



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 12:32 PM EST

PDB ID : 6DHG
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.5 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

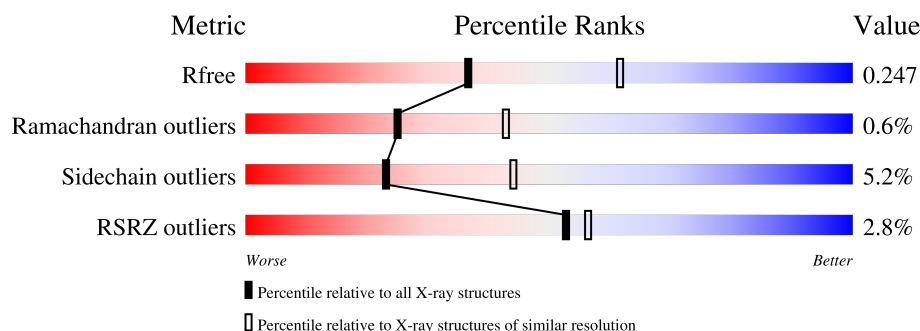
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 4661 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

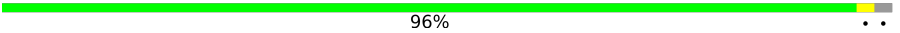
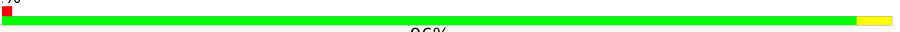
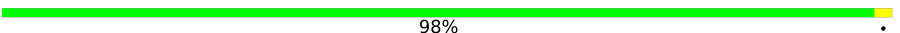




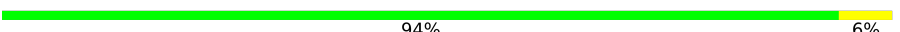





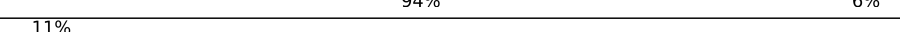



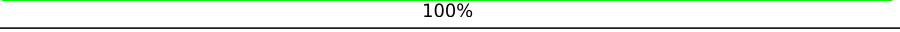







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 | 334 | <div> <div>%</div> <div>97%</div> <div>.</div> </div> |
| 1 | a | 334 | <div> <div>96%</div> <div>.</div> </div> |
| 2 | B | 505 | <div> <div>%</div> <div>96%</div> <div>.</div> </div> |
| 2 | b | 505 | <div> <div>2%</div> <div>97%</div> <div>.</div> </div> |

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.17.1

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | C | 451 |  96% |
| 3 | c | 451 |  96% |
| 4 | D | 341 |  98% |
| 4 | d | 341 |  98% |
| 5 | E | 82 |  88% 11% |
| 5 | e | 82 |  93% 7% |
| 6 | F | 34 |  100% |
| 6 | f | 34 |  94% 6% |
| 7 | H | 65 |  91% 9% |
| 7 | h | 65 |  91% 6% |
| 8 | I | 36 |  86% 14% |
| 8 | i | 36 |  94% 6% |
| 9 | J | 36 |  94% 6% |
| 9 | j | 36 |  94% 6% |
| 10 | K | 37 |  86% 14% |
| 10 | k | 37 |  89% 11% |
| 11 | L | 37 |  100% |
| 11 | l | 37 |  89% 5% |
| 12 | M | 33 |  88% 12% |
| 12 | m | 33 |  88% 9% |
| 13 | O | 244 |  90% 10% |
| 13 | o | 244 |  92% 7% |
| 14 | T | 30 |  87% 13% |
| 14 | t | 30 |  97% |
| 15 | U | 97 |  94% 6% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | u | 97 |  |
| 16 | V | 137 |  |
| 16 | v | 137 |  |
| 17 | Y | 30 |  |
| 17 | y | 30 |  |
| 18 | X | 38 |  |
| 18 | x | 38 |  |
| 19 | Z | 62 |  |
| 19 | z | 62 |  |
| 20 | R | 34 |  |
| 20 | r | 34 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CLA | A | 404 | X | - | - | - |
| 23 | CLA | A | 405 | X | - | - | - |
| 23 | CLA | A | 407 | X | - | - | - |
| 23 | CLA | B | 601 | X | - | - | - |
| 23 | CLA | B | 602 | X | - | - | - |
| 23 | CLA | B | 603 | X | - | - | - |
| 23 | CLA | B | 604 | X | - | - | - |
| 23 | CLA | B | 605 | X | - | - | - |
| 23 | CLA | B | 606 | X | - | - | - |
| 23 | CLA | B | 607 | X | - | - | - |
| 23 | CLA | B | 608 | X | - | - | - |
| 23 | CLA | B | 609 | X | - | - | - |
| 23 | CLA | B | 610 | X | - | - | - |
| 23 | CLA | B | 611 | X | - | - | - |
| 23 | CLA | B | 612 | X | - | - | - |
| 23 | CLA | B | 613 | X | - | - | - |
| 23 | CLA | B | 614 | X | - | - | - |
| 23 | CLA | B | 615 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CLA | B | 616 | X | - | - | - |
| 23 | CLA | C | 502 | X | - | - | - |
| 23 | CLA | C | 503 | X | - | - | - |
| 23 | CLA | C | 504 | X | - | - | - |
| 23 | CLA | C | 505 | X | - | - | - |
| 23 | CLA | C | 506 | X | - | - | - |
| 23 | CLA | C | 507 | X | - | - | - |
| 23 | CLA | C | 508 | X | - | - | - |
| 23 | CLA | C | 509 | X | - | - | - |
| 23 | CLA | C | 510 | X | - | - | - |
| 23 | CLA | C | 511 | X | - | - | - |
| 23 | CLA | C | 512 | X | - | - | - |
| 23 | CLA | C | 513 | X | - | - | - |
| 23 | CLA | C | 514 | X | - | - | - |
| 23 | CLA | D | 402 | X | - | - | - |
| 23 | CLA | D | 403 | X | - | - | - |
| 23 | CLA | D | 404 | X | - | - | - |
| 23 | CLA | a | 405 | X | - | - | - |
| 23 | CLA | a | 406 | X | - | - | - |
| 23 | CLA | a | 408 | X | - | - | - |
| 23 | CLA | b | 602 | X | - | - | - |
| 23 | CLA | b | 603 | X | - | - | - |
| 23 | CLA | b | 604 | X | - | - | - |
| 23 | CLA | b | 605 | X | - | - | - |
| 23 | CLA | b | 606 | X | - | - | - |
| 23 | CLA | b | 607 | X | - | - | - |
| 23 | CLA | b | 608 | X | - | - | - |
| 23 | CLA | b | 609 | X | - | - | - |
| 23 | CLA | b | 610 | X | - | - | - |
| 23 | CLA | b | 611 | X | - | - | - |
| 23 | CLA | b | 612 | X | - | - | - |
| 23 | CLA | b | 613 | X | - | - | - |
| 23 | CLA | b | 614 | X | - | - | - |
| 23 | CLA | b | 615 | X | - | - | - |
| 23 | CLA | b | 616 | X | - | - | - |
| 23 | CLA | b | 617 | X | - | - | - |
| 23 | CLA | c | 501 | X | - | - | - |
| 23 | CLA | c | 502 | X | - | - | - |
| 23 | CLA | c | 503 | X | - | - | - |
| 23 | CLA | c | 504 | X | - | - | - |
| 23 | CLA | c | 505 | X | - | - | - |
| 23 | CLA | c | 506 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CLA | c | 507 | X | - | - | - |
| 23 | CLA | c | 508 | X | - | - | - |
| 23 | CLA | c | 509 | X | - | - | - |
| 23 | CLA | c | 510 | X | - | - | - |
| 23 | CLA | c | 511 | X | - | - | - |
| 23 | CLA | c | 512 | X | - | - | - |
| 23 | CLA | c | 513 | X | - | - | - |
| 23 | CLA | d | 402 | X | - | - | - |
| 23 | CLA | d | 403 | X | - | - | - |
| 23 | CLA | d | 404 | X | - | - | - |

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103658 atoms, of which 51467 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 | 0 | 0 |
| | | | 5130 | 1717 | 2508 | 431 | 459 | 15 | | | |
| 1 | a | 334 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5118 | 1714 | 2499 | 431 | 459 | 15 | | | |

- 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 |
| | | | 7849 | 2631 | 3845 | 666 | 694 | 13 | | | |
| 2 | b | 505 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 7789 | 2610 | 3811 | 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 | 0 | 0 |
| | | | 6752 | 2244 | 3335 | 570 | 590 | 13 | | | |
| 3 | c | 451 | Total | C | H | N | O | S | 0 | 1 | 0 |
| | | | 6901 | 2286 | 3407 | 587 | 608 | 13 | | | |

- 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 | 0 | 0 |
| | | | 5330 | 1800 | 2613 | 444 | 461 | 12 | | | |
| 4 | d | 341 | Total | C | H | N | O | S | 0 | 1 | 0 |
| | | | 5342 | 1804 | 2619 | 444 | 463 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 5 | E | 81 | Total | C | H | N | O | 0 | 1 | 0 |
| | | | 1309 | 434 | 647 | 106 | 122 | | | |
| 5 | e | 82 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1311 | 434 | 647 | 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 |
| | | | 556 | 187 | 281 | 45 | 42 | | | |
| 6 | f | 34 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 556 | 187 | 281 | 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 |
| | | | 1030 | 338 | 523 | 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 |
| | | | 516 | 172 | 261 | 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 | O | 0 | 1 | 0 |
| | | | 620 | 209 | 318 | 46 | 47 | | | |

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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 |
| | | | 3730 | 1174 | 1850 | 317 | 385 | | | |
| 13 | o | 244 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 3718 | 1170 | 1844 | 317 | 383 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 14 | T | 30 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 519 | 181 | 261 | 36 | 39 | | | |
| 14 | t | 30 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 512 | 180 | 256 | 36 | 38 | | | |

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 15 | U | 97 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1546 | 491 | 772 | 129 | 154 | | | |
| 15 | u | 97 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1546 | 491 | 772 | 129 | 154 | | | |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 16 | V | 137 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2134 | 675 | 1070 | 177 | 208 | 4 | | | |
| 16 | v | 137 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2134 | 675 | 1070 | 177 | 208 | 4 | | | |

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 17 | Y | 27 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 404 | 128 | 208 | 35 | 30 | 3 | | | |
| 17 | y | 30 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 450 | 144 | 232 | 35 | 36 | 3 | | | |

- 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 | 38 | Total | C | H | N | O | | 0 | 0 | 0 |
| | | | 593 | 188 | 312 | 45 | 48 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 19 | Z | 62 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 988 | 328 | 509 | 72 | 77 | 2 | | | |
| 19 | z | 62 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 986 | 326 | 509 | 72 | 77 | 2 | | | |

- Molecule 20 is a protein called Photosystem II protein Y.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|--|---------|---------|-------|
| 20 | R | 34 | Total | C | H | N | O | | 0 | 0 | 0 |
| | | | 569 | 184 | 298 | 47 | 40 | | | | |
| 20 | r | 31 | Total | C | H | N | O | | 0 | 0 | 0 |
| | | | 461 | 154 | 234 | 40 | 33 | | | | |

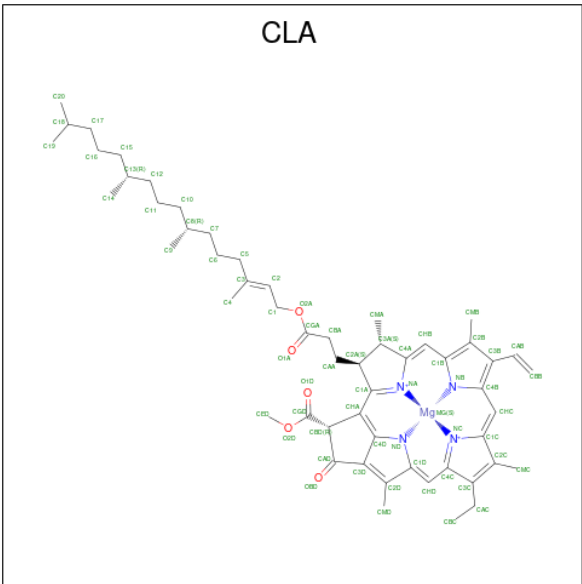
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | A | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |
| 21 | a | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 23 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 102 | 44 | 48 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | 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 |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 117 | 49 | 58 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | 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 |
|-----|-------|----------|--------------|---------|---------|---------|--------|--------|---------|---------|
| 23 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | D | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | D | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | D | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |

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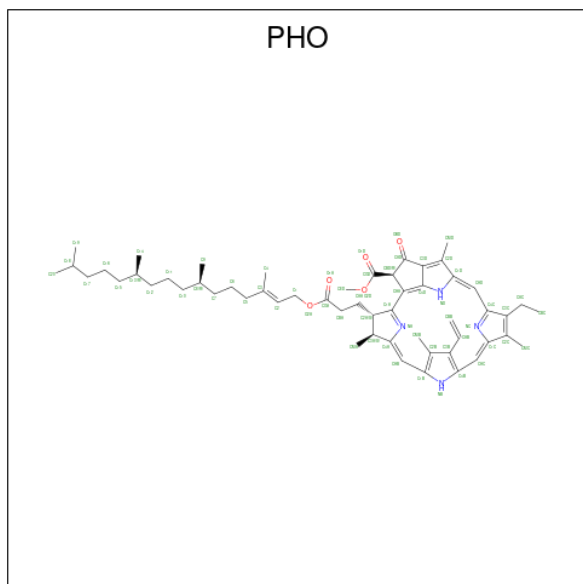
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 132 | 54 | 68 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 23 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

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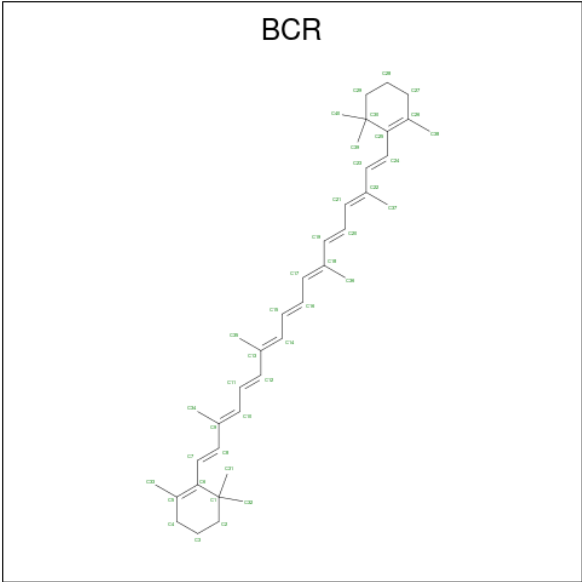
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 23 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|--|---------|---------|
| 24 | A | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 24 | D | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 24 | a | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 24 | d | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



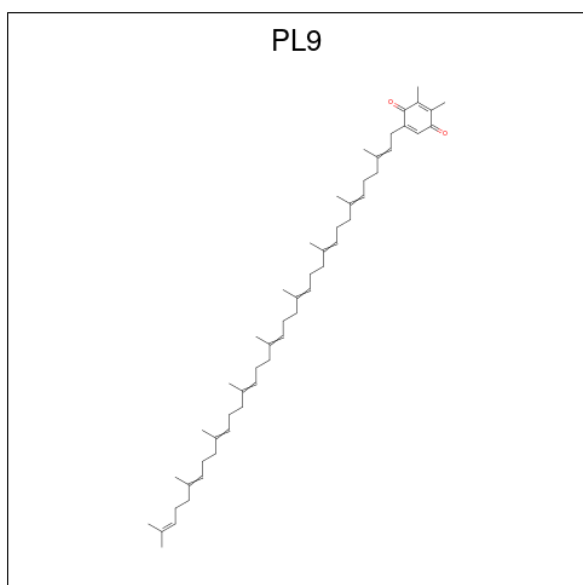
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 25 | A | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | D | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | H | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | K | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | T | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | Z | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | a | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 25 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | d | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | k | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | t | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 25 | x | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

- Molecule 26 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



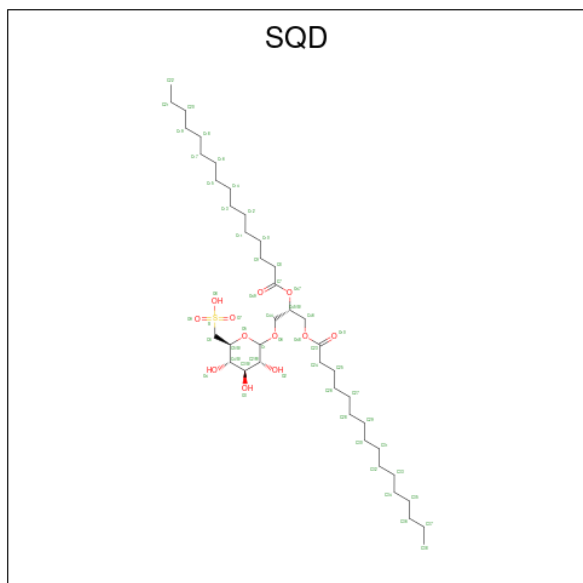
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |

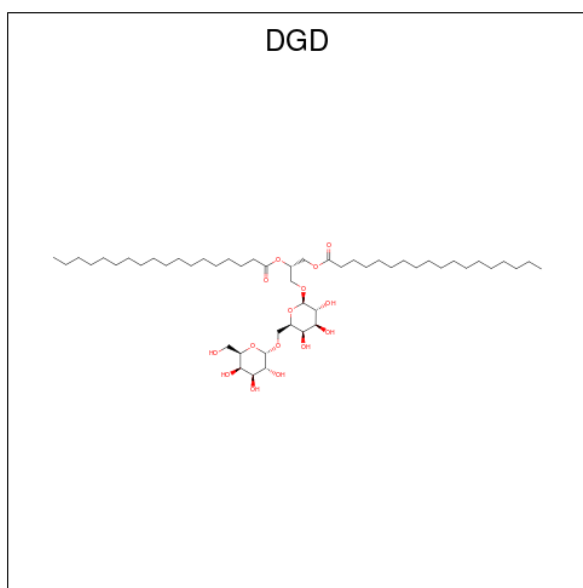
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 27 | A | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 122 | 39 | 70 | 12 | 1 | | |
| 27 | A | 1 | Total | C | H | O | | 0 | 0 |
| | | | 104 | 35 | 65 | 4 | | | |
| 27 | B | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 132 | 41 | 78 | 12 | 1 | | |
| 27 | F | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 81 | 25 | 45 | 10 | 1 | | |
| 27 | a | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 132 | 41 | 78 | 12 | 1 | | |
| 27 | a | 1 | Total | C | H | O | | 0 | 0 |
| | | | 92 | 31 | 56 | 5 | | | |
| 27 | b | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 114 | 36 | 65 | 12 | 1 | | |
| 27 | f | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 90 | 28 | 49 | 12 | 1 | | |

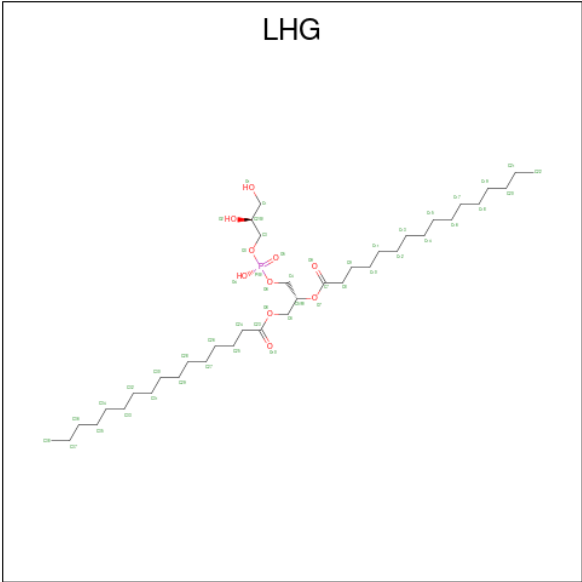
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: $C_{51}H_{96}O_{15}$).



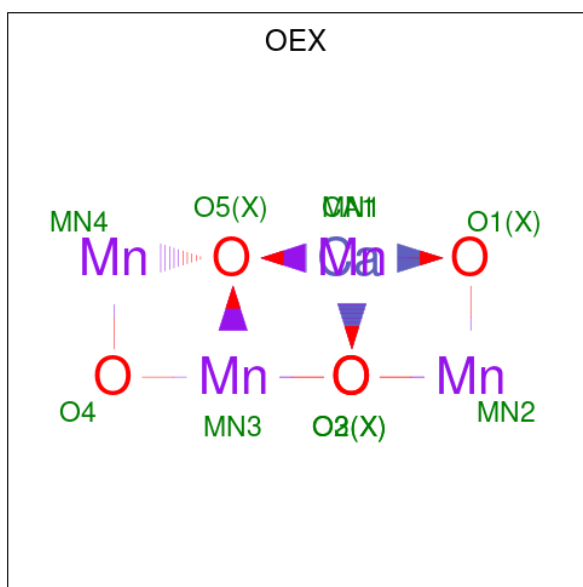
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 28 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 162 | 51 | 96 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | H | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 119 | 39 | 75 | 5 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | h | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



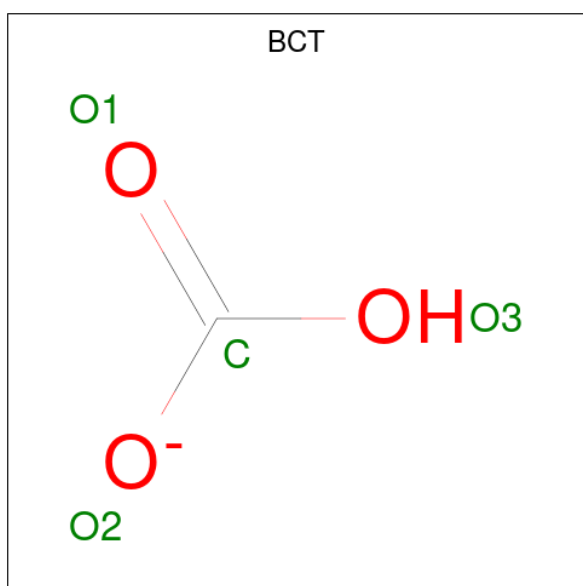
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 29 | A | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 114 | 36 | 67 | 10 | 1 | | |
| 29 | E | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | L | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 29 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 90 | 28 | 51 | 10 | 1 | | |
| 29 | e | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 99 | 31 | 57 | 10 | 1 | | |
| 29 | l | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30 | A | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |
| 30 | a | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

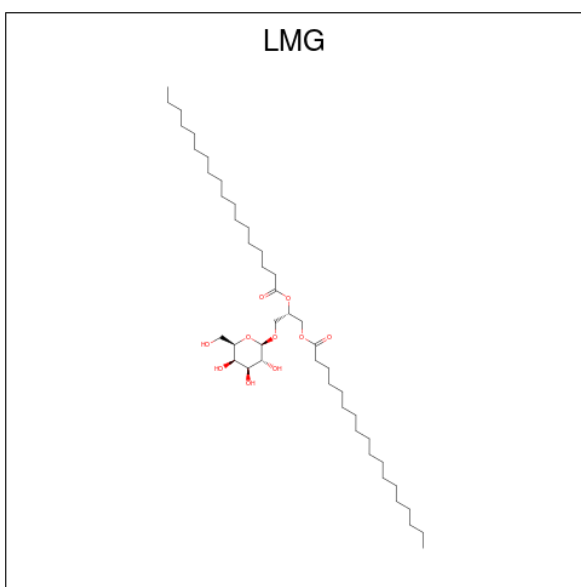


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 31 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 5 | 1 | 1 | 3 | | |
| 31 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 5 | 1 | 1 | 3 | | |

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|-----|----|---------|---------|
| 32 | B | 6 | Total | C | H | O | 0 | 0 |
| | | | 226 | 79 | 137 | 10 | | |
| 32 | C | 3 | Total | C | H | O | 0 | 0 |
| | | | 103 | 36 | 63 | 4 | | |
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 32 | E | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | H | 1 | Total | C | H | | 0 | 0 |
| | | | 53 | 18 | 35 | | | |
| 32 | I | 1 | Total | C | H | | 0 | 0 |
| | | | 41 | 15 | 26 | | | |
| 32 | J | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | M | 2 | Total | C | H | O | 0 | 0 |
| | | | 63 | 23 | 38 | 2 | | |
| 32 | T | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 32 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | b | 5 | Total | C | H | O | 0 | 0 |
| | | | 220 | 75 | 139 | 6 | | |
| 32 | c | 2 | Total | C | H | O | 0 | 0 |
| | | | 83 | 28 | 51 | 4 | | |
| 32 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 43 | 15 | 26 | 2 | | |
| 32 | j | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | l | 1 | Total | C | H | | 0 | 0 |
| | | | 53 | 18 | 35 | | | |
| 32 | m | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | t | 1 | Total | C | H | | 0 | 0 |
| | | | 26 | 10 | 16 | | | |
| 32 | x | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |

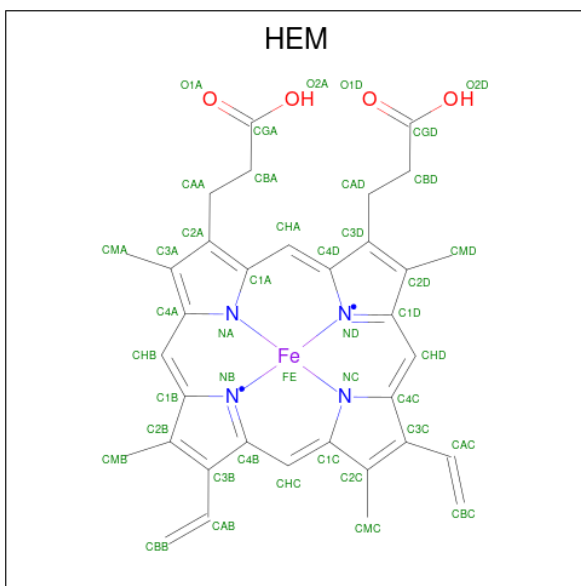
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 33 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 114 | 38 | 66 | 10 | | |
| 33 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 114 | 38 | 66 | 10 | | |
| 33 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 123 | 41 | 72 | 10 | | |
| 33 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 78 | 27 | 45 | 6 | | |
| 33 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 68 | 24 | 40 | 4 | | |
| 33 | M | 1 | Total | C | H | O | 0 | 0 |
| | | | 123 | 41 | 72 | 10 | | |
| 33 | b | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 45 | 86 | 10 | | |
| 33 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 81 | 27 | 44 | 10 | | |
| 33 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 117 | 38 | 69 | 10 | | |
| 33 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 117 | 39 | 68 | 10 | | |
| 33 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 57 | 21 | 34 | 2 | | |
| 33 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 102 | 34 | 58 | 10 | | |
| 33 | m | 1 | Total | C | H | O | 0 | 0 |
| | | | 123 | 41 | 72 | 10 | | |

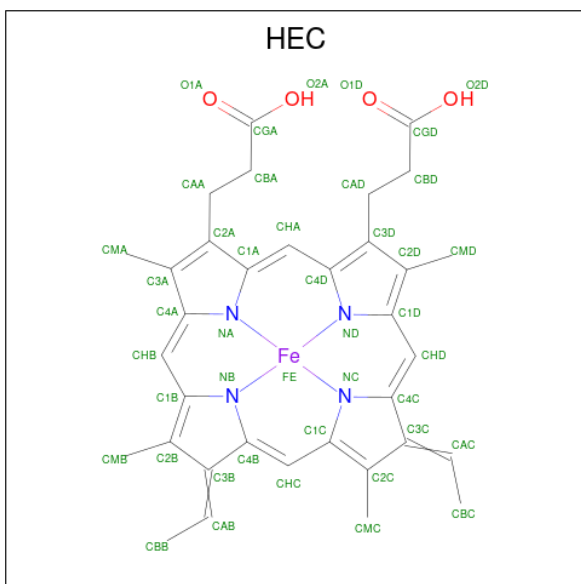
- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

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

- Molecule 36 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 36 | A | 136 | Total | O | 0 | 0 |
| | | | 136 | 136 | | |
| 36 | B | 216 | Total | O | 0 | 0 |
| | | | 216 | 216 | | |
| 36 | C | 192 | Total | O | 0 | 0 |
| | | | 192 | 192 | | |
| 36 | D | 138 | Total | O | 0 | 0 |
| | | | 138 | 138 | | |
| 36 | E | 30 | Total | O | 0 | 0 |
| | | | 30 | 30 | | |
| 36 | F | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 36 | H | 25 | Total | O | 0 | 0 |
| | | | 25 | 25 | | |
| 36 | I | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |
| 36 | J | 13 | Total | O | 0 | 0 |
| | | | 13 | 13 | | |
| 36 | L | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 36 | M | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 36 | O | 128 | Total | O | 0 | 0 |
| | | | 128 | 128 | | |
| 36 | T | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |
| 36 | U | 47 | Total | O | 0 | 0 |
| | | | 47 | 47 | | |
| 36 | V | 73 | Total | O | 0 | 0 |
| | | | 73 | 73 | | |
| 36 | Y | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 36 | X | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 36 | Z | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 36 | R | 4 | Total O 4 4 | 0 | 0 |
| 36 | a | 119 | Total O 119 119 | 0 | 0 |
| 36 | b | 190 | Total O 190 190 | 0 | 0 |
| 36 | c | 162 | Total O 162 162 | 0 | 0 |
| 36 | d | 120 | Total O 120 120 | 0 | 0 |
| 36 | e | 22 | Total O 22 22 | 0 | 0 |
| 36 | f | 4 | Total O 4 4 | 0 | 0 |
| 36 | h | 19 | Total O 19 19 | 0 | 0 |
| 36 | i | 10 | Total O 10 10 | 0 | 0 |
| 36 | j | 8 | Total O 8 8 | 0 | 0 |
| 36 | k | 5 | Total O 5 5 | 0 | 0 |
| 36 | l | 11 | Total O 11 11 | 0 | 0 |
| 36 | m | 5 | Total O 5 5 | 0 | 0 |
| 36 | o | 113 | Total O 113 113 | 0 | 0 |
| 36 | t | 11 | Total O 11 11 | 0 | 0 |
| 36 | u | 54 | Total O 54 54 | 0 | 0 |
| 36 | v | 64 | Total O 64 64 | 0 | 0 |
| 36 | y | 4 | Total O 4 4 | 0 | 0 |
| 36 | x | 13 | Total O 13 13 | 0 | 0 |
| 36 | z | 1 | Total O 1 1 | 0 | 0 |
| 36 | r | 5 | Total O 5 5 | 0 | 0 |

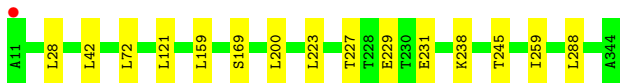
3 Residue-property plots

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.

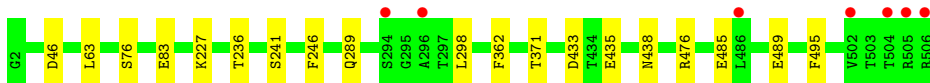
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



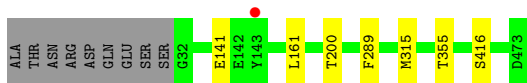
- Molecule 2: Photosystem II CP47 reaction center protein



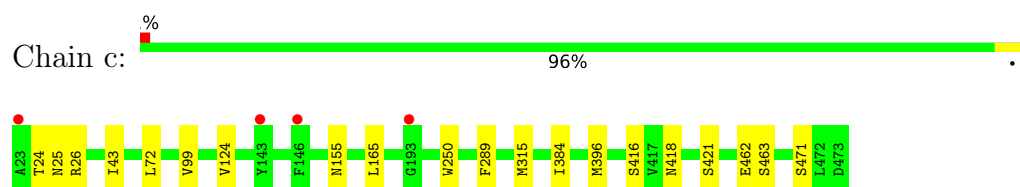
- Molecule 2: Photosystem II CP47 reaction center protein



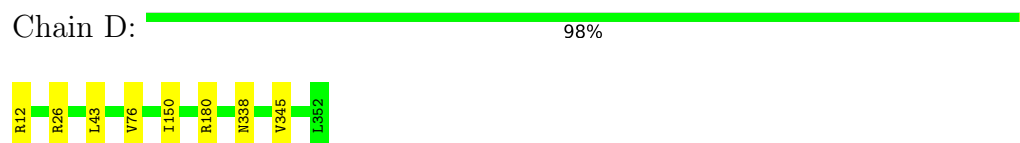
- Molecule 3: Photosystem II CP43 reaction center protein



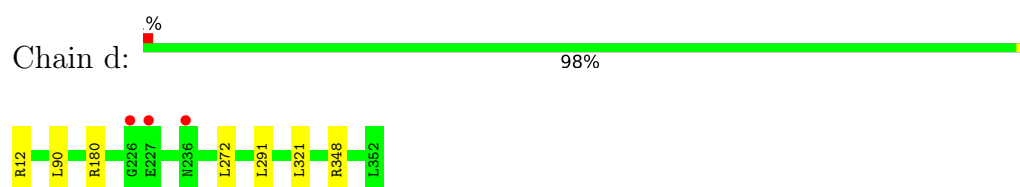
- Molecule 3: Photosystem II CP43 reaction center protein



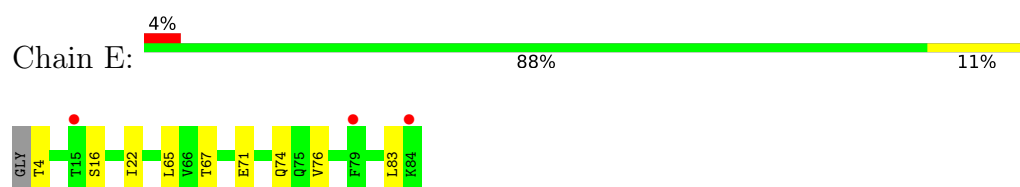
- Molecule 4: Photosystem II D2 protein



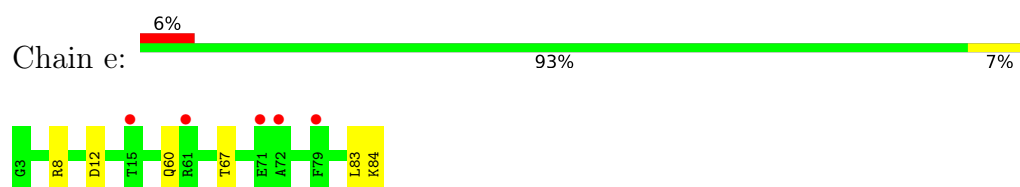
- Molecule 4: Photosystem II D2 protein



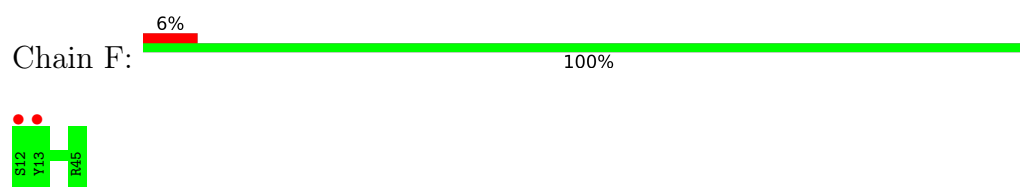
- Molecule 5: Cytochrome b559 subunit alpha



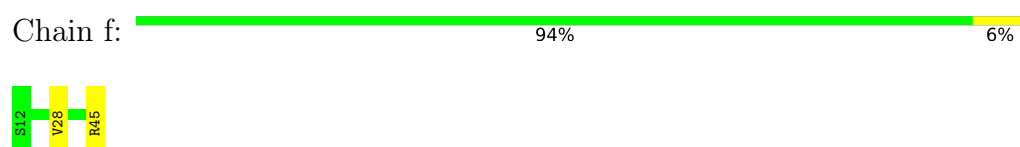
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 9%




- Molecule 7: Photosystem II reaction center protein H

Chain h:  3% 91% 6%




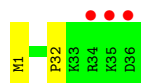
- Molecule 8: Photosystem II reaction center protein I

Chain I:  86% 14%



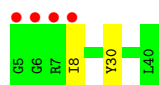
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 94% 6%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  11% 94% 6%




- Molecule 9: Photosystem II reaction center protein J

Chain j:  11% 94% 6%

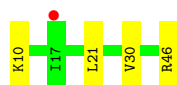
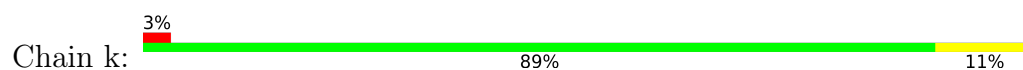


