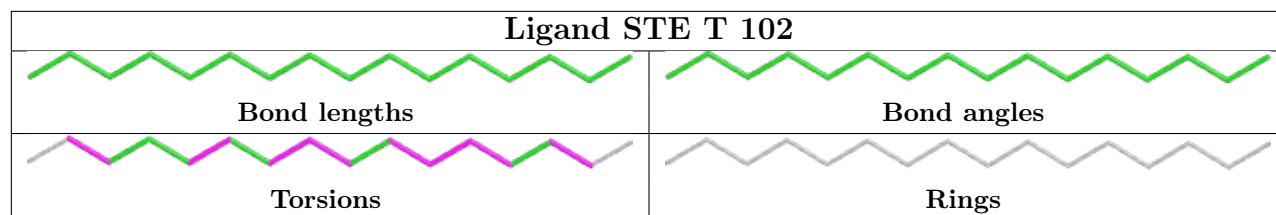
## Ligand CLA c 502



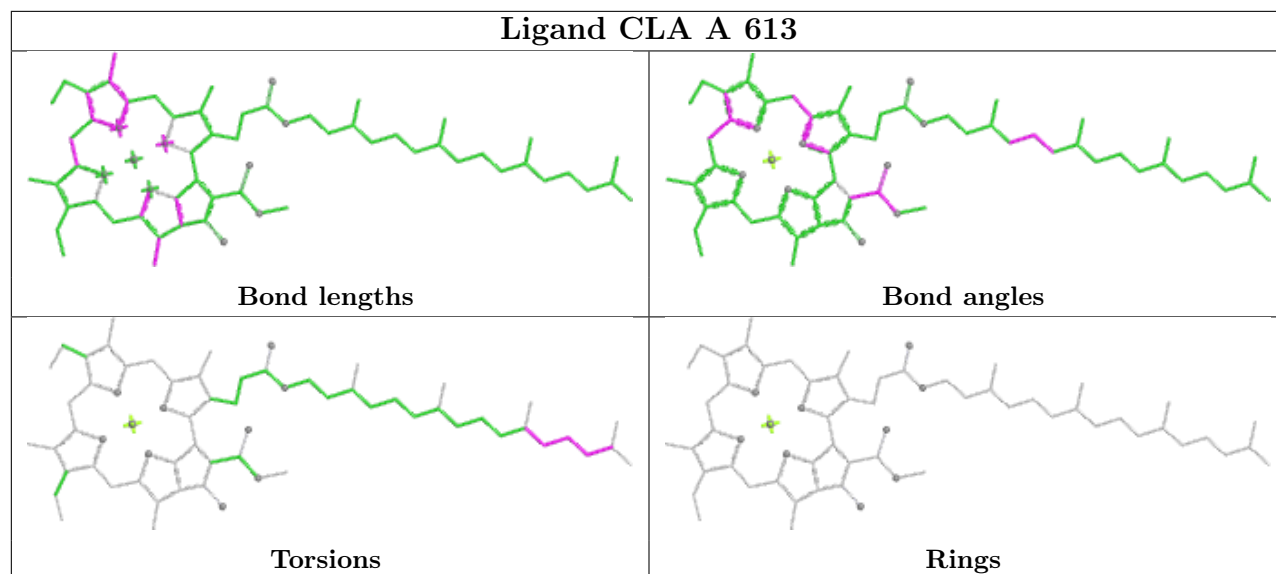
## Ligand CLA b 613



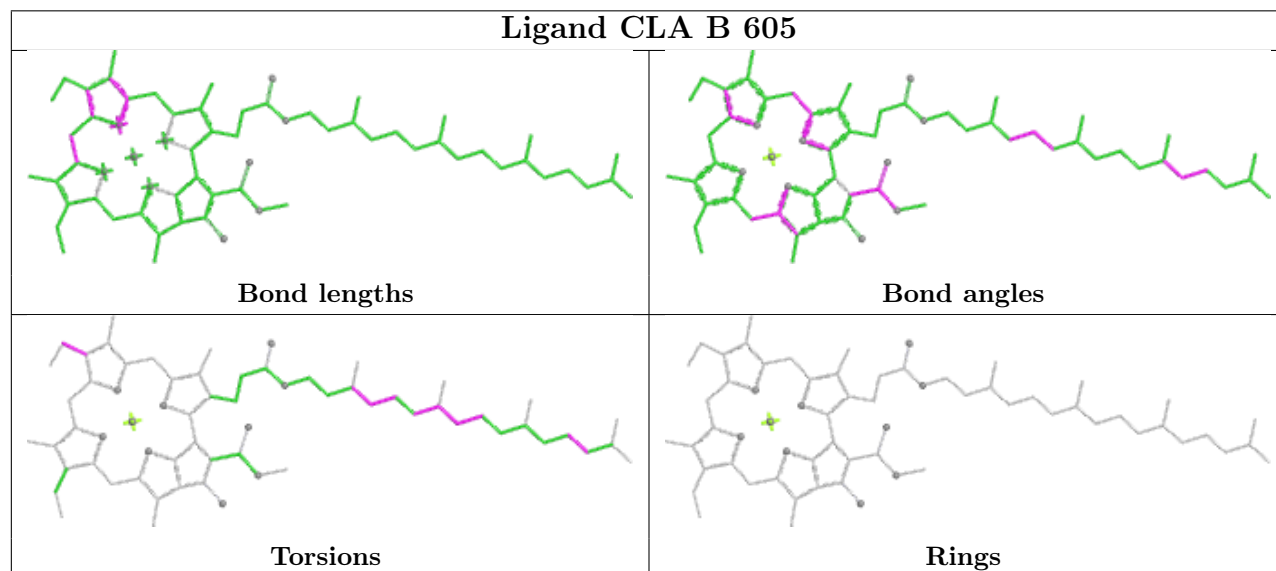




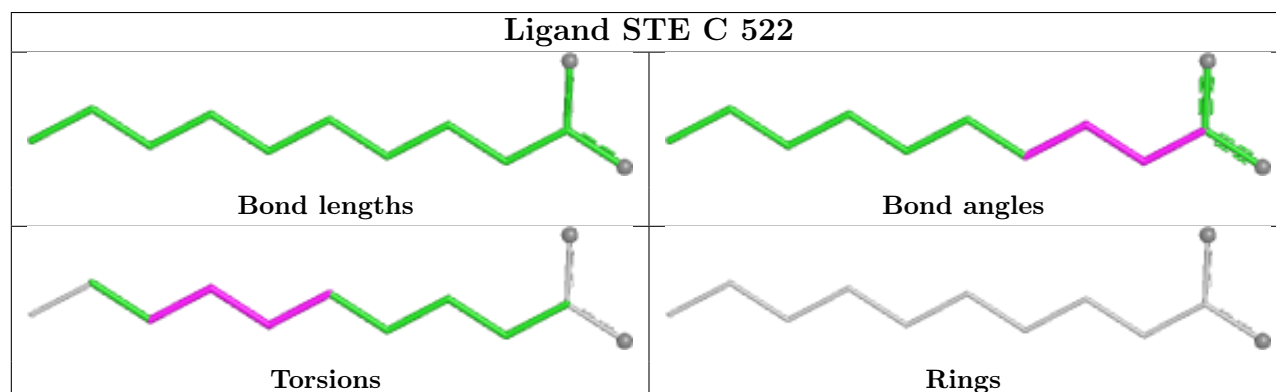
## Ligand CLA A 613

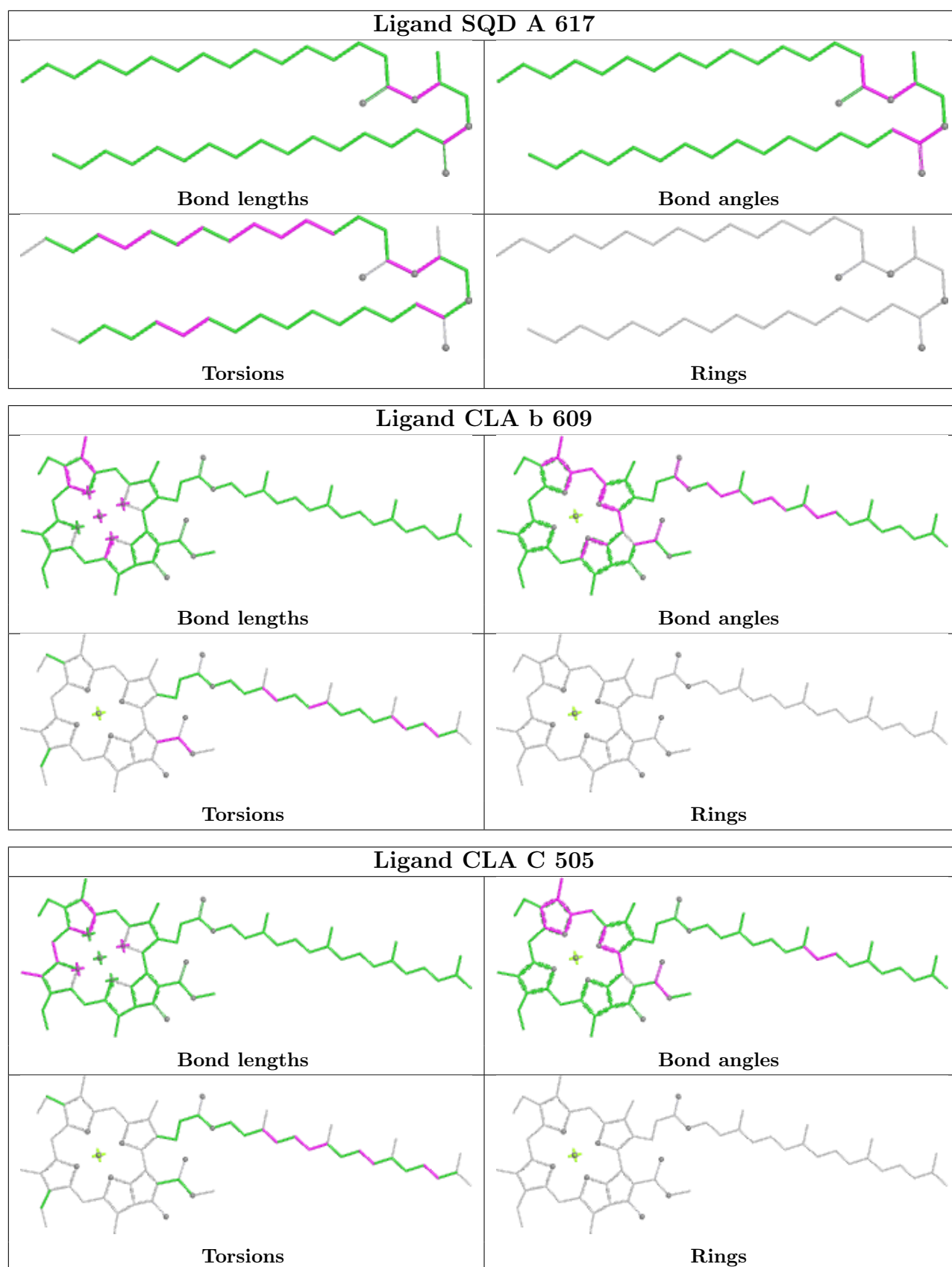


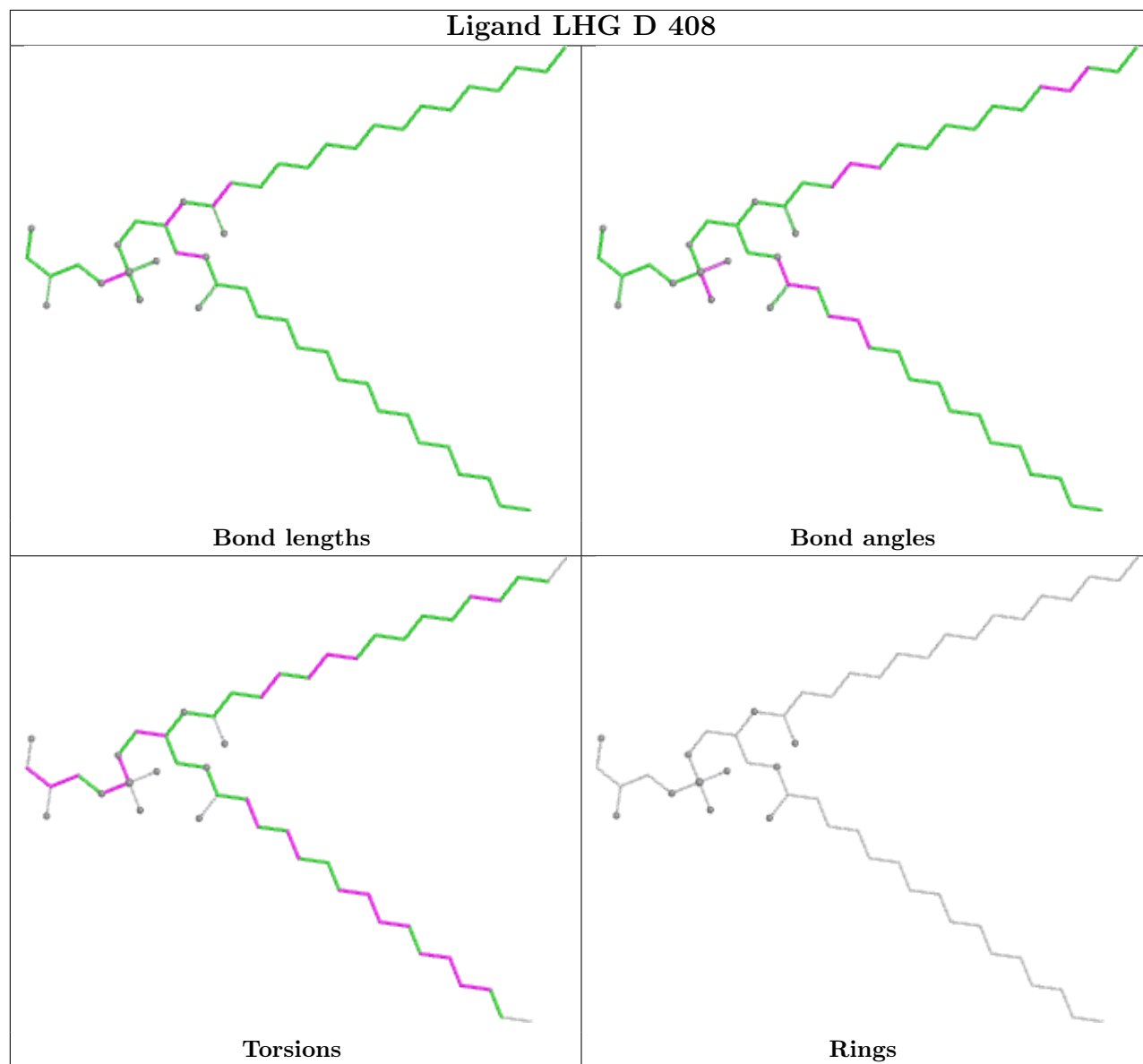
## Ligand CLA B 605

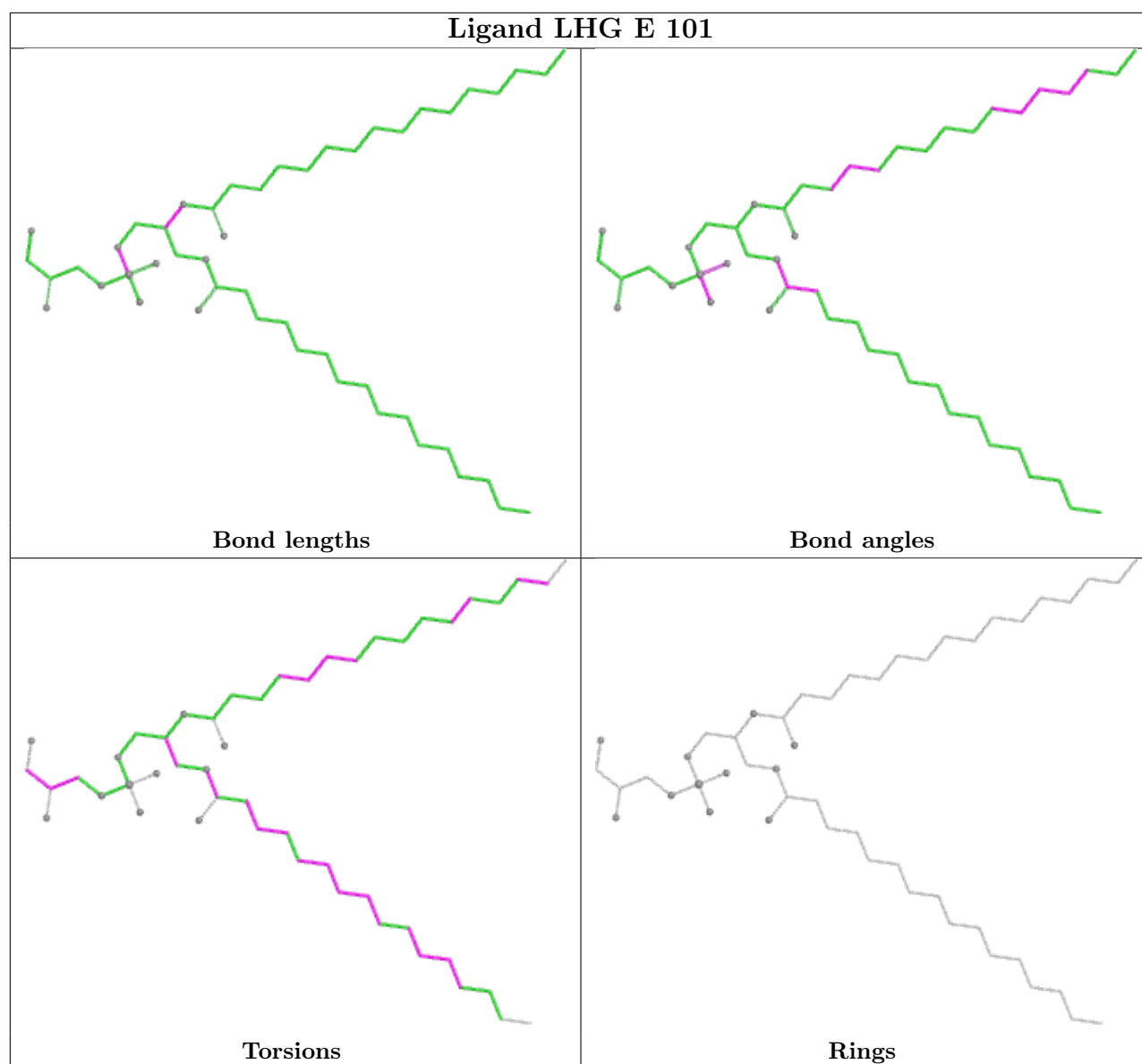


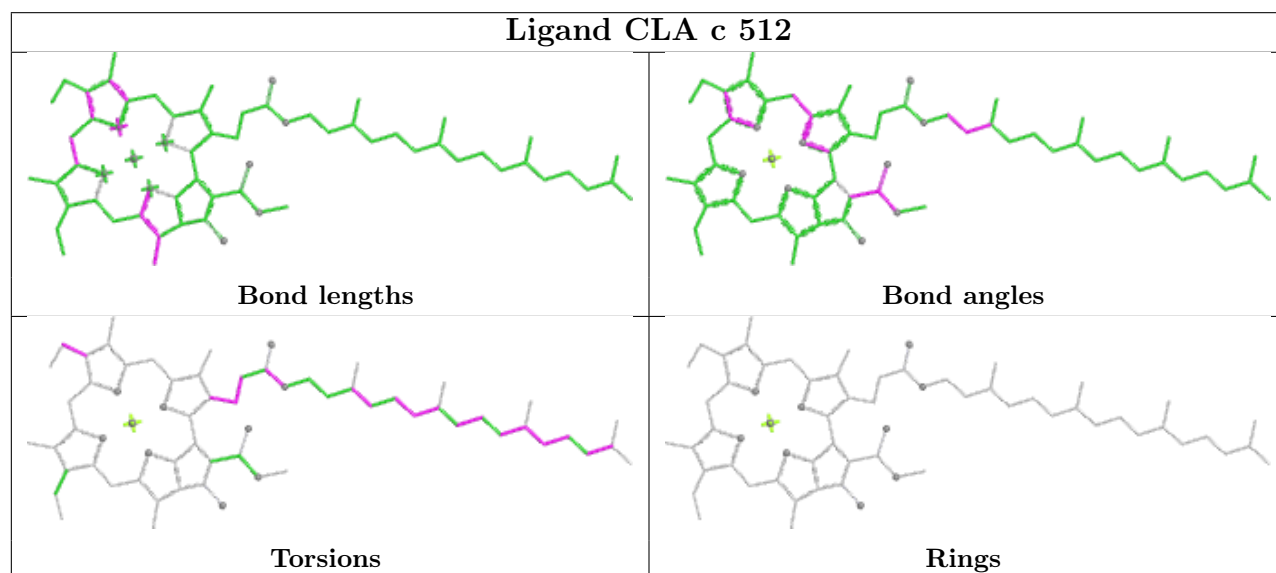
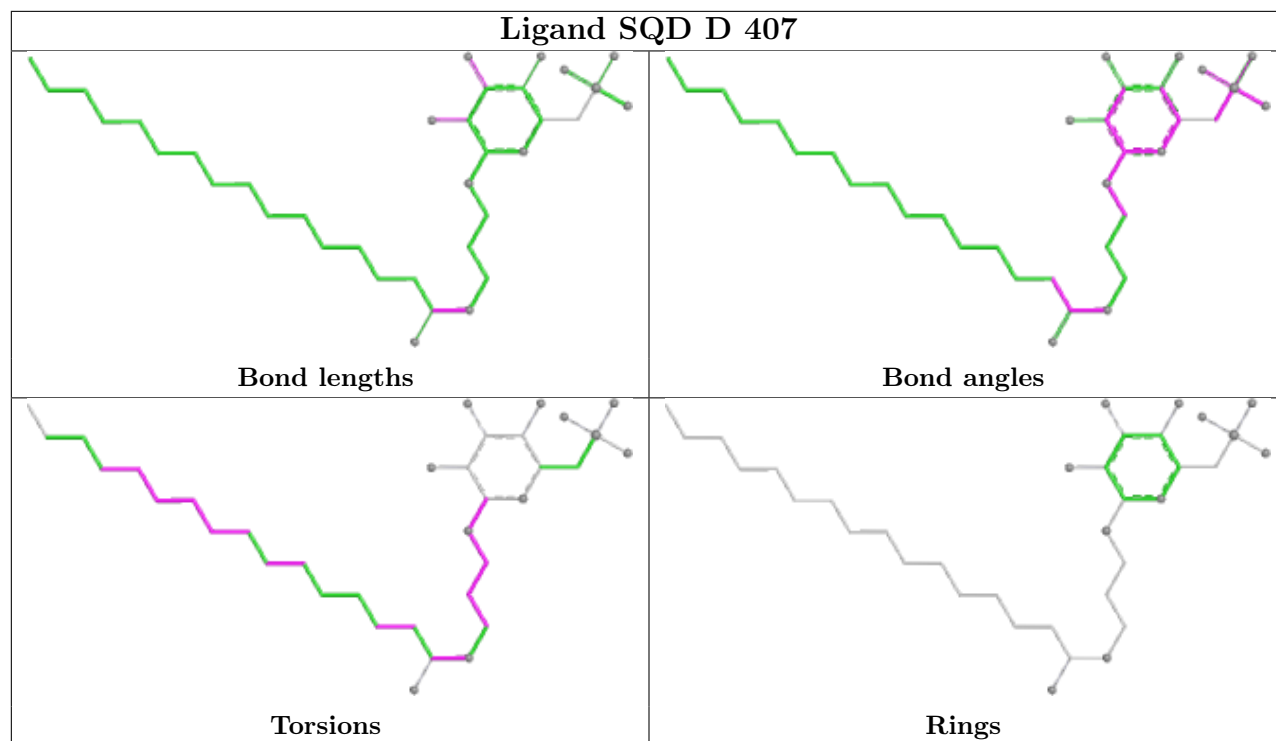
## Ligand STE C 522

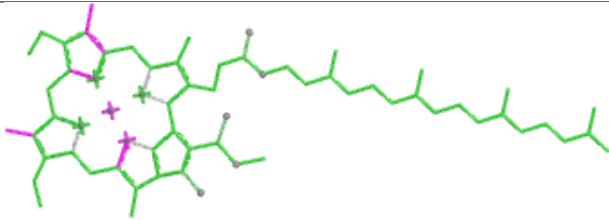
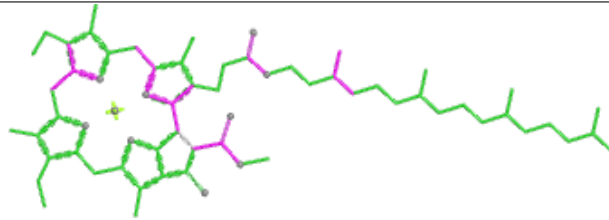
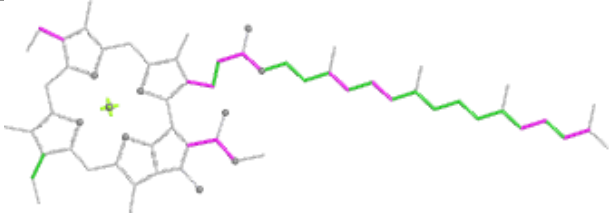
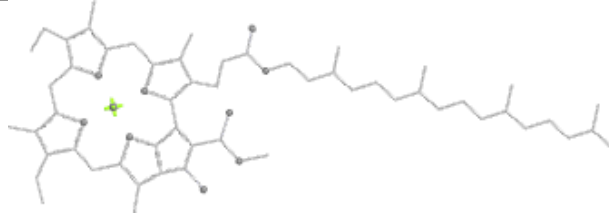


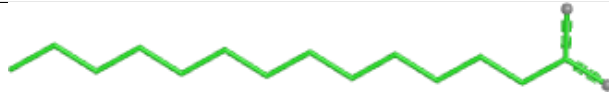
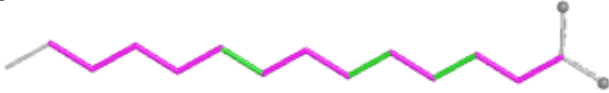
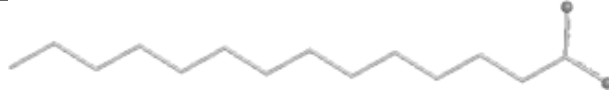


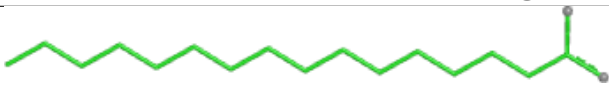
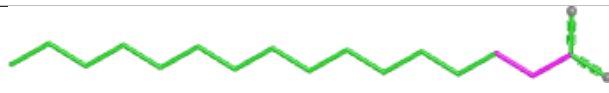
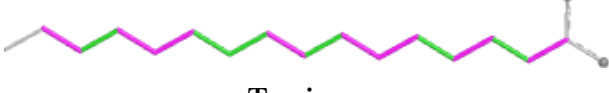
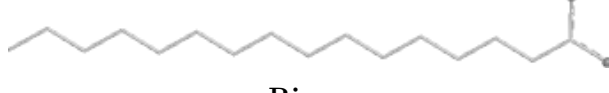


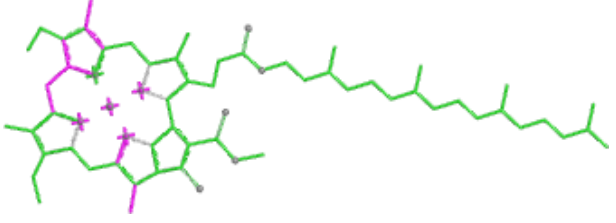
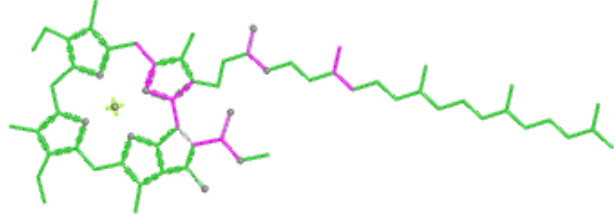
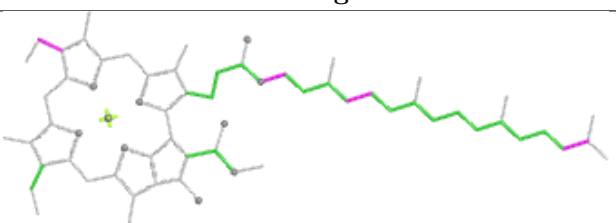
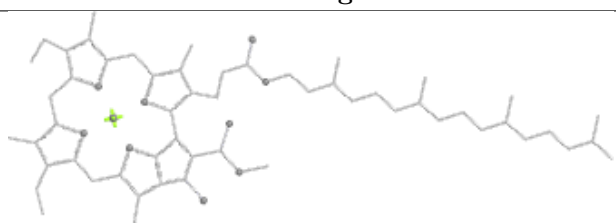
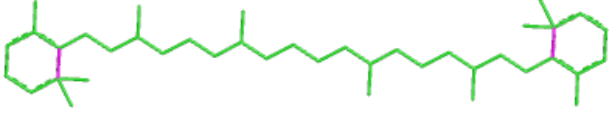
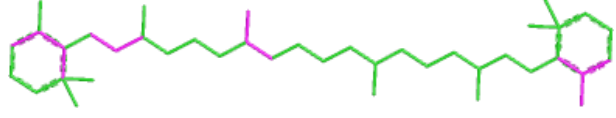
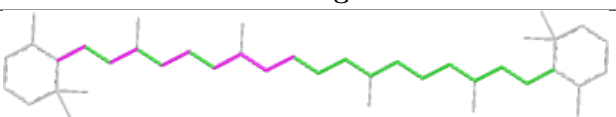
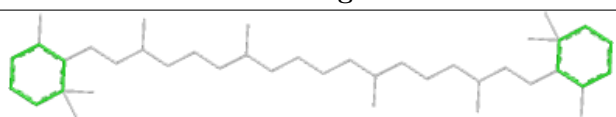
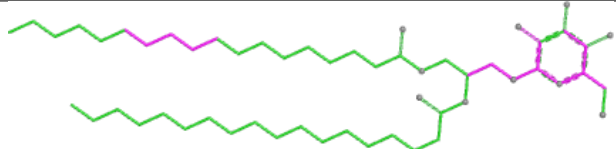
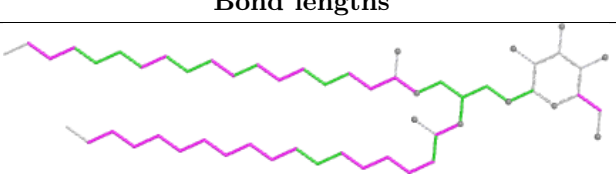
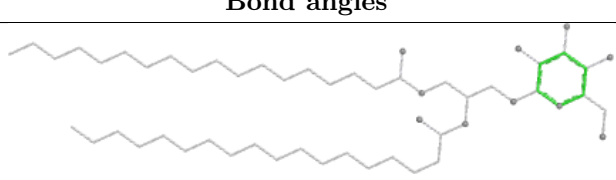




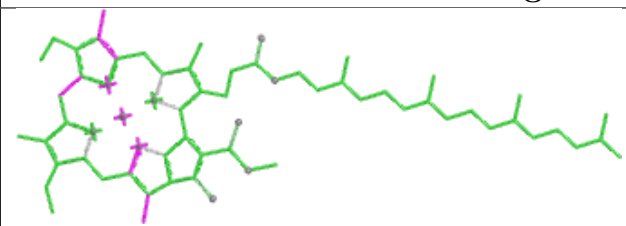
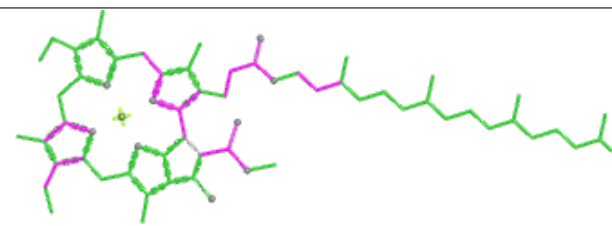
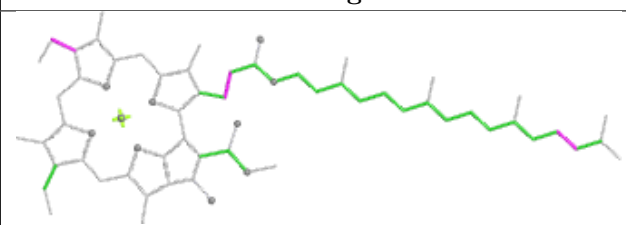
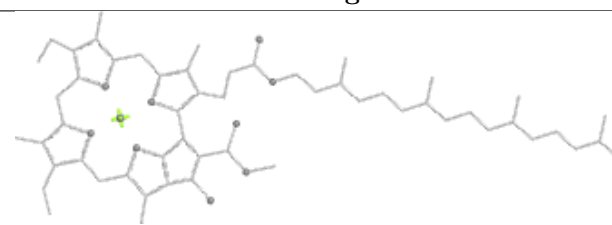
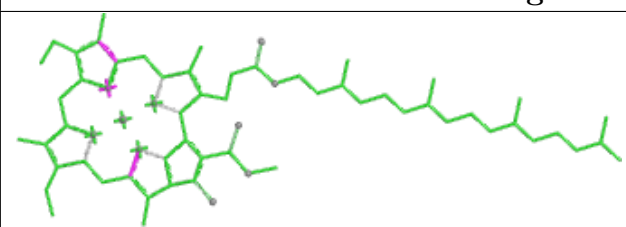
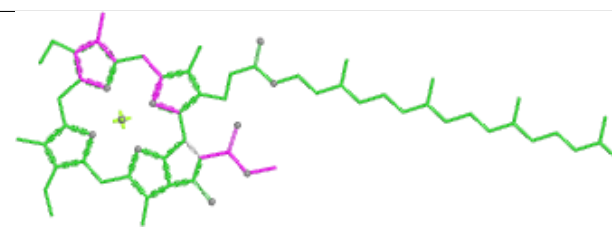
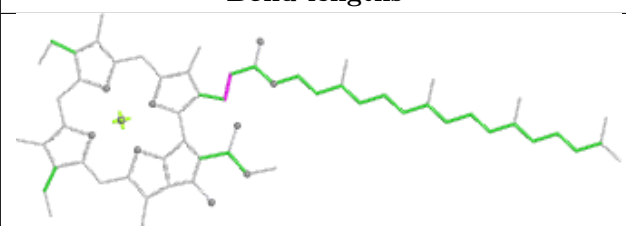
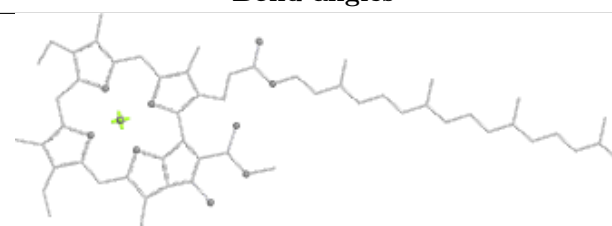
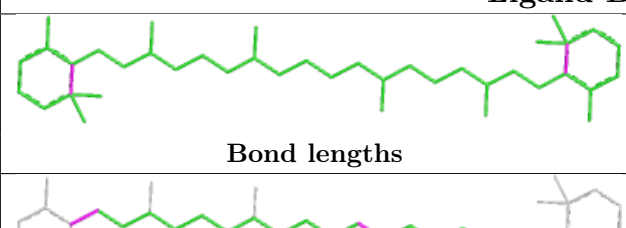
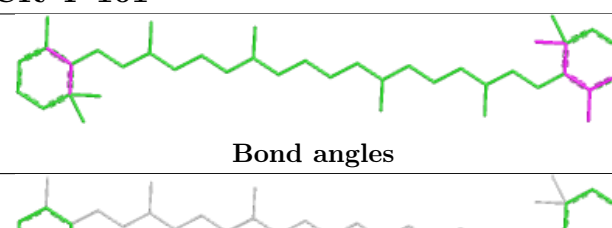
| Ligand CLA B 601                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

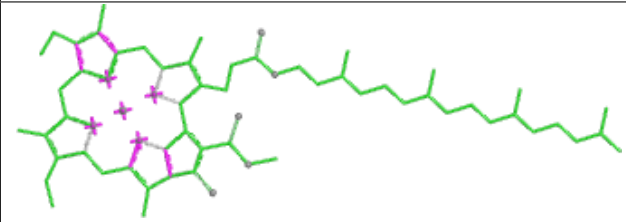
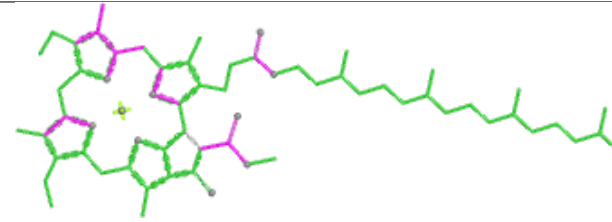
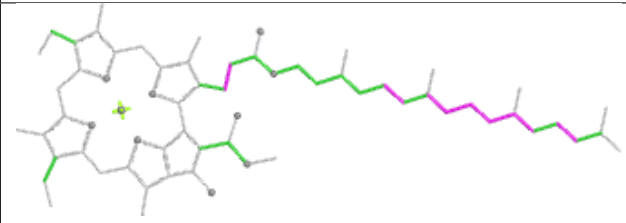
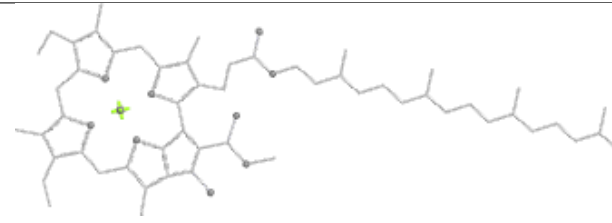
| Ligand STE b 624                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

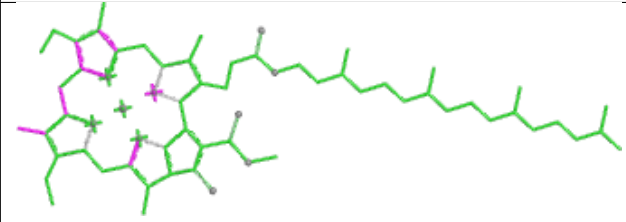
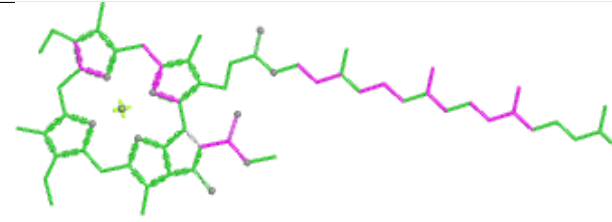
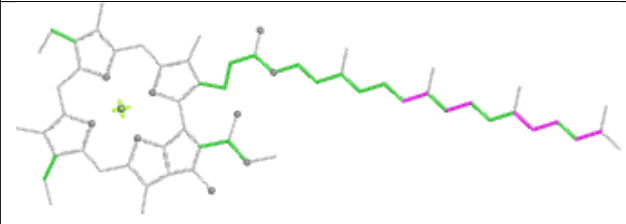
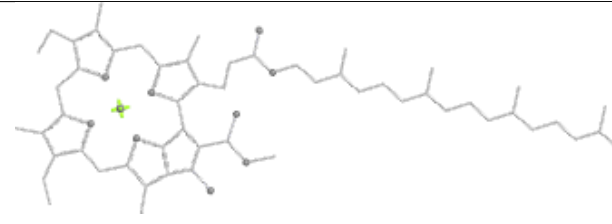
| Ligand STE t 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

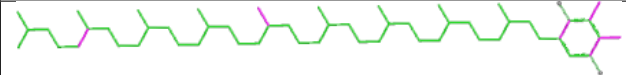
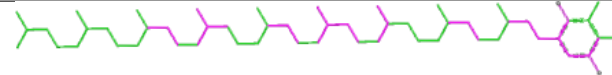
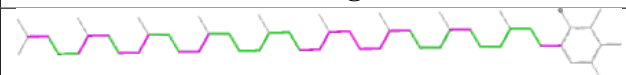
| Ligand CLA d 403                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR T 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG b 623                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

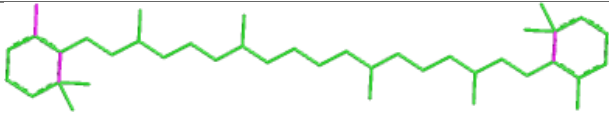
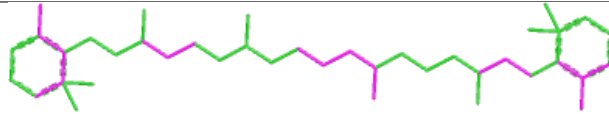
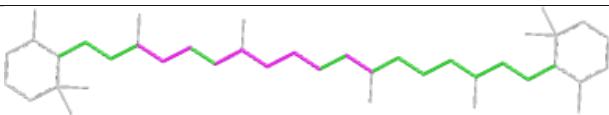
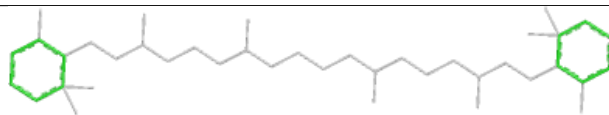


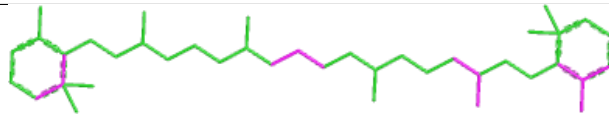
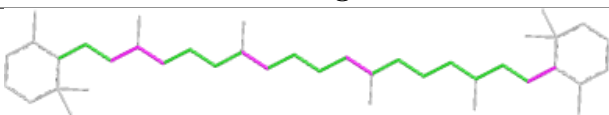
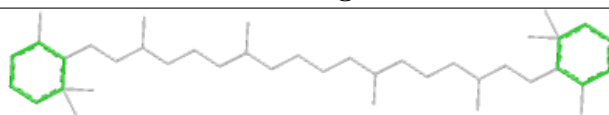
| Ligand CLA b 610                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|    |    |
| Torsions                                                                            | Rings                                                                                |
| Ligand CLA c 501                                                                    |                                                                                      |
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |
| Ligand BCR Y 101                                                                    |                                                                                      |
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

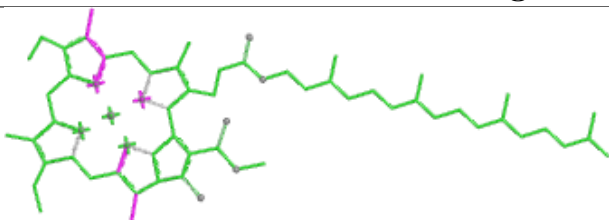
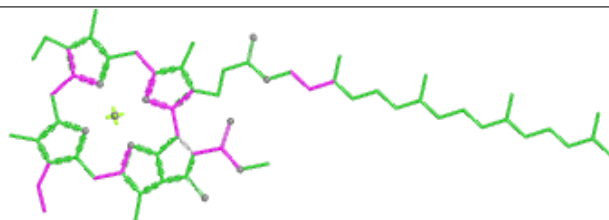
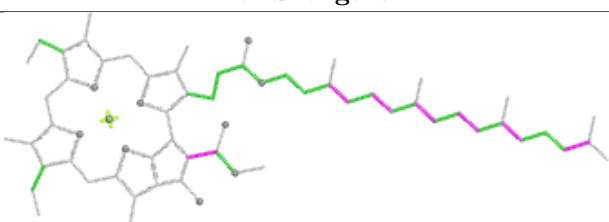
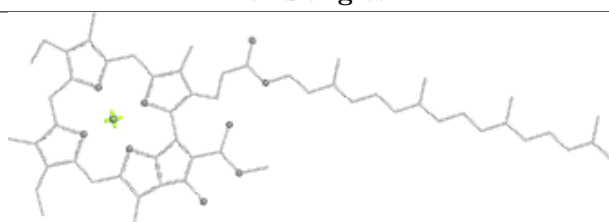
| Ligand CLA b 606                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

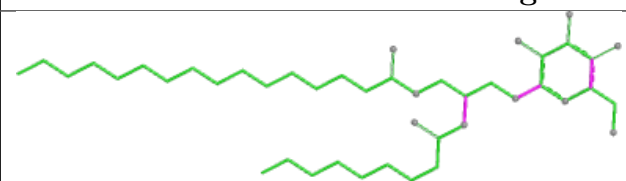
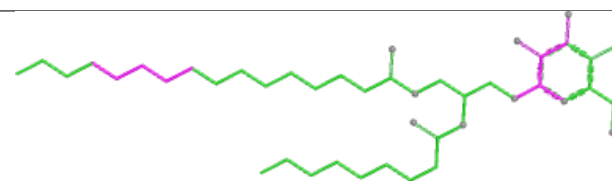
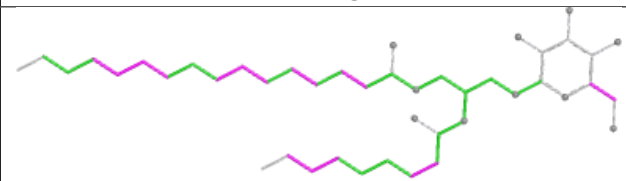
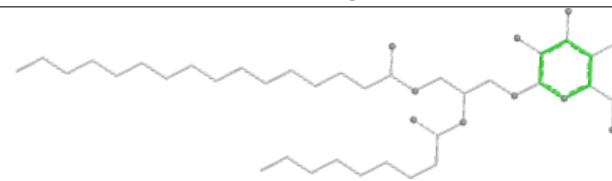
| Ligand CLA B 611                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

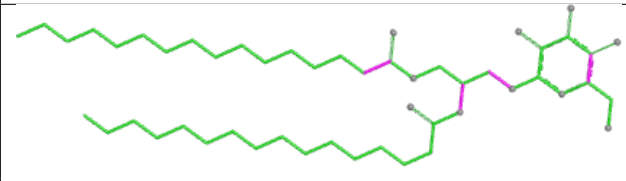
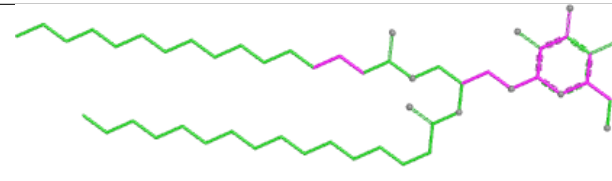
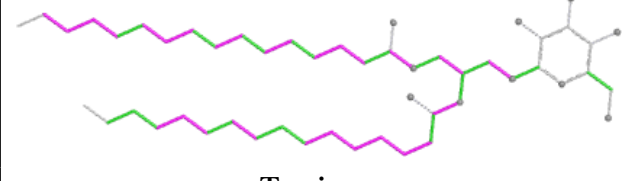
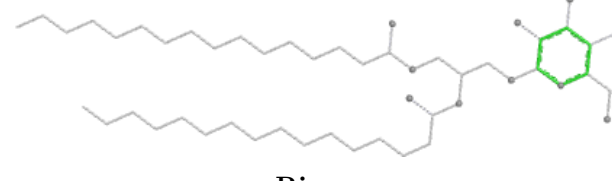
| Ligand PL9 a 611                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR C 514                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

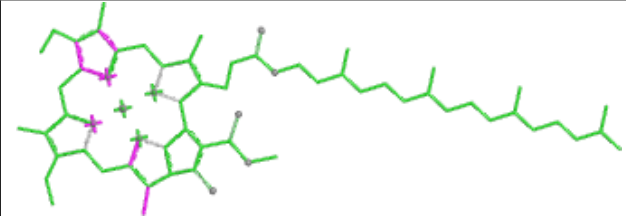
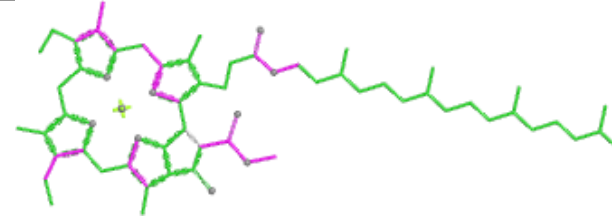
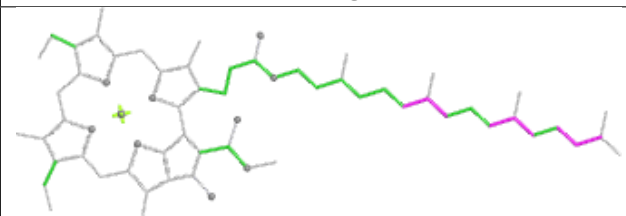
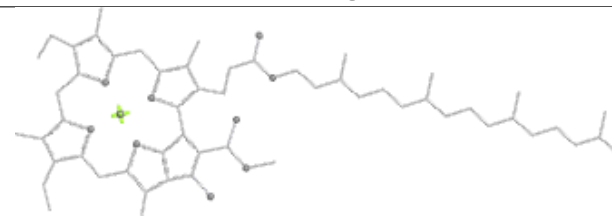
| Ligand BCR x 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

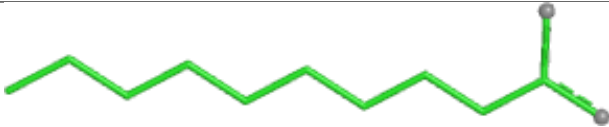
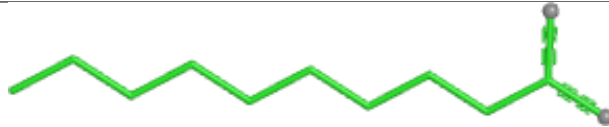
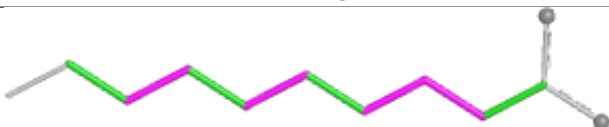
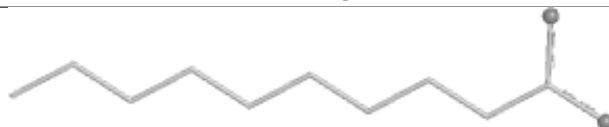
| Ligand CLA C 507                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

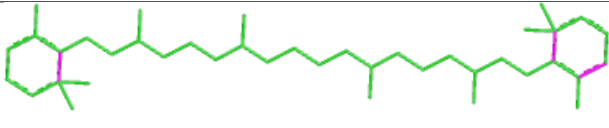
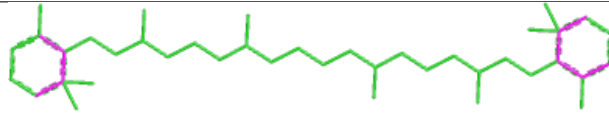
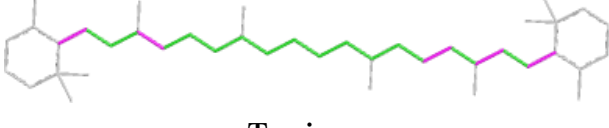
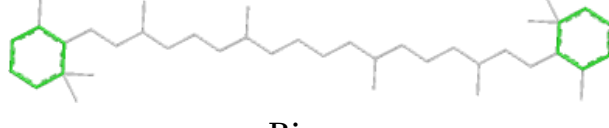
| Ligand LMG d 410                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

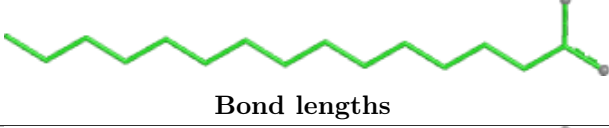
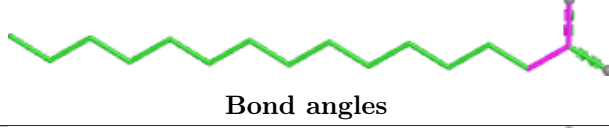
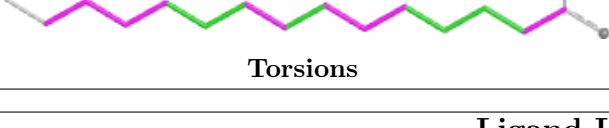
| Ligand LMG M 101                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

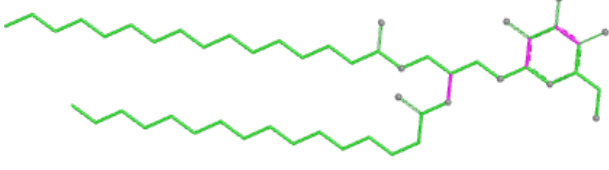
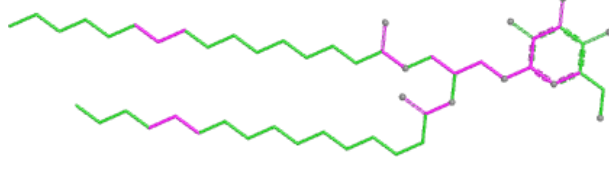
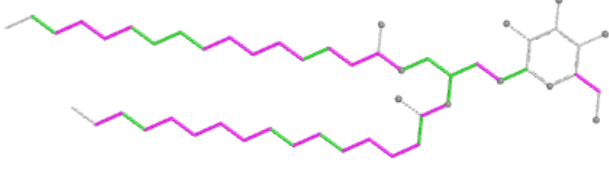
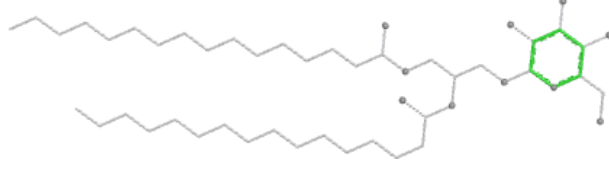
| Ligand STE l 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

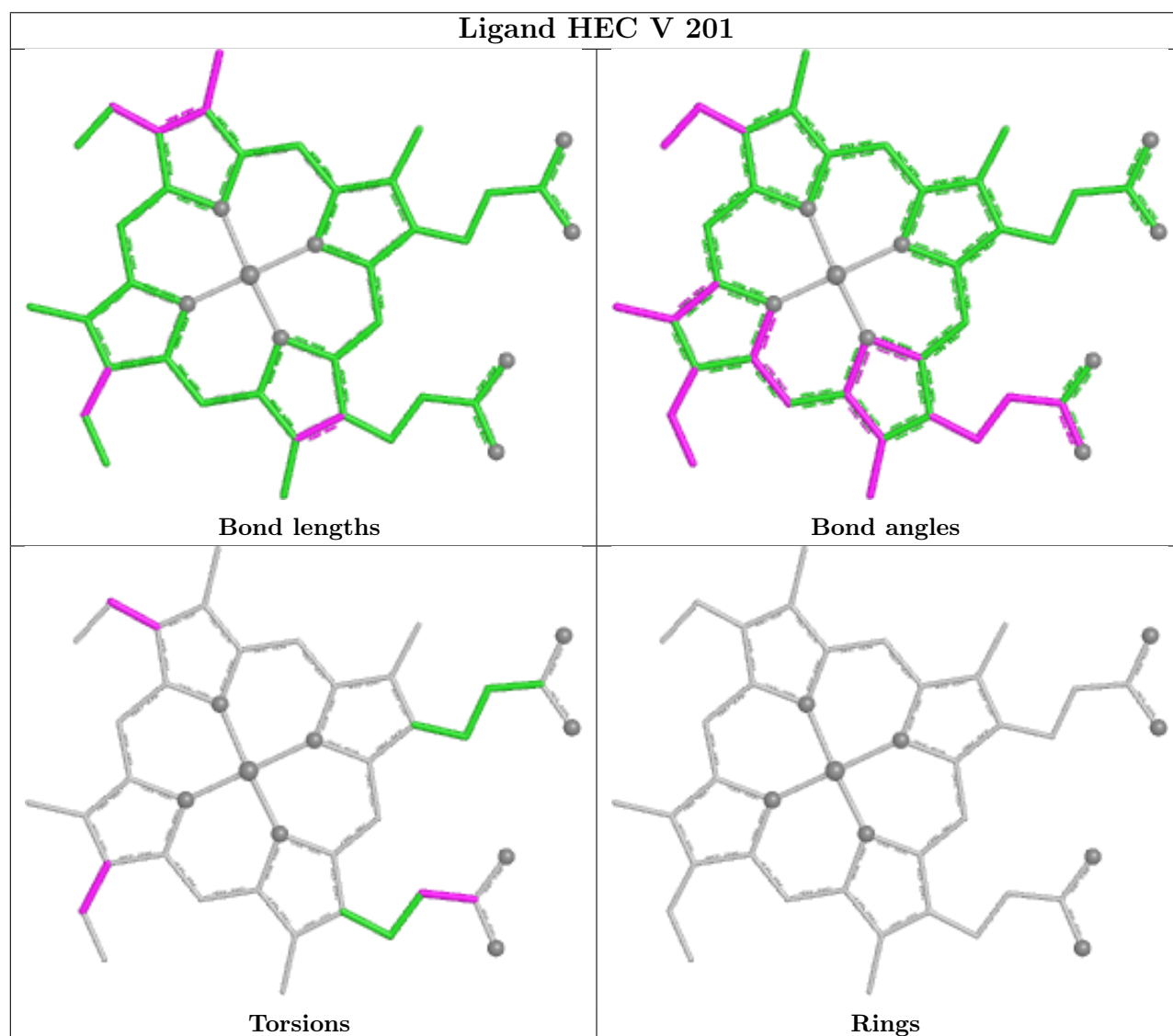
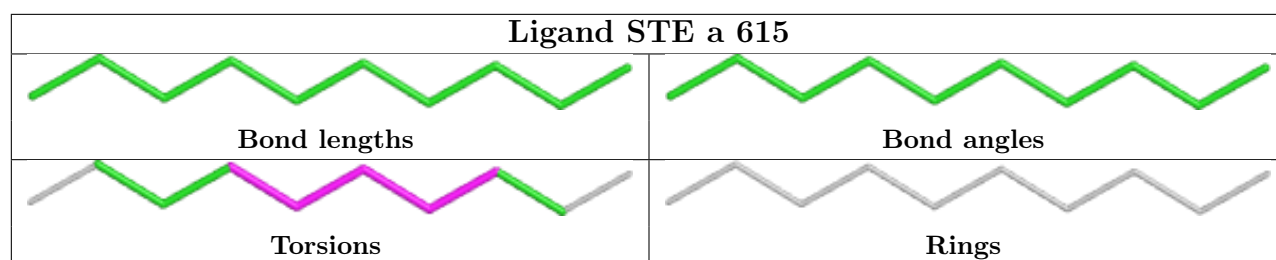
| Ligand CLA A 605                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

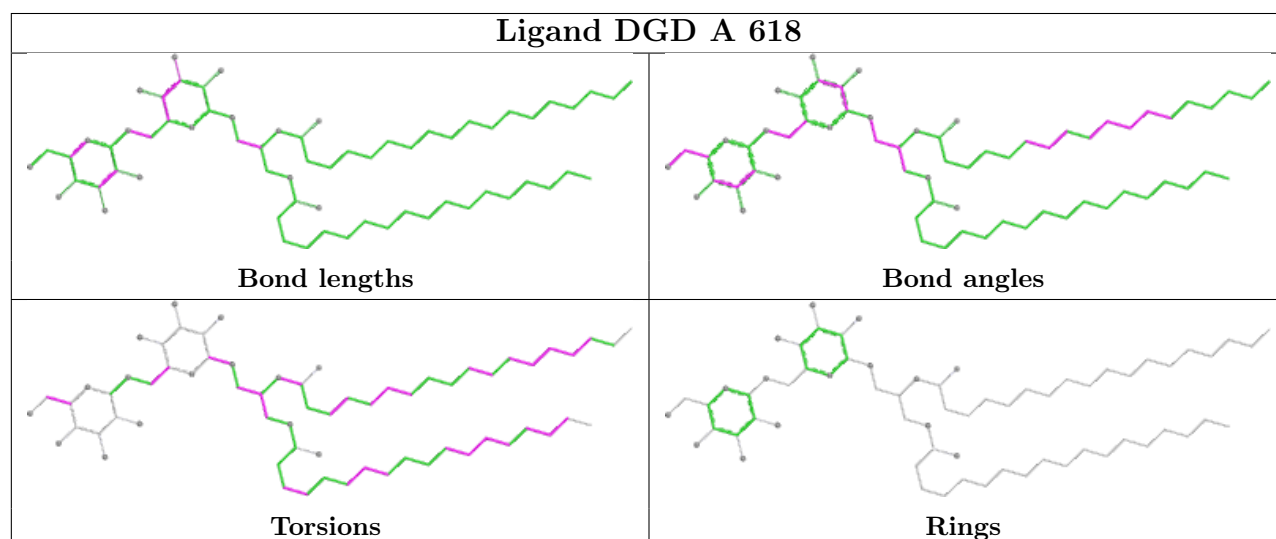
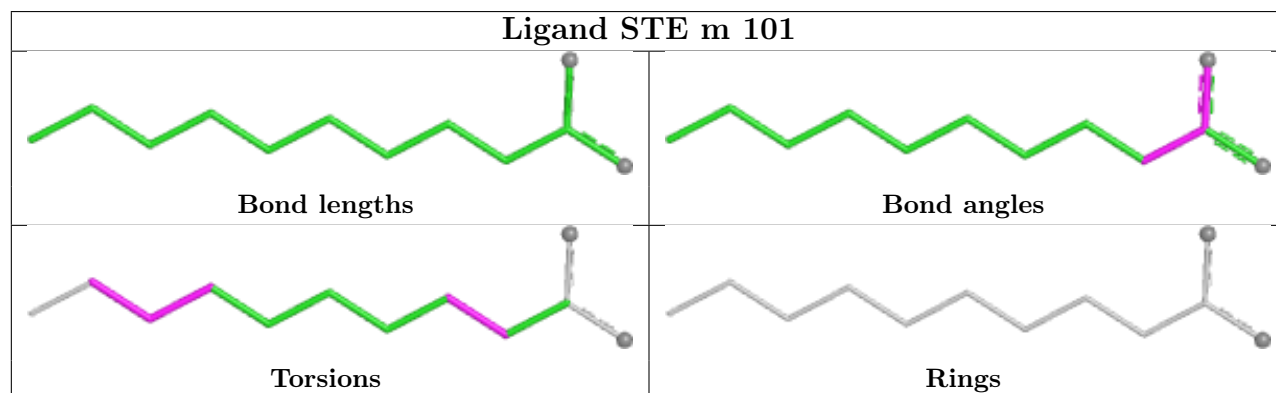
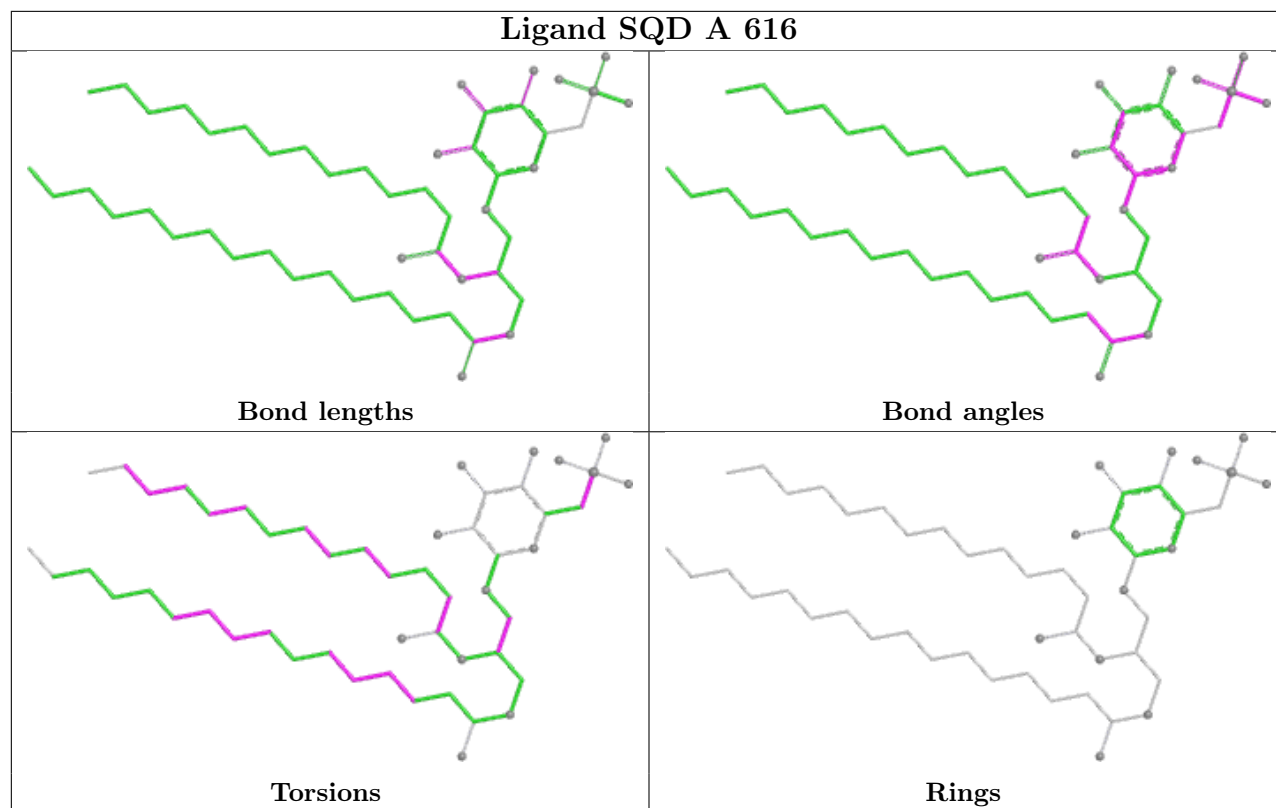
| Ligand STE k 103                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR k 102                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

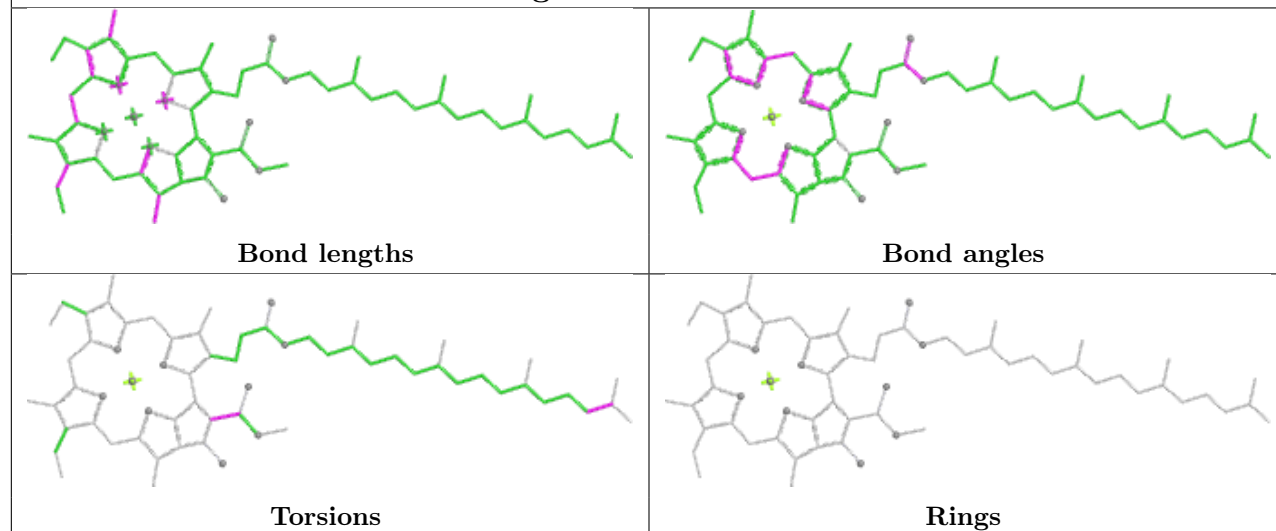
| Ligand STE d 411                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand LMG b 621                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