- Molecule 10: Photosystem II reaction center protein K

Chain K:  86% 14%



- Molecule 10: Photosystem II reaction center protein K

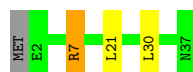
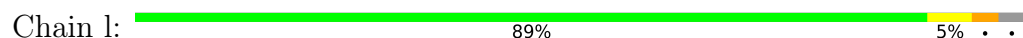


- Molecule 11: Photosystem II reaction center protein L

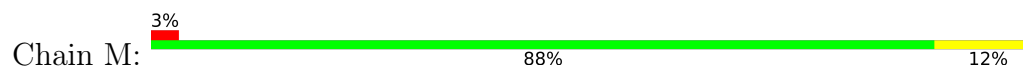


There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein L



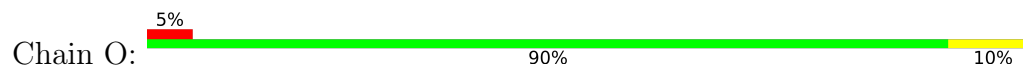
- Molecule 12: Photosystem II reaction center protein M



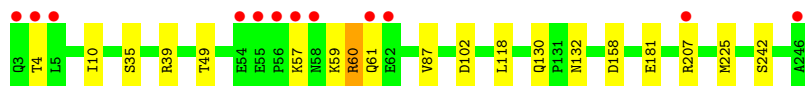
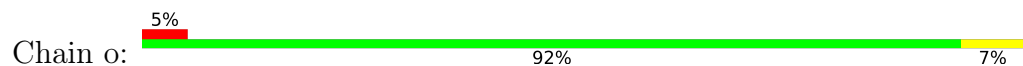
- Molecule 12: Photosystem II reaction center protein M



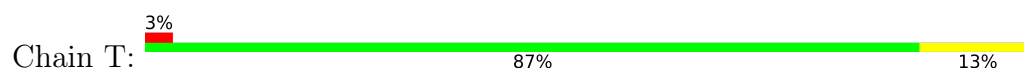
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



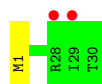
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



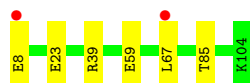
- Molecule 14: Photosystem II reaction center protein T



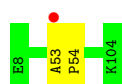
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



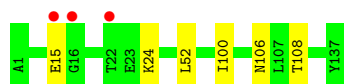
- Molecule 15: Photosystem II 12 kDa extrinsic protein



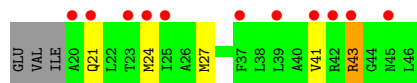
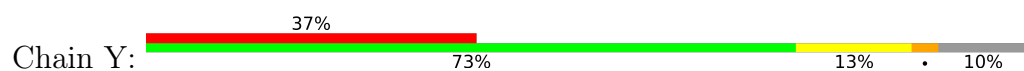
- Molecule 16: Cytochrome c-550



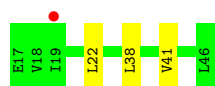
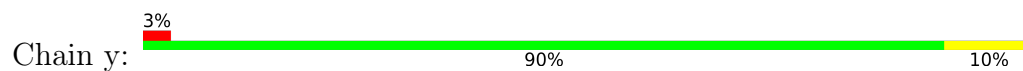
- Molecule 16: Cytochrome c-550



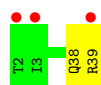
- Molecule 17: Photosystem II reaction center protein Ycf12



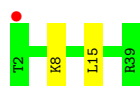
- Molecule 17: Photosystem II reaction center protein Ycf12



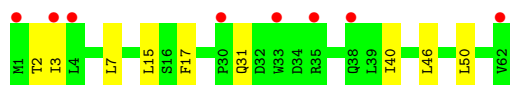
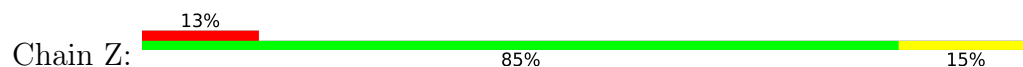
- Molecule 18: Photosystem II reaction center X protein



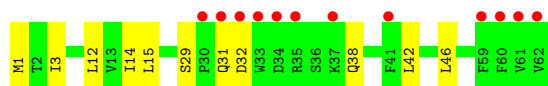
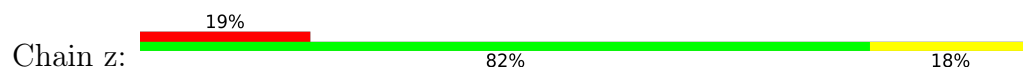
- Molecule 18: Photosystem II reaction center X protein



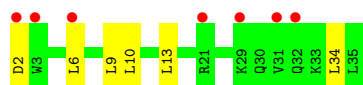
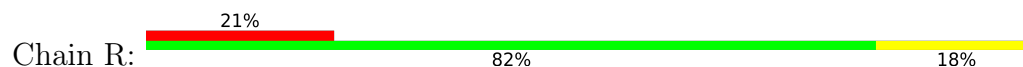
- Molecule 19: Photosystem II reaction center protein Z



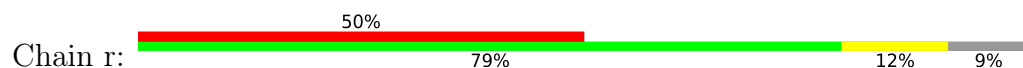
- Molecule 19: Photosystem II reaction center protein Z

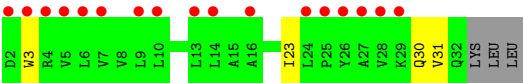


- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 117.55Å 222.69Å 309.06Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.78 – 2.50 30.78 – 2.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (30.78-2.50) 87.6 (30.78-2.50) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.98 (at 2.51Å) | Xtriage |
| Refinement program | PHENIX dev_svn | Depositor |
| R, R_{free} | 0.167 , 0.246 0.167 , 0.247 | Depositor DCC |
| R_{free} test set | 2481 reflections (0.89%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 35.5 | Xtriage |
| Anisotropy | 0.353 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 76.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 103658 | wwPDB-VP |
| Average B, all atoms (Å ²) | 53.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DGD, CL, LMG, PHO, PL9, CLA, OEX, LHG, SQD, BCT, FME, UNL, HEM, HEC, FE2, BCR

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 | 0.72 | 1/2707 (0.0%) | 0.73 | 1/3692 (0.0%) |
| 1 | a | 0.68 | 0/2704 | 0.71 | 1/3688 (0.0%) |
| 2 | B | 0.68 | 0/4160 | 0.71 | 2/5668 (0.0%) |
| 2 | b | 0.63 | 0/4118 | 0.69 | 0/5611 |
| 3 | C | 0.64 | 0/3530 | 0.68 | 0/4807 |
| 3 | c | 0.59 | 0/3610 | 0.67 | 0/4914 |
| 4 | D | 0.69 | 0/2812 | 0.70 | 0/3832 |
| 4 | d | 0.63 | 0/2821 | 0.69 | 1/3844 (0.0%) |
| 5 | E | 0.57 | 0/684 | 0.66 | 0/935 |
| 5 | e | 0.56 | 0/683 | 0.63 | 0/932 |
| 6 | F | 0.57 | 0/284 | 0.59 | 0/387 |
| 6 | f | 0.54 | 0/284 | 0.58 | 0/387 |
| 7 | H | 0.68 | 1/520 (0.2%) | 0.72 | 0/709 |
| 7 | h | 0.62 | 0/511 | 0.74 | 0/697 |
| 8 | I | 0.67 | 0/293 | 0.75 | 0/396 |
| 8 | i | 0.76 | 0/293 | 0.74 | 0/396 |
| 9 | J | 0.54 | 0/263 | 0.70 | 0/356 |
| 9 | j | 0.54 | 0/261 | 0.64 | 0/353 |
| 10 | K | 0.50 | 0/314 | 0.65 | 0/427 |
| 10 | k | 0.51 | 0/303 | 0.72 | 0/416 |
| 11 | L | 0.69 | 0/311 | 0.74 | 0/422 |
| 11 | l | 0.62 | 0/303 | 0.71 | 0/412 |
| 12 | M | 0.70 | 0/249 | 0.71 | 0/341 |
| 12 | m | 0.75 | 0/244 | 0.67 | 0/334 |
| 13 | O | 0.62 | 0/1914 | 0.77 | 2/2596 (0.1%) |
| 13 | o | 0.60 | 0/1905 | 0.76 | 3/2583 (0.1%) |
| 14 | T | 0.79 | 1/257 (0.4%) | 0.77 | 0/349 |
| 14 | t | 0.71 | 0/255 | 0.64 | 0/346 |
| 15 | U | 0.62 | 0/785 | 0.70 | 0/1064 |
| 15 | u | 0.65 | 0/785 | 0.75 | 0/1064 |
| 16 | V | 0.58 | 0/1085 | 0.69 | 0/1473 |
| 16 | v | 0.62 | 0/1085 | 0.69 | 0/1473 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | Y | 0.47 | 0/197 | 0.69 | 0/264 |
| 17 | y | 0.39 | 0/219 | 0.57 | 0/294 |
| 18 | X | 0.61 | 0/284 | 0.70 | 0/384 |
| 18 | x | 0.40 | 0/284 | 0.62 | 0/384 |
| 19 | Z | 0.53 | 0/490 | 0.64 | 0/669 |
| 19 | z | 0.48 | 0/488 | 0.56 | 0/666 |
| 20 | R | 0.39 | 0/277 | 0.57 | 0/380 |
| 20 | r | 0.39 | 0/233 | 0.55 | 0/323 |
| All | All | 0.64 | 3/42805 (0.0%) | 0.70 | 10/58268 (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 | Y | 0 | 1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14 | T | 6 | TYR | CD2-CE2 | -5.58 | 1.30 | 1.39 |
| 1 | A | 135 | TYR | CD1-CE1 | -5.56 | 1.31 | 1.39 |
| 7 | H | 41 | PHE | CB-CG | -5.18 | 1.42 | 1.51 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 13 | o | 158 | ASP | CB-CG-OD1 | 7.76 | 125.28 | 118.30 |
| 13 | O | 158 | ASP | CB-CG-OD1 | 6.08 | 123.78 | 118.30 |
| 4 | d | 348 | ARG | NE-CZ-NH2 | -5.81 | 117.39 | 120.30 |
| 13 | o | 102 | ASP | CB-CG-OD1 | 5.77 | 123.50 | 118.30 |
| 1 | A | 183 | MET | CA-CB-CG | 5.64 | 122.88 | 113.30 |
| 13 | O | 223 | ASP | CB-CG-OD2 | 5.60 | 123.34 | 118.30 |
| 13 | o | 158 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 2 | B | 433 | ASP | CB-CG-OD1 | -5.39 | 113.45 | 118.30 |
| 1 | a | 72 | LEU | CB-CG-CD1 | -5.31 | 101.97 | 111.00 |
| 2 | B | 46 | ASP | CB-CG-OD2 | -5.14 | 113.68 | 118.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 17 | Y | 21 | GLN | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 332/334 (99%) | 322 (97%) | 9 (3%) | 1 (0%) | 41 | 61 |
| 1 | a | 332/334 (99%) | 320 (96%) | 11 (3%) | 1 (0%) | 41 | 61 |
| 2 | B | 508/505 (101%) | 488 (96%) | 19 (4%) | 1 (0%) | 47 | 68 |
| 2 | b | 503/505 (100%) | 480 (95%) | 20 (4%) | 3 (1%) | 25 | 43 |
| 3 | C | 440/451 (98%) | 420 (96%) | 19 (4%) | 1 (0%) | 47 | 68 |
| 3 | c | 450/451 (100%) | 433 (96%) | 15 (3%) | 2 (0%) | 34 | 54 |
| 4 | D | 339/341 (99%) | 328 (97%) | 10 (3%) | 1 (0%) | 41 | 61 |
| 4 | d | 340/341 (100%) | 323 (95%) | 17 (5%) | 0 | 100 | 100 |
| 5 | E | 80/82 (98%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 5 | e | 80/82 (98%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | F | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 6 | f | 32/34 (94%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 7 | H | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 7 | h | 61/65 (94%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 8 | I | 34/36 (94%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | i | 34/36 (94%) | 30 (88%) | 4 (12%) | 0 | 100 | 100 |
| 9 | J | 34/36 (94%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | j | 34/36 (94%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10 | K | 35/37 (95%) | 32 (91%) | 2 (6%) | 1 (3%) | 4 | 6 |
| 10 | k | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 34/37 (92%) | 33 (97%) | 0 | 1 (3%) | 4 | 6 |
| 12 | M | 31/33 (94%) | 30 (97%) | 1 (3%) | 0 | 100 | 100 |
| 12 | m | 30/33 (91%) | 28 (93%) | 2 (7%) | 0 | 100 | 100 |
| 13 | O | 243/244 (100%) | 225 (93%) | 14 (6%) | 4 (2%) | 9 | 17 |
| 13 | o | 242/244 (99%) | 226 (93%) | 13 (5%) | 3 (1%) | 13 | 24 |
| 14 | T | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 28/30 (93%) | 26 (93%) | 2 (7%) | 0 | 100 | 100 |
| 15 | U | 95/97 (98%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 15 | u | 95/97 (98%) | 91 (96%) | 3 (3%) | 1 (1%) | 14 | 26 |
| 16 | V | 135/137 (98%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 16 | v | 135/137 (98%) | 127 (94%) | 8 (6%) | 0 | 100 | 100 |
| 17 | Y | 25/30 (83%) | 18 (72%) | 5 (20%) | 2 (8%) | 1 | 1 |
| 17 | y | 28/30 (93%) | 23 (82%) | 4 (14%) | 1 (4%) | 3 | 4 |
| 18 | X | 36/38 (95%) | 33 (92%) | 2 (6%) | 1 (3%) | 5 | 7 |
| 18 | x | 36/38 (95%) | 31 (86%) | 5 (14%) | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 54 (90%) | 6 (10%) | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 47 (78%) | 11 (18%) | 2 (3%) | 4 | 5 |
| 20 | R | 32/34 (94%) | 30 (94%) | 1 (3%) | 1 (3%) | 4 | 5 |
| 20 | r | 29/34 (85%) | 24 (83%) | 3 (10%) | 2 (7%) | 1 | 1 |
| All | All | 5235/5326 (98%) | 4963 (95%) | 243 (5%) | 29 (1%) | 25 | 43 |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 416 | SER |
| 10 | K | 16 | ALA |
| 13 | O | 62 | GLU |
| 17 | Y | 41 | VAL |
| 3 | c | 416 | SER |
| 13 | o | 60 | ARG |
| 13 | o | 61 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | u | 53 | ALA |
| 19 | z | 15 | LEU |
| 20 | r | 30 | GLN |
| 17 | Y | 43 | ARG |
| 20 | R | 34 | LEU |
| 2 | b | 85 | GLY |
| 20 | r | 31 | VAL |
| 2 | B | 438 | ASN |
| 18 | X | 38 | GLN |
| 19 | z | 14 | ILE |
| 4 | D | 338 | ASN |
| 2 | b | 127 | ARG |
| 13 | O | 138 | THR |
| 3 | c | 250 | TRP |
| 11 | l | 7 | ARG |
| 13 | o | 132 | ASN |
| 17 | y | 41 | VAL |
| 13 | O | 57 | LYS |
| 2 | b | 295 | GLY |
| 13 | O | 133 | VAL |
| 1 | A | 259 | ILE |
| 1 | a | 259 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 270/270 (100%) | 262 (97%) | 8 (3%) | 41 | 68 |
| 1 | a | 269/270 (100%) | 256 (95%) | 13 (5%) | 25 | 48 |
| 2 | B | 407/403 (101%) | 391 (96%) | 16 (4%) | 32 | 57 |
| 2 | b | 402/403 (100%) | 388 (96%) | 14 (4%) | 36 | 62 |
| 3 | C | 344/352 (98%) | 338 (98%) | 6 (2%) | 60 | 82 |
| 3 | c | 353/352 (100%) | 335 (95%) | 18 (5%) | 24 | 45 |
| 4 | D | 276/276 (100%) | 269 (98%) | 7 (2%) | 47 | 73 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | d | 277/276 (100%) | 271 (98%) | 6 (2%) | 52 | 77 |
| 5 | E | 72/72 (100%) | 62 (86%) | 10 (14%) | 3 | 6 |
| 5 | e | 71/72 (99%) | 65 (92%) | 6 (8%) | 10 | 21 |
| 6 | F | 28/28 (100%) | 28 (100%) | 0 | 100 | 100 |
| 6 | f | 28/28 (100%) | 26 (93%) | 2 (7%) | 14 | 28 |
| 7 | H | 53/54 (98%) | 48 (91%) | 5 (9%) | 8 | 17 |
| 7 | h | 53/54 (98%) | 49 (92%) | 4 (8%) | 13 | 26 |
| 8 | I | 32/32 (100%) | 28 (88%) | 4 (12%) | 4 | 8 |
| 8 | i | 32/32 (100%) | 31 (97%) | 1 (3%) | 40 | 67 |
| 9 | J | 24/24 (100%) | 22 (92%) | 2 (8%) | 11 | 22 |
| 9 | j | 23/24 (96%) | 21 (91%) | 2 (9%) | 10 | 20 |
| 10 | K | 31/30 (103%) | 26 (84%) | 5 (16%) | 2 | 4 |
| 10 | k | 30/30 (100%) | 26 (87%) | 4 (13%) | 4 | 7 |
| 11 | L | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 11 | l | 34/35 (97%) | 31 (91%) | 3 (9%) | 10 | 19 |
| 12 | M | 28/29 (97%) | 25 (89%) | 3 (11%) | 6 | 13 |
| 12 | m | 28/29 (97%) | 26 (93%) | 2 (7%) | 14 | 28 |
| 13 | O | 208/207 (100%) | 189 (91%) | 19 (9%) | 9 | 18 |
| 13 | o | 207/207 (100%) | 192 (93%) | 15 (7%) | 14 | 28 |
| 14 | T | 26/26 (100%) | 24 (92%) | 2 (8%) | 13 | 25 |
| 14 | t | 25/26 (96%) | 25 (100%) | 0 | 100 | 100 |
| 15 | U | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 28 |
| 15 | u | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 88 |
| 16 | V | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 16 | v | 117/117 (100%) | 111 (95%) | 6 (5%) | 24 | 45 |
| 17 | Y | 19/23 (83%) | 16 (84%) | 3 (16%) | 2 | 4 |
| 17 | y | 22/23 (96%) | 20 (91%) | 2 (9%) | 9 | 18 |
| 18 | X | 31/31 (100%) | 30 (97%) | 1 (3%) | 39 | 65 |
| 18 | x | 31/31 (100%) | 29 (94%) | 2 (6%) | 17 | 33 |
| 19 | Z | 52/52 (100%) | 43 (83%) | 9 (17%) | 2 | 3 |
| 19 | z | 51/52 (98%) | 42 (82%) | 9 (18%) | 2 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 20 | R | 28/29 (97%) | 23 (82%) | 5 (18%) | 2 | 3 |
| 20 | r | 19/29 (66%) | 17 (90%) | 2 (10%) | 7 | 13 |
| All | All | 4321/4348 (99%) | 4093 (95%) | 228 (5%) | 23 | 43 |

All (228) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 12 | ASN |
| 1 | A | 13 | LEU |
| 1 | A | 16 | ARG |
| 1 | A | 102 | LEU |
| 1 | A | 205 | VAL |
| 1 | A | 229 | GLU |
| 1 | A | 231 | GLU |
| 1 | A | 307 | ILE |
| 2 | B | 63 | LEU |
| 2 | B | 76 | SER |
| 2 | B | 83 | GLU |
| 2 | B | 227 | LYS |
| 2 | B | 236 | THR |
| 2 | B | 241 | SER |
| 2 | B | 246 | PHE |
| 2 | B | 289 | GLN |
| 2 | B | 298 | LEU |
| 2 | B | 362 | PHE |
| 2 | B | 371 | THR |
| 2 | B | 435 | GLU |
| 2 | B | 476 | ARG |
| 2 | B | 485 | GLU |
| 2 | B | 489 | GLU |
| 2 | B | 495 | PHE |
| 3 | C | 141 | GLU |
| 3 | C | 161 | LEU |
| 3 | C | 200 | THR |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 3 | C | 355 | THR |
| 4 | D | 12 | ARG |
| 4 | D | 26 | ARG |
| 4 | D | 43 | LEU |
| 4 | D | 76 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 4 | D | 150 | ILE |
| 4 | D | 180 | ARG |
| 4 | D | 345 | VAL |
| 5 | E | 4 | THR |
| 5 | E | 16 | SER |
| 5 | E | 22[A] | ILE |
| 5 | E | 22[B] | ILE |
| 5 | E | 65 | LEU |
| 5 | E | 67 | THR |
| 5 | E | 71 | GLU |
| 5 | E | 74 | GLN |
| 5 | E | 76 | VAL |
| 5 | E | 83 | LEU |
| 7 | H | 20 | LYS |
| 7 | H | 27 | THR |
| 7 | H | 49 | TYR |
| 7 | H | 52 | THR |
| 7 | H | 53 | LEU |
| 8 | I | 4 | LEU |
| 8 | I | 33 | LYS |
| 8 | I | 34 | ARG |
| 8 | I | 35 | LYS |
| 9 | J | 8 | ILE |
| 9 | J | 30 | TYR |
| 10 | K | 10 | LYS |
| 10 | K | 25 | LEU |
| 10 | K | 43 | VAL |
| 10 | K | 46[A] | ARG |
| 10 | K | 46[B] | ARG |
| 12 | M | 3 | VAL |
| 12 | M | 13 | LEU |
| 12 | M | 31 | SER |
| 13 | O | 3 | GLN |
| 13 | O | 4 | THR |
| 13 | O | 23 | ASP |
| 13 | O | 24 | ASP |
| 13 | O | 34 | SER |
| 13 | O | 39 | ARG |
| 13 | O | 45 | LEU |
| 13 | O | 72 | THR |
| 13 | O | 78 | LEU |
| 13 | O | 82 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 107 | THR |
| 13 | O | 118 | LEU |
| 13 | O | 134 | THR |
| 13 | O | 135 | SER |
| 13 | O | 182 | LEU |
| 13 | O | 191 | SER |
| 13 | O | 207 | ARG |
| 13 | O | 214 | THR |
| 13 | O | 217 | SER |
| 14 | T | 2 | GLU |
| 14 | T | 24 | ARG |
| 15 | U | 8 | GLU |
| 15 | U | 23 | GLU |
| 15 | U | 39 | ARG |
| 15 | U | 59 | GLU |
| 15 | U | 67 | LEU |
| 15 | U | 85 | THR |
| 16 | V | 3 | LEU |
| 16 | V | 7 | VAL |
| 16 | V | 21 | LEU |
| 16 | V | 31 | ARG |
| 16 | V | 86 | GLN |
| 17 | Y | 24 | MET |
| 17 | Y | 27 | MET |
| 17 | Y | 43 | ARG |
| 18 | X | 39 | ARG |
| 19 | Z | 2 | THR |
| 19 | Z | 3 | ILE |
| 19 | Z | 7 | LEU |
| 19 | Z | 15 | LEU |
| 19 | Z | 17 | PHE |
| 19 | Z | 31 | GLN |
| 19 | Z | 40 | ILE |
| 19 | Z | 46 | LEU |
| 19 | Z | 50 | LEU |
| 20 | R | 2 | ASP |
| 20 | R | 6 | LEU |
| 20 | R | 9 | LEU |
| 20 | R | 10 | LEU |
| 20 | R | 13 | LEU |
| 1 | a | 28 | LEU |
| 1 | a | 42 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 121 | LEU |
| 1 | a | 159 | LEU |
| 1 | a | 169 | SER |
| 1 | a | 200 | LEU |
| 1 | a | 223 | LEU |
| 1 | a | 227 | THR |
| 1 | a | 229 | GLU |
| 1 | a | 231 | GLU |
| 1 | a | 238 | LYS |
| 1 | a | 245 | THR |
| 1 | a | 288 | LEU |
| 2 | b | 81 | THR |
| 2 | b | 86 | ILE |
| 2 | b | 149 | LEU |
| 2 | b | 170 | ASP |
| 2 | b | 236 | THR |
| 2 | b | 252 | VAL |
| 2 | b | 347 | ARG |
| 2 | b | 353 | GLU |
| 2 | b | 362 | PHE |
| 2 | b | 388 | SER |
| 2 | b | 409 | GLN |
| 2 | b | 480 | SER |
| 2 | b | 490 | GLN |
| 2 | b | 492 | GLU |
| 3 | c | 24 | THR |
| 3 | c | 25 | ASN |
| 3 | c | 26 | ARG |
| 3 | c | 43 | ILE |
| 3 | c | 72 | LEU |
| 3 | c | 99 | VAL |
| 3 | c | 124 | VAL |
| 3 | c | 155 | ASN |
| 3 | c | 165 | LEU |
| 3 | c | 289 | PHE |
| 3 | c | 315 | MET |
| 3 | c | 384 | ILE |
| 3 | c | 396 | MET |
| 3 | c | 418 | ASN |
| 3 | c | 421 | SER |
| 3 | c | 462 | GLU |
| 3 | c | 463 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | c | 471 | SER |
| 4 | d | 12 | ARG |
| 4 | d | 90 | LEU |
| 4 | d | 180 | ARG |
| 4 | d | 272 | LEU |
| 4 | d | 291 | LEU |
| 4 | d | 321 | LEU |
| 5 | e | 8 | ARG |
| 5 | e | 12 | ASP |
| 5 | e | 60 | GLN |
| 5 | e | 67 | THR |
| 5 | e | 83 | LEU |
| 5 | e | 84 | LYS |
| 6 | f | 28 | VAL |
| 6 | f | 45 | ARG |
| 7 | h | 3 | ARG |
| 7 | h | 7 | LEU |
| 7 | h | 21 | VAL |
| 7 | h | 49 | TYR |
| 8 | i | 32 | PRO |
| 9 | j | 7 | ARG |
| 9 | j | 36 | LEU |
| 10 | k | 10 | LYS |
| 10 | k | 21 | LEU |
| 10 | k | 30 | VAL |
| 10 | k | 46 | ARG |
| 11 | l | 7 | ARG |
| 11 | l | 21 | LEU |
| 11 | l | 30 | LEU |
| 12 | m | 13 | LEU |
| 12 | m | 16 | LEU |
| 13 | o | 4 | THR |
| 13 | o | 10 | ILE |
| 13 | o | 35 | SER |
| 13 | o | 39 | ARG |
| 13 | o | 49 | THR |
| 13 | o | 57 | LYS |
| 13 | o | 59 | LYS |
| 13 | o | 60 | ARG |
| 13 | o | 87 | VAL |
| 13 | o | 118 | LEU |
| 13 | o | 130 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | o | 181 | GLU |
| 13 | o | 207 | ARG |
| 13 | o | 225 | MET |
| 13 | o | 242 | SER |
| 15 | u | 54 | PRO |
| 16 | v | 15 | GLU |
| 16 | v | 24 | LYS |
| 16 | v | 52 | LEU |
| 16 | v | 100 | ILE |
| 16 | v | 106 | ASN |
| 16 | v | 108 | THR |
| 17 | y | 22 | LEU |
| 17 | y | 38 | LEU |
| 18 | x | 8 | LYS |
| 18 | x | 15 | LEU |
| 19 | z | 1 | MET |
| 19 | z | 3 | ILE |
| 19 | z | 12 | LEU |
| 19 | z | 29 | SER |
| 19 | z | 31 | GLN |
| 19 | z | 32 | ASP |
| 19 | z | 38 | GLN |
| 19 | z | 42 | LEU |
| 19 | z | 46 | LEU |
| 20 | r | 3 | TRP |
| 20 | r | 23 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 285 | ASN |
| 2 | B | 289 | GLN |
| 13 | O | 82 | GLN |
| 13 | O | 231 | HIS |
| 15 | U | 37 | GLN |
| 16 | V | 86 | GLN |
| 19 | Z | 6 | GLN |
| 2 | b | 179 | GLN |
| 2 | b | 281 | GLN |
| 2 | b | 282 | GLN |
| 2 | b | 497 | GLN |
| 3 | c | 25 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | c | 28 | GLN |
| 5 | e | 74 | GLN |
| 13 | o | 58 | ASN |
| 19 | z | 38 | 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 | $\# Z > 2$ |
| 14 | FME | t | 1 | 14 | 8,9,10 | 1.07 | 1 (12%) | 7,9,11 | 1.04 | 0 |
| 12 | FME | M | 1 | 12 | 8,9,10 | 1.14 | 1 (12%) | 7,9,11 | 1.08 | 0 |
| 8 | FME | i | 1 | 8 | 8,9,10 | 1.25 | 1 (12%) | 7,9,11 | 1.06 | 0 |
| 8 | FME | I | 1 | 8 | 8,9,10 | 1.09 | 1 (12%) | 7,9,11 | 1.33 | 1 (14%) |
| 12 | FME | m | 1 | 12 | 8,9,10 | 1.06 | 1 (12%) | 7,9,11 | 0.66 | 0 |
| 14 | FME | T | 1 | 14 | 8,9,10 | 0.96 | 1 (12%) | 7,9,11 | 1.55 | 1 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 14 | FME | t | 1 | 14 | - | 2/7/9/11 | - |
| 12 | FME | M | 1 | 12 | - | 1/7/9/11 | - |
| 8 | FME | i | 1 | 8 | - | 0/7/9/11 | - |
| 8 | FME | I | 1 | 8 | - | 2/7/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 12 | FME | m | 1 | 12 | - | 0/7/9/11 | - |
| 14 | FME | T | 1 | 14 | - | 1/7/9/11 | - |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | i | 1 | FME | CA-N | -2.68 | 1.42 | 1.46 |
| 14 | t | 1 | FME | CA-N | -2.51 | 1.42 | 1.46 |
| 14 | T | 1 | FME | CA-N | -2.47 | 1.42 | 1.46 |
| 12 | m | 1 | FME | CA-N | -2.40 | 1.42 | 1.46 |
| 8 | I | 1 | FME | CA-N | -2.33 | 1.43 | 1.46 |
| 12 | M | 1 | FME | CA-N | -2.16 | 1.43 | 1.46 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | I | 1 | FME | CA-N-CN | -2.37 | 119.17 | 122.82 |
| 14 | T | 1 | FME | CA-N-CN | -2.36 | 119.19 | 122.82 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 8 | I | 1 | FME | O-C-CA-CB |
| 12 | M | 1 | FME | CB-CA-N-CN |
| 14 | t | 1 | FME | O-C-CA-CB |
| 14 | T | 1 | FME | CB-CG-SD-CE |
| 14 | t | 1 | FME | CB-CG-SD-CE |
| 8 | I | 1 | FME | C-CA-CB-CG |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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 |
| 23 | CLA | c | 510 | - | 59,73,73 | 1.34 | 6 (10%) | 67,113,113 | 1.74 | 13 (19%) |
| 23 | CLA | a | 405 | - | 59,73,73 | 1.53 | 8 (13%) | 67,113,113 | 1.55 | 11 (16%) |
| 33 | LMG | C | 519 | - | 48,48,55 | 1.03 | 6 (12%) | 56,56,63 | 1.32 | 6 (10%) |
| 23 | CLA | d | 402 | 36 | 59,73,73 | 1.63 | 8 (13%) | 67,113,113 | 1.98 | 12 (17%) |
| 23 | CLA | c | 513 | - | 59,73,73 | 1.42 | 8 (13%) | 67,113,113 | 1.33 | 11 (16%) |
| 28 | DGD | C | 518 | - | 63,63,67 | 1.11 | 7 (11%) | 77,77,81 | 1.42 | 11 (14%) |
| 23 | CLA | b | 606 | - | 59,73,73 | 1.47 | 8 (13%) | 67,113,113 | 1.90 | 19 (28%) |
| 29 | LHG | A | 413 | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 1.52 | 9 (17%) |
| 27 | SQD | F | 101 | - | 35,36,54 | 0.93 | 1 (2%) | 42,45,65 | 1.95 | 10 (23%) |
| 23 | CLA | C | 510 | - | 59,73,73 | 1.38 | 6 (10%) | 67,113,113 | 1.53 | 9 (13%) |
| 25 | BCR | D | 405 | - | 41,41,41 | 1.08 | 3 (7%) | 56,56,56 | 1.18 | 5 (8%) |
| 29 | LHG | E | 101 | - | 48,48,48 | 0.91 | 3 (6%) | 51,54,54 | 1.21 | 3 (5%) |
| 23 | CLA | b | 609 | - | 59,73,73 | 1.41 | 7 (11%) | 67,113,113 | 1.51 | 15 (22%) |
| 27 | SQD | b | 601 | - | 48,49,54 | 1.01 | 2 (4%) | 57,60,65 | 2.23 | 17 (29%) |
| 23 | CLA | C | 514 | - | 59,73,73 | 1.47 | 9 (15%) | 67,113,113 | 1.73 | 13 (19%) |
| 23 | CLA | b | 617 | - | 54,68,73 | 1.55 | 9 (16%) | 61,107,113 | 1.73 | 11 (18%) |
| 23 | CLA | D | 404 | - | 59,73,73 | 1.39 | 9 (15%) | 67,113,113 | 1.40 | 10 (14%) |
| 23 | CLA | A | 404 | - | 59,73,73 | 1.58 | 9 (15%) | 67,113,113 | 1.46 | 8 (11%) |
| 23 | CLA | c | 505 | - | 59,73,73 | 1.61 | 6 (10%) | 67,113,113 | 1.42 | 10 (14%) |
| 23 | CLA | c | 511 | 3 | 59,73,73 | 1.79 | 6 (10%) | 67,113,113 | 1.56 | 10 (14%) |
| 23 | CLA | c | 506 | - | 59,73,73 | 1.41 | 10 (16%) | 67,113,113 | 1.63 | 13 (19%) |
| 23 | CLA | b | 610 | - | 59,73,73 | 1.46 | 9 (15%) | 67,113,113 | 1.40 | 11 (16%) |
| 23 | CLA | A | 407 | - | 48,62,73 | 1.55 | 10 (20%) | 53,99,113 | 1.94 | 13 (24%) |
| 29 | LHG | D | 409 | - | 46,46,48 | 1.07 | 3 (6%) | 49,52,54 | 1.28 | 5 (10%) |
| 28 | DGD | A | 412 | - | 67,67,67 | 1.41 | 12 (17%) | 81,81,81 | 1.37 | 6 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | DGD | h | 101 | - | 63,63,67 | 1.20 | 6 (9%) | 77,77,81 | 1.59 | 17 (22%) |
| 28 | DGD | a | 413 | - | 43,43,67 | 1.46 | 4 (9%) | 45,45,81 | 1.22 | 5 (11%) |
| 33 | LMG | M | 101 | - | 51,51,55 | 0.98 | 2 (3%) | 59,59,63 | 1.48 | 9 (15%) |
| 23 | CLA | B | 609 | - | 59,73,73 | 1.66 | 11 (18%) | 67,113,113 | 1.71 | 16 (23%) |
| 23 | CLA | c | 512 | - | 59,73,73 | 1.52 | 6 (10%) | 67,113,113 | 1.48 | 11 (16%) |
| 23 | CLA | C | 509 | - | 59,73,73 | 1.62 | 9 (15%) | 67,113,113 | 1.79 | 14 (20%) |
| 27 | SQD | a | 411 | - | 53,54,54 | 0.99 | 5 (9%) | 62,65,65 | 1.90 | 9 (14%) |
| 23 | CLA | B | 602 | - | 59,73,73 | 1.56 | 8 (13%) | 67,113,113 | 1.36 | 9 (13%) |
| 33 | LMG | c | 522 | - | 48,48,55 | 1.19 | 6 (12%) | 56,56,63 | 1.36 | 5 (8%) |
| 23 | CLA | B | 603 | - | 59,73,73 | 1.57 | 10 (16%) | 67,113,113 | 1.70 | 13 (19%) |
| 26 | PL9 | A | 409 | - | 55,55,55 | 1.34 | 5 (9%) | 68,69,69 | 1.44 | 8 (11%) |
| 23 | CLA | B | 615 | - | 59,73,73 | 1.97 | 10 (16%) | 67,113,113 | 1.48 | 13 (19%) |
| 25 | BCR | c | 515 | - | 41,41,41 | 1.21 | 4 (9%) | 56,56,56 | 1.42 | 12 (21%) |
| 23 | CLA | C | 502 | - | 59,73,73 | 1.78 | 7 (11%) | 67,113,113 | 1.97 | 14 (20%) |
| 33 | LMG | b | 622 | - | 55,55,55 | 1.06 | 4 (7%) | 63,63,63 | 1.56 | 5 (7%) |
| 23 | CLA | B | 614 | - | 59,73,73 | 1.60 | 9 (15%) | 67,113,113 | 1.83 | 12 (17%) |
| 23 | CLA | b | 613 | - | 59,73,73 | 1.19 | 8 (13%) | 67,113,113 | 1.97 | 16 (23%) |
| 23 | CLA | b | 611 | 36 | 59,73,73 | 1.41 | 9 (15%) | 67,113,113 | 1.42 | 13 (19%) |
| 29 | LHG | l | 101 | - | 48,48,48 | 0.79 | 2 (4%) | 51,54,54 | 1.16 | 3 (5%) |
| 29 | LHG | d | 407 | - | 48,48,48 | 0.81 | 0 | 51,54,54 | 1.31 | 5 (9%) |
| 23 | CLA | C | 506 | - | 59,73,73 | 1.40 | 6 (10%) | 67,113,113 | 1.69 | 14 (20%) |
| 23 | CLA | c | 503 | - | 59,73,73 | 1.83 | 9 (15%) | 67,113,113 | 1.48 | 9 (13%) |
| 23 | CLA | A | 405 | 36 | 59,73,73 | 1.55 | 7 (11%) | 67,113,113 | 1.63 | 11 (16%) |
| 28 | DGD | C | 516 | - | 63,63,67 | 1.38 | 7 (11%) | 77,77,81 | 1.33 | 10 (12%) |
| 33 | LMG | c | 524 | - | 49,49,55 | 1.16 | 4 (8%) | 57,57,63 | 1.29 | 4 (7%) |
| 28 | DGD | C | 517 | - | 63,63,67 | 1.24 | 10 (15%) | 77,77,81 | 1.56 | 12 (15%) |
| 33 | LMG | d | 410 | - | 18,21,55 | 0.83 | 0 | 16,20,63 | 0.79 | 0 |
| 25 | BCR | a | 409 | - | 41,41,41 | 1.11 | 3 (7%) | 56,56,56 | 1.33 | 6 (10%) |
| 29 | LHG | e | 101 | - | 41,41,48 | 0.87 | 3 (7%) | 44,47,54 | 1.37 | 6 (13%) |
| 23 | CLA | C | 503 | - | 59,73,73 | 1.33 | 7 (11%) | 67,113,113 | 1.57 | 10 (14%) |
| 23 | CLA | B | 612 | - | 59,73,73 | 1.21 | 5 (8%) | 67,113,113 | 1.75 | 15 (22%) |
| 33 | LMG | d | 411 | - | 44,44,55 | 1.21 | 4 (9%) | 52,52,63 | 1.49 | 6 (11%) |
| 28 | DGD | H | 102 | - | 63,63,67 | 1.34 | 13 (20%) | 77,77,81 | 1.50 | 12 (15%) |
| 23 | CLA | c | 507 | 36 | 59,73,73 | 1.44 | 9 (15%) | 67,113,113 | 1.66 | 13 (19%) |
| 25 | BCR | c | 521 | - | 41,41,41 | 0.97 | 2 (4%) | 56,56,56 | 1.18 | 5 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | CLA | B | 610 | 36 | 59,73,73 | 1.52 | 8 (13%) | 67,113,113 | 1.65 | 10 (14%) |
| 23 | CLA | a | 406 | 36 | 59,73,73 | 1.33 | 8 (13%) | 67,113,113 | 1.95 | 16 (23%) |
| 25 | BCR | K | 101 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.27 | 7 (12%) |
| 31 | BCT | a | 404 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 23 | CLA | B | 604 | - | 59,73,73 | 1.65 | 8 (13%) | 67,113,113 | 1.57 | 9 (13%) |
| 23 | CLA | B | 611 | - | 59,73,73 | 1.54 | 9 (15%) | 67,113,113 | 1.56 | 11 (16%) |
| 27 | SQD | A | 410 | - | 51,52,54 | 1.10 | 6 (11%) | 60,63,65 | 2.10 | 12 (20%) |
| 33 | LMG | c | 519 | - | 37,37,55 | 1.13 | 4 (10%) | 45,45,63 | 1.30 | 6 (13%) |
| 23 | CLA | D | 402 | 36 | 59,73,73 | 1.30 | 7 (11%) | 67,113,113 | 1.27 | 9 (13%) |
| 25 | BCR | t | 101 | - | 41,41,41 | 1.06 | 3 (7%) | 56,56,56 | 1.44 | 13 (23%) |
| 29 | LHG | d | 408 | - | 48,48,48 | 0.68 | 0 | 51,54,54 | 1.20 | 4 (7%) |
| 27 | SQD | B | 621 | - | 53,54,54 | 0.96 | 3 (5%) | 62,65,65 | 1.83 | 15 (24%) |
| 23 | CLA | b | 614 | - | 59,73,73 | 1.44 | 8 (13%) | 67,113,113 | 1.75 | 14 (20%) |
| 25 | BCR | b | 619 | - | 41,41,41 | 1.29 | 2 (4%) | 56,56,56 | 1.31 | 7 (12%) |
| 23 | CLA | b | 604 | - | 59,73,73 | 1.54 | 9 (15%) | 67,113,113 | 1.61 | 11 (16%) |
| 24 | PHO | D | 401 | - | 67,69,69 | 1.28 | 9 (13%) | 85,99,99 | 1.19 | 8 (9%) |
| 23 | CLA | b | 608 | 36 | 59,73,73 | 1.31 | 8 (13%) | 67,113,113 | 1.43 | 11 (16%) |
| 23 | CLA | C | 511 | - | 59,73,73 | 1.46 | 8 (13%) | 67,113,113 | 1.56 | 8 (11%) |
| 23 | CLA | B | 616 | - | 54,68,73 | 1.60 | 9 (16%) | 61,107,113 | 1.64 | 12 (19%) |
| 25 | BCR | T | 101 | - | 41,41,41 | 1.19 | 4 (9%) | 56,56,56 | 1.45 | 9 (16%) |
| 23 | CLA | a | 408 | - | 59,73,73 | 1.72 | 9 (15%) | 67,113,113 | 1.46 | 13 (19%) |
| 30 | OEX | A | 414 | 1,3,36 | 0,15,15 | 0.00 | - | - | - | - |
| 25 | BCR | b | 618 | - | 41,41,41 | 1.16 | 3 (7%) | 56,56,56 | 1.28 | 6 (10%) |
| 23 | CLA | C | 507 | - | 59,73,73 | 1.56 | 9 (15%) | 67,113,113 | 1.59 | 16 (23%) |
| 34 | HEM | e | 102 | 6,5 | 27,50,50 | 1.84 | 4 (14%) | 17,82,82 | 2.26 | 5 (29%) |
| 26 | PL9 | a | 410 | - | 55,55,55 | 1.27 | 5 (9%) | 68,69,69 | 1.55 | 16 (23%) |
| 25 | BCR | B | 618 | - | 41,41,41 | 1.37 | 4 (9%) | 56,56,56 | 1.44 | 7 (12%) |
| 23 | CLA | d | 403 | - | 59,73,73 | 1.42 | 8 (13%) | 67,113,113 | 1.32 | 7 (10%) |
| 25 | BCR | d | 405 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.20 | 8 (14%) |
| 31 | BCT | A | 415 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 29 | LHG | D | 408 | - | 48,48,48 | 1.04 | 3 (6%) | 51,54,54 | 1.26 | 6 (11%) |
| 25 | BCR | Z | 101 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.43 | 10 (17%) |
| 24 | PHO | d | 401 | - | 67,69,69 | 1.27 | 9 (13%) | 85,99,99 | 1.22 | 9 (10%) |
| 23 | CLA | c | 508 | - | 58,72,73 | 1.34 | 8 (13%) | 65,111,113 | 1.41 | 11 (16%) |
| 25 | BCR | A | 408 | - | 41,41,41 | 1.18 | 3 (7%) | 56,56,56 | 1.51 | 10 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | PHO | a | 407 | - | 67,69,69 | 1.16 | 7 (10%) | 85,99,99 | 1.08 | 5 (5%) |
| 23 | CLA | B | 608 | - | 59,73,73 | 1.33 | 10 (16%) | 67,113,113 | 1.40 | 11 (16%) |
| 23 | CLA | b | 602 | 36 | 59,73,73 | 1.82 | 10 (16%) | 67,113,113 | 1.51 | 14 (20%) |
| 33 | LMG | D | 407 | - | 51,51,55 | 1.01 | 5 (9%) | 59,59,63 | 1.20 | 3 (5%) |
| 29 | LHG | L | 101 | - | 48,48,48 | 0.93 | 4 (8%) | 51,54,54 | 1.08 | 2 (3%) |
| 23 | CLA | C | 513 | - | 59,73,73 | 1.48 | 9 (15%) | 67,113,113 | 1.51 | 14 (20%) |
| 35 | HEC | v | 201 | 16 | 26,50,50 | 2.66 | 4 (15%) | 18,82,82 | 1.44 | 3 (16%) |
| 30 | OEX | a | 415 | 1,3,36 | 0,15,15 | 0.00 | - | - | | |
| 23 | CLA | C | 508 | 36 | 59,73,73 | 1.58 | 10 (16%) | 67,113,113 | 1.39 | 9 (13%) |
| 23 | CLA | b | 615 | - | 59,73,73 | 1.53 | 7 (11%) | 67,113,113 | 1.65 | 15 (22%) |
| 25 | BCR | C | 515 | - | 41,41,41 | 1.26 | 5 (12%) | 56,56,56 | 1.33 | 8 (14%) |
| 26 | PL9 | D | 406 | - | 55,55,55 | 1.58 | 9 (16%) | 68,69,69 | 1.65 | 14 (20%) |
| 33 | LMG | C | 501 | - | 48,48,55 | 1.17 | 6 (12%) | 56,56,63 | 1.37 | 10 (17%) |
| 24 | PHO | A | 406 | - | 67,69,69 | 1.28 | 10 (14%) | 85,99,99 | 1.04 | 4 (4%) |
| 23 | CLA | B | 607 | 36 | 59,73,73 | 1.30 | 10 (16%) | 67,113,113 | 1.36 | 9 (13%) |
| 23 | CLA | c | 502 | - | 59,73,73 | 1.33 | 5 (8%) | 67,113,113 | 1.69 | 12 (17%) |
| 28 | DGD | c | 516 | - | 63,63,67 | 1.19 | 5 (7%) | 77,77,81 | 1.55 | 15 (19%) |
| 33 | LMG | m | 101 | - | 51,51,55 | 0.96 | 4 (7%) | 59,59,63 | 1.55 | 8 (13%) |
| 23 | CLA | B | 605 | - | 59,73,73 | 1.64 | 9 (15%) | 67,113,113 | 1.50 | 15 (22%) |
| 23 | CLA | c | 501 | - | 59,73,73 | 1.54 | 7 (11%) | 67,113,113 | 2.13 | 11 (16%) |
| 23 | CLA | c | 504 | 36 | 54,68,73 | 1.61 | 7 (12%) | 61,107,113 | 1.55 | 7 (11%) |
| 25 | BCR | x | 102 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.40 | 11 (19%) |
| 25 | BCR | H | 101 | - | 41,41,41 | 1.26 | 3 (7%) | 56,56,56 | 1.34 | 7 (12%) |
| 33 | LMG | D | 411 | - | 20,26,55 | 0.53 | 0 | 18,26,63 | 1.14 | 0 |
| 28 | DGD | c | 518 | - | 63,63,67 | 1.27 | 9 (14%) | 77,77,81 | 1.53 | 12 (15%) |
| 25 | BCR | B | 617 | - | 41,41,41 | 1.28 | 4 (9%) | 56,56,56 | 1.39 | 9 (16%) |
| 23 | CLA | B | 613 | - | 59,73,73 | 1.49 | 9 (15%) | 67,113,113 | 1.81 | 16 (23%) |
| 23 | CLA | b | 612 | - | 59,73,73 | 1.54 | 10 (16%) | 67,113,113 | 1.45 | 15 (22%) |
| 35 | HEC | V | 201 | 16 | 26,50,50 | 2.60 | 6 (23%) | 18,82,82 | 1.75 | 3 (16%) |
| 23 | CLA | b | 607 | - | 59,73,73 | 1.52 | 8 (13%) | 67,113,113 | 1.56 | 14 (20%) |
| 27 | SQD | A | 411 | - | 38,38,54 | 1.09 | 4 (10%) | 40,40,65 | 1.47 | 4 (10%) |
| 28 | DGD | c | 517 | - | 63,63,67 | 1.19 | 6 (9%) | 77,77,81 | 1.34 | 8 (10%) |
| 34 | HEM | E | 103 | 6,5 | 27,50,50 | 1.91 | 5 (18%) | 17,82,82 | 1.98 | 6 (35%) |
| 23 | CLA | C | 505 | 36 | 53,67,73 | 1.51 | 8 (15%) | 59,105,113 | 1.45 | 10 (16%) |
| 25 | BCR | c | 514 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.39 | 8 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | CLA | d | 404 | - | 59,73,73 | 1.60 | 8 (13%) | 67,113,113 | 1.55 | 10 (14%) |
| 33 | LMG | D | 410 | - | 31,31,55 | 1.15 | 3 (9%) | 33,33,63 | 1.11 | 2 (6%) |
| 25 | BCR | k | 101 | - | 41,41,41 | 1.08 | 3 (7%) | 56,56,56 | 1.13 | 3 (5%) |
| 23 | CLA | B | 606 | - | 59,73,73 | 1.63 | 10 (16%) | 67,113,113 | 1.83 | 15 (22%) |
| 25 | BCR | b | 620 | - | 41,41,41 | 1.07 | 3 (7%) | 56,56,56 | 1.29 | 8 (14%) |
| 23 | CLA | b | 616 | - | 59,73,73 | 2.17 | 7 (11%) | 67,113,113 | 1.63 | 11 (16%) |
| 23 | CLA | b | 605 | - | 59,73,73 | 1.25 | 5 (8%) | 67,113,113 | 1.97 | 17 (25%) |
| 27 | SQD | a | 412 | - | 35,35,54 | 1.06 | 2 (5%) | 37,37,65 | 1.44 | 5 (13%) |
| 23 | CLA | B | 601 | 36 | 59,73,73 | 1.80 | 9 (15%) | 67,113,113 | 1.39 | 10 (14%) |
| 23 | CLA | b | 603 | - | 59,73,73 | 1.59 | 10 (16%) | 67,113,113 | 1.62 | 14 (20%) |
| 23 | CLA | C | 512 | 3 | 59,73,73 | 1.83 | 7 (11%) | 67,113,113 | 1.65 | 10 (14%) |
| 29 | LHG | d | 409 | - | 38,38,48 | 0.86 | 2 (5%) | 41,44,54 | 1.11 | 3 (7%) |
| 25 | BCR | B | 619 | - | 41,41,41 | 1.18 | 4 (9%) | 56,56,56 | 1.25 | 7 (12%) |
| 25 | BCR | C | 520 | - | 41,41,41 | 1.03 | 3 (7%) | 56,56,56 | 1.36 | 7 (12%) |
| 27 | SQD | f | 101 | - | 40,41,54 | 1.12 | 5 (12%) | 49,52,65 | 1.80 | 13 (26%) |
| 23 | CLA | C | 504 | - | 59,73,73 | 1.77 | 8 (13%) | 67,113,113 | 1.97 | 19 (28%) |
| 23 | CLA | c | 509 | - | 59,73,73 | 1.50 | 6 (10%) | 67,113,113 | 1.97 | 12 (17%) |
| 23 | CLA | D | 403 | - | 59,73,73 | 1.28 | 7 (11%) | 67,113,113 | 1.67 | 9 (13%) |
| 26 | PL9 | d | 406 | - | 55,55,55 | 1.36 | 7 (12%) | 68,69,69 | 1.79 | 19 (27%) |