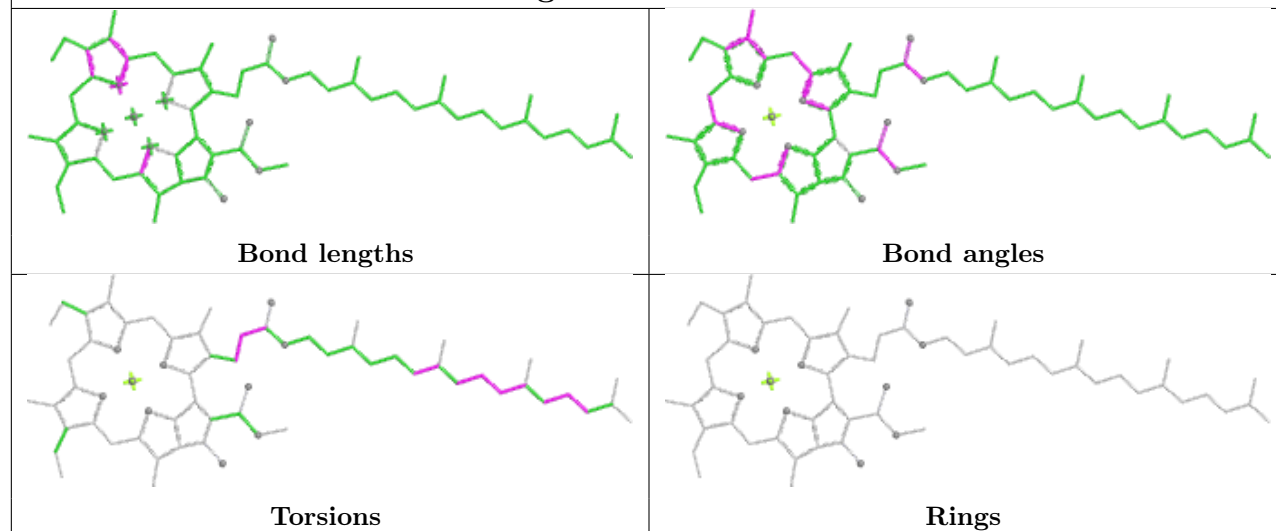




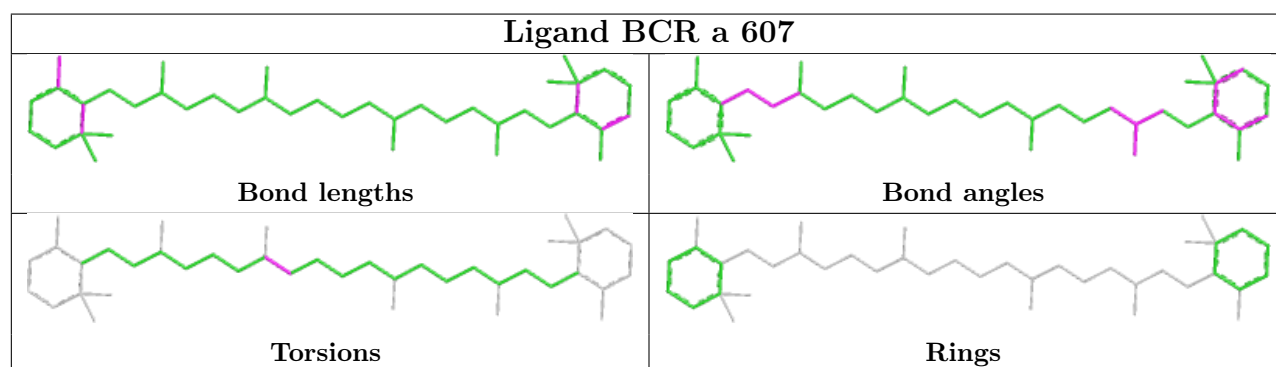
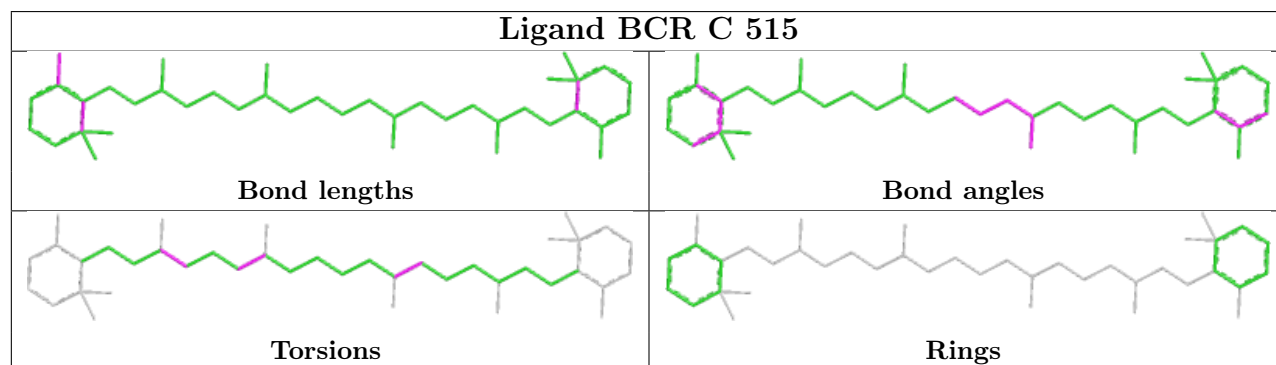
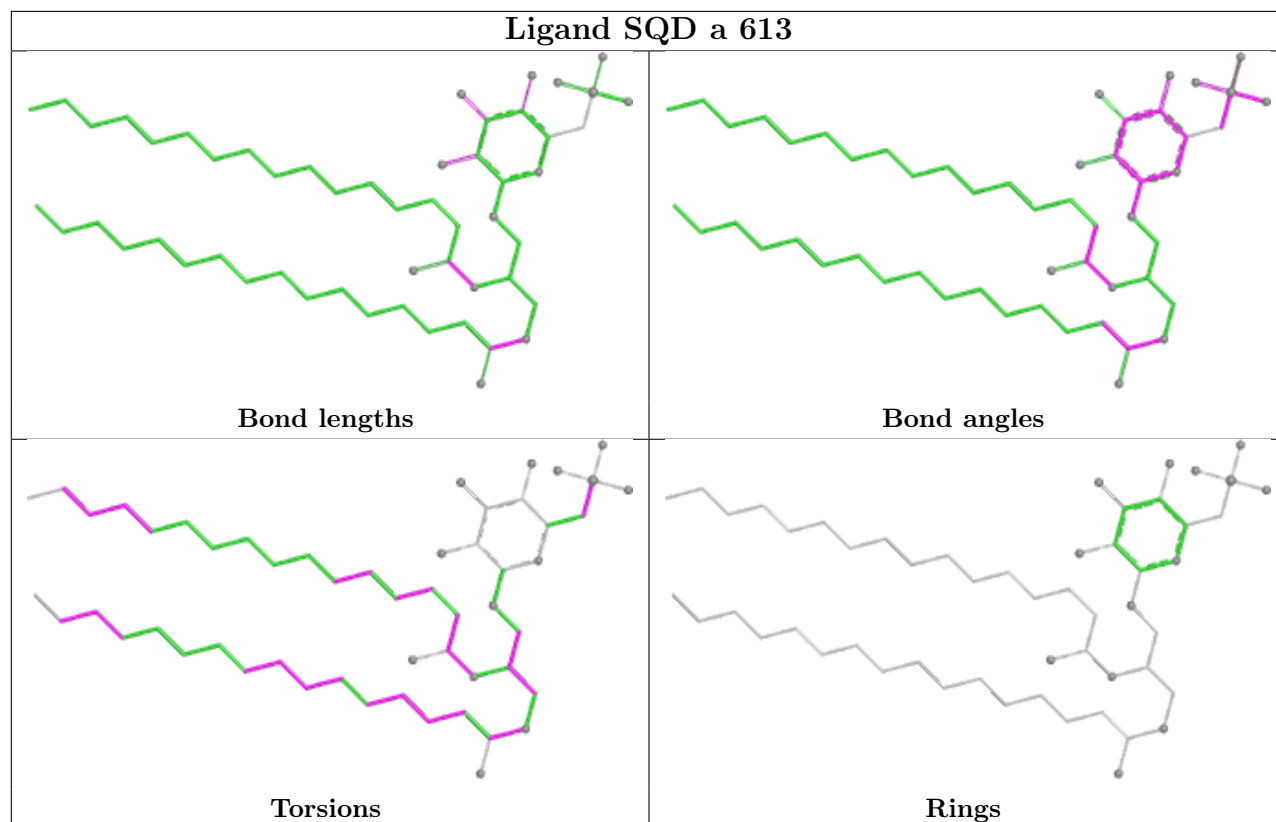
## Ligand CLA B 607

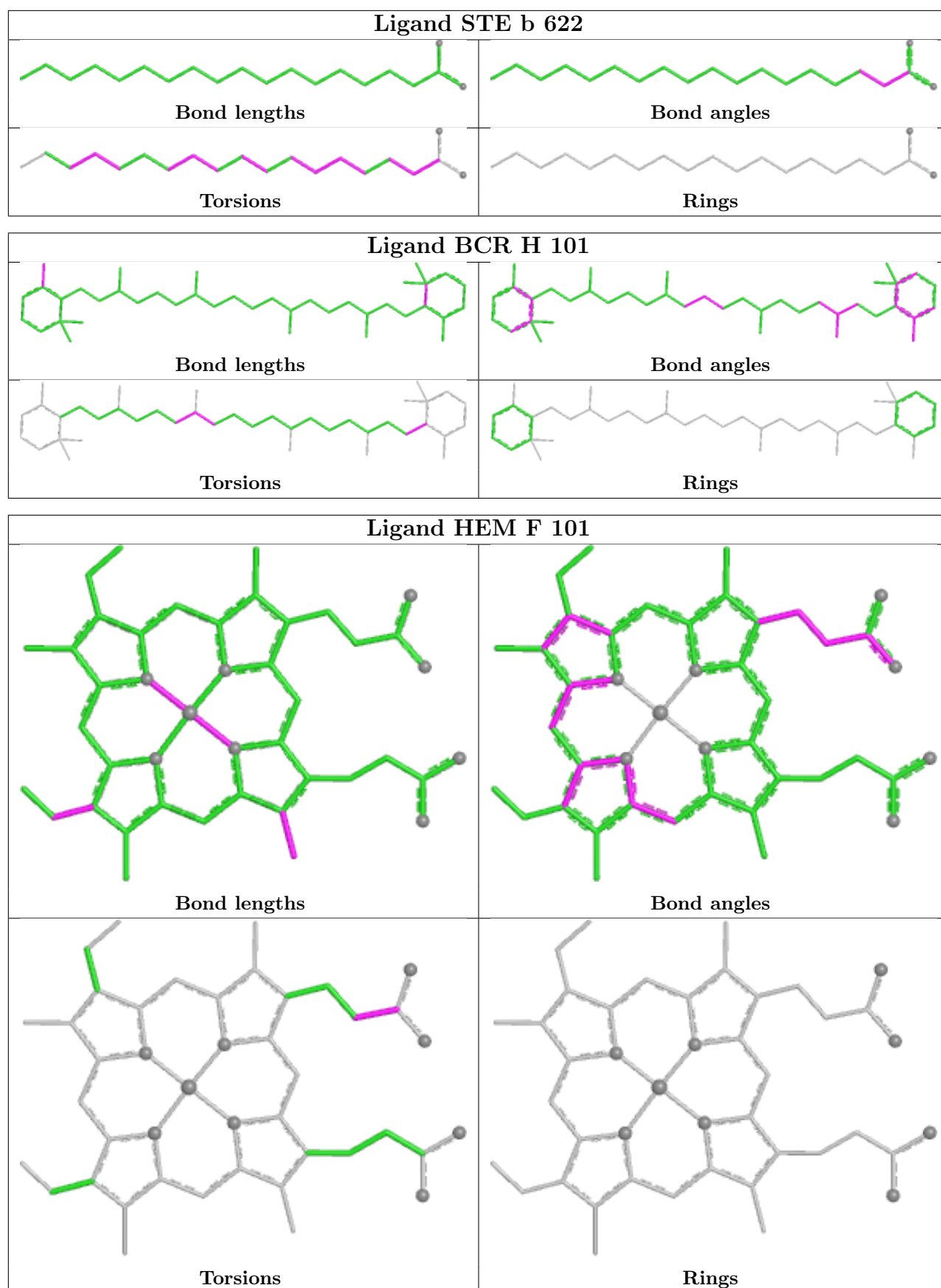


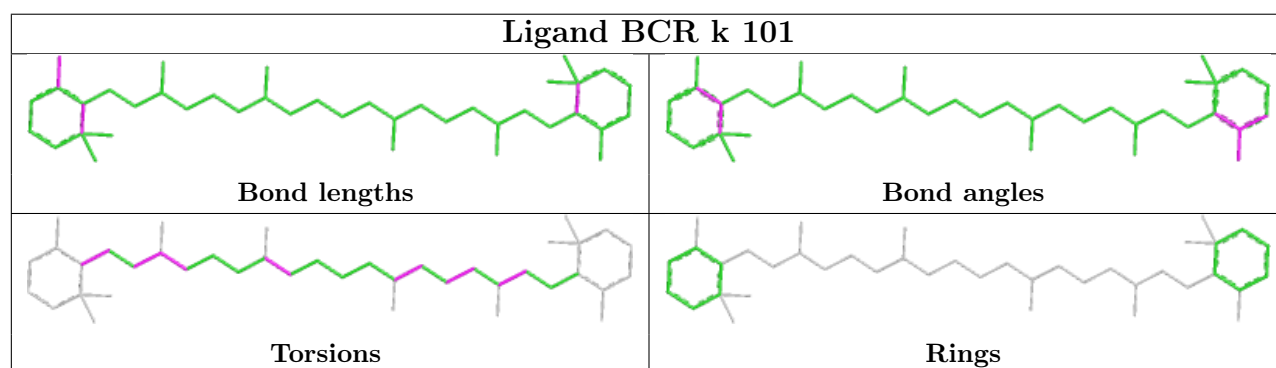
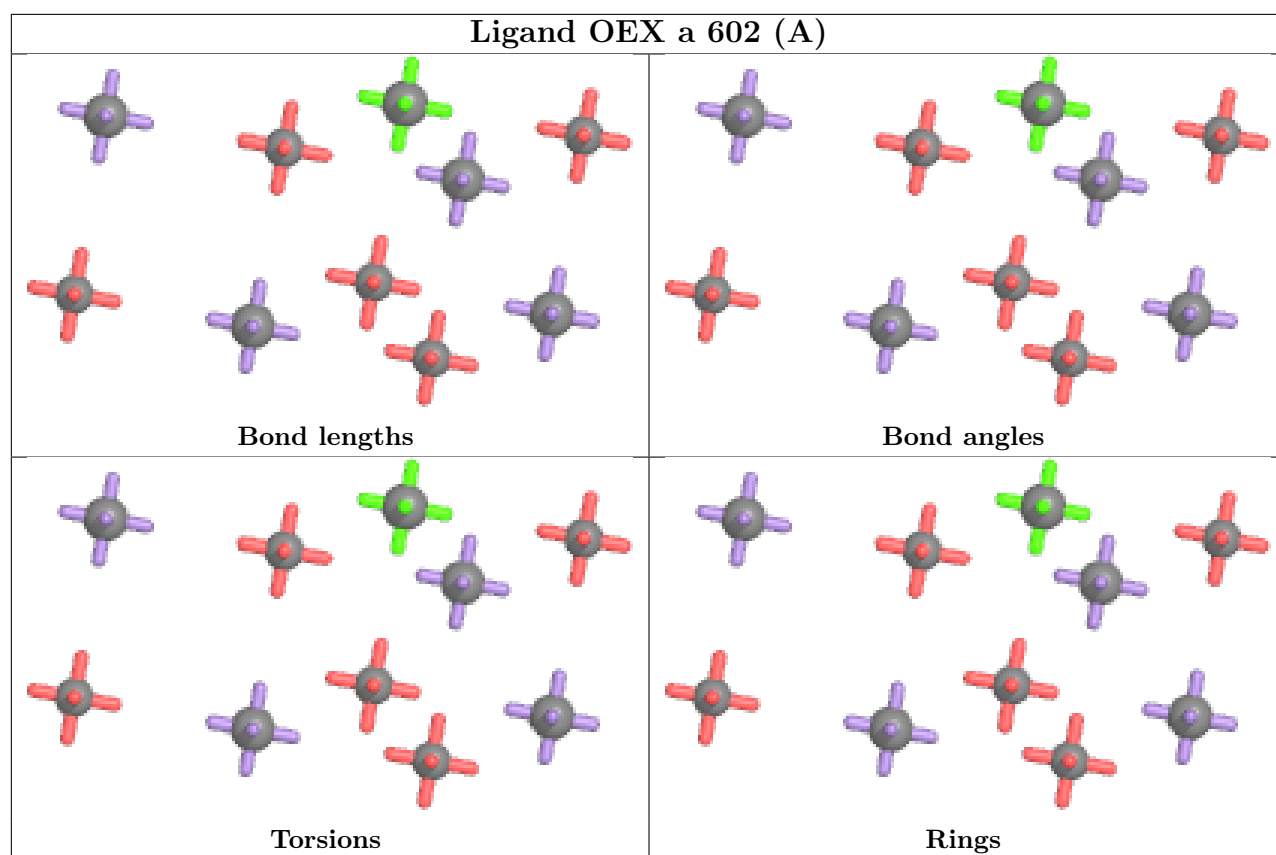
## Ligand CLA c 509

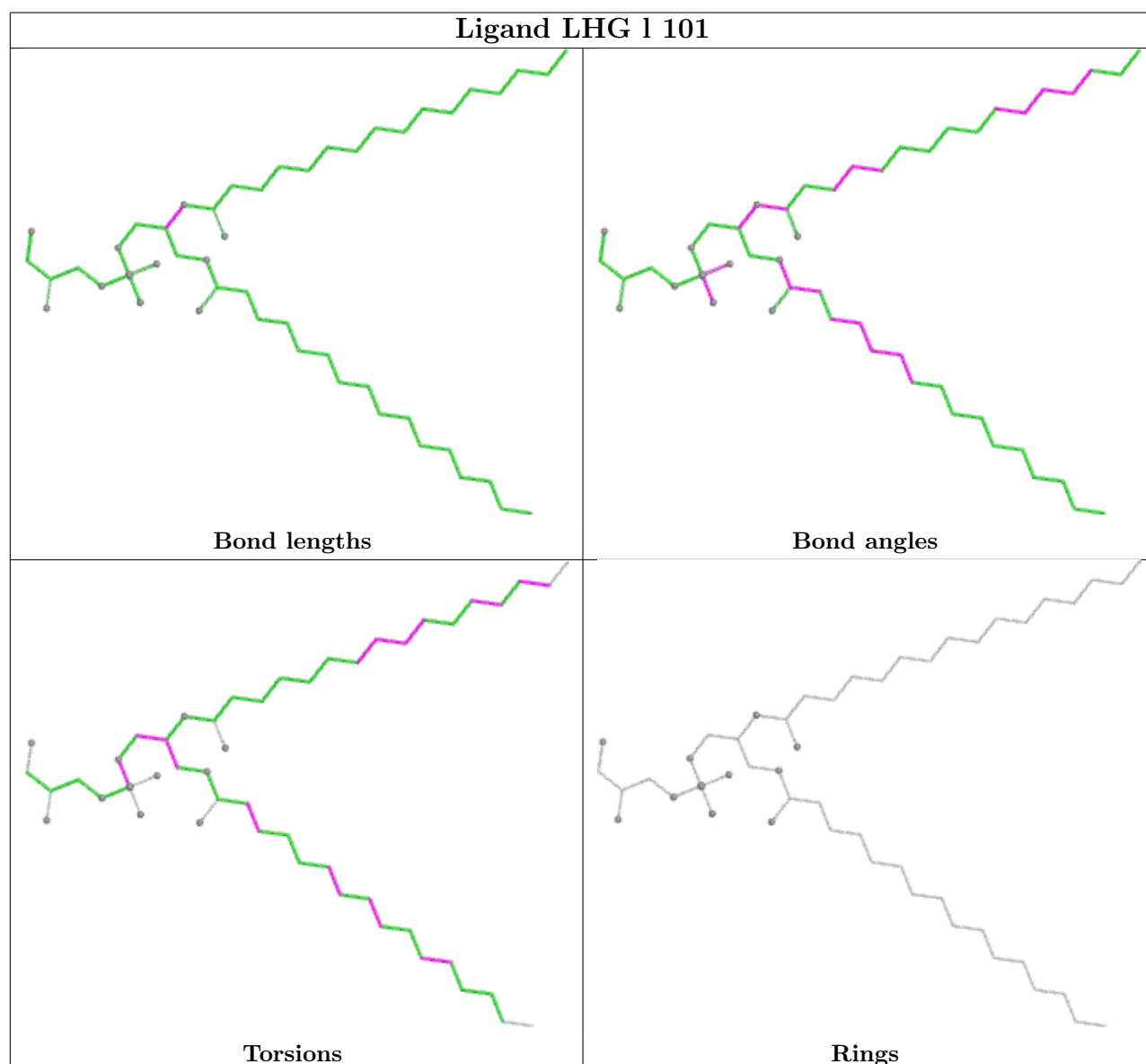
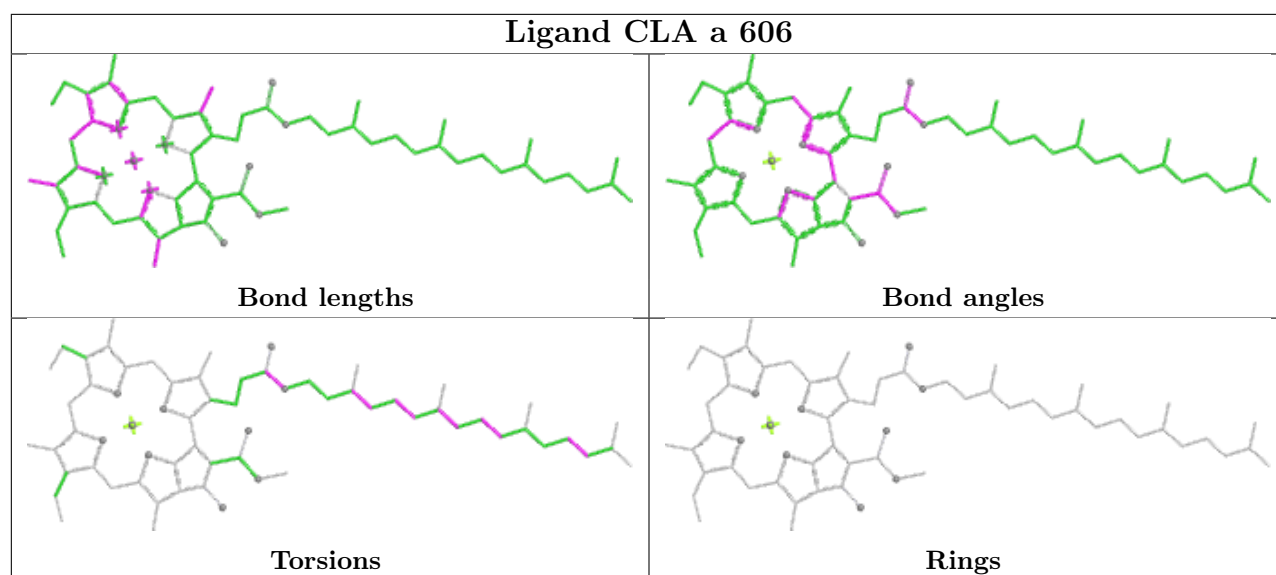


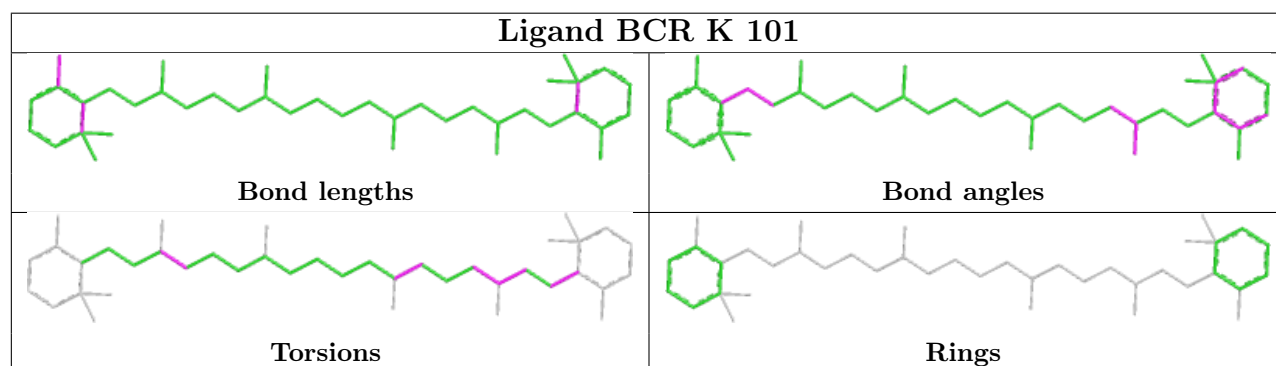
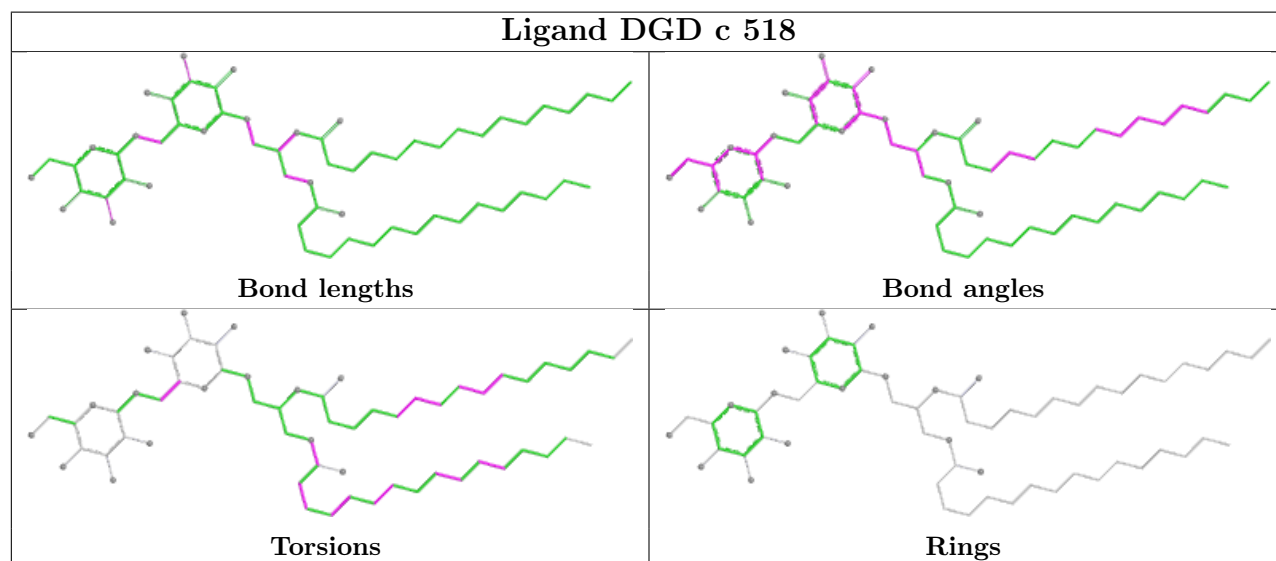
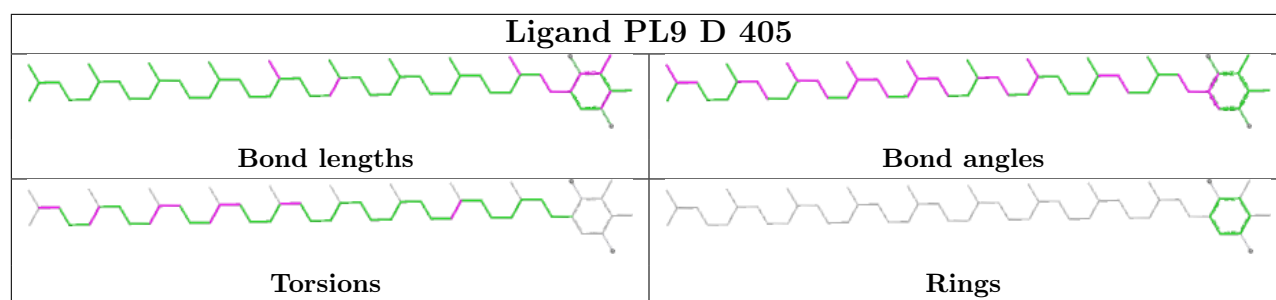


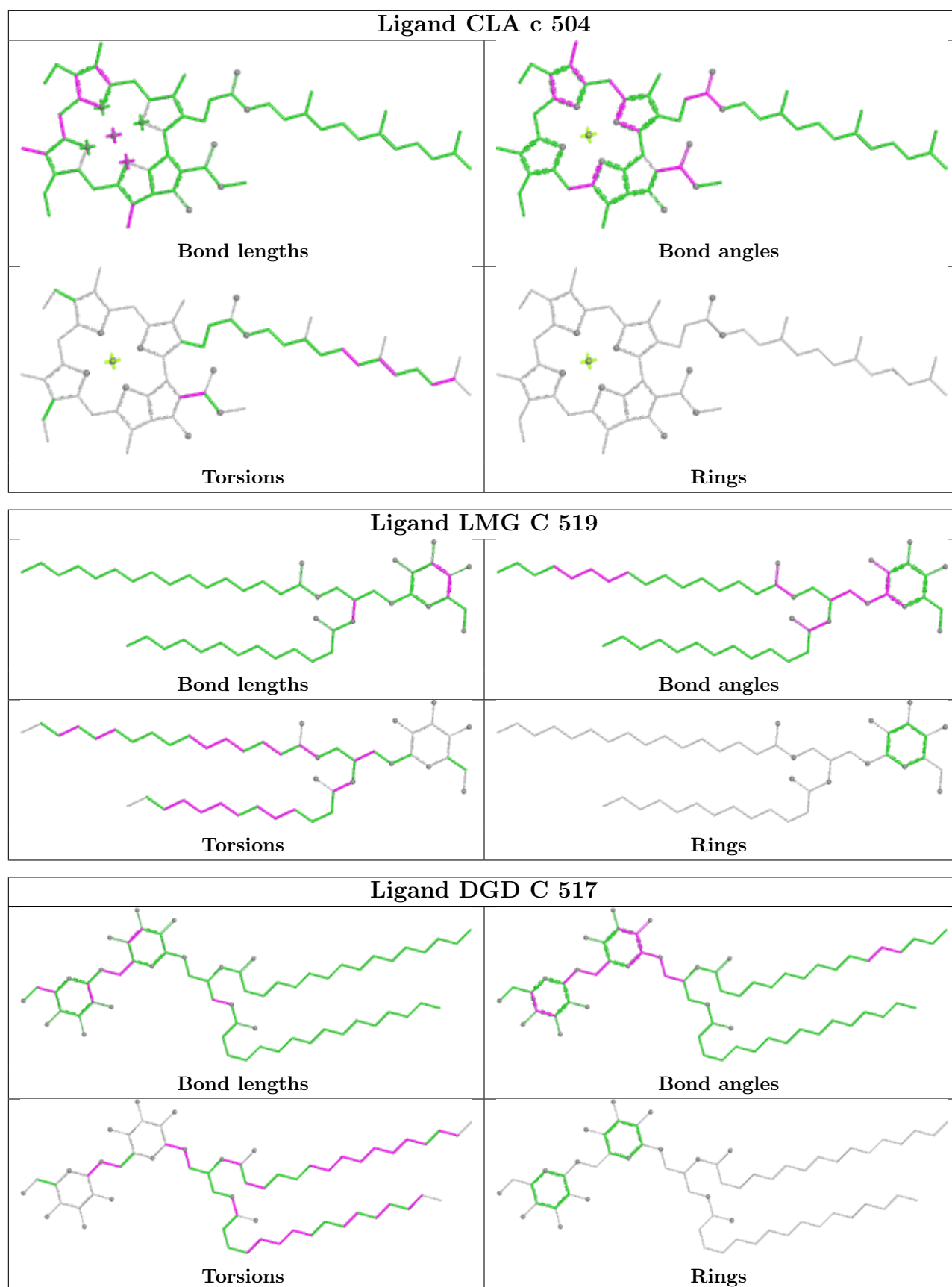


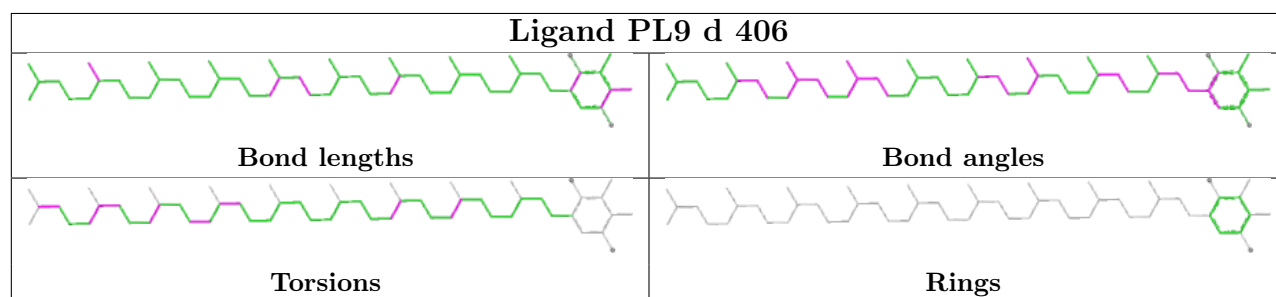
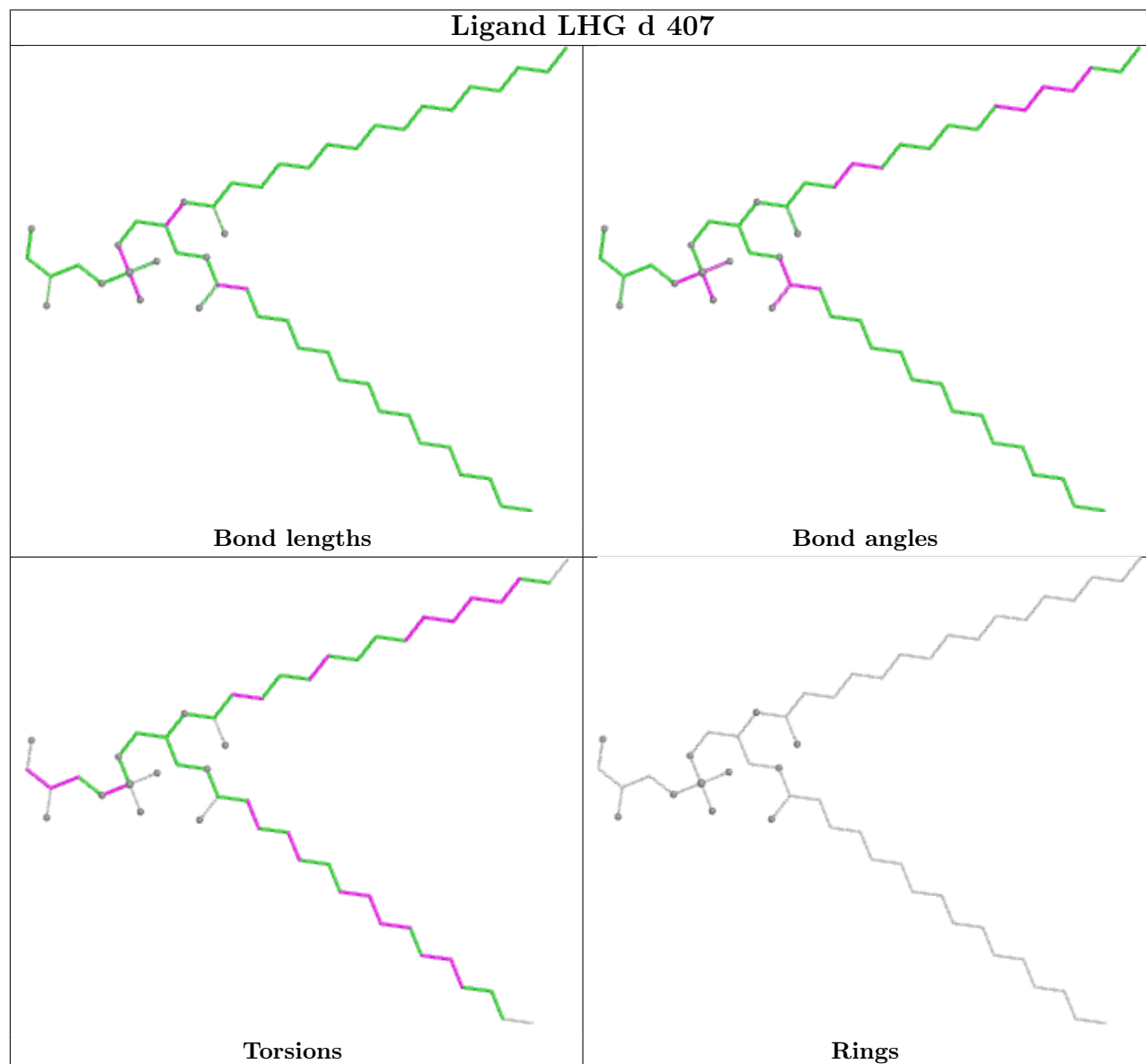
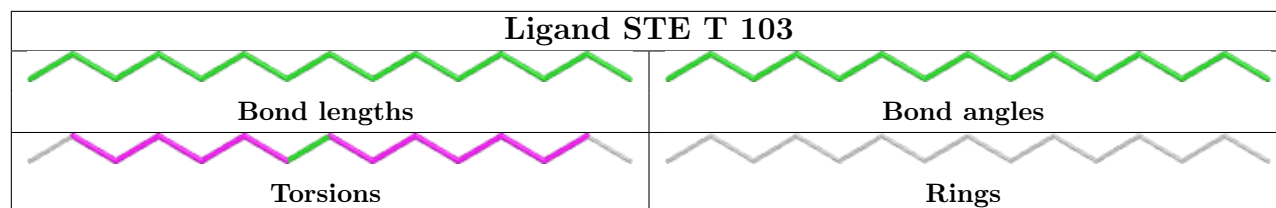


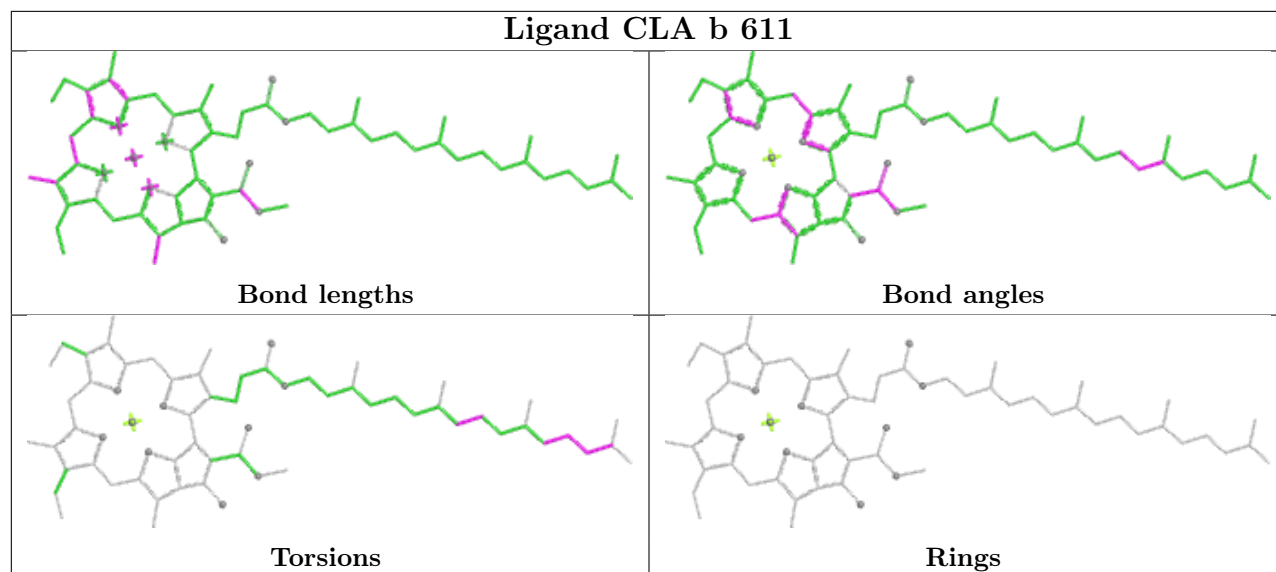
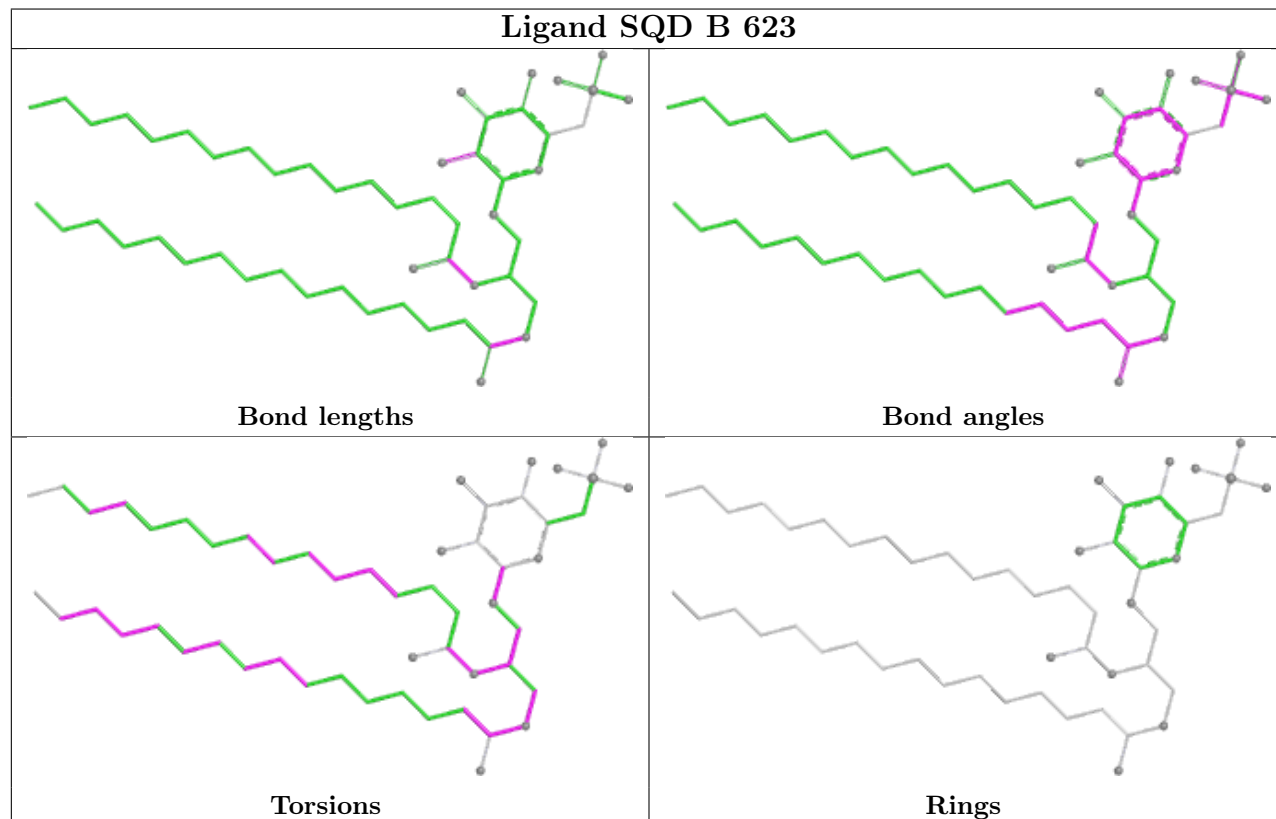




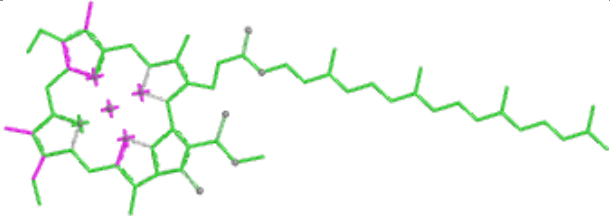
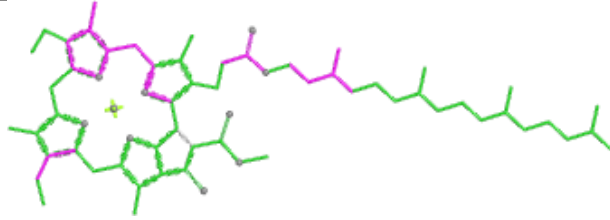
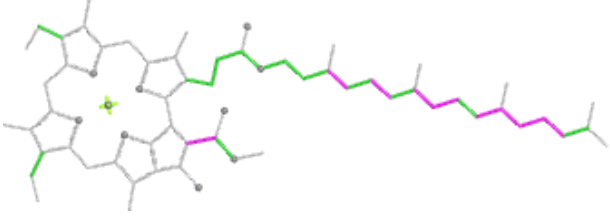
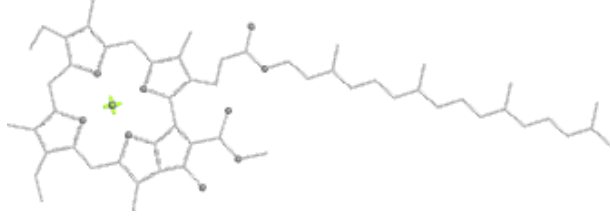
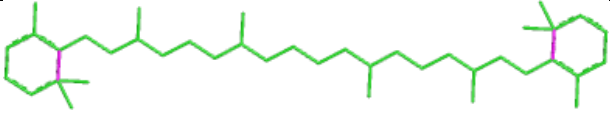
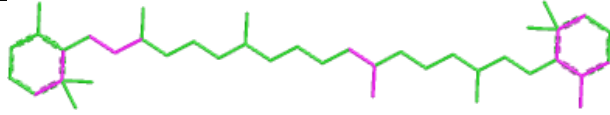
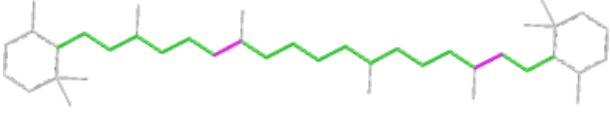
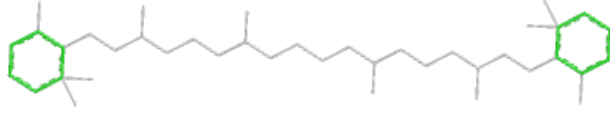
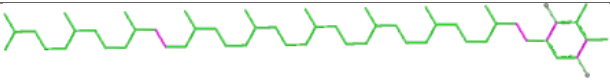
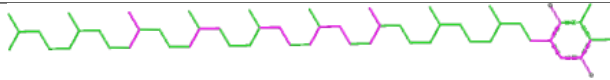
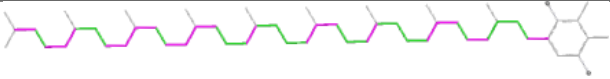
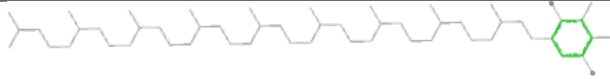




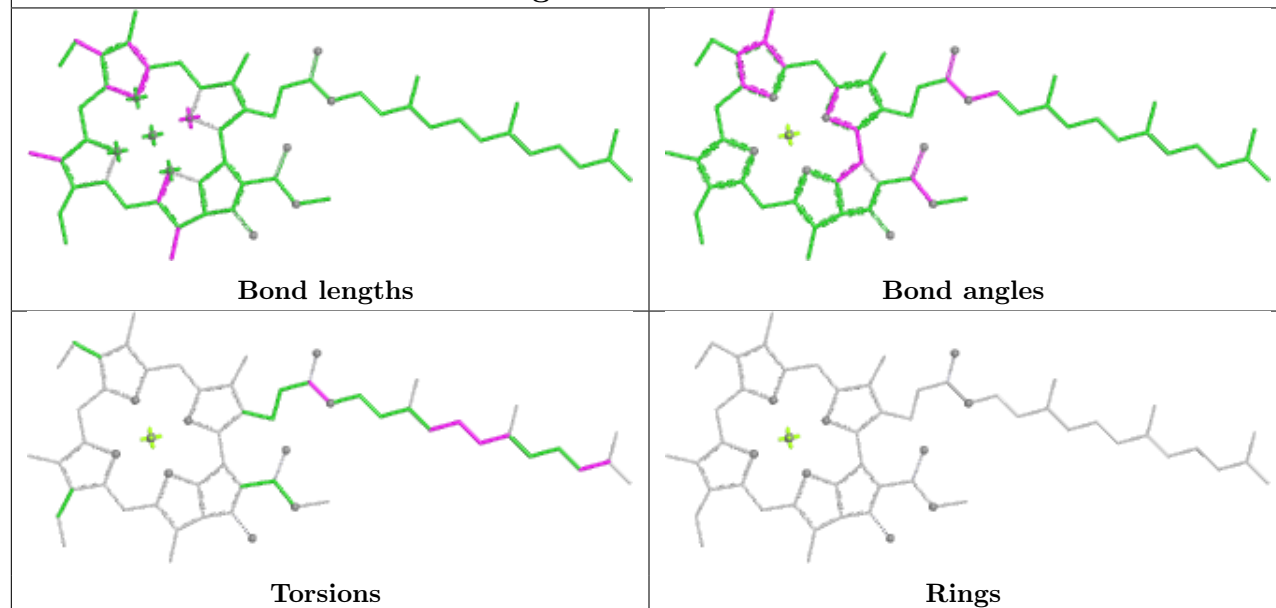


**Ligand CLA b 611****Ligand SQD B 623**

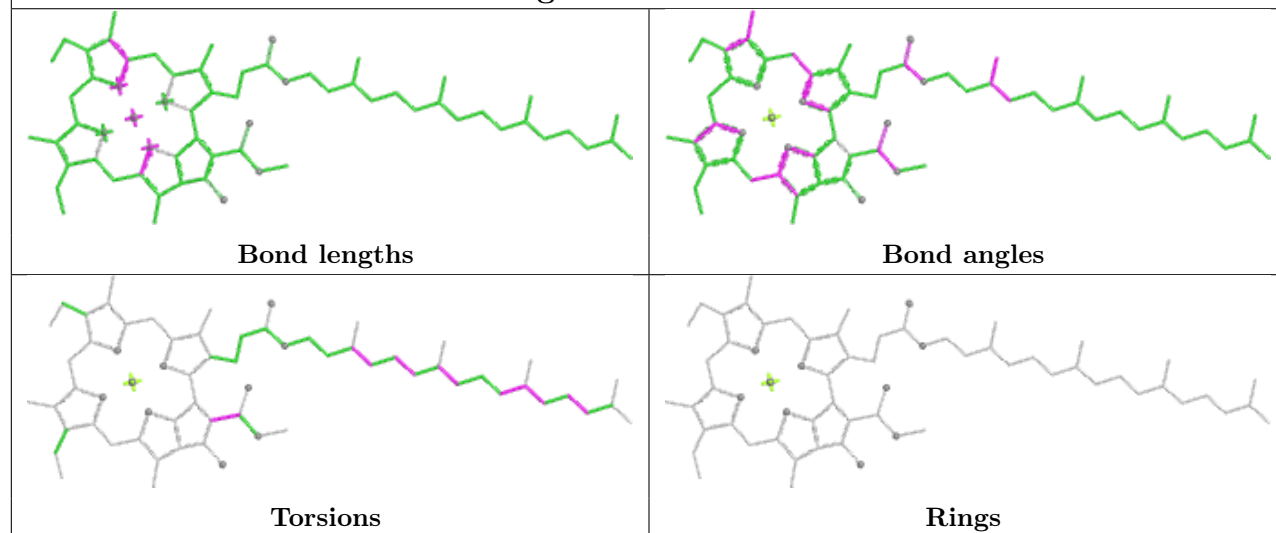


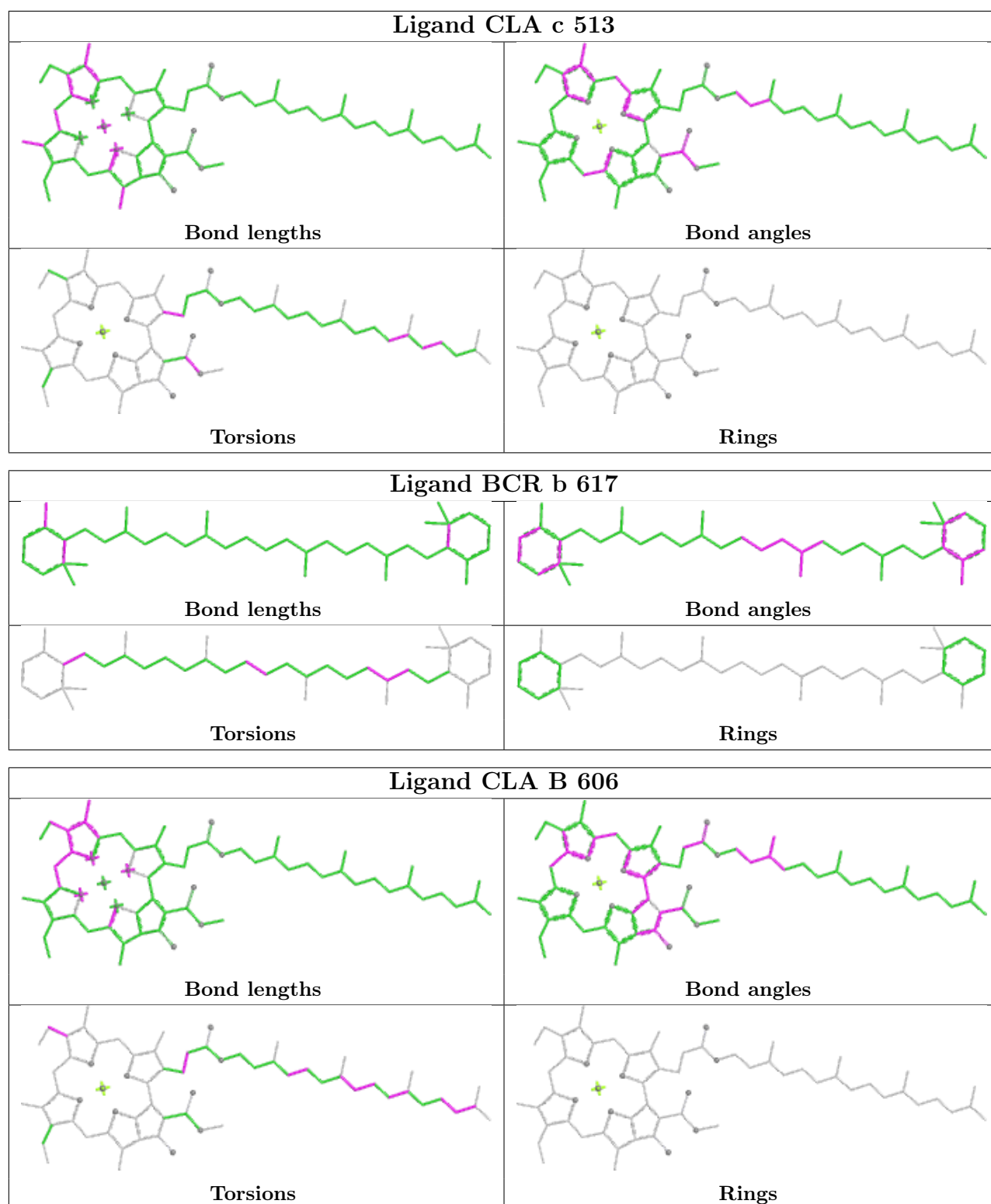
| Ligand CLA b 614                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR b 619                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand PL9 A 612                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

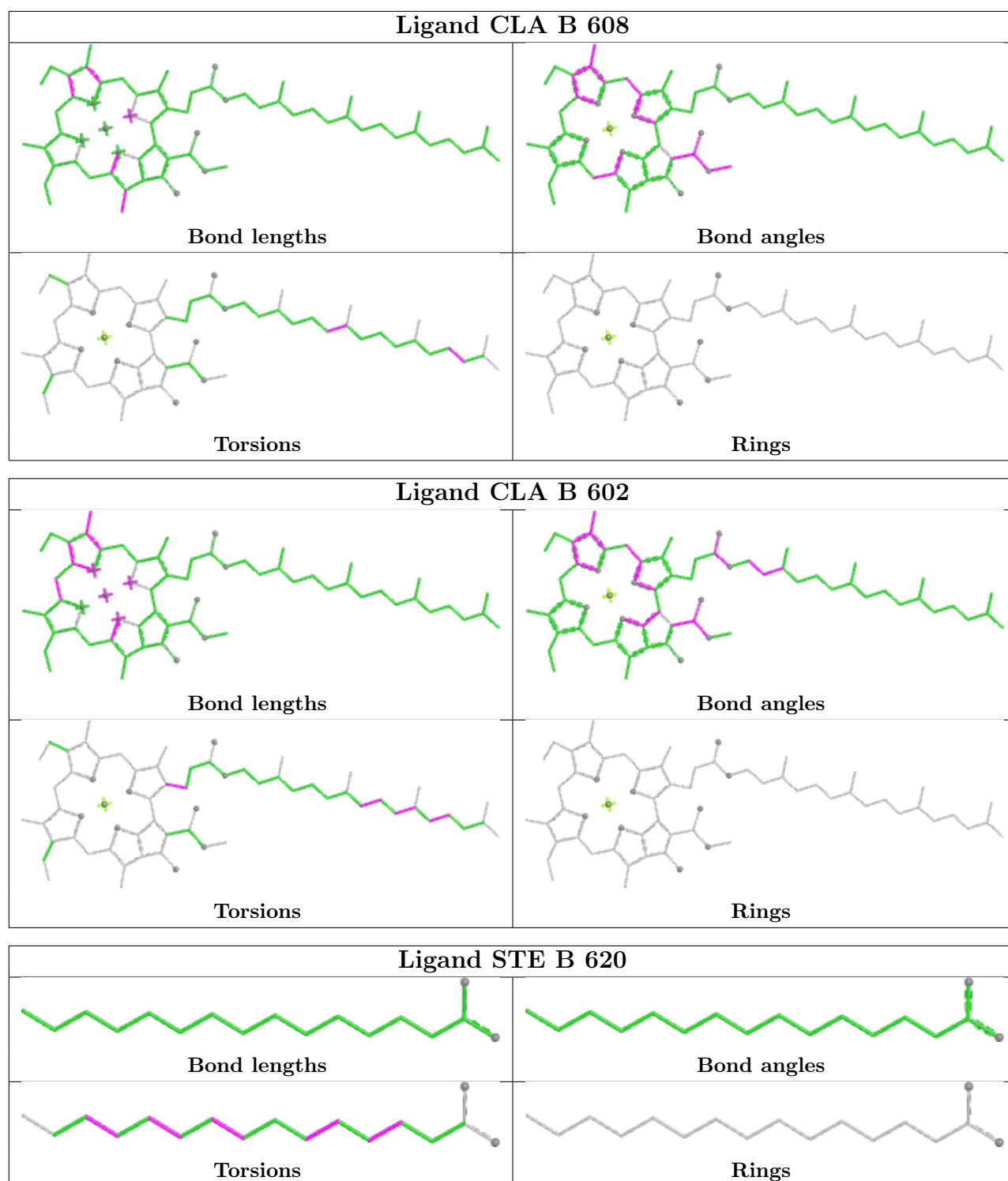
## Ligand CLA B 616

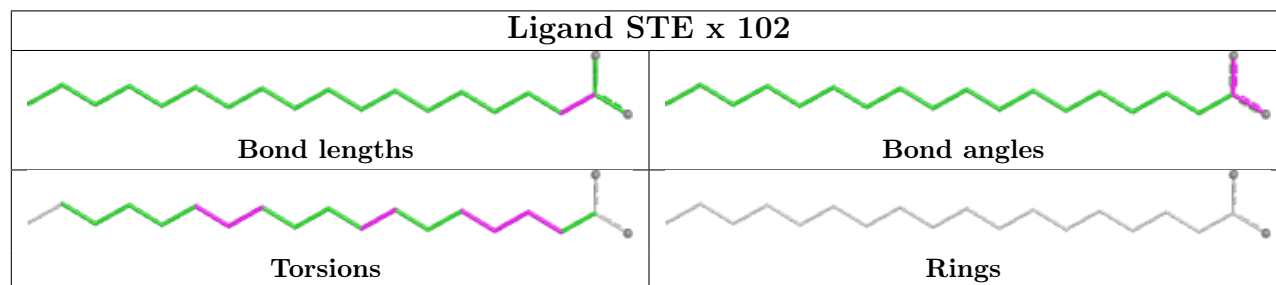
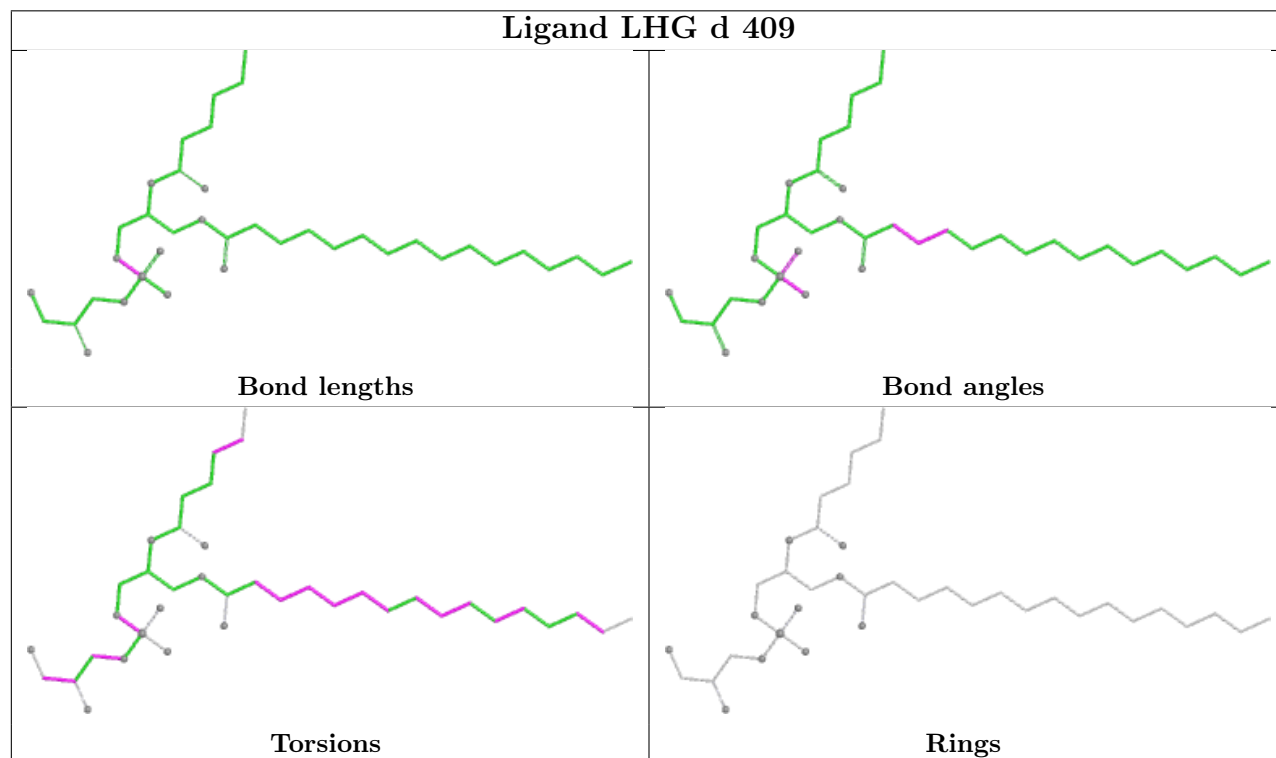
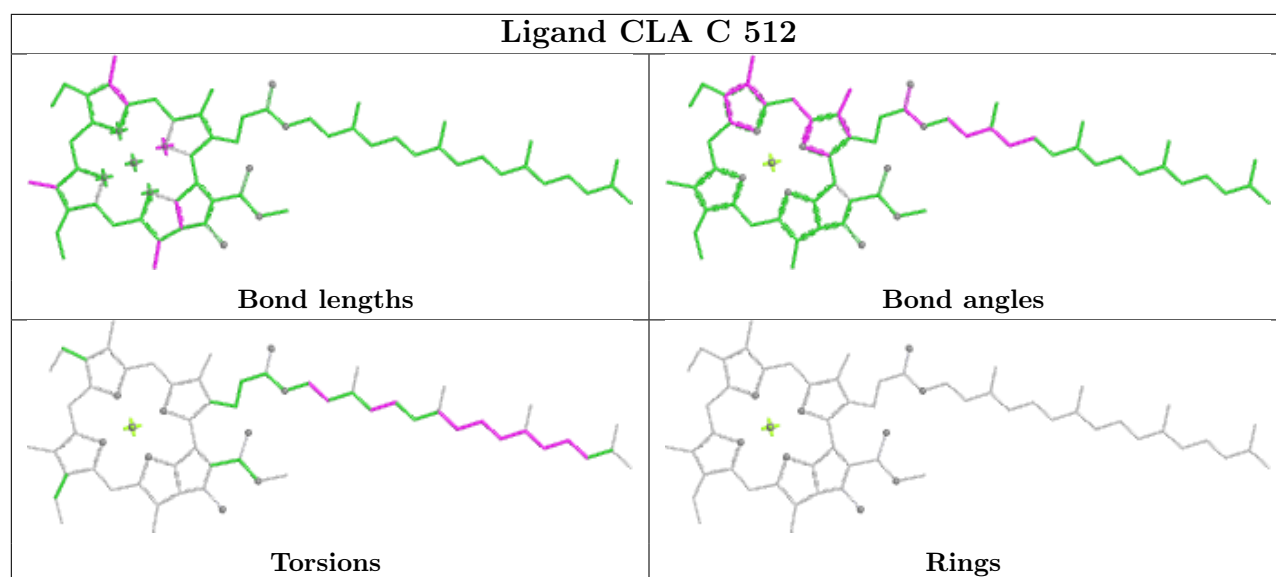


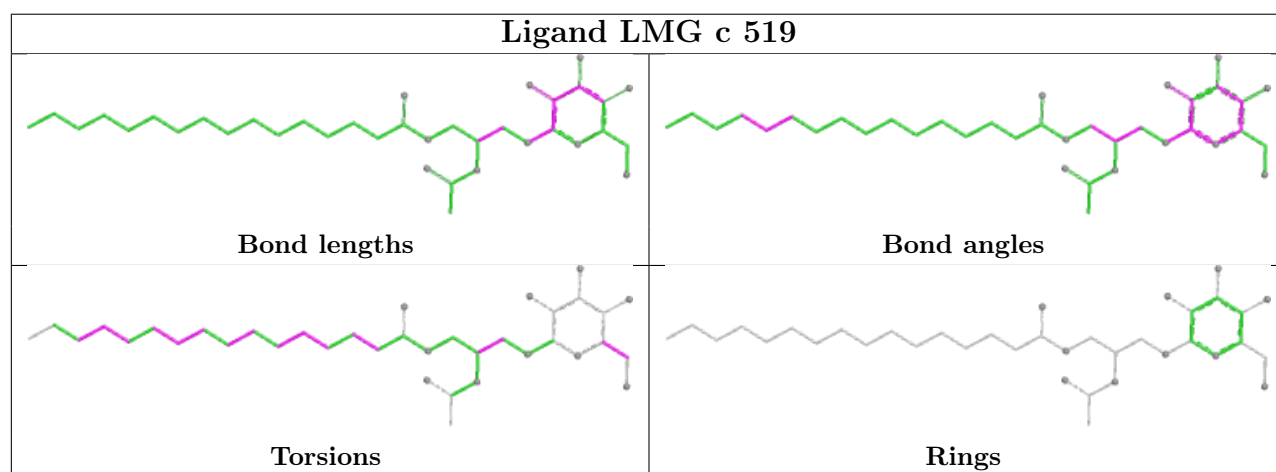
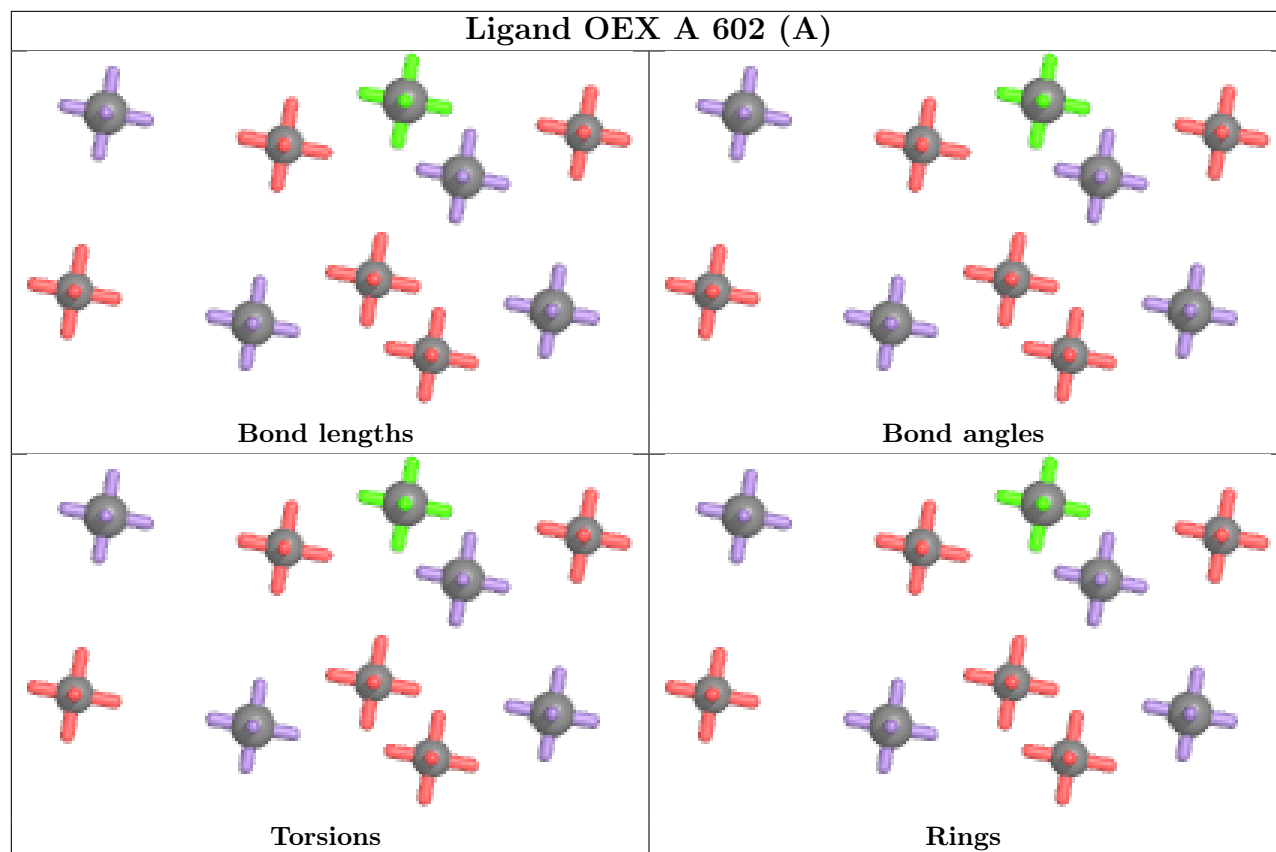
## Ligand CLA c 507

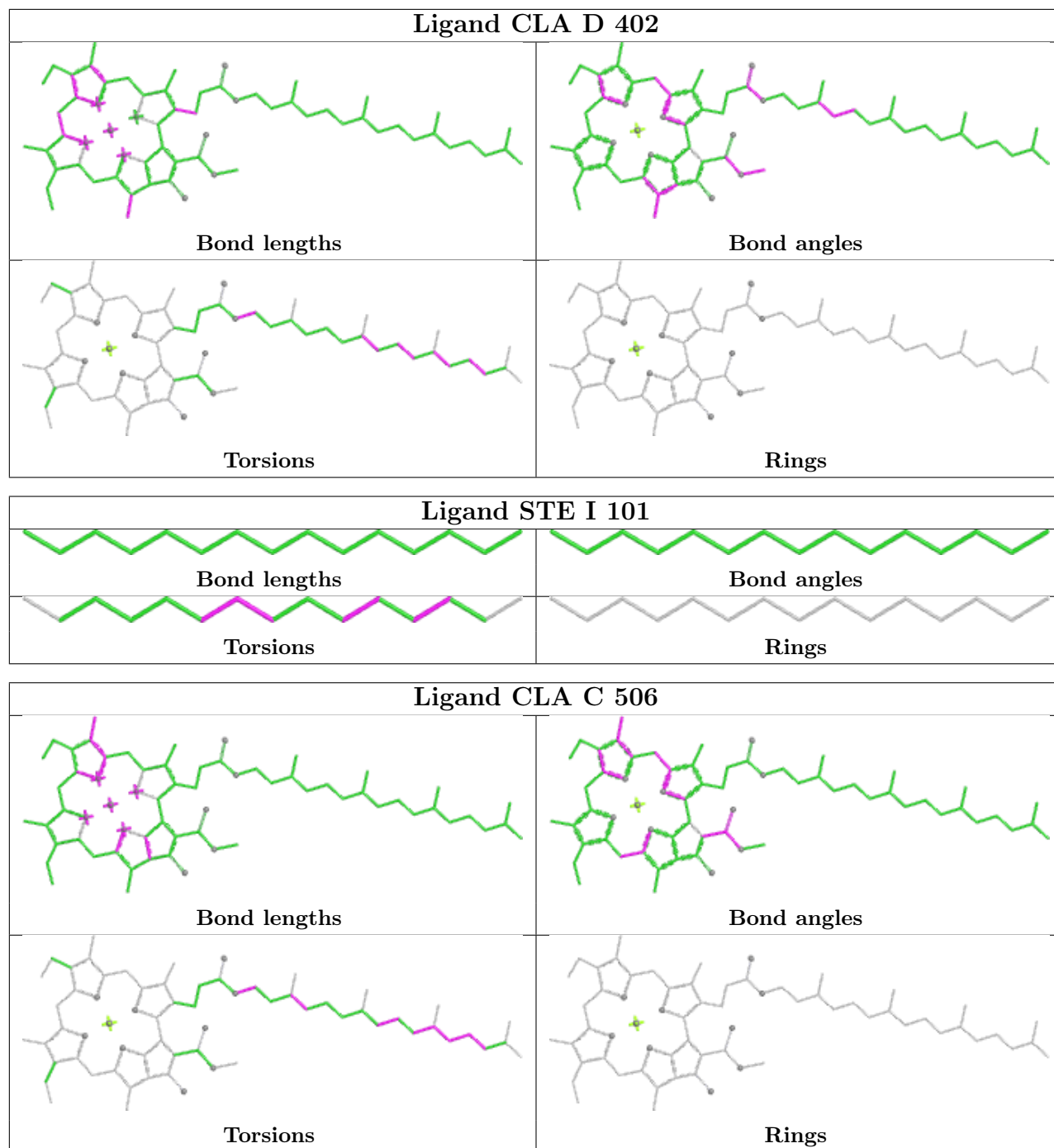


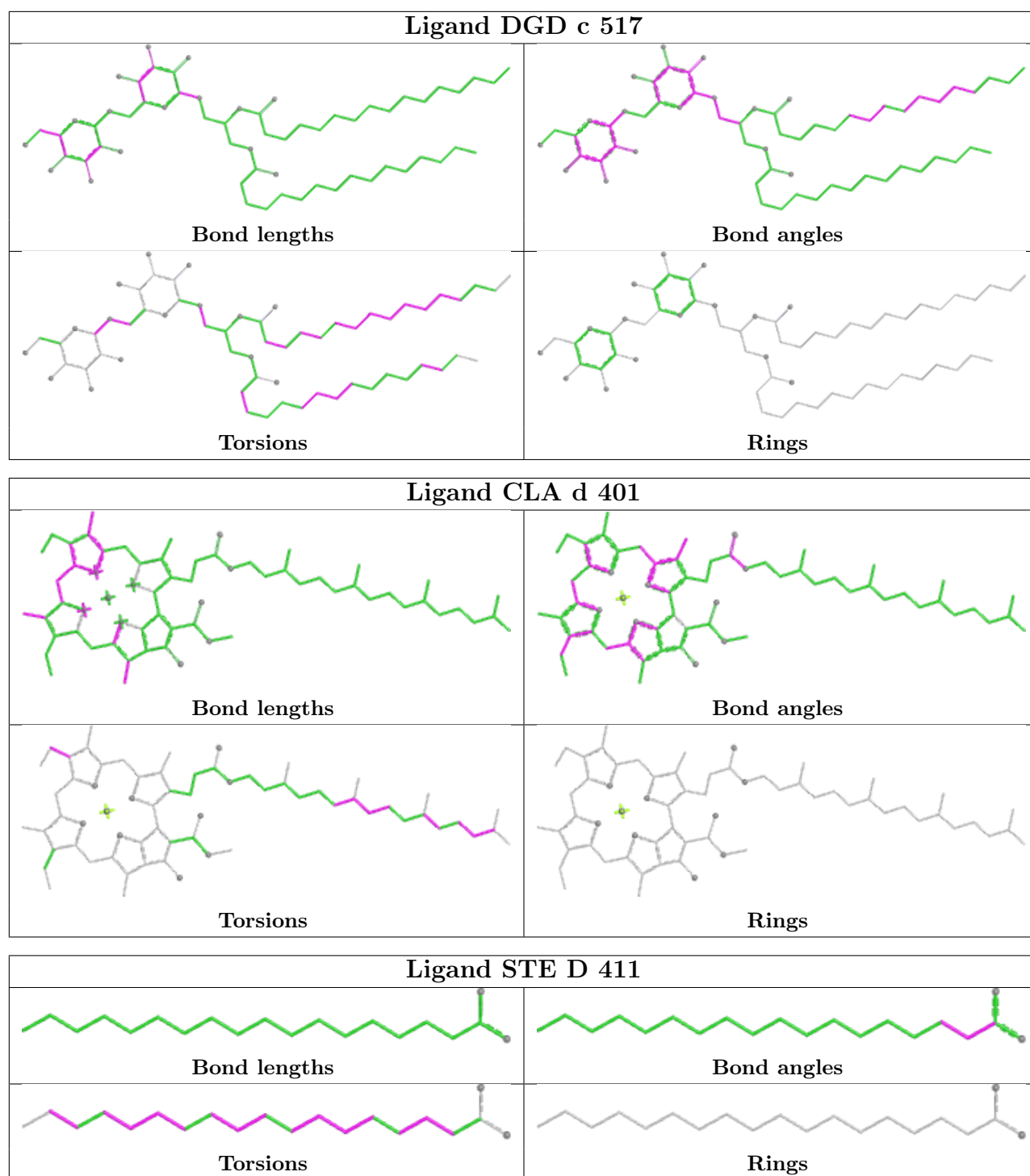




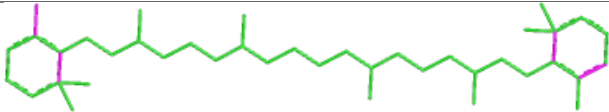
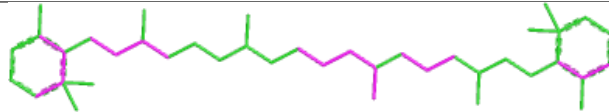
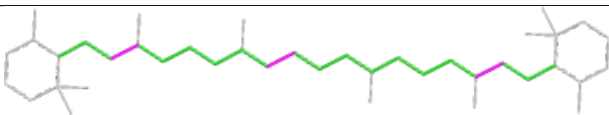
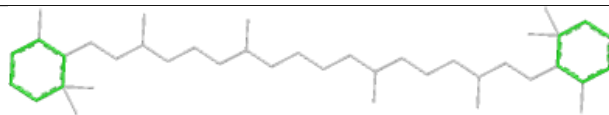


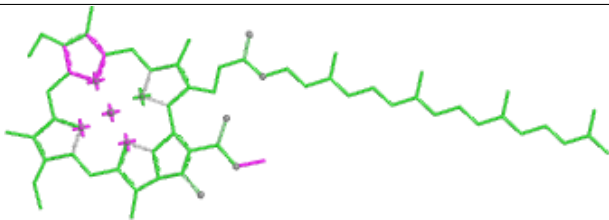
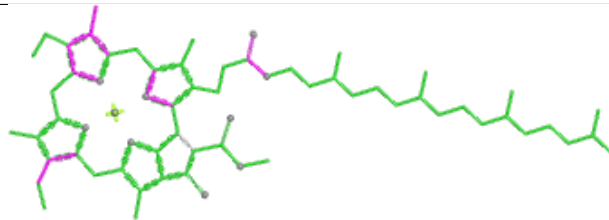
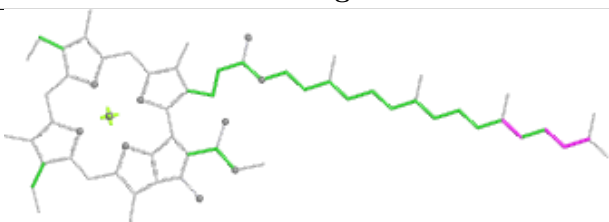
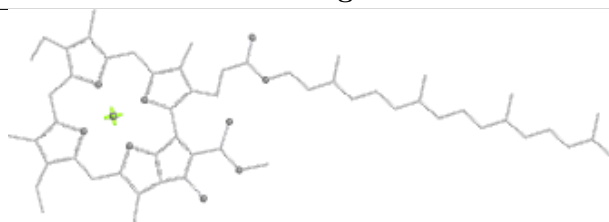


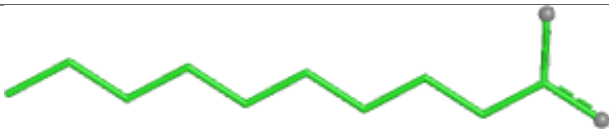
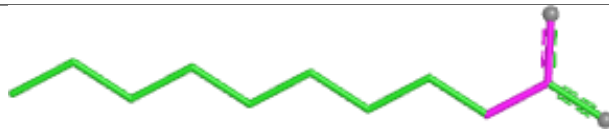
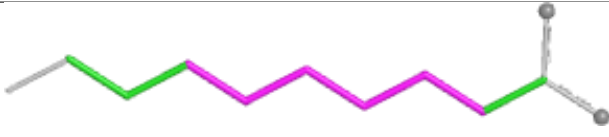
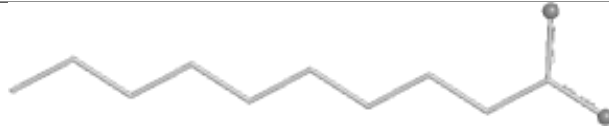


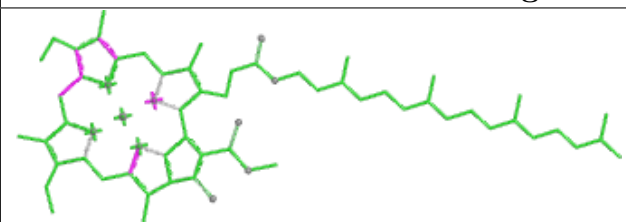
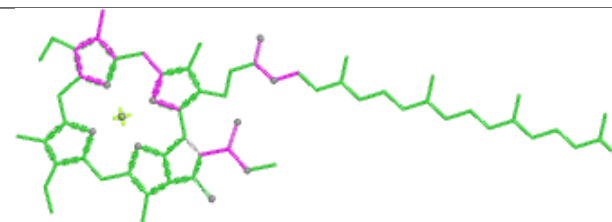
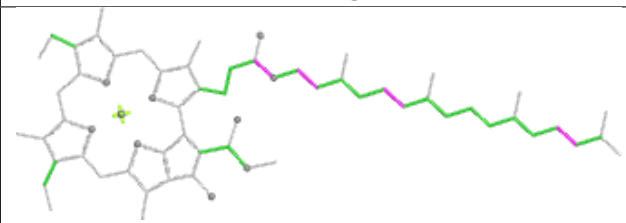
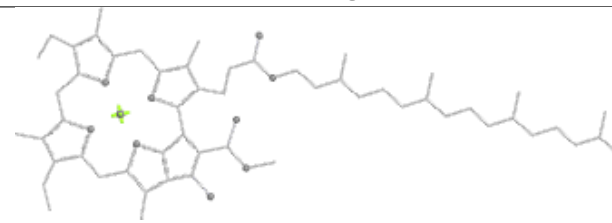




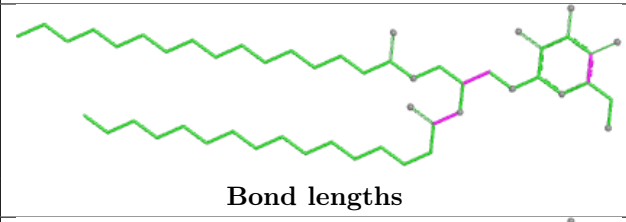
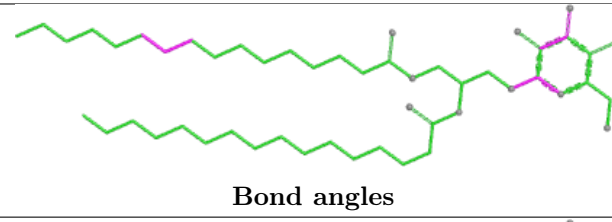
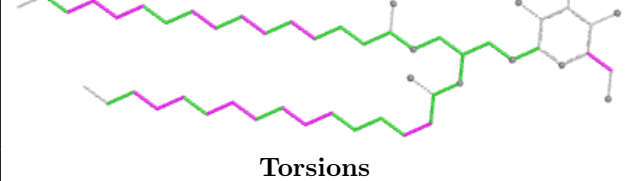
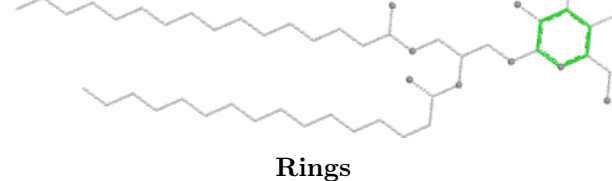
| Ligand BCR c 515                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA a 604                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

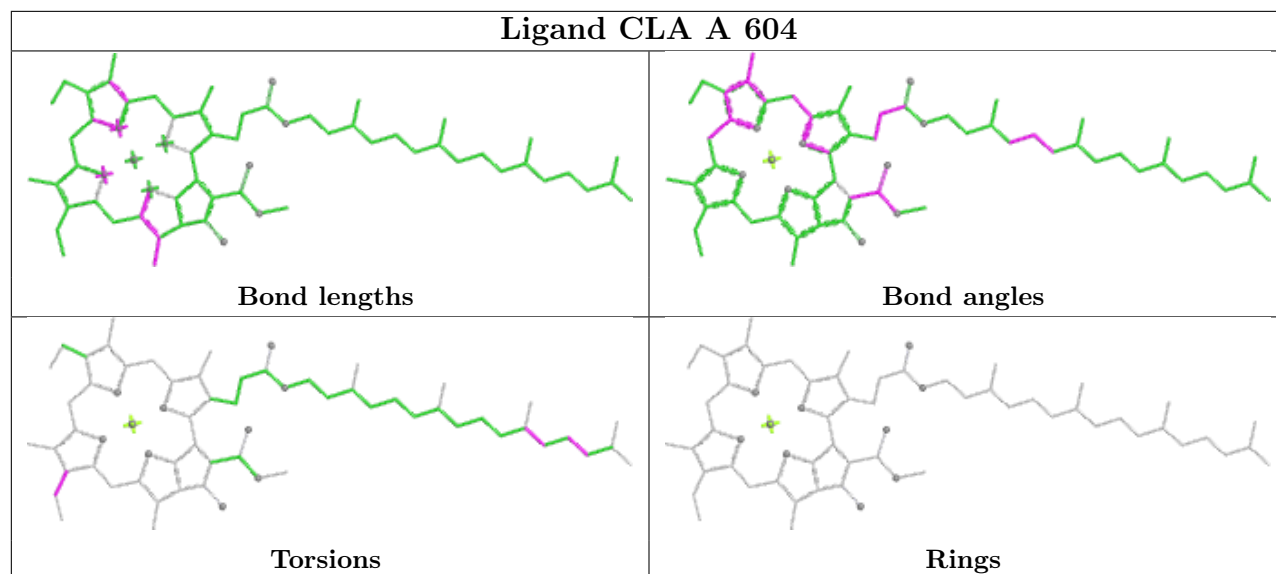
| Ligand STE B 627                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand CLA C 513                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

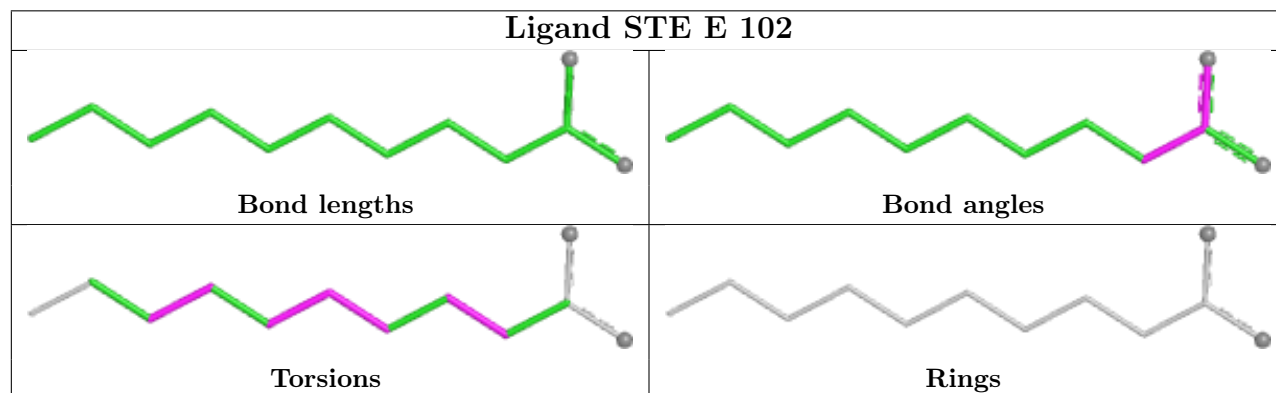
| Ligand STE M 103                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand LMG D 406                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

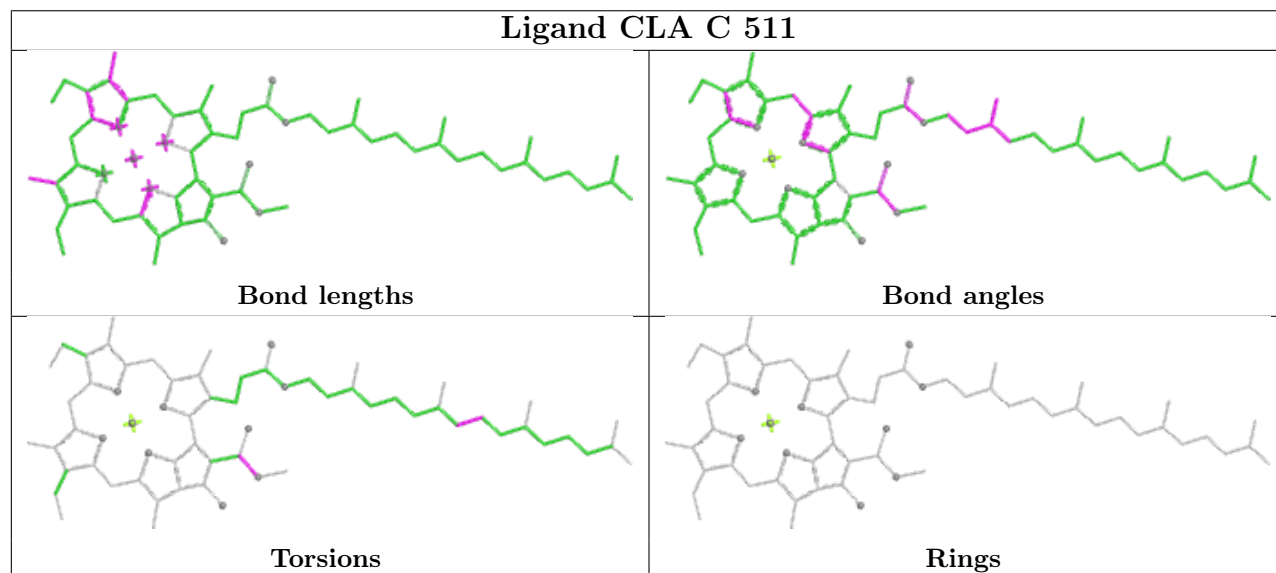
## Ligand CLA A 604

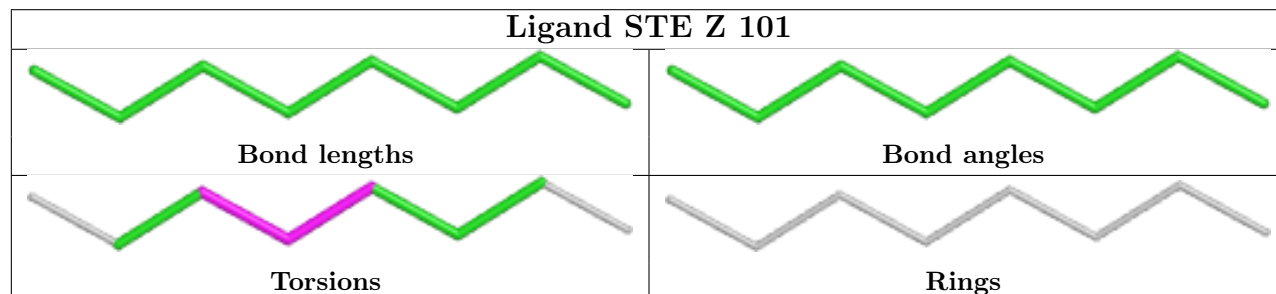
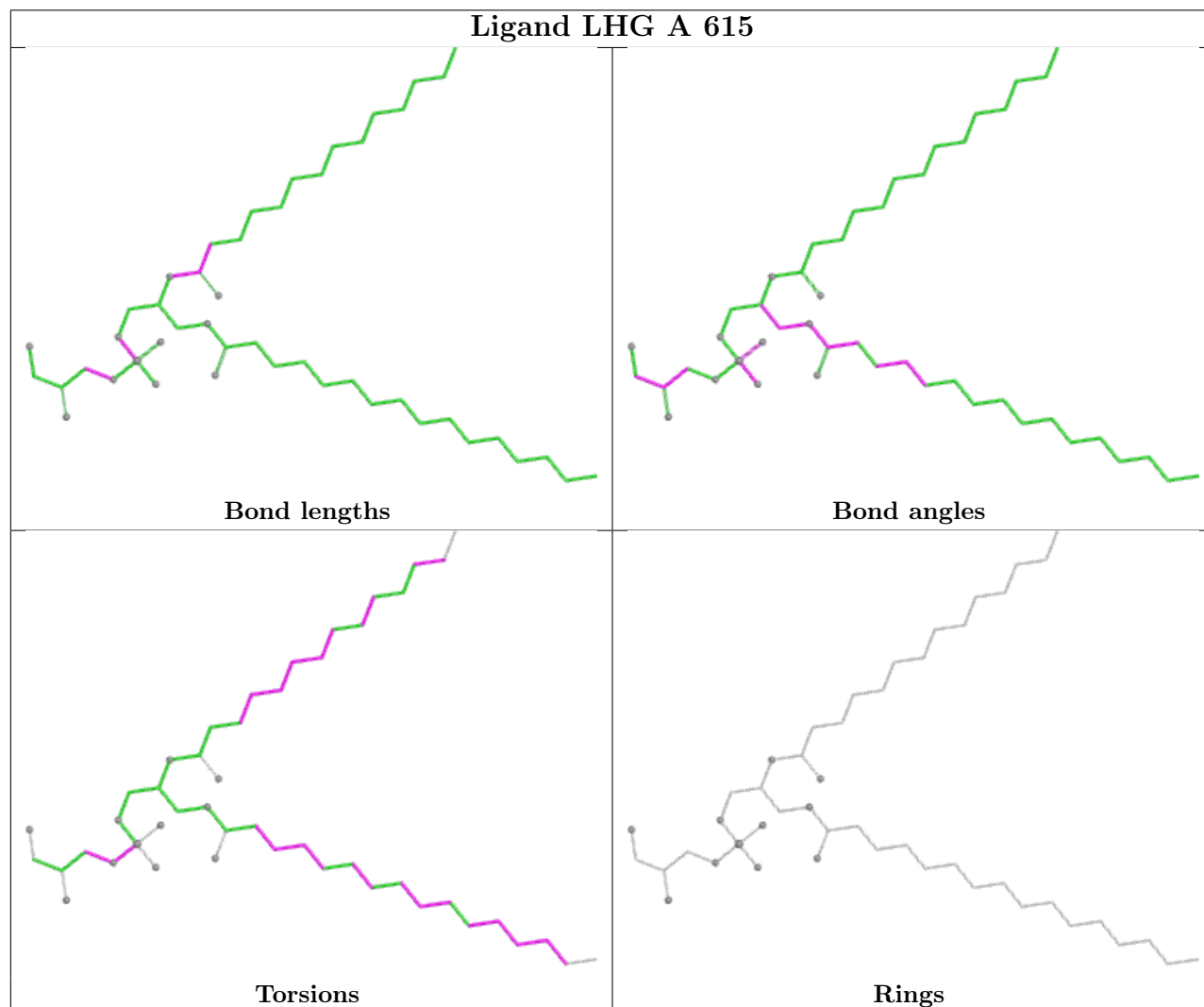
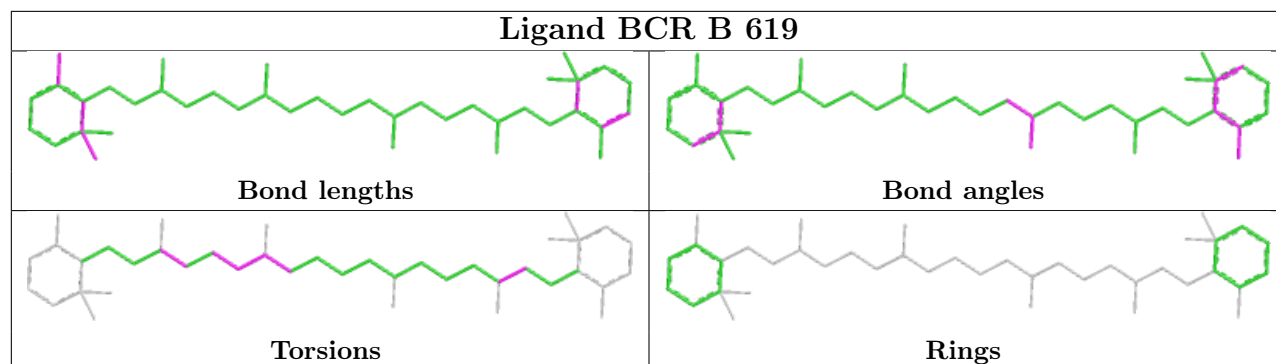


## Ligand STE E 102

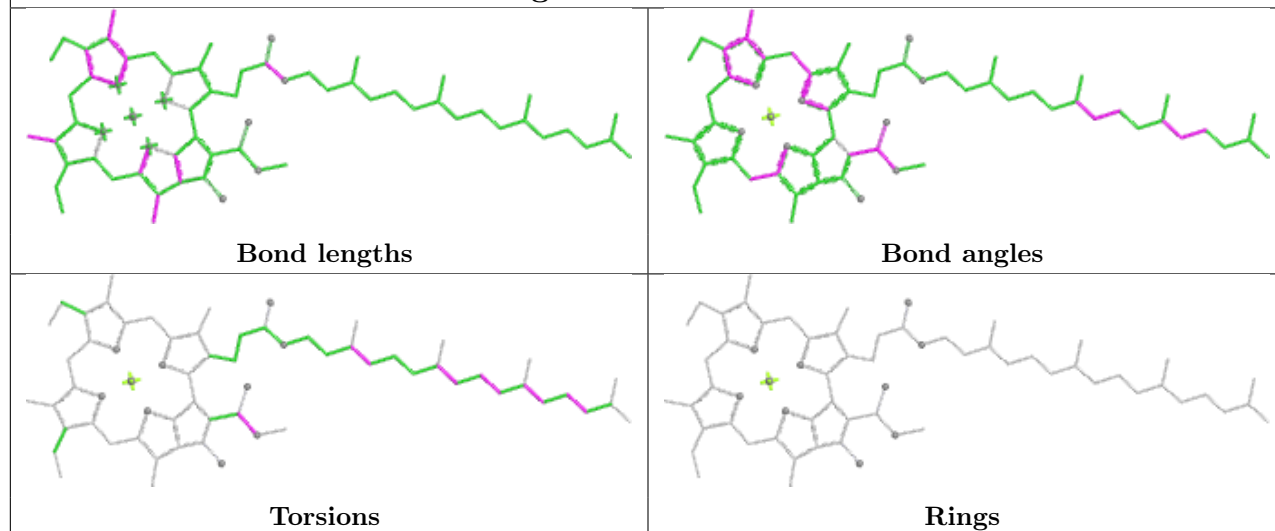


## Ligand CLA C 511

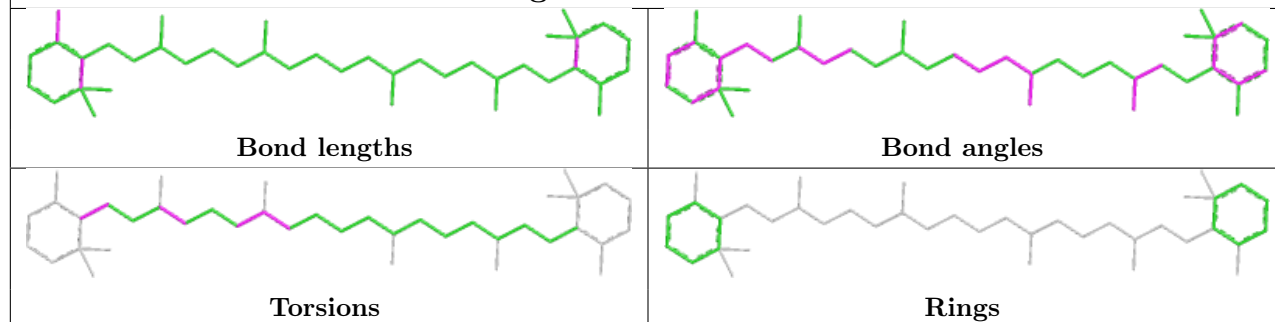




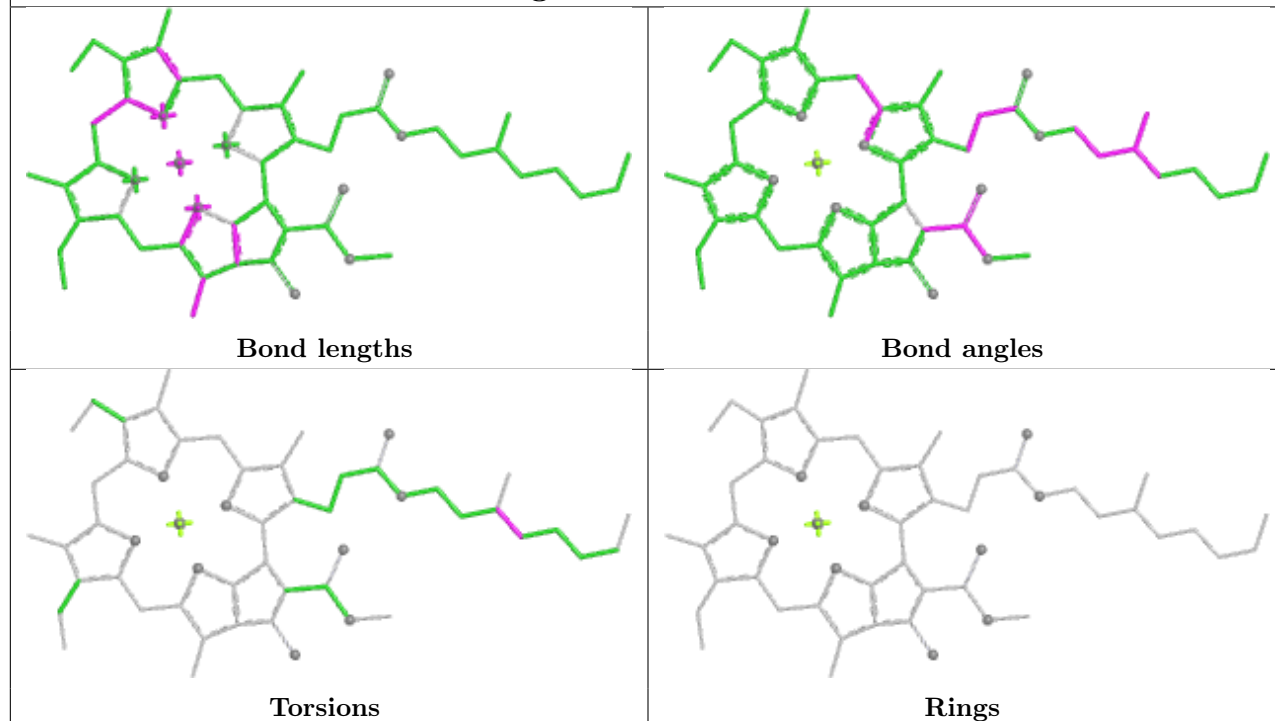
## Ligand CLA C 510



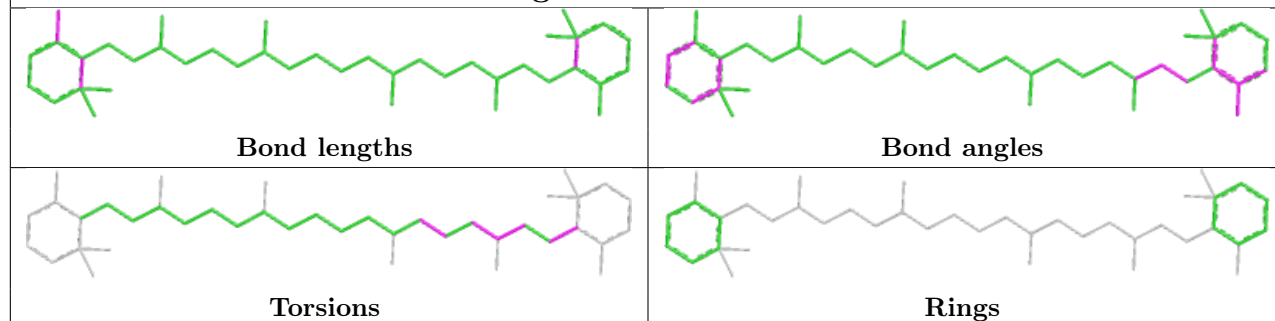
## Ligand BCR B 617



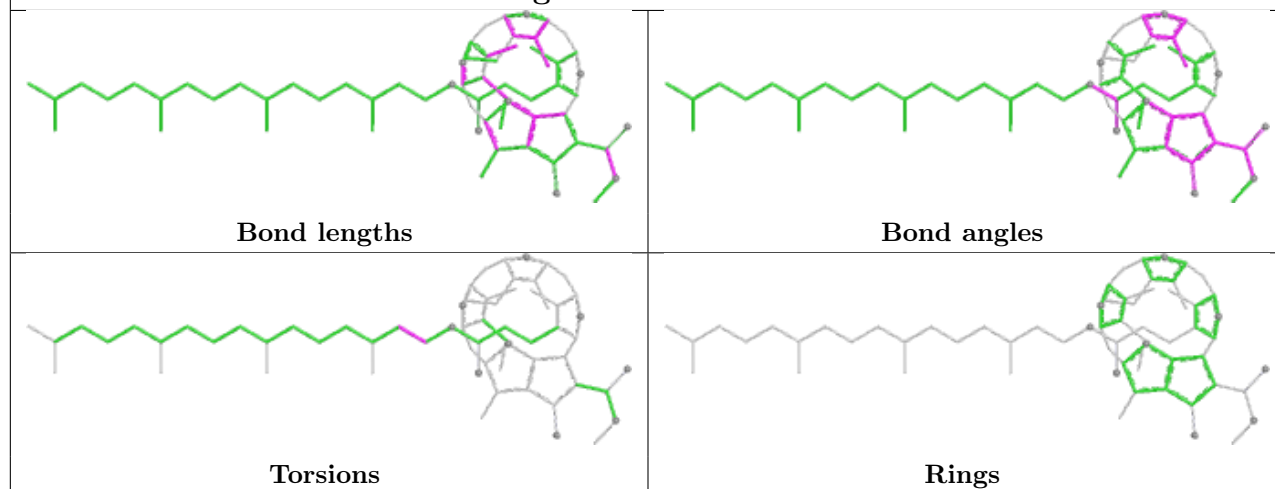
## Ligand CLA A 608



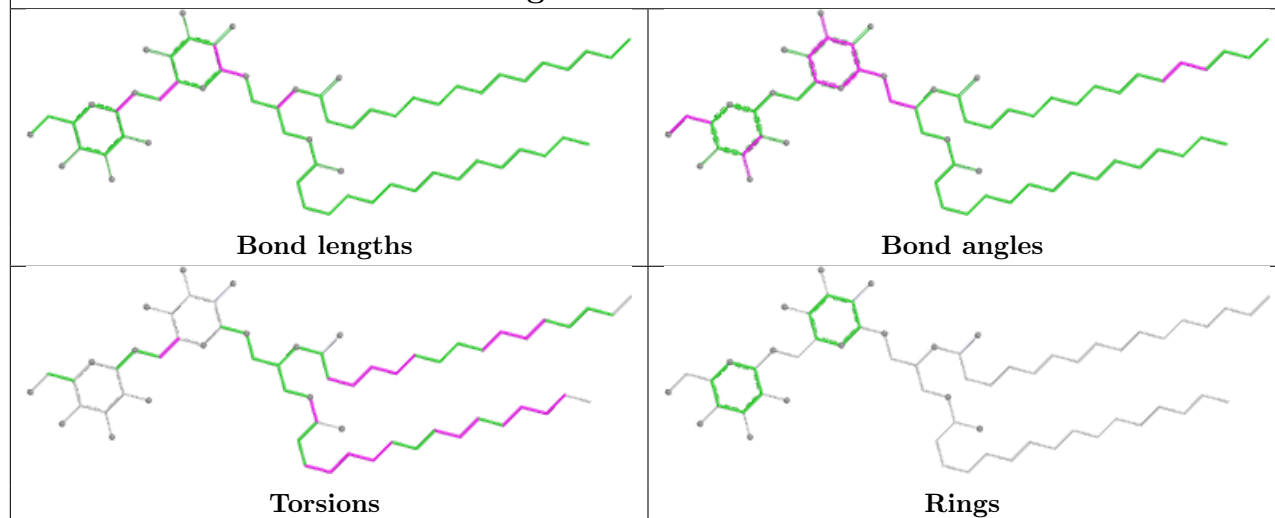
## Ligand BCR d 405

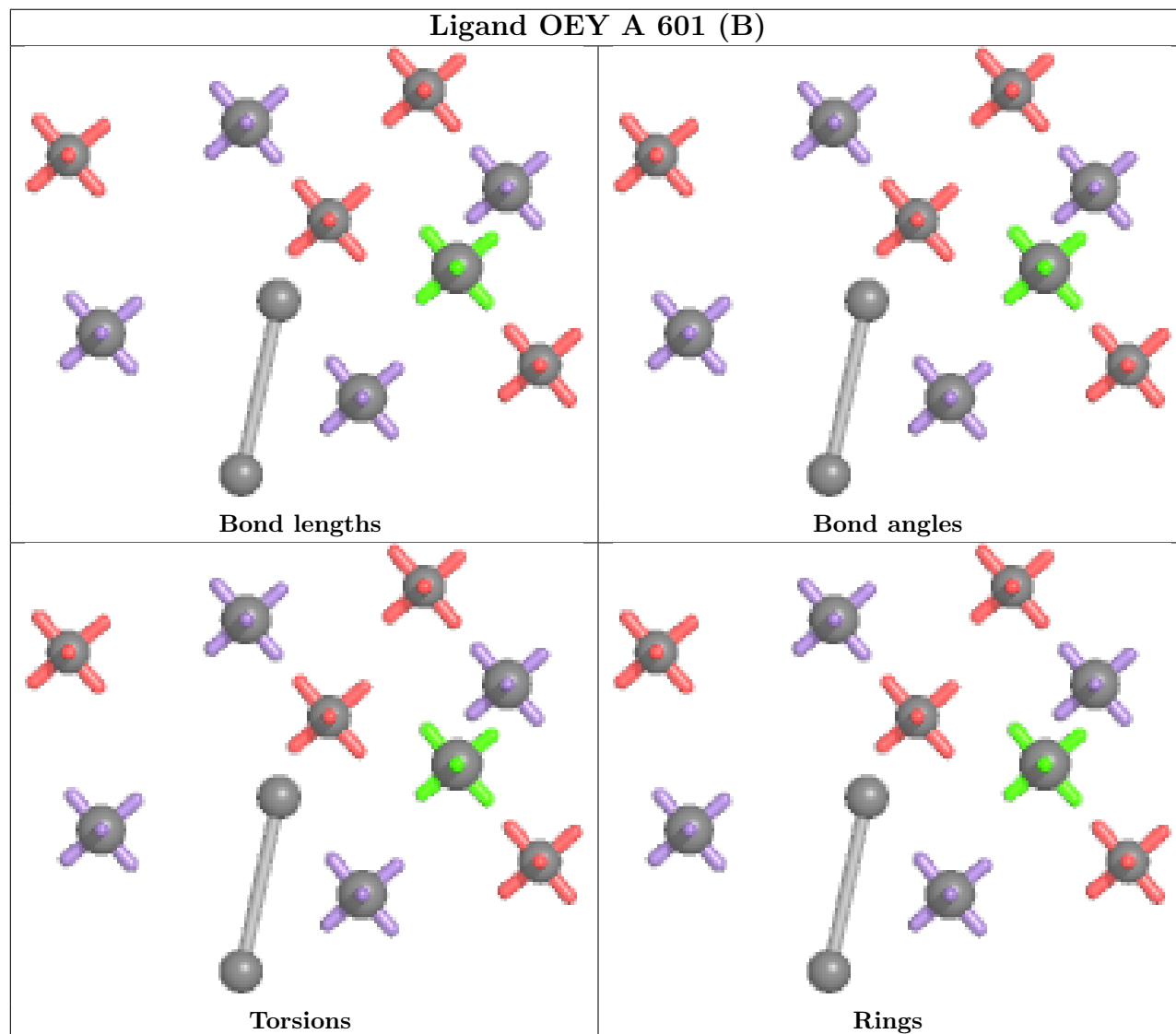
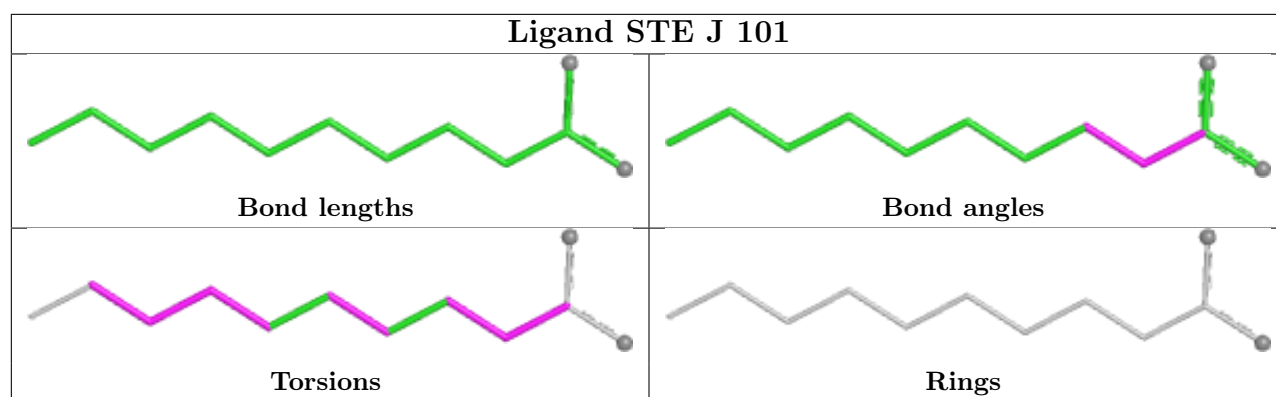


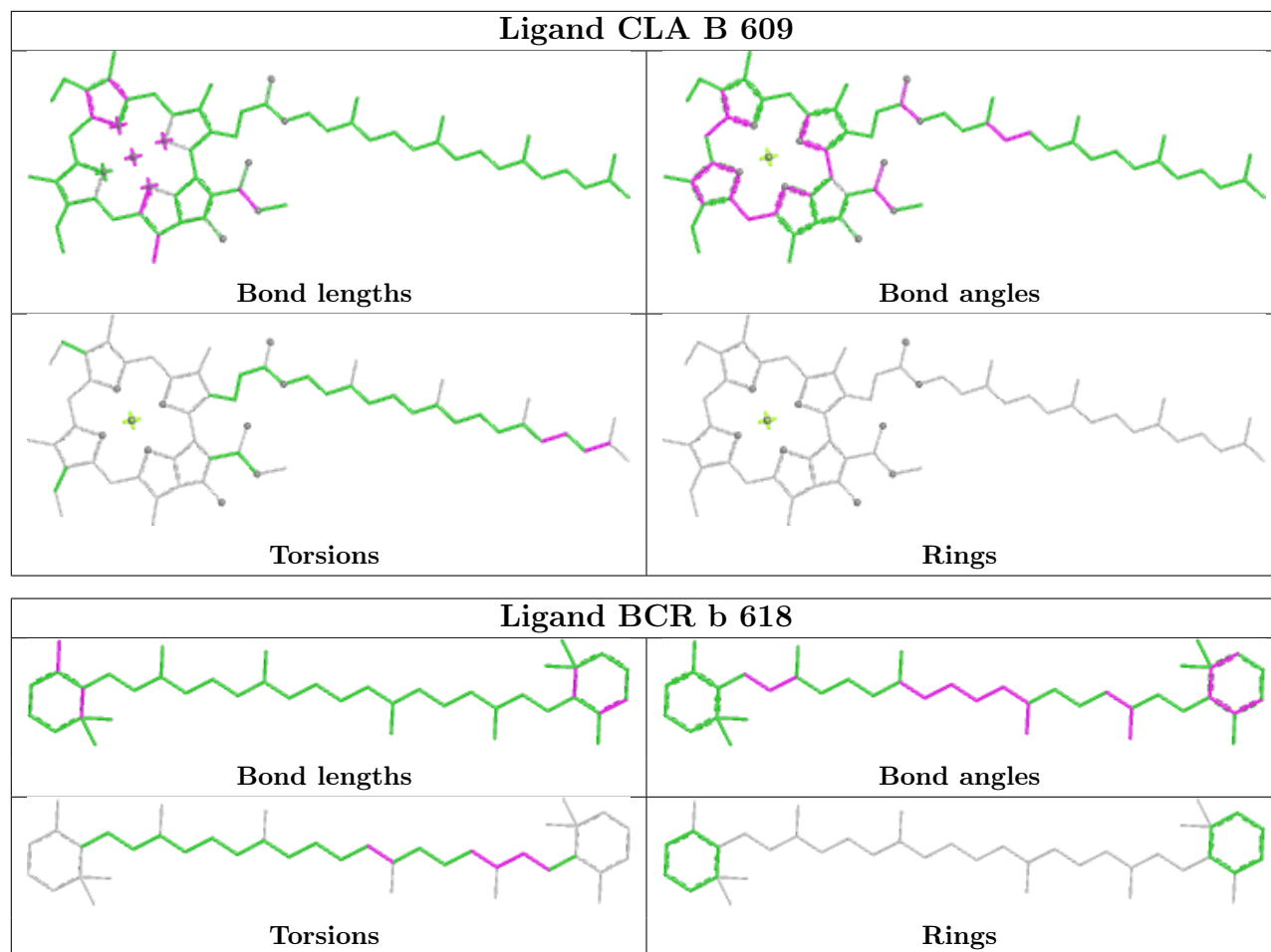
## Ligand PHO a 605



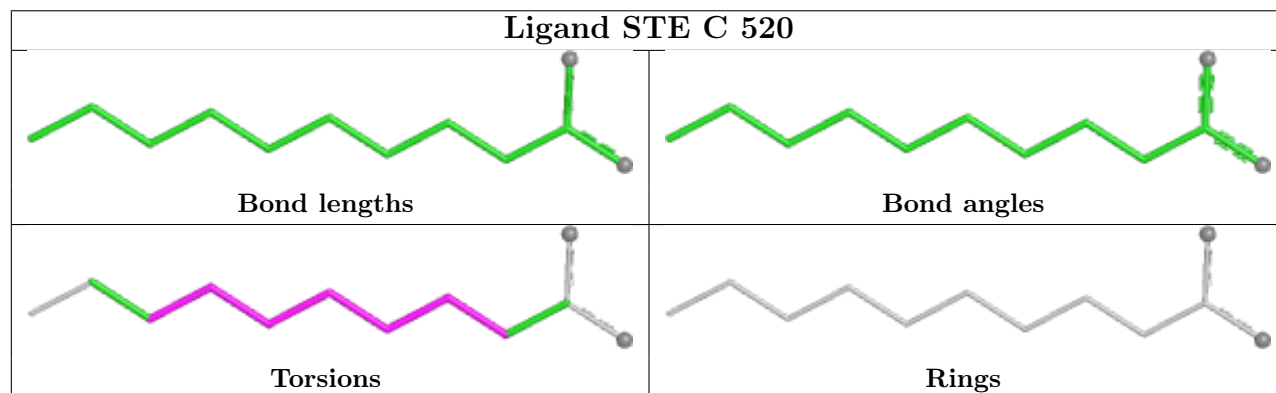
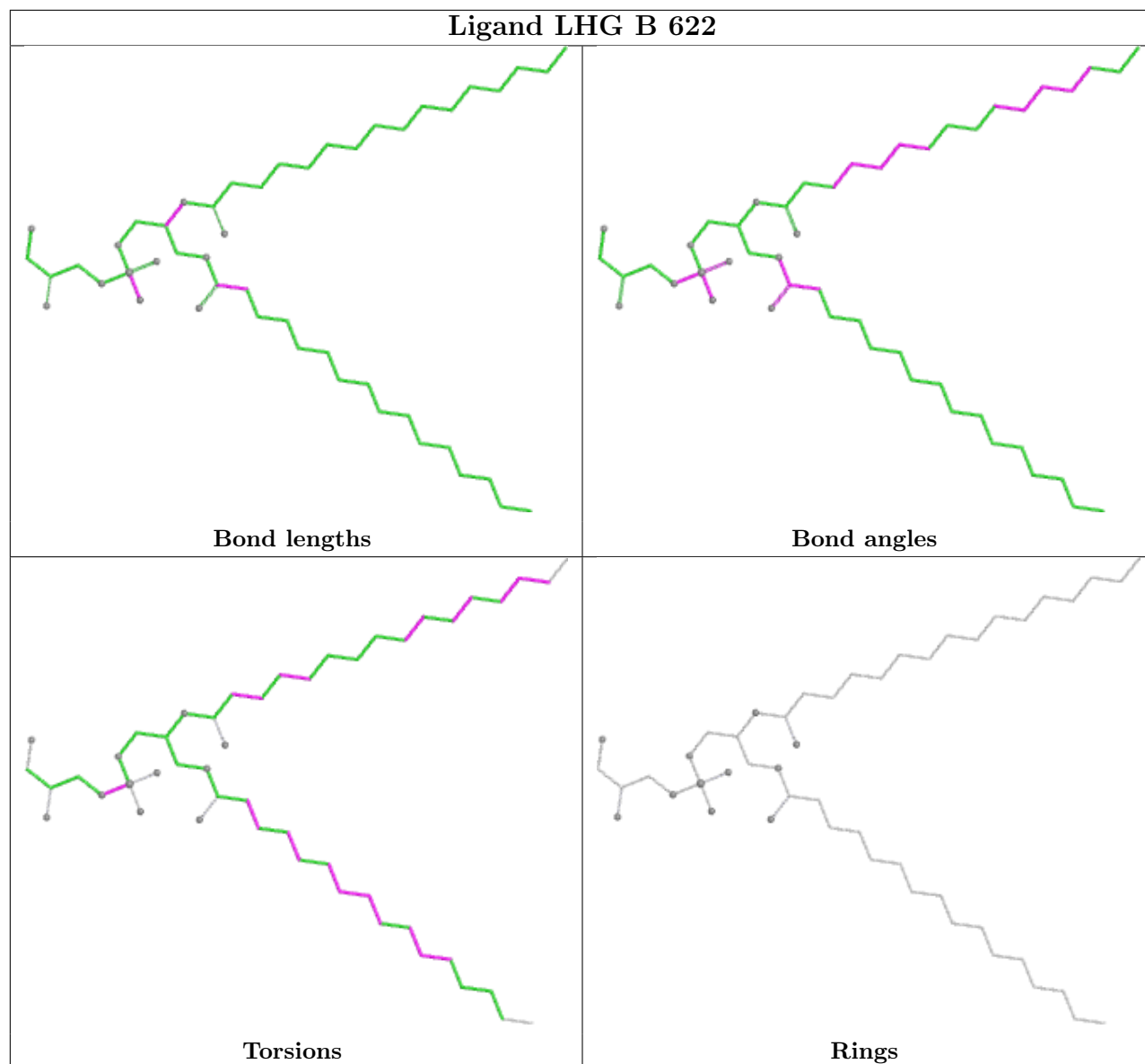
## Ligand DGD C 518



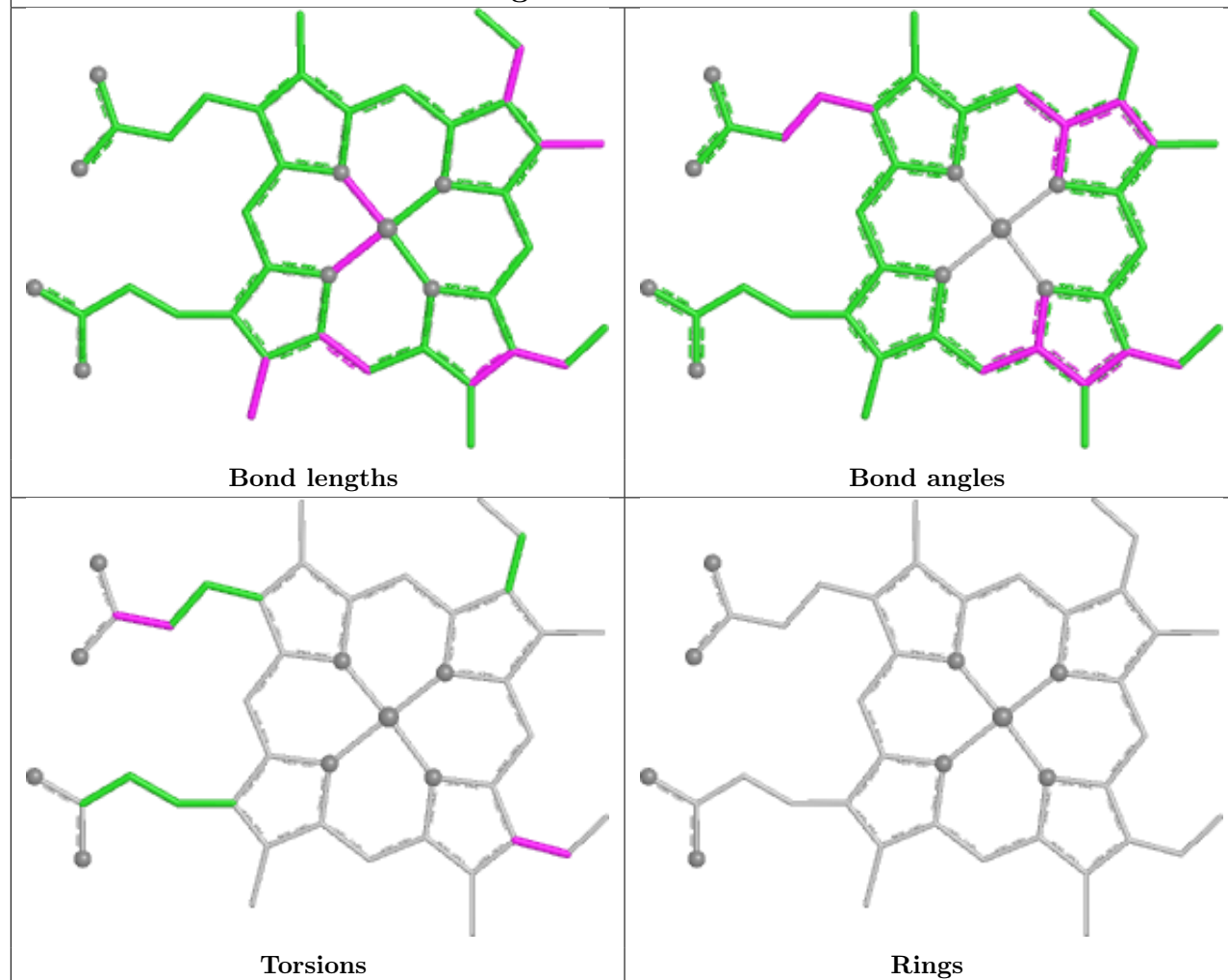




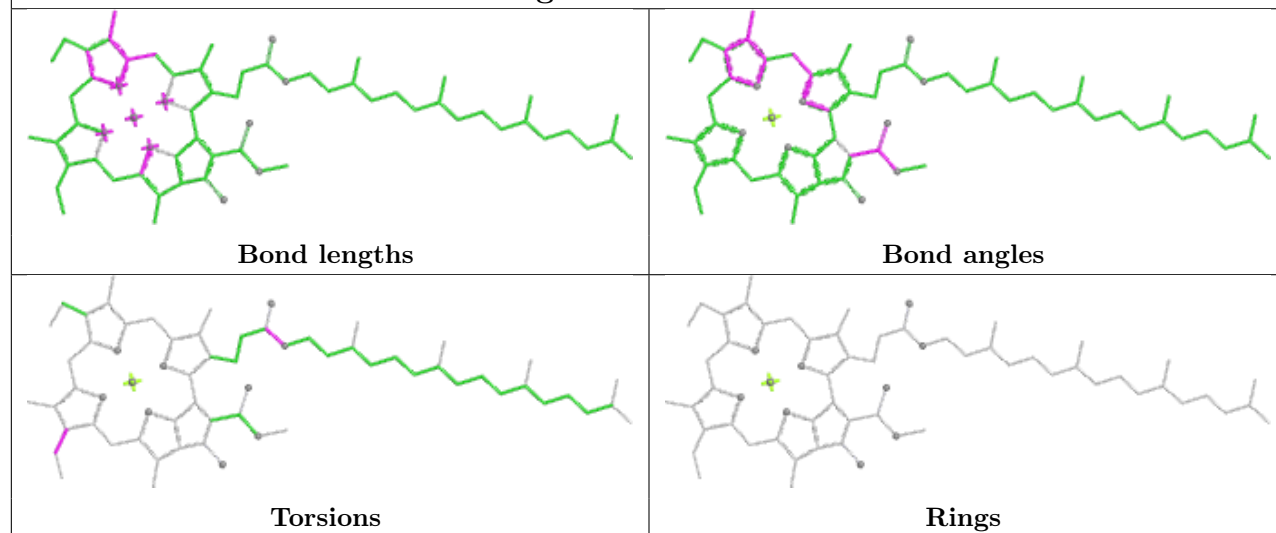




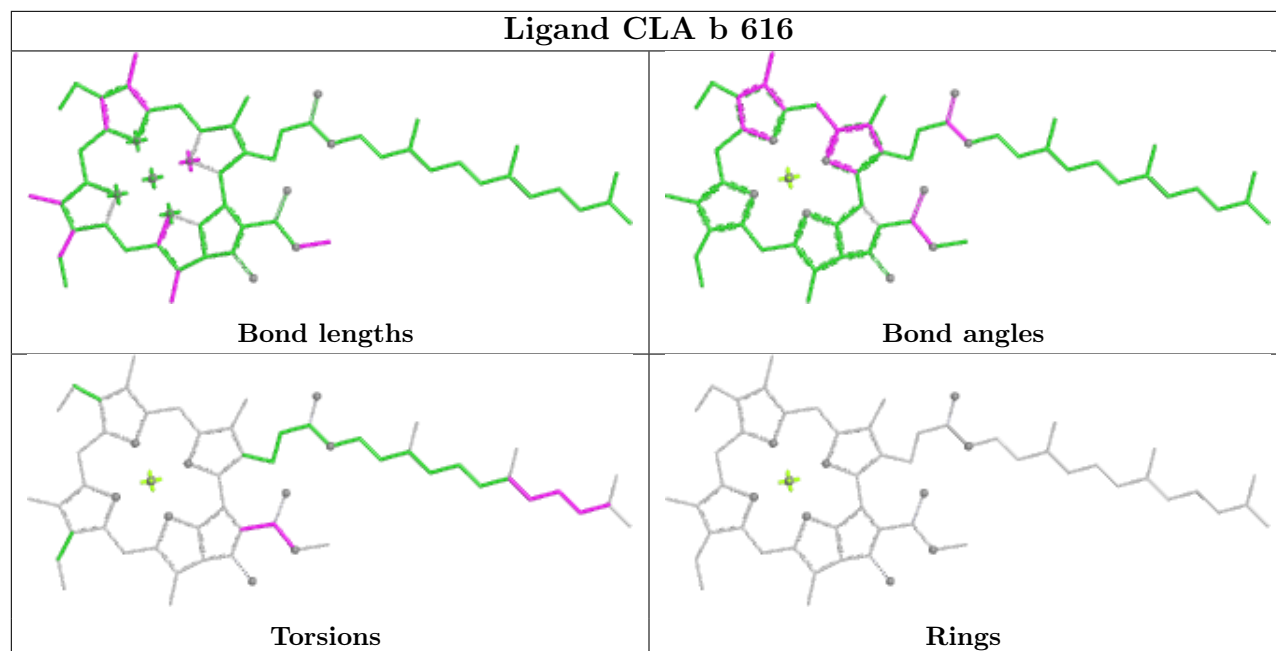
## Ligand HEM e 101



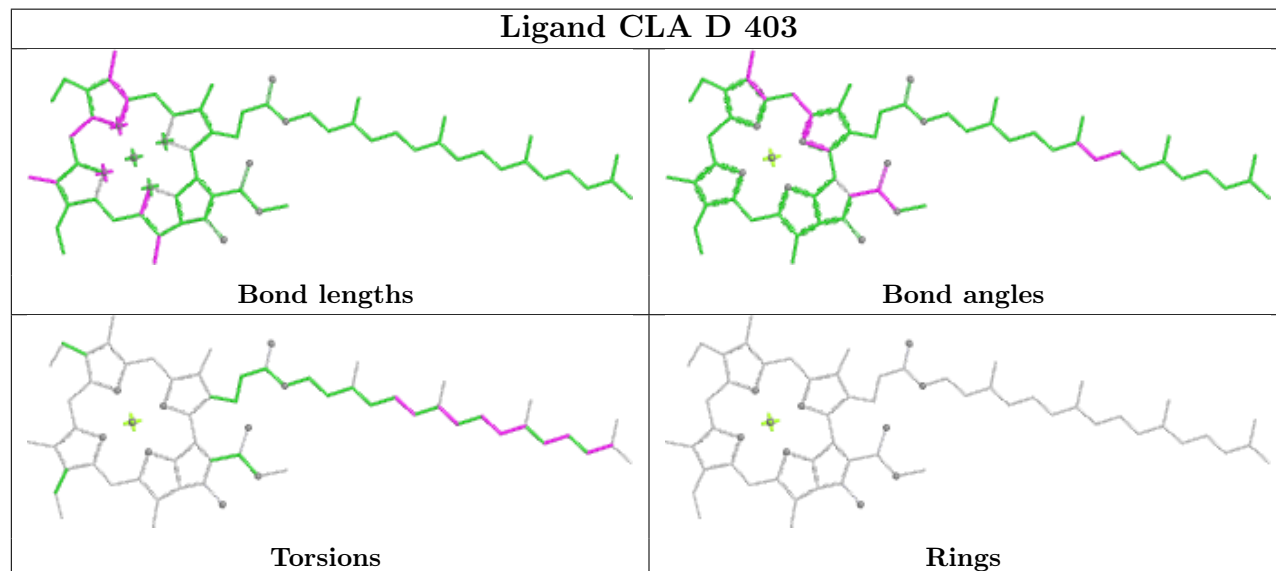
## Ligand CLA a 612

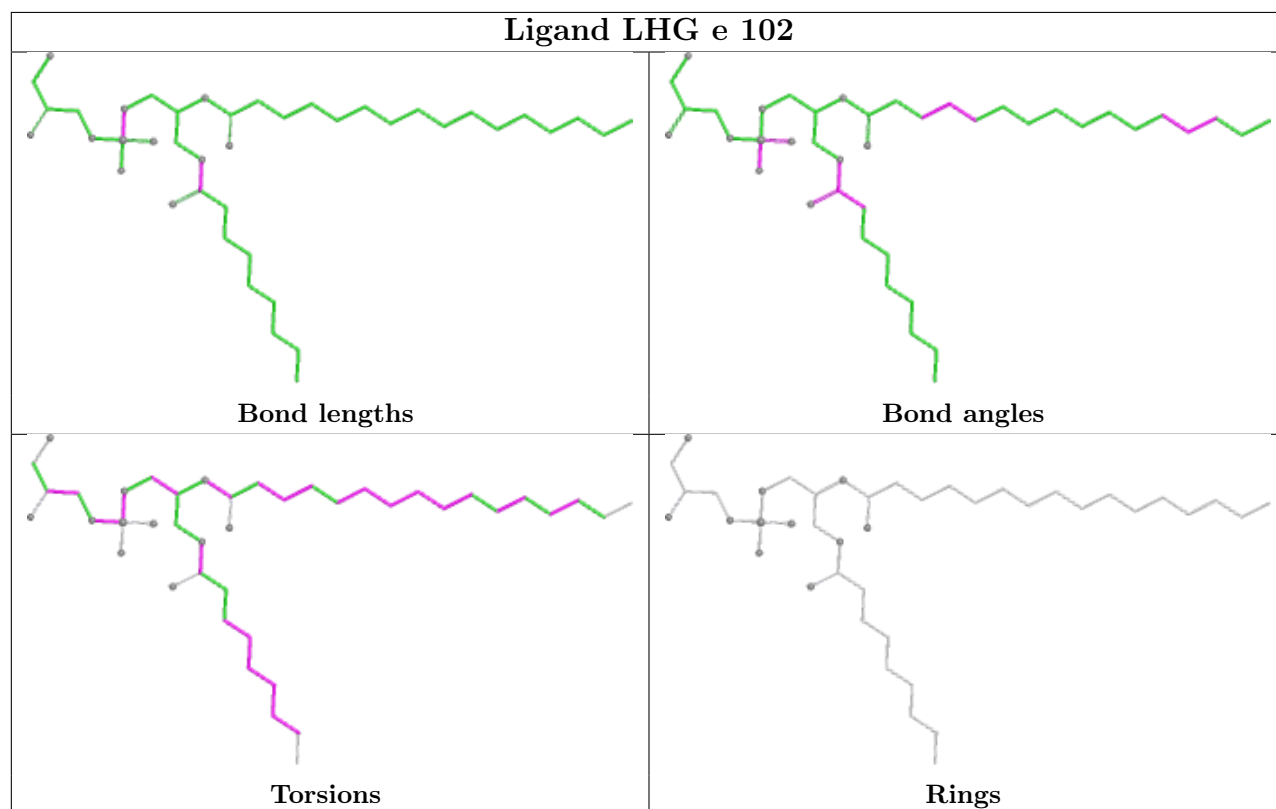
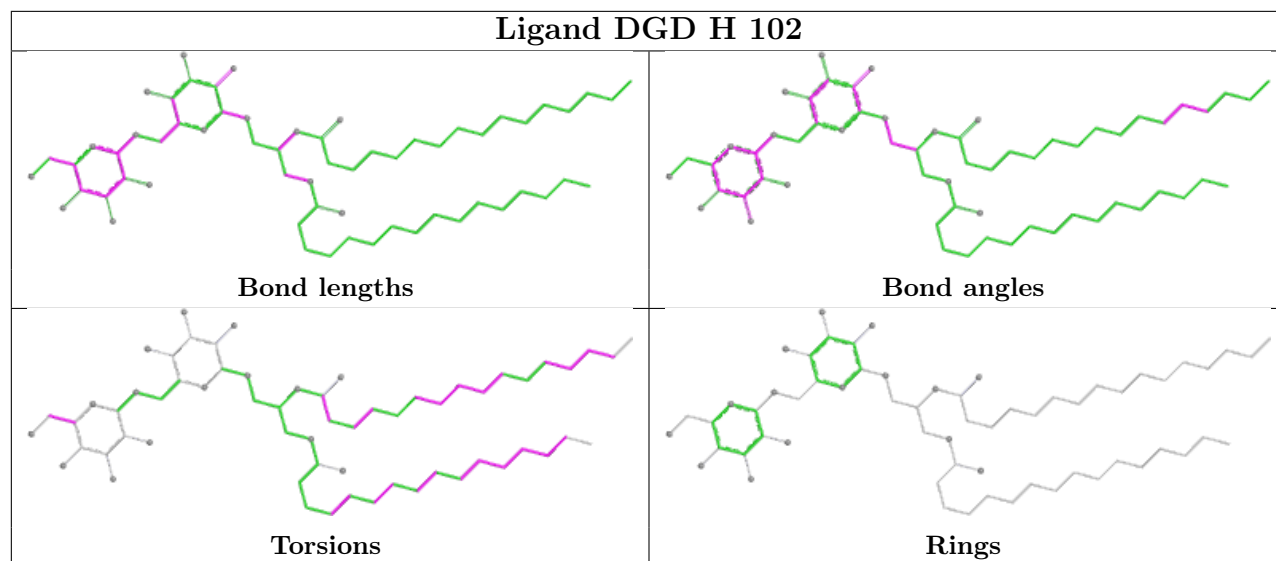