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 |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CLA | c | 510 | - | 3/3/25/25 | 15/37/135/135 | - |
| 23 | CLA | a | 405 | - | 2/2/25/25 | 6/37/135/135 | - |
| 33 | LMG | C | 519 | - | - | 16/43/63/70 | 0/1/1/1 |
| 23 | CLA | d | 402 | 36 | 3/3/25/25 | 4/37/135/135 | - |
| 23 | CLA | c | 513 | - | 3/3/25/25 | 10/37/135/135 | - |
| 28 | DGD | C | 518 | - | - | 15/51/91/95 | 0/2/2/2 |
| 23 | CLA | b | 606 | - | 3/3/25/25 | 8/37/135/135 | - |
| 29 | LHG | A | 413 | - | - | 15/53/53/53 | - |
| 27 | SQD | F | 101 | - | - | 13/28/48/69 | 0/1/1/1 |
| 23 | CLA | C | 510 | - | 3/3/25/25 | 9/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25 | BCR | D | 405 | - | - | 3/29/63/63 | 0/2/2/2 |
| 29 | LHG | E | 101 | - | - | 27/53/53/53 | - |
| 23 | CLA | b | 609 | - | 2/2/25/25 | 6/37/135/135 | - |
| 27 | SQD | b | 601 | - | - | 21/44/64/69 | 0/1/1/1 |
| 23 | CLA | C | 514 | - | 3/3/25/25 | 13/37/135/135 | - |
| 23 | CLA | b | 617 | - | 3/3/24/25 | 6/31/129/135 | - |
| 23 | CLA | D | 404 | - | 2/2/25/25 | 12/37/135/135 | - |
| 23 | CLA | A | 404 | - | 3/3/25/25 | 4/37/135/135 | - |
| 23 | CLA | c | 505 | - | 2/2/25/25 | 10/37/135/135 | - |
| 23 | CLA | c | 511 | 3 | 3/3/25/25 | 10/37/135/135 | - |
| 23 | CLA | c | 506 | - | 2/2/25/25 | 17/37/135/135 | - |
| 23 | CLA | b | 610 | - | 2/2/25/25 | 13/37/135/135 | - |
| 23 | CLA | A | 407 | - | 3/3/22/25 | 6/24/122/135 | - |
| 29 | LHG | D | 409 | - | - | 23/51/51/53 | - |
| 28 | DGD | A | 412 | - | - | 28/55/95/95 | 0/2/2/2 |
| 28 | DGD | h | 101 | - | - | 17/51/91/95 | 0/2/2/2 |
| 28 | DGD | a | 413 | - | - | 21/45/45/95 | - |
| 33 | LMG | M | 101 | - | - | 19/46/66/70 | 0/1/1/1 |
| 23 | CLA | B | 609 | - | 2/2/25/25 | 6/37/135/135 | - |
| 23 | CLA | c | 512 | - | 3/3/25/25 | 23/37/135/135 | - |
| 23 | CLA | C | 509 | - | 3/3/25/25 | 6/37/135/135 | - |
| 27 | SQD | a | 411 | - | - | 22/49/69/69 | 0/1/1/1 |
| 23 | CLA | B | 602 | - | 3/3/25/25 | 7/37/135/135 | - |
| 33 | LMG | c | 522 | - | - | 21/43/63/70 | 0/1/1/1 |
| 23 | CLA | B | 603 | - | 3/3/25/25 | 11/37/135/135 | - |
| 26 | PL9 | A | 409 | - | - | 19/53/73/73 | 0/1/1/1 |
| 23 | CLA | B | 615 | - | 3/3/25/25 | 7/37/135/135 | - |
| 25 | BCR | c | 515 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CLA | C | 502 | - | 3/3/25/25 | 4/37/135/135 | - |
| 33 | LMG | b | 622 | - | - | 20/50/70/70 | 0/1/1/1 |
| 23 | CLA | B | 614 | - | 3/3/25/25 | 13/37/135/135 | - |
| 23 | CLA | b | 613 | - | 3/3/25/25 | 11/37/135/135 | - |
| 23 | CLA | b | 611 | 36 | 3/3/25/25 | 1/37/135/135 | - |
| 29 | LHG | l | 101 | - | - | 16/53/53/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 29 | LHG | d | 407 | - | - | 21/53/53/53 | - |
| 23 | CLA | C | 506 | - | 3/3/25/25 | 13/37/135/135 | - |
| 23 | CLA | c | 503 | - | 3/3/25/25 | 9/37/135/135 | - |
| 23 | CLA | A | 405 | 36 | 3/3/25/25 | 4/37/135/135 | - |
| 28 | DGD | C | 516 | - | - | 24/51/91/95 | 0/2/2/2 |
| 33 | LMG | c | 524 | - | - | 16/44/64/70 | 0/1/1/1 |
| 28 | DGD | C | 517 | - | - | 20/51/91/95 | 0/2/2/2 |
| 33 | LMG | d | 410 | - | - | 13/15/17/70 | - |
| 25 | BCR | a | 409 | - | - | 2/29/63/63 | 0/2/2/2 |
| 29 | LHG | e | 101 | - | - | 30/46/46/53 | - |
| 23 | CLA | C | 503 | - | 3/3/25/25 | 12/37/135/135 | - |
| 23 | CLA | B | 612 | - | 3/3/25/25 | 19/37/135/135 | - |
| 33 | LMG | d | 411 | - | - | 8/39/59/70 | 0/1/1/1 |
| 28 | DGD | H | 102 | - | - | 16/51/91/95 | 0/2/2/2 |
| 23 | CLA | c | 507 | 36 | 3/3/25/25 | 10/37/135/135 | - |
| 25 | BCR | c | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 610 | 36 | 3/3/25/25 | 10/37/135/135 | - |
| 23 | CLA | a | 406 | 36 | 3/3/25/25 | 12/37/135/135 | - |
| 25 | BCR | K | 101 | - | - | 13/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 604 | - | 2/2/25/25 | 13/37/135/135 | - |
| 23 | CLA | B | 611 | - | 3/3/25/25 | 6/37/135/135 | - |
| 27 | SQD | A | 410 | - | - | 18/47/67/69 | 0/1/1/1 |
| 33 | LMG | c | 519 | - | - | 12/31/51/70 | 0/1/1/1 |
| 23 | CLA | D | 402 | 36 | 2/2/25/25 | 5/37/135/135 | - |
| 25 | BCR | t | 101 | - | - | 7/29/63/63 | 0/2/2/2 |
| 29 | LHG | d | 408 | - | - | 19/53/53/53 | - |
| 27 | SQD | B | 621 | - | - | 23/49/69/69 | 0/1/1/1 |
| 23 | CLA | b | 614 | - | 3/3/25/25 | 10/37/135/135 | - |
| 25 | BCR | b | 619 | - | - | 13/29/63/63 | 0/2/2/2 |
| 23 | CLA | b | 604 | - | 3/3/25/25 | 10/37/135/135 | - |
| 24 | PHO | D | 401 | - | - | 2/53/103/103 | 0/5/6/6 |
| 23 | CLA | b | 608 | 36 | 3/3/25/25 | 15/37/135/135 | - |
| 23 | CLA | C | 511 | - | 3/3/25/25 | 14/37/135/135 | - |
| 23 | CLA | B | 616 | - | 3/3/24/25 | 8/31/129/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25 | BCR | T | 101 | - | - | 2/29/63/63 | 0/2/2/2 |
| 23 | CLA | a | 408 | - | 3/3/25/25 | 8/37/135/135 | - |
| 25 | BCR | b | 618 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CLA | C | 507 | - | 1/1/25/25 | 19/37/135/135 | - |
| 34 | HEM | e | 102 | 6,5 | - | 0/6/54/54 | - |
| 26 | PL9 | a | 410 | - | - | 20/53/73/73 | 0/1/1/1 |
| 25 | BCR | B | 618 | - | - | 3/29/63/63 | 0/2/2/2 |
| 23 | CLA | d | 403 | - | 1/1/25/25 | 8/37/135/135 | - |
| 25 | BCR | d | 405 | - | - | 13/29/63/63 | 0/2/2/2 |
| 29 | LHG | D | 408 | - | - | 26/53/53/53 | - |
| 25 | BCR | Z | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 24 | PHO | d | 401 | - | - | 4/53/103/103 | 0/5/6/6 |
| 23 | CLA | c | 508 | - | 1/1/24/25 | 15/36/134/135 | - |
| 25 | BCR | A | 408 | - | - | 7/29/63/63 | 0/2/2/2 |
| 24 | PHO | a | 407 | - | - | 6/53/103/103 | 0/5/6/6 |
| 23 | CLA | B | 608 | - | 2/2/25/25 | 0/37/135/135 | - |
| 23 | CLA | b | 602 | 36 | 2/2/25/25 | 16/37/135/135 | - |
| 33 | LMG | D | 407 | - | - | 18/46/66/70 | 0/1/1/1 |
| 29 | LHG | L | 101 | - | - | 23/53/53/53 | - |
| 23 | CLA | C | 513 | - | 3/3/25/25 | 11/37/135/135 | - |
| 35 | HEC | v | 201 | 16 | - | 0/6/54/54 | - |
| 23 | CLA | C | 508 | 36 | 3/3/25/25 | 7/37/135/135 | - |
| 23 | CLA | b | 615 | - | 3/3/25/25 | 15/37/135/135 | - |
| 25 | BCR | C | 515 | - | - | 7/29/63/63 | 0/2/2/2 |
| 26 | PL9 | D | 406 | - | - | 11/53/73/73 | 0/1/1/1 |
| 33 | LMG | C | 501 | - | - | 21/43/63/70 | 0/1/1/1 |
| 24 | PHO | A | 406 | - | - | 9/53/103/103 | 0/5/6/6 |
| 23 | CLA | B | 607 | 36 | 3/3/25/25 | 9/37/135/135 | - |
| 23 | CLA | c | 502 | - | 2/2/25/25 | 8/37/135/135 | - |
| 28 | DGD | c | 516 | - | - | 23/51/91/95 | 0/2/2/2 |
| 33 | LMG | m | 101 | - | - | 21/46/66/70 | 0/1/1/1 |
| 23 | CLA | B | 605 | - | 3/3/25/25 | 12/37/135/135 | - |
| 23 | CLA | c | 501 | - | 3/3/25/25 | 6/37/135/135 | - |
| 23 | CLA | c | 504 | 36 | 3/3/24/25 | 9/31/129/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25 | BCR | x | 102 | - | - | 11/29/63/63 | 0/2/2/2 |
| 25 | BCR | H | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 33 | LMG | D | 411 | - | - | 11/18/22/70 | - |
| 28 | DGD | c | 518 | - | - | 22/51/91/95 | 0/2/2/2 |
| 25 | BCR | B | 617 | - | - | 11/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 613 | - | 3/3/25/25 | 6/37/135/135 | - |
| 23 | CLA | b | 612 | - | 3/3/25/25 | 14/37/135/135 | - |
| 35 | HEC | V | 201 | 16 | - | 0/6/54/54 | - |
| 23 | CLA | b | 607 | - | 3/3/25/25 | 11/37/135/135 | - |
| 27 | SQD | A | 411 | - | - | 14/39/39/69 | - |
| 28 | DGD | c | 517 | - | - | 19/51/91/95 | 0/2/2/2 |
| 34 | HEM | E | 103 | 6,5 | - | 0/6/54/54 | - |
| 23 | CLA | C | 505 | 36 | 3/3/23/25 | 8/30/128/135 | - |
| 25 | BCR | c | 514 | - | - | 15/29/63/63 | 0/2/2/2 |
| 23 | CLA | d | 404 | - | 3/3/25/25 | 7/37/135/135 | - |
| 33 | LMG | D | 410 | - | - | 17/33/33/70 | - |
| 25 | BCR | k | 101 | - | - | 13/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 606 | - | 3/3/25/25 | 13/37/135/135 | - |
| 25 | BCR | b | 620 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CLA | b | 616 | - | 3/3/25/25 | 8/37/135/135 | - |
| 23 | CLA | b | 605 | - | 3/3/25/25 | 11/37/135/135 | - |
| 27 | SQD | a | 412 | - | - | 19/37/37/69 | - |
| 23 | CLA | B | 601 | 36 | 3/3/25/25 | 12/37/135/135 | - |
| 23 | CLA | b | 603 | - | 3/3/25/25 | 10/37/135/135 | - |
| 23 | CLA | C | 512 | 3 | 3/3/25/25 | 7/37/135/135 | - |
| 29 | LHG | d | 409 | - | - | 11/43/43/53 | - |
| 25 | BCR | B | 619 | - | - | 5/29/63/63 | 0/2/2/2 |
| 25 | BCR | C | 520 | - | - | 11/29/63/63 | 0/2/2/2 |
| 27 | SQD | f | 101 | - | - | 16/36/56/69 | 0/1/1/1 |
| 23 | CLA | C | 504 | - | 1/1/25/25 | 7/37/135/135 | - |
| 23 | CLA | c | 509 | - | 3/3/25/25 | 15/37/135/135 | - |
| 23 | CLA | D | 403 | - | 1/1/25/25 | 10/37/135/135 | - |
| 26 | PL9 | d | 406 | - | - | 18/53/73/73 | 0/1/1/1 |