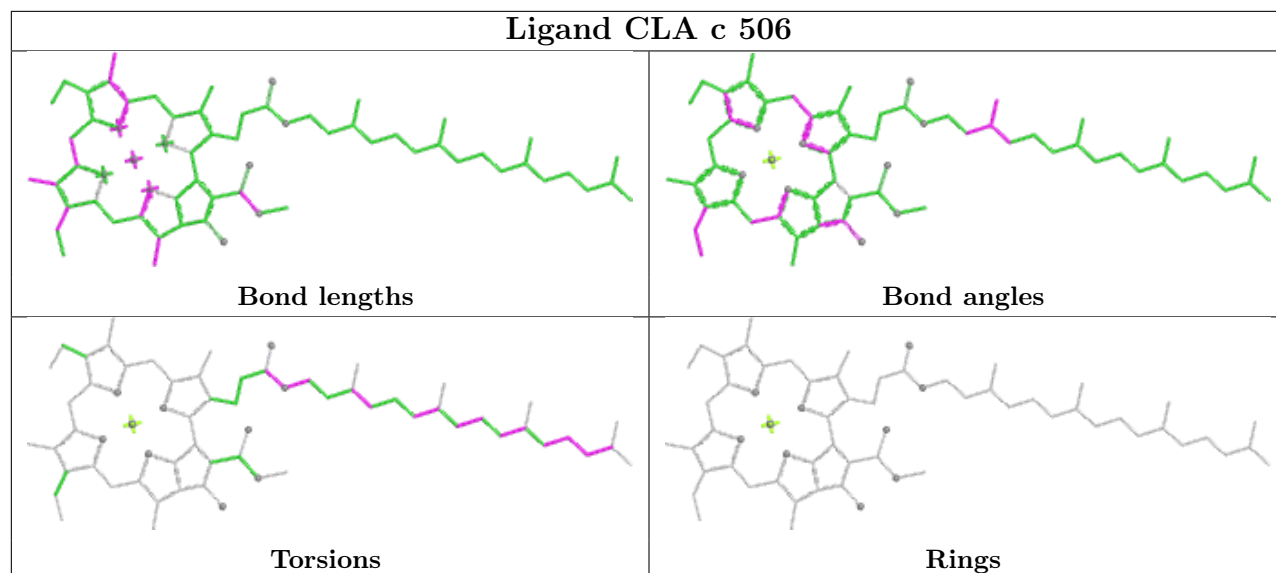
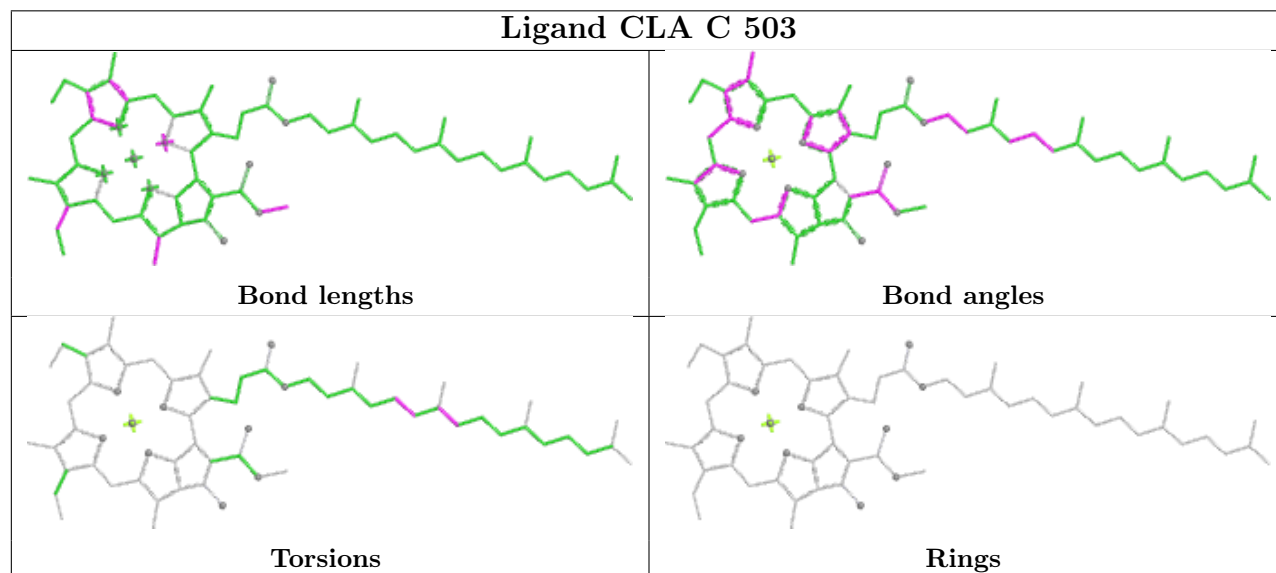
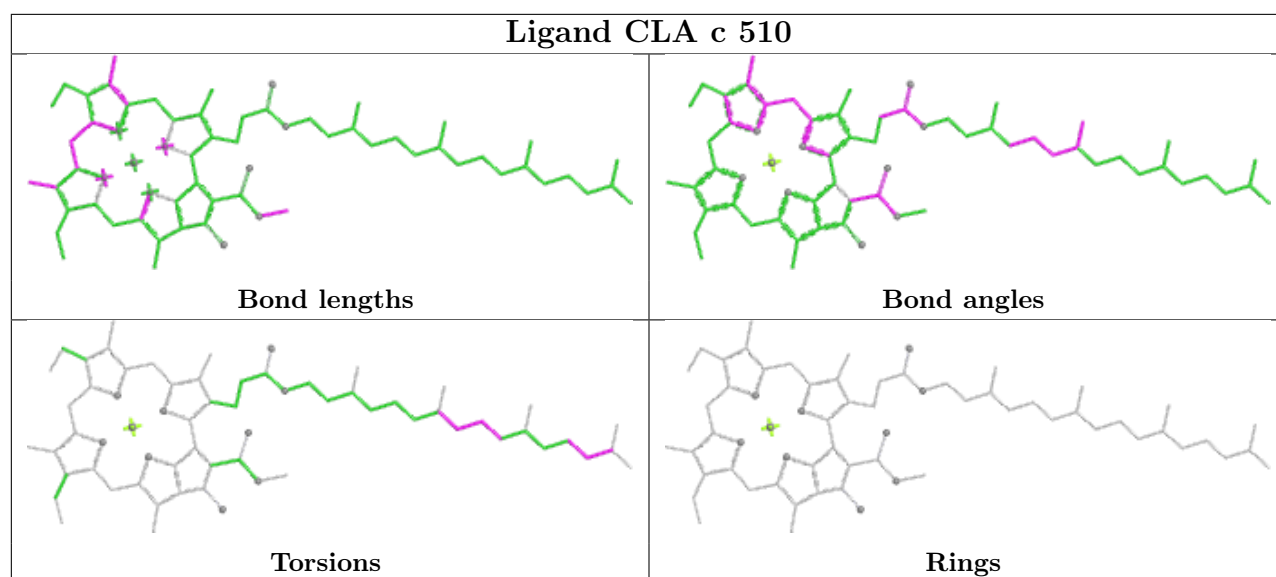
## Ligand CLA b 616



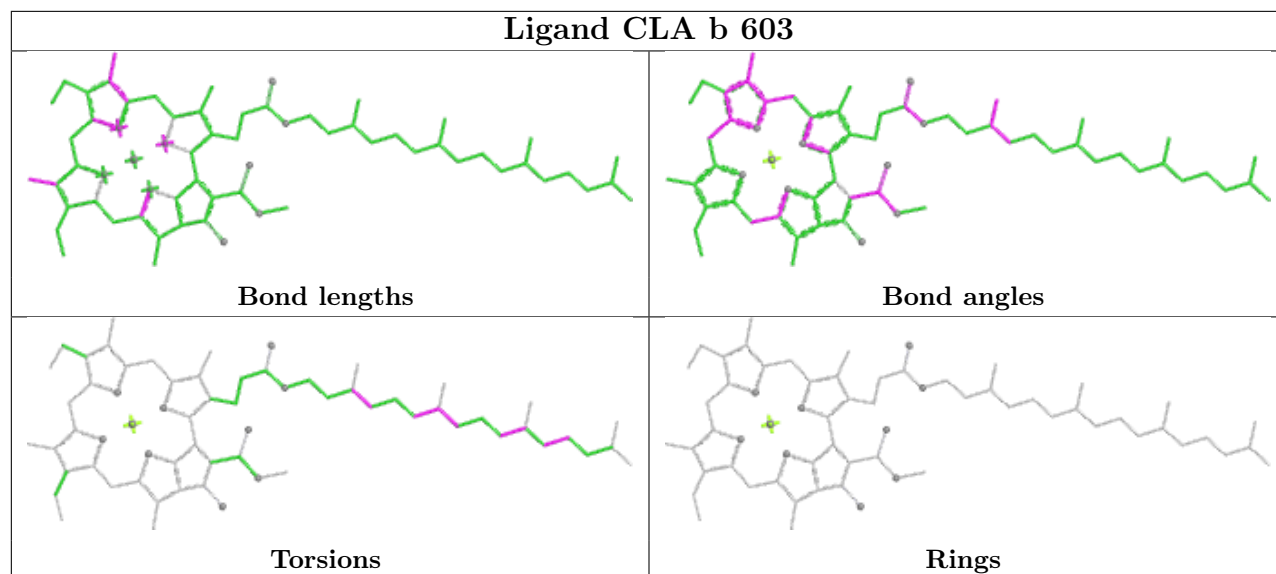
## Ligand CLA D 403



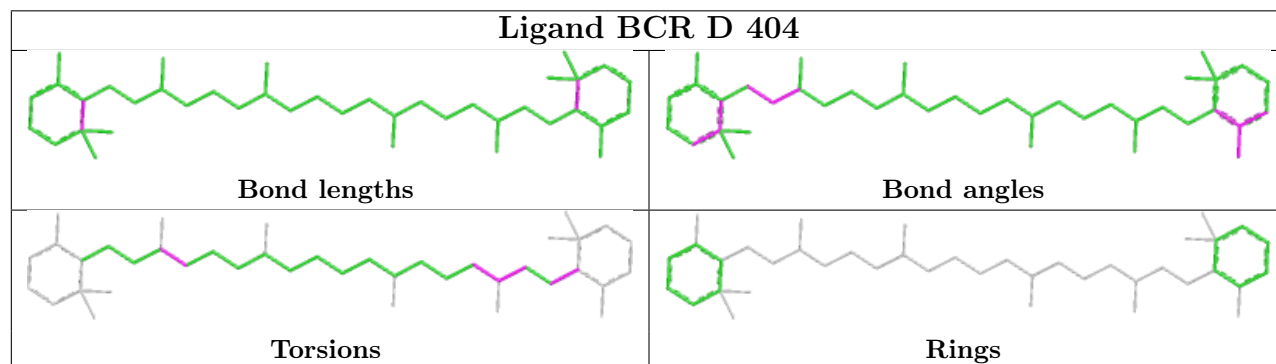




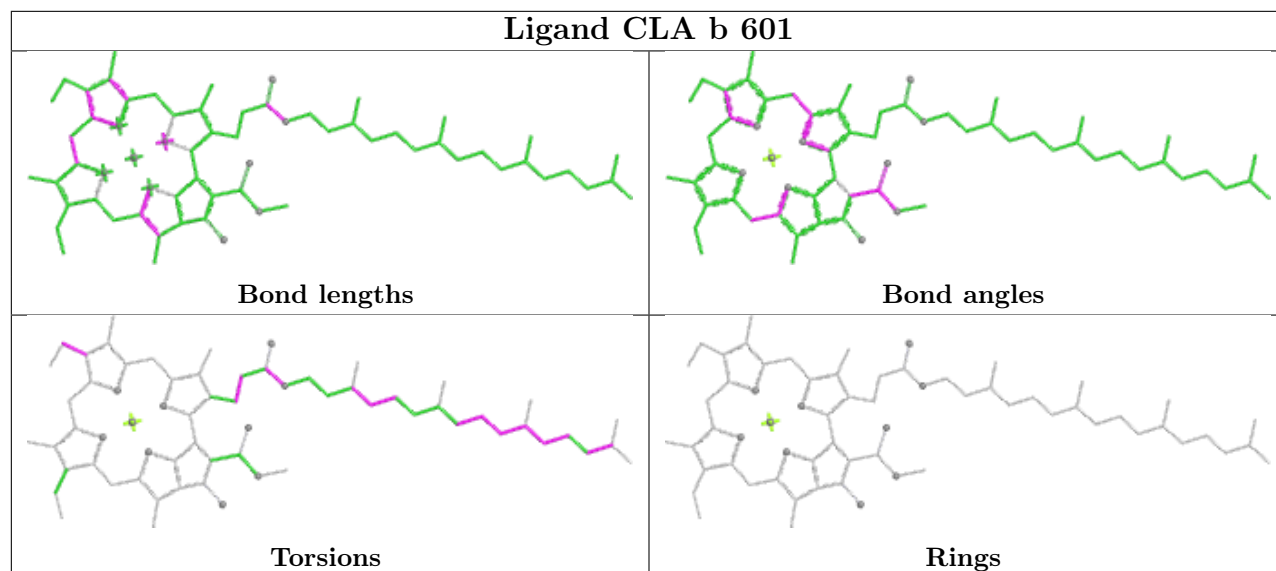
## Ligand CLA b 603

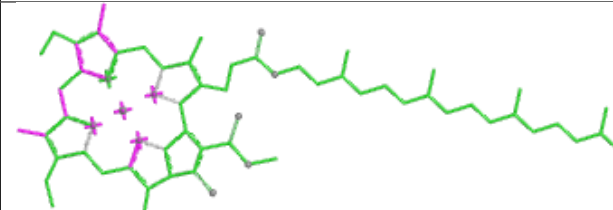
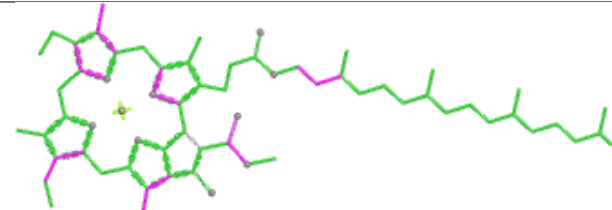
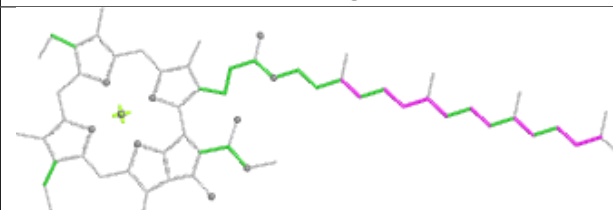
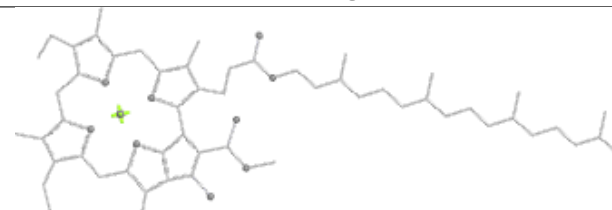


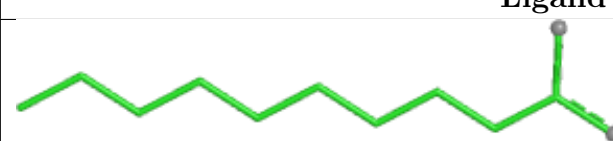
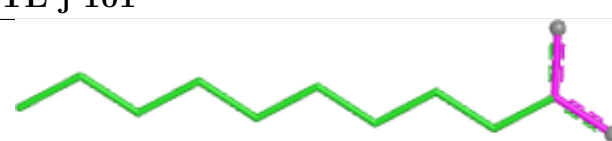
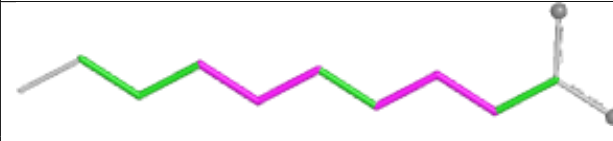
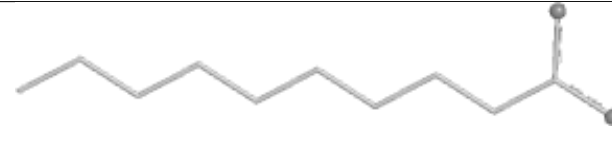
## Ligand BCR D 404



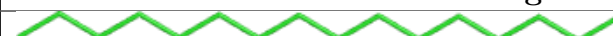
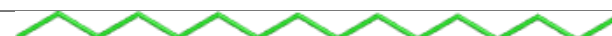
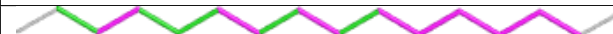
## Ligand CLA b 601

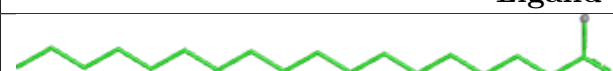
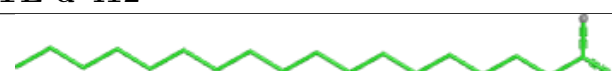
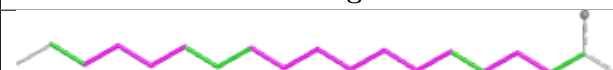


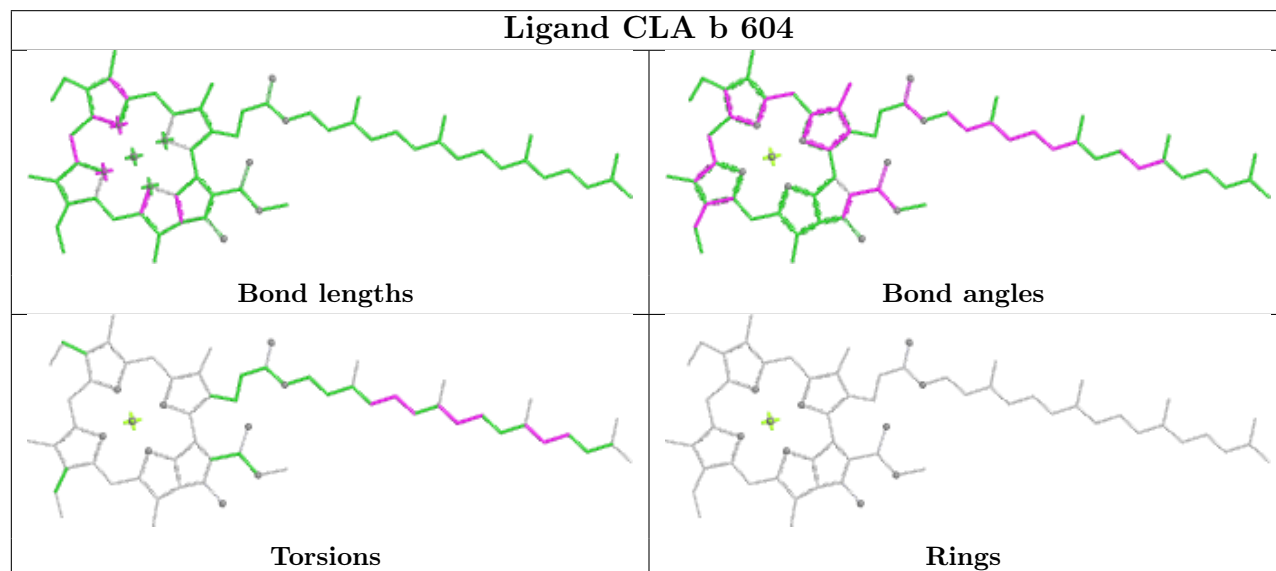
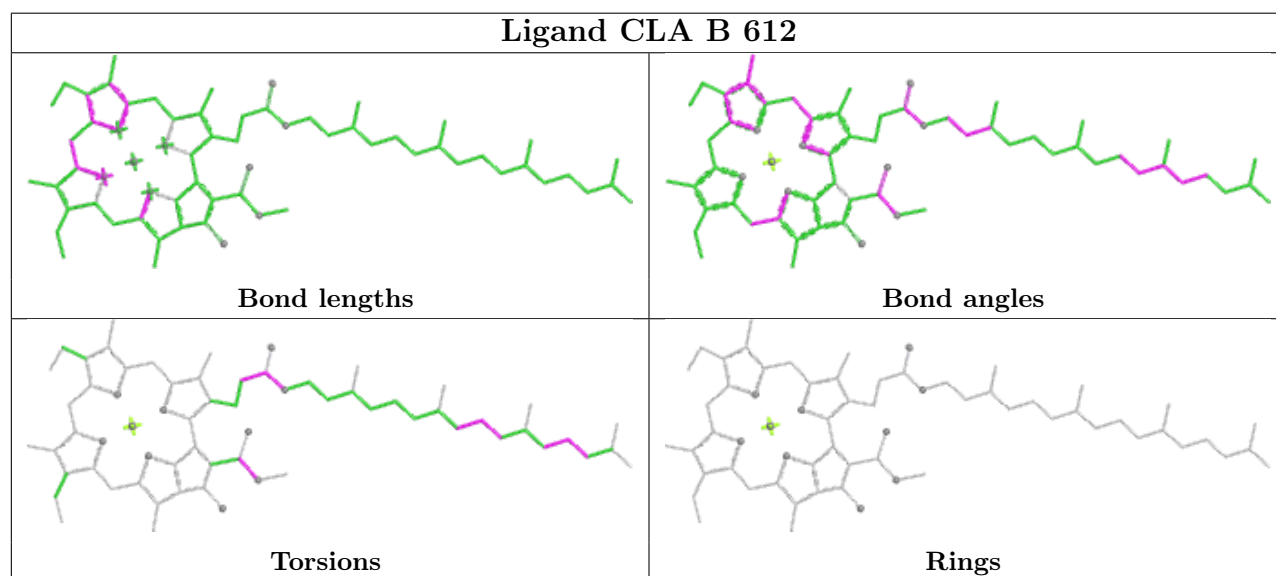
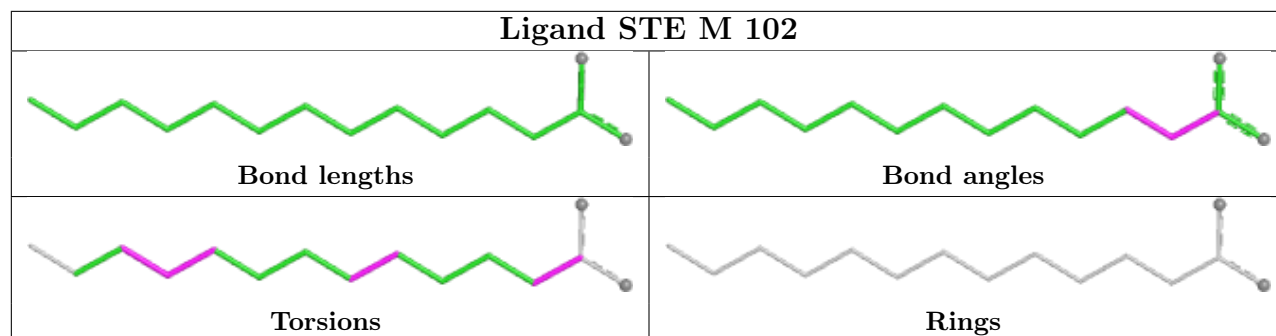
| Ligand CLA c 505                                                                  |  |                                                                                    |  |
|-----------------------------------------------------------------------------------|--|------------------------------------------------------------------------------------|--|
|  |  |  |  |
| Bond lengths                                                                      |  | Bond angles                                                                        |  |
|  |  |  |  |
| Torsions                                                                          |  | Rings                                                                              |  |

| Ligand STE j 101                                                                   |  |                                                                                     |  |
|------------------------------------------------------------------------------------|--|-------------------------------------------------------------------------------------|--|
|   |  |   |  |
| Bond lengths                                                                       |  | Bond angles                                                                         |  |
|  |  |  |  |
| Torsions                                                                           |  | Rings                                                                               |  |

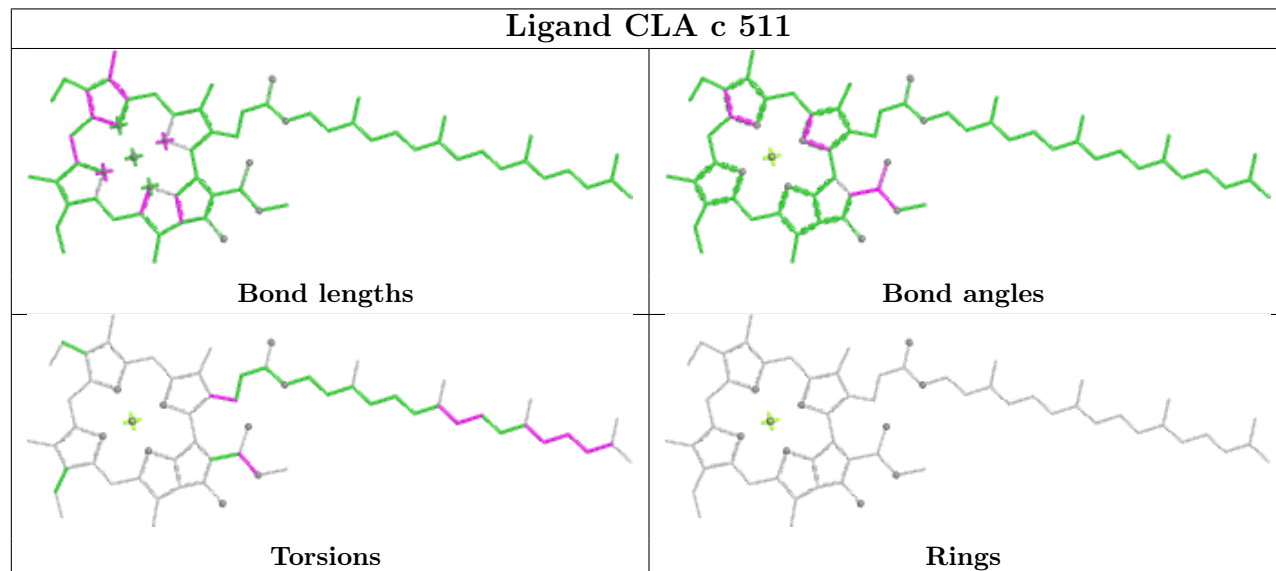
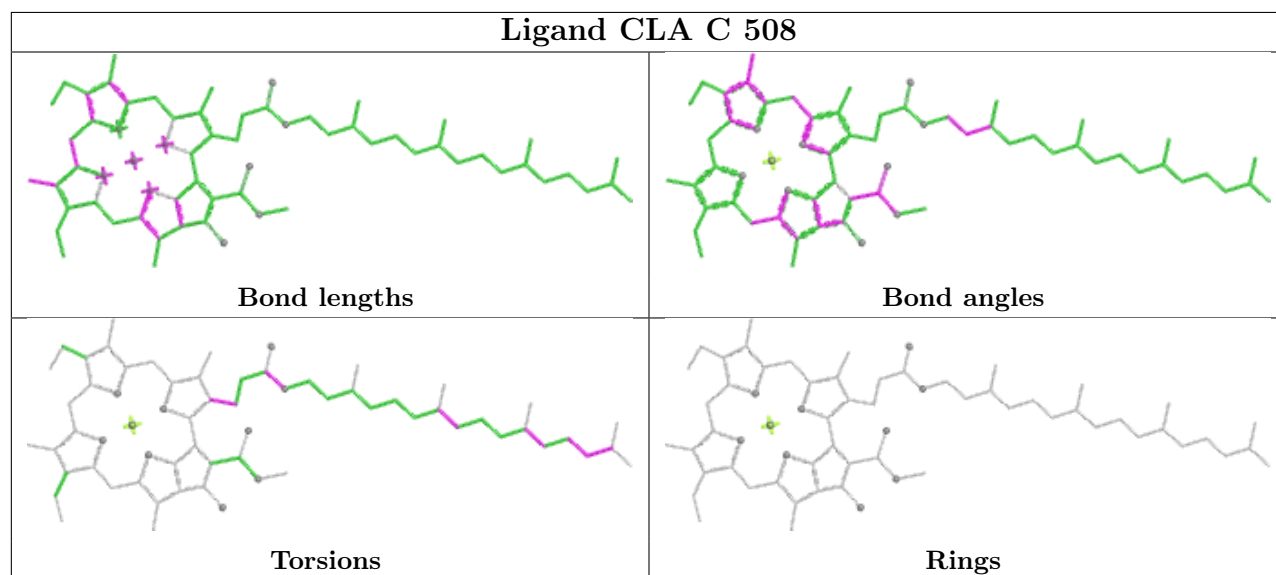
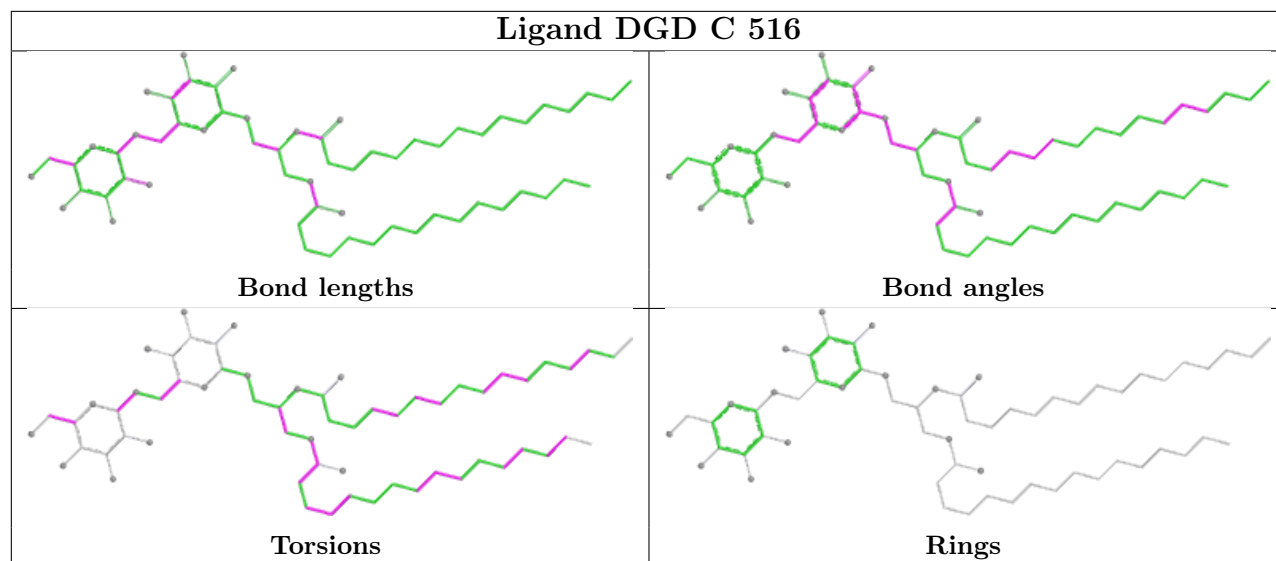
| Ligand STE H 103                                                                    |  |                                                                                      |  |
|-------------------------------------------------------------------------------------|--|--------------------------------------------------------------------------------------|--|
|  |  |  |  |
| Bond lengths                                                                        |  | Bond angles                                                                          |  |
|  |  |  |  |
| Torsions                                                                            |  | Rings                                                                                |  |

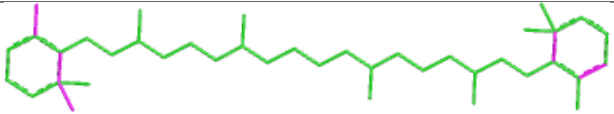
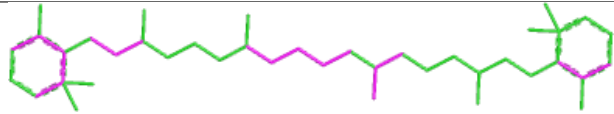
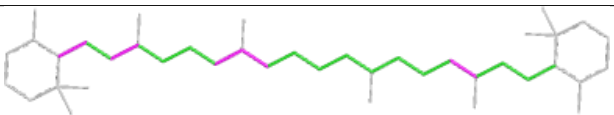
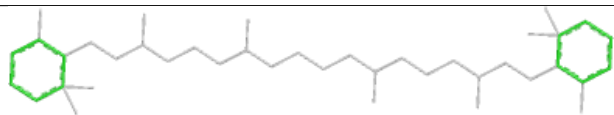
| Ligand STE B 626                                                                    |  |                                                                                      |  |
|-------------------------------------------------------------------------------------|--|--------------------------------------------------------------------------------------|--|
|  |  |  |  |
| Bond lengths                                                                        |  | Bond angles                                                                          |  |
|  |  |  |  |
| Torsions                                                                            |  | Rings                                                                                |  |

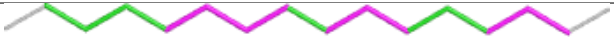
| Ligand STE d 412                                                                    |  |                                                                                      |  |
|-------------------------------------------------------------------------------------|--|--------------------------------------------------------------------------------------|--|
|  |  |  |  |
| Bond lengths                                                                        |  | Bond angles                                                                          |  |
|  |  |  |  |
| Torsions                                                                            |  | Rings                                                                                |  |

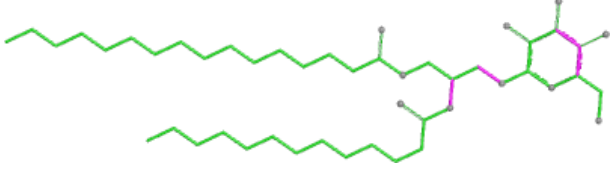
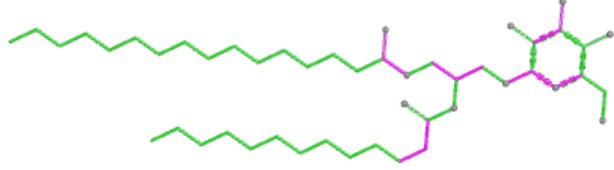
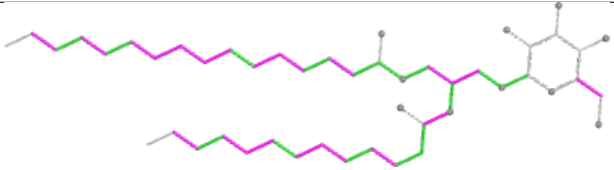
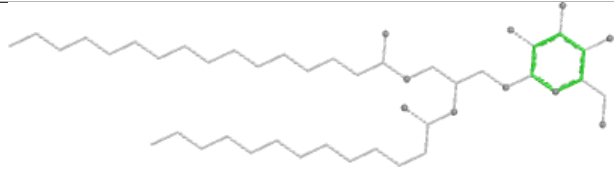


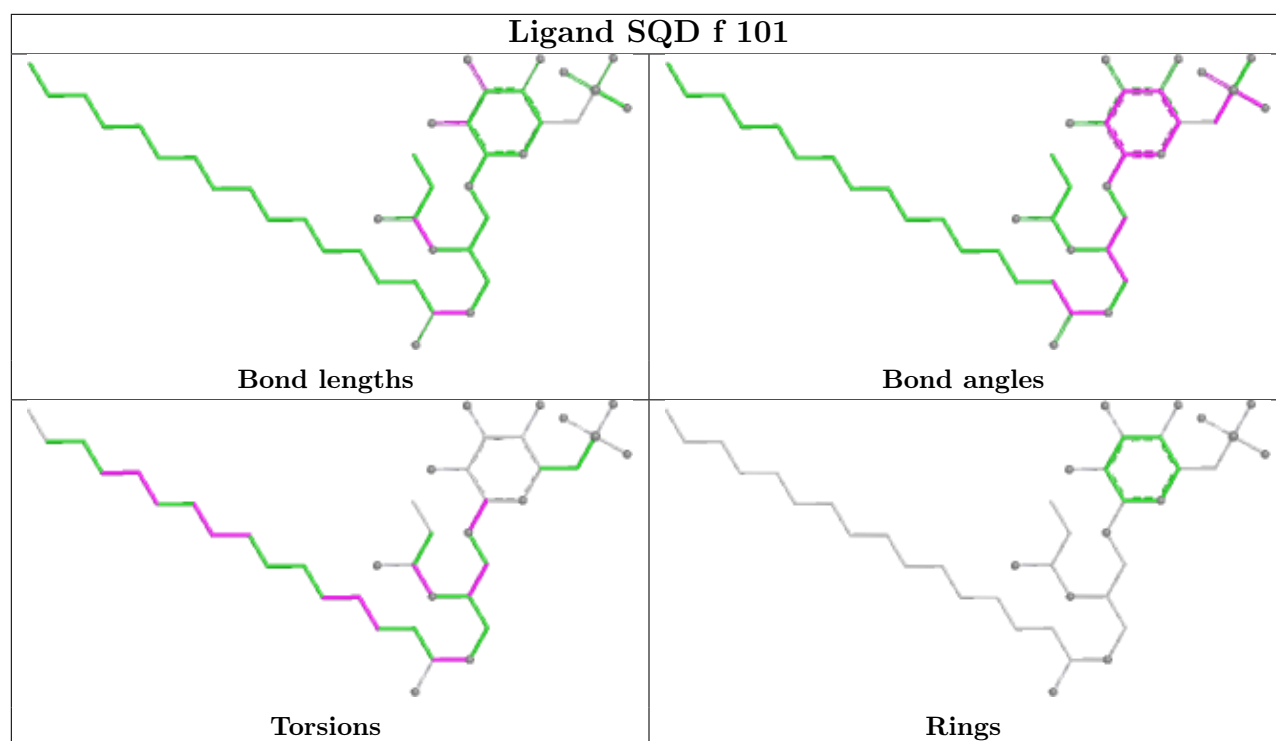


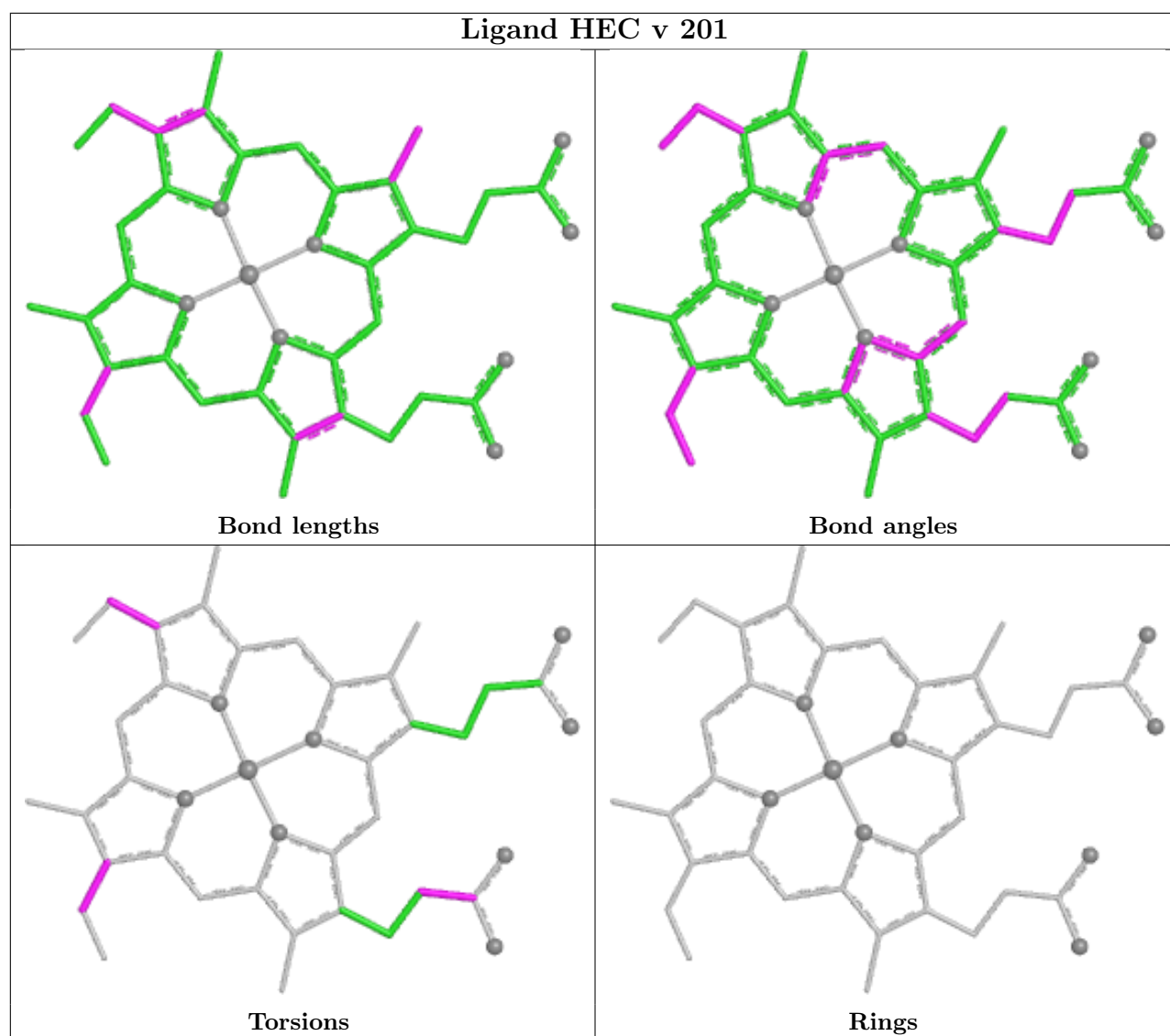


| Ligand BCR t 101                                                                                  |                                                                                                   |
|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| <br>Bond lengths | <br>Bond angles |
| <br>Torsions     | <br>Rings       |

| Ligand STE C 521                                                                                  |                                                                                                   |
|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| <br>Bond lengths | <br>Bond angles |
| <br>Torsions     | <br>Rings       |

| Ligand LMG A 614                                                                                  |                                                                                                   |
|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| <br>Bond lengths | <br>Bond angles |
| <br>Torsions   | <br>Rings     |





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|---------------|--------|--------------|-----------------------|----------|
| 1   | A     | 334/344 (97%) | -0.58  | 0 100 100    | 13, 29, 48, 83        | 64 (19%) |
| 1   | a     | 334/344 (97%) | -0.47  | 2 (0%) 85 85 | 12, 31, 57, 84        | 64 (19%) |
| 2   | B     | 505/510 (99%) | -0.46  | 3 (0%) 85 85 | 16, 34, 61, 87        | 4 (0%)   |
| 2   | b     | 505/510 (99%) | -0.30  | 2 (0%) 88 88 | 25, 38, 69, 107       | 0        |
| 3   | C     | 442/461 (95%) | -0.43  | 0 100 100    | 14, 37, 53, 80        | 11 (2%)  |
| 3   | c     | 451/461 (97%) | -0.29  | 1 (0%) 91 90 | 14, 41, 62, 101       | 12 (2%)  |
| 4   | D     | 341/352 (96%) | -0.65  | 0 100 100    | 15, 31, 47, 84        | 2 (0%)   |
| 4   | d     | 341/352 (96%) | -0.46  | 0 100 100    | 16, 34, 56, 81        | 3 (0%)   |
| 5   | E     | 82/84 (97%)   | 0.19   | 2 (2%) 59 59 | 30, 51, 69, 85        | 1 (1%)   |
| 5   | e     | 82/84 (97%)   | 0.36   | 1 (1%) 76 76 | 39, 60, 76, 92        | 0        |
| 6   | F     | 34/45 (75%)   | -0.17  | 1 (2%) 53 52 | 37, 43, 62, 83        | 0        |
| 6   | f     | 34/45 (75%)   | 0.03   | 0 100 100    | 41, 49, 77, 91        | 0        |
| 7   | H     | 65/66 (98%)   | -0.29  | 2 (3%) 51 50 | 32, 42, 58, 72        | 0        |
| 7   | h     | 63/66 (95%)   | 0.06   | 2 (3%) 50 49 | 39, 51, 65, 73        | 0        |
| 8   | I     | 35/38 (92%)   | -0.39  | 0 100 100    | 32, 40, 68, 84        | 0        |
| 8   | i     | 35/38 (92%)   | -0.18  | 1 (2%) 53 52 | 31, 42, 75, 91        | 0        |
| 9   | J     | 36/40 (90%)   | -0.08  | 1 (2%) 55 54 | 34, 51, 72, 91        | 0        |
| 9   | j     | 36/40 (90%)   | 0.10   | 1 (2%) 55 54 | 38, 53, 91, 107       | 0        |
| 10  | K     | 37/46 (80%)   | -0.02  | 0 100 100    | 41, 52, 73, 77        | 0        |
| 10  | k     | 37/46 (80%)   | 0.19   | 0 100 100    | 47, 57, 71, 80        | 0        |
| 11  | L     | 37/37 (100%)  | -0.57  | 0 100 100    | 25, 32, 61, 68        | 0        |
| 11  | l     | 36/37 (97%)   | -0.49  | 0 100 100    | 26, 32, 74, 90        | 0        |
| 12  | M     | 32/36 (88%)   | -0.50  | 0 100 100    | 25, 36, 56, 68        | 0        |
| 12  | m     | 31/36 (86%)   | -0.47  | 0 100 100    | 27, 36, 50, 69        | 0        |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 13  | O     | 244/272 (89%)   | -0.14  | 4 (1%) 70 70  | 25, 44, 82, 136       | 1 (0%)   |
| 13  | o     | 244/272 (89%)   | -0.17  | 3 (1%) 76 76  | 26, 42, 78, 135       | 0        |
| 14  | R     | 28/41 (68%)     | 0.72   | 0 100 100     | 61, 71, 87, 91        | 0        |
| 14  | r     | 28/41 (68%)     | 1.14   | 1 (3%) 46 45  | 69, 87, 104, 114      | 0        |
| 15  | T     | 29/32 (90%)     | -0.53  | 1 (3%) 48 47  | 27, 32, 61, 75        | 0        |
| 15  | t     | 29/32 (90%)     | -0.36  | 2 (6%) 23 21  | 29, 33, 78, 85        | 0        |
| 16  | U     | 97/134 (72%)    | -0.21  | 0 100 100     | 33, 44, 72, 88        | 0        |
| 16  | u     | 97/134 (72%)    | -0.28  | 0 100 100     | 30, 41, 56, 86        | 0        |
| 17  | V     | 137/163 (84%)   | -0.36  | 0 100 100     | 30, 41, 57, 77        | 0        |
| 17  | v     | 137/163 (84%)   | -0.11  | 1 (0%) 84 84  | 34, 48, 69, 86        | 0        |
| 18  | X     | 38/41 (92%)     | -0.05  | 0 100 100     | 37, 50, 67, 77        | 0        |
| 18  | x     | 39/41 (95%)     | 0.26   | 1 (2%) 57 56  | 48, 58, 86, 100       | 0        |
| 19  | Y     | 27/46 (58%)     | 1.11   | 4 (14%) 5 5   | 52, 70, 96, 99        | 0        |
| 19  | y     | 30/46 (65%)     | 0.84   | 0 100 100     | 60, 72, 91, 100       | 0        |
| 20  | Z     | 62/62 (100%)    | 0.76   | 1 (1%) 70 70  | 53, 68, 119, 126      | 0        |
| 20  | z     | 62/62 (100%)    | 0.76   | 2 (3%) 50 49  | 59, 73, 111, 121      | 0        |
| All | All   | 5293/5700 (92%) | -0.28  | 39 (0%) 84 84 | 12, 39, 74, 136       | 162 (3%) |

All (39) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | o     | 58  | ASN  | 5.0  |
| 13  | O     | 59  | LYS  | 4.1  |
| 5   | e     | 79  | PHE  | 3.7  |
| 20  | Z     | 62  | VAL  | 3.7  |
| 15  | t     | 30  | THR  | 3.7  |
| 2   | b     | 495 | PHE  | 3.4  |
| 18  | x     | 40  | SER  | 3.2  |
| 14  | r     | 20  | VAL  | 3.1  |
| 7   | H     | 41  | PHE  | 3.1  |
| 19  | Y     | 22  | LEU  | 3.0  |
| 20  | z     | 33  | TRP  | 2.9  |
| 19  | Y     | 20  | ALA  | 2.9  |
| 2   | B     | 495 | PHE  | 2.9  |
| 15  | T     | 30  | THR  | 2.8  |
| 5   | E     | 84  | LYS  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | h     | 41  | PHE  | 2.7  |
| 13  | O     | 60  | ARG  | 2.7  |
| 19  | Y     | 25  | ILE  | 2.7  |
| 3   | c     | 24  | THR  | 2.7  |
| 2   | B     | 490 | GLN  | 2.6  |
| 1   | a     | 11  | ALA  | 2.6  |
| 13  | O     | 58  | ASN  | 2.6  |
| 9   | J     | 5   | GLY  | 2.6  |
| 1   | a     | 250 | ALA  | 2.3  |
| 7   | h     | 64  | ALA  | 2.3  |
| 13  | o     | 56  | PRO  | 2.2  |
| 17  | v     | 113 | VAL  | 2.2  |
| 13  | o     | 57  | LYS  | 2.2  |
| 19  | Y     | 24  | MET  | 2.2  |
| 6   | F     | 12  | SER  | 2.2  |
| 13  | O     | 56  | PRO  | 2.1  |
| 20  | z     | 30  | PRO  | 2.1  |
| 9   | j     | 6   | GLY  | 2.1  |
| 8   | i     | 36  | ASP  | 2.1  |
| 15  | t     | 29  | ILE  | 2.1  |
| 2   | b     | 487 | SER  | 2.1  |
| 5   | E     | 79  | PHE  | 2.0  |
| 7   | H     | 65  | LEU  | 2.0  |
| 2   | B     | 494 | GLY  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 12  | FME  | M     | 1   | 10/11 | 0.94 | 0.09 | 37,48,67,75                | 0     |
| 15  | FME  | t     | 1   | 10/11 | 0.94 | 0.08 | 31,44,66,66                | 0     |
| 8   | FME  | I     | 1   | 10/11 | 0.95 | 0.09 | 35,46,65,66                | 0     |
| 12  | FME  | m     | 1   | 10/11 | 0.96 | 0.09 | 34,42,59,71                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.96 | 0.08 | 33,48,59,64                | 0     |
| 15  | FME  | T     | 1   | 10/11 | 0.97 | 0.06 | 28,45,61,61                | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 33  | STE  | a     | 616 | 12/20 | 0.74 | 0.15 | 45,61,68,71                | 0     |
| 33  | STE  | H     | 103 | 18/20 | 0.75 | 0.17 | 49,67,78,81                | 0     |
| 33  | STE  | b     | 626 | 10/20 | 0.76 | 0.17 | 42,54,62,63                | 0     |
| 33  | STE  | d     | 412 | 20/20 | 0.76 | 0.16 | 41,65,84,85                | 0     |
| 33  | STE  | b     | 625 | 20/20 | 0.78 | 0.14 | 47,62,72,76                | 0     |
| 29  | LMG  | a     | 618 | 55/55 | 0.79 | 0.14 | 38,58,72,83                | 0     |
| 33  | STE  | a     | 615 | 10/20 | 0.79 | 0.16 | 40,60,68,69                | 0     |
| 29  | LMG  | b     | 623 | 55/55 | 0.79 | 0.16 | 51,68,87,91                | 0     |
| 33  | STE  | a     | 617 | 15/20 | 0.80 | 0.18 | 38,57,69,77                | 0     |
| 33  | STE  | m     | 101 | 12/20 | 0.80 | 0.15 | 45,61,75,76                | 0     |
| 29  | LMG  | c     | 521 | 48/55 | 0.81 | 0.14 | 50,71,93,96                | 0     |
| 33  | STE  | b     | 627 | 14/20 | 0.81 | 0.15 | 50,65,77,78                | 0     |
| 33  | STE  | I     | 101 | 15/20 | 0.81 | 0.15 | 40,55,75,80                | 0     |
| 30  | LHG  | e     | 102 | 42/49 | 0.81 | 0.13 | 52,77,103,111              | 0     |
| 33  | STE  | B     | 627 | 12/20 | 0.82 | 0.15 | 47,60,73,74                | 0     |
| 33  | STE  | k     | 103 | 12/20 | 0.82 | 0.12 | 49,67,78,80                | 0     |
| 33  | STE  | E     | 102 | 12/20 | 0.82 | 0.16 | 56,72,77,83                | 0     |
| 30  | LHG  | E     | 101 | 49/49 | 0.83 | 0.13 | 46,71,102,108              | 0     |
| 33  | STE  | B     | 626 | 16/20 | 0.83 | 0.14 | 45,58,70,74                | 0     |
| 33  | STE  | T     | 103 | 15/20 | 0.83 | 0.14 | 43,55,68,71                | 0     |
| 31  | SQD  | a     | 614 | 36/54 | 0.84 | 0.13 | 33,61,81,83                | 0     |
| 33  | STE  | j     | 101 | 12/20 | 0.84 | 0.12 | 45,58,67,70                | 0     |
| 33  | STE  | C     | 520 | 12/20 | 0.84 | 0.12 | 44,56,64,64                | 0     |
| 24  | CLA  | b     | 601 | 65/65 | 0.84 | 0.12 | 47,65,83,96                | 0     |
| 33  | STE  | T     | 102 | 16/20 | 0.85 | 0.12 | 30,48,62,65                | 0     |
| 33  | STE  | b     | 624 | 16/20 | 0.85 | 0.13 | 45,61,70,73                | 0     |
| 33  | STE  | B     | 620 | 17/20 | 0.85 | 0.12 | 36,51,64,65                | 0     |
| 33  | STE  | x     | 102 | 20/20 | 0.85 | 0.11 | 38,55,68,71                | 0     |
| 33  | STE  | C     | 522 | 12/20 | 0.86 | 0.12 | 39,49,57,58                | 0     |
| 33  | STE  | Z     | 101 | 8/20  | 0.86 | 0.17 | 41,57,64,64                | 0     |
| 29  | LMG  | A     | 614 | 48/55 | 0.86 | 0.11 | 37,55,74,84                | 0     |
| 31  | SQD  | A     | 617 | 39/54 | 0.86 | 0.13 | 40,59,87,92                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 29  | LMG  | D     | 409 | 33/55 | 0.86 | 0.13 | 37,56,77,84                 | 0     |
| 33  | STE  | J     | 101 | 12/20 | 0.86 | 0.12 | 45,55,63,65                 | 0     |
| 33  | STE  | t     | 102 | 18/20 | 0.86 | 0.12 | 42,55,72,77                 | 0     |
| 32  | DGD  | A     | 618 | 66/66 | 0.86 | 0.11 | 43,61,74,82                 | 0     |
| 33  | STE  | b     | 622 | 20/20 | 0.87 | 0.11 | 38,53,67,67                 | 0     |
| 29  | LMG  | c     | 522 | 49/55 | 0.87 | 0.11 | 37,56,81,96                 | 0     |
| 33  | STE  | B     | 624 | 14/20 | 0.87 | 0.11 | 36,51,61,63                 | 0     |
| 33  | STE  | l     | 102 | 18/20 | 0.87 | 0.12 | 36,49,76,78                 | 0     |
| 29  | LMG  | c     | 519 | 37/55 | 0.87 | 0.12 | 44,63,80,85                 | 0     |
| 28  | PL9  | A     | 612 | 55/55 | 0.87 | 0.13 | 33,62,82,85                 | 0     |
| 33  | STE  | c     | 520 | 20/20 | 0.87 | 0.11 | 36,55,71,76                 | 0     |
| 28  | PL9  | a     | 611 | 55/55 | 0.88 | 0.13 | 32,65,80,88                 | 0     |
| 31  | SQD  | B     | 623 | 54/54 | 0.88 | 0.10 | 39,57,81,90                 | 0     |
| 29  | LMG  | C     | 519 | 48/55 | 0.88 | 0.12 | 39,67,85,89                 | 0     |
| 33  | STE  | M     | 103 | 10/20 | 0.89 | 0.13 | 33,43,52,58                 | 0     |
| 33  | STE  | C     | 521 | 16/20 | 0.89 | 0.11 | 37,51,64,71                 | 0     |
| 33  | STE  | B     | 625 | 12/20 | 0.89 | 0.10 | 37,51,59,66                 | 0     |
| 26  | BCR  | C     | 514 | 40/40 | 0.89 | 0.12 | 38,55,68,71                 | 0     |
| 33  | STE  | d     | 411 | 17/20 | 0.90 | 0.11 | 41,52,64,65                 | 0     |
| 29  | LMG  | D     | 410 | 28/55 | 0.90 | 0.11 | 36,50,61,63                 | 0     |
| 24  | CLA  | B     | 601 | 65/65 | 0.90 | 0.11 | 32,58,84,95                 | 0     |
| 31  | SQD  | D     | 407 | 36/54 | 0.90 | 0.11 | 41,65,80,82                 | 0     |
| 33  | STE  | D     | 411 | 20/20 | 0.90 | 0.10 | 35,49,68,72                 | 0     |
| 29  | LMG  | b     | 621 | 51/55 | 0.90 | 0.10 | 35,51,70,76                 | 0     |
| 31  | SQD  | b     | 620 | 49/54 | 0.90 | 0.09 | 38,54,87,97                 | 0     |
| 31  | SQD  | f     | 101 | 41/54 | 0.90 | 0.12 | 54,77,98,101                | 0     |
| 26  | BCR  | d     | 405 | 40/40 | 0.91 | 0.10 | 37,52,87,93                 | 0     |
| 31  | SQD  | a     | 613 | 54/54 | 0.91 | 0.10 | 38,60,79,84                 | 0     |
| 29  | LMG  | M     | 101 | 51/55 | 0.91 | 0.09 | 31,47,64,73                 | 0     |
| 24  | CLA  | C     | 513 | 65/65 | 0.91 | 0.10 | 41,62,84,92                 | 0     |
| 26  | BCR  | D     | 404 | 40/40 | 0.91 | 0.10 | 28,43,79,87                 | 0     |
| 26  | BCR  | H     | 101 | 40/40 | 0.92 | 0.08 | 30,46,59,63                 | 0     |
| 32  | DGD  | H     | 102 | 62/66 | 0.92 | 0.08 | 25,43,55,60                 | 0     |
| 26  | BCR  | k     | 101 | 40/40 | 0.92 | 0.09 | 39,56,68,69                 | 0     |
| 26  | BCR  | x     | 101 | 40/40 | 0.92 | 0.09 | 37,52,71,75                 | 0     |
| 26  | BCR  | Y     | 101 | 40/40 | 0.92 | 0.09 | 32,50,62,69                 | 0     |
| 26  | BCR  | c     | 514 | 40/40 | 0.92 | 0.09 | 46,59,68,70                 | 0     |
| 32  | DGD  | c     | 517 | 62/66 | 0.93 | 0.08 | 31,51,87,90                 | 0     |
| 32  | DGD  | h     | 101 | 62/66 | 0.93 | 0.08 | 31,45,57,64                 | 0     |
| 24  | CLA  | c     | 512 | 65/65 | 0.93 | 0.10 | 41,56,88,94                 | 0     |
| 24  | CLA  | c     | 513 | 65/65 | 0.93 | 0.11 | 44,65,100,105               | 0     |
| 29  | LMG  | D     | 406 | 51/55 | 0.93 | 0.10 | 26,52,75,84                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24  | CLA  | C     | 512 | 65/65 | 0.93 | 0.10 | 33,51,81,86                 | 0     |
| 26  | BCR  | b     | 617 | 40/40 | 0.93 | 0.07 | 29,40,51,54                 | 0     |
| 29  | LMG  | d     | 410 | 44/55 | 0.93 | 0.10 | 33,51,79,86                 | 0     |
| 26  | BCR  | b     | 618 | 40/40 | 0.93 | 0.07 | 26,39,51,54                 | 0     |
| 30  | LHG  | d     | 407 | 49/49 | 0.93 | 0.11 | 34,47,70,74                 | 0     |
| 32  | DGD  | C     | 517 | 62/66 | 0.93 | 0.09 | 27,47,92,108                | 0     |
| 26  | BCR  | b     | 619 | 40/40 | 0.93 | 0.08 | 26,47,61,69                 | 0     |
| 26  | BCR  | B     | 618 | 40/40 | 0.94 | 0.07 | 23,38,49,49                 | 0     |
| 24  | CLA  | c     | 509 | 65/65 | 0.94 | 0.09 | 32,46,61,69                 | 0     |
| 33  | STE  | M     | 102 | 15/20 | 0.94 | 0.08 | 36,47,59,62                 | 0     |
| 26  | BCR  | C     | 515 | 40/40 | 0.94 | 0.08 | 27,40,50,61                 | 0     |
| 24  | CLA  | C     | 511 | 65/65 | 0.94 | 0.09 | 30,48,65,70                 | 0     |
| 24  | CLA  | b     | 606 | 65/65 | 0.94 | 0.08 | 25,39,70,73                 | 0     |
| 26  | BCR  | k     | 102 | 40/40 | 0.94 | 0.10 | 39,51,63,68                 | 0     |
| 32  | DGD  | C     | 516 | 62/66 | 0.94 | 0.09 | 21,40,77,80                 | 0     |
| 26  | BCR  | T     | 101 | 40/40 | 0.94 | 0.07 | 25,37,50,52                 | 0     |
| 31  | SQD  | A     | 616 | 52/54 | 0.94 | 0.10 | 34,54,90,95                 | 0     |
| 26  | BCR  | A     | 609 | 40/40 | 0.94 | 0.07 | 21,34,42,44                 | 0     |
| 26  | BCR  | B     | 617 | 40/40 | 0.94 | 0.07 | 26,38,56,60                 | 0     |
| 30  | LHG  | d     | 409 | 39/49 | 0.95 | 0.08 | 30,44,67,68                 | 0     |
| 26  | BCR  | t     | 101 | 40/40 | 0.95 | 0.06 | 27,37,50,54                 | 0     |
| 24  | CLA  | C     | 507 | 65/65 | 0.95 | 0.07 | 25,38,53,57                 | 0     |
| 26  | BCR  | B     | 619 | 40/40 | 0.95 | 0.07 | 25,41,54,62                 | 0     |
| 28  | PL9  | D     | 405 | 55/55 | 0.95 | 0.06 | 19,31,46,47                 | 0     |
| 24  | CLA  | b     | 608 | 65/65 | 0.95 | 0.08 | 25,42,61,66                 | 0     |
| 28  | PL9  | d     | 406 | 55/55 | 0.95 | 0.06 | 20,34,42,44                 | 0     |
| 24  | CLA  | b     | 609 | 65/65 | 0.95 | 0.08 | 29,43,62,68                 | 0     |
| 24  | CLA  | c     | 504 | 60/65 | 0.95 | 0.08 | 31,43,78,85                 | 0     |
| 24  | CLA  | c     | 506 | 65/65 | 0.95 | 0.09 | 31,48,89,90                 | 0     |
| 26  | BCR  | K     | 101 | 40/40 | 0.95 | 0.08 | 34,49,65,65                 | 0     |
| 24  | CLA  | c     | 508 | 64/65 | 0.95 | 0.09 | 29,43,83,98                 | 0     |
| 24  | CLA  | C     | 510 | 65/65 | 0.95 | 0.07 | 26,41,61,62                 | 0     |
| 32  | DGD  | C     | 518 | 62/66 | 0.95 | 0.08 | 24,46,75,85                 | 0     |
| 26  | BCR  | a     | 607 | 40/40 | 0.95 | 0.06 | 23,33,43,49                 | 0     |
| 32  | DGD  | c     | 516 | 62/66 | 0.95 | 0.08 | 21,41,67,74                 | 0     |
| 24  | CLA  | c     | 511 | 65/65 | 0.95 | 0.09 | 33,50,70,75                 | 0     |
| 32  | DGD  | c     | 518 | 62/66 | 0.95 | 0.09 | 25,49,80,86                 | 0     |
| 24  | CLA  | B     | 610 | 65/65 | 0.95 | 0.07 | 20,32,42,45                 | 0     |
| 24  | CLA  | C     | 503 | 65/65 | 0.95 | 0.06 | 27,39,48,51                 | 0     |
| 24  | CLA  | d     | 404 | 65/65 | 0.95 | 0.09 | 28,47,81,87                 | 0     |
| 26  | BCR  | c     | 515 | 40/40 | 0.95 | 0.07 | 27,42,58,61                 | 0     |
| 25  | PHO  | d     | 402 | 64/64 | 0.95 | 0.06 | 26,35,45,49                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 30  | LHG  | A     | 615 | 47/49 | 0.95 | 0.10 | 27,48,77,88                 | 0     |
| 30  | LHG  | B     | 622 | 49/49 | 0.95 | 0.08 | 29,43,64,69                 | 0     |
| 24  | CLA  | C     | 504 | 59/65 | 0.95 | 0.08 | 28,40,79,80                 | 0     |
| 24  | CLA  | C     | 506 | 65/65 | 0.95 | 0.09 | 26,42,78,84                 | 0     |
| 34  | BCT  | a     | 610 | 4/4   | 0.95 | 0.09 | 28,33,39,47                 | 0     |
| 24  | CLA  | B     | 605 | 65/65 | 0.96 | 0.07 | 20,31,47,50                 | 0     |
| 24  | CLA  | c     | 505 | 65/65 | 0.96 | 0.08 | 25,38,66,72                 | 0     |
| 24  | CLA  | C     | 505 | 65/65 | 0.96 | 0.08 | 23,39,65,81                 | 0     |
| 24  | CLA  | c     | 507 | 65/65 | 0.96 | 0.07 | 26,43,58,64                 | 0     |
| 24  | CLA  | B     | 606 | 65/65 | 0.96 | 0.07 | 23,34,65,71                 | 0     |
| 24  | CLA  | B     | 609 | 65/65 | 0.96 | 0.07 | 24,36,58,66                 | 0     |
| 24  | CLA  | c     | 510 | 65/65 | 0.96 | 0.07 | 28,45,58,71                 | 0     |
| 24  | CLA  | C     | 508 | 65/65 | 0.96 | 0.07 | 26,38,98,109                | 0     |
| 24  | CLA  | C     | 509 | 65/65 | 0.96 | 0.08 | 26,42,60,64                 | 0     |
| 24  | CLA  | A     | 604 | 65/65 | 0.96 | 0.06 | 15,26,44,54                 | 0     |
| 24  | CLA  | d     | 401 | 65/65 | 0.96 | 0.08 | 24,37,86,90                 | 0     |
| 24  | CLA  | B     | 613 | 65/65 | 0.96 | 0.07 | 17,31,65,70                 | 0     |
| 25  | PHO  | A     | 606 | 64/64 | 0.96 | 0.05 | 17,27,35,41                 | 0     |
| 25  | PHO  | A     | 607 | 64/64 | 0.96 | 0.05 | 22,31,40,42                 | 0     |
| 24  | CLA  | B     | 614 | 65/65 | 0.96 | 0.08 | 20,35,70,80                 | 0     |
| 24  | CLA  | B     | 615 | 65/65 | 0.96 | 0.07 | 22,36,59,63                 | 0     |
| 24  | CLA  | a     | 604 | 65/65 | 0.96 | 0.05 | 18,28,45,55                 | 0     |
| 24  | CLA  | a     | 606 | 65/65 | 0.96 | 0.08 | 19,36,78,84                 | 0     |
| 30  | LHG  | B     | 621 | 49/49 | 0.96 | 0.07 | 26,40,54,61                 | 0     |
| 24  | CLA  | a     | 612 | 65/65 | 0.96 | 0.06 | 20,29,46,51                 | 0     |
| 24  | CLA  | B     | 616 | 60/65 | 0.96 | 0.08 | 23,37,88,95                 | 0     |
| 24  | CLA  | b     | 602 | 65/65 | 0.96 | 0.07 | 27,41,57,62                 | 0     |
| 24  | CLA  | b     | 603 | 65/65 | 0.96 | 0.07 | 23,36,60,68                 | 0     |
| 24  | CLA  | b     | 605 | 65/65 | 0.96 | 0.06 | 21,34,49,54                 | 0     |
| 30  | LHG  | l     | 101 | 49/49 | 0.96 | 0.06 | 30,42,51,57                 | 0     |
| 24  | CLA  | C     | 501 | 65/65 | 0.96 | 0.06 | 21,35,48,51                 | 0     |
| 24  | CLA  | b     | 607 | 65/65 | 0.96 | 0.07 | 20,35,62,68                 | 0     |
| 24  | CLA  | C     | 502 | 65/65 | 0.96 | 0.06 | 25,39,52,59                 | 0     |
| 24  | CLA  | B     | 602 | 65/65 | 0.96 | 0.06 | 23,35,54,61                 | 0     |
| 24  | CLA  | b     | 610 | 65/65 | 0.96 | 0.07 | 22,37,50,54                 | 0     |
| 24  | CLA  | b     | 611 | 65/65 | 0.96 | 0.06 | 22,33,52,62                 | 0     |
| 24  | CLA  | b     | 612 | 65/65 | 0.96 | 0.07 | 21,34,47,56                 | 0     |
| 24  | CLA  | b     | 613 | 65/65 | 0.96 | 0.07 | 17,33,66,74                 | 0     |
| 24  | CLA  | b     | 614 | 65/65 | 0.96 | 0.07 | 24,38,68,76                 | 0     |
| 24  | CLA  | b     | 615 | 65/65 | 0.96 | 0.07 | 26,39,57,63                 | 0     |
| 24  | CLA  | b     | 616 | 60/65 | 0.96 | 0.08 | 26,41,81,83                 | 0     |
| 24  | CLA  | c     | 501 | 65/65 | 0.96 | 0.06 | 28,39,51,55                 | 0     |

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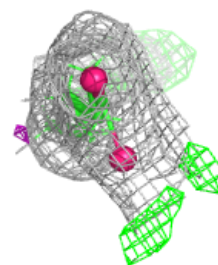
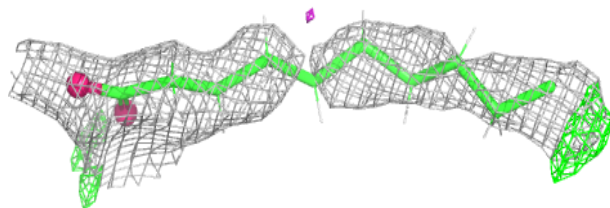
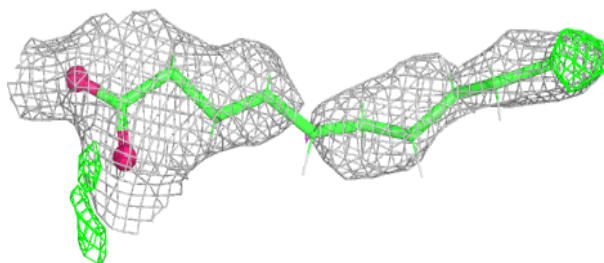
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 24  | CLA  | c     | 502    | 65/65 | 0.96 | 0.06 | 29,40,55,62                 | 0     |
| 24  | CLA  | c     | 503    | 65/65 | 0.96 | 0.07 | 28,42,53,61                 | 0     |
| 30  | LHG  | D     | 408    | 49/49 | 0.97 | 0.07 | 21,40,52,57                 | 0     |
| 24  | CLA  | B     | 612    | 65/65 | 0.97 | 0.06 | 19,32,49,53                 | 0     |
| 24  | CLA  | A     | 605    | 65/65 | 0.97 | 0.08 | 23,33,83,91                 | 0     |
| 30  | LHG  | d     | 408    | 49/49 | 0.97 | 0.07 | 24,41,51,60                 | 0     |
| 24  | CLA  | D     | 402    | 65/65 | 0.97 | 0.06 | 17,28,54,56                 | 0     |
| 24  | CLA  | D     | 403    | 65/65 | 0.97 | 0.08 | 22,42,105,112               | 0     |
| 24  | CLA  | d     | 403    | 65/65 | 0.97 | 0.06 | 20,32,54,64                 | 0     |
| 24  | CLA  | A     | 613    | 65/65 | 0.97 | 0.06 | 18,28,47,53                 | 0     |
| 24  | CLA  | B     | 607    | 65/65 | 0.97 | 0.07 | 17,32,57,67                 | 0     |
| 24  | CLA  | B     | 608    | 65/65 | 0.97 | 0.06 | 18,33,54,56                 | 0     |
| 25  | PHO  | a     | 605    | 64/64 | 0.97 | 0.05 | 18,29,37,46                 | 0     |
| 24  | CLA  | B     | 603    | 65/65 | 0.97 | 0.06 | 20,32,61,63                 | 0     |
| 24  | CLA  | B     | 604    | 65/65 | 0.97 | 0.07 | 21,32,68,71                 | 0     |
| 24  | CLA  | B     | 611    | 65/65 | 0.97 | 0.06 | 19,31,49,52                 | 0     |
| 34  | BCT  | D     | 401    | 4/4   | 0.97 | 0.06 | 27,28,31,38                 | 0     |
| 24  | CLA  | b     | 604    | 65/65 | 0.97 | 0.07 | 19,35,79,89                 | 0     |
| 35  | HEM  | F     | 101    | 43/43 | 0.97 | 0.08 | 34,46,60,62                 | 0     |
| 35  | HEM  | e     | 101    | 43/43 | 0.97 | 0.09 | 41,53,73,73                 | 0     |
| 27  | CL   | A     | 611    | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 24  | CLA  | A     | 608    | 54/65 | 0.98 | 0.06 | 17,32,67,69                 | 0     |
| 36  | HEC  | V     | 201    | 43/43 | 0.98 | 0.05 | 23,31,40,40                 | 0     |
| 36  | HEC  | v     | 201    | 43/43 | 0.98 | 0.06 | 26,36,46,46                 | 0     |
| 22  | OEX  | a     | 602[A] | 10/10 | 0.99 | 0.03 | 27,32,35,35                 | 10    |
| 23  | FE2  | a     | 603    | 1/1   | 0.99 | 0.03 | 29,29,29,29                 | 0     |
| 27  | CL   | A     | 610    | 1/1   | 0.99 | 0.03 | 28,28,28,28                 | 0     |
| 21  | OEY  | a     | 601[B] | 11/11 | 0.99 | 0.03 | 15,21,24,26                 | 11    |
| 27  | CL   | a     | 608    | 1/1   | 0.99 | 0.04 | 25,25,25,25                 | 0     |
| 27  | CL   | a     | 609    | 1/1   | 0.99 | 0.06 | 25,25,25,25                 | 0     |
| 22  | OEX  | A     | 602[A] | 10/10 | 0.99 | 0.03 | 29,31,35,35                 | 10    |
| 21  | OEY  | A     | 601[B] | 11/11 | 1.00 | 0.03 | 15,20,23,26                 | 11    |
| 23  | FE2  | A     | 603    | 1/1   | 1.00 | 0.01 | 24,24,24,24                 | 0     |

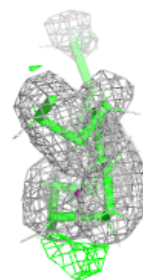
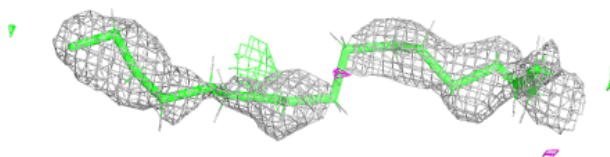
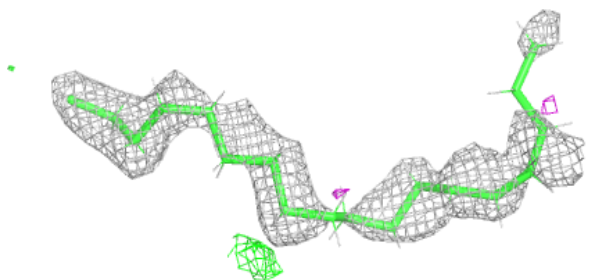
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around STE a 616:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

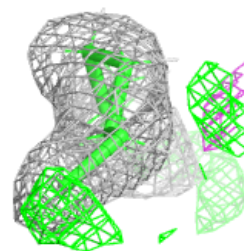
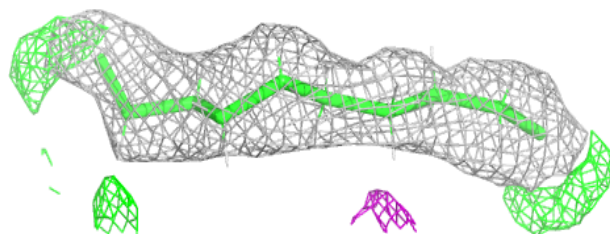
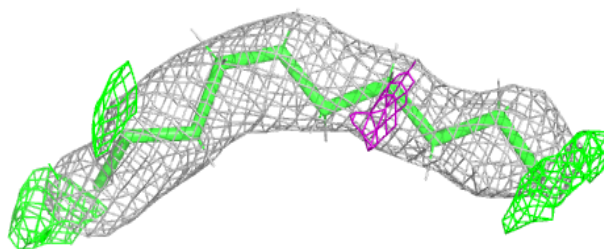
**Electron density around STE H 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

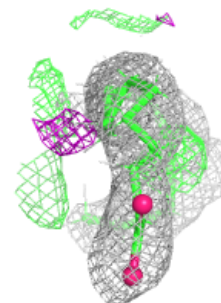
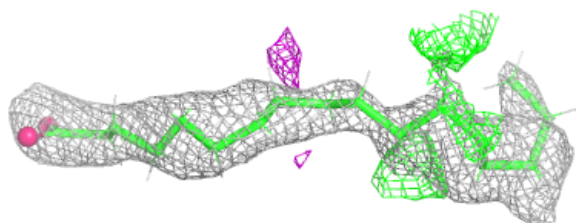
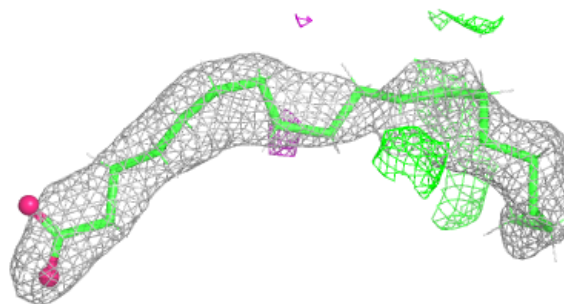


**Electron density around STE b 626:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STE d 412:**

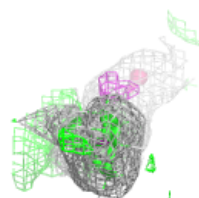
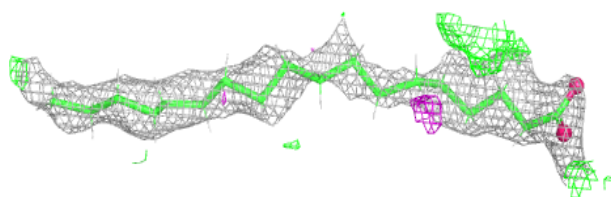
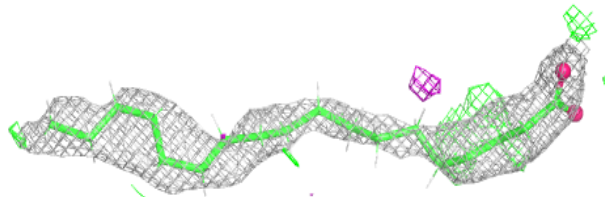
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



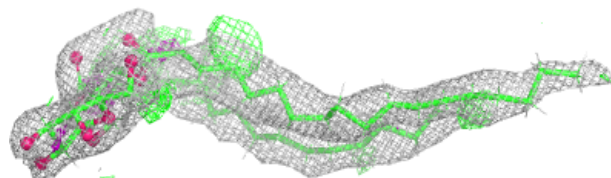
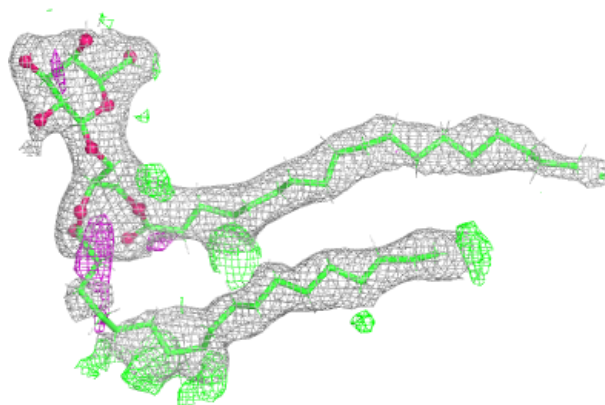


**Electron density around STE b 625:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

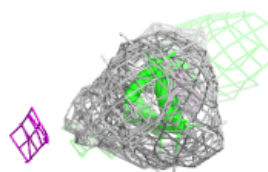
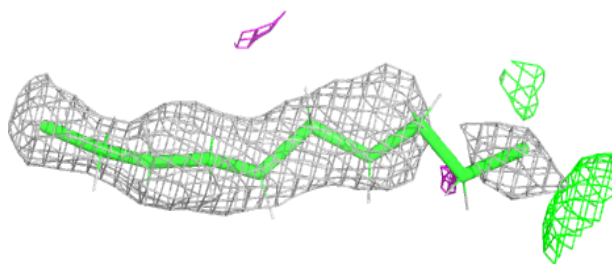
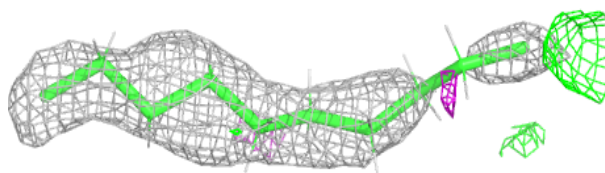
**Electron density around LMG a 618:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

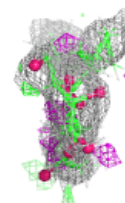
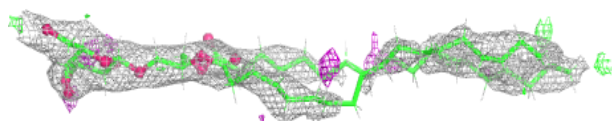
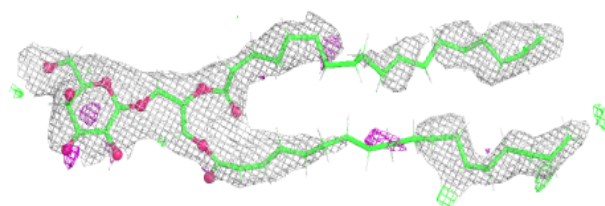


**Electron density around STE a 615:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG b 623:**

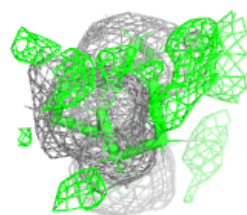
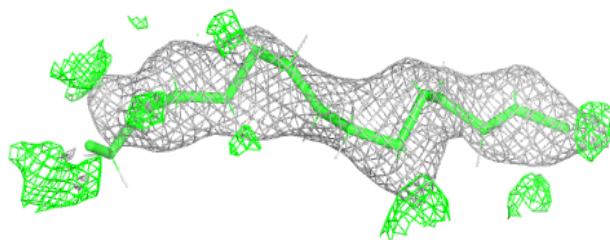
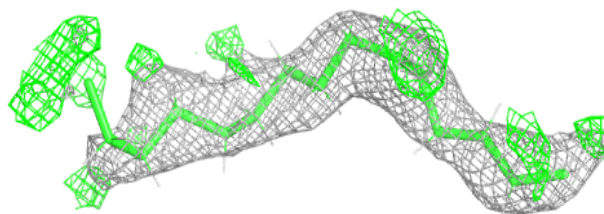
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



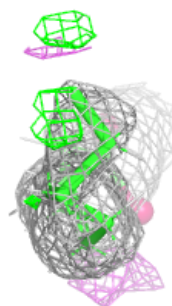
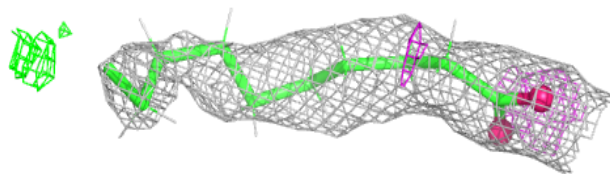
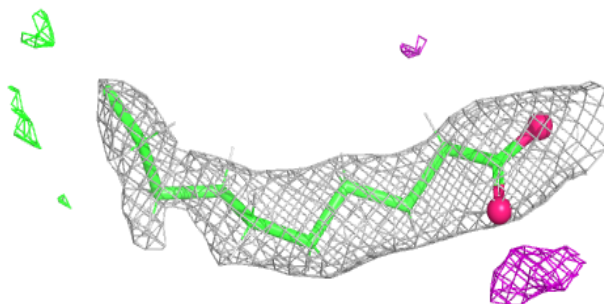


**Electron density around STE a 617:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

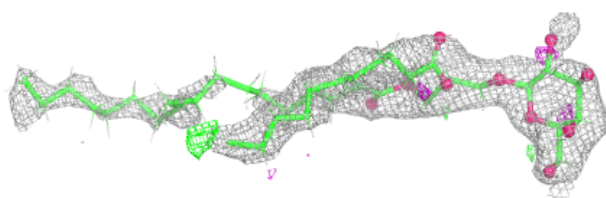
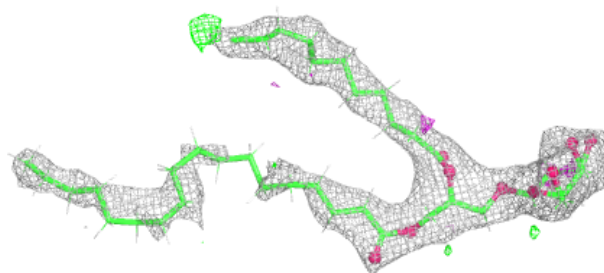
**Electron density around STE m 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

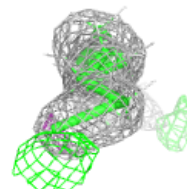
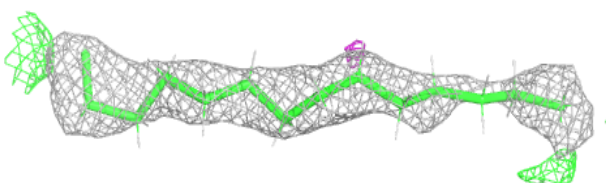
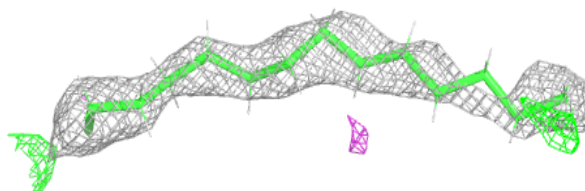


**Electron density around LMG c 521:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

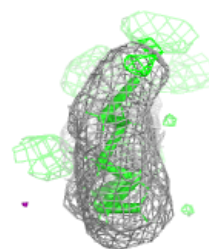
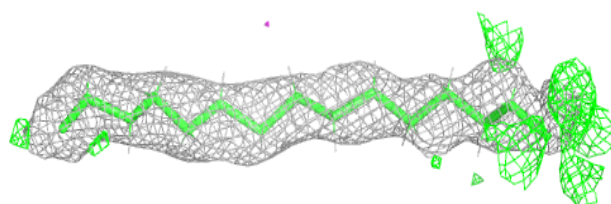
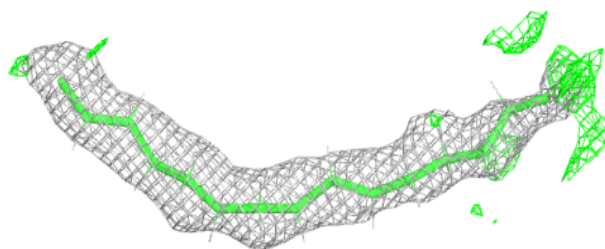
**Electron density around STE b 627:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

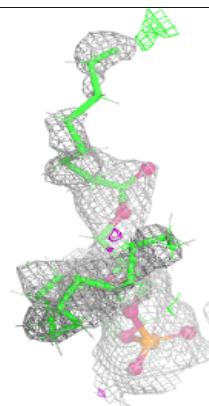
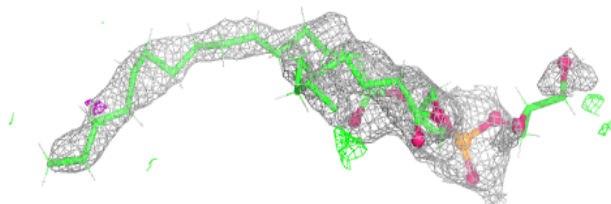
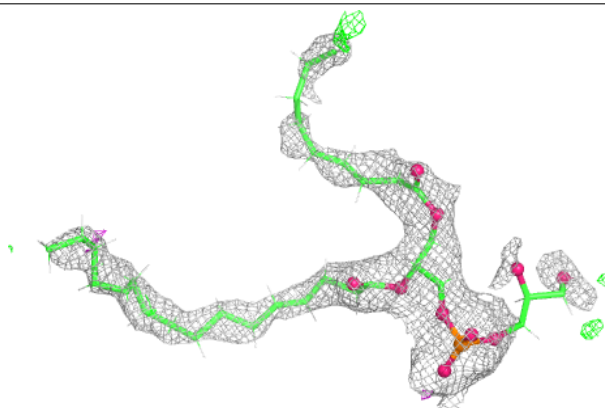


**Electron density around STE I 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

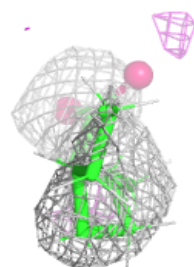
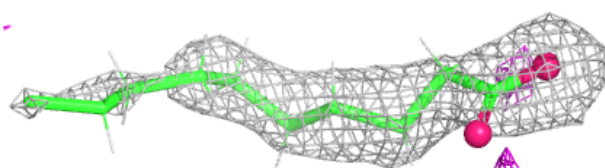
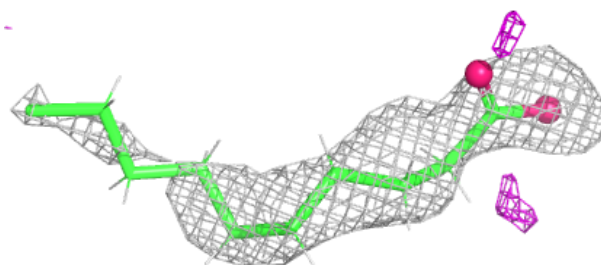
**Electron density around LHG e 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

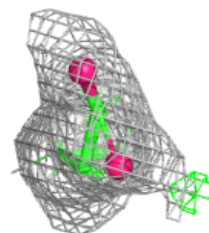
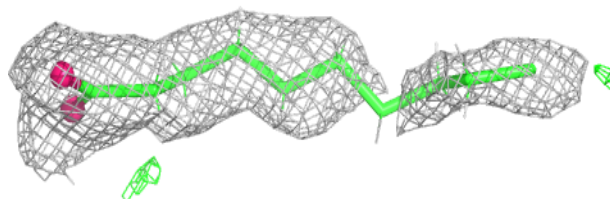
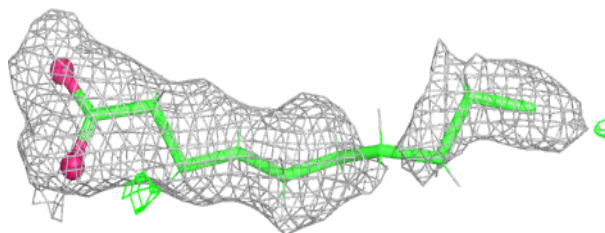


**Electron density around STE B 627:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

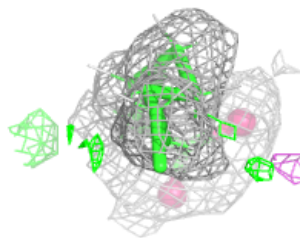
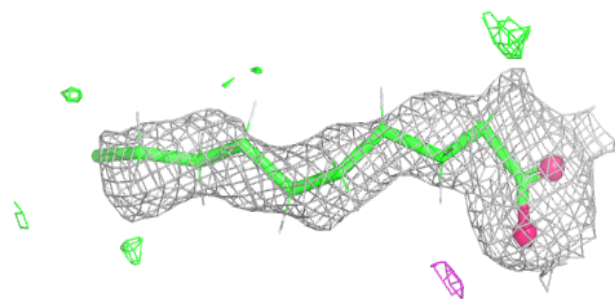
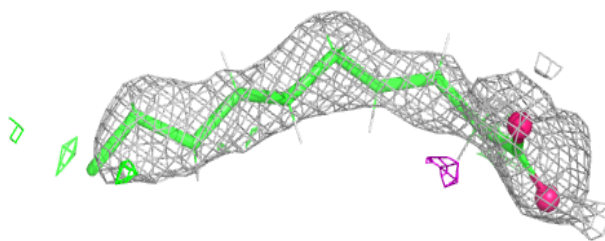
**Electron density around STE k 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



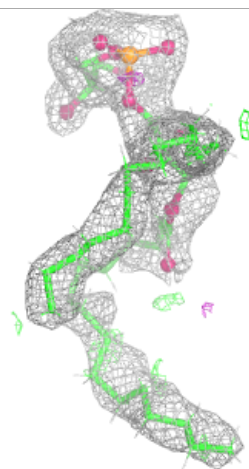
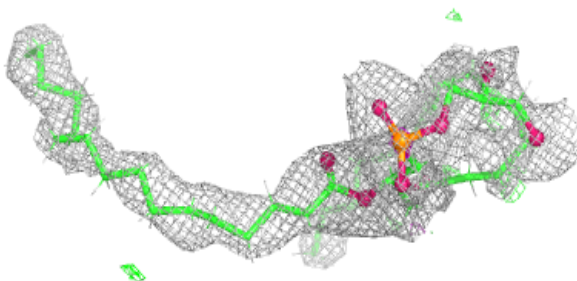
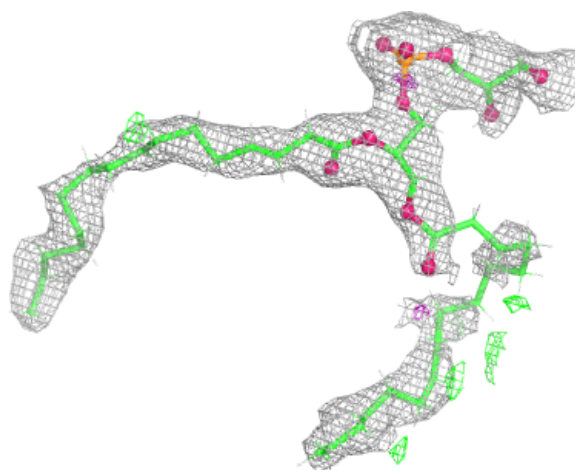
**Electron density around STE E 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG E 101:**

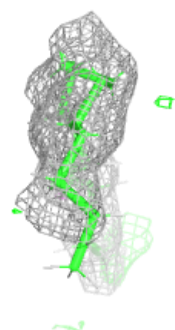
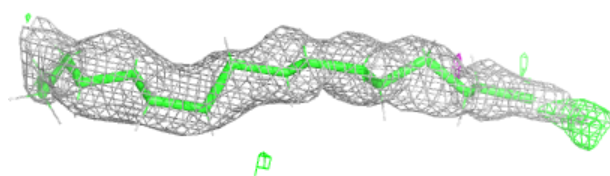
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



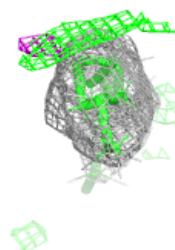
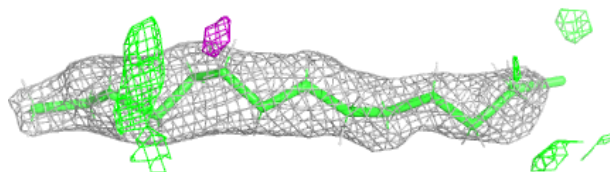
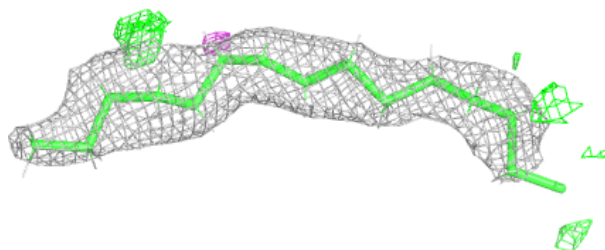


**Electron density around STE B 626:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

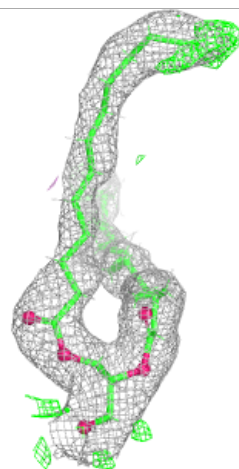
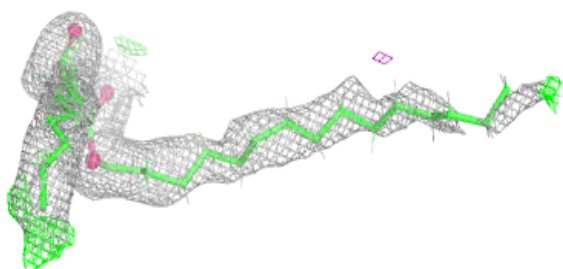
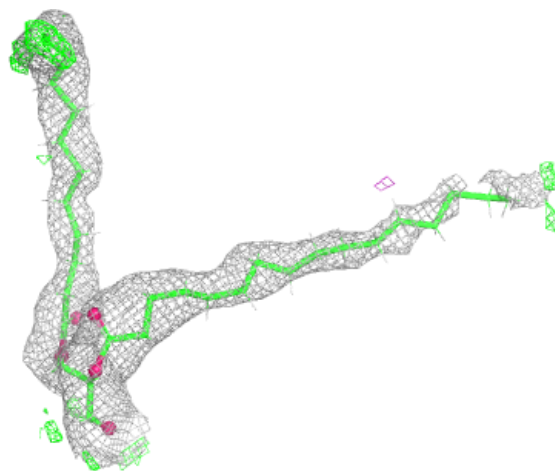
**Electron density around STE T 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SQD a 614:**

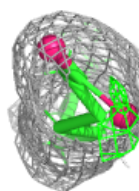
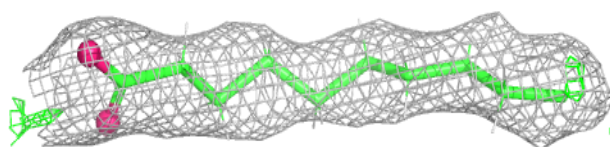
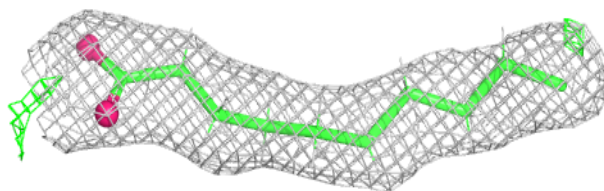
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



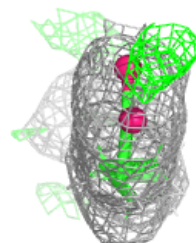
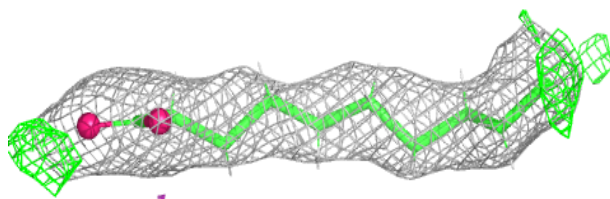
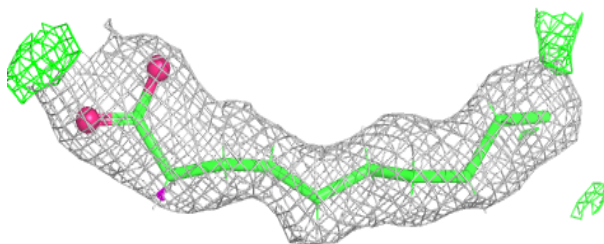


**Electron density around STE j 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

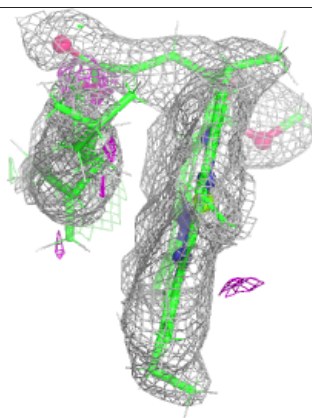
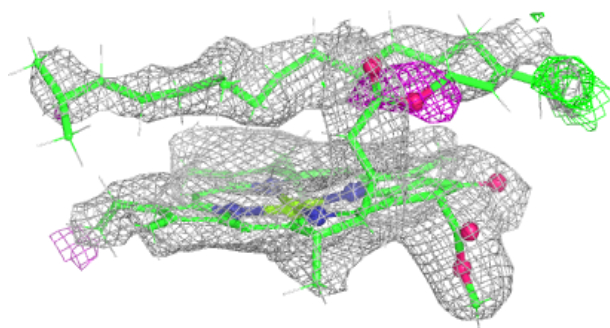
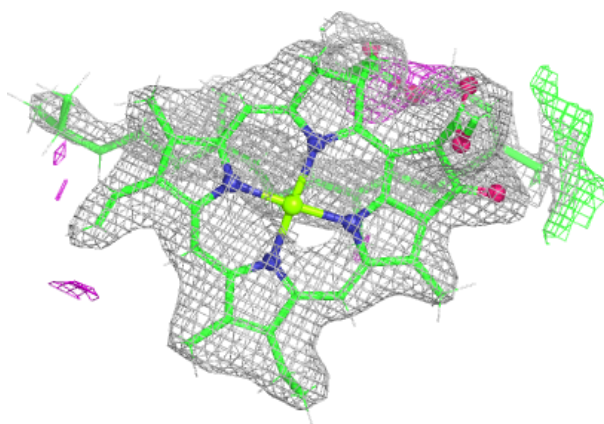
**Electron density around STE C 520:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

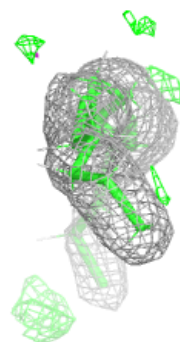
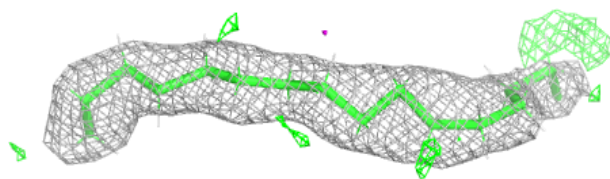
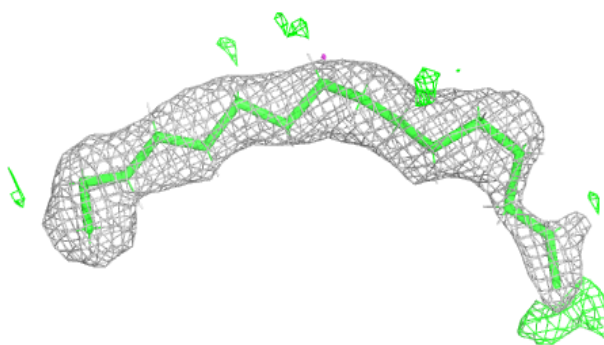


**Electron density around CLA b 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

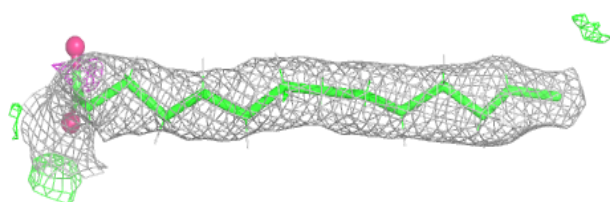
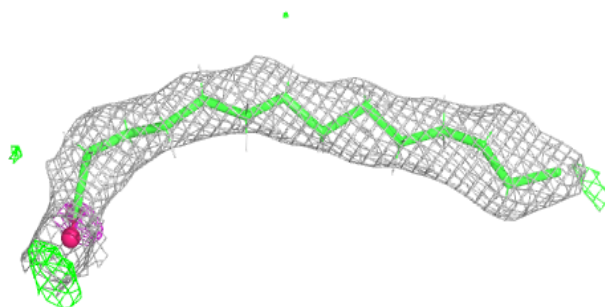
**Electron density around STE T 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

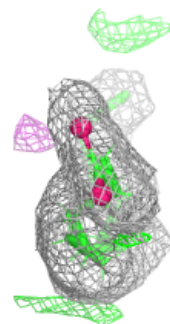
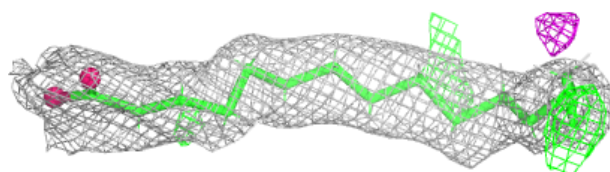
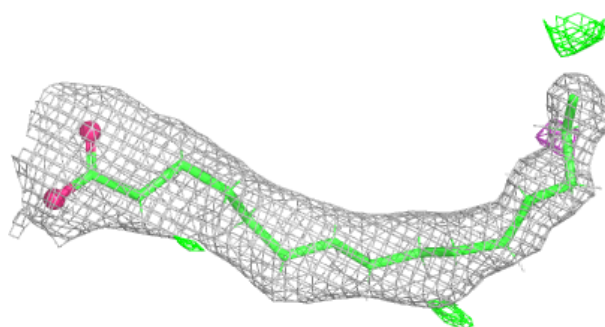


**Electron density around STE b 624:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

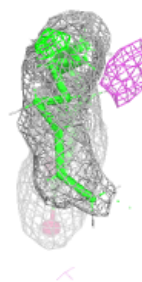
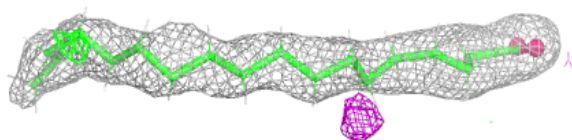
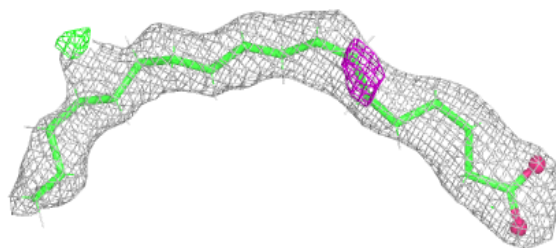
**Electron density around STE B 620:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

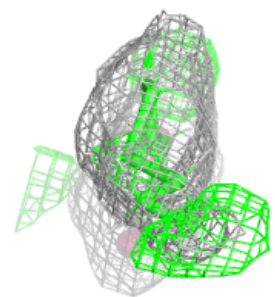
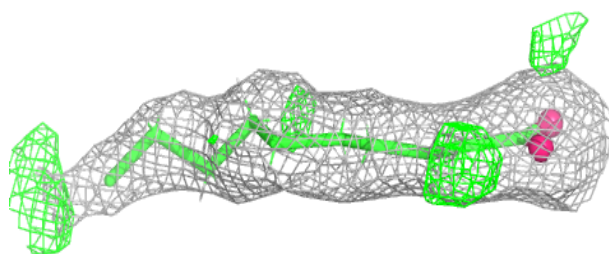
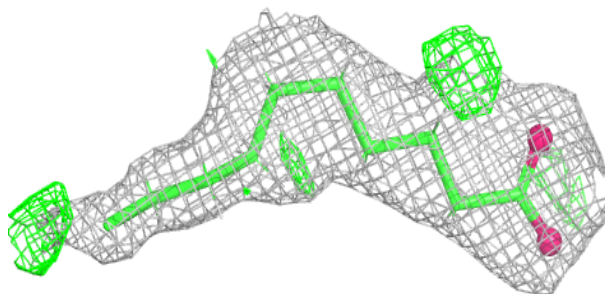


**Electron density around STE x 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

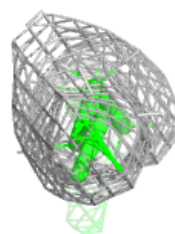
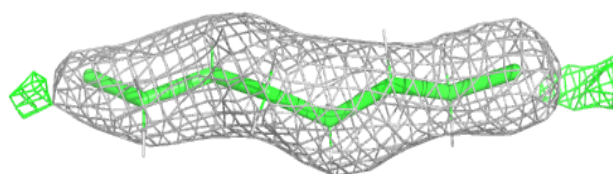
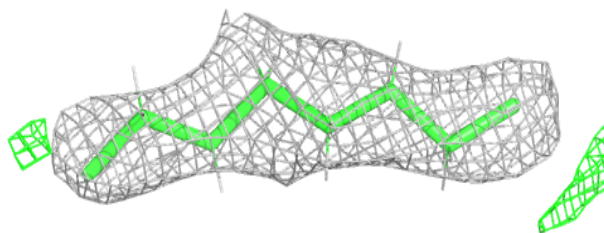
**Electron density around STE C 522:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

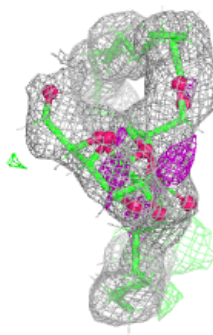
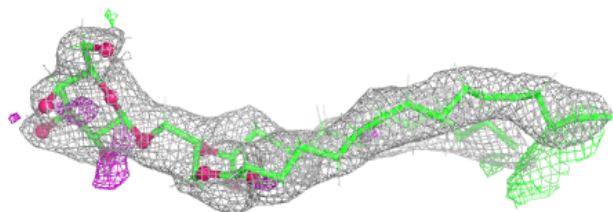
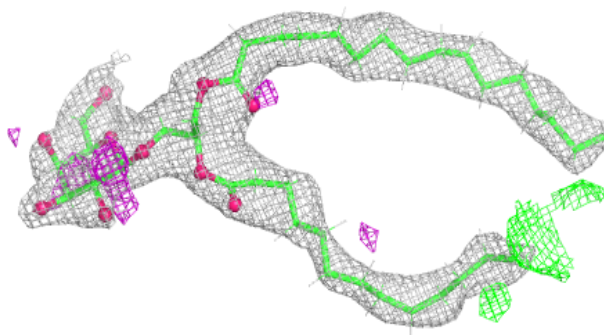


**Electron density around STE Z 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG A 614:**

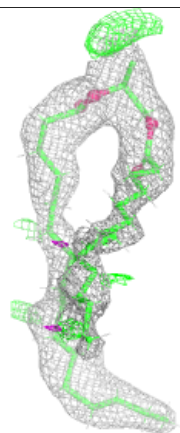
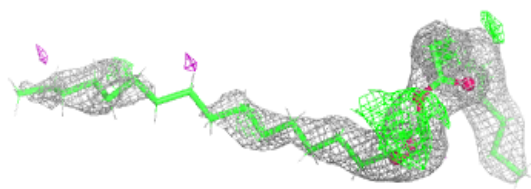
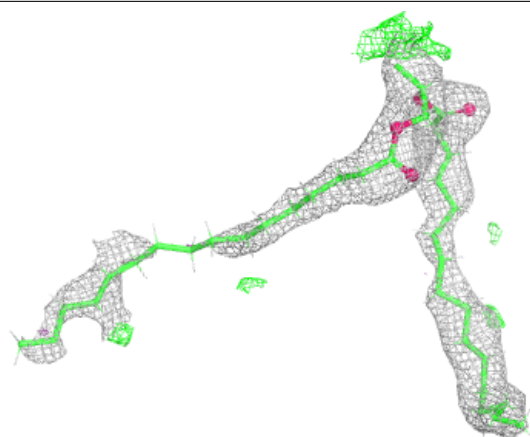
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



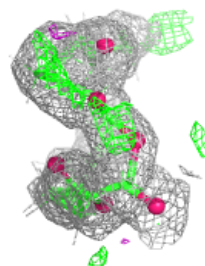
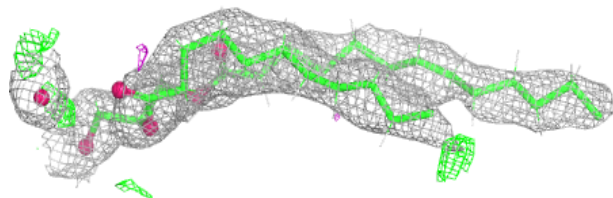
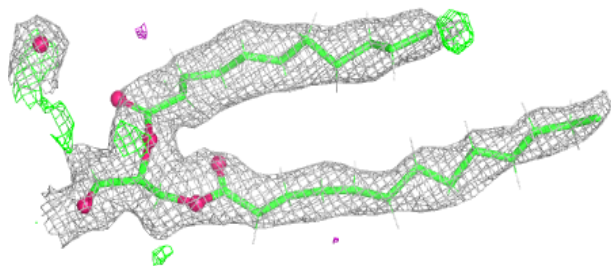


**Electron density around SQD A 617:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

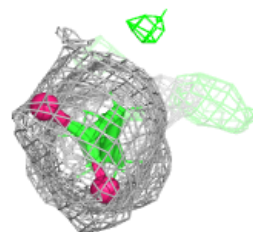
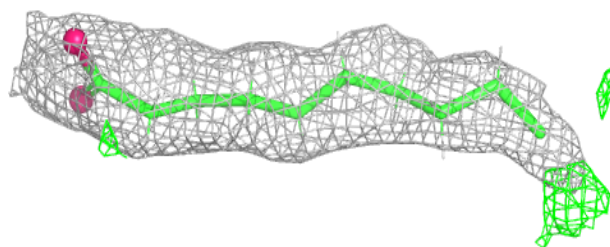
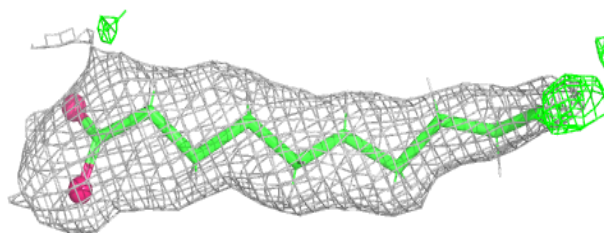
**Electron density around LMG D 409:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

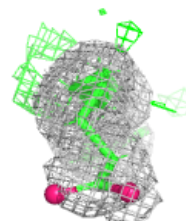
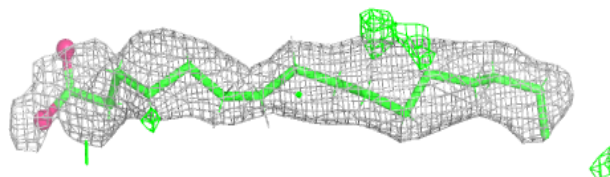
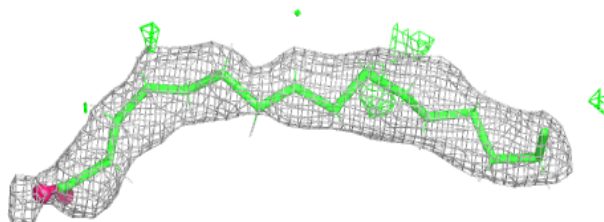


**Electron density around STE J 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

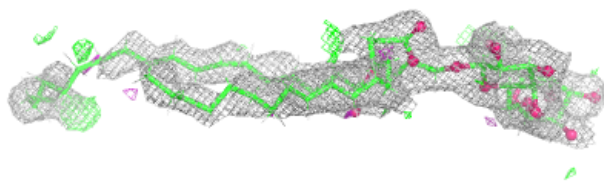
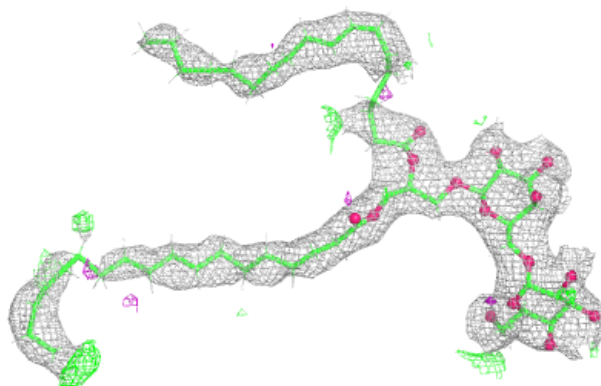
**Electron density around STE t 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

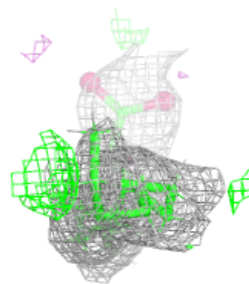
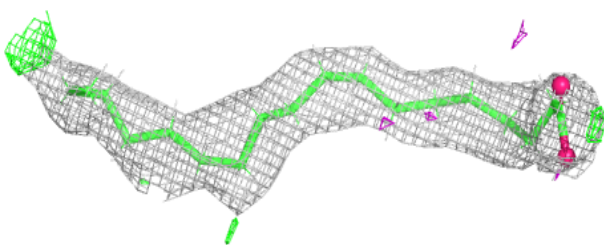
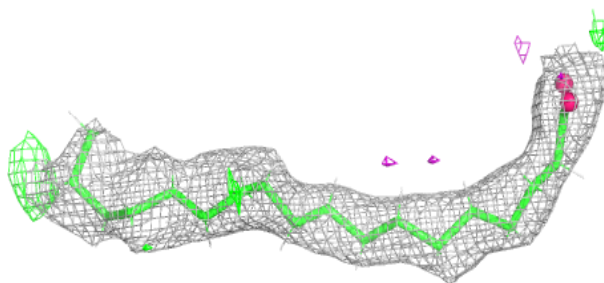


**Electron density around DGD A 618:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STE b 622:**

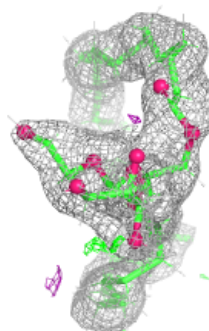
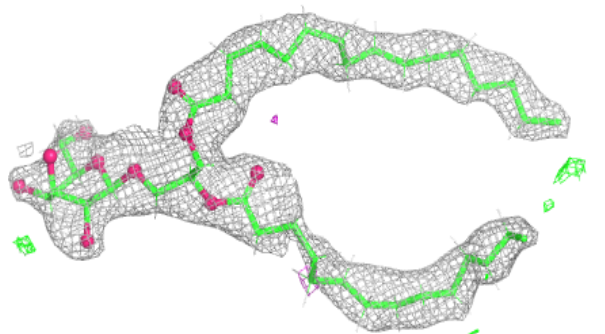
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



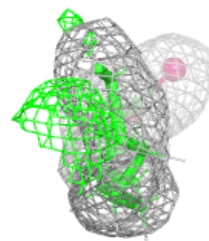
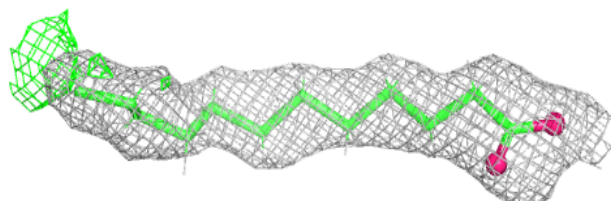
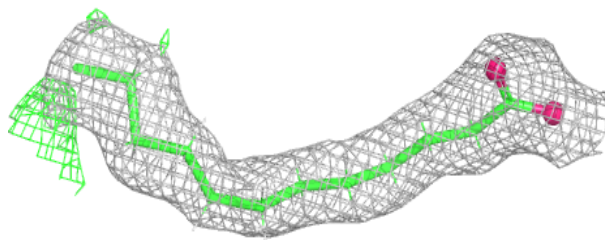


**Electron density around LMG c 522:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

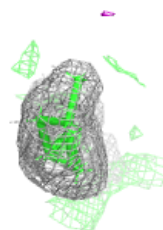
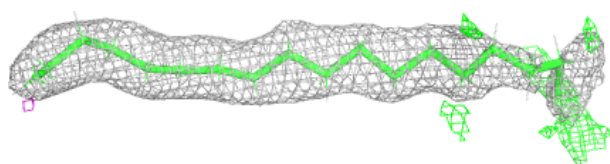
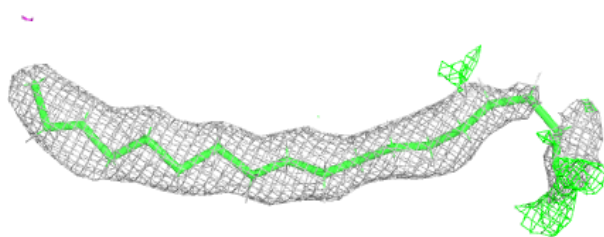
**Electron density around STE B 624:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

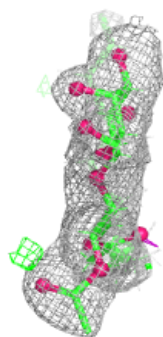
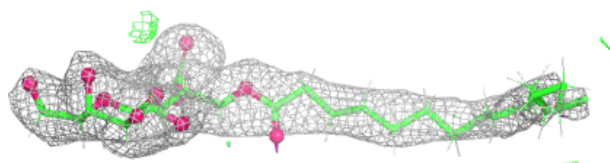
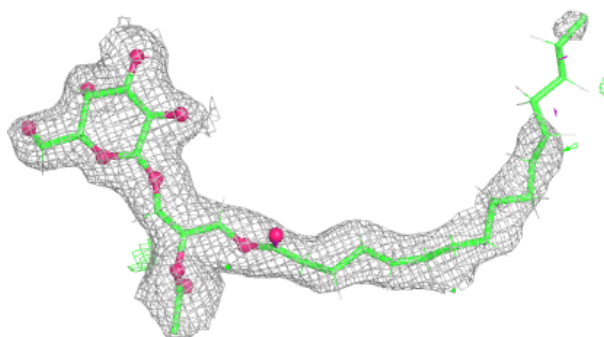


**Electron density around STE l 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

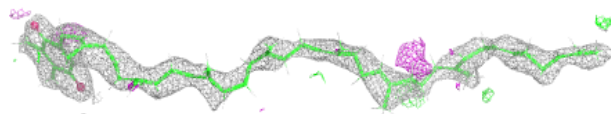
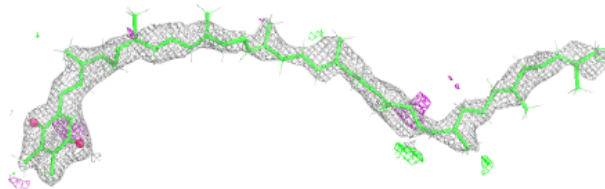
**Electron density around LMG c 519:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

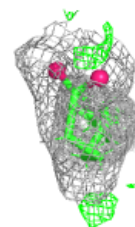
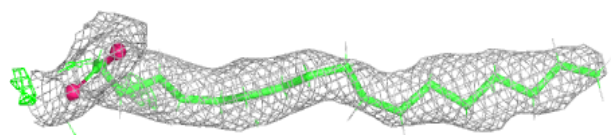
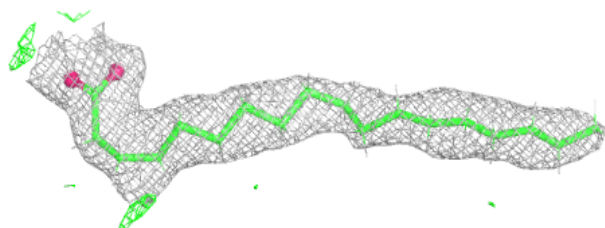


**Electron density around PL9 A 612:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

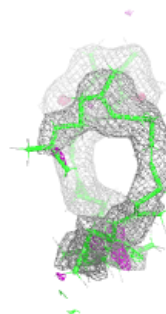
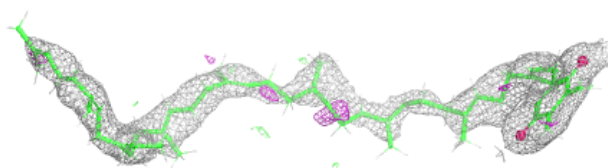
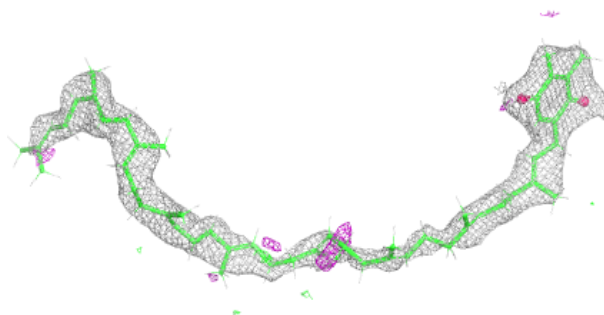
**Electron density around STE c 520:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

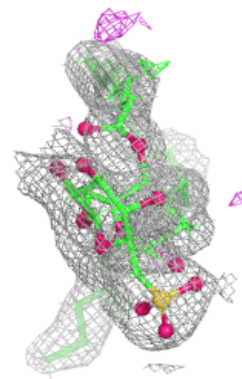
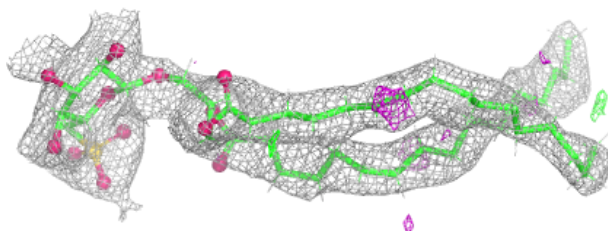
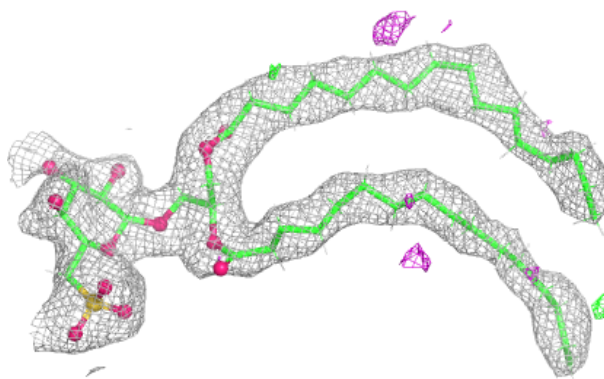


**Electron density around PL9 a 611:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

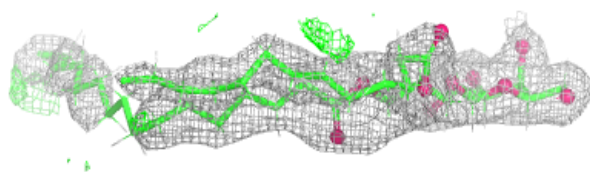
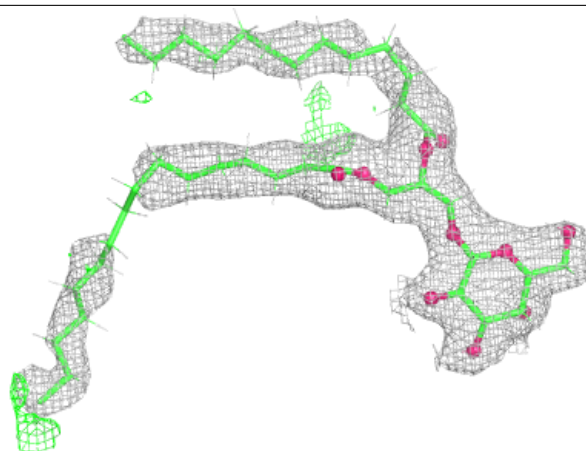
**Electron density around SQD B 623:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

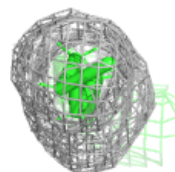
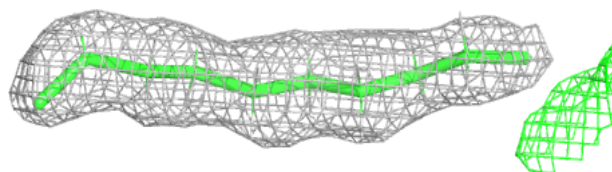
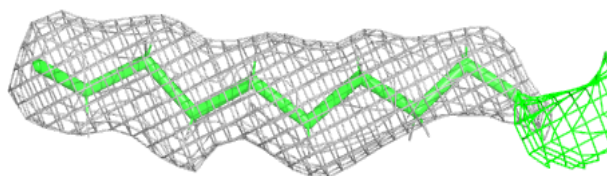


**Electron density around LMG C 519:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around STE M 103:**

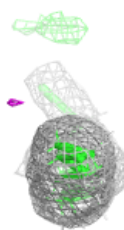
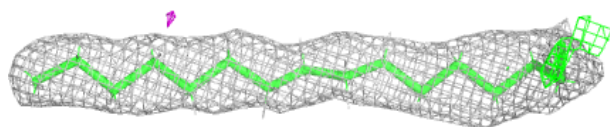
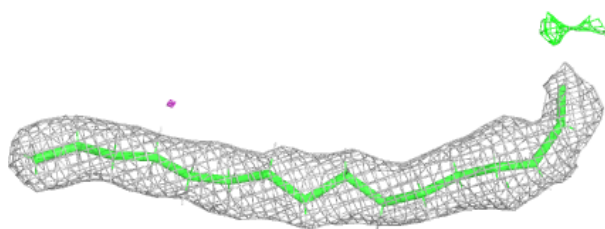
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



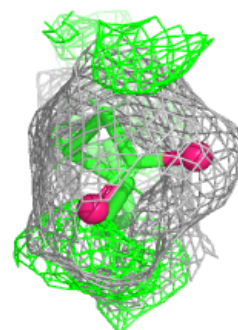
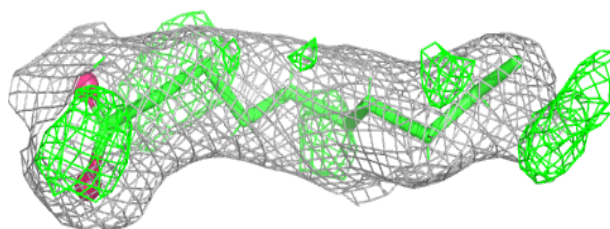
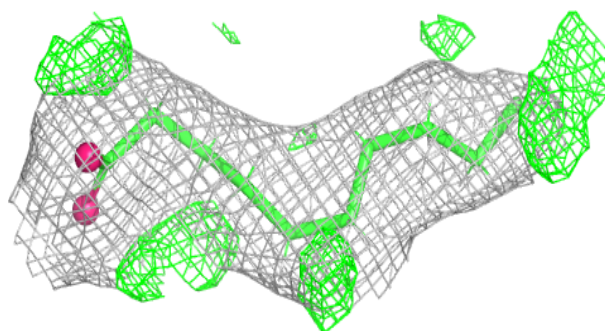


**Electron density around STE C 521:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

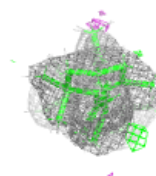
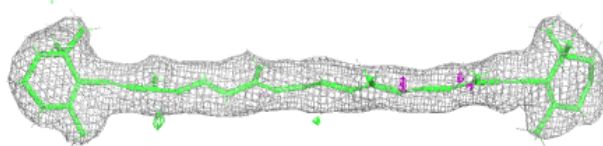
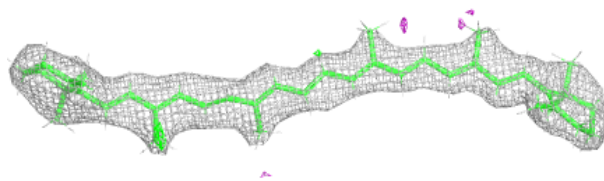
**Electron density around STE B 625:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

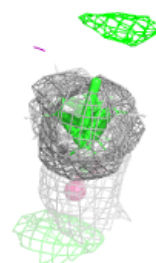
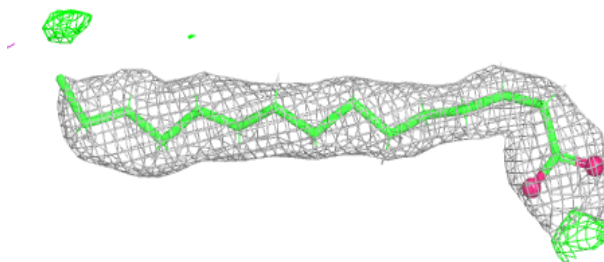


**Electron density around BCR C 514:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

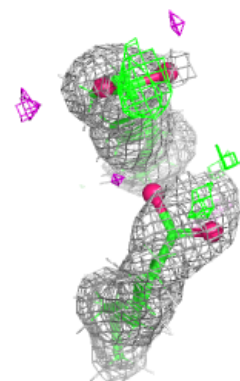
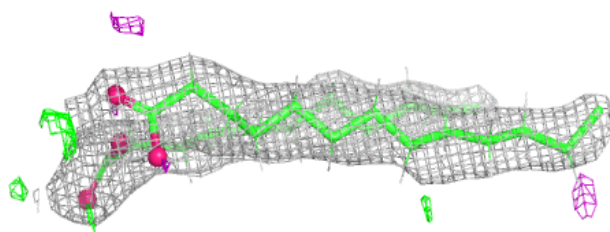
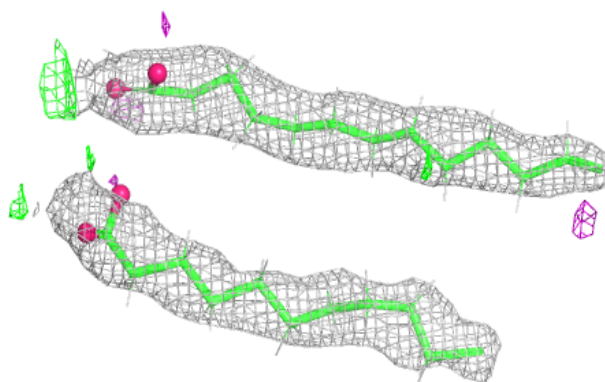
**Electron density around STE d 411:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