All (892) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | b | 616 | CLA | MG-NA | 11.51 | 2.33 | 2.06 |
| 23 | B | 615 | CLA | C4B-NB | 9.83 | 1.44 | 1.35 |
| 23 | c | 503 | CLA | C4B-NB | 9.41 | 1.43 | 1.35 |
| 23 | C | 512 | CLA | MG-NA | 8.81 | 2.27 | 2.06 |
| 35 | v | 201 | HEC | C3B-C2B | -8.55 | 1.31 | 1.40 |
| 23 | c | 504 | CLA | C4B-NB | 8.29 | 1.42 | 1.35 |
| 23 | B | 601 | CLA | C4B-NB | 8.29 | 1.42 | 1.35 |
| 23 | C | 504 | CLA | MG-NA | 8.14 | 2.25 | 2.06 |
| 23 | c | 505 | CLA | C4B-NB | 8.10 | 1.42 | 1.35 |
| 23 | c | 511 | CLA | C4B-NB | 8.10 | 1.42 | 1.35 |
| 35 | V | 201 | HEC | C3B-C2B | -7.99 | 1.32 | 1.40 |
| 23 | B | 614 | CLA | C4B-NB | 7.95 | 1.42 | 1.35 |
| 23 | B | 616 | CLA | C4B-NB | 7.80 | 1.42 | 1.35 |
| 23 | a | 405 | CLA | C4B-NB | 7.73 | 1.42 | 1.35 |
| 23 | d | 404 | CLA | C4B-NB | 7.72 | 1.42 | 1.35 |
| 23 | C | 502 | CLA | MG-NA | 7.70 | 2.24 | 2.06 |
| 23 | c | 512 | CLA | C4B-NB | 7.69 | 1.42 | 1.35 |
| 23 | b | 615 | CLA | C4B-NB | 7.68 | 1.42 | 1.35 |
| 23 | b | 603 | CLA | C4B-NB | 7.64 | 1.42 | 1.35 |
| 23 | C | 502 | CLA | C4B-NB | 7.60 | 1.42 | 1.35 |
| 23 | b | 602 | CLA | C4B-NB | 7.57 | 1.42 | 1.35 |
| 23 | B | 610 | CLA | C4B-NB | 7.57 | 1.42 | 1.35 |
| 23 | B | 604 | CLA | MG-NA | 7.45 | 2.24 | 2.06 |
| 23 | B | 602 | CLA | C4B-NB | 7.36 | 1.41 | 1.35 |
| 23 | b | 616 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 23 | b | 606 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 23 | C | 512 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 35 | V | 201 | HEC | C3C-C2C | -7.31 | 1.33 | 1.40 |
| 23 | a | 408 | CLA | MG-NC | -7.30 | 1.88 | 2.06 |
| 23 | d | 402 | CLA | C4B-NB | 7.24 | 1.41 | 1.35 |
| 23 | b | 610 | CLA | C4B-NB | 7.17 | 1.41 | 1.35 |
| 23 | b | 604 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 23 | b | 602 | CLA | MG-NA | 7.14 | 2.23 | 2.06 |
| 23 | B | 605 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 23 | c | 511 | CLA | MG-NA | 7.07 | 2.23 | 2.06 |
| 23 | C | 504 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 23 | B | 609 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 23 | c | 501 | CLA | MG-NA | 6.90 | 2.22 | 2.06 |
| 23 | C | 510 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 23 | c | 509 | CLA | C4B-NB | 6.80 | 1.41 | 1.35 |
| 23 | A | 404 | CLA | C4B-NB | 6.79 | 1.41 | 1.35 |
| 23 | C | 506 | CLA | C4B-NB | 6.71 | 1.41 | 1.35 |
| 35 | v | 201 | HEC | C3C-C2C | -6.66 | 1.33 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | C | 511 | CLA | C4B-NB | 6.61 | 1.41 | 1.35 |
| 23 | B | 603 | CLA | MG-NA | 6.61 | 2.22 | 2.06 |
| 23 | C | 514 | CLA | C4B-NB | 6.50 | 1.41 | 1.35 |
| 23 | c | 513 | CLA | C4B-NB | 6.46 | 1.41 | 1.35 |
| 23 | C | 508 | CLA | C4B-NB | 6.43 | 1.40 | 1.35 |
| 23 | b | 607 | CLA | C4B-NB | 6.41 | 1.40 | 1.35 |
| 23 | C | 509 | CLA | C4B-NB | 6.36 | 1.40 | 1.35 |
| 23 | B | 606 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 23 | B | 611 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 23 | b | 614 | CLA | C4B-NB | 6.23 | 1.40 | 1.35 |
| 23 | B | 613 | CLA | C4B-NB | 6.23 | 1.40 | 1.35 |
| 23 | C | 507 | CLA | C4B-NB | 6.22 | 1.40 | 1.35 |
| 23 | B | 601 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 23 | C | 505 | CLA | C4B-NB | 6.18 | 1.40 | 1.35 |
| 23 | A | 405 | CLA | C4B-NB | 6.11 | 1.40 | 1.35 |
| 23 | b | 609 | CLA | C4B-NB | 6.11 | 1.40 | 1.35 |
| 23 | C | 503 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 23 | c | 501 | CLA | C4B-NB | 5.81 | 1.40 | 1.35 |
| 23 | d | 403 | CLA | C4B-NB | 5.81 | 1.40 | 1.35 |
| 26 | D | 406 | PL9 | C6-C1 | -5.79 | 1.38 | 1.48 |
| 23 | A | 407 | CLA | C4B-NB | 5.79 | 1.40 | 1.35 |
| 23 | b | 617 | CLA | C4B-NB | 5.78 | 1.40 | 1.35 |
| 23 | a | 408 | CLA | C4B-NB | 5.76 | 1.40 | 1.35 |
| 23 | c | 510 | CLA | C4B-NB | 5.67 | 1.40 | 1.35 |
| 23 | a | 406 | CLA | C4B-NB | 5.66 | 1.40 | 1.35 |
| 23 | B | 615 | CLA | MG-NC | 5.58 | 2.19 | 2.06 |
| 23 | c | 507 | CLA | C4B-NB | 5.50 | 1.40 | 1.35 |
| 23 | b | 605 | CLA | C4B-NB | 5.46 | 1.40 | 1.35 |
| 34 | e | 102 | HEM | C3B-C2B | -5.43 | 1.32 | 1.40 |
| 28 | a | 413 | DGD | O2G-C1B | 5.42 | 1.49 | 1.34 |
| 23 | b | 616 | CLA | MG-NC | -5.41 | 1.93 | 2.06 |
| 23 | d | 402 | CLA | MG-NA | 5.35 | 2.19 | 2.06 |
| 23 | c | 506 | CLA | C4B-NB | 5.33 | 1.40 | 1.35 |
| 23 | B | 606 | CLA | C4B-NB | 5.33 | 1.40 | 1.35 |
| 23 | B | 603 | CLA | C4B-NB | 5.28 | 1.39 | 1.35 |
| 23 | c | 508 | CLA | C4B-NB | 5.28 | 1.39 | 1.35 |
| 26 | A | 409 | PL9 | C7-C3 | -5.23 | 1.46 | 1.51 |
| 23 | c | 502 | CLA | C4B-NB | 5.23 | 1.39 | 1.35 |
| 23 | b | 608 | CLA | C4B-NB | 5.19 | 1.39 | 1.35 |
| 23 | b | 611 | CLA | C4B-NB | 5.18 | 1.39 | 1.35 |
| 23 | C | 513 | CLA | C4B-NB | 5.14 | 1.39 | 1.35 |
| 34 | E | 103 | HEM | C3B-C2B | -5.14 | 1.33 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | A | 405 | CLA | MG-NC | 5.10 | 2.18 | 2.06 |
| 23 | D | 402 | CLA | C4B-NB | 5.10 | 1.39 | 1.35 |
| 23 | B | 609 | CLA | MG-NC | -5.09 | 1.94 | 2.06 |
| 28 | C | 516 | DGD | C4E-C3E | 4.99 | 1.65 | 1.52 |
| 26 | d | 406 | PL9 | C7-C3 | -4.98 | 1.46 | 1.51 |
| 23 | b | 612 | CLA | C4B-NB | 4.94 | 1.39 | 1.35 |
| 23 | b | 607 | CLA | MG-NA | 4.89 | 2.17 | 2.06 |
| 25 | B | 618 | BCR | C30-C25 | -4.86 | 1.47 | 1.53 |
| 23 | b | 612 | CLA | MG-NA | 4.83 | 2.17 | 2.06 |
| 23 | C | 507 | CLA | MG-NA | 4.72 | 2.17 | 2.06 |
| 23 | C | 509 | CLA | MG-NA | 4.70 | 2.17 | 2.06 |
| 33 | d | 411 | LMG | O1-C7 | -4.68 | 1.35 | 1.43 |
| 23 | c | 503 | CLA | MG-NC | 4.67 | 2.17 | 2.06 |
| 34 | E | 103 | HEM | C3C-C2C | -4.64 | 1.33 | 1.40 |
| 23 | B | 607 | CLA | C4B-NB | 4.57 | 1.39 | 1.35 |
| 23 | c | 509 | CLA | MG-NC | 4.53 | 2.17 | 2.06 |
| 23 | B | 613 | CLA | MG-NA | 4.40 | 2.16 | 2.06 |
| 23 | A | 405 | CLA | MG-NA | -4.39 | 1.95 | 2.06 |
| 28 | A | 412 | DGD | C4D-C5D | 4.38 | 1.62 | 1.53 |
| 23 | A | 404 | CLA | MG-NC | -4.30 | 1.96 | 2.06 |
| 23 | B | 606 | CLA | C3B-C2B | -4.29 | 1.34 | 1.40 |
| 25 | B | 617 | BCR | C1-C6 | -4.23 | 1.48 | 1.53 |
| 23 | B | 611 | CLA | C4B-NB | 4.20 | 1.39 | 1.35 |
| 25 | K | 101 | BCR | C1-C6 | -4.19 | 1.48 | 1.53 |
| 23 | B | 612 | CLA | C4B-NB | 4.18 | 1.38 | 1.35 |
| 25 | b | 619 | BCR | C30-C25 | -4.18 | 1.48 | 1.53 |
| 23 | C | 508 | CLA | MG-NA | 4.18 | 2.16 | 2.06 |
| 25 | H | 101 | BCR | C1-C6 | -4.15 | 1.48 | 1.53 |
| 23 | B | 608 | CLA | C4B-NB | 4.14 | 1.38 | 1.35 |
| 23 | D | 404 | CLA | C4B-NB | 4.14 | 1.38 | 1.35 |
| 23 | c | 505 | CLA | CHC-C1C | 4.13 | 1.45 | 1.35 |
| 29 | D | 409 | LHG | P-O6 | 4.11 | 1.76 | 1.59 |
| 23 | C | 514 | CLA | MG-NC | 4.11 | 2.16 | 2.06 |
| 23 | D | 403 | CLA | C4B-NB | 4.11 | 1.38 | 1.35 |
| 35 | V | 201 | HEC | CBB-CAB | -4.05 | 1.34 | 1.49 |
| 23 | c | 507 | CLA | C3B-C2B | -4.01 | 1.34 | 1.40 |
| 23 | B | 605 | CLA | MG-NC | -3.99 | 1.96 | 2.06 |
| 35 | v | 201 | HEC | CBB-CAB | -3.97 | 1.34 | 1.49 |
| 33 | D | 410 | LMG | C7-C8 | 3.95 | 1.61 | 1.51 |
| 25 | H | 101 | BCR | C30-C25 | -3.94 | 1.48 | 1.53 |
| 35 | v | 201 | HEC | CBC-CAC | -3.93 | 1.34 | 1.49 |
| 23 | b | 617 | CLA | MG-NC | 3.92 | 2.15 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 511 | CLA | CHC-C1C | 3.91 | 1.45 | 1.35 |
| 26 | D | 406 | PL9 | C52-C5 | -3.90 | 1.42 | 1.50 |
| 23 | c | 509 | CLA | CHC-C1C | 3.89 | 1.44 | 1.35 |
| 25 | b | 618 | BCR | C1-C6 | -3.89 | 1.48 | 1.53 |
| 23 | b | 613 | CLA | C4B-NB | 3.88 | 1.38 | 1.35 |
| 25 | K | 101 | BCR | C30-C25 | -3.87 | 1.48 | 1.53 |
| 25 | B | 619 | BCR | C1-C6 | -3.87 | 1.48 | 1.53 |
| 35 | V | 201 | HEC | CBC-CAC | -3.87 | 1.35 | 1.49 |
| 23 | b | 614 | CLA | MG-NA | 3.86 | 2.15 | 2.06 |
| 25 | x | 102 | BCR | C30-C25 | -3.84 | 1.48 | 1.53 |
| 23 | B | 605 | CLA | CHC-C1C | 3.83 | 1.44 | 1.35 |
| 23 | b | 609 | CLA | CHC-C1C | 3.83 | 1.44 | 1.35 |
| 23 | c | 504 | CLA | CHC-C1C | 3.82 | 1.44 | 1.35 |
| 28 | a | 413 | DGD | C3G-C2G | 3.82 | 1.60 | 1.51 |
| 23 | D | 404 | CLA | C3B-C2B | -3.76 | 1.35 | 1.40 |
| 27 | b | 601 | SQD | O48-C23 | 3.76 | 1.44 | 1.33 |
| 34 | e | 102 | HEM | C3C-C2C | -3.75 | 1.35 | 1.40 |
| 23 | B | 611 | CLA | MG-NC | -3.74 | 1.97 | 2.06 |
| 23 | C | 511 | CLA | CHC-C1C | 3.73 | 1.44 | 1.35 |
| 25 | C | 515 | BCR | C1-C6 | -3.71 | 1.48 | 1.53 |
| 33 | c | 524 | LMG | C4-C5 | 3.70 | 1.60 | 1.53 |
| 23 | d | 402 | CLA | CHC-C1C | 3.69 | 1.44 | 1.35 |
| 23 | B | 615 | CLA | CMB-C2B | -3.67 | 1.44 | 1.51 |
| 28 | c | 517 | DGD | C6E-C5E | 3.66 | 1.64 | 1.51 |
| 23 | a | 405 | CLA | C1B-NB | 3.64 | 1.38 | 1.35 |
| 23 | B | 610 | CLA | CHC-C1C | 3.64 | 1.44 | 1.35 |
| 25 | b | 619 | BCR | C1-C6 | -3.62 | 1.48 | 1.53 |
| 28 | A | 412 | DGD | C4E-C5E | 3.59 | 1.60 | 1.53 |
| 23 | b | 615 | CLA | CMB-C2B | -3.58 | 1.44 | 1.51 |
| 28 | H | 102 | DGD | O1G-C1G | -3.58 | 1.37 | 1.45 |
| 28 | h | 101 | DGD | O2D-C2D | -3.57 | 1.34 | 1.43 |
| 23 | c | 513 | CLA | MG-NA | 3.56 | 2.14 | 2.06 |
| 23 | b | 602 | CLA | CHC-C1C | 3.56 | 1.44 | 1.35 |
| 27 | a | 412 | SQD | O48-C23 | 3.54 | 1.43 | 1.33 |
| 23 | b | 611 | CLA | MG-NA | 3.53 | 2.14 | 2.06 |
| 23 | C | 506 | CLA | CHC-C1C | 3.52 | 1.44 | 1.35 |
| 23 | B | 604 | CLA | C4B-NB | 3.52 | 1.38 | 1.35 |
| 23 | C | 513 | CLA | CHC-C1C | 3.52 | 1.44 | 1.35 |
| 23 | B | 604 | CLA | C1D-C2D | 3.51 | 1.50 | 1.42 |
| 25 | A | 408 | BCR | C1-C6 | -3.51 | 1.48 | 1.53 |
| 23 | c | 512 | CLA | CHC-C1C | 3.51 | 1.44 | 1.35 |
| 25 | Z | 101 | BCR | C30-C25 | -3.51 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | D | 406 | PL9 | C11-C9 | -3.50 | 1.44 | 1.51 |
| 23 | B | 616 | CLA | MG-NC | 3.50 | 2.14 | 2.06 |
| 23 | d | 403 | CLA | MG-NA | 3.50 | 2.14 | 2.06 |
| 23 | A | 407 | CLA | MG-NA | -3.49 | 1.98 | 2.06 |
| 23 | A | 404 | CLA | CHC-C1C | 3.49 | 1.43 | 1.35 |
| 23 | C | 505 | CLA | MG-NA | 3.49 | 2.14 | 2.06 |
| 25 | d | 405 | BCR | C1-C6 | -3.47 | 1.49 | 1.53 |
| 29 | D | 408 | LHG | O8-C6 | -3.47 | 1.37 | 1.45 |
| 23 | A | 404 | CLA | MG-NA | 3.47 | 2.14 | 2.06 |
| 23 | C | 502 | CLA | CHC-C1C | 3.46 | 1.43 | 1.35 |
| 23 | B | 614 | CLA | MG-NA | 3.43 | 2.14 | 2.06 |
| 23 | B | 605 | CLA | C3B-C2B | -3.42 | 1.35 | 1.40 |
| 23 | B | 601 | CLA | C3B-C2B | -3.41 | 1.35 | 1.40 |
| 23 | B | 605 | CLA | MG-NA | 3.39 | 2.14 | 2.06 |
| 23 | b | 606 | CLA | MG-NC | -3.39 | 1.98 | 2.06 |
| 23 | C | 508 | CLA | MG-NC | -3.38 | 1.98 | 2.06 |
| 23 | B | 604 | CLA | CHC-C1C | 3.36 | 1.43 | 1.35 |
| 23 | a | 408 | CLA | CMD-C2D | -3.36 | 1.43 | 1.51 |
| 23 | B | 601 | CLA | CMB-C2B | -3.35 | 1.44 | 1.51 |
| 23 | b | 602 | CLA | C1B-NB | 3.35 | 1.38 | 1.35 |
| 28 | c | 518 | DGD | C6D-C5D | 3.34 | 1.62 | 1.51 |
| 23 | b | 603 | CLA | CHC-C1C | 3.34 | 1.43 | 1.35 |
| 23 | B | 605 | CLA | CMB-C2B | -3.33 | 1.44 | 1.51 |
| 23 | C | 512 | CLA | C1D-C2D | 3.33 | 1.50 | 1.42 |
| 27 | A | 411 | SQD | O48-C23 | 3.33 | 1.43 | 1.33 |
| 23 | b | 604 | CLA | MG-NC | 3.33 | 2.14 | 2.06 |
| 23 | C | 513 | CLA | MG-NA | 3.31 | 2.14 | 2.06 |
| 27 | f | 101 | SQD | O47-C7 | 3.31 | 1.43 | 1.34 |
| 28 | c | 517 | DGD | C3E-C2E | 3.30 | 1.60 | 1.52 |
| 24 | a | 407 | PHO | CHD-C4C | -3.30 | 1.32 | 1.40 |
| 23 | B | 601 | CLA | C1D-C2D | 3.30 | 1.50 | 1.42 |
| 23 | c | 506 | CLA | MG-NA | 3.29 | 2.14 | 2.06 |
| 23 | C | 509 | CLA | CMB-C2B | -3.29 | 1.44 | 1.51 |
| 27 | A | 411 | SQD | O47-C7 | 3.29 | 1.43 | 1.34 |
| 23 | c | 505 | CLA | MG-NA | 3.28 | 2.14 | 2.06 |
| 23 | a | 406 | CLA | C3B-C2B | -3.28 | 1.35 | 1.40 |
| 26 | d | 406 | PL9 | C3-C4 | -3.27 | 1.44 | 1.49 |
| 23 | D | 402 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 25 | T | 101 | BCR | C30-C25 | -3.26 | 1.49 | 1.53 |
| 23 | b | 615 | CLA | C1D-C2D | 3.26 | 1.49 | 1.42 |
| 24 | A | 406 | PHO | CHC-C1C | 3.25 | 1.45 | 1.38 |
| 23 | B | 608 | CLA | C1B-NB | -3.25 | 1.32 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | C | 513 | CLA | MG-NC | 3.25 | 2.14 | 2.06 |
| 23 | B | 610 | CLA | CMB-C2B | -3.24 | 1.44 | 1.51 |
| 23 | B | 615 | CLA | C3B-C2B | -3.24 | 1.35 | 1.40 |
| 23 | c | 510 | CLA | CHC-C1C | 3.24 | 1.43 | 1.35 |
| 28 | c | 516 | DGD | O3G-C3G | -3.23 | 1.37 | 1.43 |
| 28 | c | 518 | DGD | O2G-C1B | 3.22 | 1.43 | 1.34 |
| 23 | C | 505 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 23 | b | 612 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 23 | a | 405 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 27 | B | 621 | SQD | O47-C7 | 3.21 | 1.43 | 1.34 |
| 23 | C | 507 | CLA | C3B-CAB | -3.21 | 1.41 | 1.47 |
| 23 | a | 408 | CLA | C4B-CHC | -3.20 | 1.32 | 1.41 |
| 27 | a | 412 | SQD | O47-C7 | 3.19 | 1.43 | 1.34 |
| 23 | b | 617 | CLA | MG-NA | -3.19 | 1.98 | 2.06 |
| 27 | a | 411 | SQD | O48-C23 | 3.18 | 1.42 | 1.33 |
| 33 | C | 501 | LMG | C4-C5 | 3.18 | 1.59 | 1.53 |
| 23 | B | 609 | CLA | MG-NA | 3.18 | 2.13 | 2.06 |
| 23 | B | 610 | CLA | C3B-C2B | -3.18 | 1.36 | 1.40 |
| 23 | B | 614 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 24 | d | 401 | PHO | CHC-C1C | 3.18 | 1.44 | 1.38 |
| 23 | d | 403 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 23 | C | 510 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 23 | c | 502 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 27 | B | 621 | SQD | O48-C23 | 3.17 | 1.42 | 1.33 |
| 25 | C | 520 | BCR | C30-C25 | -3.17 | 1.49 | 1.53 |
| 23 | C | 513 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 23 | b | 613 | CLA | MG-NA | -3.16 | 1.98 | 2.06 |
| 27 | b | 601 | SQD | O47-C7 | 3.15 | 1.43 | 1.34 |
| 25 | k | 101 | BCR | C30-C25 | -3.14 | 1.49 | 1.53 |
| 28 | A | 412 | DGD | C3G-C2G | 3.14 | 1.60 | 1.50 |
| 23 | B | 602 | CLA | MG-NA | 3.14 | 2.13 | 2.06 |
| 25 | b | 618 | BCR | C30-C25 | -3.13 | 1.49 | 1.53 |
| 23 | c | 505 | CLA | CMB-C2B | -3.13 | 1.45 | 1.51 |
| 23 | C | 511 | CLA | MG-NA | 3.13 | 2.13 | 2.06 |
| 33 | c | 522 | LMG | C7-C8 | 3.13 | 1.60 | 1.50 |
| 23 | c | 508 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 27 | A | 410 | SQD | O48-C23 | 3.11 | 1.42 | 1.33 |
| 27 | f | 101 | SQD | O48-C23 | 3.11 | 1.42 | 1.33 |
| 23 | B | 609 | CLA | C3B-C2B | -3.10 | 1.36 | 1.40 |
| 34 | E | 103 | HEM | C3B-CAB | 3.10 | 1.54 | 1.47 |
| 23 | D | 404 | CLA | MG-NA | -3.10 | 1.98 | 2.06 |
| 23 | a | 406 | CLA | CMB-C2B | -3.10 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 507 | CLA | CMB-C2B | -3.09 | 1.45 | 1.51 |
| 24 | A | 406 | PHO | O2D-CGD | 3.09 | 1.40 | 1.33 |
| 26 | A | 409 | PL9 | C37-C38 | 3.09 | 1.60 | 1.50 |
| 23 | b | 614 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 28 | h | 101 | DGD | C1E-C2E | 3.08 | 1.61 | 1.52 |
| 33 | D | 410 | LMG | C9-C8 | 3.08 | 1.60 | 1.50 |
| 23 | D | 404 | CLA | CMD-C2D | -3.08 | 1.44 | 1.51 |
| 23 | b | 617 | CLA | C3B-CAB | -3.07 | 1.41 | 1.47 |
| 23 | B | 602 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 33 | C | 501 | LMG | C4-C3 | 3.07 | 1.60 | 1.52 |
| 23 | c | 506 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 28 | A | 412 | DGD | C6E-C5E | 3.06 | 1.62 | 1.51 |
| 23 | C | 509 | CLA | C1D-C2D | 3.06 | 1.49 | 1.42 |
| 23 | c | 503 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 23 | c | 507 | CLA | C3B-CAB | -3.06 | 1.41 | 1.47 |
| 33 | d | 411 | LMG | O7-C8 | -3.06 | 1.38 | 1.46 |
| 23 | B | 603 | CLA | C3B-C2B | -3.05 | 1.36 | 1.40 |
| 28 | A | 412 | DGD | C1E-C2E | 3.04 | 1.61 | 1.52 |
| 25 | c | 515 | BCR | C1-C6 | -3.04 | 1.49 | 1.53 |
| 28 | c | 518 | DGD | C4E-C5E | 3.04 | 1.59 | 1.53 |
| 27 | A | 411 | SQD | O47-C45 | -3.04 | 1.41 | 1.47 |
| 23 | B | 604 | CLA | C1B-NB | 3.04 | 1.37 | 1.35 |
| 23 | B | 606 | CLA | CMB-C2B | -3.03 | 1.45 | 1.51 |
| 33 | b | 622 | LMG | C4-C3 | 3.03 | 1.60 | 1.52 |
| 23 | b | 604 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 28 | C | 517 | DGD | C4D-C3D | 3.03 | 1.60 | 1.52 |
| 23 | c | 508 | CLA | MG-NA | 3.03 | 2.13 | 2.06 |
| 23 | C | 504 | CLA | CMB-C2B | -3.03 | 1.45 | 1.51 |
| 23 | C | 512 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 33 | C | 519 | LMG | O7-C8 | -3.03 | 1.39 | 1.46 |
| 23 | C | 503 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 28 | C | 516 | DGD | C3D-C2D | 3.02 | 1.60 | 1.52 |
| 28 | c | 516 | DGD | C4D-C3D | 3.02 | 1.60 | 1.52 |
| 25 | D | 405 | BCR | C1-C6 | -3.01 | 1.49 | 1.53 |
| 23 | B | 612 | CLA | CMC-C2C | -3.01 | 1.44 | 1.50 |
| 26 | d | 406 | PL9 | C6-C1 | -3.00 | 1.43 | 1.48 |
| 23 | c | 503 | CLA | C1D-C2D | 3.00 | 1.49 | 1.42 |
| 23 | b | 609 | CLA | C3B-CAB | -3.00 | 1.41 | 1.47 |
| 25 | b | 620 | BCR | C1-C6 | -3.00 | 1.49 | 1.53 |
| 23 | B | 611 | CLA | CMB-C2B | -3.00 | 1.45 | 1.51 |
| 24 | d | 401 | PHO | C3B-C4B | 3.00 | 1.49 | 1.43 |
| 25 | a | 409 | BCR | C30-C25 | -2.99 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | b | 610 | CLA | MG-NA | 2.99 | 2.13 | 2.06 |
| 23 | b | 609 | CLA | C1D-C2D | 2.98 | 1.49 | 1.42 |
| 25 | T | 101 | BCR | C38-C26 | -2.98 | 1.46 | 1.50 |
| 23 | d | 404 | CLA | MG-NA | 2.98 | 2.13 | 2.06 |
| 23 | c | 502 | CLA | MG-NA | 2.98 | 2.13 | 2.06 |
| 29 | A | 413 | LHG | O7-C5 | -2.97 | 1.39 | 1.46 |
| 23 | D | 403 | CLA | MG-NA | 2.97 | 2.13 | 2.06 |
| 23 | B | 615 | CLA | C3B-CAB | -2.97 | 1.41 | 1.47 |
| 23 | b | 611 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 23 | b | 602 | CLA | C1D-C2D | 2.95 | 1.49 | 1.42 |
| 23 | c | 506 | CLA | C3B-C2B | -2.95 | 1.36 | 1.40 |
| 33 | m | 101 | LMG | O7-C8 | -2.95 | 1.39 | 1.46 |
| 23 | d | 402 | CLA | C3B-C2B | -2.95 | 1.36 | 1.40 |
| 23 | b | 605 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 26 | a | 410 | PL9 | C53-C6 | -2.94 | 1.44 | 1.50 |
| 23 | D | 402 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 23 | b | 617 | CLA | CMB-C2B | -2.94 | 1.45 | 1.51 |
| 23 | B | 607 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 23 | B | 605 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 26 | a | 410 | PL9 | C3-C4 | -2.94 | 1.44 | 1.49 |
| 26 | d | 406 | PL9 | C30-C29 | -2.93 | 1.43 | 1.50 |
| 23 | b | 615 | CLA | CMC-C2C | -2.93 | 1.44 | 1.50 |
| 23 | b | 612 | CLA | C1D-C2D | 2.92 | 1.49 | 1.42 |
| 33 | c | 524 | LMG | O6-C5 | -2.92 | 1.37 | 1.44 |
| 24 | d | 401 | PHO | C4C-NC | 2.92 | 1.43 | 1.36 |
| 23 | b | 607 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 23 | C | 507 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 33 | c | 522 | LMG | C1-C2 | 2.91 | 1.60 | 1.52 |
| 23 | d | 402 | CLA | C1D-C2D | 2.91 | 1.49 | 1.42 |
| 24 | A | 406 | PHO | C4C-C3C | 2.91 | 1.50 | 1.45 |
| 23 | B | 614 | CLA | MG-NC | 2.90 | 2.13 | 2.06 |
| 24 | D | 401 | PHO | C1C-NC | -2.90 | 1.32 | 1.38 |
| 23 | c | 510 | CLA | C1D-C2D | 2.90 | 1.49 | 1.42 |
| 27 | A | 410 | SQD | O47-C7 | 2.89 | 1.42 | 1.34 |
| 23 | B | 608 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 25 | a | 409 | BCR | C1-C6 | -2.89 | 1.49 | 1.53 |
| 28 | c | 517 | DGD | O4E-C4E | -2.89 | 1.36 | 1.43 |
| 23 | c | 506 | CLA | CAC-C3C | -2.89 | 1.43 | 1.51 |
| 23 | c | 513 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 23 | b | 603 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 28 | c | 518 | DGD | C2A-C1A | -2.88 | 1.42 | 1.50 |
| 23 | C | 509 | CLA | MG-NC | 2.88 | 2.13 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | A | 407 | CLA | C4B-CHC | -2.88 | 1.33 | 1.41 |
| 23 | b | 615 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 23 | B | 612 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 23 | c | 503 | CLA | CMB-C2B | -2.87 | 1.45 | 1.51 |
| 23 | C | 508 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 23 | b | 604 | CLA | C1D-C2D | 2.86 | 1.49 | 1.42 |
| 25 | c | 515 | BCR | C30-C25 | -2.85 | 1.49 | 1.53 |
| 23 | c | 503 | CLA | C3B-CAB | -2.85 | 1.42 | 1.47 |
| 33 | D | 407 | LMG | C6-C5 | 2.85 | 1.61 | 1.51 |
| 23 | C | 513 | CLA | C1D-C2D | 2.84 | 1.49 | 1.42 |
| 23 | b | 607 | CLA | C3B-C2B | -2.84 | 1.36 | 1.40 |
| 23 | B | 615 | CLA | MG-NA | 2.84 | 2.13 | 2.06 |
| 27 | F | 101 | SQD | O48-C23 | 2.84 | 1.41 | 1.33 |
| 26 | a | 410 | PL9 | C11-C9 | -2.83 | 1.45 | 1.51 |
| 28 | H | 102 | DGD | O3D-C3D | -2.83 | 1.36 | 1.43 |
| 23 | D | 403 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 24 | D | 401 | PHO | C4C-NC | 2.82 | 1.43 | 1.36 |
| 23 | b | 613 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 23 | b | 617 | CLA | C3B-C2B | -2.82 | 1.36 | 1.40 |
| 23 | B | 603 | CLA | CMA-C3A | -2.82 | 1.47 | 1.53 |
| 23 | b | 602 | CLA | O2A-CGA | 2.82 | 1.41 | 1.33 |
| 25 | D | 405 | BCR | C30-C25 | -2.81 | 1.49 | 1.53 |
| 28 | A | 412 | DGD | O5D-C1E | 2.81 | 1.45 | 1.40 |
| 23 | D | 404 | CLA | C3B-CAB | -2.80 | 1.42 | 1.47 |
| 23 | c | 503 | CLA | C3B-C2B | -2.80 | 1.36 | 1.40 |
| 25 | c | 521 | BCR | C1-C6 | -2.80 | 1.49 | 1.53 |
| 23 | D | 403 | CLA | C1C-NC | -2.79 | 1.33 | 1.37 |
| 23 | b | 616 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 33 | c | 522 | LMG | O1-C1 | 2.79 | 1.44 | 1.40 |
| 28 | C | 518 | DGD | C1G-C2G | 2.79 | 1.59 | 1.50 |
| 24 | a | 407 | PHO | C3B-C4B | 2.79 | 1.49 | 1.43 |
| 27 | A | 410 | SQD | O2-C2 | -2.78 | 1.36 | 1.43 |
| 23 | C | 506 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 27 | a | 411 | SQD | O47-C7 | 2.78 | 1.42 | 1.34 |
| 23 | B | 609 | CLA | CMD-C2D | -2.78 | 1.45 | 1.51 |
| 23 | D | 404 | CLA | MG-NC | 2.77 | 2.12 | 2.06 |
| 23 | B | 611 | CLA | CMD-C2D | -2.77 | 1.45 | 1.51 |
| 23 | B | 602 | CLA | C1D-C2D | 2.77 | 1.48 | 1.42 |
| 23 | d | 404 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 23 | b | 612 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 23 | B | 616 | CLA | CMC-C2C | -2.77 | 1.44 | 1.50 |
| 23 | b | 608 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | c | 515 | BCR | C33-C5 | -2.76 | 1.46 | 1.50 |
| 23 | B | 607 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 23 | B | 609 | CLA | C4B-CHC | -2.76 | 1.33 | 1.41 |
| 23 | D | 404 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 23 | C | 508 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 23 | B | 615 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 24 | D | 401 | PHO | C1A-NA | 2.76 | 1.43 | 1.37 |
| 23 | B | 607 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 23 | b | 617 | CLA | CMD-C2D | -2.76 | 1.45 | 1.51 |
| 33 | c | 519 | LMG | C4-C5 | 2.75 | 1.58 | 1.53 |
| 28 | h | 101 | DGD | O1G-C1G | -2.75 | 1.38 | 1.45 |
| 23 | b | 606 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 23 | c | 511 | CLA | MG-NC | 2.75 | 2.12 | 2.06 |
| 23 | b | 603 | CLA | CMD-C2D | -2.75 | 1.45 | 1.51 |
| 23 | B | 613 | CLA | C3B-CAB | -2.75 | 1.42 | 1.47 |
| 26 | D | 406 | PL9 | C30-C29 | -2.74 | 1.43 | 1.50 |
| 23 | c | 504 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 23 | B | 603 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 23 | d | 404 | CLA | CMD-C2D | -2.74 | 1.45 | 1.51 |
| 23 | c | 512 | CLA | MG-NC | 2.74 | 2.12 | 2.06 |
| 23 | a | 406 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 25 | k | 101 | BCR | C1-C6 | -2.73 | 1.50 | 1.53 |
| 33 | d | 411 | LMG | O2-C2 | -2.73 | 1.36 | 1.43 |
| 23 | d | 404 | CLA | C3B-CAB | -2.73 | 1.42 | 1.47 |
| 23 | B | 611 | CLA | C1B-NB | 2.73 | 1.37 | 1.35 |
| 23 | b | 607 | CLA | C1D-C2D | 2.72 | 1.48 | 1.42 |
| 23 | B | 613 | CLA | C4B-CHC | -2.72 | 1.33 | 1.41 |
| 23 | a | 408 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 23 | d | 404 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 24 | A | 406 | PHO | C4C-NC | 2.71 | 1.42 | 1.36 |
| 34 | e | 102 | HEM | C3C-CAC | 2.71 | 1.53 | 1.47 |
| 23 | c | 503 | CLA | MG-NA | 2.71 | 2.12 | 2.06 |
| 23 | b | 611 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 28 | H | 102 | DGD | C1E-C2E | 2.71 | 1.60 | 1.52 |
| 23 | b | 606 | CLA | C1D-C2D | 2.71 | 1.48 | 1.42 |
| 25 | Z | 101 | BCR | C1-C6 | -2.71 | 1.50 | 1.53 |
| 23 | A | 407 | CLA | MG-NC | -2.71 | 1.99 | 2.06 |
| 28 | H | 102 | DGD | O2D-C2D | -2.70 | 1.36 | 1.43 |
| 23 | B | 609 | CLA | CMC-C2C | -2.70 | 1.45 | 1.50 |
| 23 | A | 405 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 25 | B | 618 | BCR | C1-C6 | -2.69 | 1.50 | 1.53 |
| 23 | C | 504 | CLA | C4B-CHC | -2.69 | 1.33 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | C | 507 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 28 | C | 516 | DGD | O1G-C1A | 2.69 | 1.41 | 1.33 |
| 23 | B | 615 | CLA | C1D-C2D | 2.68 | 1.48 | 1.42 |
| 24 | D | 401 | PHO | CMC-C2C | -2.68 | 1.45 | 1.50 |
| 23 | C | 506 | CLA | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 23 | B | 608 | CLA | CMD-C2D | -2.68 | 1.45 | 1.51 |
| 23 | c | 501 | CLA | CAC-C3C | -2.68 | 1.44 | 1.51 |
| 23 | B | 608 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 23 | B | 616 | CLA | CMD-C2D | -2.67 | 1.45 | 1.51 |
| 28 | c | 516 | DGD | C3D-C2D | 2.67 | 1.59 | 1.52 |
| 23 | c | 501 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 23 | b | 612 | CLA | C3B-C2B | -2.66 | 1.36 | 1.40 |
| 23 | a | 408 | CLA | CMC-C2C | -2.66 | 1.45 | 1.50 |
| 23 | A | 404 | CLA | C1D-C2D | 2.66 | 1.48 | 1.42 |
| 28 | H | 102 | DGD | C4D-C5D | 2.66 | 1.58 | 1.53 |
| 29 | e | 101 | LHG | O7-C5 | -2.66 | 1.39 | 1.46 |
| 23 | C | 514 | CLA | C1D-C2D | 2.66 | 1.48 | 1.42 |
| 23 | B | 609 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 25 | T | 101 | BCR | C1-C6 | -2.65 | 1.50 | 1.53 |
| 29 | E | 101 | LHG | O7-C5 | -2.65 | 1.40 | 1.46 |
| 23 | D | 402 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 33 | c | 522 | LMG | C4-C3 | 2.65 | 1.59 | 1.52 |
| 28 | A | 412 | DGD | O2G-C1B | 2.65 | 1.41 | 1.34 |
| 23 | C | 509 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 23 | C | 502 | CLA | C1D-C2D | 2.64 | 1.48 | 1.42 |
| 23 | C | 509 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 23 | C | 508 | CLA | C1D-C2D | 2.64 | 1.48 | 1.42 |
| 25 | C | 515 | BCR | C33-C5 | -2.64 | 1.46 | 1.50 |