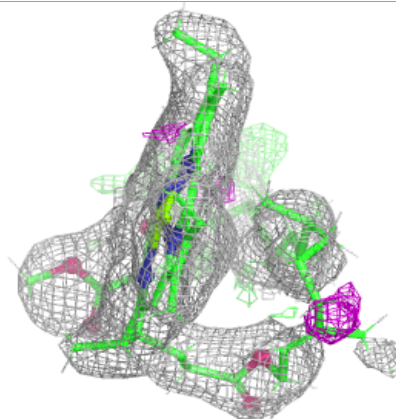
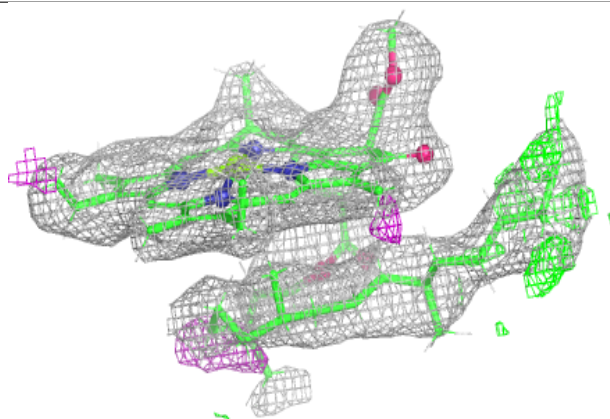
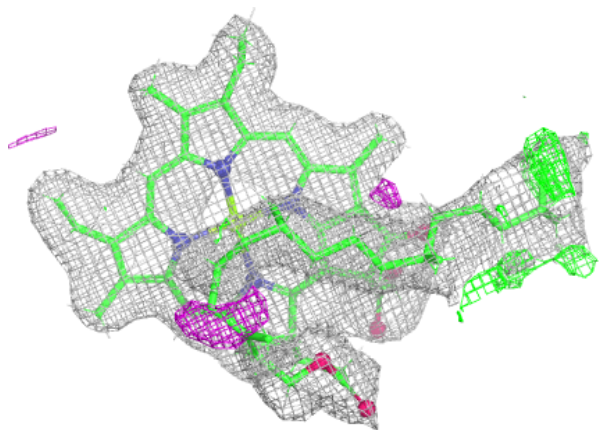


**Electron density around LMG D 410:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 601:**

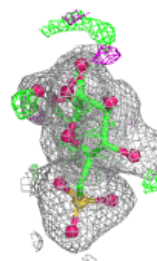
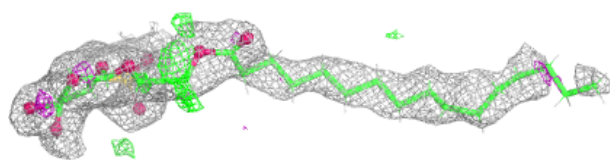
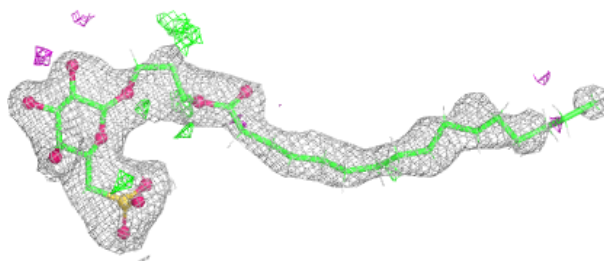
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



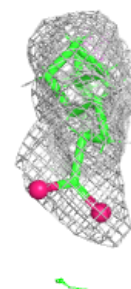
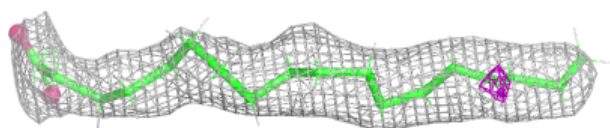
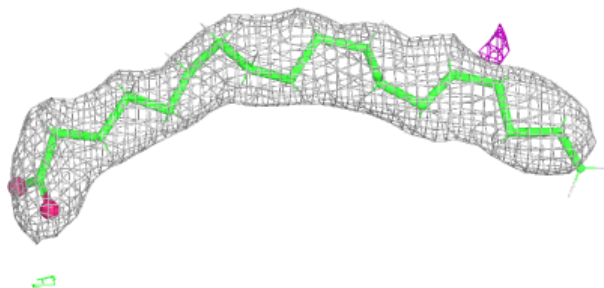


**Electron density around SQD D 407:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

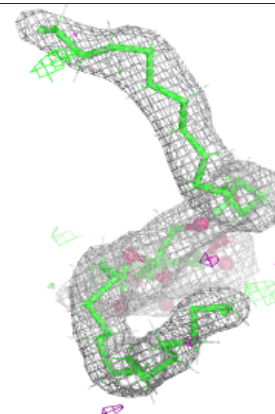
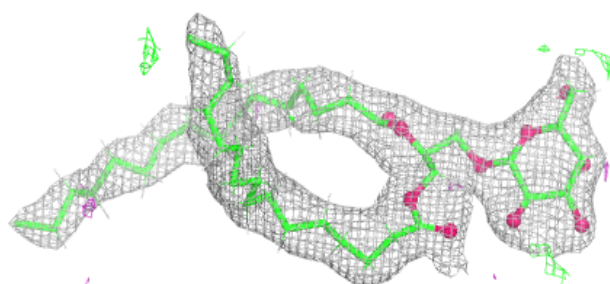
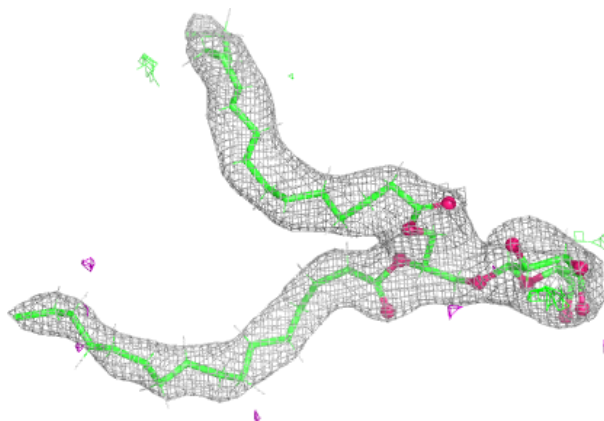
**Electron density around STE D 411:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

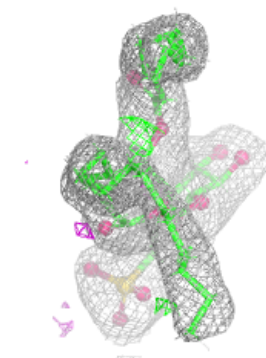
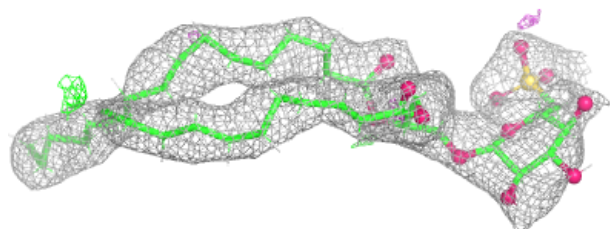
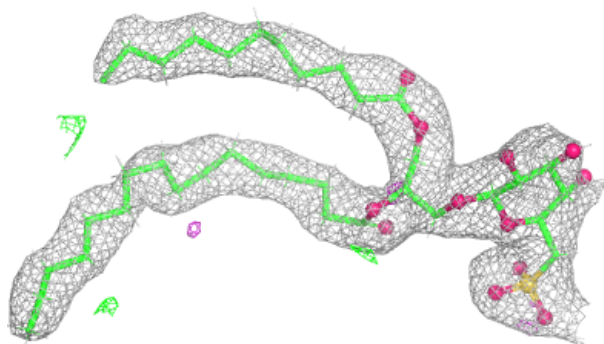


**Electron density around LMG b 621:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

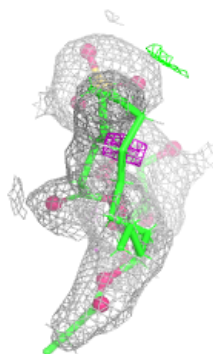
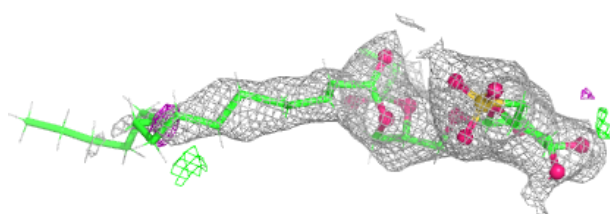
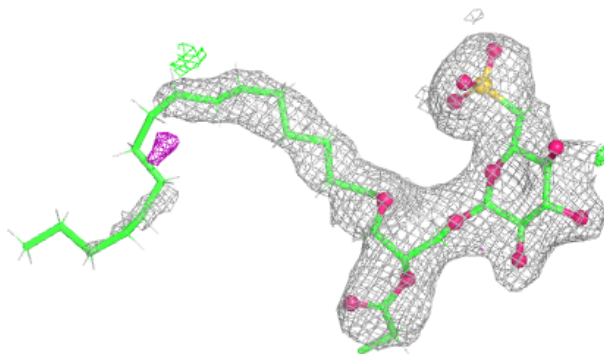
**Electron density around SQD b 620:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

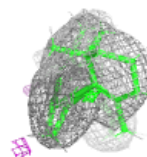
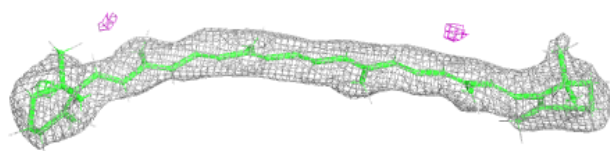


**Electron density around SQD f 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

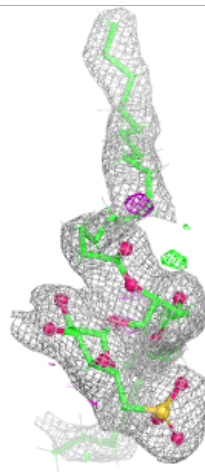
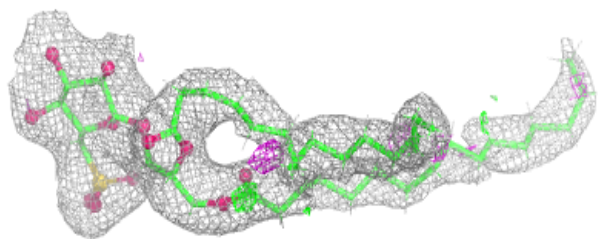
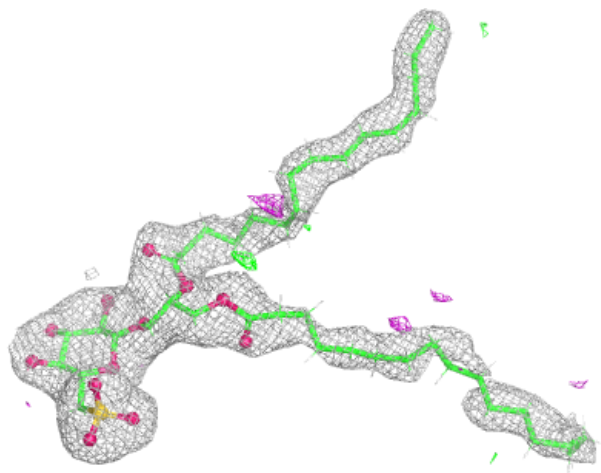
**Electron density around BCR d 405:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



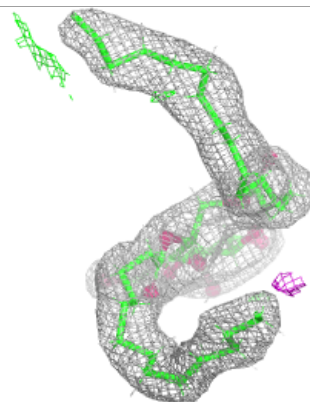
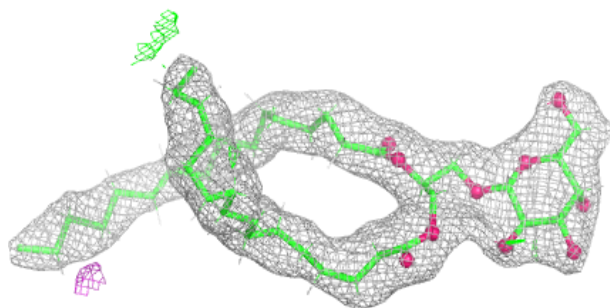
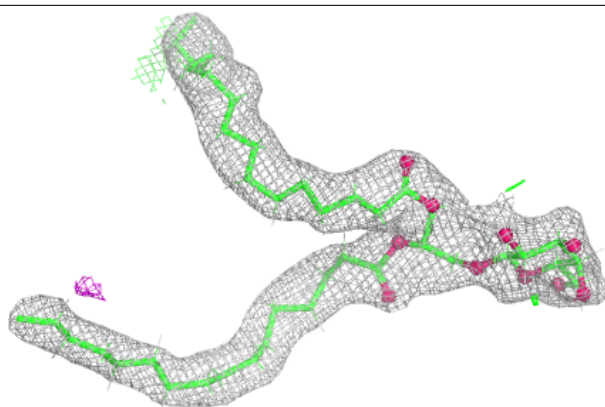
**Electron density around SQD a 613:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

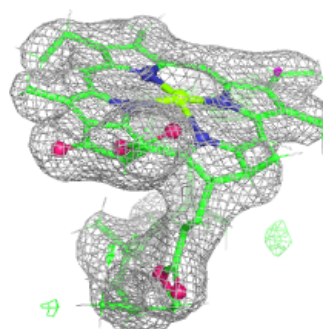
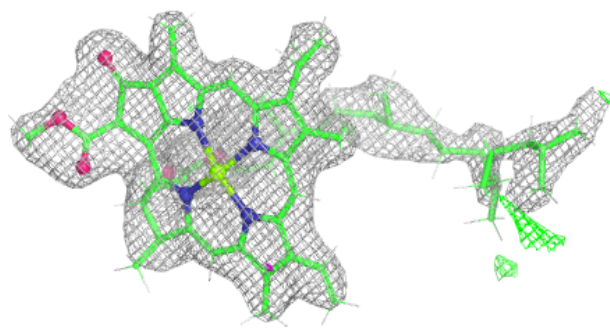
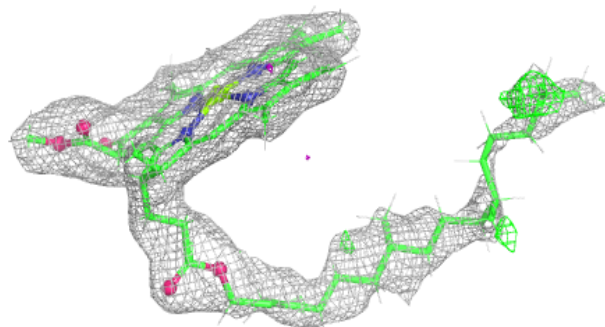


**Electron density around LMG M 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA C 513:**

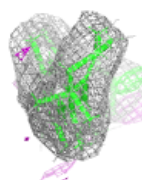
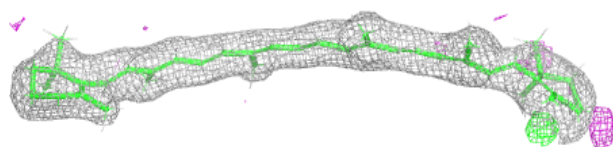
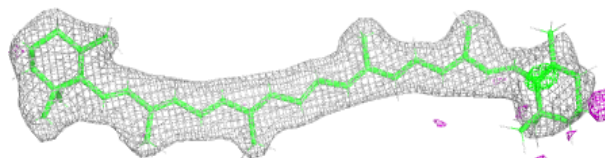
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



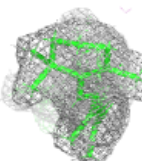
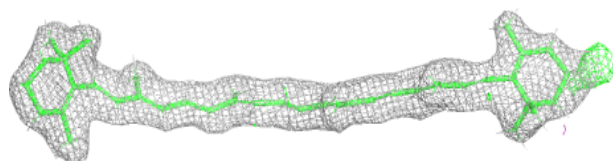
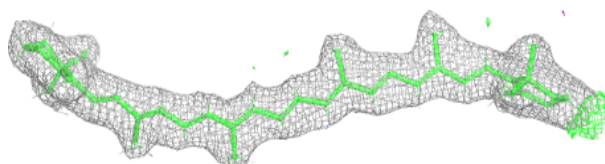


**Electron density around BCR D 404:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

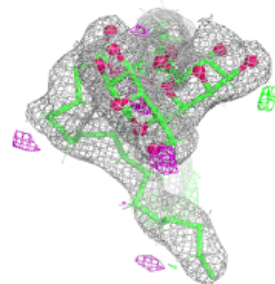
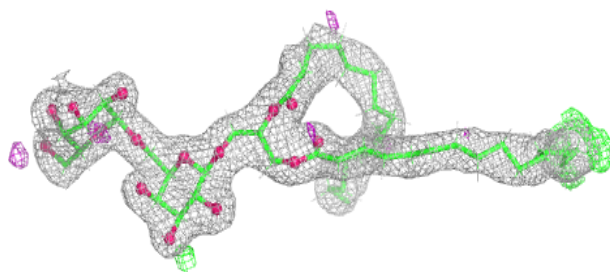
**Electron density around BCR H 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

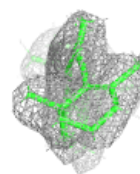
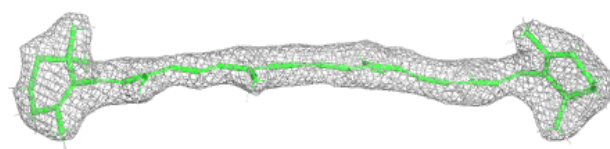
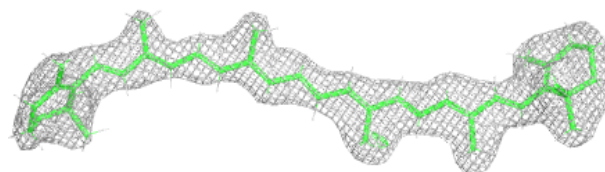


**Electron density around DGD H 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

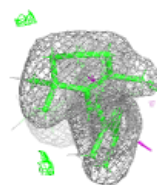
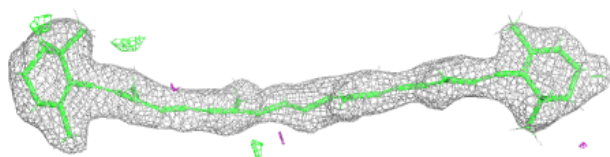
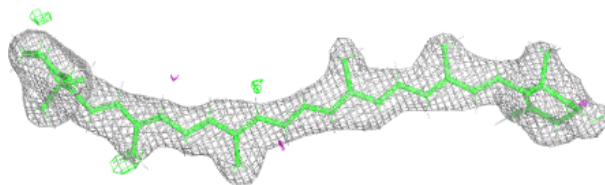
**Electron density around BCR k 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

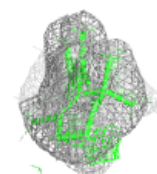
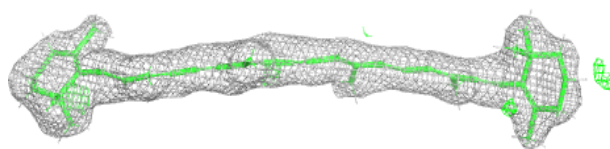


**Electron density around BCR x 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR Y 101:**

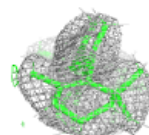
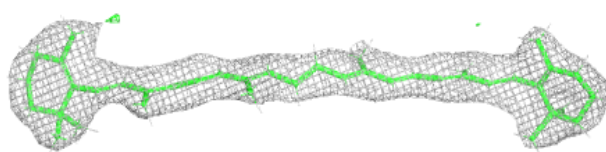
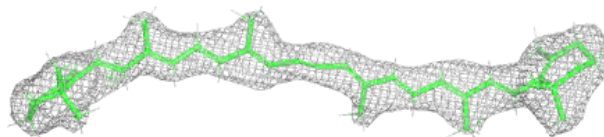
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



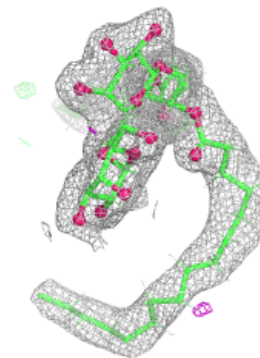
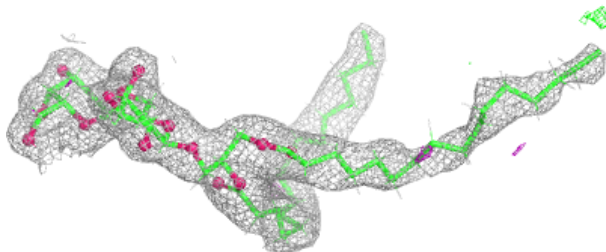
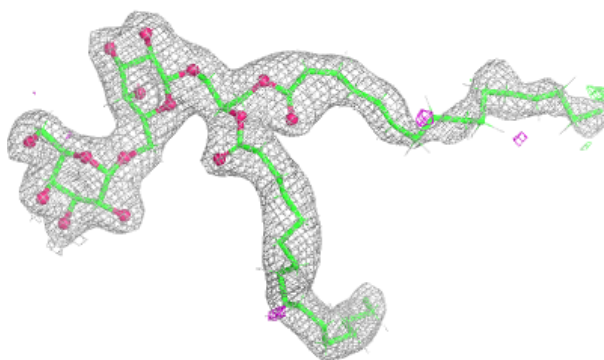


**Electron density around BCR c 514:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

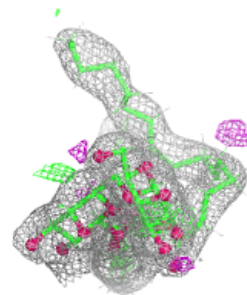
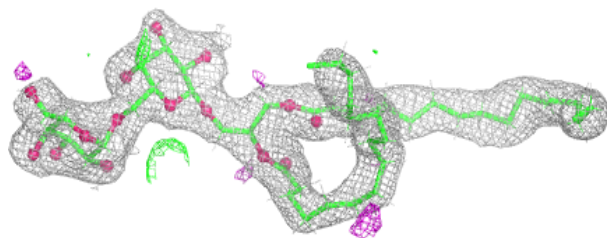
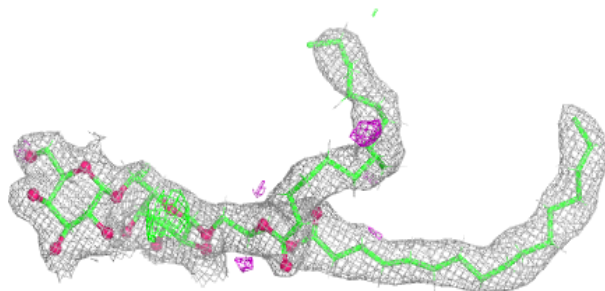
**Electron density around DGD c 517:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



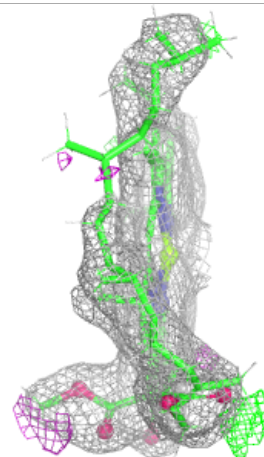
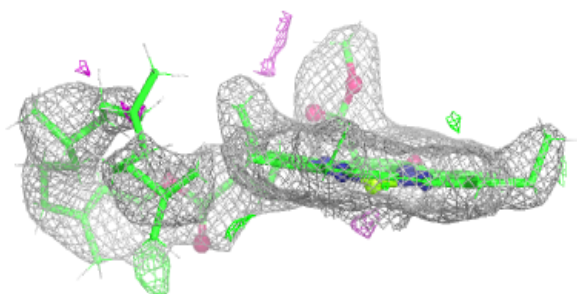
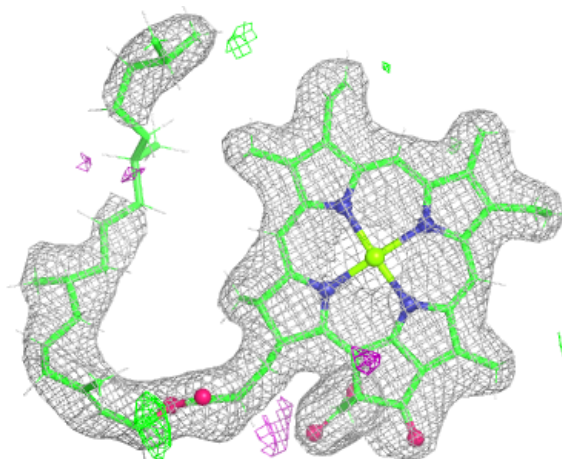
**Electron density around DGD h 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



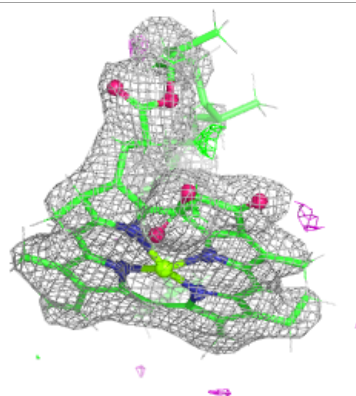
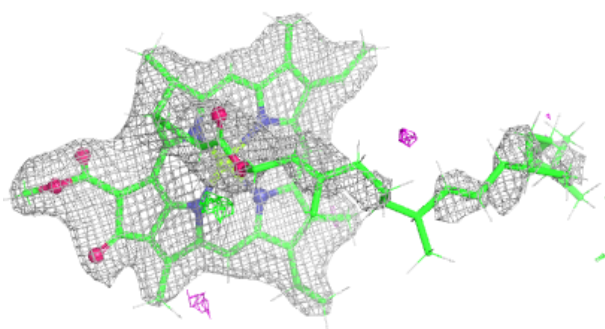
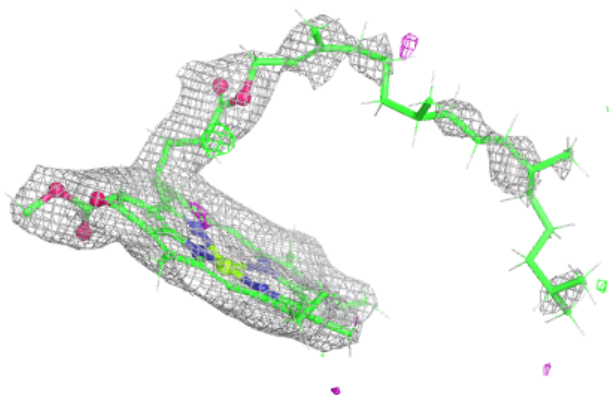
**Electron density around CLA c 512:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

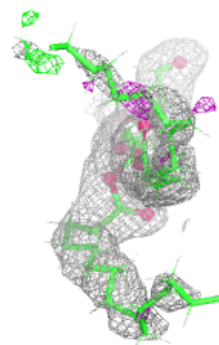
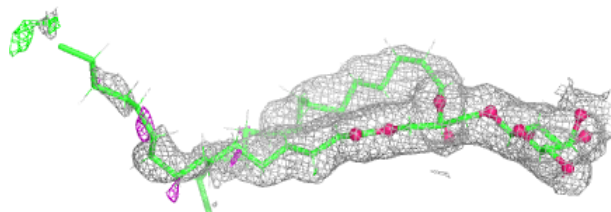
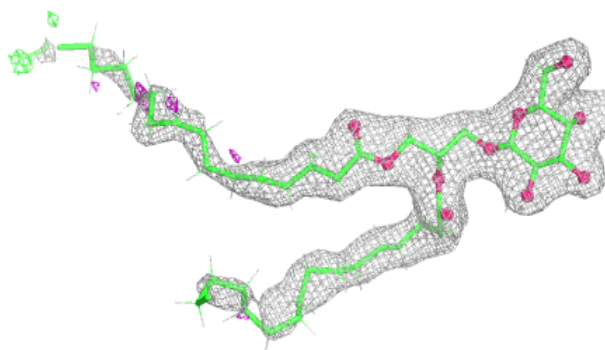


**Electron density around CLA c 513:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

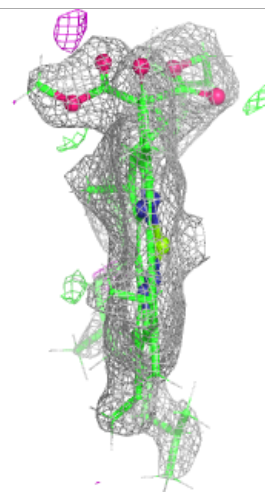
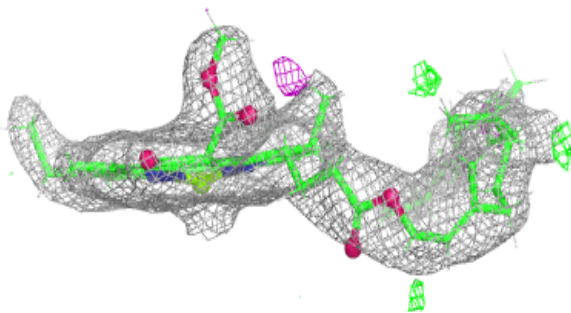
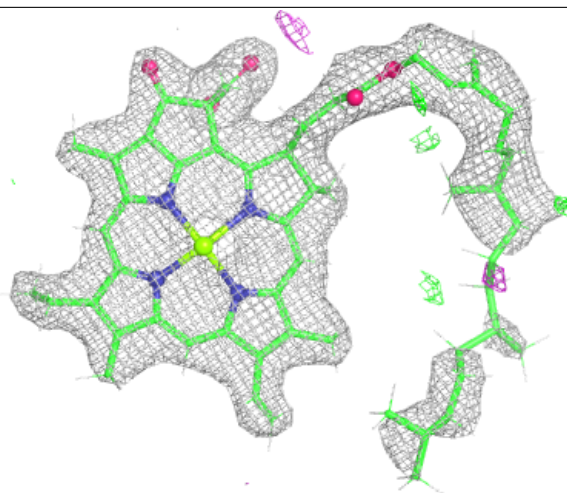
**Electron density around LMG D 406:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



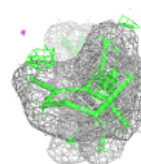
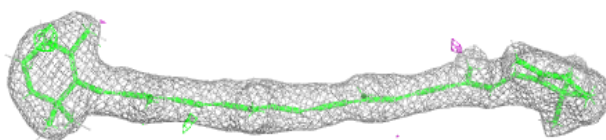
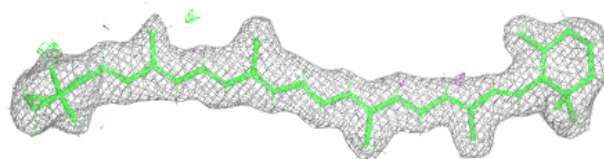
**Electron density around CLA C 512:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

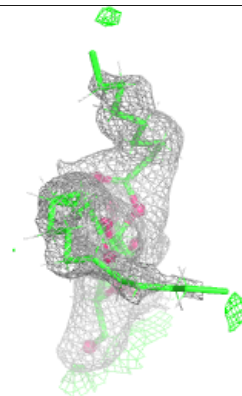
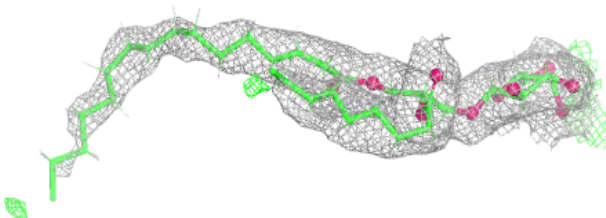
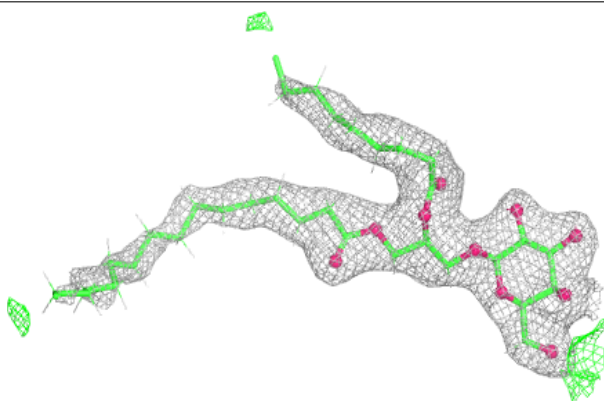


**Electron density around BCR b 617:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG d 410:**

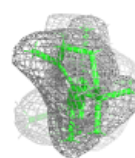
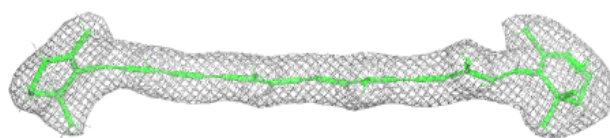
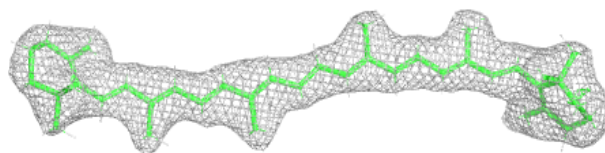
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



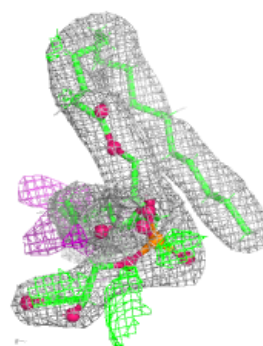
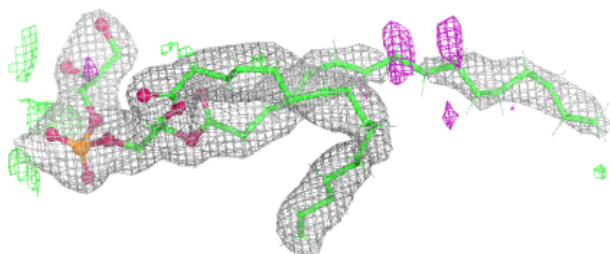
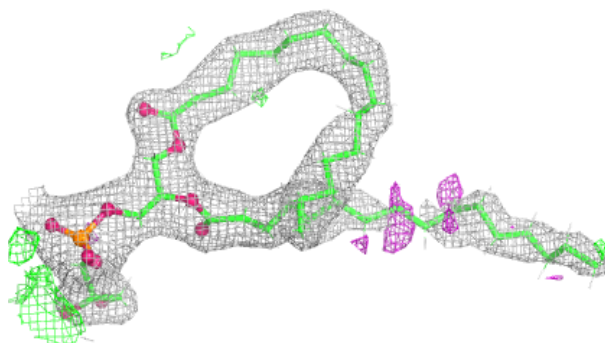


**Electron density around BCR b 618:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

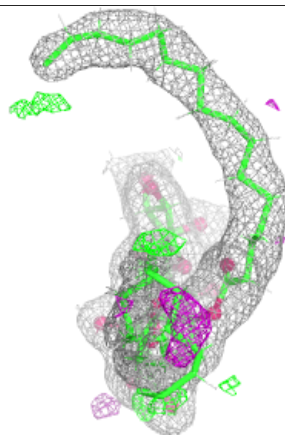
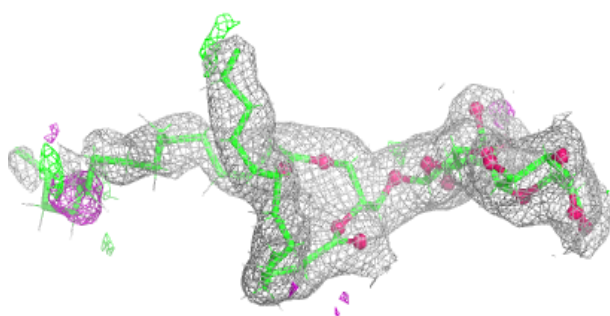
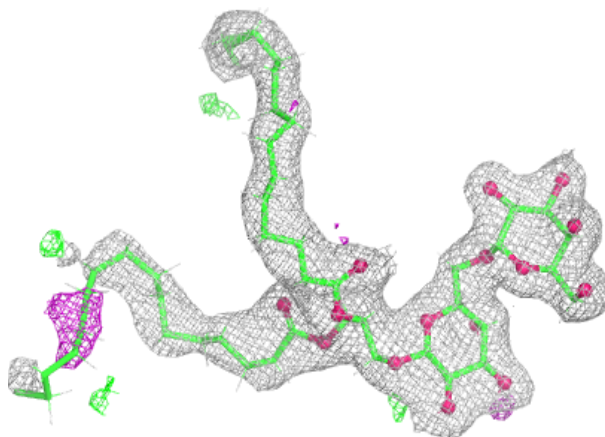
**Electron density around LHG d 407:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

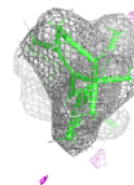
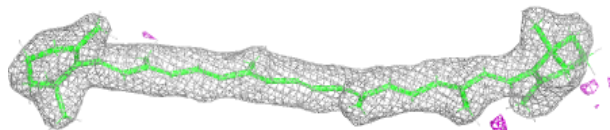
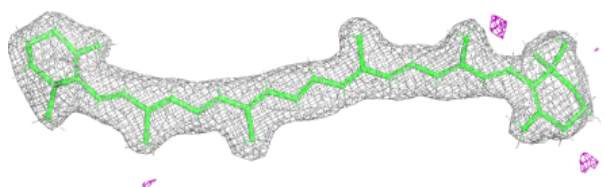


**Electron density around DGD C 517:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR b 619:**

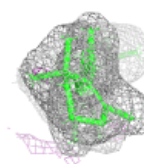
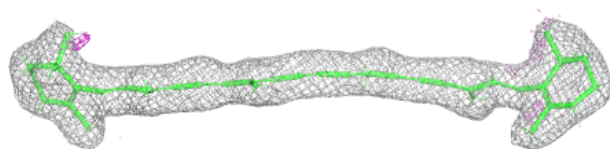
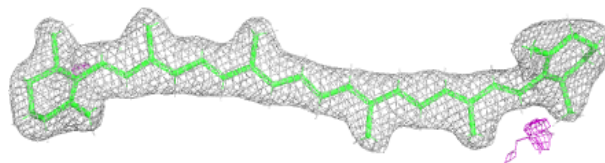
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





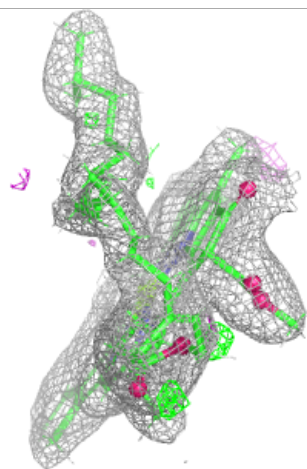
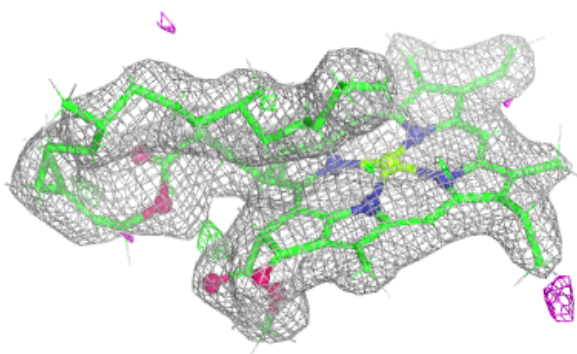
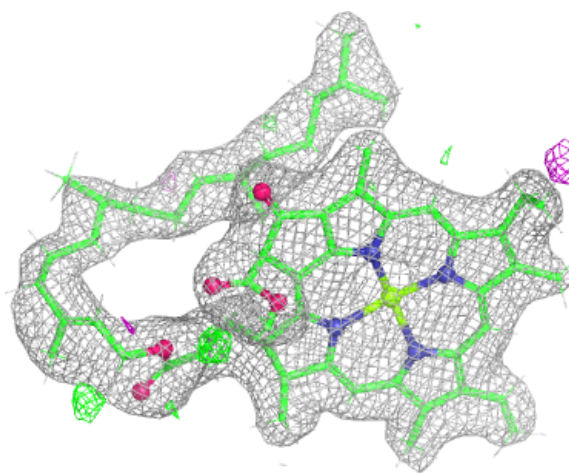
**Electron density around BCR B 618:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



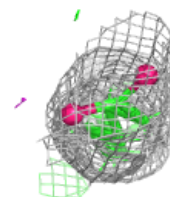
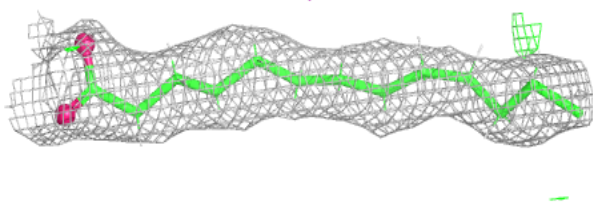
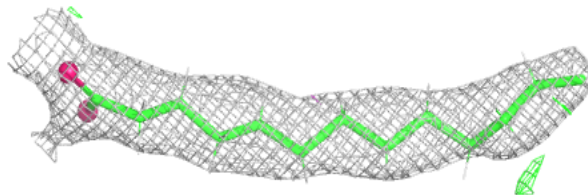
**Electron density around CLA c 509:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

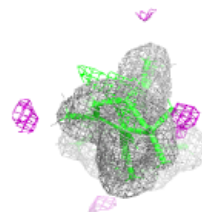
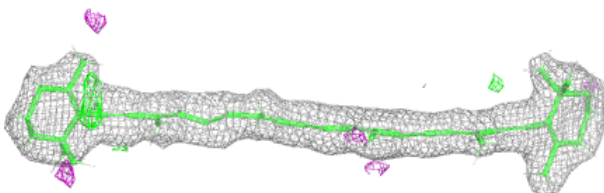
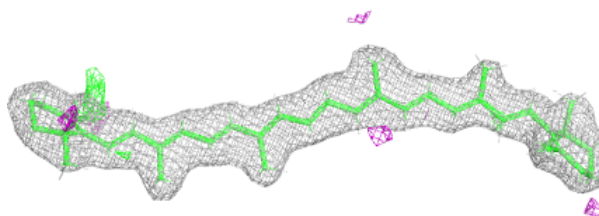


**Electron density around STE M 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

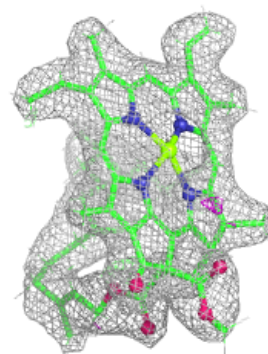
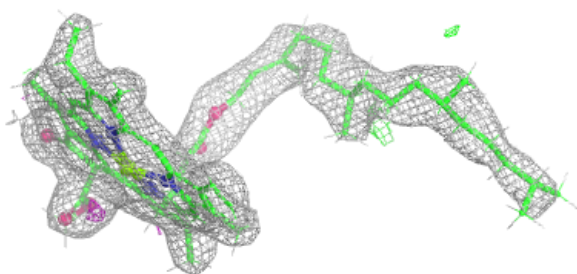
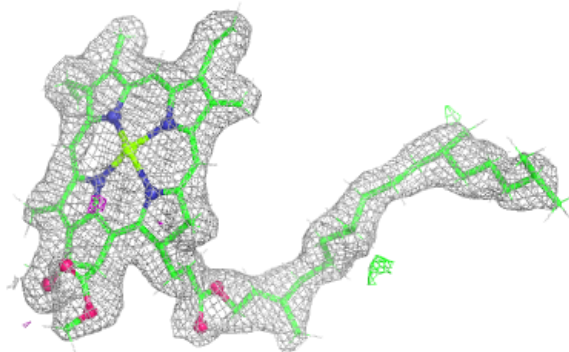
**Electron density around BCR C 515:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

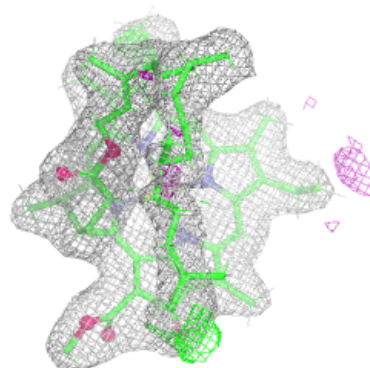
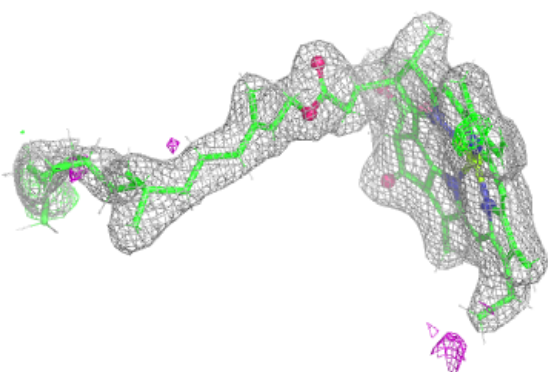
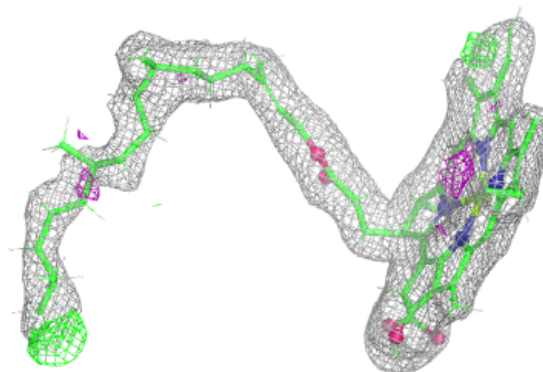


**Electron density around CLA C 511:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

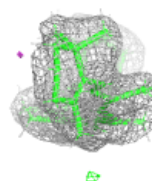
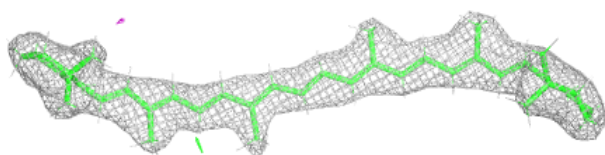
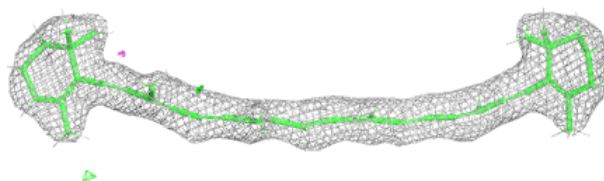
**Electron density around CLA b 606:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

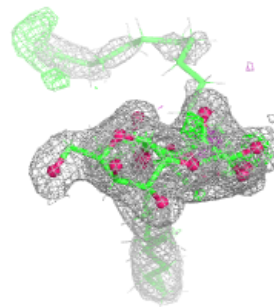
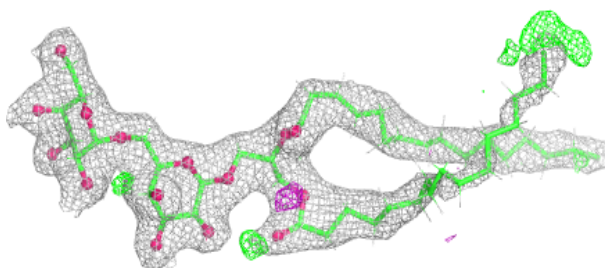
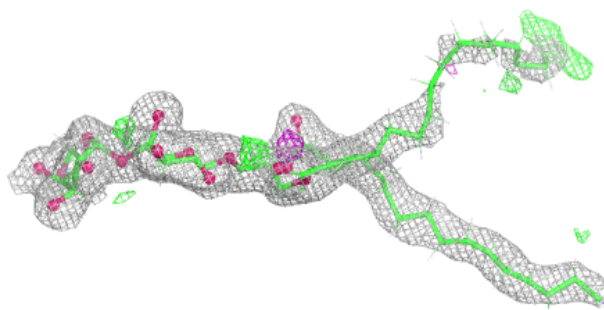


**Electron density around BCR k 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

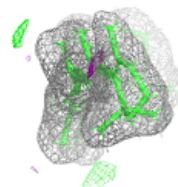
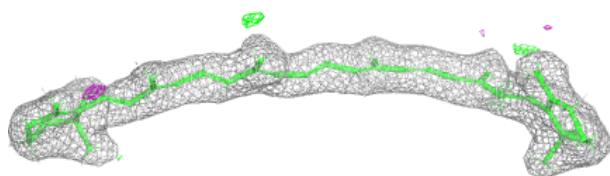
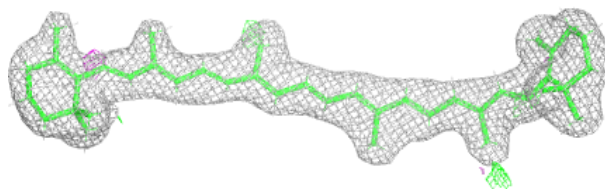
**Electron density around DGD C 516:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



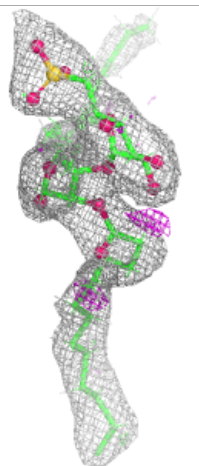
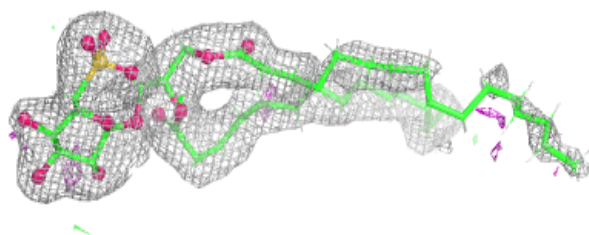
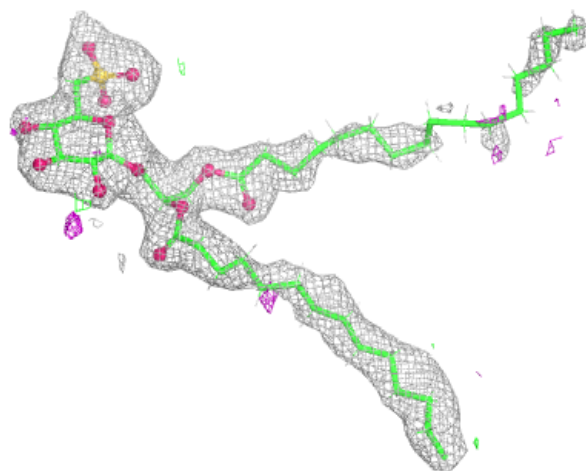
**Electron density around BCR T 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SQD A 616:**

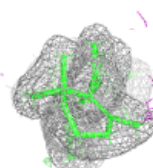
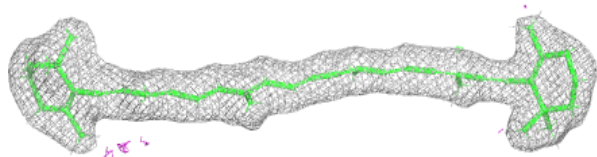
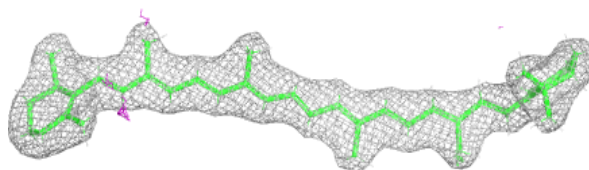
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



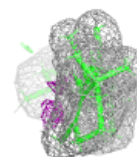
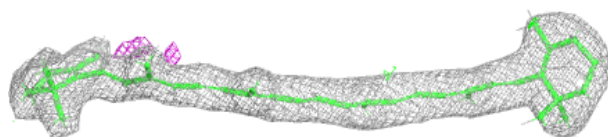
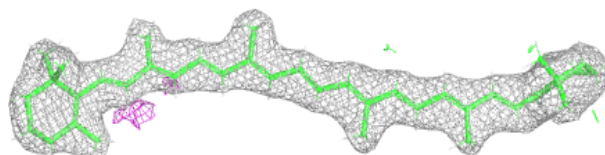


**Electron density around BCR A 609:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR B 617:**

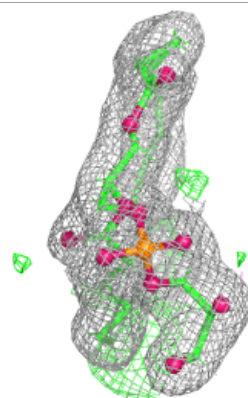
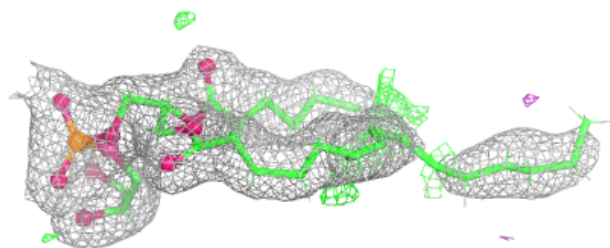
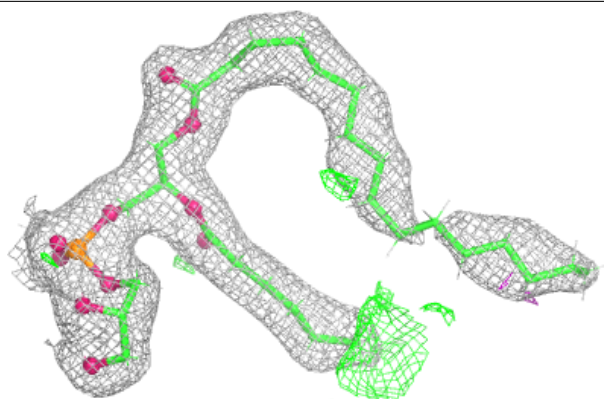
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



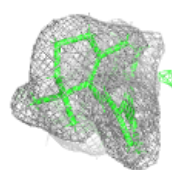
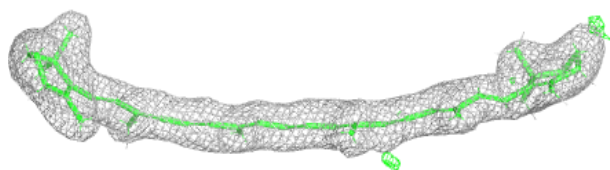
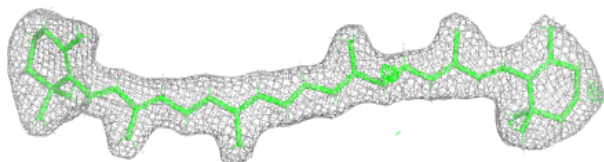


**Electron density around LHG d 409:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

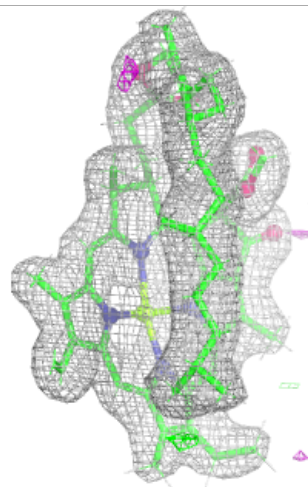
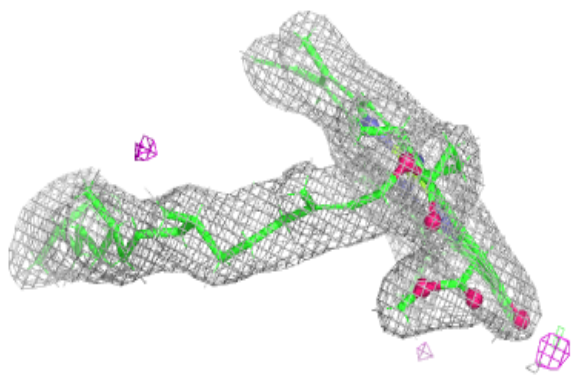
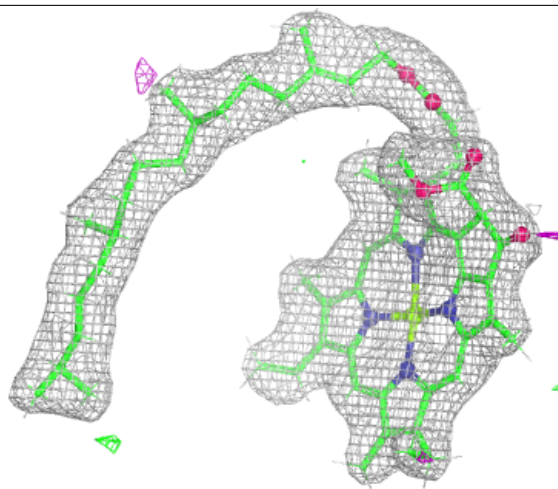
**Electron density around BCR t 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



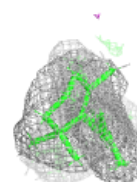
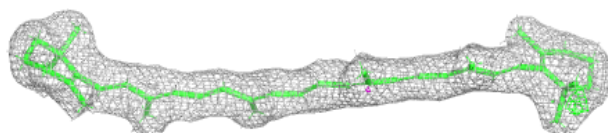
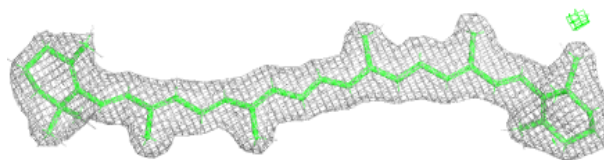
**Electron density around CLA C 507:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

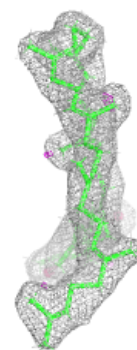
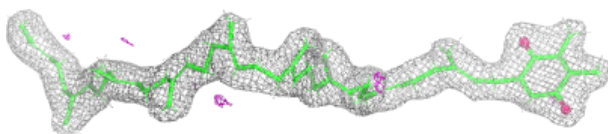
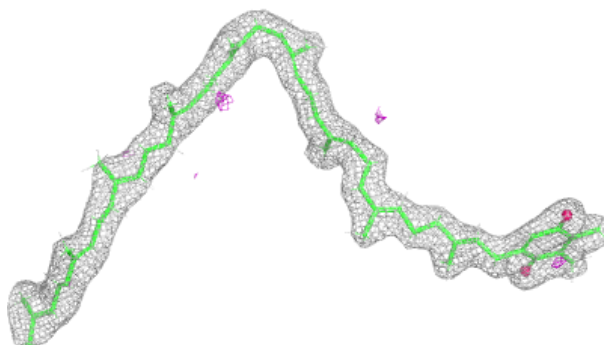


**Electron density around BCR B 619:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

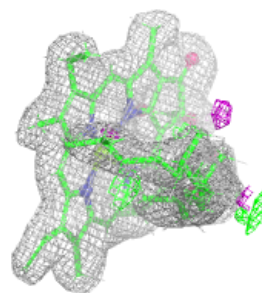
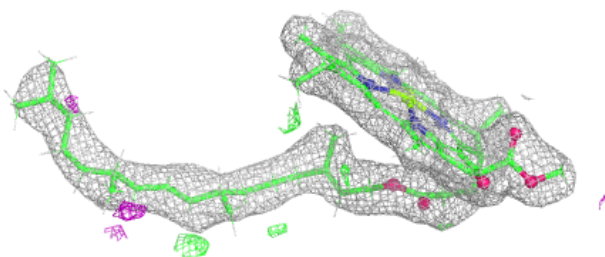
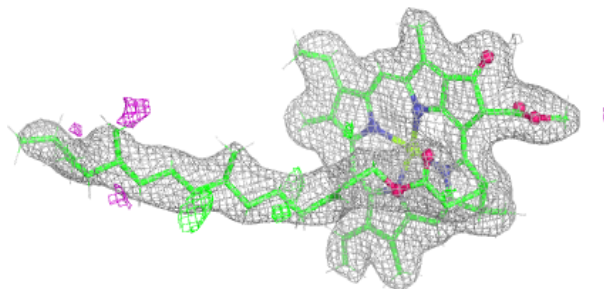
**Electron density around PL9 D 405:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

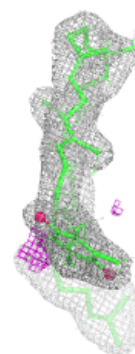
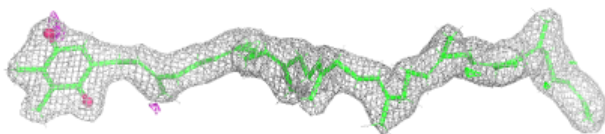
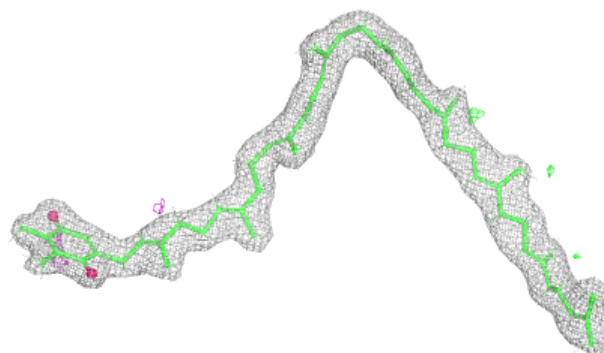


**Electron density around CLA b 608:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

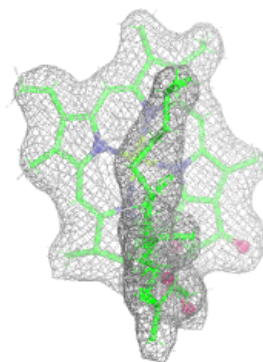
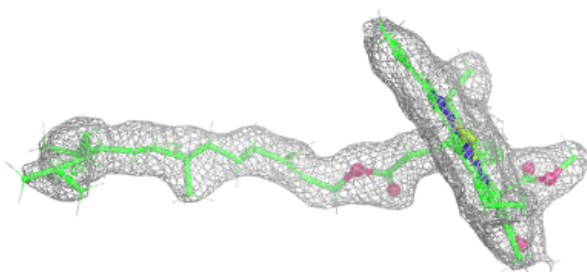
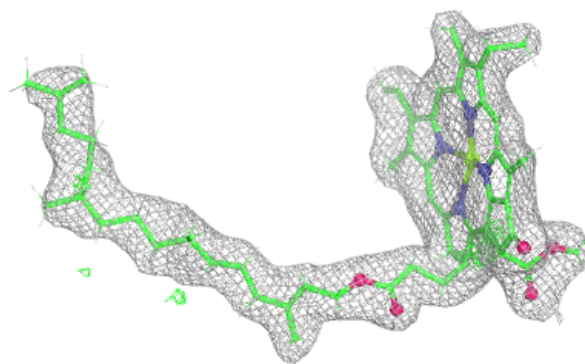
**Electron density around PL9 d 406:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

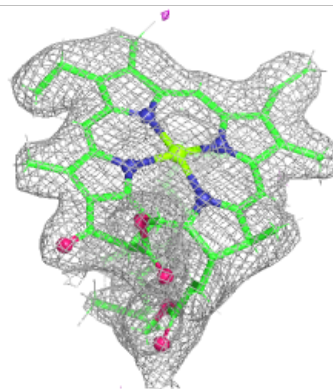
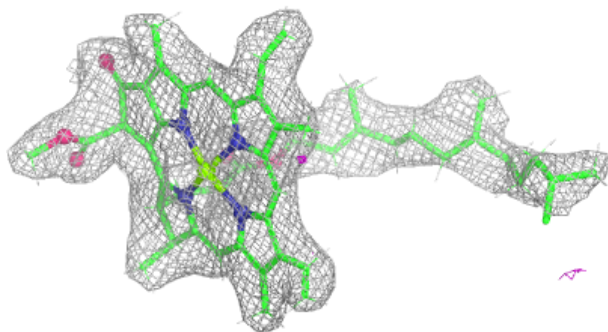
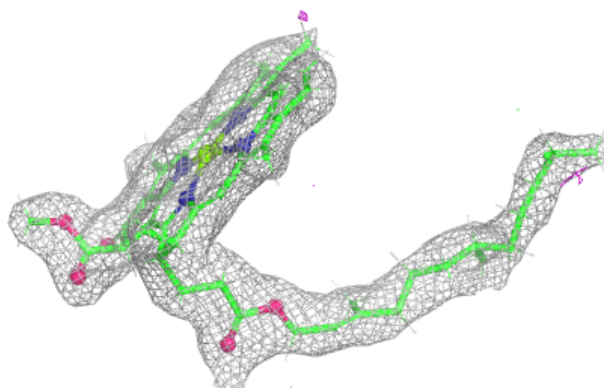


**Electron density around CLA b 609:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA c 504:**

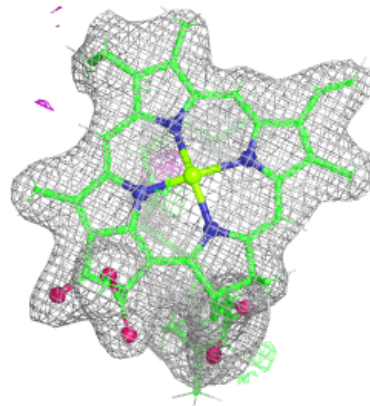
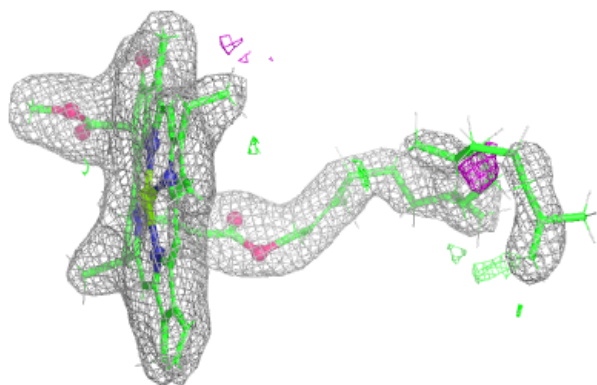
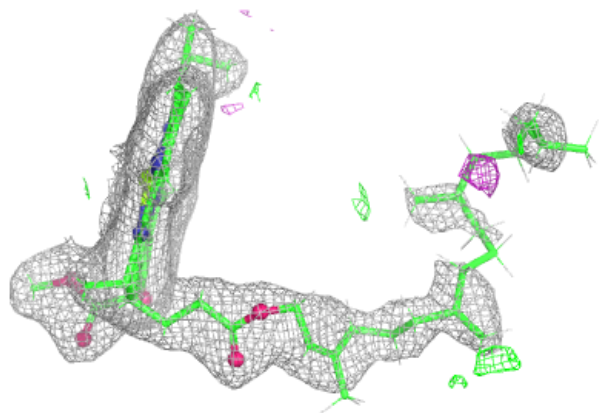
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



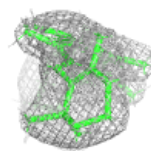
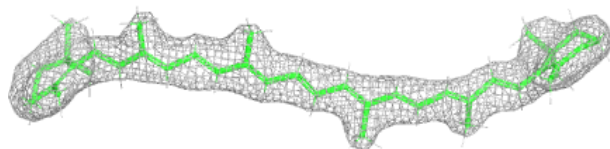
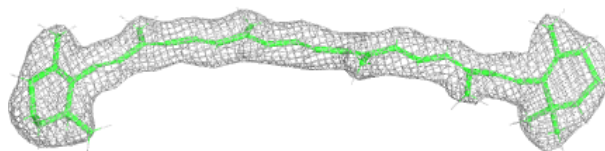


**Electron density around CLA c 506:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

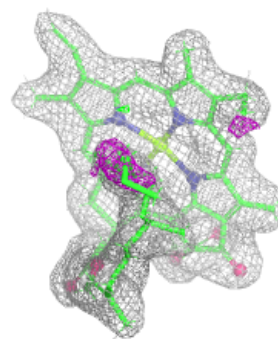
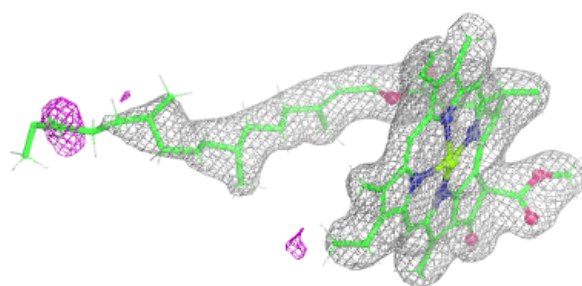
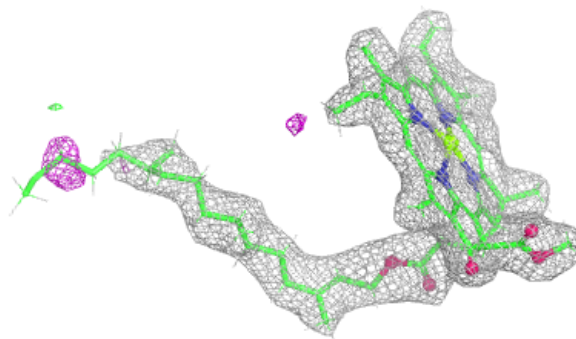
**Electron density around BCR K 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