| 23 | C | 513 | CLA | C3B-C2B | -2.63 | 1.36 | 1.40 |
| 28 | C | 518 | DGD | O2G-C2G | -2.63 | 1.40 | 1.46 |
| 23 | B | 601 | CLA | C3B-CAB | -2.63 | 1.42 | 1.47 |
| 23 | c | 504 | CLA | MG-NC | 2.63 | 2.12 | 2.06 |
| 23 | c | 507 | CLA | MG-NA | -2.63 | 2.00 | 2.06 |
| 23 | C | 503 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 23 | D | 403 | CLA | CMD-C2D | -2.62 | 1.45 | 1.51 |
| 23 | c | 512 | CLA | C3B-CAB | -2.62 | 1.42 | 1.47 |
| 25 | d | 405 | BCR | C30-C25 | -2.62 | 1.50 | 1.53 |
| 23 | c | 507 | CLA | C4B-CHC | -2.62 | 1.33 | 1.41 |
| 24 | a | 407 | PHO | CHC-C4B | -2.62 | 1.34 | 1.40 |
| 23 | C | 514 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 23 | b | 614 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 23 | B | 613 | CLA | C1C-NC | -2.61 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 512 | CLA | C1D-C2D | 2.61 | 1.48 | 1.42 |
| 23 | c | 503 | CLA | CMC-C2C | -2.61 | 1.45 | 1.50 |
| 23 | C | 508 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 23 | b | 604 | CLA | C3B-C2B | -2.61 | 1.36 | 1.40 |
| 23 | a | 405 | CLA | MG-NA | 2.61 | 2.12 | 2.06 |
| 23 | C | 504 | CLA | C1D-C2D | 2.61 | 1.48 | 1.42 |
| 23 | c | 511 | CLA | C1D-C2D | 2.61 | 1.48 | 1.42 |
| 24 | A | 406 | PHO | CMD-C2D | -2.60 | 1.45 | 1.50 |
| 23 | b | 608 | CLA | C1C-NC | -2.60 | 1.33 | 1.37 |
| 23 | b | 610 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 23 | B | 609 | CLA | C3B-CAB | -2.59 | 1.42 | 1.47 |
| 23 | a | 405 | CLA | CMD-C2D | -2.59 | 1.45 | 1.51 |
| 28 | H | 102 | DGD | O5D-C6D | -2.59 | 1.39 | 1.43 |
| 25 | c | 514 | BCR | C1-C6 | -2.59 | 1.50 | 1.53 |
| 25 | B | 617 | BCR | C33-C5 | -2.58 | 1.46 | 1.50 |
| 23 | A | 407 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 24 | D | 401 | PHO | CHD-C1D | 2.58 | 1.43 | 1.38 |
| 23 | C | 514 | CLA | MG-NA | 2.58 | 2.12 | 2.06 |
| 23 | B | 616 | CLA | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 23 | B | 606 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 23 | c | 508 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 23 | B | 611 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 23 | C | 503 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 23 | C | 514 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 23 | C | 503 | CLA | C1D-C2D | 2.57 | 1.48 | 1.42 |
| 28 | h | 101 | DGD | C4E-C3E | 2.57 | 1.58 | 1.52 |
| 23 | b | 603 | CLA | MG-NA | 2.57 | 2.12 | 2.06 |
| 23 | C | 502 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 23 | d | 402 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 24 | d | 401 | PHO | C1A-NA | 2.57 | 1.42 | 1.37 |
| 23 | b | 616 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 23 | B | 614 | CLA | C1D-C2D | 2.56 | 1.48 | 1.42 |
| 29 | L | 101 | LHG | O8-C23 | 2.56 | 1.40 | 1.33 |
| 29 | l | 101 | LHG | O8-C23 | 2.56 | 1.40 | 1.33 |
| 34 | e | 102 | HEM | C3B-CAB | 2.56 | 1.53 | 1.47 |
| 23 | C | 513 | CLA | CMD-C2D | -2.56 | 1.45 | 1.51 |
| 24 | d | 401 | PHO | CMC-C2C | -2.55 | 1.45 | 1.50 |
| 28 | C | 518 | DGD | O3E-C3E | -2.55 | 1.37 | 1.43 |
| 23 | b | 612 | CLA | MG-NC | -2.55 | 2.00 | 2.06 |
| 28 | A | 412 | DGD | C4D-C3D | 2.55 | 1.58 | 1.52 |
| 28 | H | 102 | DGD | O5D-C1E | 2.55 | 1.44 | 1.40 |
| 28 | C | 518 | DGD | C4E-C3E | 2.54 | 1.58 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 513 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 23 | A | 404 | CLA | C3B-CAB | -2.53 | 1.42 | 1.47 |
| 23 | A | 405 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 23 | C | 505 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 26 | a | 410 | PL9 | C6-C1 | -2.53 | 1.44 | 1.48 |
| 23 | A | 404 | CLA | C1B-NB | 2.53 | 1.37 | 1.35 |
| 28 | C | 516 | DGD | O2G-C2G | -2.53 | 1.40 | 1.46 |
| 33 | C | 519 | LMG | O3-C3 | -2.52 | 1.37 | 1.43 |
| 24 | d | 401 | PHO | CAA-C2A | -2.52 | 1.49 | 1.54 |
| 23 | A | 407 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 33 | M | 101 | LMG | C1-C2 | 2.51 | 1.59 | 1.52 |
| 23 | b | 611 | CLA | CMD-C2D | -2.51 | 1.45 | 1.51 |
| 23 | a | 408 | CLA | CMA-C3A | -2.51 | 1.47 | 1.53 |
| 23 | B | 608 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 23 | b | 604 | CLA | CMD-C2D | -2.51 | 1.45 | 1.51 |
| 27 | A | 410 | SQD | O3-C3 | -2.51 | 1.37 | 1.43 |
| 26 | a | 410 | PL9 | C7-C3 | -2.51 | 1.48 | 1.51 |
| 29 | E | 101 | LHG | O8-C23 | 2.50 | 1.40 | 1.33 |
| 33 | C | 519 | LMG | O4-C4 | -2.50 | 1.37 | 1.43 |
| 23 | b | 604 | CLA | CMC-C2C | -2.50 | 1.45 | 1.50 |
| 23 | B | 603 | CLA | C3B-CAB | -2.50 | 1.42 | 1.47 |
| 23 | b | 604 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 23 | d | 403 | CLA | CAA-C2A | -2.49 | 1.49 | 1.54 |
| 23 | a | 408 | CLA | C3B-C2B | -2.49 | 1.36 | 1.40 |
| 26 | d | 406 | PL9 | C53-C6 | -2.49 | 1.45 | 1.50 |
| 23 | B | 616 | CLA | C3B-CAB | -2.49 | 1.42 | 1.47 |
| 23 | C | 510 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 23 | b | 611 | CLA | CHC-C1C | 2.49 | 1.41 | 1.35 |
| 23 | b | 608 | CLA | CMD-C2D | -2.48 | 1.45 | 1.51 |
| 23 | b | 608 | CLA | C3B-C2B | -2.48 | 1.36 | 1.40 |
| 23 | b | 606 | CLA | CHC-C1C | 2.48 | 1.41 | 1.35 |
| 28 | C | 517 | DGD | C3E-C2E | 2.48 | 1.58 | 1.52 |
| 23 | B | 607 | CLA | C3B-CAB | -2.47 | 1.42 | 1.47 |
| 23 | c | 502 | CLA | C1D-C2D | 2.47 | 1.48 | 1.42 |
| 23 | c | 508 | CLA | CMC-C2C | -2.47 | 1.45 | 1.50 |
| 23 | B | 601 | CLA | CHC-C1C | 2.47 | 1.41 | 1.35 |
| 34 | E | 103 | HEM | C3C-CAC | 2.47 | 1.52 | 1.47 |
| 23 | b | 603 | CLA | CAC-C3C | -2.46 | 1.44 | 1.51 |
| 23 | b | 605 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 27 | f | 101 | SQD | O2-C2 | -2.46 | 1.37 | 1.43 |
| 23 | c | 508 | CLA | C1D-C2D | 2.45 | 1.48 | 1.42 |
| 24 | D | 401 | PHO | CHC-C1C | 2.45 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 512 | CLA | CMD-C2D | -2.45 | 1.45 | 1.51 |
| 23 | a | 405 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 23 | c | 507 | CLA | CMC-C2C | -2.44 | 1.45 | 1.50 |
| 29 | D | 408 | LHG | C24-C23 | 2.44 | 1.57 | 1.50 |
| 23 | c | 505 | CLA | C3B-CAB | -2.44 | 1.43 | 1.47 |
| 23 | C | 504 | CLA | CHC-C1C | 2.44 | 1.41 | 1.35 |
| 23 | c | 506 | CLA | MG-NC | 2.44 | 2.12 | 2.06 |
| 23 | A | 405 | CLA | CMD-C2D | -2.44 | 1.45 | 1.51 |
| 23 | B | 606 | CLA | C1D-C2D | 2.44 | 1.48 | 1.42 |
| 33 | c | 519 | LMG | O2-C2 | -2.44 | 1.37 | 1.43 |
| 28 | C | 517 | DGD | O4E-C4E | -2.44 | 1.37 | 1.43 |
| 23 | b | 613 | CLA | C1D-C2D | 2.43 | 1.48 | 1.42 |
| 23 | b | 605 | CLA | MG-NC | 2.43 | 2.12 | 2.06 |
| 33 | m | 101 | LMG | O6-C5 | -2.43 | 1.38 | 1.44 |
| 23 | B | 607 | CLA | MG-NC | 2.43 | 2.12 | 2.06 |
| 33 | c | 522 | LMG | C3-C2 | 2.43 | 1.58 | 1.52 |
| 25 | c | 515 | BCR | C38-C26 | -2.42 | 1.47 | 1.50 |
| 28 | h | 101 | DGD | C4D-C5D | 2.42 | 1.58 | 1.53 |
| 23 | B | 602 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 23 | C | 504 | CLA | C3B-C2B | -2.42 | 1.37 | 1.40 |
| 33 | c | 522 | LMG | O6-C5 | -2.42 | 1.38 | 1.44 |
| 33 | D | 407 | LMG | O2-C2 | -2.41 | 1.37 | 1.43 |
| 23 | C | 511 | CLA | C1D-C2D | 2.41 | 1.48 | 1.42 |
| 23 | C | 508 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 23 | B | 613 | CLA | CMD-C2D | -2.41 | 1.45 | 1.51 |
| 23 | c | 513 | CLA | C1D-C2D | 2.41 | 1.48 | 1.42 |
| 28 | A | 412 | DGD | C3E-C2E | 2.41 | 1.58 | 1.52 |
| 24 | a | 407 | PHO | C1C-NC | -2.41 | 1.33 | 1.38 |
| 23 | a | 406 | CLA | C3B-CAB | -2.40 | 1.43 | 1.47 |
| 24 | d | 401 | PHO | CHC-C4B | -2.40 | 1.34 | 1.40 |
| 28 | C | 517 | DGD | O3G-C3G | -2.40 | 1.39 | 1.43 |
| 23 | C | 510 | CLA | C1D-C2D | 2.40 | 1.48 | 1.42 |
| 23 | b | 607 | CLA | C4B-CHC | -2.39 | 1.34 | 1.41 |
| 25 | C | 515 | BCR | C30-C25 | -2.39 | 1.50 | 1.53 |
| 28 | C | 517 | DGD | C1E-C2E | 2.38 | 1.59 | 1.52 |
| 28 | a | 413 | DGD | C1G-C2G | 2.38 | 1.58 | 1.50 |
| 23 | C | 507 | CLA | C1D-C2D | 2.38 | 1.48 | 1.42 |
| 23 | A | 407 | CLA | CMD-C2D | -2.38 | 1.45 | 1.51 |
| 23 | C | 502 | CLA | CMD-C2D | -2.38 | 1.45 | 1.51 |
| 28 | C | 516 | DGD | O2D-C2D | -2.38 | 1.37 | 1.43 |
| 23 | d | 403 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 23 | B | 613 | CLA | CMC-C2C | -2.38 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33 | d | 411 | LMG | C4-C5 | 2.38 | 1.58 | 1.53 |
| 25 | c | 521 | BCR | C38-C26 | -2.38 | 1.47 | 1.50 |
| 23 | c | 501 | CLA | CMD-C2D | -2.38 | 1.45 | 1.51 |
| 23 | B | 601 | CLA | CMD-C2D | -2.37 | 1.45 | 1.51 |
| 33 | b | 622 | LMG | O1-C7 | -2.37 | 1.39 | 1.43 |
| 23 | B | 604 | CLA | O2A-CGA | 2.37 | 1.40 | 1.33 |
| 23 | b | 612 | CLA | C3B-CAB | -2.37 | 1.43 | 1.47 |
| 23 | D | 403 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 23 | B | 607 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 23 | C | 511 | CLA | O2A-CGA | 2.37 | 1.40 | 1.33 |
| 25 | B | 617 | BCR | C30-C25 | -2.37 | 1.50 | 1.53 |
| 23 | B | 606 | CLA | C3B-CAB | -2.37 | 1.43 | 1.47 |
| 23 | C | 503 | CLA | MG-NA | 2.37 | 2.11 | 2.06 |
| 28 | C | 516 | DGD | C4D-C3D | 2.36 | 1.58 | 1.52 |
| 25 | b | 618 | BCR | C33-C5 | -2.36 | 1.47 | 1.50 |
| 33 | C | 501 | LMG | C7-C8 | 2.36 | 1.57 | 1.50 |
| 33 | b | 622 | LMG | C4-C5 | 2.36 | 1.58 | 1.53 |
| 23 | b | 609 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 23 | c | 513 | CLA | CMD-C2D | -2.36 | 1.46 | 1.51 |
| 23 | b | 602 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 24 | D | 401 | PHO | CHC-C4B | -2.36 | 1.34 | 1.40 |
| 23 | c | 506 | CLA | C3B-CAB | -2.35 | 1.43 | 1.47 |
| 23 | b | 613 | CLA | C1B-NB | -2.35 | 1.33 | 1.35 |
| 28 | A | 412 | DGD | O6D-C1D | 2.35 | 1.47 | 1.41 |
| 24 | A | 406 | PHO | C1C-NC | -2.35 | 1.33 | 1.38 |
| 23 | B | 603 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 26 | A | 409 | PL9 | C10-C9 | -2.34 | 1.44 | 1.50 |
| 29 | L | 101 | LHG | O7-C5 | -2.34 | 1.40 | 1.46 |
| 23 | B | 613 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 35 | V | 201 | HEC | C2A-C3A | -2.34 | 1.30 | 1.37 |
| 23 | c | 501 | CLA | MG-NC | 2.34 | 2.11 | 2.06 |
| 23 | b | 603 | CLA | C4B-CHC | -2.33 | 1.34 | 1.41 |
| 33 | D | 410 | LMG | O8-C28 | 2.33 | 1.40 | 1.33 |
| 33 | m | 101 | LMG | O1-C7 | -2.33 | 1.39 | 1.43 |
| 23 | C | 507 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 28 | c | 518 | DGD | O6E-C1E | -2.33 | 1.35 | 1.41 |
| 29 | L | 101 | LHG | P-O6 | 2.33 | 1.68 | 1.59 |
| 23 | B | 614 | CLA | C1B-NB | 2.32 | 1.37 | 1.35 |
| 27 | f | 101 | SQD | O3-C3 | -2.32 | 1.37 | 1.43 |
| 28 | c | 518 | DGD | O2D-C2D | -2.32 | 1.37 | 1.43 |
| 23 | D | 403 | CLA | CMB-C2B | -2.32 | 1.46 | 1.51 |
| 23 | B | 614 | CLA | CMB-C2B | -2.31 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | c | 507 | CLA | C1D-C2D | 2.31 | 1.47 | 1.42 |
| 23 | b | 617 | CLA | C1D-C2D | 2.31 | 1.47 | 1.42 |
| 23 | b | 616 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 29 | D | 409 | LHG | O7-C7 | 2.31 | 1.40 | 1.34 |
| 23 | a | 405 | CLA | C1D-C2D | 2.31 | 1.47 | 1.42 |
| 23 | b | 605 | CLA | C1D-C2D | 2.30 | 1.47 | 1.42 |
| 33 | D | 407 | LMG | O8-C28 | 2.30 | 1.40 | 1.33 |
| 33 | C | 519 | LMG | C3-C2 | 2.30 | 1.58 | 1.52 |
| 23 | B | 608 | CLA | CHC-C1C | 2.29 | 1.40 | 1.35 |
| 23 | b | 609 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 27 | A | 410 | SQD | O4-C4 | -2.29 | 1.37 | 1.43 |
| 29 | D | 408 | LHG | O7-C5 | -2.29 | 1.40 | 1.46 |
| 23 | B | 616 | CLA | CMB-C2B | -2.29 | 1.46 | 1.51 |
| 33 | C | 501 | LMG | O7-C8 | -2.29 | 1.40 | 1.46 |
| 23 | B | 606 | CLA | CMD-C2D | -2.29 | 1.46 | 1.51 |
| 23 | b | 614 | CLA | C5-C3 | -2.29 | 1.46 | 1.51 |
| 28 | c | 517 | DGD | C4E-C5E | 2.28 | 1.57 | 1.53 |
| 23 | B | 609 | CLA | CAC-C3C | -2.28 | 1.45 | 1.51 |
| 23 | c | 508 | CLA | CMD-C2D | -2.28 | 1.46 | 1.51 |
| 23 | C | 508 | CLA | CMD-C2D | -2.28 | 1.46 | 1.51 |
| 28 | H | 102 | DGD | C4E-C3E | 2.28 | 1.58 | 1.52 |
| 23 | D | 404 | CLA | C1D-C2D | 2.28 | 1.47 | 1.42 |
| 29 | e | 101 | LHG | P-O6 | 2.28 | 1.68 | 1.59 |
| 27 | a | 411 | SQD | O3-C3 | -2.27 | 1.37 | 1.43 |
| 23 | a | 408 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 23 | B | 604 | CLA | MG-NC | -2.27 | 2.00 | 2.06 |
| 23 | D | 402 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 23 | b | 610 | CLA | C1D-C2D | 2.27 | 1.47 | 1.42 |
| 29 | e | 101 | LHG | O8-C23 | 2.27 | 1.40 | 1.33 |
| 24 | A | 406 | PHO | C1C-C2C | 2.27 | 1.50 | 1.45 |
| 29 | d | 409 | LHG | P-O6 | 2.27 | 1.68 | 1.59 |
| 33 | b | 622 | LMG | C7-C8 | 2.27 | 1.57 | 1.50 |
| 25 | B | 619 | BCR | C30-C25 | -2.26 | 1.50 | 1.53 |
| 23 | b | 610 | CLA | CHC-C1C | 2.26 | 1.40 | 1.35 |
| 23 | C | 511 | CLA | CMD-C2D | -2.26 | 1.46 | 1.51 |
| 26 | D | 406 | PL9 | C41-C39 | -2.26 | 1.46 | 1.51 |
| 23 | B | 612 | CLA | C1D-C2D | 2.26 | 1.47 | 1.42 |
| 24 | d | 401 | PHO | C1C-NC | -2.26 | 1.33 | 1.38 |
| 28 | C | 517 | DGD | O3D-C3D | -2.26 | 1.37 | 1.43 |
| 23 | A | 407 | CLA | C1D-C2D | 2.26 | 1.47 | 1.42 |
| 23 | B | 605 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 25 | T | 101 | BCR | C27-C26 | -2.26 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | A | 409 | PL9 | C21-C19 | 2.26 | 1.56 | 1.51 |
| 23 | B | 603 | CLA | C1A-CHA | -2.26 | 1.33 | 1.43 |
| 23 | C | 505 | CLA | CMD-C2D | -2.26 | 1.46 | 1.51 |
| 23 | D | 404 | CLA | C4B-CHC | -2.26 | 1.34 | 1.41 |
| 28 | C | 517 | DGD | O6D-C5D | -2.25 | 1.38 | 1.44 |
| 26 | d | 406 | PL9 | C7-C8 | -2.25 | 1.47 | 1.50 |
| 23 | C | 512 | CLA | CMB-C2B | -2.25 | 1.47 | 1.51 |
| 23 | b | 603 | CLA | C1B-NB | 2.25 | 1.37 | 1.35 |
| 23 | c | 506 | CLA | C4B-CHC | -2.25 | 1.34 | 1.41 |
| 24 | D | 401 | PHO | C3B-C4B | 2.25 | 1.47 | 1.43 |
| 28 | A | 412 | DGD | O1G-C1A | 2.25 | 1.39 | 1.33 |
| 23 | B | 606 | CLA | C4B-CHC | -2.24 | 1.34 | 1.41 |
| 28 | H | 102 | DGD | C6D-C5D | 2.24 | 1.58 | 1.51 |
| 29 | D | 409 | LHG | O3-C3 | -2.24 | 1.36 | 1.44 |
| 25 | A | 408 | BCR | C33-C5 | -2.24 | 1.47 | 1.50 |
| 23 | b | 614 | CLA | C3B-CAB | -2.24 | 1.43 | 1.47 |
| 23 | B | 603 | CLA | CHC-C1C | 2.24 | 1.40 | 1.35 |
| 33 | D | 407 | LMG | O6-C5 | -2.24 | 1.38 | 1.44 |
| 23 | b | 614 | CLA | C1D-C2D | 2.23 | 1.47 | 1.42 |
| 25 | t | 101 | BCR | C30-C25 | -2.23 | 1.50 | 1.53 |
| 23 | a | 406 | CLA | C1D-C2D | 2.23 | 1.47 | 1.42 |
| 23 | c | 513 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 28 | H | 102 | DGD | C4E-C5E | 2.22 | 1.57 | 1.53 |
| 23 | B | 612 | CLA | CMD-C2D | -2.22 | 1.46 | 1.51 |
| 23 | b | 608 | CLA | C1D-C2D | 2.22 | 1.47 | 1.42 |
| 35 | V | 201 | HEC | CMD-C2D | 2.22 | 1.56 | 1.51 |
| 28 | c | 518 | DGD | C1E-C2E | 2.22 | 1.58 | 1.52 |
| 23 | c | 505 | CLA | CMD-C2D | -2.22 | 1.46 | 1.51 |
| 23 | C | 505 | CLA | MG-NC | 2.21 | 2.11 | 2.06 |
| 23 | B | 614 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 23 | b | 606 | CLA | CMD-C2D | -2.21 | 1.46 | 1.51 |
| 28 | C | 518 | DGD | O2E-C2E | -2.21 | 1.37 | 1.43 |
| 23 | b | 604 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 28 | a | 413 | DGD | O1G-C1A | 2.21 | 1.39 | 1.33 |
| 33 | C | 501 | LMG | O1-C1 | 2.20 | 1.43 | 1.40 |
| 26 | D | 406 | PL9 | C27-C28 | -2.20 | 1.43 | 1.50 |
| 27 | B | 621 | SQD | O2-C2 | -2.20 | 1.37 | 1.43 |
| 23 | b | 612 | CLA | CMD-C2D | -2.20 | 1.46 | 1.51 |
| 25 | C | 515 | BCR | C38-C26 | -2.20 | 1.47 | 1.50 |
| 25 | C | 515 | BCR | C34-C9 | -2.20 | 1.46 | 1.50 |
| 23 | A | 407 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 25 | b | 620 | BCR | C30-C25 | -2.19 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | b | 616 | CLA | CMD-C2D | -2.19 | 1.46 | 1.51 |
| 23 | B | 615 | CLA | CMD-C2D | -2.19 | 1.46 | 1.51 |
| 23 | b | 611 | CLA | C1D-C2D | 2.19 | 1.47 | 1.42 |
| 23 | C | 510 | CLA | MG-NA | 2.19 | 2.11 | 2.06 |
| 23 | b | 617 | CLA | CHC-C1C | 2.19 | 1.40 | 1.35 |
| 24 | a | 407 | PHO | C4C-NC | 2.18 | 1.41 | 1.36 |
| 27 | a | 411 | SQD | O2-C2 | -2.18 | 1.37 | 1.43 |
| 29 | E | 101 | LHG | P-O6 | 2.18 | 1.68 | 1.59 |
| 28 | C | 517 | DGD | C1G-C2G | 2.18 | 1.57 | 1.50 |
| 23 | b | 602 | CLA | CMD-C2D | -2.18 | 1.46 | 1.51 |
| 28 | c | 516 | DGD | O3E-C3E | -2.18 | 1.37 | 1.43 |
| 23 | C | 511 | CLA | MG-NC | 2.18 | 2.11 | 2.06 |
| 28 | h | 101 | DGD | C3G-C2G | 2.18 | 1.57 | 1.50 |
| 23 | C | 504 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 29 | A | 413 | LHG | O6-C4 | -2.17 | 1.36 | 1.44 |
| 23 | b | 606 | CLA | MG-NA | 2.17 | 2.11 | 2.06 |
| 28 | C | 516 | DGD | C2B-C1B | -2.17 | 1.44 | 1.50 |
| 27 | A | 410 | SQD | O47-C45 | -2.17 | 1.41 | 1.46 |
| 25 | D | 405 | BCR | C27-C26 | -2.17 | 1.46 | 1.51 |
| 23 | b | 603 | CLA | CMB-C2B | -2.17 | 1.47 | 1.51 |
| 33 | m | 101 | LMG | O4-C4 | -2.17 | 1.37 | 1.43 |
| 23 | c | 506 | CLA | CMB-C2B | -2.17 | 1.47 | 1.51 |
| 28 | c | 518 | DGD | C3G-C2G | 2.17 | 1.57 | 1.50 |
| 23 | B | 608 | CLA | MG-NA | -2.17 | 2.01 | 2.06 |
| 23 | C | 509 | CLA | CMD-C2D | -2.17 | 1.46 | 1.51 |
| 23 | b | 615 | CLA | C1A-CHA | -2.16 | 1.34 | 1.43 |
| 23 | c | 504 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 28 | c | 518 | DGD | O1G-C1G | -2.16 | 1.40 | 1.45 |
| 23 | B | 610 | CLA | CMA-C3A | -2.16 | 1.48 | 1.53 |
| 23 | B | 615 | CLA | C5-C3 | -2.16 | 1.46 | 1.51 |
| 23 | B | 607 | CLA | CAC-C3C | -2.16 | 1.45 | 1.51 |
| 23 | A | 404 | CLA | C3D-C2D | -2.16 | 1.35 | 1.39 |
| 28 | C | 518 | DGD | C2A-C1A | -2.16 | 1.44 | 1.50 |
| 23 | b | 608 | CLA | CHC-C1C | 2.16 | 1.40 | 1.35 |
| 25 | C | 520 | BCR | C38-C26 | -2.15 | 1.47 | 1.50 |
| 23 | c | 509 | CLA | C1D-C2D | 2.15 | 1.47 | 1.42 |
| 23 | b | 615 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | C | 520 | BCR | C1-C6 | -2.15 | 1.50 | 1.53 |
| 26 | D | 406 | PL9 | C5-C4 | -2.15 | 1.39 | 1.47 |
| 26 | d | 406 | PL9 | C46-C44 | -2.14 | 1.46 | 1.51 |
| 23 | C | 508 | CLA | C1B-NB | -2.14 | 1.33 | 1.35 |
| 23 | B | 608 | CLA | C4B-CHC | -2.14 | 1.35 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | b | 607 | CLA | CMB-C2B | -2.14 | 1.47 | 1.51 |
| 23 | b | 611 | CLA | C1C-NC | -2.14 | 1.34 | 1.37 |
| 24 | d | 401 | PHO | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 23 | B | 603 | CLA | C3C-C2C | 2.14 | 1.41 | 1.36 |
| 26 | A | 409 | PL9 | C3-C4 | -2.14 | 1.46 | 1.49 |
| 23 | b | 613 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 28 | c | 516 | DGD | O5D-C1E | 2.13 | 1.43 | 1.40 |
| 23 | c | 509 | CLA | C3C-C2C | 2.13 | 1.41 | 1.36 |
| 25 | B | 619 | BCR | C38-C26 | -2.13 | 1.47 | 1.50 |
| 29 | l | 101 | LHG | P-O6 | 2.13 | 1.67 | 1.59 |
| 23 | c | 510 | CLA | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 23 | C | 505 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 28 | A | 412 | DGD | O1G-C1G | -2.13 | 1.40 | 1.45 |
| 23 | c | 502 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 23 | b | 613 | CLA | O2D-CED | -2.13 | 1.40 | 1.45 |
| 25 | B | 618 | BCR | C39-C30 | -2.13 | 1.49 | 1.53 |
| 23 | C | 506 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 23 | C | 507 | CLA | C1A-CHA | -2.12 | 1.34 | 1.43 |
| 23 | B | 607 | CLA | C4B-CHC | -2.12 | 1.35 | 1.41 |
| 27 | a | 411 | SQD | O4-C4 | -2.12 | 1.38 | 1.43 |
| 23 | B | 606 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 23 | a | 405 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 23 | b | 610 | CLA | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 24 | A | 406 | PHO | C3B-C4B | 2.12 | 1.47 | 1.43 |
| 23 | C | 514 | CLA | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 23 | C | 511 | CLA | CAA-C2A | -2.12 | 1.50 | 1.54 |
| 29 | d | 409 | LHG | C3-C2 | 2.12 | 1.58 | 1.51 |
| 27 | A | 411 | SQD | C46-C45 | 2.12 | 1.55 | 1.50 |
| 23 | b | 603 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 25 | A | 408 | BCR | C27-C26 | -2.12 | 1.46 | 1.51 |
| 33 | D | 407 | LMG | C4-C3 | 2.11 | 1.57 | 1.52 |
| 23 | d | 403 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 23 | b | 613 | CLA | CMB-C2B | -2.11 | 1.47 | 1.51 |
| 23 | D | 402 | CLA | C4B-CHC | -2.11 | 1.35 | 1.41 |
| 23 | C | 512 | CLA | C1B-NB | 2.11 | 1.37 | 1.35 |
| 23 | B | 604 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 33 | c | 519 | LMG | O8-C9 | -2.10 | 1.40 | 1.45 |
| 33 | C | 519 | LMG | C4-C3 | 2.10 | 1.57 | 1.52 |
| 23 | C | 507 | CLA | CMA-C3A | -2.10 | 1.48 | 1.53 |
| 23 | B | 610 | CLA | C1D-C2D | 2.10 | 1.47 | 1.42 |
| 23 | b | 610 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 23 | c | 504 | CLA | CMD-C2D | -2.10 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | L | 101 | LHG | C4-C5 | 2.10 | 1.57 | 1.50 |
| 23 | b | 614 | CLA | CMD-C2D | -2.10 | 1.46 | 1.51 |
| 24 | A | 406 | PHO | CHD-C4C | -2.10 | 1.35 | 1.40 |
| 23 | b | 606 | CLA | C4B-CHC | -2.10 | 1.35 | 1.41 |
| 23 | C | 514 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 23 | d | 404 | CLA | C3D-C2D | -2.09 | 1.35 | 1.39 |
| 23 | c | 510 | CLA | C5-C3 | -2.09 | 1.46 | 1.51 |
| 25 | x | 102 | BCR | C1-C6 | -2.09 | 1.50 | 1.53 |
| 23 | B | 602 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 23 | b | 608 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 28 | H | 102 | DGD | O2G-C2G | -2.09 | 1.41 | 1.46 |
| 23 | B | 605 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |
| 23 | C | 512 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 28 | C | 517 | DGD | O2G-C2G | -2.09 | 1.41 | 1.46 |
| 23 | B | 611 | CLA | C1D-C2D | 2.09 | 1.47 | 1.42 |
| 23 | B | 610 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 23 | C | 510 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |
| 26 | D | 406 | PL9 | C7-C8 | -2.08 | 1.47 | 1.50 |
| 23 | b | 607 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 23 | c | 511 | CLA | C3C-C2C | 2.08 | 1.41 | 1.36 |
| 23 | D | 402 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 23 | B | 609 | CLA | C1D-C2D | 2.08 | 1.47 | 1.42 |
| 23 | d | 403 | CLA | MG-NC | 2.08 | 2.11 | 2.06 |
| 23 | c | 501 | CLA | C4B-CHC | -2.08 | 1.35 | 1.41 |
| 23 | B | 602 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | B | 617 | BCR | C38-C26 | -2.08 | 1.47 | 1.50 |
| 28 | H | 102 | DGD | O2G-C1B | 2.08 | 1.40 | 1.34 |
| 23 | B | 602 | CLA | OBD-CAD | 2.08 | 1.25 | 1.22 |
| 33 | C | 519 | LMG | C4-C5 | 2.07 | 1.57 | 1.53 |
| 25 | a | 409 | BCR | C35-C13 | -2.07 | 1.46 | 1.50 |
| 23 | d | 404 | CLA | CHC-C1C | 2.07 | 1.40 | 1.35 |
| 23 | B | 616 | CLA | C1D-C2D | 2.07 | 1.47 | 1.42 |
| 25 | b | 620 | BCR | C38-C26 | -2.07 | 1.47 | 1.50 |
| 33 | c | 524 | LMG | C1-C2 | 2.07 | 1.58 | 1.52 |
| 25 | k | 101 | BCR | C33-C5 | -2.07 | 1.47 | 1.50 |
| 26 | D | 406 | PL9 | C21-C19 | -2.06 | 1.47 | 1.51 |
| 27 | f | 101 | SQD | O4-C4 | -2.06 | 1.38 | 1.43 |
| 33 | C | 501 | LMG | C1-C2 | 2.06 | 1.58 | 1.52 |
| 23 | b | 602 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 23 | B | 614 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 23 | A | 407 | CLA | CAC-C3C | -2.06 | 1.45 | 1.51 |
| 23 | C | 505 | CLA | C4B-CHC | -2.05 | 1.35 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28 | c | 517 | DGD | O1G-C1A | 2.05 | 1.39 | 1.33 |
| 28 | C | 517 | DGD | C4E-C5E | 2.05 | 1.57 | 1.53 |
| 24 | a | 407 | PHO | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 23 | C | 514 | CLA | C4B-CHC | -2.05 | 1.35 | 1.41 |
| 25 | t | 101 | BCR | C1-C6 | -2.05 | 1.50 | 1.53 |
| 23 | a | 406 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 23 | B | 608 | CLA | O2D-CED | -2.05 | 1.40 | 1.45 |
| 33 | c | 519 | LMG | O7-C8 | -2.05 | 1.41 | 1.46 |
| 28 | C | 518 | DGD | O1G-C1G | -2.04 | 1.40 | 1.45 |
| 24 | D | 401 | PHO | C1B-C2B | 2.04 | 1.50 | 1.45 |
| 23 | c | 509 | CLA | O1D-CGD | 2.04 | 1.26 | 1.21 |
| 23 | c | 506 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 23 | b | 611 | CLA | CMA-C3A | -2.04 | 1.48 | 1.53 |
| 25 | t | 101 | BCR | C33-C5 | -2.04 | 1.47 | 1.50 |
| 23 | B | 613 | CLA | C1D-C2D | 2.04 | 1.47 | 1.42 |
| 23 | c | 508 | CLA | C4B-CHC | -2.03 | 1.35 | 1.41 |
| 23 | B | 607 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 33 | c | 524 | LMG | O8-C28 | 2.03 | 1.39 | 1.33 |
| 33 | M | 101 | LMG | C9-C8 | 2.03 | 1.56 | 1.50 |
| 23 | b | 602 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 23 | C | 513 | CLA | C1A-CHA | -2.03 | 1.34 | 1.43 |
| 23 | b | 610 | CLA | C1A-CHA | -2.03 | 1.34 | 1.43 |
| 23 | C | 506 | CLA | C4B-CHC | -2.03 | 1.35 | 1.41 |
| 24 | a | 407 | PHO | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 23 | d | 403 | CLA | CMD-C2D | -2.03 | 1.46 | 1.51 |
| 28 | H | 102 | DGD | O3E-C3E | -2.03 | 1.38 | 1.43 |
| 23 | C | 509 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 23 | b | 610 | CLA | CMA-C3A | -2.02 | 1.48 | 1.53 |
| 23 | B | 616 | CLA | CHC-C1C | 2.02 | 1.40 | 1.35 |
| 23 | c | 507 | CLA | CHC-C1C | 2.02 | 1.40 | 1.35 |
| 23 | B | 601 | CLA | CAA-C2A | -2.02 | 1.50 | 1.54 |
| 23 | c | 504 | CLA | C1D-C2D | 2.02 | 1.47 | 1.42 |
| 23 | b | 609 | CLA | CBD-CGD | -2.02 | 1.46 | 1.52 |
| 23 | d | 402 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 23 | c | 510 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 25 | H | 101 | BCR | C33-C5 | -2.02 | 1.47 | 1.50 |
| 28 | c | 517 | DGD | O2G-C2G | -2.01 | 1.41 | 1.46 |
| 23 | B | 611 | CLA | C4B-CHC | -2.01 | 1.35 | 1.41 |
| 23 | C | 502 | CLA | CMB-C2B | -2.01 | 1.47 | 1.51 |
| 23 | A | 404 | CLA | O2D-CGD | 2.01 | 1.38 | 1.33 |
| 23 | C | 503 | CLA | CMD-C2D | -2.01 | 1.46 | 1.51 |
| 23 | B | 610 | CLA | CMD-C2D | -2.01 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | A | 405 | CLA | CAA-C2A | -2.01 | 1.50 | 1.54 |
| 25 | B | 618 | BCR | C33-C5 | -2.01 | 1.47 | 1.50 |
| 34 | E | 103 | HEM | C4A-CHB | -2.01 | 1.35 | 1.41 |
| 23 | b | 612 | CLA | C3D-C2D | -2.01 | 1.35 | 1.39 |
| 23 | d | 402 | CLA | C1B-NB | 2.00 | 1.37 | 1.35 |
| 23 | a | 406 | CLA | C4B-CHC | -2.00 | 1.35 | 1.41 |
| 23 | c | 513 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 25 | B | 619 | BCR | C33-C5 | -2.00 | 1.47 | 1.50 |
| 24 | A | 406 | PHO | CHB-C1B | -2.00 | 1.34 | 1.38 |

All (1425) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | c | 509 | CLA | C4A-NA-C1A | 11.10 | 111.69 | 106.71 |
| 23 | c | 501 | CLA | C4A-NA-C1A | 10.59 | 111.47 | 106.71 |
| 23 | C | 502 | CLA | C4A-NA-C1A | 10.55 | 111.45 | 106.71 |
| 23 | d | 402 | CLA | C4A-NA-C1A | 10.41 | 111.38 | 106.71 |
| 27 | A | 410 | SQD | O6-C1-C2 | 10.12 | 124.11 | 108.30 |
| 23 | C | 504 | CLA | C4A-NA-C1A | 9.22 | 110.85 | 106.71 |
| 23 | D | 403 | CLA | C4A-NA-C1A | 8.97 | 110.74 | 106.71 |
| 23 | B | 606 | CLA | C4A-NA-C1A | 8.58 | 110.56 | 106.71 |
| 23 | C | 514 | CLA | C4A-NA-C1A | 8.41 | 110.49 | 106.71 |
| 27 | b | 601 | SQD | O6-C1-C2 | 8.37 | 121.37 | 108.30 |
| 23 | C | 509 | CLA | C4A-NA-C1A | 8.10 | 110.35 | 106.71 |
| 23 | C | 512 | CLA | C4A-NA-C1A | 7.99 | 110.30 | 106.71 |
| 27 | a | 411 | SQD | O6-C1-C2 | 7.93 | 120.69 | 108.30 |
| 23 | C | 511 | CLA | C4A-NA-C1A | 7.75 | 110.19 | 106.71 |
| 23 | B | 612 | CLA | C4A-NA-C1A | 7.69 | 110.16 | 106.71 |
| 23 | B | 613 | CLA | C4A-NA-C1A | 7.45 | 110.06 | 106.71 |
| 23 | c | 511 | CLA | C4A-NA-C1A | 7.35 | 110.01 | 106.71 |
| 23 | B | 610 | CLA | C4A-NA-C1A | 7.33 | 110.00 | 106.71 |
| 23 | b | 613 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 23 | b | 606 | CLA | C4A-NA-C1A | 6.81 | 109.77 | 106.71 |
| 33 | b | 622 | LMG | O1-C1-C2 | -6.79 | 97.70 | 108.30 |
| 23 | c | 502 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 23 | b | 605 | CLA | OBD-CAD-CBD | -6.64 | 116.41 | 125.89 |
| 23 | b | 616 | CLA | C4A-NA-C1A | 6.50 | 109.63 | 106.71 |
| 23 | c | 507 | CLA | C4A-NA-C1A | 6.47 | 109.62 | 106.71 |
| 23 | c | 504 | CLA | C4A-NA-C1A | 6.33 | 109.55 | 106.71 |
| 23 | C | 510 | CLA | C4A-NA-C1A | 6.31 | 109.54 | 106.71 |
| 27 | b | 601 | SQD | O7-S-C6 | 6.14 | 114.24 | 106.94 |
| 27 | A | 410 | SQD | O7-S-C6 | 6.12 | 114.22 | 106.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | a | 405 | CLA | C4A-NA-C1A | 6.09 | 109.45 | 106.71 |
| 23 | A | 407 | CLA | O2D-CGD-O1D | -5.97 | 112.16 | 123.84 |
| 27 | a | 411 | SQD | O9-S-C6 | 5.95 | 114.01 | 106.94 |
| 23 | A | 404 | CLA | C4A-NA-C1A | 5.95 | 109.38 | 106.71 |
| 23 | B | 604 | CLA | C4A-NA-C1A | 5.94 | 109.38 | 106.71 |
| 23 | B | 616 | CLA | C4A-NA-C1A | 5.84 | 109.33 | 106.71 |
| 27 | F | 101 | SQD | O8-S-C6 | 5.84 | 115.05 | 105.74 |
| 23 | B | 603 | CLA | O2D-CGD-O1D | -5.84 | 112.42 | 123.84 |
| 23 | B | 614 | CLA | C4A-NA-C1A | 5.84 | 109.33 | 106.71 |
| 27 | B | 621 | SQD | O6-C1-C2 | 5.78 | 117.33 | 108.30 |
| 23 | c | 503 | CLA | C4A-NA-C1A | 5.76 | 109.30 | 106.71 |
| 26 | D | 406 | PL9 | C7-C3-C4 | 5.75 | 121.55 | 116.88 |
| 23 | c | 501 | CLA | O2D-CGD-O1D | -5.70 | 112.69 | 123.84 |
| 23 | B | 614 | CLA | O2D-CGD-O1D | -5.70 | 112.70 | 123.84 |
| 23 | B | 611 | CLA | C4A-NA-C1A | 5.59 | 109.22 | 106.71 |
| 27 | B | 621 | SQD | O47-C7-C8 | 5.56 | 123.48 | 111.50 |
| 27 | F | 101 | SQD | O6-C1-C2 | 5.54 | 116.96 | 108.30 |
| 23 | b | 617 | CLA | O2D-CGD-O1D | -5.54 | 113.01 | 123.84 |
| 23 | c | 506 | CLA | C4A-NA-C1A | 5.53 | 109.19 | 106.71 |
| 23 | b | 605 | CLA | C4D-C3D-CAD | -5.53 | 105.39 | 108.47 |
| 23 | b | 607 | CLA | C4A-NA-C1A | 5.52 | 109.19 | 106.71 |
| 27 | f | 101 | SQD | O6-C1-C2 | 5.50 | 116.89 | 108.30 |
| 23 | a | 406 | CLA | CHB-C4A-NA | 5.48 | 132.09 | 124.51 |
| 28 | H | 102 | DGD | O3G-C3G-C2G | -5.47 | 97.71 | 110.90 |
| 34 | e | 102 | HEM | CBD-CAD-C3D | -5.45 | 102.44 | 112.48 |
| 23 | b | 613 | CLA | CMB-C2B-C1B | -5.42 | 120.13 | 128.46 |
| 26 | a | 410 | PL9 | C7-C3-C4 | 5.39 | 121.26 | 116.88 |
| 27 | F | 101 | SQD | O9-S-C6 | 5.35 | 113.30 | 106.94 |
| 23 | B | 614 | CLA | CMB-C2B-C1B | -5.18 | 120.51 | 128.46 |
| 23 | b | 615 | CLA | C4A-NA-C1A | 5.17 | 109.03 | 106.71 |
| 23 | b | 613 | CLA | CMB-C2B-C3B | 5.16 | 134.33 | 124.68 |
| 23 | c | 512 | CLA | C4A-NA-C1A | 5.13 | 109.01 | 106.71 |
| 27 | a | 412 | SQD | O47-C7-C8 | 5.10 | 122.49 | 111.50 |
| 26 | A | 409 | PL9 | C7-C3-C4 | 5.07 | 121.00 | 116.88 |
| 23 | c | 501 | CLA | CMB-C2B-C1B | -5.04 | 120.72 | 128.46 |
| 23 | b | 605 | CLA | OBD-CAD-C3D | 5.03 | 136.33 | 127.98 |
| 23 | A | 407 | CLA | CMB-C2B-C1B | -4.89 | 120.95 | 128.46 |
| 26 | d | 406 | PL9 | C40-C39-C41 | 4.84 | 123.42 | 115.27 |
| 23 | b | 614 | CLA | CMB-C2B-C1B | -4.81 | 121.07 | 128.46 |
| 23 | b | 616 | CLA | CMB-C2B-C1B | -4.81 | 121.07 | 128.46 |
| 23 | b | 614 | CLA | C4A-NA-C1A | 4.80 | 108.86 | 106.71 |
| 23 | D | 404 | CLA | O2D-CGD-O1D | -4.77 | 114.51 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 502 | CLA | O2D-CGD-CBD | 4.75 | 119.71 | 111.27 |
| 23 | c | 501 | CLA | O2D-CGD-CBD | 4.71 | 119.64 | 111.27 |
| 23 | C | 503 | CLA | C4D-C3D-CAD | -4.67 | 105.87 | 108.47 |
| 23 | b | 617 | CLA | C4A-NA-C1A | 4.66 | 108.80 | 106.71 |
| 23 | a | 406 | CLA | O2D-CGD-CBD | 4.64 | 119.51 | 111.27 |
| 23 | B | 609 | CLA | C4A-NA-C1A | 4.63 | 108.79 | 106.71 |
| 23 | b | 603 | CLA | O2D-CGD-O1D | -4.63 | 114.79 | 123.84 |
| 23 | b | 615 | CLA | CMB-C2B-C1B | -4.62 | 121.36 | 128.46 |
| 23 | B | 608 | CLA | C4A-NA-C1A | 4.61 | 108.78 | 106.71 |
| 23 | B | 609 | CLA | CMB-C2B-C1B | -4.61 | 121.39 | 128.46 |
| 23 | b | 608 | CLA | C4A-NA-C1A | 4.60 | 108.77 | 106.71 |
| 23 | b | 604 | CLA | C4A-NA-C1A | 4.59 | 108.77 | 106.71 |
| 23 | a | 406 | CLA | C4D-C3D-CAD | -4.58 | 105.92 | 108.47 |
| 23 | c | 504 | CLA | CMB-C2B-C1B | -4.57 | 121.44 | 128.46 |
| 29 | A | 413 | LHG | O4-P-O5 | 4.56 | 134.81 | 112.24 |
| 23 | a | 406 | CLA | C4A-NA-C1A | 4.55 | 108.75 | 106.71 |
| 23 | B | 609 | CLA | OBD-CAD-CBD | -4.51 | 119.46 | 125.89 |
| 33 | c | 522 | LMG | O6-C1-O1 | -4.51 | 99.30 | 109.97 |
| 23 | C | 508 | CLA | CMB-C2B-C1B | -4.48 | 121.58 | 128.46 |
| 23 | B | 601 | CLA | C4A-NA-C1A | 4.48 | 108.72 | 106.71 |
| 23 | A | 404 | CLA | CHB-C4A-NA | 4.47 | 130.69 | 124.51 |
| 23 | b | 606 | CLA | CMB-C2B-C1B | -4.46 | 121.61 | 128.46 |
| 28 | C | 518 | DGD | O3G-C3G-C2G | -4.44 | 100.19 | 110.90 |
| 23 | b | 606 | CLA | O2D-CGD-O1D | -4.43 | 115.17 | 123.84 |
| 23 | C | 509 | CLA | O2D-CGD-O1D | -4.41 | 115.22 | 123.84 |
| 23 | A | 405 | CLA | O2D-CGD-O1D | -4.38 | 115.27 | 123.84 |
| 27 | A | 411 | SQD | O47-C7-C8 | 4.37 | 120.93 | 111.50 |
| 23 | A | 405 | CLA | CMB-C2B-C1B | -4.37 | 121.75 | 128.46 |
| 23 | b | 603 | CLA | O2D-CGD-CBD | 4.37 | 119.03 | 111.27 |
| 23 | A | 405 | CLA | O2D-CGD-CBD | 4.35 | 119.00 | 111.27 |
| 23 | B | 610 | CLA | O2D-CGD-O1D | -4.35 | 115.34 | 123.84 |
| 28 | C | 517 | DGD | O3G-C3G-C2G | -4.35 | 100.41 | 110.90 |
| 23 | C | 505 | CLA | CMB-C2B-C1B | -4.34 | 121.80 | 128.46 |
| 25 | B | 618 | BCR | C35-C13-C14 | -4.33 | 116.85 | 122.92 |
| 23 | b | 604 | CLA | O2D-CGD-O1D | -4.31 | 115.42 | 123.84 |
| 23 | d | 402 | CLA | O2D-CGD-O1D | -4.29 | 115.45 | 123.84 |
| 28 | A | 412 | DGD | C3G-C2G-C1G | -4.27 | 101.70 | 111.79 |
| 27 | f | 101 | SQD | O8-S-C6 | 4.26 | 112.52 | 105.74 |
| 23 | b | 615 | CLA | OBD-CAD-CBD | -4.25 | 119.82 | 125.89 |
| 27 | b | 601 | SQD | O8-S-C6 | 4.24 | 112.50 | 105.74 |
| 23 | c | 506 | CLA | CBC-CAC-C3C | -4.23 | 100.78 | 112.43 |
| 23 | c | 510 | CLA | O2D-CGD-O1D | -4.23 | 115.58 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | b | 604 | CLA | O2D-CGD-CBD | 4.22 | 118.77 | 111.27 |
| 29 | e | 101 | LHG | O4-P-O5 | 4.22 | 133.09 | 112.24 |
| 23 | c | 513 | CLA | C4A-NA-C1A | 4.21 | 108.60 | 106.71 |
| 29 | d | 407 | LHG | O4-P-O5 | 4.20 | 133.00 | 112.24 |
| 23 | c | 510 | CLA | CMB-C2B-C3B | 4.20 | 132.53 | 124.68 |
| 23 | b | 610 | CLA | CMB-C2B-C1B | -4.19 | 122.03 | 128.46 |
| 34 | e | 102 | HEM | CBA-CAA-C2A | -4.18 | 104.77 | 112.49 |
| 23 | C | 504 | CLA | O2D-CGD-O1D | -4.17 | 115.68 | 123.84 |
| 29 | E | 101 | LHG | O4-P-O5 | 4.17 | 132.87 | 112.24 |
| 23 | A | 407 | CLA | CMB-C2B-C3B | 4.17 | 132.47 | 124.68 |
| 29 | D | 408 | LHG | O4-P-O5 | 4.16 | 132.83 | 112.24 |
| 29 | d | 409 | LHG | O4-P-O5 | 4.15 | 132.74 | 112.24 |
| 27 | b | 601 | SQD | O5-C5-C4 | 4.14 | 117.22 | 109.69 |
| 23 | B | 612 | CLA | CHB-C4A-NA | 4.14 | 130.23 | 124.51 |
| 23 | B | 601 | CLA | O2D-CGD-O1D | -4.13 | 115.76 | 123.84 |
| 27 | b | 601 | SQD | C1-C2-C3 | -4.11 | 101.43 | 110.00 |
| 23 | B | 614 | CLA | C1D-CHD-C4C | 4.11 | 127.98 | 122.56 |
| 33 | d | 411 | LMG | O6-C5-C4 | 4.11 | 117.15 | 109.69 |
| 23 | c | 509 | CLA | C4D-C3D-CAD | -4.09 | 106.19 | 108.47 |
| 23 | c | 501 | CLA | CMB-C2B-C3B | 4.08 | 132.31 | 124.68 |
| 33 | d | 411 | LMG | O1-C1-C2 | -4.07 | 101.94 | 108.30 |
| 23 | a | 406 | CLA | CMA-C3A-C4A | -4.07 | 100.84 | 111.77 |
| 28 | c | 516 | DGD | O3G-C3G-C2G | -4.07 | 101.09 | 110.90 |
| 23 | b | 614 | CLA | OBD-CAD-CBD | -4.05 | 120.11 | 125.89 |
| 23 | c | 505 | CLA | CMD-C2D-C3D | 4.04 | 132.24 | 124.68 |
| 23 | b | 613 | CLA | CHB-C4A-NA | 4.04 | 130.09 | 124.51 |
| 23 | c | 502 | CLA | CMB-C2B-C1B | -4.03 | 122.26 | 128.46 |
| 23 | c | 510 | CLA | CMB-C2B-C1B | -4.03 | 122.27 | 128.46 |
| 28 | c | 516 | DGD | C3G-C2G-C1G | -4.02 | 102.29 | 111.79 |
| 29 | d | 408 | LHG | O4-P-O5 | 4.02 | 132.09 | 112.24 |
| 23 | b | 603 | CLA | CHB-C4A-NA | 4.01 | 130.06 | 124.51 |
| 23 | C | 506 | CLA | CMD-C2D-C3D | 4.01 | 132.19 | 124.68 |
| 29 | D | 409 | LHG | O4-P-O5 | 4.01 | 132.04 | 112.24 |
| 23 | C | 513 | CLA | CHB-C4A-NA | 4.00 | 130.05 | 124.51 |
| 23 | B | 614 | CLA | CMB-C2B-C3B | 4.00 | 132.16 | 124.68 |
| 23 | c | 508 | CLA | CMB-C2B-C1B | -3.99 | 122.32 | 128.46 |
| 23 | C | 507 | CLA | OBD-CAD-CBD | -3.98 | 120.21 | 125.89 |
| 23 | c | 507 | CLA | C1B-CHB-C4A | -3.97 | 122.25 | 130.12 |
| 23 | c | 502 | CLA | CMB-C2B-C3B | 3.97 | 132.11 | 124.68 |
| 23 | c | 510 | CLA | C4A-NA-C1A | 3.96 | 108.49 | 106.71 |
| 23 | d | 403 | CLA | C4A-NA-C1A | 3.96 | 108.49 | 106.71 |
| 23 | a | 406 | CLA | O2D-CGD-O1D | -3.95 | 116.12 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | A | 410 | SQD | C1-C2-C3 | -3.95 | 101.78 | 110.00 |
| 28 | c | 518 | DGD | C3G-C2G-C1G | -3.94 | 102.47 | 111.79 |
| 27 | B | 621 | SQD | O8-S-C6 | 3.92 | 111.99 | 105.74 |
| 23 | d | 404 | CLA | CMB-C2B-C1B | -3.92 | 122.44 | 128.46 |
| 23 | b | 613 | CLA | CMD-C2D-C3D | 3.91 | 131.99 | 124.68 |
| 23 | A | 405 | CLA | CMB-C2B-C3B | 3.91 | 131.99 | 124.68 |
| 23 | b | 605 | CLA | CMD-C2D-C3D | 3.89 | 131.95 | 124.68 |
| 23 | b | 609 | CLA | C1B-CHB-C4A | -3.89 | 122.42 | 130.12 |
| 28 | H | 102 | DGD | C1D-O6D-C5D | -3.88 | 106.08 | 113.69 |
| 23 | B | 607 | CLA | C4A-NA-C1A | 3.88 | 108.45 | 106.71 |
| 29 | l | 101 | LHG | O4-P-O5 | 3.88 | 131.40 | 112.24 |
| 33 | m | 101 | LMG | O7-C10-O9 | -3.86 | 114.38 | 123.70 |
| 23 | A | 407 | CLA | C1B-CHB-C4A | -3.86 | 122.48 | 130.12 |
| 23 | b | 617 | CLA | CHB-C4A-NA | 3.86 | 129.84 | 124.51 |
| 28 | C | 517 | DGD | C1D-C2D-C3D | -3.85 | 101.98 | 110.00 |
| 23 | B | 603 | CLA | C4D-C3D-CAD | -3.84 | 106.33 | 108.47 |
| 23 | B | 615 | CLA | CMB-C2B-C1B | -3.83 | 122.58 | 128.46 |
| 23 | b | 604 | CLA | OBD-CAD-CBD | -3.82 | 120.43 | 125.89 |
| 23 | b | 616 | CLA | CMD-C2D-C3D | 3.82 | 131.82 | 124.68 |
| 23 | C | 506 | CLA | CMB-C2B-C1B | -3.82 | 122.60 | 128.46 |
| 23 | C | 505 | CLA | C4A-NA-C1A | 3.81 | 108.42 | 106.71 |
| 23 | c | 510 | CLA | CHB-C4A-NA | 3.81 | 129.78 | 124.51 |
| 23 | b | 603 | CLA | CHC-C1C-NC | 3.81 | 129.98 | 124.20 |
| 23 | c | 511 | CLA | OBD-CAD-CBD | -3.81 | 120.45 | 125.89 |
| 23 | B | 615 | CLA | C4A-NA-C1A | 3.80 | 108.42 | 106.71 |
| 23 | B | 603 | CLA | C4A-NA-C1A | 3.79 | 108.41 | 106.71 |
| 23 | C | 508 | CLA | CMB-C2B-C3B | 3.78 | 131.75 | 124.68 |
| 27 | B | 621 | SQD | C1-O5-C5 | -3.77 | 106.29 | 113.69 |
| 23 | b | 606 | CLA | C1-C2-C3 | -3.76 | 119.54 | 126.04 |
| 23 | C | 510 | CLA | O2D-CGD-O1D | -3.76 | 116.49 | 123.84 |
| 25 | T | 101 | BCR | C27-C26-C25 | 3.76 | 128.19 | 122.73 |
| 23 | C | 502 | CLA | O2D-CGD-O1D | -3.76 | 116.50 | 123.84 |
| 27 | A | 410 | SQD | O47-C7-C8 | 3.75 | 119.58 | 111.50 |
| 27 | a | 411 | SQD | O9-S-O7 | -3.74 | 101.00 | 113.95 |
| 25 | b | 618 | BCR | C33-C5-C6 | -3.74 | 120.33 | 124.53 |
| 25 | b | 618 | BCR | C2-C1-C6 | 3.73 | 116.22 | 110.48 |
| 23 | C | 506 | CLA | OBD-CAD-CBD | -3.73 | 120.57 | 125.89 |
| 23 | b | 614 | CLA | CMB-C2B-C3B | 3.73 | 131.65 | 124.68 |
| 23 | b | 617 | CLA | O1D-CGD-CBD | 3.73 | 132.11 | 124.48 |
| 35 | V | 201 | HEC | CMC-C2C-C1C | -3.72 | 122.75 | 128.46 |
| 23 | c | 508 | CLA | C4A-NA-C1A | 3.72 | 108.38 | 106.71 |
| 23 | C | 513 | CLA | CMB-C2B-C1B | -3.71 | 122.76 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | c | 509 | CLA | CHB-C4A-NA | 3.70 | 129.63 | 124.51 |
| 26 | d | 406 | PL9 | C30-C29-C31 | -3.70 | 109.05 | 115.27 |
| 23 | B | 604 | CLA | C1D-CHD-C4C | 3.69 | 127.43 | 122.56 |
| 23 | A | 407 | CLA | O2D-CGD-CBD | 3.69 | 117.83 | 111.27 |
| 25 | A | 408 | BCR | C37-C22-C21 | -3.69 | 117.75 | 122.92 |
| 27 | f | 101 | SQD | O9-S-C6 | 3.69 | 111.32 | 106.94 |
| 23 | b | 603 | CLA | CMB-C2B-C1B | -3.68 | 122.81 | 128.46 |
| 33 | b | 622 | LMG | O2-C2-C1 | -3.68 | 101.12 | 110.05 |
| 33 | m | 101 | LMG | O1-C7-C8 | -3.66 | 102.06 | 110.90 |
| 28 | h | 101 | DGD | C4E-C3E-C2E | -3.66 | 104.43 | 110.82 |
| 23 | d | 404 | CLA | O2A-CGA-O1A | -3.65 | 114.37 | 123.59 |
| 23 | B | 603 | CLA | O2D-CGD-CBD | 3.64 | 117.74 | 111.27 |
| 23 | C | 503 | CLA | CMB-C2B-C1B | -3.64 | 122.86 | 128.46 |
| 26 | a | 410 | PL9 | C7-C3-C2 | -3.63 | 118.52 | 123.30 |
| 23 | C | 507 | CLA | C4A-NA-C1A | 3.63 | 108.34 | 106.71 |
| 34 | E | 103 | HEM | CBD-CAD-C3D | -3.63 | 105.79 | 112.48 |
| 23 | c | 502 | CLA | C4D-C3D-CAD | -3.63 | 106.45 | 108.47 |
| 23 | a | 405 | CLA | C1B-CHB-C4A | -3.62 | 122.94 | 130.12 |
| 28 | C | 518 | DGD | O6D-C1D-O3G | -3.62 | 101.39 | 109.97 |
| 23 | b | 614 | CLA | C4D-C3D-CAD | -3.62 | 106.45 | 108.47 |
| 23 | C | 508 | CLA | O2D-CGD-CBD | 3.61 | 117.69 | 111.27 |
| 23 | C | 503 | CLA | C1D-CHD-C4C | 3.61 | 127.32 | 122.56 |
| 23 | B | 602 | CLA | CMB-C2B-C3B | 3.61 | 131.42 | 124.68 |
| 23 | d | 404 | CLA | CMB-C2B-C3B | 3.61 | 131.42 | 124.68 |
| 24 | D | 401 | PHO | O1D-CGD-CBD | 3.59 | 131.83 | 124.48 |
| 23 | B | 614 | CLA | O1D-CGD-CBD | 3.59 | 131.83 | 124.48 |
| 23 | a | 406 | CLA | OBD-CAD-CBD | -3.59 | 120.77 | 125.89 |
| 23 | B | 616 | CLA | CMB-C2B-C1B | -3.59 | 122.95 | 128.46 |
| 23 | c | 505 | CLA | CMB-C2B-C1B | -3.58 | 122.97 | 128.46 |
| 26 | d | 406 | PL9 | C45-C44-C46 | -3.58 | 109.25 | 115.27 |
| 28 | A | 412 | DGD | O5D-C1E-C2E | 3.57 | 113.88 | 108.30 |
| 25 | B | 618 | BCR | C15-C16-C17 | -3.57 | 116.16 | 123.47 |
| 23 | B | 605 | CLA | OBD-CAD-CBD | -3.57 | 120.79 | 125.89 |
| 23 | b | 614 | CLA | CMD-C2D-C3D | 3.56 | 131.35 | 124.68 |
| 23 | C | 503 | CLA | O2D-CGD-O1D | -3.56 | 116.87 | 123.84 |
| 23 | b | 602 | CLA | O2D-CGD-O1D | -3.56 | 116.87 | 123.84 |
| 23 | b | 604 | CLA | C7-C6-C5 | -3.56 | 103.69 | 113.36 |
| 23 | c | 509 | CLA | O2A-CGA-O1A | -3.56 | 114.61 | 123.59 |
| 23 | B | 602 | CLA | CHB-C4A-NA | 3.55 | 129.43 | 124.51 |
| 27 | A | 411 | SQD | C45-O47-C7 | 3.55 | 122.45 | 117.88 |
| 23 | a | 406 | CLA | CED-O2D-CGD | -3.55 | 107.91 | 115.94 |
| 23 | b | 605 | CLA | C4A-NA-C1A | 3.55 | 108.30 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | c | 524 | LMG | C1-O6-C5 | -3.55 | 106.72 | 113.69 |
| 26 | d | 406 | PL9 | C7-C3-C4 | 3.54 | 119.76 | 116.88 |
| 23 | C | 507 | CLA | CMB-C2B-C3B | 3.54 | 131.29 | 124.68 |
| 28 | c | 516 | DGD | C3E-C4E-C5E | -3.54 | 103.93 | 110.24 |
| 27 | a | 411 | SQD | C1-C2-C3 | -3.53 | 102.65 | 110.00 |
| 23 | d | 402 | CLA | C4D-C3D-CAD | -3.53 | 106.50 | 108.47 |
| 23 | C | 507 | CLA | CMB-C2B-C1B | -3.53 | 123.04 | 128.46 |
| 27 | A | 410 | SQD | O9-S-O7 | -3.53 | 101.75 | 113.95 |
| 23 | b | 609 | CLA | CMA-C3A-C4A | -3.52 | 102.30 | 111.77 |
| 23 | B | 616 | CLA | O2D-CGD-O1D | -3.52 | 116.95 | 123.84 |
| 23 | B | 602 | CLA | CMB-C2B-C1B | -3.52 | 123.06 | 128.46 |
| 23 | c | 507 | CLA | CHB-C4A-NA | 3.52 | 129.38 | 124.51 |
| 23 | B | 606 | CLA | C2A-C1A-CHA | 3.51 | 130.00 | 123.86 |
| 26 | A | 409 | PL9 | C7-C3-C2 | -3.51 | 118.68 | 123.30 |
| 23 | b | 605 | CLA | C1D-CHD-C4C | 3.51 | 127.18 | 122.56 |
| 23 | b | 610 | CLA | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 23 | B | 602 | CLA | O2D-CGD-CBD | 3.50 | 117.49 | 111.27 |
| 23 | b | 616 | CLA | CMB-C2B-C3B | 3.50 | 131.22 | 124.68 |
| 23 | b | 611 | CLA | O2D-CGD-O1D | -3.49 | 117.01 | 123.84 |
| 23 | B | 616 | CLA | C1-O2A-CGA | 3.49 | 125.60 | 116.44 |
| 33 | d | 411 | LMG | O2-C2-C1 | -3.48 | 101.59 | 110.05 |
| 29 | A | 413 | LHG | O8-C23-C24 | 3.48 | 122.83 | 111.91 |
| 29 | L | 101 | LHG | O4-P-O5 | 3.47 | 129.41 | 112.24 |
| 28 | h | 101 | DGD | O3G-C3G-C2G | -3.46 | 102.54 | 110.90 |
| 23 | C | 512 | CLA | C1D-CHD-C4C | 3.46 | 127.13 | 122.56 |
| 26 | d | 406 | PL9 | C22-C23-C24 | -3.46 | 119.33 | 127.66 |
| 23 | b | 602 | CLA | O2A-C1-C2 | 3.45 | 117.72 | 108.64 |
| 35 | V | 201 | HEC | CMB-C2B-C1B | -3.45 | 123.16 | 128.46 |
| 29 | d | 407 | LHG | O8-C23-C24 | 3.44 | 122.70 | 111.91 |
| 23 | B | 603 | CLA | OBD-CAD-CBD | -3.44 | 120.98 | 125.89 |
| 23 | B | 609 | CLA | CMB-C2B-C3B | 3.44 | 131.11 | 124.68 |
| 23 | c | 509 | CLA | CMB-C2B-C1B | -3.44 | 123.18 | 128.46 |
| 23 | C | 506 | CLA | CAC-C3C-C4C | 3.43 | 129.26 | 124.81 |
| 26 | D | 406 | PL9 | C37-C38-C39 | -3.43 | 119.40 | 127.66 |
| 23 | b | 611 | CLA | CAA-CBA-CGA | -3.43 | 103.24 | 113.25 |
| 25 | Z | 101 | BCR | C15-C16-C17 | -3.42 | 116.46 | 123.47 |
| 23 | c | 503 | CLA | O2D-CGD-O1D | -3.42 | 117.14 | 123.84 |
| 34 | E | 103 | HEM | C1D-C2D-C3D | 3.42 | 109.37 | 107.00 |
| 23 | b | 612 | CLA | C1D-CHD-C4C | 3.41 | 127.06 | 122.56 |
| 34 | e | 102 | HEM | CMC-C2C-C3C | 3.41 | 131.07 | 124.68 |
| 23 | d | 403 | CLA | CMD-C2D-C3D | 3.41 | 131.05 | 124.68 |
| 23 | b | 608 | CLA | CHB-C4A-NA | 3.41 | 129.22 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | f | 101 | SQD | O47-C7-C8 | 3.40 | 120.29 | 110.80 |
| 23 | B | 613 | CLA | C4-C3-C5 | 3.40 | 120.99 | 115.27 |
| 23 | A | 405 | CLA | CAC-C3C-C4C | 3.40 | 129.22 | 124.81 |
| 23 | b | 602 | CLA | C4A-NA-C1A | 3.40 | 108.23 | 106.71 |
| 28 | c | 518 | DGD | O6E-C5E-C4E | 3.39 | 115.85 | 109.69 |
| 23 | d | 404 | CLA | CHA-C1A-NA | -3.39 | 118.64 | 126.40 |
| 25 | b | 619 | BCR | C8-C7-C6 | -3.39 | 117.69 | 127.20 |
| 27 | F | 101 | SQD | O5-C5-C4 | 3.38 | 115.84 | 109.69 |
| 23 | b | 615 | CLA | CMB-C2B-C3B | 3.38 | 131.00 | 124.68 |
| 23 | b | 609 | CLA | CMB-C2B-C3B | 3.38 | 131.00 | 124.68 |
| 28 | h | 101 | DGD | C1E-O6E-C5E | 3.38 | 120.32 | 113.69 |
| 23 | C | 504 | CLA | O2A-C1-C2 | -3.37 | 99.77 | 108.64 |
| 27 | a | 412 | SQD | O48-C23-C24 | 3.37 | 122.49 | 111.91 |
| 23 | c | 504 | CLA | CMD-C2D-C3D | 3.37 | 130.98 | 124.68 |
| 23 | B | 604 | CLA | O2A-C1-C2 | 3.36 | 117.48 | 108.64 |
| 25 | b | 619 | BCR | C30-C25-C26 | -3.36 | 117.88 | 122.61 |
| 23 | B | 611 | CLA | C1-C2-C3 | -3.36 | 120.22 | 126.04 |
| 26 | A | 409 | PL9 | C20-C19-C21 | 3.36 | 120.92 | 115.27 |
| 25 | C | 520 | BCR | C37-C22-C21 | -3.36 | 118.22 | 122.92 |
| 28 | c | 517 | DGD | O6D-C1D-O3G | -3.36 | 102.03 | 109.97 |
| 26 | d | 406 | PL9 | C7-C8-C9 | -3.35 | 121.21 | 126.79 |
| 27 | A | 410 | SQD | O47-C7-O49 | -3.35 | 115.60 | 123.70 |
| 23 | B | 604 | CLA | O2A-CGA-O1A | -3.34 | 115.15 | 123.59 |
| 23 | B | 614 | CLA | CMD-C2D-C3D | 3.34 | 130.93 | 124.68 |
| 23 | A | 407 | CLA | C4-C3-C5 | 3.34 | 120.89 | 115.27 |
| 23 | B | 612 | CLA | CMD-C2D-C3D | 3.34 | 130.93 | 124.68 |
| 23 | c | 511 | CLA | C1D-CHD-C4C | 3.33 | 126.95 | 122.56 |
| 33 | m | 101 | LMG | O6-C1-O1 | -3.32 | 102.12 | 109.97 |
| 23 | C | 506 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 23 | A | 407 | CLA | C2C-C1C-NC | 3.31 | 113.07 | 109.97 |
| 23 | C | 508 | CLA | C4A-NA-C1A | 3.31 | 108.19 | 106.71 |
| 23 | b | 602 | CLA | CMB-C2B-C1B | -3.31 | 123.38 | 128.46 |
| 23 | D | 403 | CLA | O2D-CGD-O1D | -3.31 | 117.37 | 123.84 |
| 23 | C | 511 | CLA | CHB-C4A-NA | 3.31 | 129.08 | 124.51 |
| 23 | b | 617 | CLA | CMB-C2B-C3B | 3.30 | 130.84 | 124.68 |
| 23 | B | 613 | CLA | CHB-C4A-NA | 3.29 | 129.07 | 124.51 |
| 27 | B | 621 | SQD | O7-S-C6 | 3.29 | 110.85 | 106.94 |
| 25 | B | 618 | BCR | C15-C14-C13 | -3.29 | 122.62 | 127.31 |
| 29 | A | 413 | LHG | O3-P-O5 | -3.29 | 96.22 | 109.07 |
| 25 | C | 520 | BCR | C15-C16-C17 | -3.28 | 116.75 | 123.47 |
| 23 | C | 509 | CLA | CMB-C2B-C1B | -3.28 | 123.42 | 128.46 |
| 23 | d | 402 | CLA | CHB-C4A-NA | 3.28 | 129.04 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 607 | CLA | CMB-C2B-C1B | -3.28 | 123.43 | 128.46 |
| 33 | C | 519 | LMG | O1-C7-C8 | -3.28 | 103.00 | 110.90 |
| 28 | C | 517 | DGD | O5D-C1E-C2E | 3.27 | 113.42 | 108.30 |
| 27 | b | 601 | SQD | O9-S-O7 | -3.27 | 102.62 | 113.95 |
| 23 | c | 512 | CLA | CMD-C2D-C3D | 3.27 | 130.80 | 124.68 |
| 25 | Z | 101 | BCR | C35-C13-C14 | -3.27 | 118.34 | 122.92 |
| 25 | c | 515 | BCR | C33-C5-C6 | -3.27 | 120.86 | 124.53 |
| 23 | b | 608 | CLA | O1D-CGD-CBD | 3.27 | 131.17 | 124.48 |
| 23 | B | 609 | CLA | OBD-CAD-C3D | 3.27 | 133.40 | 127.98 |
| 23 | B | 609 | CLA | C2C-C1C-NC | 3.26 | 113.03 | 109.97 |
| 27 | a | 411 | SQD | O47-C7-O49 | -3.26 | 115.82 | 123.70 |
| 23 | B | 615 | CLA | C1B-CHB-C4A | -3.26 | 123.66 | 130.12 |
| 23 | c | 509 | CLA | CMD-C2D-C3D | 3.26 | 130.78 | 124.68 |
| 25 | b | 620 | BCR | C37-C22-C21 | -3.26 | 118.36 | 122.92 |
| 23 | B | 612 | CLA | C4D-C3D-CAD | -3.26 | 106.65 | 108.47 |
| 33 | d | 411 | LMG | C6-C5-C4 | -3.25 | 105.38 | 113.00 |
| 25 | A | 408 | BCR | C38-C26-C27 | -3.25 | 107.36 | 113.62 |
| 23 | b | 607 | CLA | O2D-CGD-O1D | -3.25 | 117.48 | 123.84 |
| 23 | C | 510 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 23 | C | 502 | CLA | OBD-CAD-C3D | 3.25 | 133.38 | 127.98 |
| 25 | x | 102 | BCR | C27-C26-C25 | 3.25 | 127.44 | 122.73 |
| 25 | c | 521 | BCR | C11-C10-C9 | -3.24 | 122.68 | 127.31 |
| 23 | b | 613 | CLA | C1B-CHB-C4A | -3.24 | 123.71 | 130.12 |
| 26 | D | 406 | PL9 | C31-C32-C33 | -3.24 | 101.25 | 111.88 |
| 23 | B | 611 | CLA | O2D-CGD-CBD | 3.24 | 117.02 | 111.27 |
| 33 | c | 519 | LMG | O6-C1-O1 | -3.23 | 102.32 | 109.97 |
| 23 | C | 509 | CLA | O2D-CGD-CBD | 3.23 | 117.01 | 111.27 |
| 23 | C | 504 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 23 | b | 615 | CLA | O2D-CGD-O1D | -3.23 | 117.52 | 123.84 |
| 23 | c | 513 | CLA | CMB-C2B-C1B | -3.22 | 123.51 | 128.46 |
| 23 | B | 608 | CLA | CMB-C2B-C1B | -3.21 | 123.52 | 128.46 |
| 23 | B | 609 | CLA | O2D-CGD-O1D | -3.21 | 117.56 | 123.84 |
| 28 | A | 412 | DGD | C1D-C2D-C3D | -3.21 | 103.31 | 110.00 |
| 23 | C | 505 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 25 | T | 101 | BCR | C7-C8-C9 | -3.21 | 121.39 | 126.23 |
| 33 | c | 524 | LMG | O6-C1-O1 | -3.21 | 102.37 | 109.97 |
| 28 | c | 518 | DGD | O3G-C3G-C2G | -3.20 | 103.17 | 110.90 |
| 23 | c | 504 | CLA | CMB-C2B-C3B | 3.20 | 130.66 | 124.68 |
| 23 | d | 404 | CLA | O2A-C1-C2 | -3.20 | 100.23 | 108.64 |
| 23 | a | 406 | CLA | C1D-CHD-C4C | 3.20 | 126.78 | 122.56 |
| 23 | c | 513 | CLA | O2D-CGD-O1D | -3.20 | 117.58 | 123.84 |
| 23 | c | 509 | CLA | CMB-C2B-C3B | 3.19 | 130.65 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | t | 101 | BCR | C29-C30-C25 | 3.19 | 115.39 | 110.48 |
| 23 | A | 405 | CLA | C1B-CHB-C4A | -3.19 | 123.81 | 130.12 |
| 27 | F | 101 | SQD | O9-S-O7 | -3.18 | 102.94 | 113.95 |
| 23 | B | 606 | CLA | OBD-CAD-CBD | -3.18 | 121.36 | 125.89 |