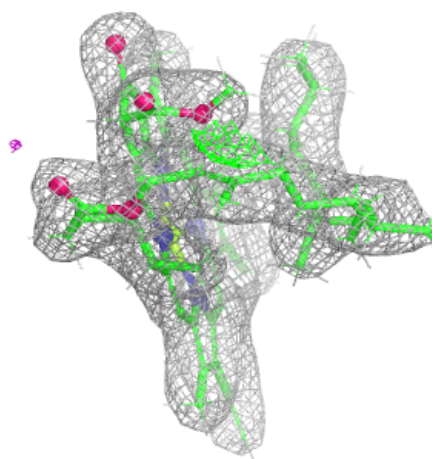
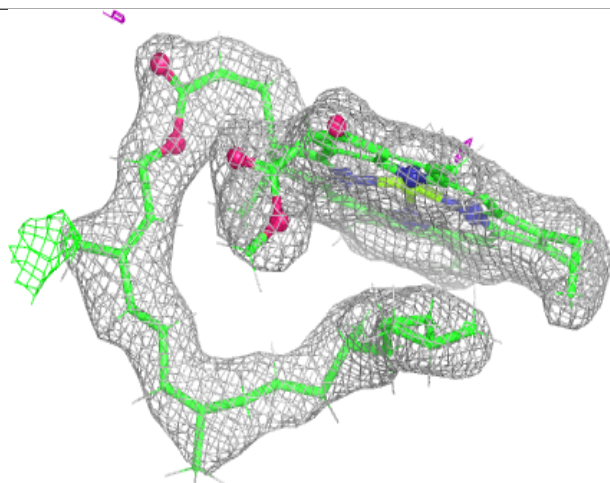
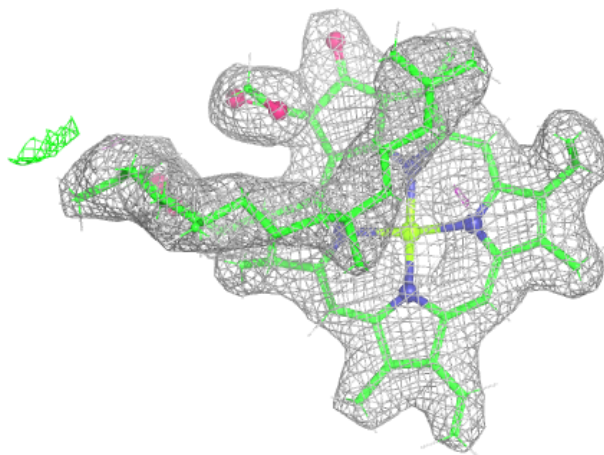
**Electron density around CLA c 508:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 510:**

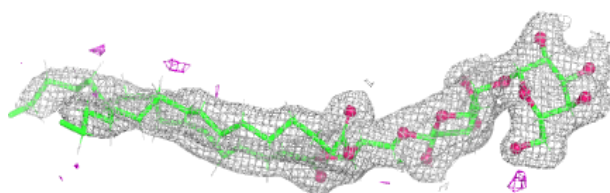
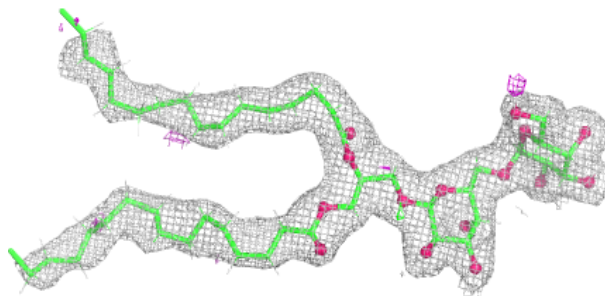
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



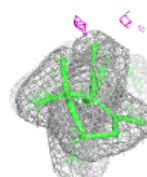
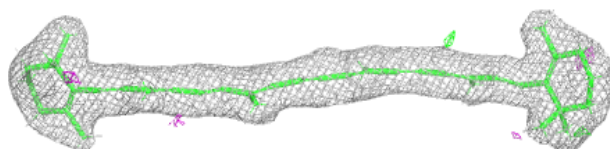
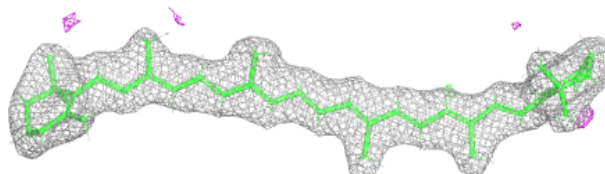


**Electron density around DGD C 518:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

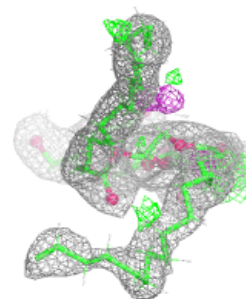
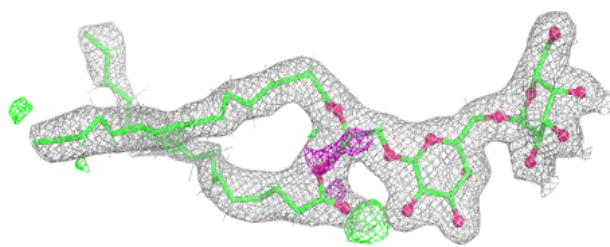
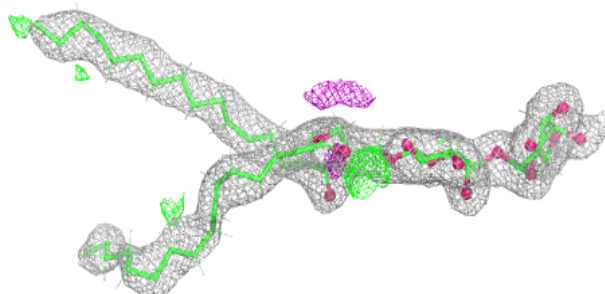
**Electron density around BCR a 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

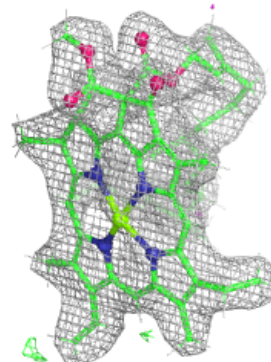
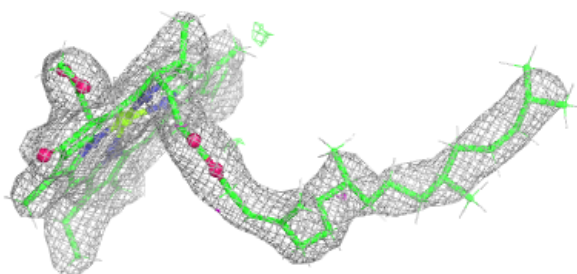
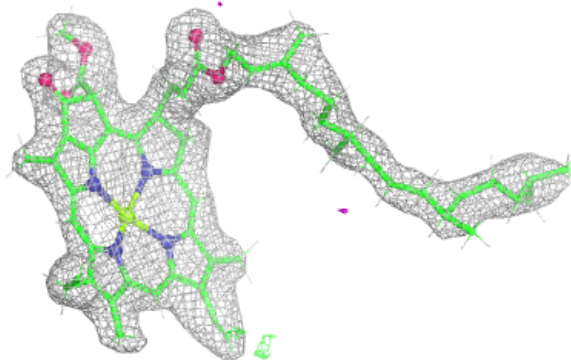


**Electron density around DGD c 516:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

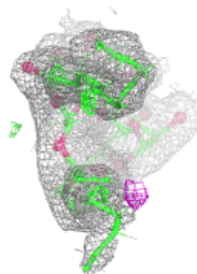
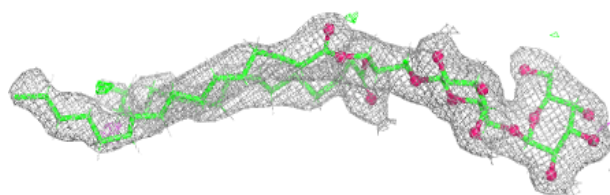
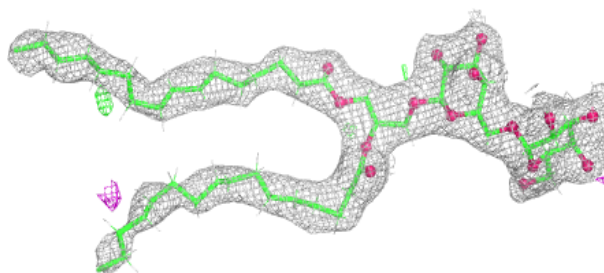
**Electron density around CLA c 511:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

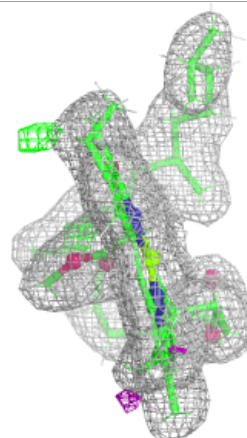
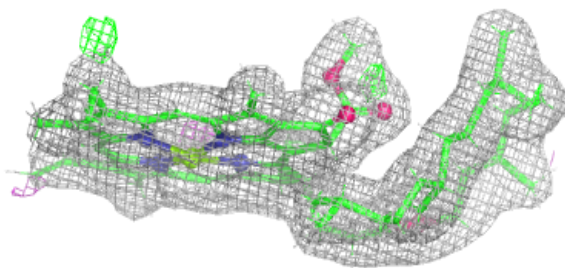
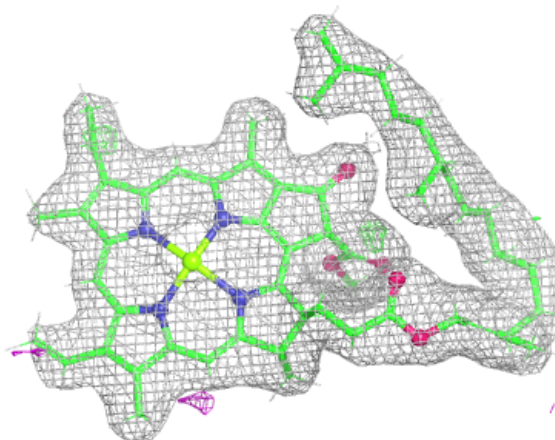


**Electron density around DGD c 518:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

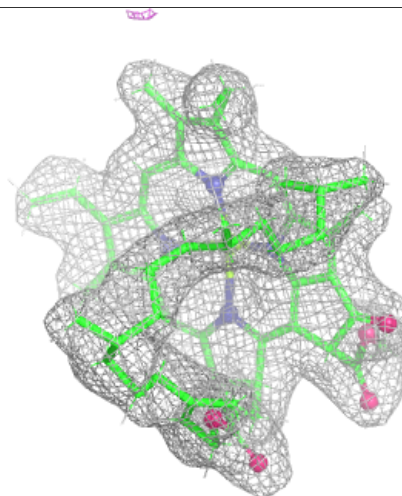
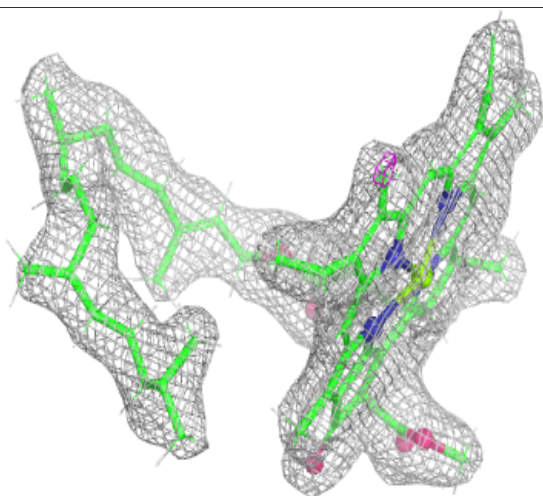
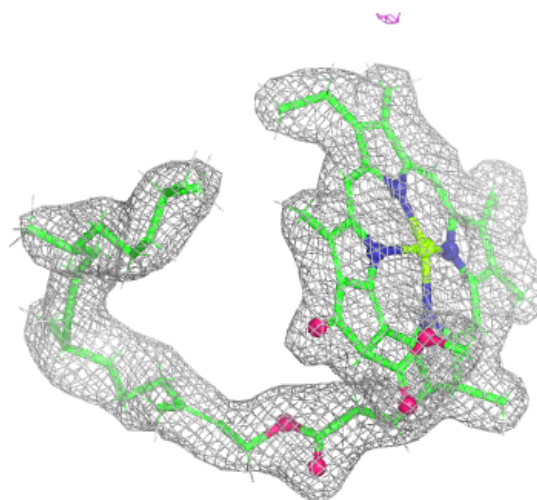
**Electron density around CLA B 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



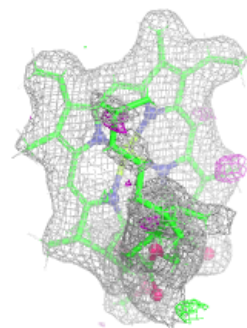
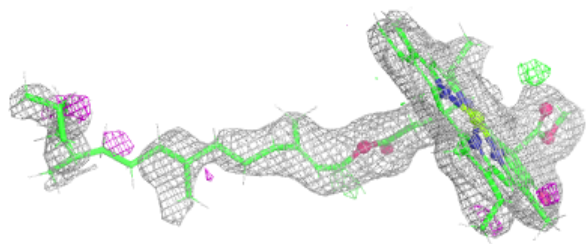
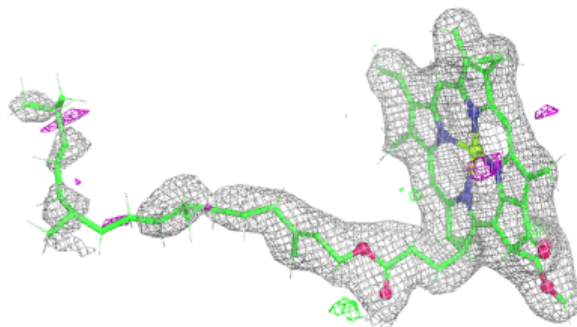
**Electron density around CLA C 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

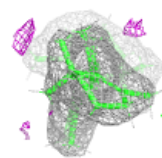
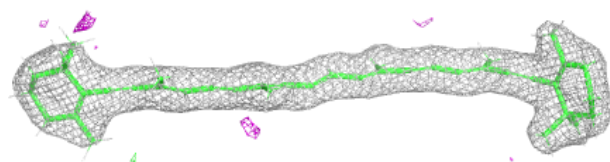


**Electron density around CLA d 404:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR c 515:**

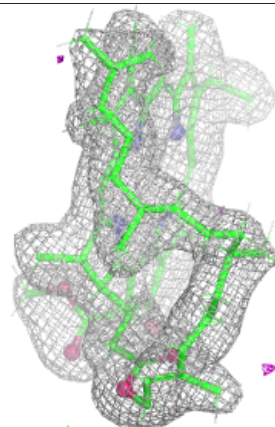
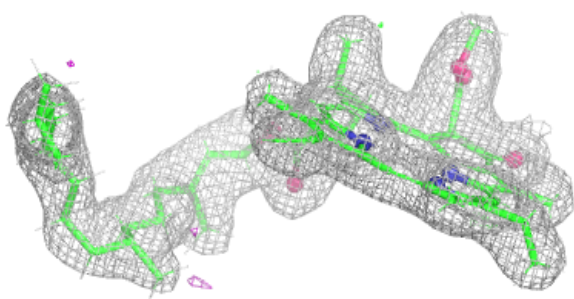
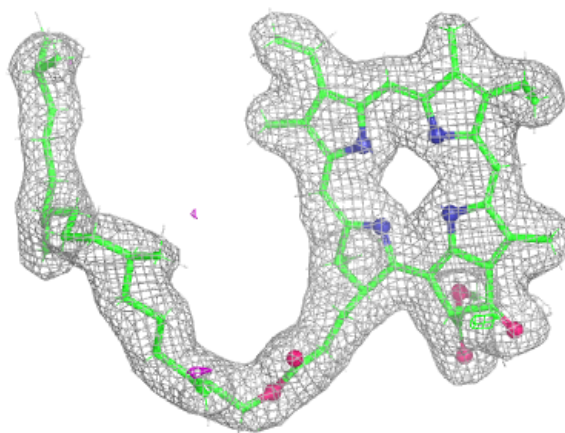
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



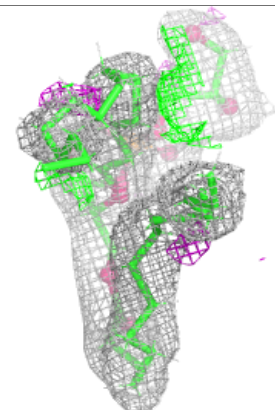
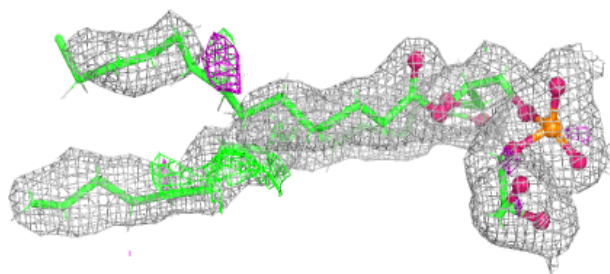
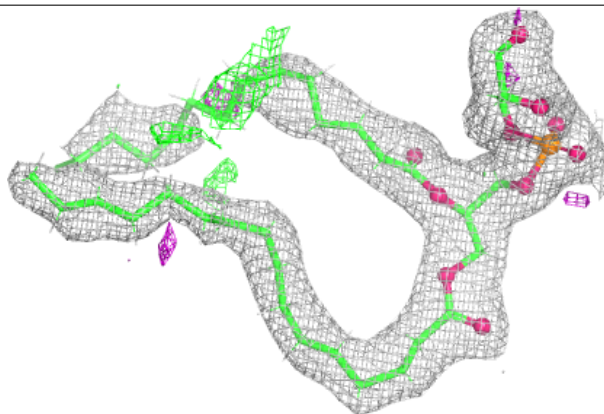


**Electron density around PHO d 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

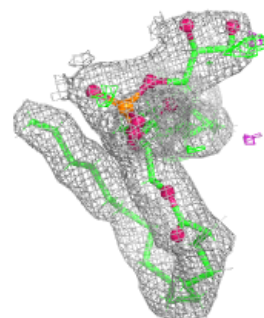
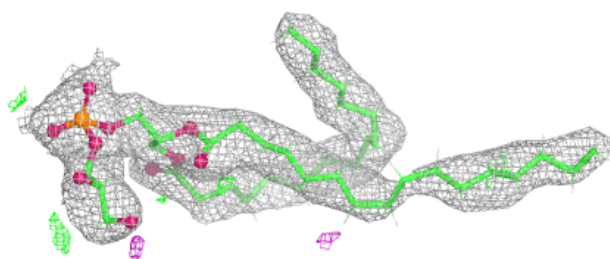
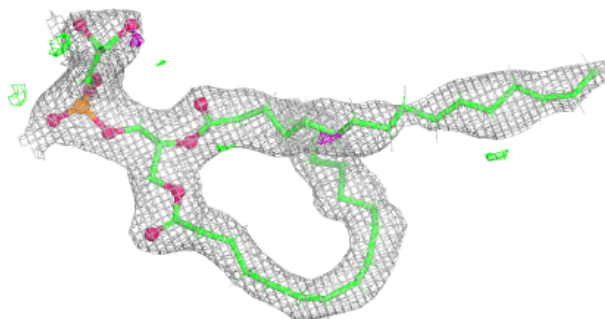
**Electron density around LHG A 615:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

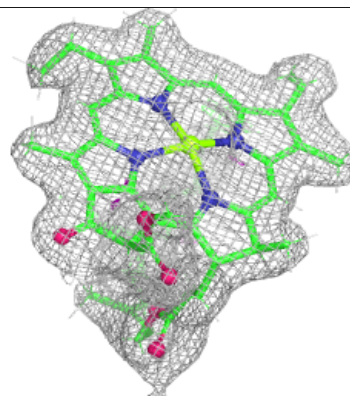
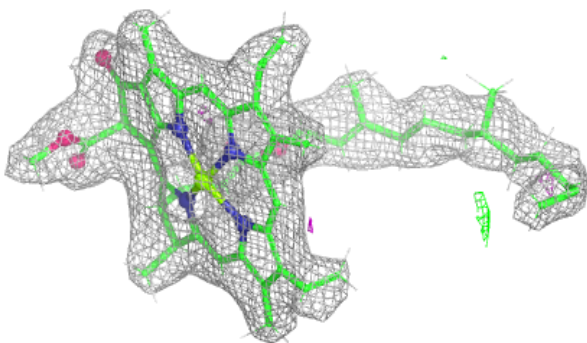
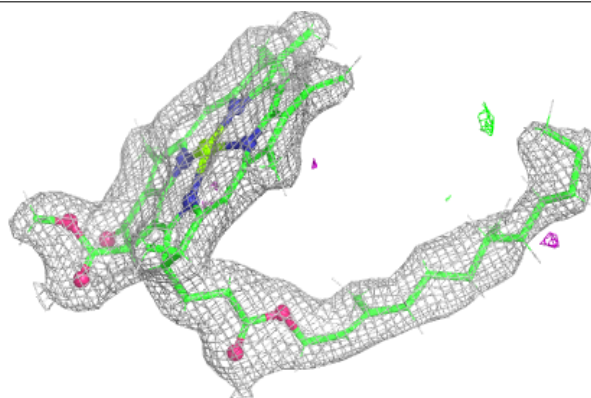


**Electron density around LHG B 622:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

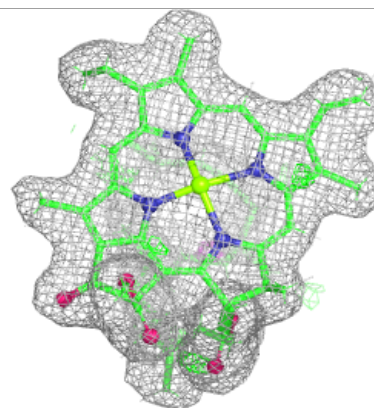
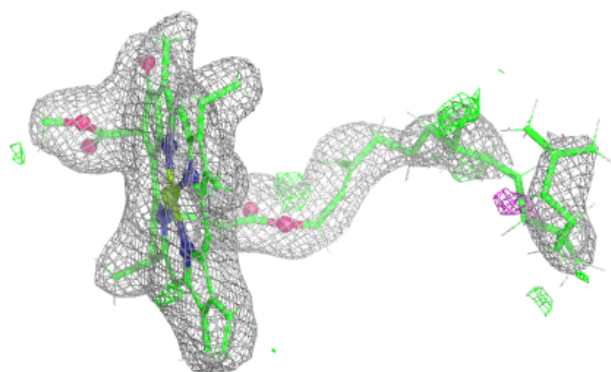
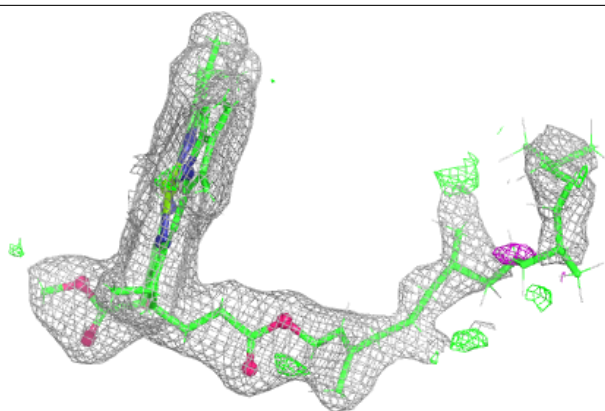
**Electron density around CLA C 504:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

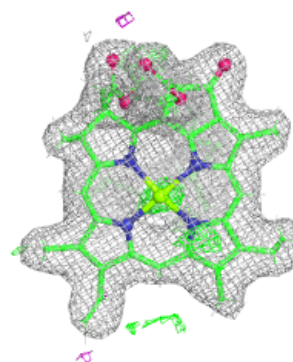
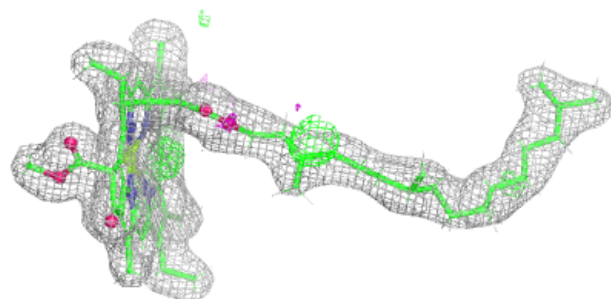
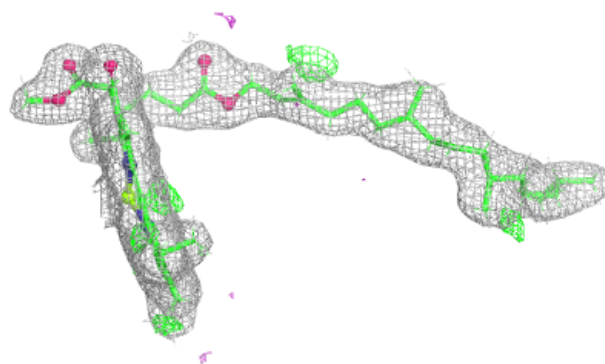


**Electron density around CLA C 506:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 605:**

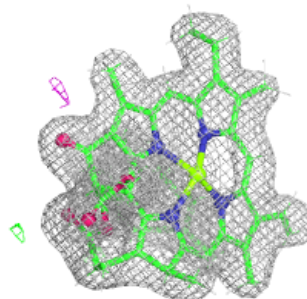
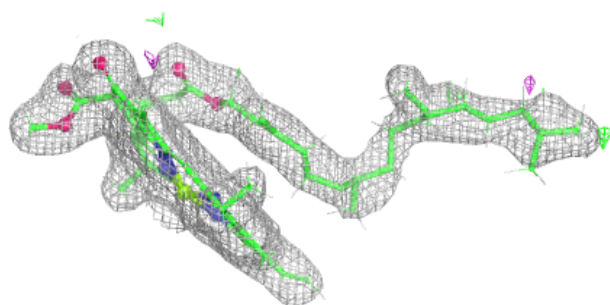
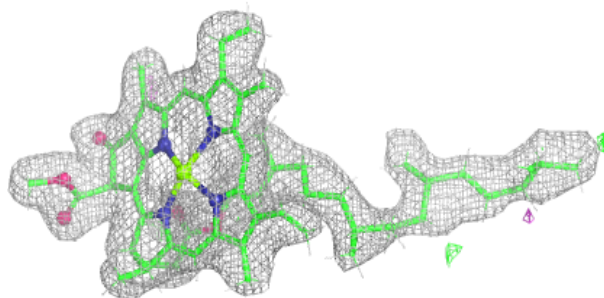
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



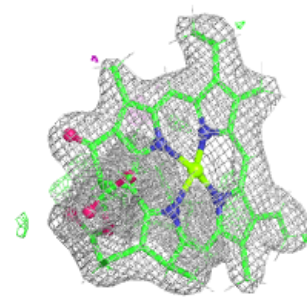
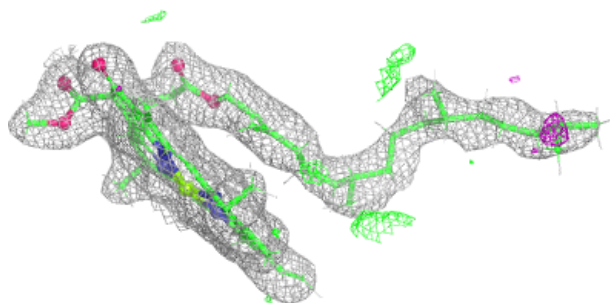
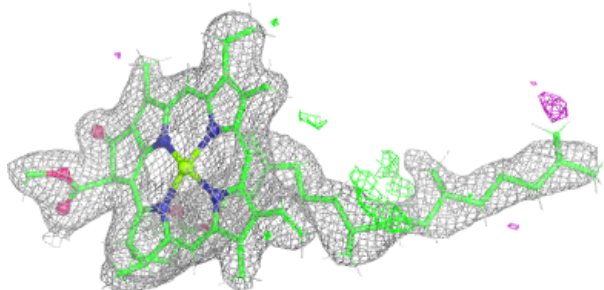


**Electron density around CLA c 505:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

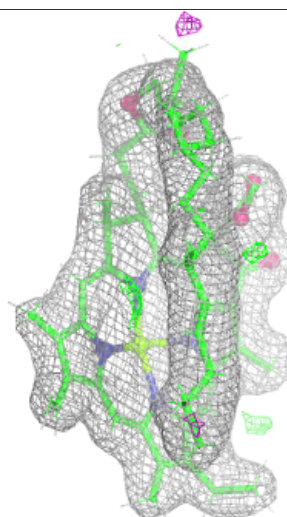
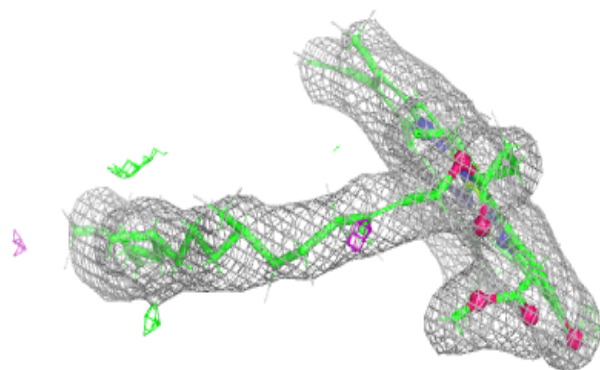
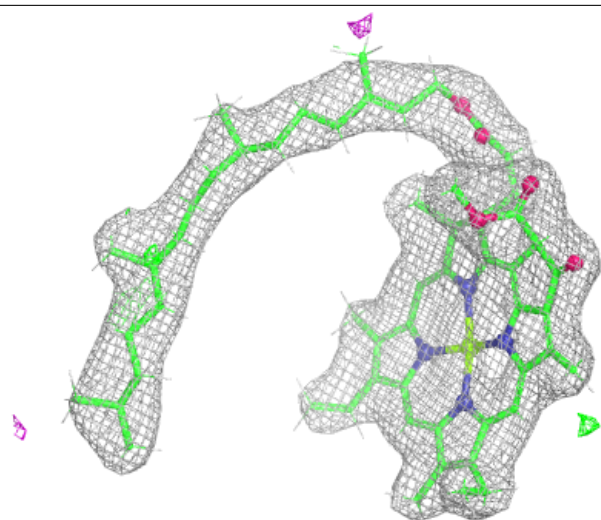
**Electron density around CLA C 505:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



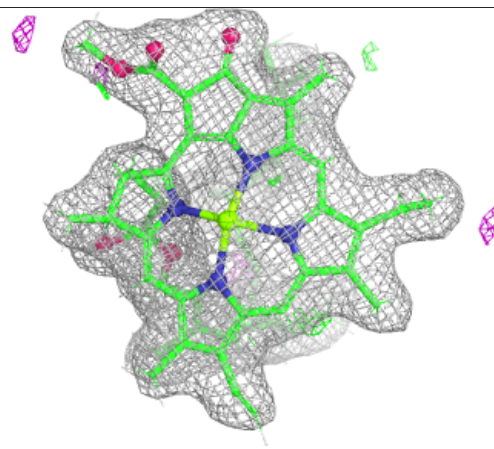
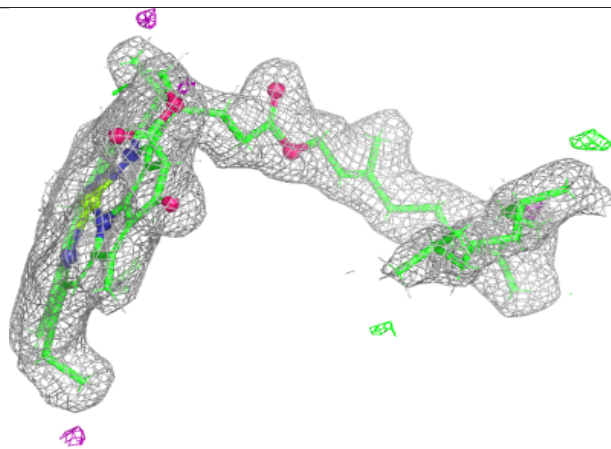
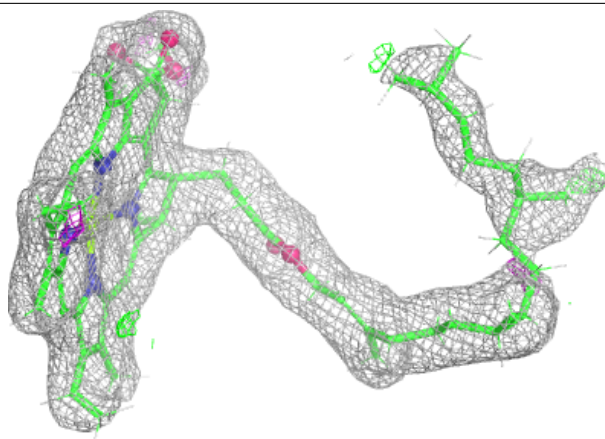
**Electron density around CLA c 507:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



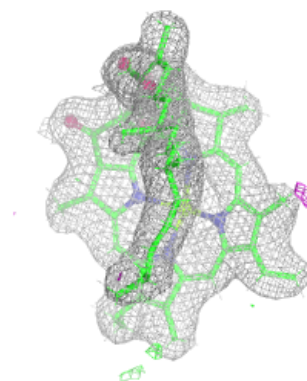
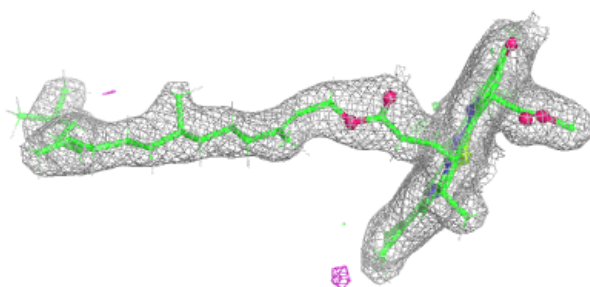
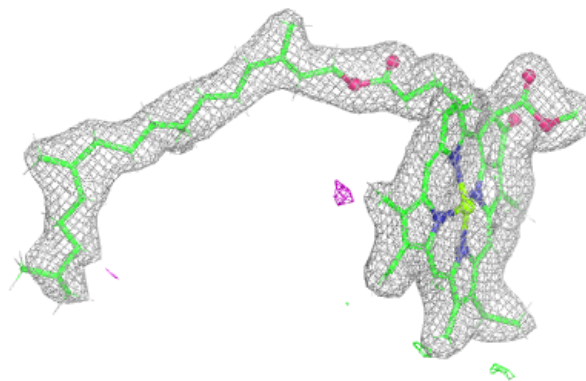
**Electron density around CLA B 606:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



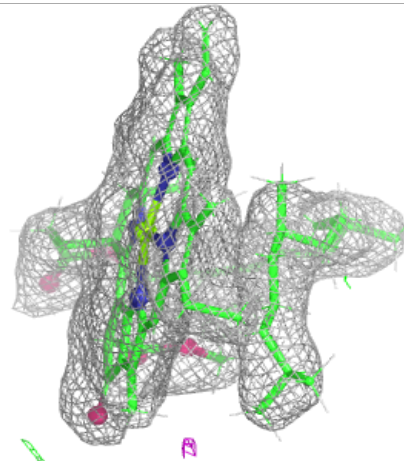
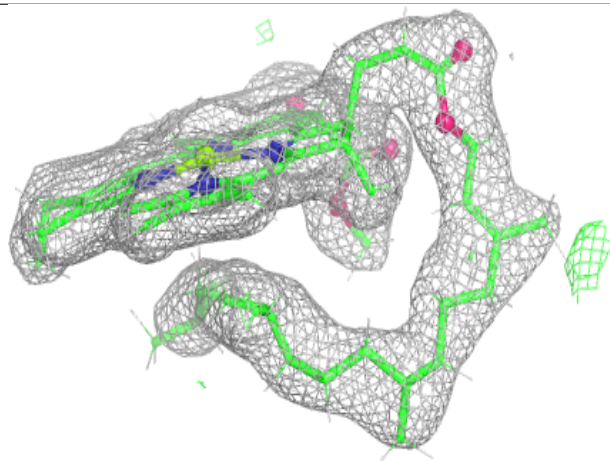
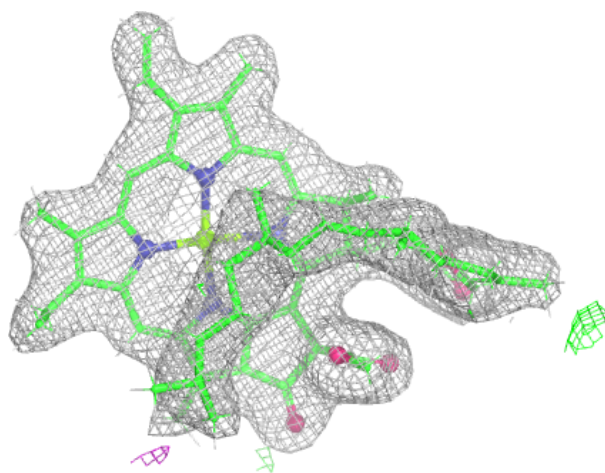
**Electron density around CLA B 609:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



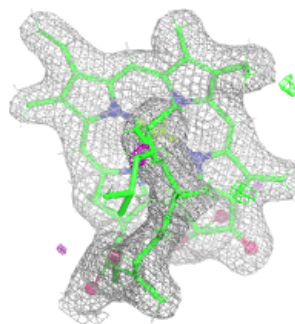
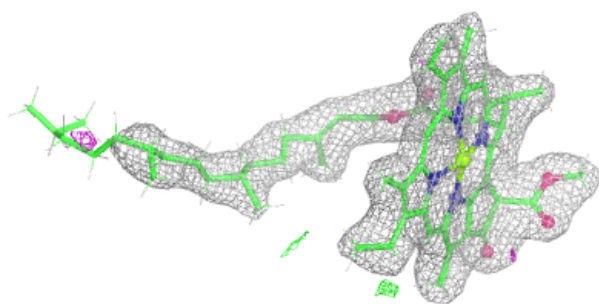
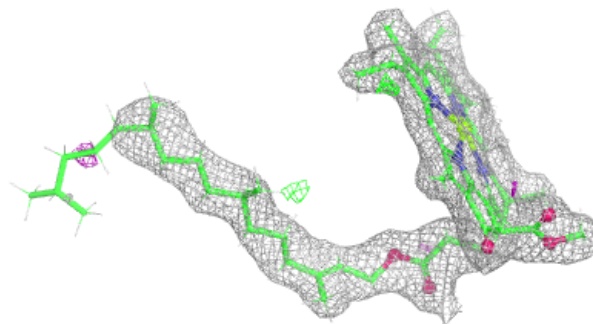
**Electron density around CLA c 510:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 508:**

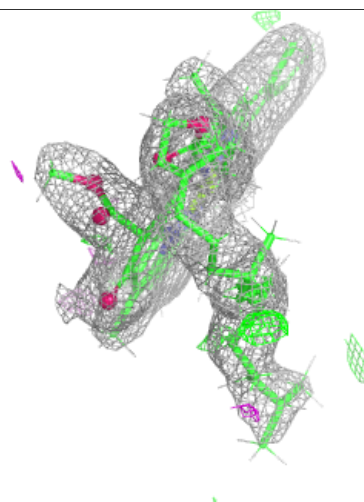
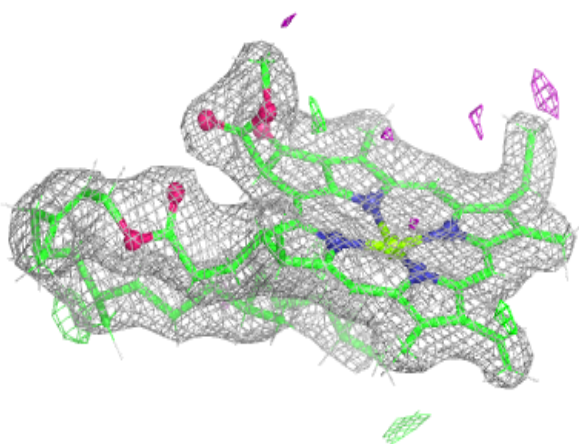
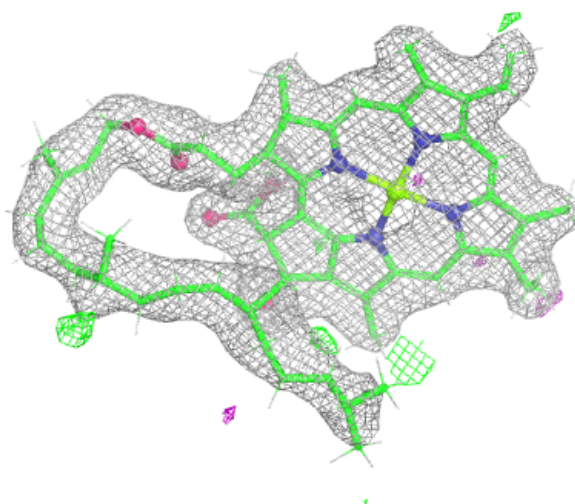
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





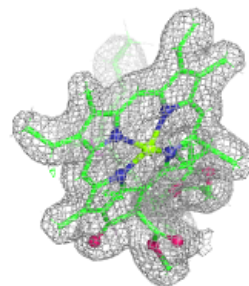
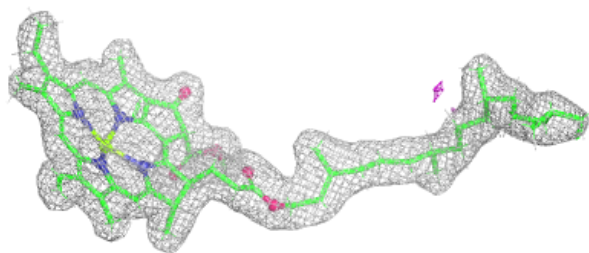
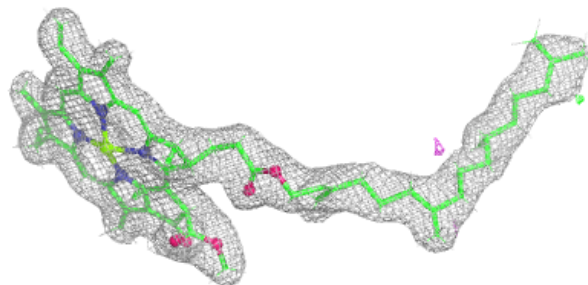
**Electron density around CLA C 509:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

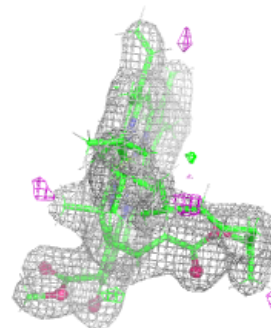
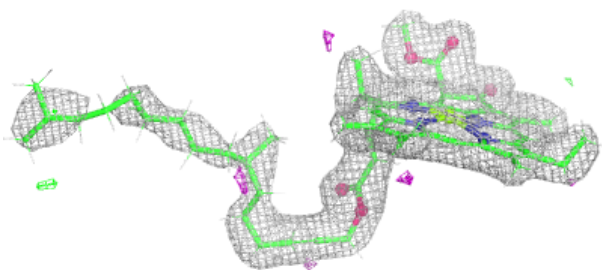
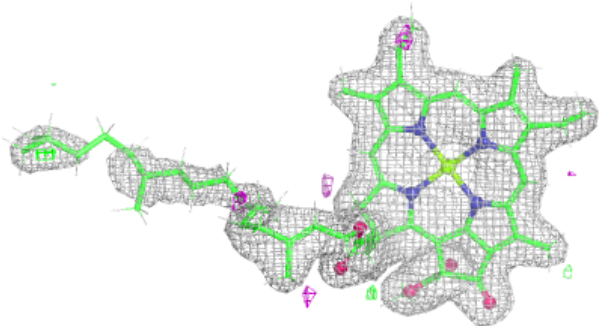


**Electron density around CLA A 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA d 401:**

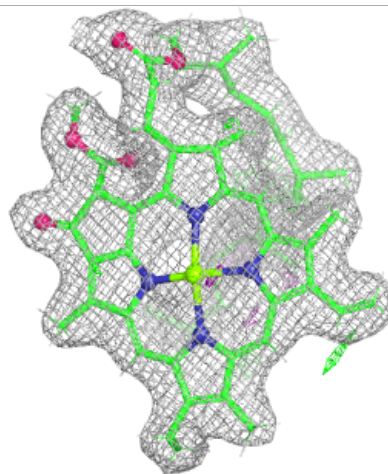
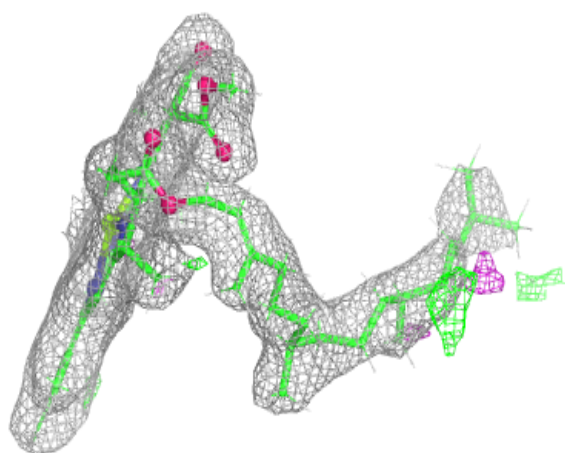
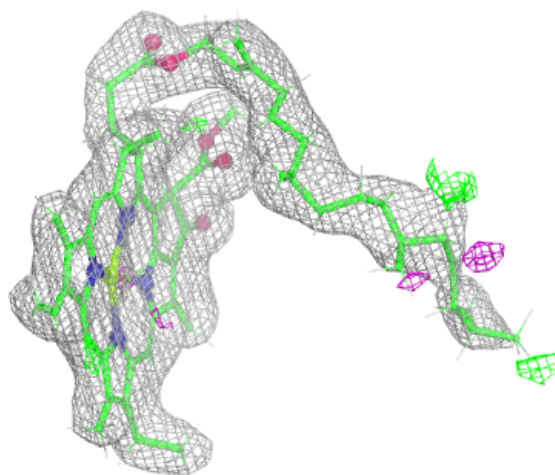
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





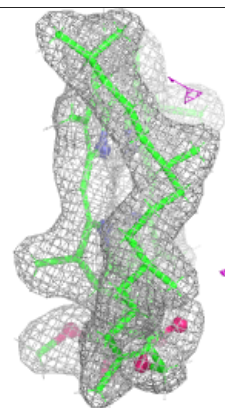
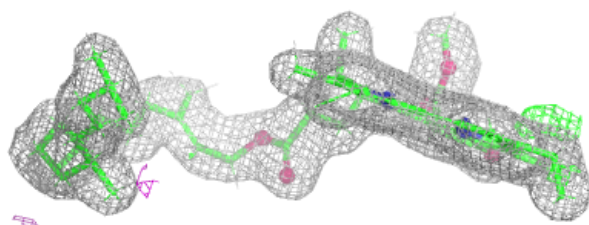
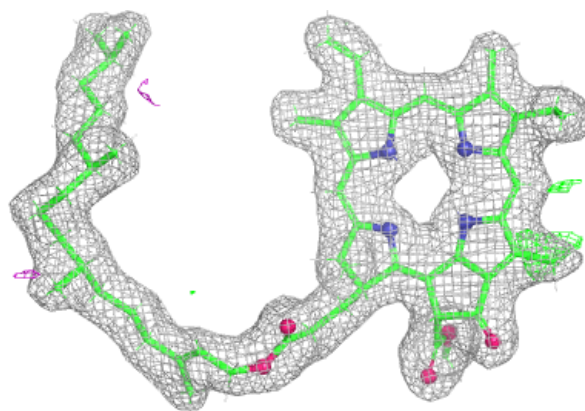
**Electron density around CLA B 613:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



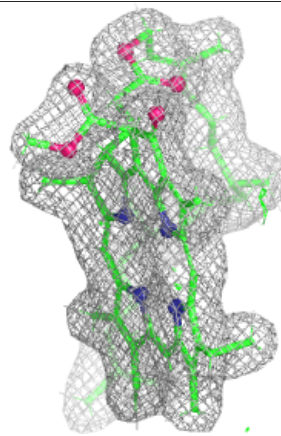
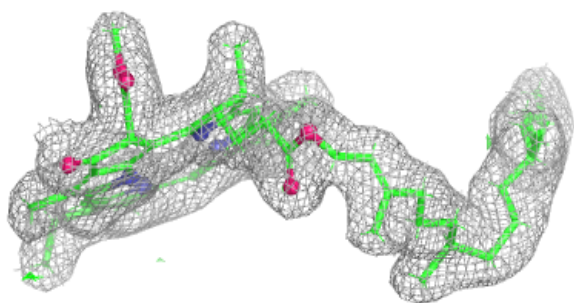
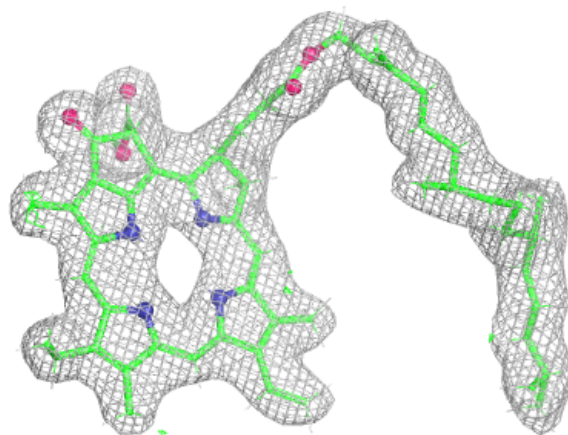
**Electron density around PHO A 606:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

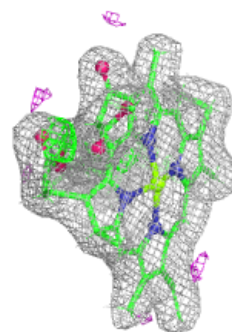
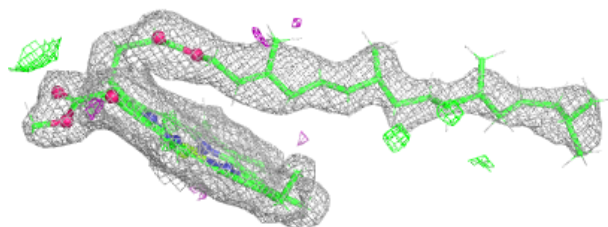
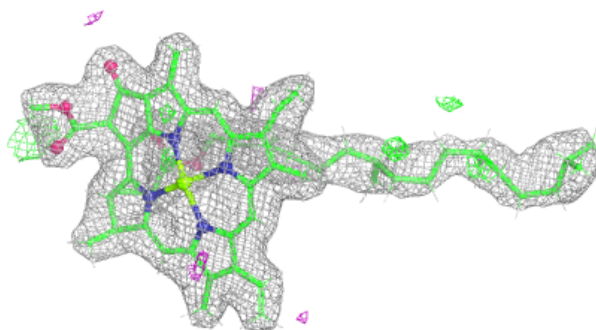


**Electron density around PHO A 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

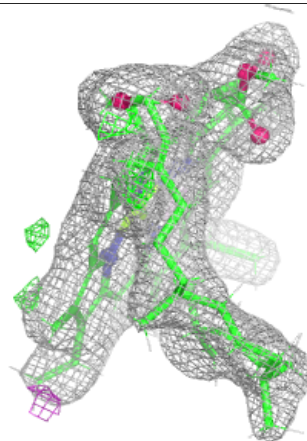
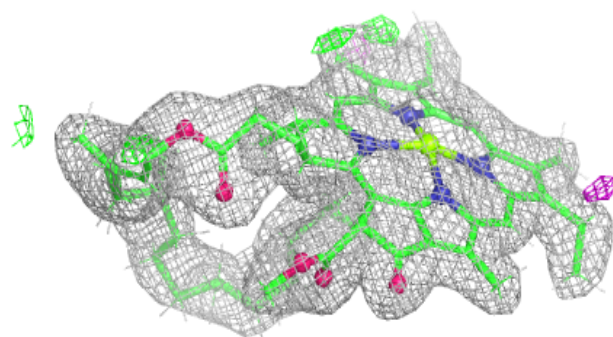
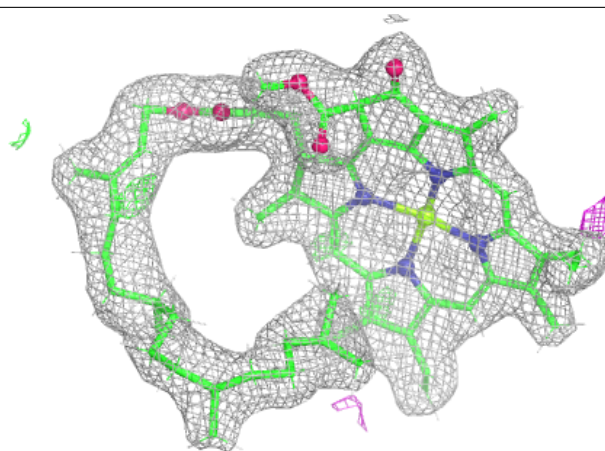
**Electron density around CLA B 614:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



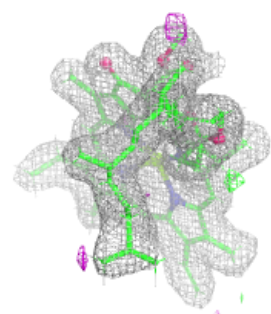
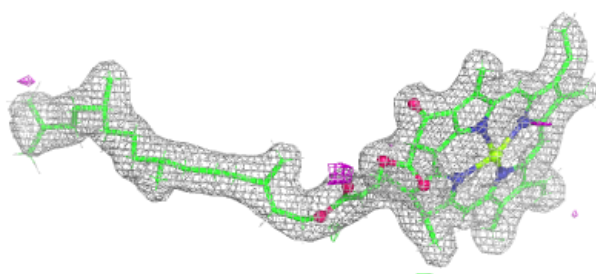
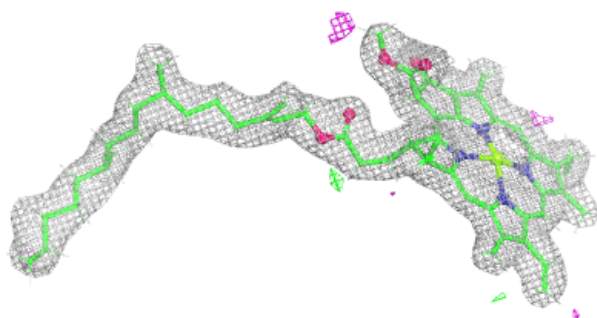
**Electron density around CLA B 615:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



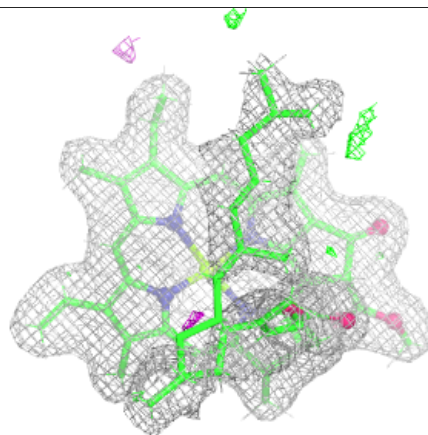
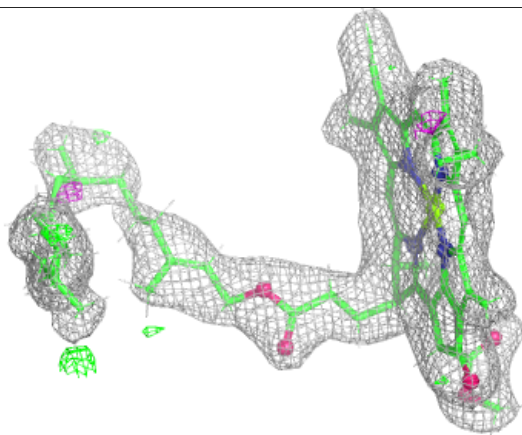
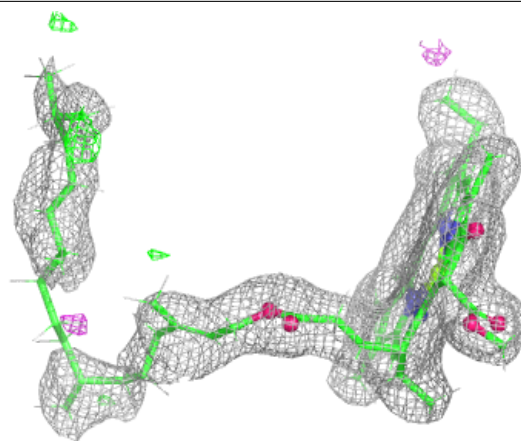
**Electron density around CLA a 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA a 606:**

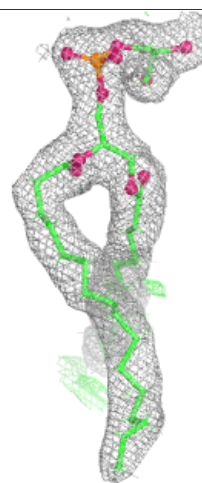
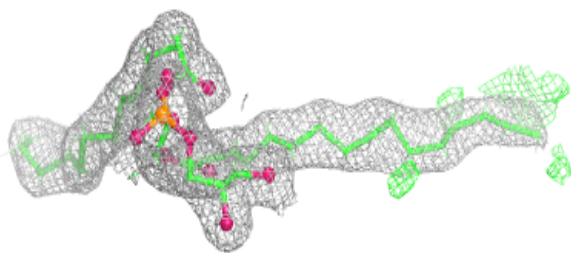
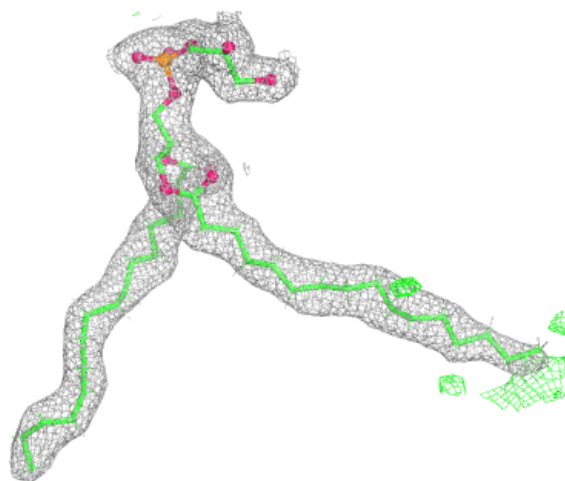
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





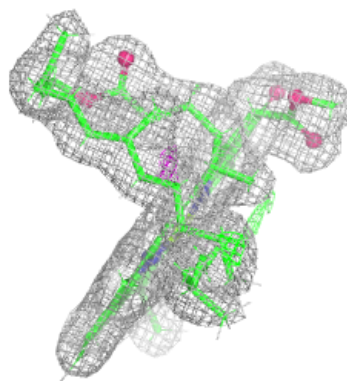
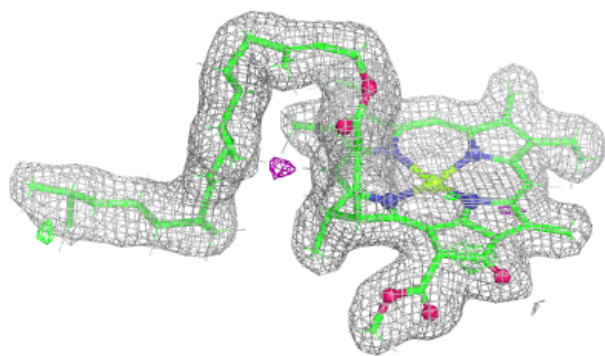
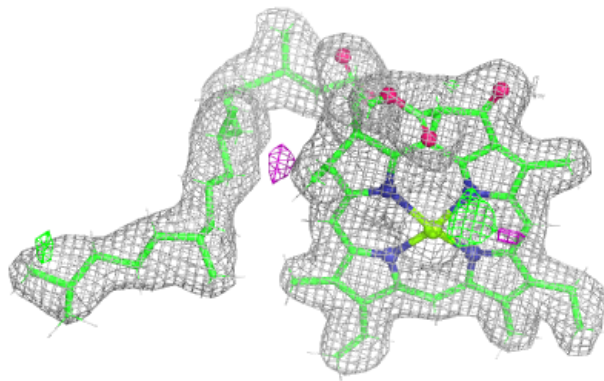
**Electron density around LHG B 621:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA a 612:**

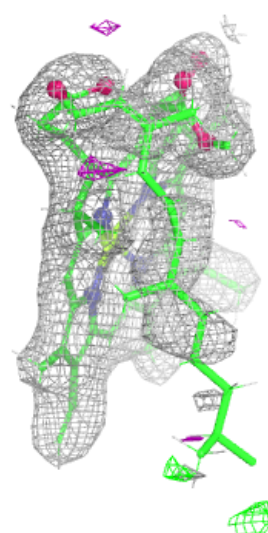
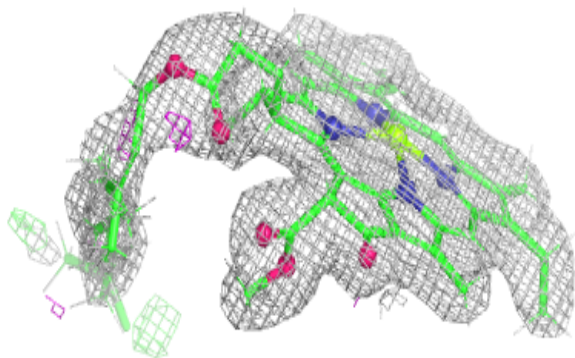
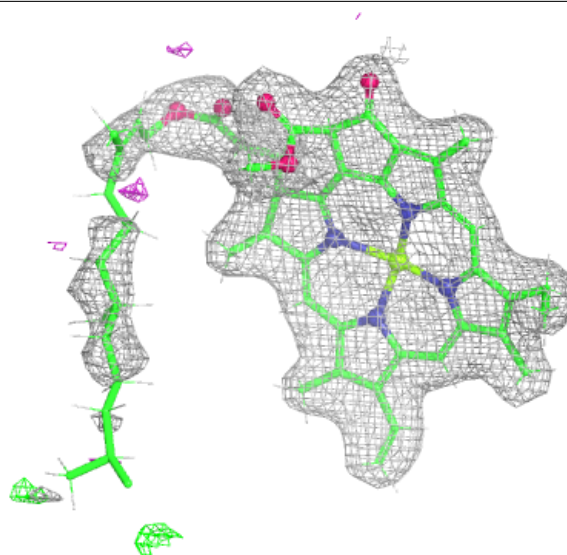
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





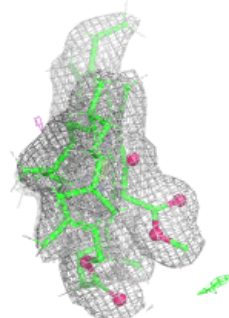
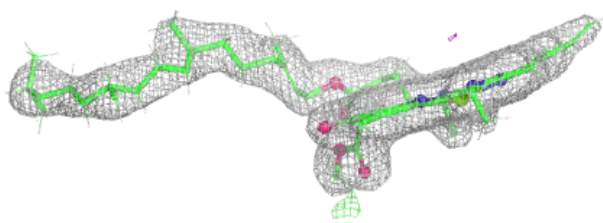
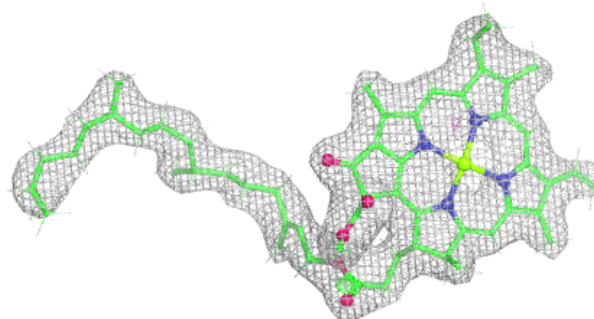
**Electron density around CLA B 616:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

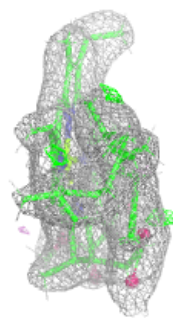
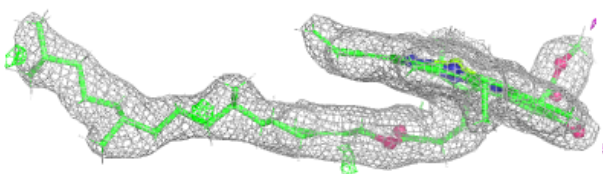
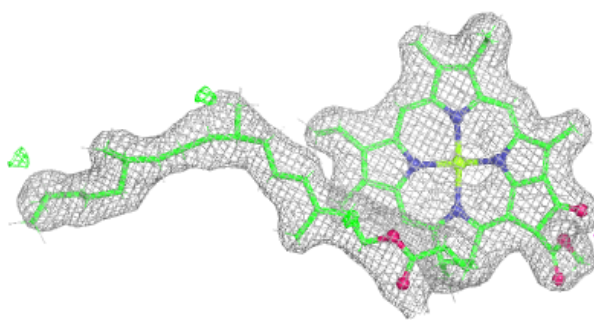


**Electron density around CLA b 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

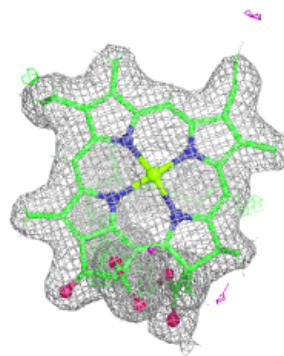
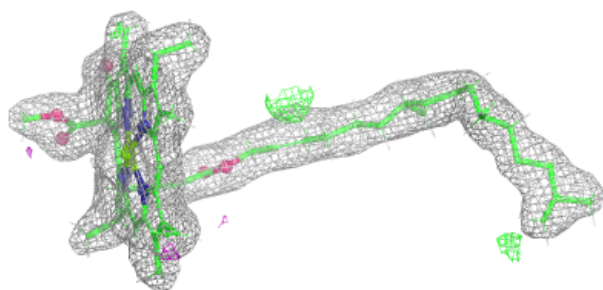
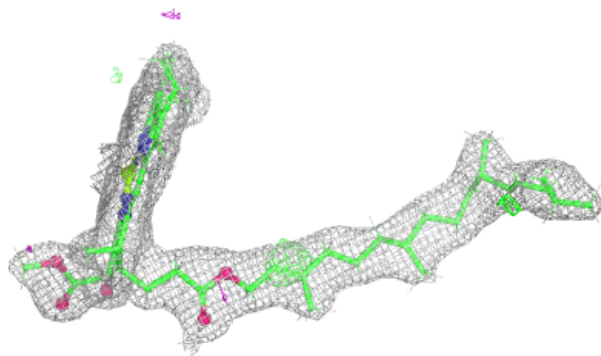
**Electron density around CLA b 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



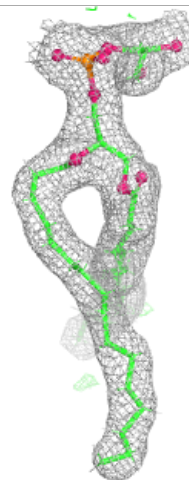
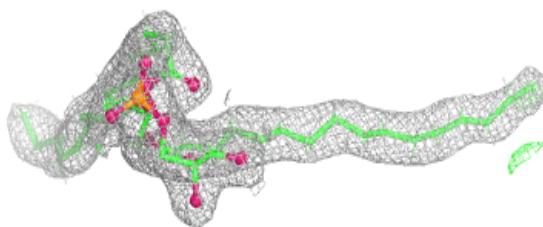
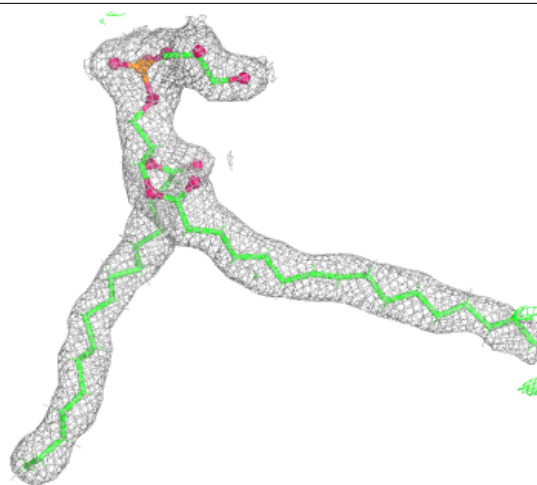
**Electron density around CLA b 605:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



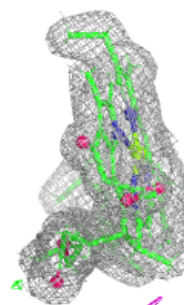
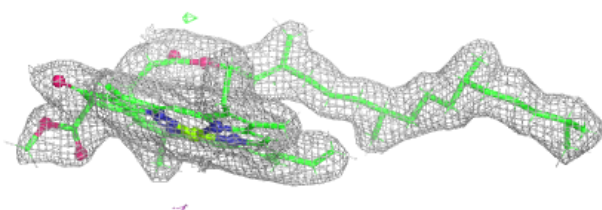
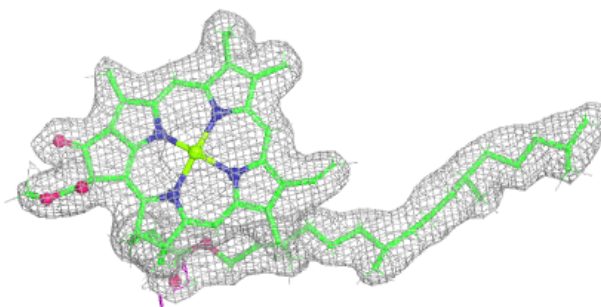
**Electron density around LHG 1 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