| 23 | c | 506 | CLA | C4-C3-C5 | 3.18 | 120.61 | 115.27 |
| 23 | B | 606 | CLA | O2D-CGD-O1D | -3.17 | 117.63 | 123.84 |
| 23 | c | 508 | CLA | C4D-C3D-CAD | -3.17 | 106.70 | 108.47 |
| 28 | C | 517 | DGD | C1D-O6D-C5D | -3.17 | 107.47 | 113.69 |
| 23 | b | 609 | CLA | OBD-CAD-CBD | -3.17 | 121.37 | 125.89 |
| 23 | B | 605 | CLA | C4-C3-C5 | 3.17 | 120.60 | 115.27 |
| 23 | C | 509 | CLA | C1D-CHD-C4C | 3.16 | 126.73 | 122.56 |
| 28 | h | 101 | DGD | C4D-C3D-C2D | -3.16 | 105.31 | 110.82 |
| 23 | b | 606 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 34 | e | 102 | HEM | CMD-C2D-C1D | -3.16 | 123.61 | 128.46 |
| 33 | m | 101 | LMG | O3-C3-C2 | -3.16 | 103.05 | 110.35 |
| 23 | D | 403 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 23 | B | 610 | CLA | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 23 | b | 613 | CLA | C4D-C3D-CAD | -3.15 | 106.71 | 108.47 |
| 23 | B | 611 | CLA | O2D-CGD-O1D | -3.15 | 117.68 | 123.84 |
| 23 | c | 501 | CLA | C2C-C1C-NC | 3.15 | 112.92 | 109.97 |
| 23 | D | 404 | CLA | OBD-CAD-CBD | -3.15 | 121.40 | 125.89 |
| 23 | C | 503 | CLA | OBD-CAD-CBD | -3.14 | 121.40 | 125.89 |
| 23 | C | 506 | CLA | O1D-CGD-CBD | 3.14 | 130.92 | 124.48 |
| 25 | H | 101 | BCR | C29-C30-C25 | 3.14 | 115.32 | 110.48 |
| 23 | c | 502 | CLA | CMD-C2D-C3D | 3.14 | 130.56 | 124.68 |
| 23 | b | 614 | CLA | C7-C6-C5 | -3.14 | 104.83 | 113.36 |
| 23 | c | 511 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 23 | B | 604 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 25 | Z | 101 | BCR | C2-C1-C6 | 3.14 | 115.31 | 110.48 |
| 23 | b | 609 | CLA | CHB-C4A-NA | 3.14 | 128.85 | 124.51 |
| 25 | c | 515 | BCR | C27-C26-C25 | 3.14 | 127.28 | 122.73 |
| 29 | d | 408 | LHG | O8-C23-C24 | 3.13 | 121.73 | 111.91 |
| 23 | C | 506 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 23 | C | 514 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 23 | b | 605 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 25 | H | 101 | BCR | C30-C25-C26 | -3.12 | 118.21 | 122.61 |
| 25 | c | 514 | BCR | C27-C26-C25 | 3.12 | 127.27 | 122.73 |
| 23 | B | 610 | CLA | CMD-C2D-C3D | 3.12 | 130.52 | 124.68 |
| 23 | C | 510 | CLA | O1D-CGD-CBD | 3.12 | 130.88 | 124.48 |
| 34 | E | 103 | HEM | CAD-CBD-CGD | 3.12 | 117.91 | 112.67 |
| 23 | c | 503 | CLA | CMB-C2B-C1B | -3.12 | 123.67 | 128.46 |
| 28 | h | 101 | DGD | O3E-C3E-C4E | 3.12 | 117.56 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | c | 521 | BCR | C27-C26-C25 | 3.12 | 127.26 | 122.73 |
| 23 | B | 605 | CLA | OBD-CAD-C3D | 3.11 | 133.15 | 127.98 |
| 23 | c | 506 | CLA | OBD-CAD-CBD | -3.11 | 121.45 | 125.89 |
| 29 | A | 413 | LHG | O8-C23-O10 | -3.11 | 115.74 | 123.59 |
| 23 | b | 610 | CLA | O1D-CGD-CBD | 3.11 | 130.84 | 124.48 |
| 23 | c | 512 | CLA | C1-C2-C3 | -3.11 | 120.67 | 126.04 |
| 23 | C | 505 | CLA | CMD-C2D-C3D | 3.10 | 130.48 | 124.68 |
| 23 | a | 408 | CLA | CHB-C4A-NA | 3.10 | 128.80 | 124.51 |
| 23 | b | 614 | CLA | CED-O2D-CGD | 3.10 | 122.94 | 115.94 |
| 24 | d | 401 | PHO | C1B-NB-C4B | 3.10 | 112.35 | 106.51 |
| 23 | b | 606 | CLA | O1D-CGD-CBD | 3.09 | 130.81 | 124.48 |
| 23 | b | 607 | CLA | CHD-C4C-NC | 3.09 | 129.07 | 124.20 |
| 27 | B | 621 | SQD | O9-S-O7 | -3.09 | 103.25 | 113.95 |
| 35 | v | 201 | HEC | CBD-CAD-C3D | -3.09 | 106.79 | 112.49 |
| 23 | c | 510 | CLA | C1D-CHD-C4C | 3.09 | 126.63 | 122.56 |
| 23 | B | 613 | CLA | CMB-C2B-C1B | -3.09 | 123.72 | 128.46 |
| 23 | b | 616 | CLA | C1-O2A-CGA | 3.08 | 124.53 | 116.44 |
| 23 | d | 402 | CLA | C2A-C1A-CHA | 3.08 | 129.25 | 123.86 |
| 23 | d | 402 | CLA | CMC-C2C-C1C | 3.08 | 129.73 | 125.04 |
| 23 | B | 605 | CLA | O2D-CGD-O1D | -3.07 | 117.84 | 123.84 |
| 23 | c | 502 | CLA | C3A-C2A-C1A | 3.07 | 105.93 | 101.34 |
| 23 | B | 615 | CLA | C7-C6-C5 | -3.06 | 105.05 | 113.36 |
| 23 | c | 502 | CLA | C1B-CHB-C4A | -3.06 | 124.06 | 130.12 |
| 25 | K | 101 | BCR | C23-C22-C21 | -3.06 | 114.25 | 118.94 |
| 23 | c | 505 | CLA | CMB-C2B-C3B | 3.05 | 130.38 | 124.68 |
| 27 | a | 411 | SQD | O47-C7-C8 | 3.05 | 118.07 | 111.50 |
| 23 | b | 611 | CLA | C4A-NA-C1A | 3.05 | 108.08 | 106.71 |
| 23 | c | 511 | CLA | CMD-C2D-C3D | 3.05 | 130.38 | 124.68 |
| 29 | E | 101 | LHG | O8-C23-C24 | 3.04 | 121.45 | 111.91 |
| 28 | H | 102 | DGD | O3E-C3E-C2E | -3.04 | 103.32 | 110.35 |
| 23 | B | 616 | CLA | CMB-C2B-C3B | 3.04 | 130.37 | 124.68 |
| 23 | b | 617 | CLA | CMB-C2B-C1B | -3.04 | 123.79 | 128.46 |
| 23 | B | 608 | CLA | CHB-C4A-NA | 3.04 | 128.71 | 124.51 |
| 23 | b | 603 | CLA | OBD-CAD-CBD | -3.03 | 121.56 | 125.89 |
| 26 | D | 406 | PL9 | C7-C3-C2 | -3.03 | 119.31 | 123.30 |
| 23 | d | 404 | CLA | C1B-CHB-C4A | -3.03 | 124.11 | 130.12 |
| 26 | a | 410 | PL9 | C22-C23-C24 | -3.03 | 120.37 | 127.66 |
| 27 | a | 412 | SQD | O48-C23-O10 | -3.03 | 115.95 | 123.59 |
| 28 | C | 516 | DGD | O2D-C2D-C1D | -3.02 | 102.71 | 110.05 |
| 23 | C | 510 | CLA | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 23 | b | 606 | CLA | CHD-C4C-NC | 3.02 | 128.96 | 124.20 |
| 23 | d | 403 | CLA | O2A-CGA-O1A | -3.02 | 115.98 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | C | 520 | BCR | C27-C26-C25 | 3.02 | 127.11 | 122.73 |
| 27 | A | 411 | SQD | O48-C23-O10 | -3.01 | 115.99 | 123.59 |
| 23 | a | 406 | CLA | CMD-C2D-C3D | 3.01 | 130.31 | 124.68 |
| 28 | h | 101 | DGD | C3G-C2G-C1G | -3.01 | 104.67 | 111.79 |
| 23 | c | 501 | CLA | C1C-C2C-C3C | -3.01 | 103.79 | 106.96 |
| 25 | B | 618 | BCR | C27-C26-C25 | 3.00 | 127.09 | 122.73 |
| 24 | A | 406 | PHO | C1B-NB-C4B | 3.00 | 112.17 | 106.51 |
| 33 | D | 407 | LMG | O3-C3-C2 | -3.00 | 103.41 | 110.35 |
| 33 | D | 407 | LMG | O6-C1-O1 | -3.00 | 102.86 | 109.97 |
| 23 | a | 405 | CLA | C3A-C2A-C1A | 3.00 | 105.83 | 101.34 |
| 23 | B | 613 | CLA | C1-C2-C3 | -3.00 | 120.86 | 126.04 |
| 23 | C | 514 | CLA | CMB-C2B-C1B | -3.00 | 123.86 | 128.46 |
| 23 | C | 506 | CLA | CMB-C2B-C3B | 3.00 | 130.28 | 124.68 |
| 28 | C | 517 | DGD | O6E-C1E-O5D | -3.00 | 102.88 | 109.97 |
| 23 | a | 408 | CLA | CAA-CBA-CGA | -2.99 | 104.52 | 113.25 |
| 23 | C | 513 | CLA | CMB-C2B-C3B | 2.99 | 130.27 | 124.68 |
| 25 | B | 617 | BCR | C30-C25-C26 | -2.99 | 118.41 | 122.61 |
| 23 | b | 611 | CLA | O2A-C1-C2 | 2.99 | 116.48 | 108.64 |
| 23 | b | 603 | CLA | CMB-C2B-C3B | 2.99 | 130.26 | 124.68 |
| 23 | b | 613 | CLA | O2D-CGD-O1D | -2.98 | 118.00 | 123.84 |
| 23 | A | 407 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 23 | B | 612 | CLA | O2A-CGA-O1A | -2.98 | 116.07 | 123.59 |
| 25 | D | 405 | BCR | C28-C27-C26 | -2.97 | 108.77 | 114.08 |
| 23 | B | 614 | CLA | OBD-CAD-CBD | -2.97 | 121.66 | 125.89 |
| 23 | a | 408 | CLA | CMB-C2B-C1B | -2.97 | 123.90 | 128.46 |
| 26 | D | 406 | PL9 | C11-C12-C13 | -2.96 | 102.15 | 111.88 |
| 23 | b | 612 | CLA | CHD-C4C-NC | 2.96 | 128.87 | 124.20 |
| 23 | D | 402 | CLA | C16-C15-C13 | -2.96 | 106.36 | 115.92 |
| 25 | c | 515 | BCR | C35-C13-C14 | -2.96 | 118.78 | 122.92 |
| 23 | b | 613 | CLA | C11-C12-C13 | -2.96 | 106.36 | 115.92 |
| 33 | C | 501 | LMG | O6-C1-C2 | -2.96 | 104.09 | 110.35 |
| 33 | C | 501 | LMG | C38-C37-C36 | -2.95 | 99.42 | 114.42 |
| 24 | d | 401 | PHO | O1D-CGD-CBD | 2.95 | 130.53 | 124.48 |
| 23 | b | 615 | CLA | C4D-C3D-CAD | -2.95 | 106.82 | 108.47 |
| 23 | a | 406 | CLA | C1B-CHB-C4A | -2.95 | 124.27 | 130.12 |
| 23 | C | 502 | CLA | OBD-CAD-CBD | -2.95 | 121.68 | 125.89 |
| 29 | D | 409 | LHG | O8-C23-O10 | -2.95 | 116.14 | 123.59 |
| 23 | C | 503 | CLA | C4A-NA-C1A | 2.95 | 108.03 | 106.71 |
| 33 | M | 101 | LMG | O1-C1-C2 | -2.94 | 103.71 | 108.30 |
| 23 | b | 610 | CLA | C4A-NA-C1A | 2.94 | 108.03 | 106.71 |
| 28 | C | 517 | DGD | O2D-C2D-C1D | -2.94 | 102.90 | 110.05 |
| 23 | b | 605 | CLA | CMB-C2B-C1B | -2.94 | 123.94 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | a | 408 | CLA | CMD-C2D-C3D | 2.94 | 130.18 | 124.68 |
| 27 | B | 621 | SQD | O5-C5-C4 | 2.94 | 115.03 | 109.69 |
| 23 | B | 605 | CLA | C16-C15-C13 | -2.94 | 106.43 | 115.92 |
| 23 | c | 512 | CLA | CHB-C4A-NA | 2.93 | 128.57 | 124.51 |
| 28 | C | 516 | DGD | C4E-C3E-C2E | -2.93 | 105.70 | 110.82 |
| 23 | D | 404 | CLA | O1D-CGD-CBD | 2.93 | 130.48 | 124.48 |
| 25 | x | 102 | BCR | C35-C13-C14 | -2.93 | 118.82 | 122.92 |
| 23 | c | 505 | CLA | C6-C7-C8 | -2.93 | 106.45 | 115.92 |
| 23 | B | 604 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 23 | c | 505 | CLA | C4A-NA-C1A | 2.92 | 108.02 | 106.71 |
| 23 | D | 404 | CLA | C1B-CHB-C4A | -2.92 | 124.33 | 130.12 |
| 23 | C | 504 | CLA | C7-C6-C5 | -2.92 | 105.42 | 113.36 |
| 25 | H | 101 | BCR | C27-C26-C25 | 2.92 | 126.97 | 122.73 |
| 27 | b | 601 | SQD | O47-C45-C46 | 2.92 | 118.98 | 108.40 |
| 23 | B | 613 | CLA | CMB-C2B-C3B | 2.92 | 130.15 | 124.68 |
| 23 | B | 616 | CLA | C1B-CHB-C4A | -2.92 | 124.33 | 130.12 |
| 27 | A | 410 | SQD | O2-C2-C1 | 2.92 | 117.14 | 110.05 |
| 23 | B | 602 | CLA | C1B-CHB-C4A | -2.92 | 124.33 | 130.12 |
| 24 | D | 401 | PHO | O2D-CGD-CBD | -2.91 | 106.09 | 111.27 |
| 25 | b | 620 | BCR | C29-C30-C25 | 2.91 | 114.96 | 110.48 |
| 29 | d | 407 | LHG | C11-C10-C9 | -2.91 | 99.67 | 114.42 |
| 23 | c | 502 | CLA | C1-C2-C3 | -2.90 | 121.02 | 126.04 |
| 23 | b | 602 | CLA | C1D-CHD-C4C | 2.90 | 126.38 | 122.56 |
| 23 | C | 506 | CLA | C1D-CHD-C4C | 2.90 | 126.38 | 122.56 |
| 33 | m | 101 | LMG | O1-C1-C2 | -2.90 | 103.78 | 108.30 |
| 28 | H | 102 | DGD | O3D-C3D-C4D | -2.89 | 103.66 | 110.35 |
| 23 | b | 612 | CLA | O2D-CGD-CBD | 2.89 | 116.41 | 111.27 |
| 25 | C | 515 | BCR | C27-C26-C25 | 2.89 | 126.93 | 122.73 |
| 23 | d | 402 | CLA | CMD-C2D-C3D | 2.89 | 130.08 | 124.68 |
| 23 | c | 503 | CLA | C1B-CHB-C4A | -2.89 | 124.40 | 130.12 |
| 23 | b | 617 | CLA | C1B-CHB-C4A | -2.89 | 124.40 | 130.12 |
| 23 | C | 506 | CLA | C4A-NA-C1A | 2.88 | 108.00 | 106.71 |
| 23 | a | 406 | CLA | CMB-C2B-C1B | -2.88 | 124.03 | 128.46 |
| 23 | b | 609 | CLA | CMB-C2B-C1B | -2.88 | 124.03 | 128.46 |
| 25 | K | 101 | BCR | C33-C5-C6 | -2.88 | 121.29 | 124.53 |
| 26 | D | 406 | PL9 | C36-C34-C33 | -2.88 | 115.29 | 121.12 |
| 25 | t | 101 | BCR | C35-C13-C14 | -2.88 | 118.89 | 122.92 |
| 27 | b | 601 | SQD | O47-C7-C8 | 2.88 | 117.70 | 111.50 |
| 23 | C | 512 | CLA | OBD-CAD-CBD | -2.87 | 121.79 | 125.89 |
| 28 | c | 518 | DGD | O5E-C6E-C5E | -2.87 | 101.44 | 111.29 |
| 23 | c | 501 | CLA | O2A-CGA-O1A | -2.87 | 116.35 | 123.59 |
| 23 | b | 609 | CLA | O2A-CGA-O1A | -2.87 | 116.36 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | b | 611 | CLA | C1B-CHB-C4A | -2.87 | 124.44 | 130.12 |
| 23 | b | 617 | CLA | CGD-CBD-CAD | -2.86 | 101.46 | 110.73 |
| 25 | a | 409 | BCR | C35-C13-C14 | -2.86 | 118.91 | 122.92 |
| 25 | T | 101 | BCR | C38-C26-C27 | -2.86 | 108.12 | 113.62 |
| 26 | D | 406 | PL9 | C20-C19-C21 | 2.86 | 120.08 | 115.27 |
| 29 | D | 408 | LHG | O8-C23-C24 | 2.86 | 120.89 | 111.91 |
| 27 | b | 601 | SQD | O2-C2-C1 | 2.86 | 116.99 | 110.05 |
| 23 | C | 504 | CLA | C6-C5-C3 | 2.86 | 120.95 | 113.45 |
| 23 | b | 606 | CLA | C4D-C3D-CAD | -2.86 | 106.88 | 108.47 |
| 23 | b | 604 | CLA | OBD-CAD-C3D | 2.86 | 132.72 | 127.98 |
| 23 | b | 602 | CLA | O2D-CGD-CBD | 2.85 | 116.34 | 111.27 |
| 25 | B | 617 | BCR | C2-C1-C6 | 2.85 | 114.87 | 110.48 |
| 28 | H | 102 | DGD | C8B-C7B-C6B | -2.85 | 99.95 | 114.42 |
| 25 | c | 514 | BCR | C30-C25-C26 | -2.85 | 118.60 | 122.61 |
| 25 | H | 101 | BCR | C2-C1-C6 | 2.85 | 114.86 | 110.48 |
| 23 | d | 402 | CLA | O2D-CGD-CBD | 2.85 | 116.33 | 111.27 |
| 23 | A | 404 | CLA | CMB-C2B-C3B | 2.85 | 130.00 | 124.68 |
| 33 | b | 622 | LMG | C8-O7-C10 | 2.84 | 124.79 | 117.79 |
| 23 | C | 507 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 27 | b | 601 | SQD | C1-O5-C5 | 2.84 | 119.27 | 113.69 |
| 25 | Z | 101 | BCR | C7-C8-C9 | -2.84 | 121.94 | 126.23 |
| 23 | A | 404 | CLA | C1D-CHD-C4C | 2.84 | 126.30 | 122.56 |
| 23 | b | 606 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 23 | b | 608 | CLA | C1B-CHB-C4A | -2.84 | 124.50 | 130.12 |
| 23 | b | 605 | CLA | O2A-CGA-O1A | -2.84 | 116.43 | 123.59 |
| 23 | b | 605 | CLA | CMB-C2B-C3B | 2.84 | 129.98 | 124.68 |
| 23 | b | 606 | CLA | C11-C12-C13 | -2.83 | 106.76 | 115.92 |
| 27 | F | 101 | SQD | O48-C23-C24 | 2.83 | 120.80 | 111.91 |
| 25 | B | 617 | BCR | C27-C26-C25 | 2.83 | 126.84 | 122.73 |
| 23 | b | 602 | CLA | C1B-CHB-C4A | -2.83 | 124.51 | 130.12 |
| 23 | b | 612 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 33 | M | 101 | LMG | O3-C3-C2 | -2.83 | 103.82 | 110.35 |
| 23 | D | 402 | CLA | C4A-NA-C1A | 2.82 | 107.98 | 106.71 |
| 27 | a | 411 | SQD | O8-S-C6 | 2.82 | 110.24 | 105.74 |
| 23 | B | 602 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 28 | C | 517 | DGD | C6D-O5D-C1E | 2.82 | 119.24 | 113.74 |
| 23 | c | 513 | CLA | CMB-C2B-C3B | 2.82 | 129.95 | 124.68 |
| 25 | A | 408 | BCR | C29-C30-C25 | 2.82 | 114.82 | 110.48 |
| 25 | c | 515 | BCR | C30-C25-C26 | -2.82 | 118.65 | 122.61 |
| 23 | b | 604 | CLA | C1B-CHB-C4A | -2.82 | 124.54 | 130.12 |
| 23 | C | 513 | CLA | O2D-CGD-O1D | -2.81 | 118.33 | 123.84 |
| 23 | b | 613 | CLA | OBD-CAD-CBD | -2.81 | 121.88 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 510 | CLA | C4D-C3D-CAD | -2.81 | 106.90 | 108.47 |
| 23 | b | 612 | CLA | C4A-NA-C1A | 2.81 | 107.97 | 106.71 |
| 28 | c | 516 | DGD | O3E-C3E-C2E | -2.81 | 103.86 | 110.35 |
| 23 | b | 602 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 23 | b | 615 | CLA | O1D-CGD-CBD | 2.80 | 130.22 | 124.48 |
| 23 | B | 606 | CLA | CHA-C1A-NA | -2.80 | 120.00 | 126.40 |
| 25 | a | 409 | BCR | C33-C5-C6 | -2.79 | 121.39 | 124.53 |
| 23 | d | 404 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 27 | a | 411 | SQD | C1-O5-C5 | -2.79 | 108.22 | 113.69 |
| 23 | C | 504 | CLA | CMD-C2D-C3D | 2.79 | 129.89 | 124.68 |
| 29 | D | 408 | LHG | O8-C23-O10 | -2.79 | 116.56 | 123.59 |
| 23 | D | 402 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 23 | c | 510 | CLA | O1D-CGD-CBD | 2.78 | 130.18 | 124.48 |
| 23 | B | 616 | CLA | CMD-C2D-C3D | 2.78 | 129.89 | 124.68 |
| 28 | c | 516 | DGD | CDB-CCB-CBB | -2.78 | 100.30 | 114.42 |
| 25 | k | 101 | BCR | C27-C26-C25 | 2.78 | 126.77 | 122.73 |
| 23 | D | 403 | CLA | CMB-C2B-C1B | -2.78 | 124.19 | 128.46 |
| 23 | B | 609 | CLA | C1B-CHB-C4A | -2.78 | 124.61 | 130.12 |
| 29 | e | 101 | LHG | O8-C23-C24 | 2.78 | 120.63 | 111.91 |
| 27 | f | 101 | SQD | O5-C5-C4 | 2.77 | 114.73 | 109.69 |
| 23 | b | 614 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 23 | B | 607 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 23 | B | 613 | CLA | C2C-C1C-NC | 2.77 | 112.56 | 109.97 |
| 23 | b | 602 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 23 | c | 510 | CLA | OBD-CAD-CBD | -2.77 | 121.94 | 125.89 |
| 23 | c | 511 | CLA | C4D-C3D-CAD | -2.76 | 106.93 | 108.47 |
| 23 | b | 605 | CLA | C1-C2-C3 | -2.76 | 121.27 | 126.04 |
| 28 | h | 101 | DGD | C6D-O5D-C1E | 2.76 | 119.13 | 113.74 |
| 23 | B | 613 | CLA | CED-O2D-CGD | 2.76 | 122.18 | 115.94 |
| 23 | b | 607 | CLA | C4D-C3D-CAD | -2.76 | 106.93 | 108.47 |
| 28 | C | 518 | DGD | CDB-CCB-CBB | -2.75 | 100.45 | 114.42 |
| 23 | c | 508 | CLA | O2A-CGA-O1A | -2.75 | 116.65 | 123.59 |
| 23 | c | 509 | CLA | C1B-CHB-C4A | -2.75 | 124.67 | 130.12 |
| 28 | C | 516 | DGD | C3D-C4D-C5D | -2.75 | 105.34 | 110.24 |
| 23 | B | 610 | CLA | C1B-CHB-C4A | -2.75 | 124.67 | 130.12 |
| 23 | C | 502 | CLA | C1D-CHD-C4C | 2.75 | 126.18 | 122.56 |
| 27 | A | 411 | SQD | O48-C46-C45 | 2.75 | 116.29 | 108.38 |
| 23 | b | 612 | CLA | C11-C10-C8 | -2.74 | 107.05 | 115.92 |
| 29 | e | 101 | LHG | O8-C23-O10 | -2.74 | 116.67 | 123.59 |
| 25 | b | 618 | BCR | C27-C26-C25 | 2.74 | 126.71 | 122.73 |
| 23 | c | 508 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 23 | D | 404 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | B | 621 | SQD | O47-C7-O49 | -2.74 | 117.09 | 123.70 |
| 23 | C | 505 | CLA | CHA-C1A-NA | -2.74 | 120.13 | 126.40 |
| 33 | C | 501 | LMG | C1-O6-C5 | -2.73 | 108.32 | 113.69 |
| 25 | c | 515 | BCR | C2-C1-C6 | 2.73 | 114.69 | 110.48 |
| 25 | C | 515 | BCR | C15-C16-C17 | -2.73 | 117.88 | 123.47 |
| 23 | C | 504 | CLA | O1D-CGD-CBD | 2.73 | 130.07 | 124.48 |
| 25 | c | 514 | BCR | C15-C14-C13 | -2.73 | 123.42 | 127.31 |
| 23 | C | 510 | CLA | CMB-C2B-C3B | 2.73 | 129.78 | 124.68 |
| 23 | B | 615 | CLA | C1D-CHD-C4C | 2.72 | 126.15 | 122.56 |
| 23 | c | 507 | CLA | O2A-CGA-O1A | -2.72 | 116.73 | 123.59 |
| 23 | c | 507 | CLA | C4D-C3D-CAD | -2.72 | 106.95 | 108.47 |
| 23 | C | 513 | CLA | OBD-CAD-CBD | -2.72 | 122.01 | 125.89 |
| 23 | d | 404 | CLA | CBC-CAC-C3C | -2.72 | 104.94 | 112.43 |
| 25 | C | 515 | BCR | C2-C1-C6 | 2.71 | 114.66 | 110.48 |
| 23 | B | 606 | CLA | C1D-CHD-C4C | 2.71 | 126.14 | 122.56 |
| 23 | b | 609 | CLA | C3B-C4B-NB | -2.71 | 105.70 | 109.21 |
| 28 | H | 102 | DGD | C1D-C2D-C3D | -2.71 | 104.36 | 110.00 |
| 23 | b | 609 | CLA | C4D-C3D-CAD | -2.71 | 106.96 | 108.47 |
| 27 | B | 621 | SQD | C45-O47-C7 | 2.71 | 124.46 | 117.79 |
| 23 | B | 606 | CLA | CMB-C2B-C1B | -2.71 | 124.31 | 128.46 |
| 23 | B | 603 | CLA | CMD-C2D-C3D | 2.70 | 129.74 | 124.68 |
| 26 | A | 409 | PL9 | O1-C4-C3 | -2.70 | 117.75 | 120.72 |
| 23 | C | 511 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 23 | a | 406 | CLA | O2A-CGA-O1A | -2.70 | 116.78 | 123.59 |
| 23 | C | 508 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 23 | C | 512 | CLA | O2D-CGD-O1D | -2.70 | 118.57 | 123.84 |
| 23 | a | 405 | CLA | CMB-C2B-C1B | -2.69 | 124.32 | 128.46 |
| 23 | B | 612 | CLA | CED-O2D-CGD | -2.69 | 109.84 | 115.94 |
| 23 | c | 506 | CLA | CGD-CBD-CAD | -2.69 | 102.01 | 110.73 |
| 23 | b | 605 | CLA | C11-C10-C8 | -2.69 | 107.22 | 115.92 |
| 28 | h | 101 | DGD | C3D-C4D-C5D | -2.69 | 105.44 | 110.24 |
| 23 | b | 607 | CLA | O2D-CGD-CBD | 2.69 | 116.04 | 111.27 |
| 23 | B | 613 | CLA | CAC-C3C-C4C | 2.69 | 128.29 | 124.81 |
| 26 | d | 406 | PL9 | C46-C47-C48 | -2.68 | 103.06 | 111.88 |
| 23 | C | 503 | CLA | CMB-C2B-C3B | 2.68 | 129.70 | 124.68 |
| 23 | D | 404 | CLA | C1-C2-C3 | -2.68 | 121.41 | 126.04 |
| 25 | A | 408 | BCR | C27-C26-C25 | 2.68 | 126.62 | 122.73 |
| 23 | c | 507 | CLA | CMB-C2B-C1B | -2.68 | 124.34 | 128.46 |
| 23 | C | 510 | CLA | CMD-C2D-C3D | 2.68 | 129.69 | 124.68 |
| 23 | C | 514 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 25 | c | 515 | BCR | C29-C30-C25 | 2.68 | 114.60 | 110.48 |
| 25 | k | 101 | BCR | C30-C25-C26 | -2.67 | 118.85 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 613 | CLA | CMD-C2D-C3D | 2.67 | 129.68 | 124.68 |
| 23 | c | 508 | CLA | CHD-C4C-NC | 2.67 | 128.41 | 124.20 |
| 23 | C | 509 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 25 | Z | 101 | BCR | C15-C14-C13 | -2.67 | 123.50 | 127.31 |
| 28 | a | 413 | DGD | O2G-C1B-C2B | 2.66 | 117.24 | 111.50 |
| 35 | v | 201 | HEC | CBA-CAA-C2A | -2.66 | 107.57 | 112.48 |
| 23 | C | 514 | CLA | CMB-C2B-C3B | 2.66 | 129.66 | 124.68 |
| 23 | C | 507 | CLA | CMD-C2D-C3D | 2.66 | 129.66 | 124.68 |
| 23 | b | 615 | CLA | C1B-CHB-C4A | -2.66 | 124.85 | 130.12 |
| 27 | A | 410 | SQD | O5-C1-C2 | -2.66 | 104.72 | 110.35 |
| 23 | b | 613 | CLA | C1-C2-C3 | -2.66 | 121.44 | 126.04 |
| 23 | C | 507 | CLA | C2A-C3A-C4A | 2.66 | 106.17 | 101.87 |
| 26 | a | 410 | PL9 | C37-C38-C39 | -2.66 | 121.26 | 127.66 |
| 23 | c | 513 | CLA | O1D-CGD-CBD | 2.66 | 129.92 | 124.48 |
| 23 | C | 505 | CLA | O2A-CGA-O1A | -2.66 | 116.89 | 123.59 |
| 23 | b | 611 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 25 | H | 101 | BCR | C16-C15-C14 | -2.66 | 118.03 | 123.47 |
| 27 | B | 621 | SQD | C1-C2-C3 | -2.66 | 104.47 | 110.00 |
| 23 | B | 605 | CLA | CHD-C4C-NC | 2.65 | 128.39 | 124.20 |
| 33 | M | 101 | LMG | C40-C39-C38 | -2.65 | 100.95 | 114.42 |
| 25 | c | 514 | BCR | C15-C16-C17 | -2.65 | 118.04 | 123.47 |
| 25 | A | 408 | BCR | C40-C30-C25 | 2.65 | 114.60 | 110.30 |
| 23 | b | 606 | CLA | C16-C15-C13 | -2.65 | 107.35 | 115.92 |
| 26 | a | 410 | PL9 | C35-C34-C36 | 2.65 | 119.73 | 115.27 |
| 25 | H | 101 | BCR | C35-C13-C14 | -2.65 | 119.21 | 122.92 |
| 29 | e | 101 | LHG | C5-O7-C7 | -2.65 | 111.27 | 117.79 |
| 23 | b | 602 | CLA | CBA-CAA-C2A | 2.65 | 121.67 | 113.86 |
| 25 | a | 409 | BCR | C29-C30-C25 | 2.64 | 114.55 | 110.48 |
| 27 | a | 411 | SQD | O48-C23-C24 | 2.64 | 120.20 | 111.91 |
| 23 | d | 404 | CLA | C1-C2-C3 | -2.64 | 121.48 | 126.04 |
| 27 | f | 101 | SQD | C1-O5-C5 | -2.64 | 108.51 | 113.69 |
| 27 | f | 101 | SQD | O9-S-O7 | -2.64 | 104.82 | 113.95 |
| 23 | c | 507 | CLA | CMB-C2B-C3B | 2.64 | 129.61 | 124.68 |
| 25 | B | 619 | BCR | C33-C5-C6 | -2.64 | 121.57 | 124.53 |
| 23 | d | 403 | CLA | CMB-C2B-C3B | 2.63 | 129.60 | 124.68 |
| 28 | c | 517 | DGD | C3G-O3G-C1D | 2.63 | 118.88 | 113.74 |
| 23 | A | 407 | CLA | O1D-CGD-CBD | 2.63 | 129.87 | 124.48 |
| 27 | f | 101 | SQD | O48-C23-O10 | -2.63 | 116.95 | 123.59 |
| 25 | x | 102 | BCR | C34-C9-C8 | -2.63 | 113.93 | 118.08 |
| 25 | b | 619 | BCR | C27-C26-C25 | 2.63 | 126.55 | 122.73 |
| 24 | a | 407 | PHO | CMB-C2B-C1B | -2.62 | 121.02 | 125.06 |
| 27 | B | 621 | SQD | C3-C4-C5 | 2.62 | 114.92 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 603 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 23 | d | 402 | CLA | O2A-CGA-O1A | -2.62 | 116.98 | 123.59 |
| 28 | c | 518 | DGD | O3G-C1D-C2D | -2.62 | 104.21 | 108.30 |
| 33 | C | 501 | LMG | O3-C3-C2 | -2.62 | 104.29 | 110.35 |
| 23 | b | 612 | CLA | CGD-CBD-CAD | -2.62 | 102.25 | 110.73 |
| 23 | c | 505 | CLA | CED-O2D-CGD | -2.62 | 110.02 | 115.94 |
| 26 | d | 406 | PL9 | C50-C49-C48 | -2.62 | 115.08 | 122.65 |
| 23 | D | 402 | CLA | C1B-CHB-C4A | -2.62 | 124.94 | 130.12 |
| 23 | B | 603 | CLA | O1D-CGD-CBD | 2.62 | 129.84 | 124.48 |
| 33 | c | 522 | LMG | C9-C8-C7 | -2.62 | 105.60 | 111.79 |
| 29 | d | 409 | LHG | O8-C6-C5 | -2.62 | 100.82 | 108.43 |
| 23 | b | 606 | CLA | CHC-C1C-NC | 2.61 | 128.17 | 124.20 |
| 23 | C | 514 | CLA | C3A-C2A-C1A | 2.61 | 105.25 | 101.34 |
| 23 | B | 611 | CLA | CMD-C2D-C3D | 2.61 | 129.56 | 124.68 |
| 23 | c | 512 | CLA | C4D-C3D-CAD | -2.61 | 107.01 | 108.47 |
| 23 | C | 503 | CLA | CHA-C1A-NA | -2.61 | 120.42 | 126.40 |
| 33 | C | 501 | LMG | O8-C28-O10 | -2.61 | 117.00 | 123.59 |
| 25 | x | 102 | BCR | C30-C25-C26 | -2.61 | 118.94 | 122.61 |
| 23 | B | 604 | CLA | CGD-CBD-CAD | -2.61 | 102.28 | 110.73 |
| 23 | b | 613 | CLA | C6-C5-C3 | -2.61 | 106.62 | 113.45 |
| 23 | c | 505 | CLA | O2D-CGD-O1D | -2.61 | 118.74 | 123.84 |
| 25 | c | 514 | BCR | C39-C30-C25 | 2.60 | 114.52 | 110.30 |
| 28 | a | 413 | DGD | C5B-C4B-C3B | -2.60 | 101.21 | 114.42 |
| 23 | A | 405 | CLA | C4A-NA-C1A | 2.60 | 107.88 | 106.71 |
| 23 | b | 608 | CLA | C2C-C1C-NC | 2.60 | 112.41 | 109.97 |
| 23 | b | 616 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 23 | b | 612 | CLA | C3C-C4C-NC | -2.60 | 107.65 | 110.57 |
| 26 | d | 406 | PL9 | C37-C38-C39 | -2.60 | 121.40 | 127.66 |
| 23 | B | 606 | CLA | CGD-CBD-CAD | -2.60 | 102.31 | 110.73 |
| 23 | c | 503 | CLA | CAC-C3C-C4C | 2.60 | 128.18 | 124.81 |
| 28 | c | 516 | DGD | O2D-C2D-C1D | -2.60 | 103.74 | 110.05 |
| 25 | d | 405 | BCR | C8-C7-C6 | -2.59 | 119.91 | 127.20 |
| 23 | A | 404 | CLA | C7-C6-C5 | -2.59 | 106.32 | 113.36 |
| 28 | a | 413 | DGD | O1G-C1A-O1A | -2.59 | 117.05 | 123.59 |
| 23 | B | 605 | CLA | O1D-CGD-CBD | 2.59 | 129.79 | 124.48 |