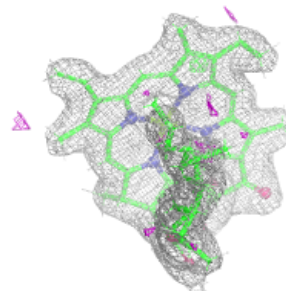
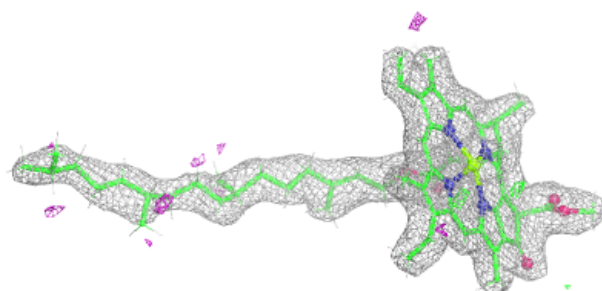
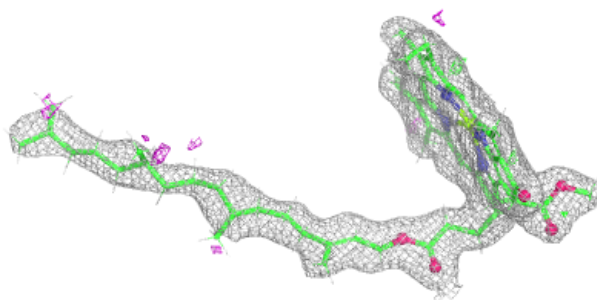


**Electron density around CLA C 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

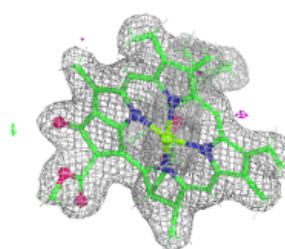
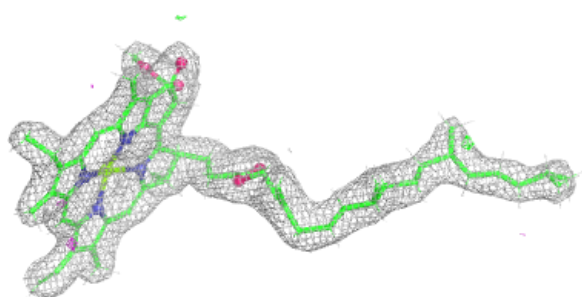
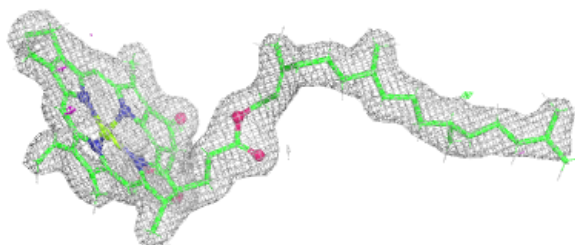
**Electron density around CLA b 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

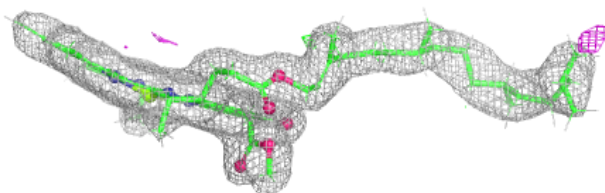
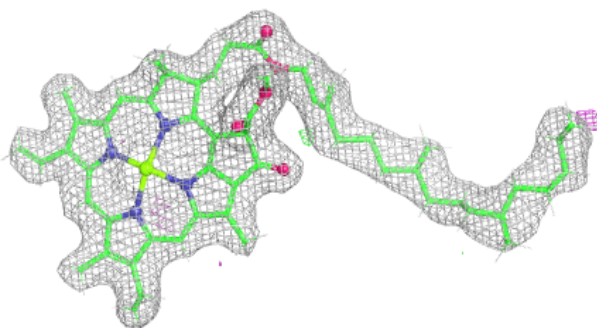


**Electron density around CLA C 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 602:**

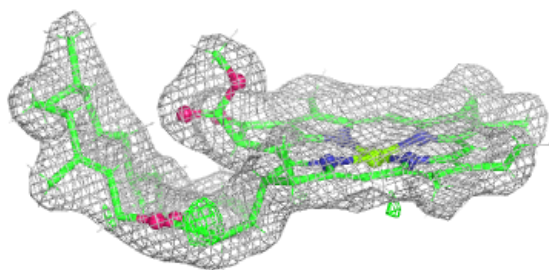
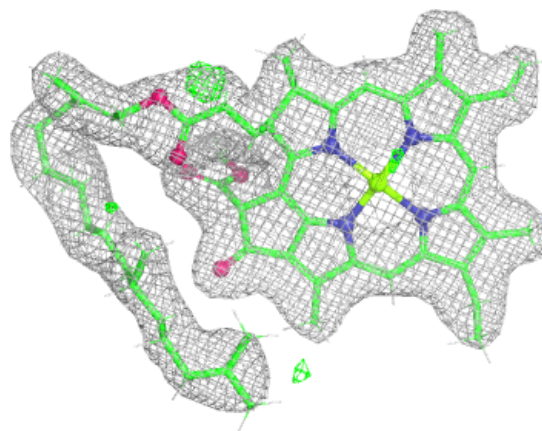
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





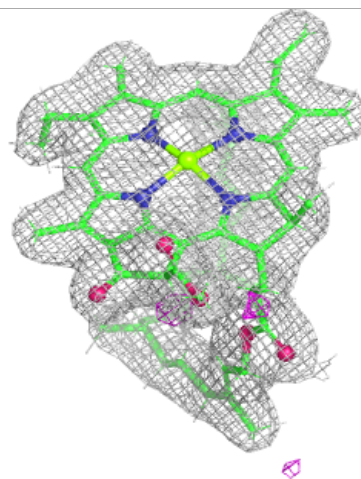
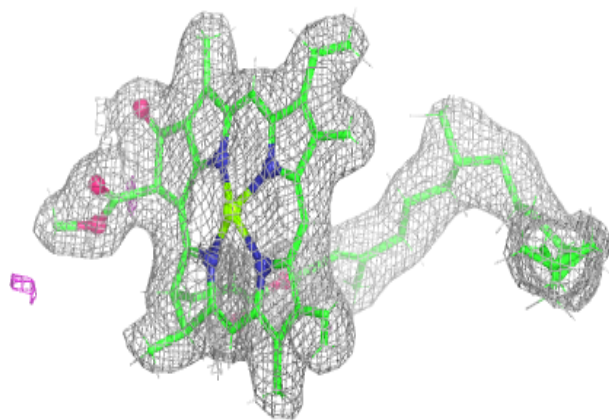
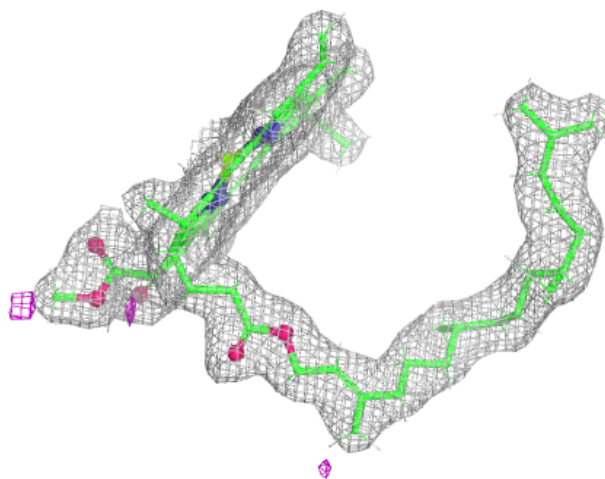
**Electron density around CLA b 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 611:**

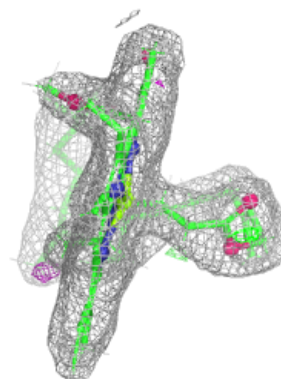
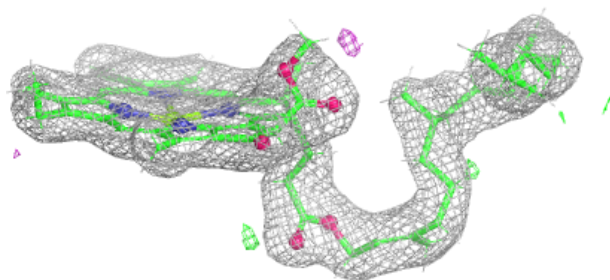
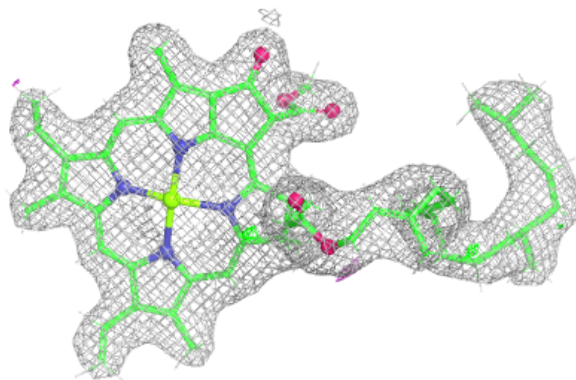
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





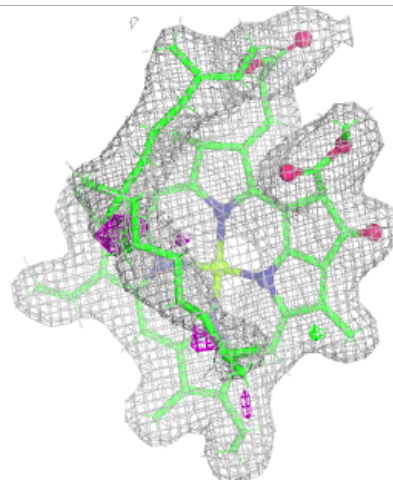
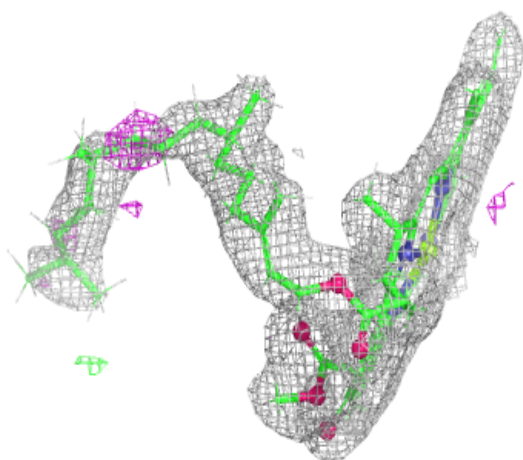
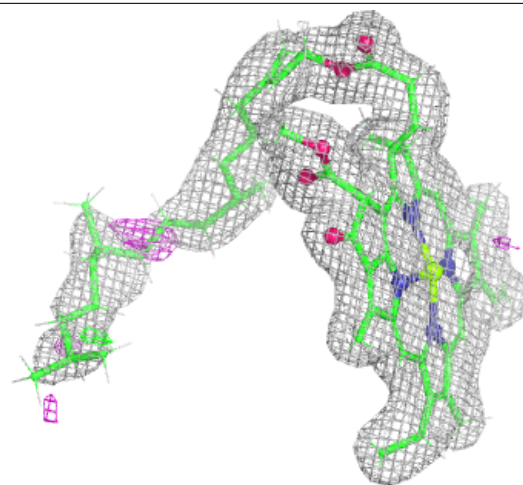
**Electron density around CLA b 612:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



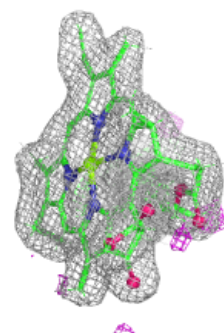
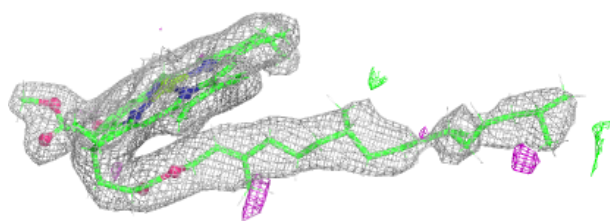
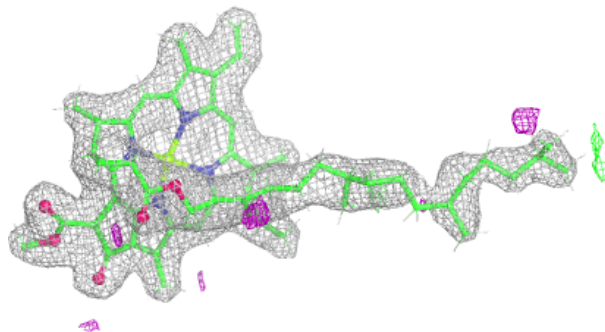
**Electron density around CLA b 613:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



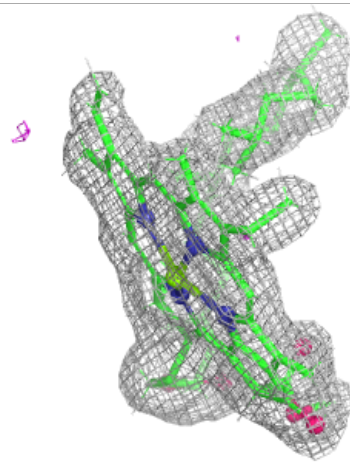
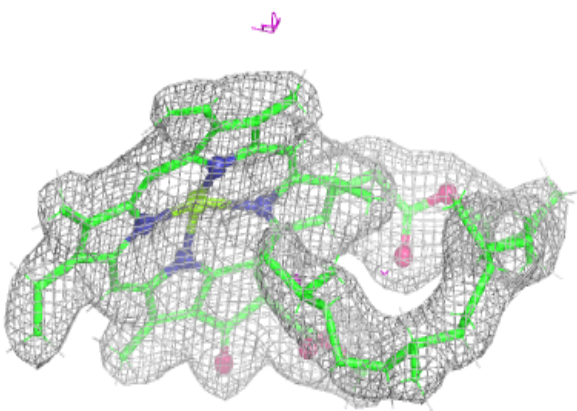
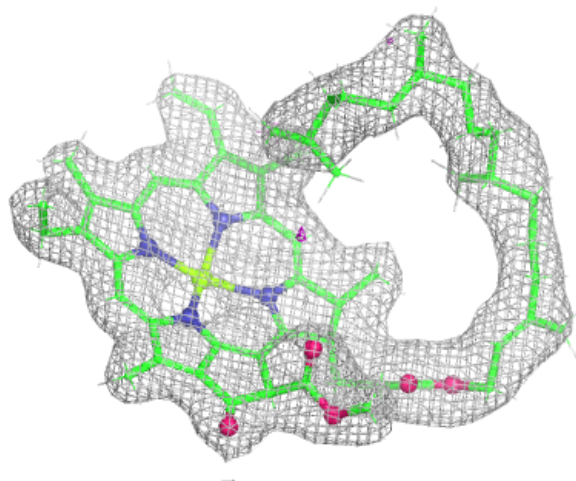
**Electron density around CLA b 614:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



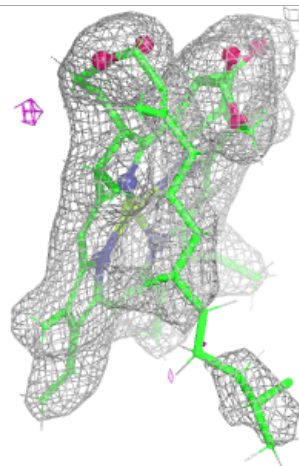
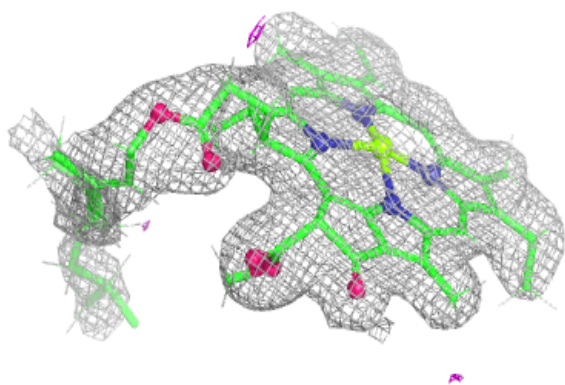
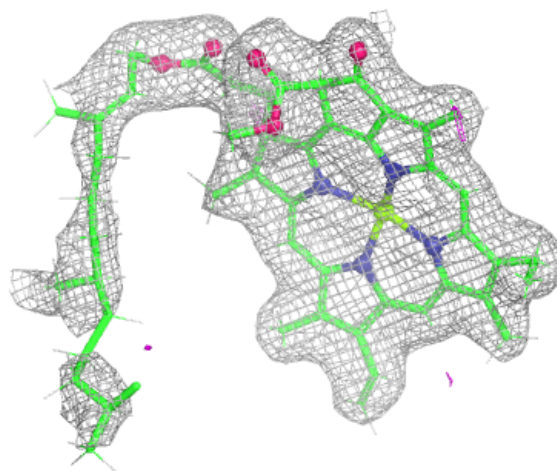
**Electron density around CLA b 615:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



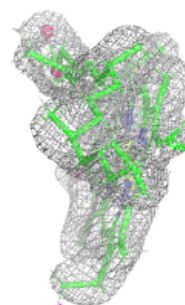
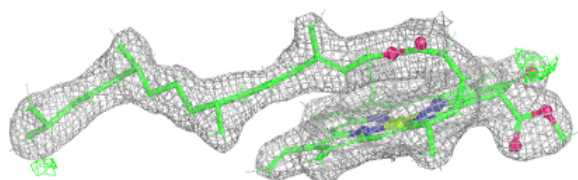
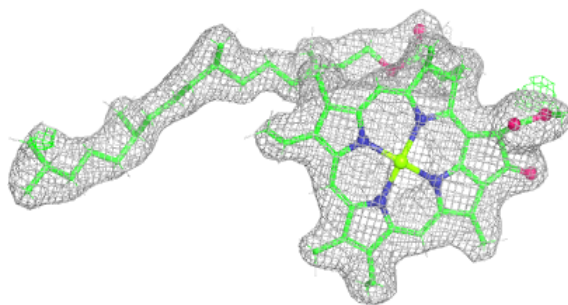
**Electron density around CLA b 616:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

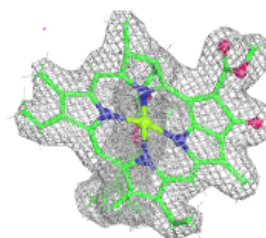
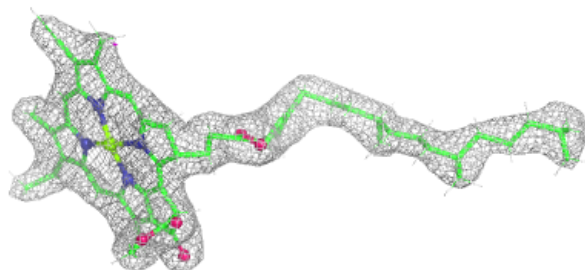
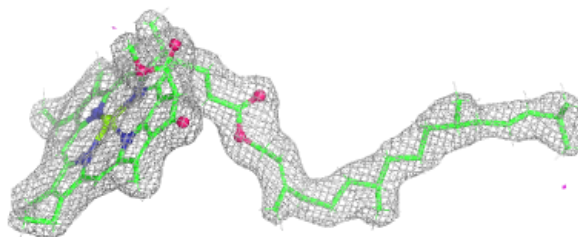


**Electron density around CLA c 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA c 502:**

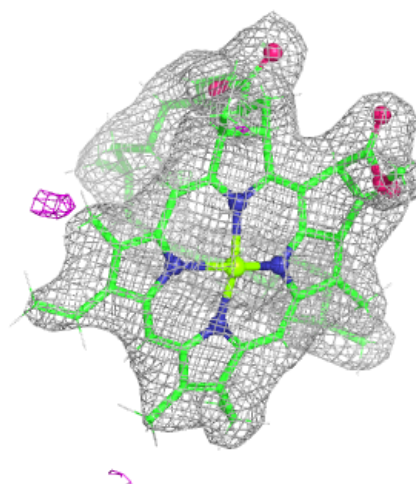
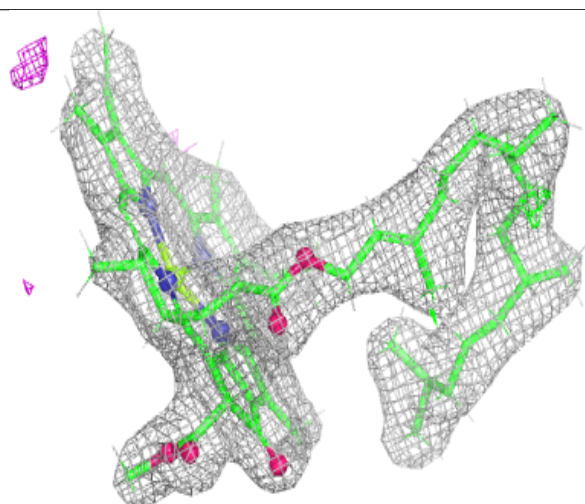
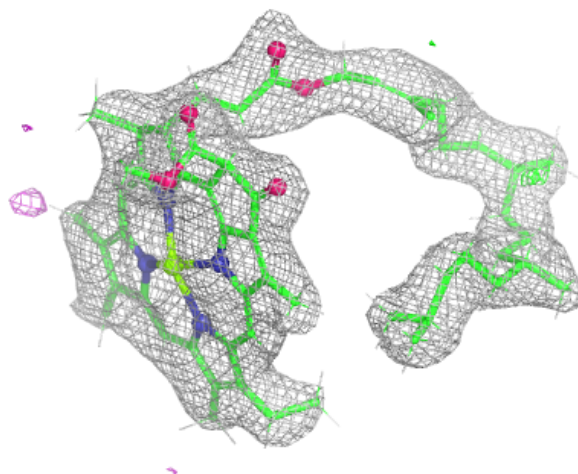
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





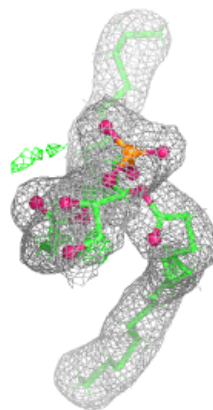
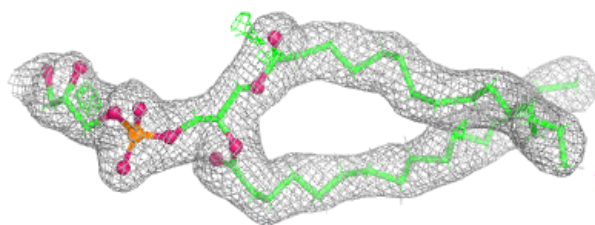
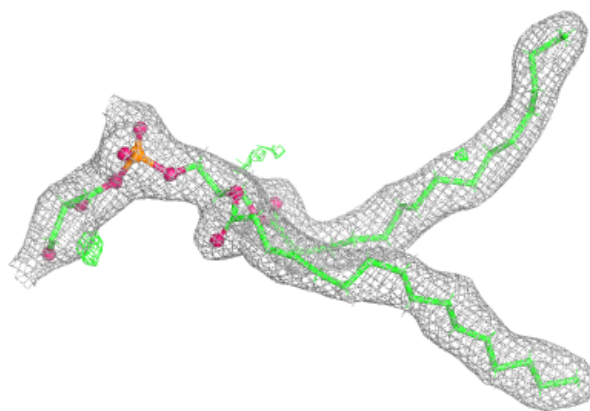
**Electron density around CLA c 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

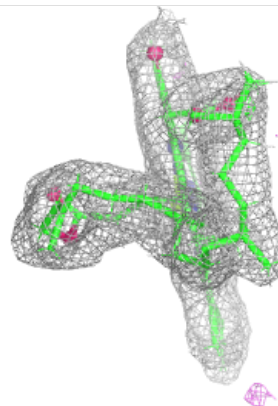
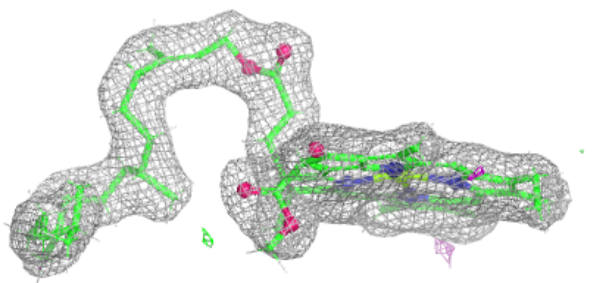
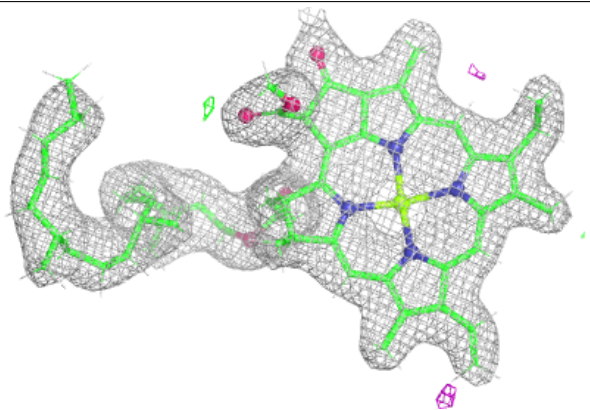


**Electron density around LHG D 408:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 612:**

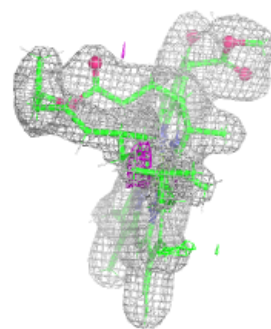
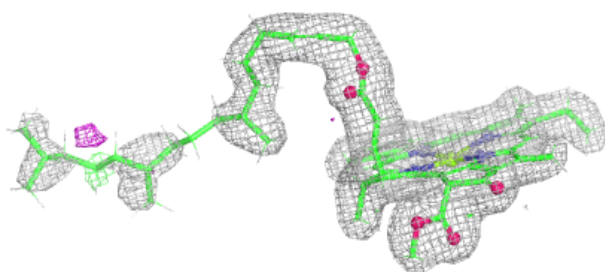
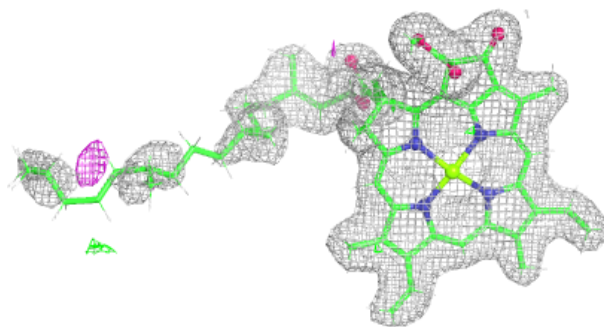
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



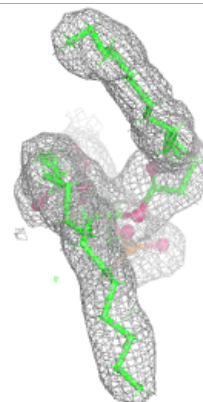
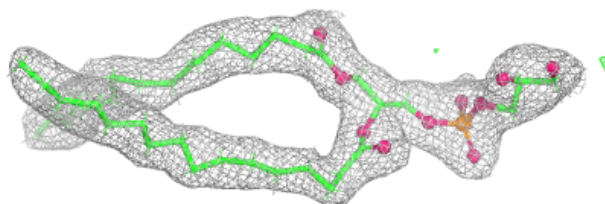
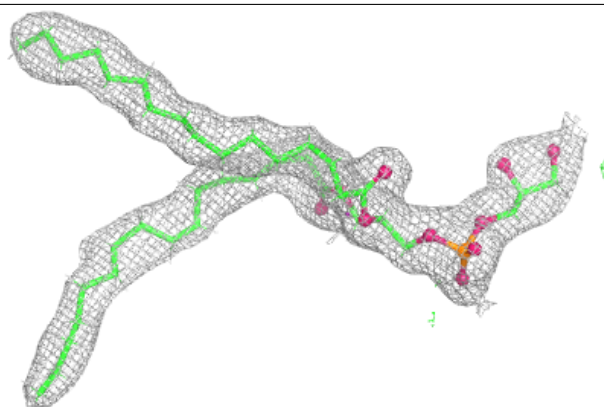


**Electron density around CLA A 605:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

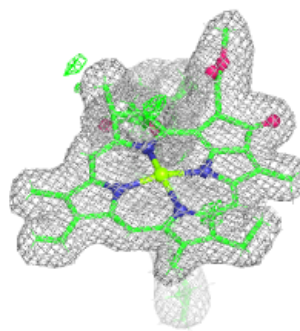
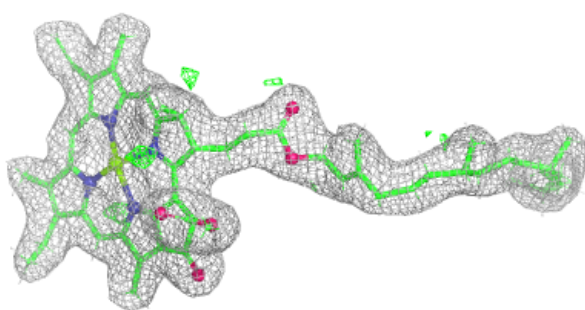
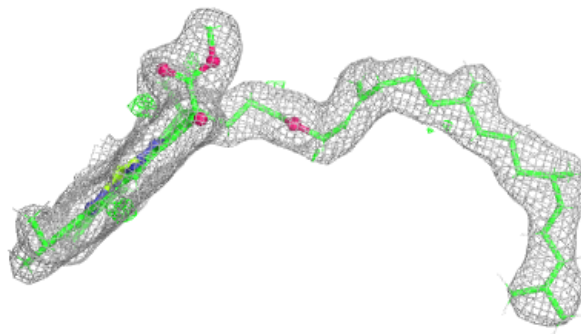
**Electron density around LHG d 408:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

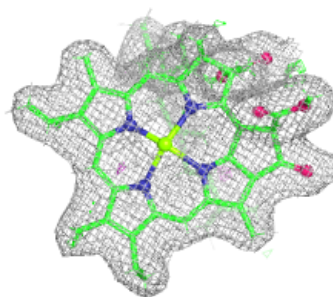
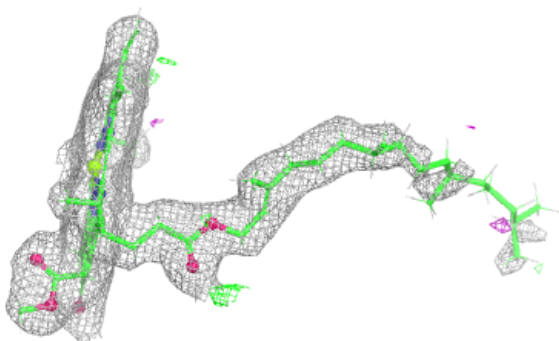
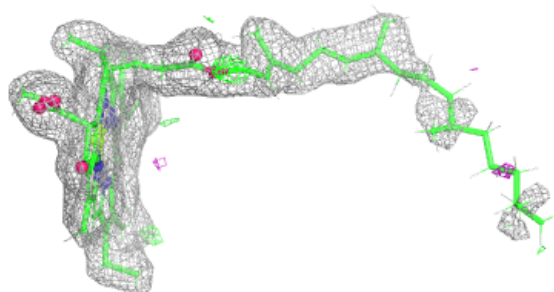


**Electron density around CLA D 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

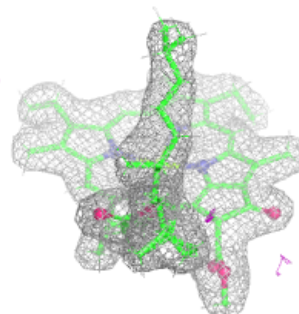
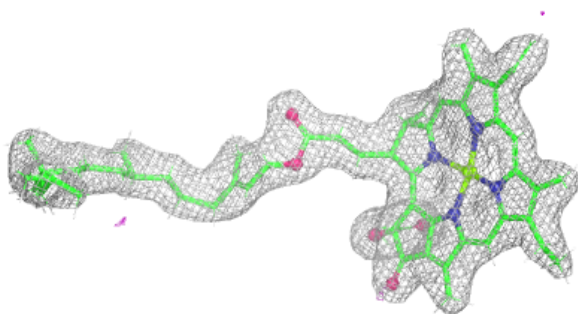
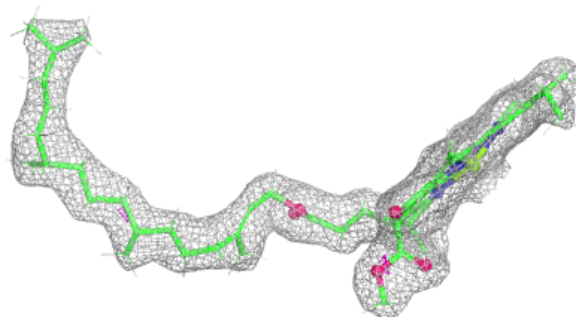
**Electron density around CLA D 403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

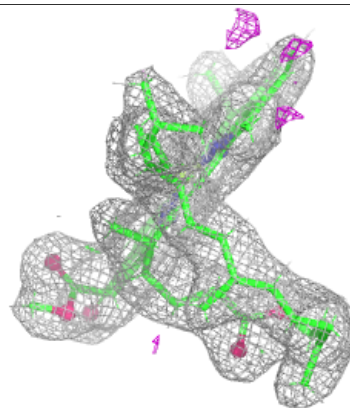
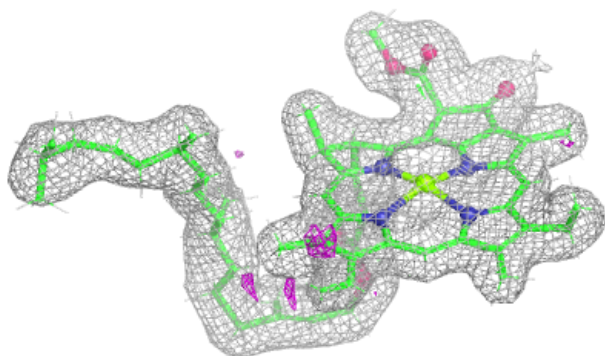
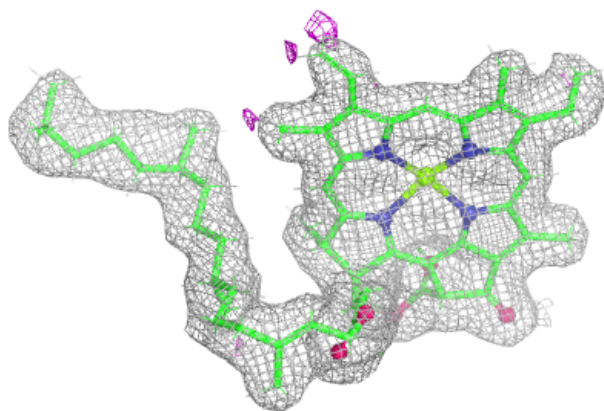


**Electron density around CLA d 403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

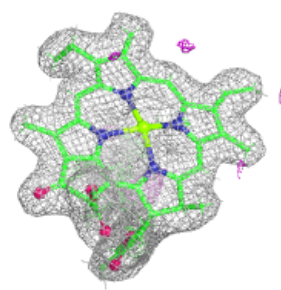
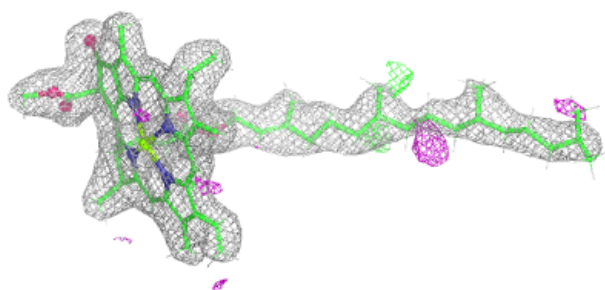
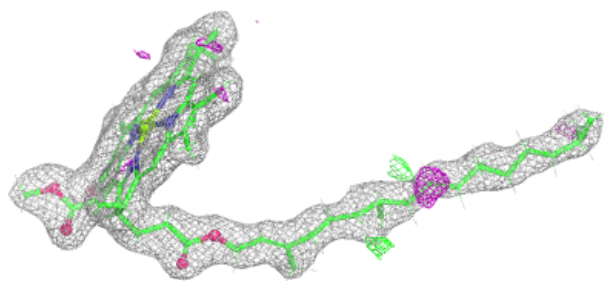
**Electron density around CLA A 613:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

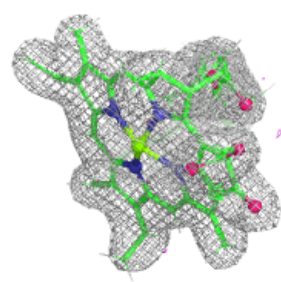
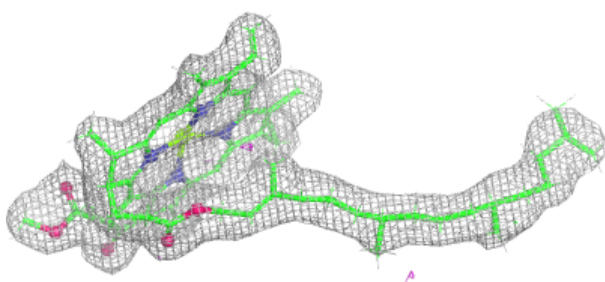
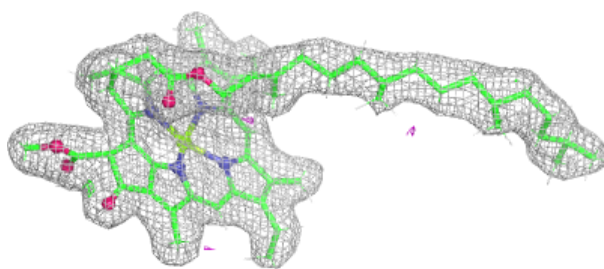


**Electron density around CLA B 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 608:**

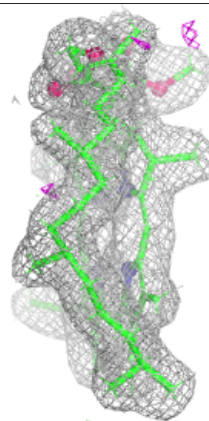
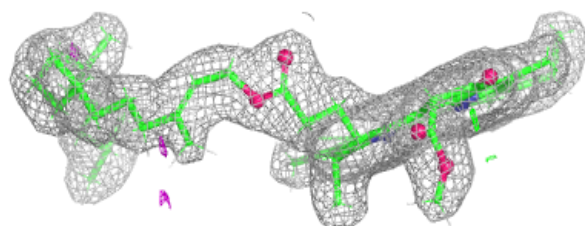
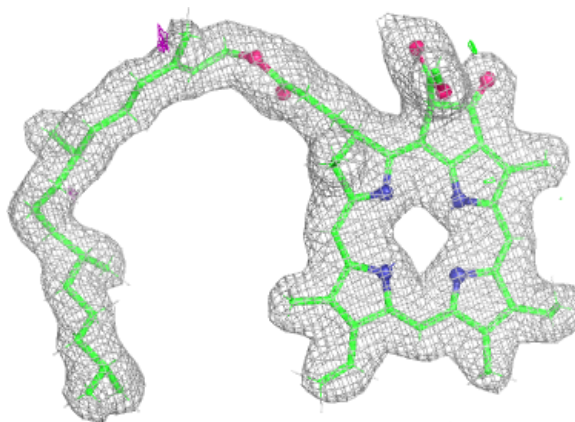
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



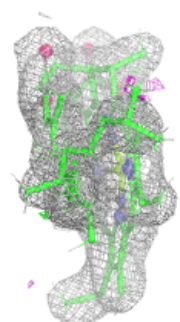
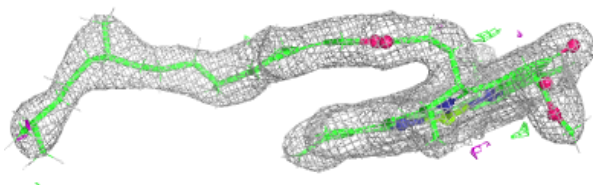
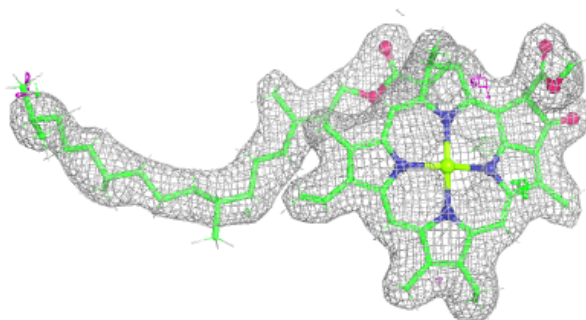


**Electron density around PHO a 605:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

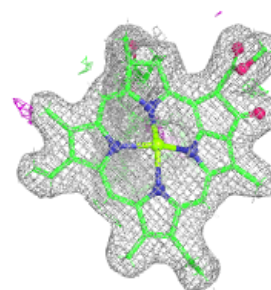
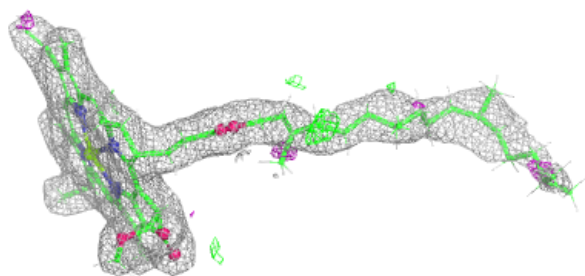
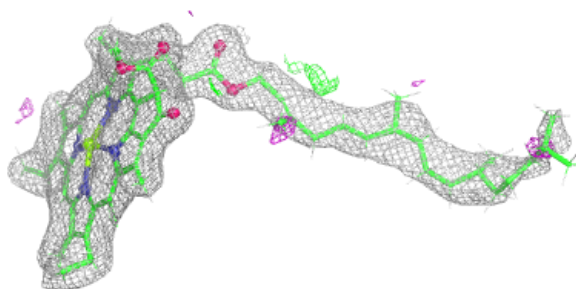
**Electron density around CLA B 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



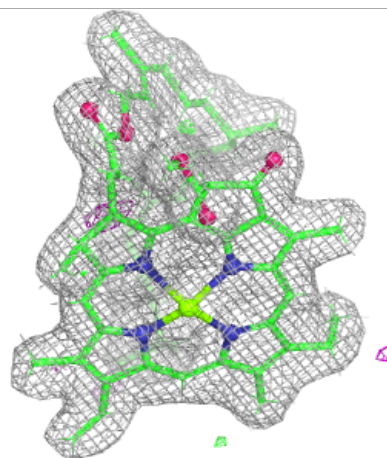
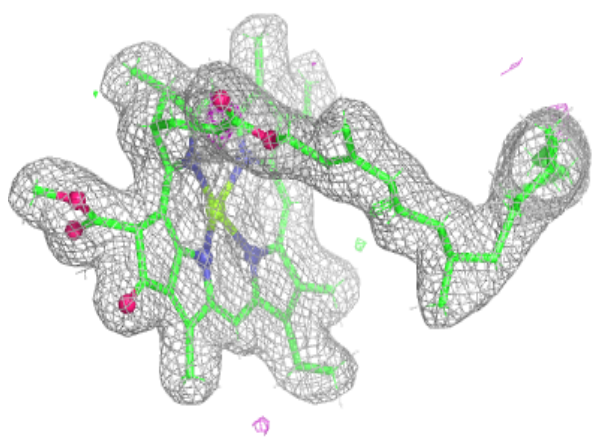
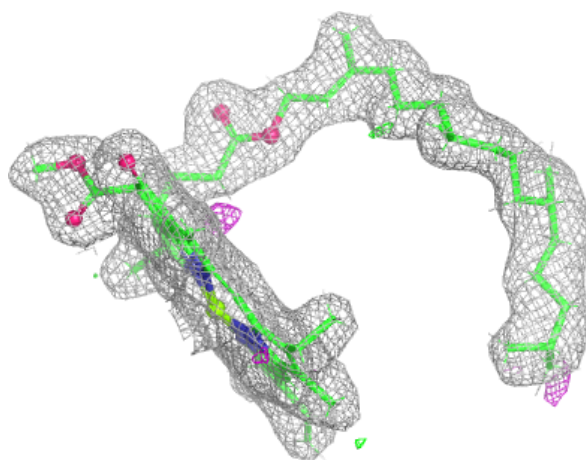
**Electron density around CLA B 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



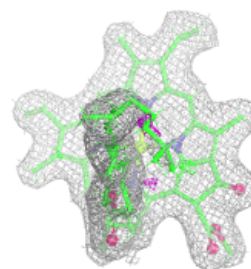
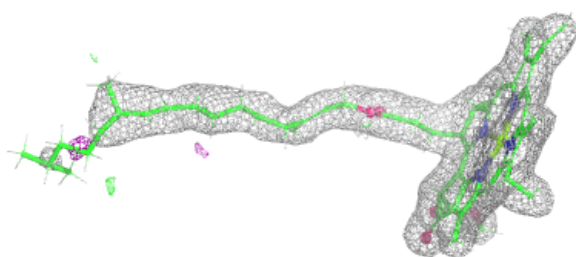
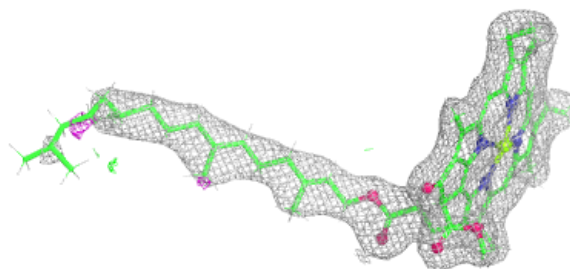
**Electron density around CLA B 611:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 604:**

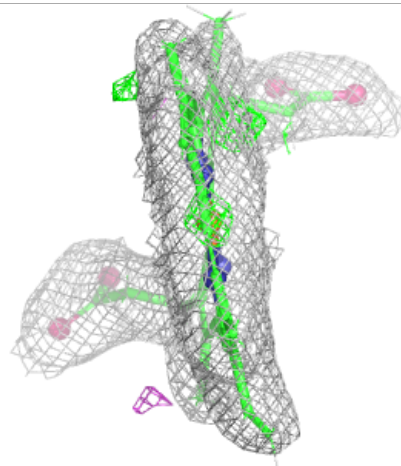
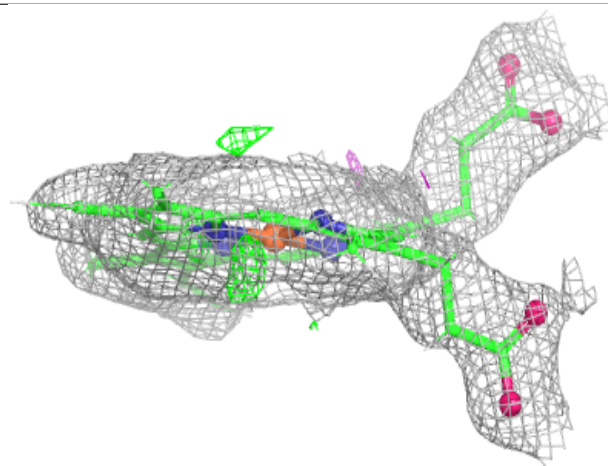
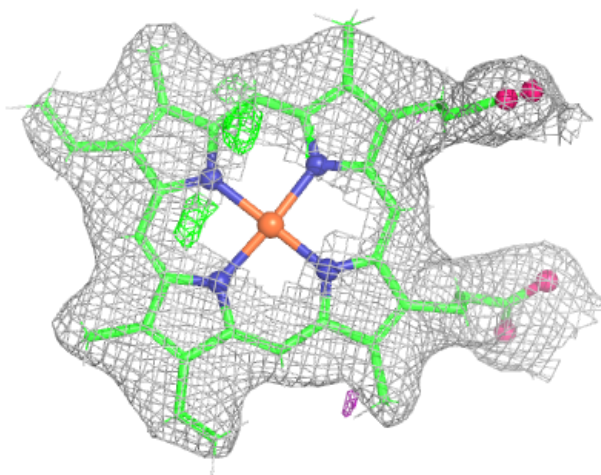
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





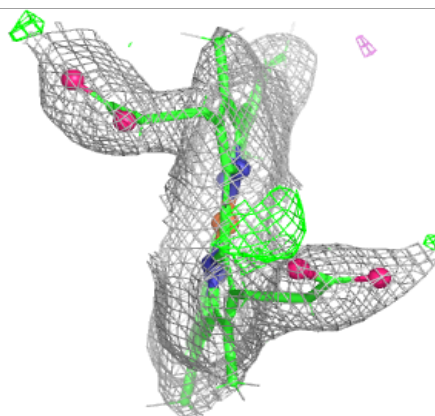
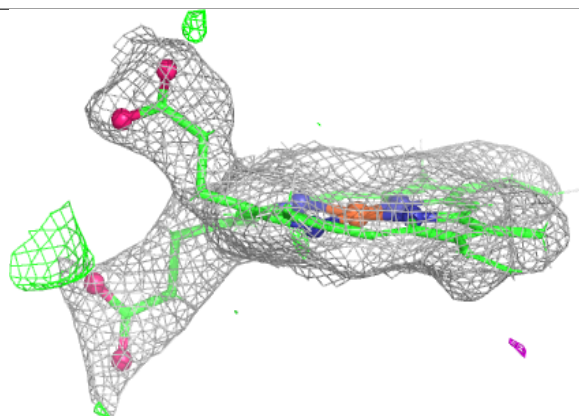
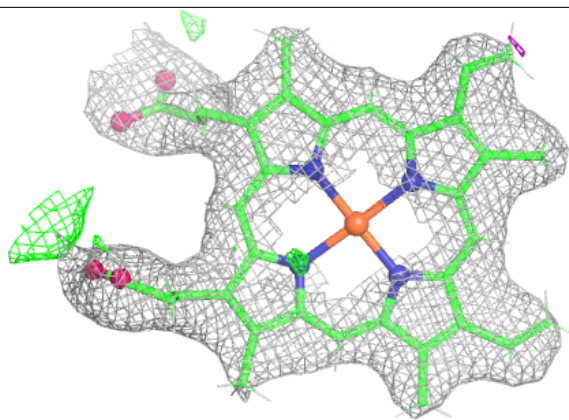
**Electron density around HEM F 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

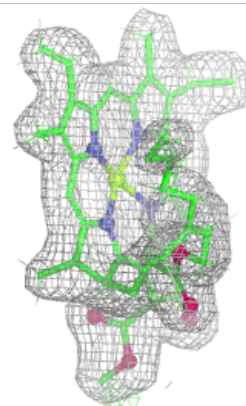
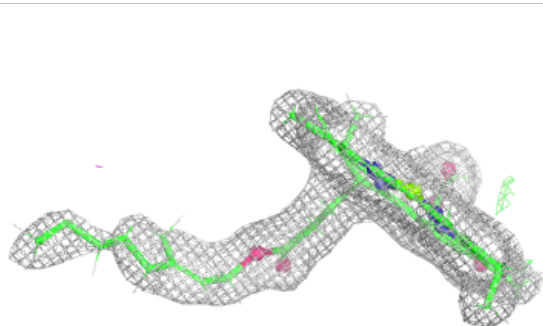
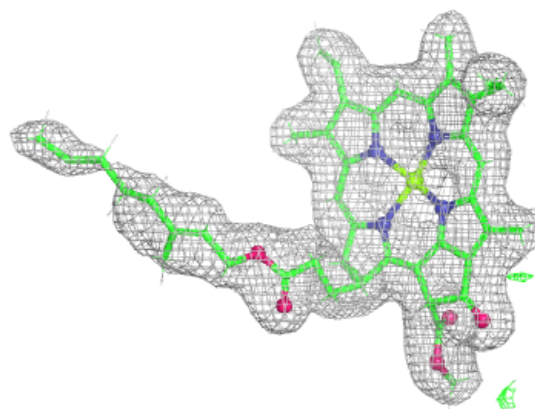


**Electron density around HEM e 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

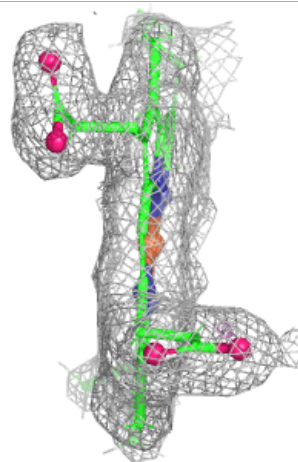
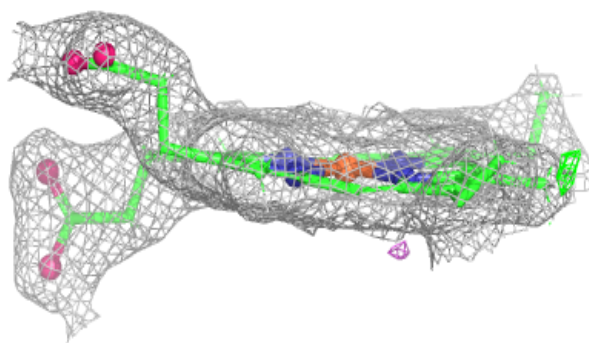
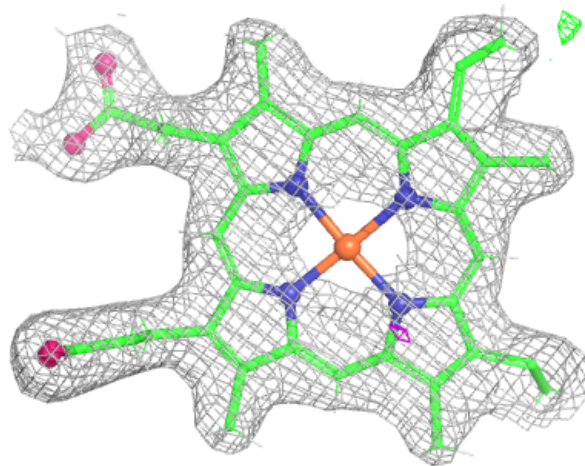
**Electron density around CLA A 608:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



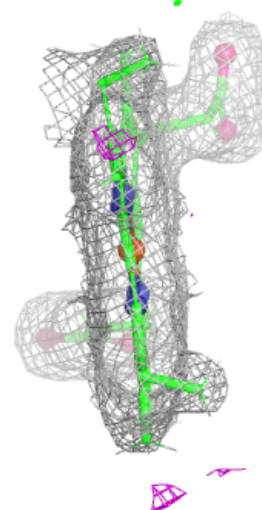
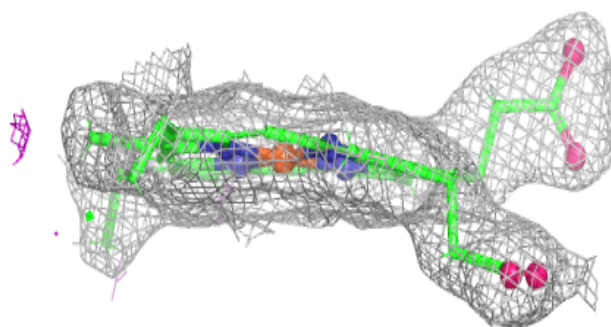
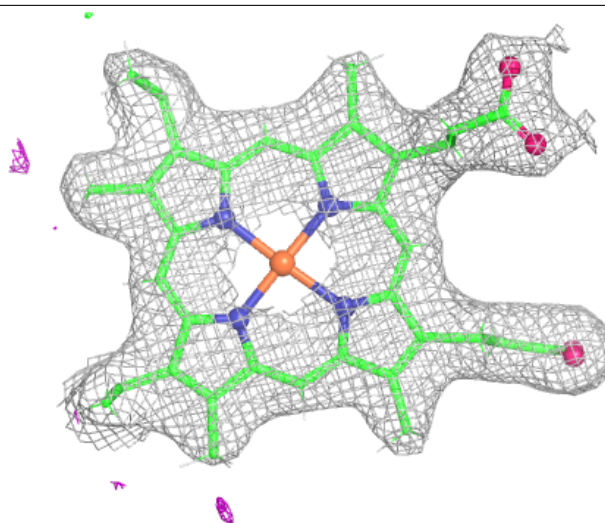
**Electron density around HEC V 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



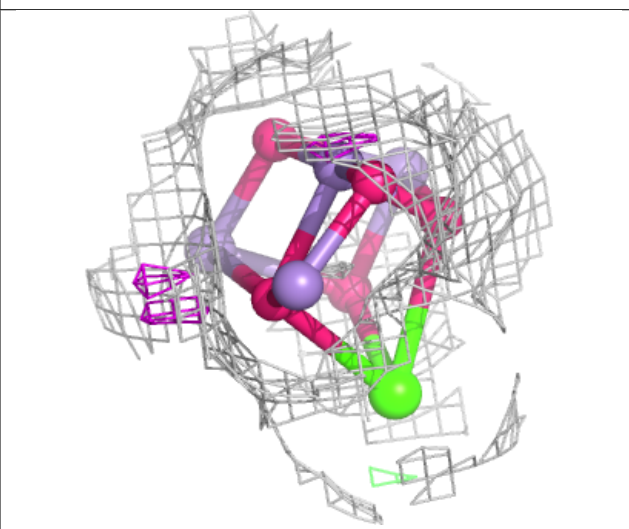
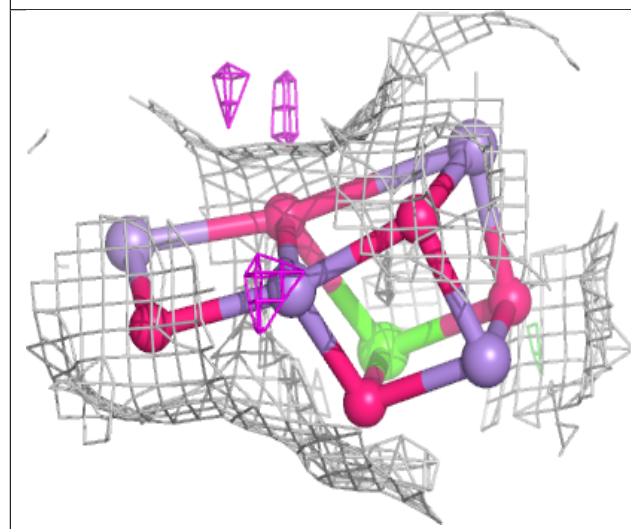
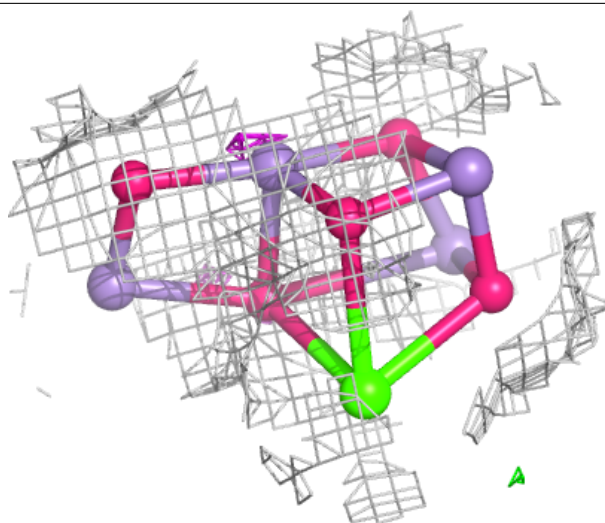
**Electron density around HEC v 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around OEX a 602 (A):**

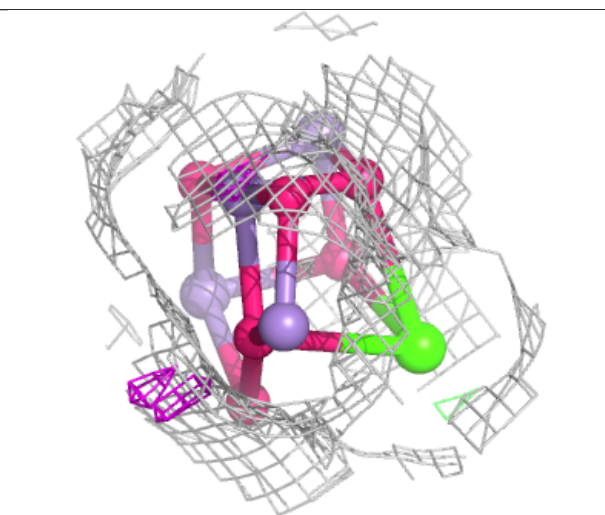
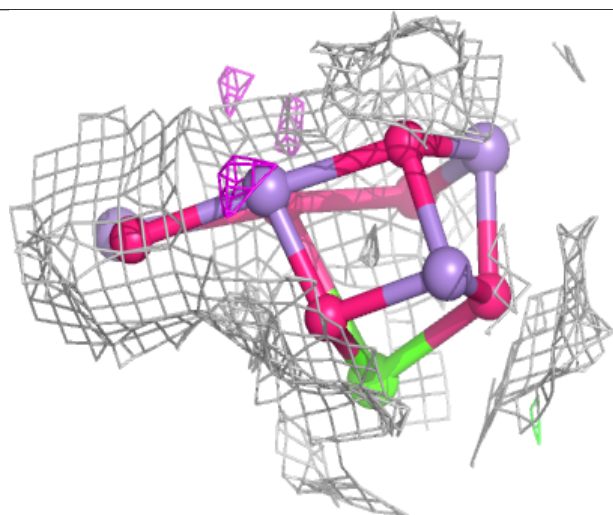
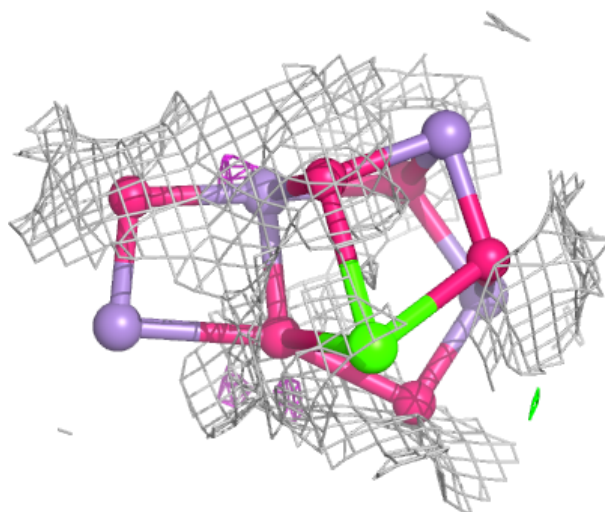
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





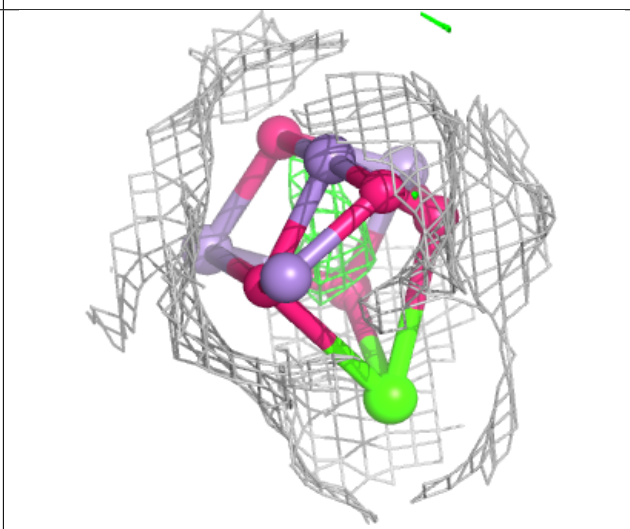
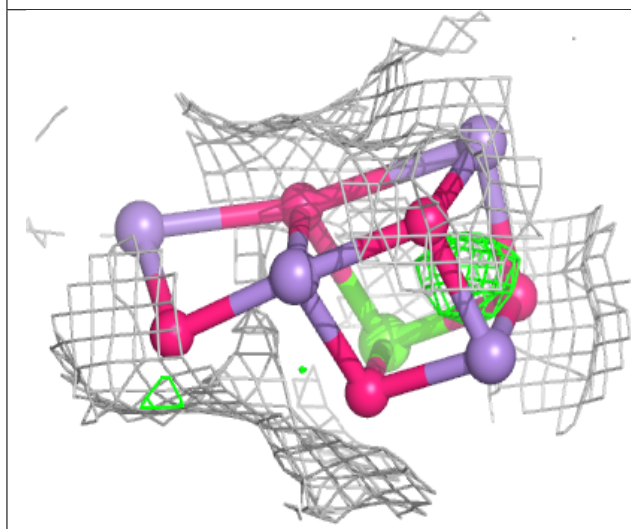
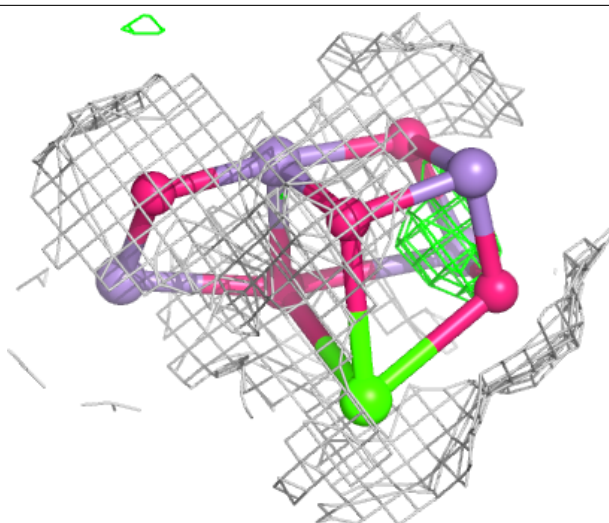
**Electron density around OEY a 601 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



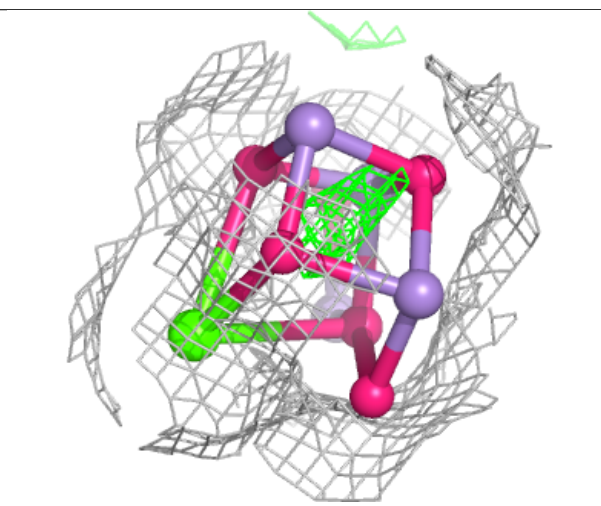
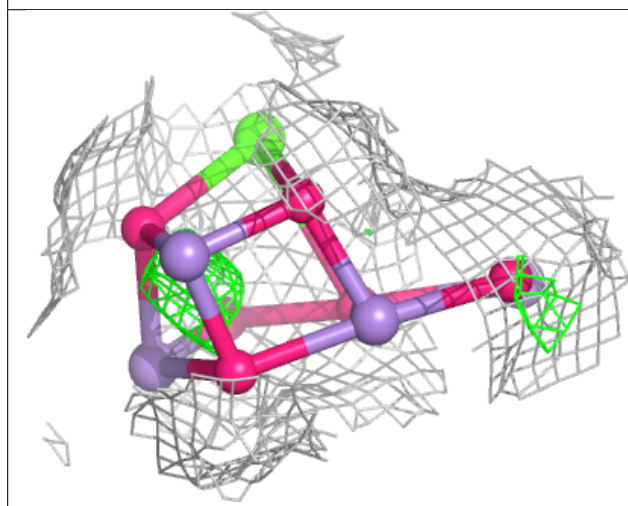
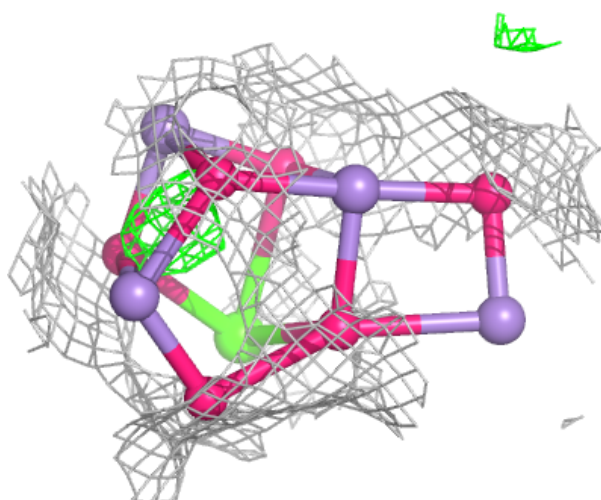
**Electron density around OEX A 602 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around OEY A 601 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.