| 23 | C | 511 | CLA | C16-C15-C13 | -2.59 | 107.55 | 115.92 |
| 25 | T | 101 | BCR | C37-C22-C21 | -2.59 | 119.30 | 122.92 |
| 26 | d | 406 | PL9 | C8-C7-C3 | 2.59 | 119.29 | 111.98 |
| 29 | D | 408 | LHG | C20-C19-C18 | -2.58 | 101.31 | 114.42 |
| 23 | c | 501 | CLA | OBD-CAD-CBD | -2.58 | 122.20 | 125.89 |
| 28 | c | 517 | DGD | C8B-C7B-C6B | -2.58 | 101.31 | 114.42 |
| 23 | B | 613 | CLA | CHA-C1A-NA | -2.58 | 120.49 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | c | 503 | CLA | C1D-CHD-C4C | 2.58 | 125.96 | 122.56 |
| 35 | v | 201 | HEC | CMC-C2C-C1C | -2.58 | 124.50 | 128.46 |
| 23 | c | 505 | CLA | C11-C10-C8 | -2.58 | 107.58 | 115.92 |
| 23 | D | 402 | CLA | CMD-C2D-C3D | 2.58 | 129.50 | 124.68 |
| 25 | A | 408 | BCR | C33-C5-C6 | -2.58 | 121.63 | 124.53 |
| 23 | B | 605 | CLA | CHD-C4C-C3C | -2.58 | 121.05 | 124.84 |
| 23 | B | 615 | CLA | C6-C5-C3 | -2.58 | 106.70 | 113.45 |
| 25 | T | 101 | BCR | C15-C16-C17 | -2.58 | 118.20 | 123.47 |
| 23 | B | 608 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 26 | A | 409 | PL9 | C36-C34-C33 | -2.57 | 115.91 | 121.12 |
| 23 | b | 605 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 27 | b | 601 | SQD | C3-C4-C5 | 2.57 | 114.83 | 110.24 |
| 27 | f | 101 | SQD | O5-C1-C2 | -2.57 | 104.91 | 110.35 |
| 23 | D | 402 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 23 | d | 402 | CLA | C1D-CHD-C4C | 2.57 | 125.94 | 122.56 |
| 28 | H | 102 | DGD | C3E-C4E-C5E | -2.56 | 105.66 | 110.24 |
| 23 | a | 406 | CLA | CAC-C3C-C4C | 2.56 | 128.13 | 124.81 |
| 26 | a | 410 | PL9 | C27-C28-C29 | -2.56 | 121.50 | 127.66 |
| 23 | c | 512 | CLA | CMB-C2B-C3B | 2.56 | 129.46 | 124.68 |
| 23 | B | 605 | CLA | C4A-NA-C1A | 2.56 | 107.86 | 106.71 |
| 25 | B | 618 | BCR | C2-C1-C6 | 2.55 | 114.41 | 110.48 |
| 25 | B | 619 | BCR | C30-C25-C26 | -2.55 | 119.02 | 122.61 |
| 24 | d | 401 | PHO | CBA-CAA-C2A | -2.55 | 106.33 | 113.86 |
| 29 | d | 409 | LHG | C25-C24-C23 | 2.55 | 122.90 | 113.62 |
| 28 | c | 516 | DGD | O3D-C3D-C4D | -2.55 | 104.45 | 110.35 |
| 23 | B | 608 | CLA | OBD-CAD-CBD | -2.55 | 122.25 | 125.89 |
| 23 | C | 508 | CLA | C1B-CHB-C4A | -2.55 | 125.06 | 130.12 |
| 24 | A | 406 | PHO | CED-O2D-CGD | 2.55 | 121.71 | 115.94 |
| 23 | A | 405 | CLA | CED-O2D-CGD | -2.55 | 110.17 | 115.94 |
| 23 | c | 513 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 23 | b | 610 | CLA | CHB-C4A-NA | 2.55 | 128.03 | 124.51 |
| 23 | C | 506 | CLA | O2A-CGA-O1A | -2.55 | 117.17 | 123.59 |
| 33 | M | 101 | LMG | C3-C4-C5 | -2.55 | 105.70 | 110.24 |
| 23 | c | 510 | CLA | C7-C6-C5 | -2.54 | 106.45 | 113.36 |
| 23 | C | 505 | CLA | C4D-C3D-CAD | -2.54 | 107.05 | 108.47 |
| 23 | A | 405 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 23 | c | 506 | CLA | C1B-CHB-C4A | -2.54 | 125.08 | 130.12 |
| 24 | a | 407 | PHO | C1-C2-C3 | -2.54 | 121.65 | 126.04 |
| 23 | d | 403 | CLA | CMB-C2B-C1B | -2.54 | 124.56 | 128.46 |
| 23 | c | 502 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 23 | B | 613 | CLA | OBD-CAD-CBD | -2.54 | 122.27 | 125.89 |
| 23 | C | 506 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | b | 619 | BCR | C39-C30-C25 | -2.54 | 106.19 | 110.30 |
| 23 | b | 606 | CLA | OBD-CAD-CBD | -2.53 | 122.28 | 125.89 |
| 28 | c | 518 | DGD | O6D-C1D-O3G | -2.53 | 103.98 | 109.97 |
| 23 | C | 509 | CLA | CED-O2D-CGD | -2.53 | 110.21 | 115.94 |
| 23 | B | 603 | CLA | O2A-CGA-O1A | -2.53 | 117.21 | 123.59 |
| 28 | C | 518 | DGD | O3E-C3E-C2E | -2.53 | 104.51 | 110.35 |
| 25 | C | 520 | BCR | C35-C13-C12 | 2.53 | 122.06 | 118.08 |
| 26 | D | 406 | PL9 | C22-C23-C24 | -2.53 | 121.58 | 127.66 |
| 23 | d | 403 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 23 | c | 506 | CLA | CMD-C2D-C3D | 2.52 | 129.40 | 124.68 |
| 25 | t | 101 | BCR | C1-C6-C5 | -2.52 | 119.06 | 122.61 |
| 23 | C | 504 | CLA | CMC-C2C-C1C | -2.52 | 121.20 | 125.04 |
| 23 | c | 508 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 28 | C | 517 | DGD | O6E-C5E-C4E | 2.52 | 114.27 | 109.69 |
| 23 | b | 608 | CLA | CMB-C2B-C1B | -2.52 | 124.59 | 128.46 |
| 34 | e | 102 | HEM | CAA-CBA-CGA | -2.52 | 108.44 | 112.67 |
| 29 | d | 408 | LHG | C20-C19-C18 | -2.52 | 101.65 | 114.42 |
| 23 | a | 408 | CLA | O2A-C1-C2 | -2.52 | 102.02 | 108.64 |
| 23 | b | 615 | CLA | O2A-CGA-O1A | -2.51 | 117.25 | 123.59 |
| 33 | b | 622 | LMG | C1-O6-C5 | -2.51 | 108.76 | 113.69 |
| 28 | A | 412 | DGD | CDB-CCB-CBB | -2.51 | 101.67 | 114.42 |
| 23 | a | 408 | CLA | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 29 | D | 409 | LHG | O8-C23-C24 | 2.51 | 119.78 | 111.91 |
| 23 | B | 610 | CLA | O2A-CGA-O1A | -2.51 | 117.26 | 123.59 |
| 23 | c | 506 | CLA | C4D-C3D-CAD | -2.51 | 107.07 | 108.47 |
| 23 | C | 503 | CLA | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 23 | B | 613 | CLA | C2A-C1A-CHA | 2.50 | 128.24 | 123.86 |
| 34 | E | 103 | HEM | C4C-C3C-C2C | 2.50 | 108.64 | 106.90 |
| 27 | F | 101 | SQD | C3-C4-C5 | 2.50 | 114.70 | 110.24 |
| 25 | B | 618 | BCR | C3-C4-C5 | -2.50 | 109.61 | 114.08 |
| 23 | b | 610 | CLA | CHA-C1A-NA | -2.50 | 120.68 | 126.40 |
| 23 | b | 602 | CLA | C3C-C4C-NC | -2.50 | 107.77 | 110.57 |
| 23 | B | 607 | CLA | O2A-CGA-O1A | -2.50 | 117.29 | 123.59 |
| 23 | b | 603 | CLA | C4A-NA-C1A | 2.50 | 107.83 | 106.71 |
| 23 | c | 511 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 25 | x | 102 | BCR | C2-C1-C6 | 2.50 | 114.32 | 110.48 |
| 23 | B | 616 | CLA | C4D-C3D-CAD | -2.49 | 107.08 | 108.47 |
| 23 | B | 609 | CLA | O2A-CGA-O1A | -2.49 | 117.30 | 123.59 |
| 24 | D | 401 | PHO | C1B-NB-C4B | 2.49 | 111.21 | 106.51 |
| 28 | C | 516 | DGD | C1E-O6E-C5E | 2.49 | 118.58 | 113.69 |
| 23 | C | 507 | CLA | O2A-CGA-O1A | -2.49 | 117.30 | 123.59 |
| 28 | C | 516 | DGD | O3G-C3G-C2G | -2.49 | 104.89 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 506 | CLA | C4D-C3D-CAD | -2.49 | 107.08 | 108.47 |
| 23 | B | 610 | CLA | O2D-CGD-CBD | 2.49 | 115.69 | 111.27 |
| 28 | h | 101 | DGD | C3E-C4E-C5E | -2.49 | 105.80 | 110.24 |
| 23 | B | 607 | CLA | C1D-CHD-C4C | 2.49 | 125.84 | 122.56 |
| 23 | C | 514 | CLA | C1D-CHD-C4C | 2.49 | 125.84 | 122.56 |
| 23 | a | 406 | CLA | CMB-C2B-C3B | 2.49 | 129.33 | 124.68 |
| 23 | C | 507 | CLA | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 28 | c | 518 | DGD | CAB-C9B-C8B | -2.49 | 101.80 | 114.42 |
| 23 | c | 512 | CLA | C1D-CHD-C4C | 2.48 | 125.83 | 122.56 |
| 23 | c | 508 | CLA | CMD-C2D-C3D | 2.48 | 129.32 | 124.68 |
| 28 | C | 518 | DGD | O3G-C1D-C2D | -2.48 | 104.43 | 108.30 |
| 23 | C | 513 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 25 | c | 521 | BCR | C33-C5-C6 | -2.48 | 121.75 | 124.53 |
| 25 | c | 514 | BCR | C2-C1-C6 | 2.48 | 114.29 | 110.48 |
| 23 | B | 601 | CLA | C1D-CHD-C4C | 2.48 | 125.83 | 122.56 |
| 24 | D | 401 | PHO | C2B-C1B-NB | -2.48 | 106.06 | 109.79 |
| 23 | B | 604 | CLA | O2A-CGA-CBA | 2.48 | 119.68 | 111.91 |
| 25 | Z | 101 | BCR | C33-C5-C6 | -2.48 | 121.75 | 124.53 |
| 28 | c | 516 | DGD | C3D-C4D-C5D | -2.48 | 105.82 | 110.24 |
| 33 | c | 522 | LMG | O7-C10-O9 | -2.47 | 117.72 | 123.70 |
| 23 | C | 502 | CLA | C3B-C4B-NB | -2.47 | 106.01 | 109.21 |
| 27 | b | 601 | SQD | O48-C23-C24 | 2.47 | 119.67 | 111.91 |
| 27 | a | 412 | SQD | O49-C7-C8 | -2.47 | 114.10 | 123.73 |
| 25 | d | 405 | BCR | C38-C26-C25 | -2.46 | 121.76 | 124.53 |
| 25 | B | 619 | BCR | C27-C26-C25 | 2.46 | 126.31 | 122.73 |
| 25 | H | 101 | BCR | C33-C5-C6 | -2.46 | 121.76 | 124.53 |
| 23 | b | 609 | CLA | C6-C7-C8 | -2.46 | 107.96 | 115.92 |
| 23 | b | 610 | CLA | O2D-CGD-CBD | -2.46 | 106.89 | 111.27 |
| 25 | a | 409 | BCR | C2-C1-C6 | 2.46 | 114.27 | 110.48 |
| 23 | B | 609 | CLA | CHA-C1A-NA | -2.46 | 120.77 | 126.40 |
| 25 | T | 101 | BCR | C37-C22-C23 | 2.46 | 121.95 | 118.08 |
| 23 | D | 403 | CLA | C1-C2-C3 | -2.46 | 121.79 | 126.04 |
| 25 | b | 618 | BCR | C29-C30-C25 | 2.46 | 114.26 | 110.48 |
| 27 | f | 101 | SQD | C1-C2-C3 | -2.46 | 104.88 | 110.00 |
| 23 | a | 405 | CLA | CAC-C3C-C4C | 2.45 | 128.00 | 124.81 |
| 28 | c | 517 | DGD | O5D-C6D-C5D | -2.45 | 104.51 | 109.05 |
| 28 | c | 516 | DGD | O2G-C1B-C2B | -2.45 | 106.21 | 111.50 |
| 23 | C | 509 | CLA | O2A-CGA-O1A | -2.45 | 117.40 | 123.59 |
| 23 | B | 606 | CLA | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 23 | A | 407 | CLA | O2A-CGA-O1A | -2.45 | 117.41 | 123.59 |
| 26 | D | 406 | PL9 | C30-C29-C31 | -2.45 | 111.15 | 115.27 |
| 23 | C | 504 | CLA | C6-C7-C8 | -2.45 | 108.01 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | c | 524 | LMG | O8-C28-O10 | -2.45 | 117.42 | 123.59 |
| 26 | a | 410 | PL9 | C40-C39-C38 | -2.44 | 117.41 | 123.68 |
| 23 | B | 611 | CLA | O2A-CGA-O1A | -2.44 | 117.42 | 123.59 |
| 23 | C | 513 | CLA | C16-C15-C13 | -2.44 | 108.02 | 115.92 |
| 23 | B | 601 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 27 | B | 621 | SQD | O10-C23-C24 | -2.44 | 114.20 | 123.73 |
| 24 | d | 401 | PHO | CHB-C4A-NA | 2.44 | 129.14 | 124.94 |
| 23 | a | 408 | CLA | CHD-C4C-NC | 2.44 | 128.05 | 124.20 |
| 23 | C | 513 | CLA | C1D-CHD-C4C | 2.44 | 125.78 | 122.56 |
| 33 | c | 522 | LMG | O3-C3-C2 | -2.44 | 104.72 | 110.35 |
| 28 | h | 101 | DGD | C1D-C2D-C3D | -2.44 | 104.92 | 110.00 |
| 23 | B | 605 | CLA | O2A-CGA-O1A | -2.43 | 117.45 | 123.59 |
| 23 | b | 602 | CLA | CMD-C2D-C3D | 2.43 | 129.23 | 124.68 |
| 23 | b | 607 | CLA | OBD-CAD-CBD | -2.43 | 122.42 | 125.89 |
| 34 | E | 103 | HEM | CAA-CBA-CGA | -2.43 | 108.59 | 112.67 |
| 25 | Z | 101 | BCR | C27-C26-C25 | 2.43 | 126.26 | 122.73 |
| 23 | b | 617 | CLA | C2A-C3A-C4A | 2.43 | 105.80 | 101.87 |
| 23 | B | 601 | CLA | OBD-CAD-CBD | -2.43 | 122.42 | 125.89 |
| 28 | H | 102 | DGD | C3G-C2G-C1G | -2.43 | 106.04 | 111.79 |
| 26 | a | 410 | PL9 | C11-C12-C13 | -2.43 | 103.89 | 111.88 |
| 23 | b | 615 | CLA | CHD-C4C-NC | 2.43 | 128.03 | 124.20 |
| 23 | b | 605 | CLA | CGD-CBD-CAD | -2.43 | 102.87 | 110.73 |
| 26 | d | 406 | PL9 | C7-C3-C2 | -2.43 | 120.11 | 123.30 |
| 25 | d | 405 | BCR | C27-C26-C25 | 2.43 | 126.26 | 122.73 |
| 23 | C | 512 | CLA | C3C-C4C-NC | -2.43 | 107.85 | 110.57 |
| 23 | c | 510 | CLA | C16-C15-C13 | -2.43 | 108.08 | 115.92 |
| 28 | c | 517 | DGD | O2E-C2E-C1E | -2.42 | 104.16 | 110.05 |
| 23 | C | 514 | CLA | CMD-C2D-C3D | 2.42 | 129.21 | 124.68 |
| 23 | C | 507 | CLA | CHA-C1A-NA | -2.42 | 120.85 | 126.40 |
| 23 | b | 614 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 23 | b | 609 | CLA | CHA-C1A-NA | -2.42 | 120.85 | 126.40 |
| 25 | b | 620 | BCR | C27-C26-C25 | 2.42 | 126.24 | 122.73 |
| 23 | b | 611 | CLA | C11-C10-C8 | -2.42 | 108.10 | 115.92 |
| 25 | T | 101 | BCR | C4-C5-C6 | 2.41 | 126.23 | 122.73 |
| 23 | c | 505 | CLA | C1B-CHB-C4A | -2.41 | 125.34 | 130.12 |
| 27 | b | 601 | SQD | C45-O47-C7 | 2.41 | 123.73 | 117.79 |
| 23 | b | 614 | CLA | CHA-C1A-NA | -2.41 | 120.88 | 126.40 |
| 33 | M | 101 | LMG | C38-C37-C36 | -2.41 | 102.19 | 114.42 |
| 26 | a | 410 | PL9 | O2-C1-C2 | -2.41 | 116.27 | 121.78 |
| 33 | C | 501 | LMG | O5-C6-C5 | -2.41 | 103.04 | 111.29 |
| 25 | C | 515 | BCR | C40-C30-C25 | 2.40 | 114.20 | 110.30 |
| 23 | c | 513 | CLA | CAC-C3C-C4C | 2.40 | 127.92 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | C | 515 | BCR | C34-C9-C10 | -2.40 | 119.56 | 122.92 |
| 23 | c | 512 | CLA | OBD-CAD-CBD | -2.40 | 122.47 | 125.89 |
| 28 | C | 517 | DGD | CDB-CCB-CBB | -2.40 | 102.25 | 114.42 |
| 25 | B | 619 | BCR | C34-C9-C10 | -2.40 | 119.56 | 122.92 |
| 23 | b | 606 | CLA | O1A-CGA-CBA | 2.40 | 133.08 | 123.73 |
| 28 | c | 517 | DGD | CDB-CCB-CBB | -2.39 | 102.27 | 114.42 |
| 28 | c | 517 | DGD | O3G-C3G-C2G | -2.39 | 105.12 | 110.90 |
| 23 | a | 408 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 28 | h | 101 | DGD | O6D-C1D-O3G | -2.39 | 104.31 | 109.97 |
| 25 | b | 620 | BCR | C16-C15-C14 | -2.39 | 118.58 | 123.47 |
| 24 | D | 401 | PHO | C1-C2-C3 | -2.39 | 121.91 | 126.04 |
| 24 | a | 407 | PHO | C1B-NB-C4B | 2.39 | 111.02 | 106.51 |
| 23 | B | 613 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 28 | H | 102 | DGD | O6D-C1D-O3G | -2.39 | 104.32 | 109.97 |
| 23 | b | 612 | CLA | CMB-C2B-C1B | -2.39 | 124.79 | 128.46 |
| 23 | D | 403 | CLA | C1B-CHB-C4A | -2.39 | 125.39 | 130.12 |
| 23 | a | 405 | CLA | C4-C3-C5 | 2.39 | 119.29 | 115.27 |
| 33 | m | 101 | LMG | C40-C39-C38 | -2.39 | 102.31 | 114.42 |
| 23 | b | 606 | CLA | O2A-CGA-O1A | -2.38 | 117.58 | 123.59 |
| 23 | A | 404 | CLA | CMB-C2B-C1B | -2.38 | 124.80 | 128.46 |
| 25 | c | 515 | BCR | C36-C18-C17 | -2.38 | 119.58 | 122.92 |
| 23 | c | 504 | CLA | O2A-CGA-O1A | -2.38 | 117.58 | 123.59 |
| 25 | A | 408 | BCR | C31-C1-C6 | -2.38 | 106.44 | 110.30 |
| 23 | D | 403 | CLA | CMB-C2B-C3B | 2.38 | 129.13 | 124.68 |
| 23 | C | 509 | CLA | CHA-C1A-NA | -2.38 | 120.95 | 126.40 |
| 25 | t | 101 | BCR | C15-C14-C13 | -2.38 | 123.92 | 127.31 |
| 23 | a | 408 | CLA | CHD-C4C-C3C | -2.38 | 121.35 | 124.84 |
| 23 | b | 607 | CLA | CMB-C2B-C1B | -2.37 | 124.81 | 128.46 |
| 23 | A | 407 | CLA | CHC-C1C-C2C | -2.37 | 120.16 | 126.72 |
| 25 | B | 619 | BCR | C29-C30-C25 | 2.37 | 114.13 | 110.48 |
| 23 | B | 607 | CLA | O2D-CGD-O1D | -2.37 | 119.20 | 123.84 |
| 28 | C | 516 | DGD | O6D-C1D-O3G | -2.37 | 104.36 | 109.97 |
| 23 | b | 610 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 23 | a | 408 | CLA | OBD-CAD-CBD | -2.37 | 122.51 | 125.89 |
| 25 | b | 619 | BCR | C3-C4-C5 | -2.37 | 109.84 | 114.08 |
| 23 | c | 510 | CLA | C4D-C3D-CAD | -2.37 | 107.15 | 108.47 |
| 23 | b | 608 | CLA | C1D-CHD-C4C | 2.37 | 125.69 | 122.56 |
| 23 | C | 512 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 23 | c | 503 | CLA | CMB-C2B-C3B | 2.37 | 129.11 | 124.68 |
| 26 | a | 410 | PL9 | C31-C29-C28 | 2.37 | 125.91 | 121.12 |
| 23 | B | 615 | CLA | CHA-C1A-NA | -2.37 | 120.98 | 126.40 |
| 23 | c | 502 | CLA | O1D-CGD-CBD | 2.37 | 129.32 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 614 | CLA | O2D-CGD-CBD | 2.37 | 115.47 | 111.27 |
| 24 | a | 407 | PHO | O1D-CGD-CBD | 2.36 | 129.32 | 124.48 |
| 23 | B | 615 | CLA | C6-C7-C8 | -2.36 | 108.28 | 115.92 |
| 23 | B | 601 | CLA | CAA-C2A-C3A | -2.36 | 106.31 | 112.78 |
| 23 | b | 613 | CLA | C11-C10-C8 | -2.36 | 108.28 | 115.92 |
| 23 | B | 606 | CLA | C7-C6-C5 | -2.36 | 106.94 | 113.36 |
| 23 | B | 602 | CLA | CHA-C1A-NA | -2.36 | 120.99 | 126.40 |
| 35 | V | 201 | HEC | CMD-C2D-C1D | -2.36 | 124.83 | 128.46 |
| 23 | C | 507 | CLA | OBD-CAD-C3D | 2.36 | 131.89 | 127.98 |
| 25 | D | 405 | BCR | C1-C6-C5 | -2.36 | 119.30 | 122.61 |
| 27 | b | 601 | SQD | O9-S-C6 | 2.36 | 109.74 | 106.94 |
| 23 | C | 504 | CLA | CMC-C2C-C3C | 2.35 | 132.50 | 126.12 |
| 23 | B | 609 | CLA | CHC-C1C-C2C | -2.35 | 120.22 | 126.72 |
| 25 | b | 620 | BCR | C11-C10-C9 | -2.35 | 123.95 | 127.31 |
| 23 | a | 405 | CLA | CMB-C2B-C3B | 2.35 | 129.08 | 124.68 |
| 23 | D | 404 | CLA | C6-C7-C8 | -2.35 | 108.32 | 115.92 |
| 25 | K | 101 | BCR | C8-C7-C6 | -2.35 | 120.60 | 127.20 |
| 28 | h | 101 | DGD | CDB-CCB-CBB | -2.35 | 102.50 | 114.42 |
| 23 | b | 603 | CLA | CGD-CBD-CAD | -2.35 | 103.13 | 110.73 |
| 28 | c | 516 | DGD | O4D-C4D-C3D | 2.35 | 115.78 | 110.35 |
| 25 | t | 101 | BCR | C36-C18-C19 | 2.35 | 121.78 | 118.08 |
| 26 | d | 406 | PL9 | C40-C39-C38 | -2.35 | 117.66 | 123.68 |
| 29 | A | 413 | LHG | C18-C17-C16 | -2.35 | 102.52 | 114.42 |
| 23 | D | 403 | CLA | O2A-CGA-O1A | -2.35 | 117.67 | 123.59 |
| 27 | b | 601 | SQD | O48-C23-O10 | -2.35 | 117.67 | 123.59 |
| 28 | h | 101 | DGD | O3E-C3E-C2E | -2.35 | 104.93 | 110.35 |
| 23 | c | 504 | CLA | CMC-C2C-C1C | 2.34 | 128.60 | 125.04 |
| 23 | B | 601 | CLA | O1D-CGD-CBD | 2.34 | 129.27 | 124.48 |
| 23 | a | 405 | CLA | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 25 | t | 101 | BCR | C37-C22-C21 | -2.34 | 119.64 | 122.92 |
| 25 | c | 514 | BCR | C35-C13-C14 | -2.34 | 119.65 | 122.92 |
| 23 | b | 607 | CLA | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 23 | C | 512 | CLA | CAC-C3C-C4C | 2.34 | 127.84 | 124.81 |
| 28 | c | 516 | DGD | CBB-CAB-C9B | -2.34 | 102.56 | 114.42 |
| 23 | b | 607 | CLA | CHC-C1C-NC | 2.34 | 127.75 | 124.20 |
| 23 | b | 612 | CLA | CHB-C4A-NA | 2.34 | 127.74 | 124.51 |
| 23 | b | 602 | CLA | O2A-CGA-O1A | -2.33 | 117.70 | 123.59 |
| 28 | C | 518 | DGD | O3D-C3D-C4D | -2.33 | 104.96 | 110.35 |
| 26 | d | 406 | PL9 | C42-C43-C44 | -2.33 | 122.05 | 127.66 |
| 26 | D | 406 | PL9 | C35-C34-C36 | 2.33 | 119.18 | 115.27 |
| 23 | C | 514 | CLA | C3C-C4C-NC | -2.33 | 107.96 | 110.57 |
| 23 | C | 502 | CLA | CAC-C3C-C4C | 2.32 | 127.83 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28 | c | 518 | DGD | O1G-C1A-C2A | -2.32 | 104.61 | 111.91 |
| 23 | c | 508 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 23 | b | 615 | CLA | C3C-C4C-NC | -2.32 | 107.97 | 110.57 |
| 25 | d | 405 | BCR | C30-C25-C26 | -2.32 | 119.35 | 122.61 |
| 23 | B | 603 | CLA | O1A-CGA-CBA | 2.32 | 132.78 | 123.73 |
| 23 | b | 614 | CLA | CGD-CBD-CAD | -2.32 | 103.22 | 110.73 |
| 23 | c | 507 | CLA | CHD-C4C-NC | 2.32 | 127.86 | 124.20 |
| 23 | B | 609 | CLA | C4D-C3D-CAD | -2.32 | 107.18 | 108.47 |
| 26 | d | 406 | PL9 | C36-C34-C33 | -2.32 | 116.43 | 121.12 |
| 33 | M | 101 | LMG | O6-C1-O1 | -2.31 | 104.49 | 109.97 |
| 25 | k | 101 | BCR | C2-C1-C6 | 2.31 | 114.04 | 110.48 |
| 23 | B | 616 | CLA | C2C-C1C-NC | 2.31 | 112.14 | 109.97 |
| 23 | c | 506 | CLA | C4-C3-C2 | -2.31 | 117.75 | 123.68 |
| 23 | B | 608 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 23 | B | 615 | CLA | C4-C3-C2 | 2.31 | 129.60 | 123.68 |
| 23 | D | 404 | CLA | OBD-CAD-C3D | 2.31 | 131.81 | 127.98 |
| 23 | b | 603 | CLA | CHC-C1C-C2C | -2.31 | 120.34 | 126.72 |
| 25 | Z | 101 | BCR | C24-C23-C22 | -2.31 | 122.75 | 126.23 |
| 28 | h | 101 | DGD | CBB-CAB-C9B | -2.31 | 102.72 | 114.42 |
| 26 | a | 410 | PL9 | O2-C1-C6 | 2.31 | 124.58 | 120.59 |
| 33 | b | 622 | LMG | O7-C10-O9 | -2.31 | 118.13 | 123.70 |
| 23 | c | 502 | CLA | C1-O2A-CGA | 2.30 | 122.49 | 116.44 |
| 23 | b | 613 | CLA | CHD-C4C-C3C | -2.30 | 121.45 | 124.84 |
| 23 | b | 604 | CLA | CMB-C2B-C1B | -2.30 | 124.93 | 128.46 |
| 23 | C | 511 | CLA | C3A-C2A-C1A | 2.30 | 104.78 | 101.34 |
| 25 | B | 618 | BCR | C30-C25-C26 | -2.30 | 119.37 | 122.61 |
| 28 | C | 516 | DGD | O1G-C1A-C2A | -2.30 | 104.70 | 111.91 |
| 23 | B | 606 | CLA | OBD-CAD-C3D | 2.30 | 131.79 | 127.98 |
| 23 | B | 603 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 23 | b | 616 | CLA | CAA-CBA-CGA | -2.30 | 106.54 | 113.25 |
| 23 | d | 402 | CLA | C1B-CHB-C4A | -2.29 | 125.57 | 130.12 |
| 23 | C | 507 | CLA | C4D-C3D-CAD | -2.29 | 107.19 | 108.47 |
| 27 | A | 410 | SQD | O48-C23-C24 | 2.29 | 119.10 | 111.91 |
| 23 | b | 608 | CLA | C1-C2-C3 | -2.29 | 122.08 | 126.04 |
| 25 | b | 620 | BCR | C2-C1-C6 | 2.29 | 114.01 | 110.48 |
| 23 | D | 403 | CLA | O2D-CGD-CBD | 2.29 | 115.34 | 111.27 |
| 23 | C | 513 | CLA | CAA-CBA-CGA | -2.29 | 106.57 | 113.25 |
| 23 | C | 507 | CLA | O1D-CGD-CBD | 2.29 | 129.16 | 124.48 |
| 26 | D | 406 | PL9 | C11-C9-C8 | -2.29 | 116.49 | 121.12 |
| 27 | f | 101 | SQD | O48-C23-C24 | 2.29 | 119.08 | 111.91 |
| 23 | a | 405 | CLA | CAA-C2A-C1A | -2.29 | 104.48 | 111.97 |
| 26 | A | 409 | PL9 | C22-C23-C24 | -2.29 | 122.16 | 127.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 509 | CLA | CMB-C2B-C3B | 2.28 | 128.95 | 124.68 |
| 23 | b | 609 | CLA | CMD-C2D-C3D | 2.28 | 128.95 | 124.68 |
| 23 | B | 605 | CLA | C3A-C2A-C1A | 2.28 | 104.76 | 101.34 |
| 23 | c | 507 | CLA | C3A-C2A-C1A | 2.28 | 104.75 | 101.34 |
| 33 | c | 519 | LMG | O7-C10-O9 | -2.28 | 118.44 | 122.96 |
| 28 | H | 102 | DGD | CDB-CCB-CBB | -2.28 | 102.86 | 114.42 |
| 23 | B | 615 | CLA | CMD-C2D-C3D | 2.28 | 128.94 | 124.68 |
| 25 | C | 515 | BCR | C3-C4-C5 | -2.27 | 110.02 | 114.08 |
| 27 | A | 410 | SQD | C1-O5-C5 | -2.27 | 109.22 | 113.69 |
| 25 | t | 101 | BCR | C2-C1-C6 | 2.27 | 113.98 | 110.48 |
| 33 | M | 101 | LMG | C8-O7-C10 | 2.27 | 123.39 | 117.79 |
| 25 | b | 620 | BCR | C36-C18-C17 | -2.27 | 119.74 | 122.92 |
| 23 | B | 612 | CLA | CMC-C2C-C1C | -2.27 | 121.58 | 125.04 |
| 28 | h | 101 | DGD | C6D-C5D-C4D | 2.27 | 116.83 | 112.09 |
| 25 | B | 617 | BCR | C16-C15-C14 | -2.27 | 118.83 | 123.47 |
| 23 | c | 510 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 26 | a | 410 | PL9 | C21-C19-C18 | -2.27 | 116.53 | 121.12 |
| 33 | d | 411 | LMG | C40-C39-C38 | -2.27 | 102.92 | 114.42 |
| 23 | a | 405 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 23 | b | 612 | CLA | C1C-C2C-C3C | -2.27 | 104.57 | 106.96 |
| 23 | b | 616 | CLA | CED-O2D-CGD | 2.27 | 121.06 | 115.94 |
| 25 | C | 520 | BCR | C38-C26-C25 | -2.27 | 121.98 | 124.53 |
| 23 | a | 408 | CLA | O2D-CGD-O1D | -2.26 | 119.41 | 123.84 |
| 23 | d | 404 | CLA | C2C-C1C-NC | 2.26 | 112.09 | 109.97 |
| 24 | A | 406 | PHO | O2A-CGA-O1A | -2.26 | 117.88 | 123.59 |
| 25 | a | 409 | BCR | C16-C15-C14 | -2.26 | 118.84 | 123.47 |
| 25 | B | 617 | BCR | C16-C17-C18 | -2.26 | 124.08 | 127.31 |
| 23 | c | 512 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 27 | B | 621 | SQD | O5-C1-O6 | 2.26 | 115.33 | 109.97 |
| 23 | B | 603 | CLA | CMB-C2B-C1B | -2.26 | 124.99 | 128.46 |
| 23 | b | 603 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 23 | B | 614 | CLA | C4D-C3D-CAD | -2.26 | 107.21 | 108.47 |
| 25 | b | 620 | BCR | C30-C25-C26 | -2.26 | 119.44 | 122.61 |
| 23 | B | 611 | CLA | CGD-CBD-CAD | -2.26 | 103.43 | 110.73 |
| 23 | C | 511 | CLA | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 33 | c | 519 | LMG | C9-C8-C7 | -2.25 | 106.46 | 111.79 |
| 23 | c | 505 | CLA | C4D-C3D-CAD | -2.25 | 107.21 | 108.47 |
| 23 | b | 607 | CLA | O2A-CGA-O1A | -2.25 | 117.91 | 123.59 |
| 23 | B | 616 | CLA | O2D-CGD-CBD | 2.25 | 115.27 | 111.27 |
| 25 | K | 101 | BCR | C27-C26-C25 | 2.25 | 126.00 | 122.73 |
| 29 | d | 408 | LHG | C18-C17-C16 | -2.25 | 103.00 | 114.42 |
| 24 | D | 401 | PHO | C3A-C4A-CHB | -2.25 | 117.94 | 121.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | A | 413 | LHG | C20-C19-C18 | -2.25 | 103.01 | 114.42 |
| 23 | C | 505 | CLA | C2A-C1A-CHA | 2.25 | 127.79 | 123.86 |
| 33 | c | 524 | LMG | O7-C10-O9 | -2.25 | 118.28 | 123.70 |
| 23 | D | 402 | CLA | CMB-C2B-C3B | 2.24 | 128.88 | 124.68 |
| 23 | A | 407 | CLA | C6-C5-C3 | 2.24 | 119.34 | 113.45 |
| 23 | B | 605 | CLA | O1A-CGA-CBA | 2.24 | 132.49 | 123.73 |
| 33 | D | 410 | LMG | O1-C7-C8 | -2.24 | 105.83 | 111.78 |
| 23 | B | 604 | CLA | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |
| 24 | D | 401 | PHO | C3C-C4C-NC | -2.24 | 106.80 | 110.28 |
| 25 | A | 408 | BCR | C15-C16-C17 | -2.24 | 118.88 | 123.47 |
| 25 | B | 619 | BCR | C1-C6-C5 | -2.24 | 119.46 | 122.61 |
| 23 | C | 513 | CLA | O2A-CGA-O1A | -2.24 | 117.94 | 123.59 |
| 23 | C | 507 | CLA | C6-C7-C8 | -2.24 | 108.68 | 115.92 |
| 33 | C | 501 | LMG | O6-C1-O1 | -2.24 | 104.67 | 109.97 |
| 23 | b | 613 | CLA | OBD-CAD-C3D | 2.24 | 131.69 | 127.98 |
| 23 | B | 612 | CLA | C11-C12-C13 | -2.23 | 108.70 | 115.92 |
| 23 | C | 509 | CLA | C7-C6-C5 | -2.23 | 107.29 | 113.36 |
| 33 | d | 411 | LMG | O5-C6-C5 | -2.23 | 103.63 | 111.29 |
| 26 | a | 410 | PL9 | C12-C13-C14 | -2.23 | 122.28 | 127.66 |
| 23 | b | 606 | CLA | CHC-C1C-C2C | -2.23 | 120.55 | 126.72 |
| 28 | A | 412 | DGD | C4E-C3E-C2E | -2.23 | 106.93 | 110.82 |
| 23 | B | 615 | CLA | C3D-CAD-CBD | -2.23 | 104.67 | 107.61 |
| 23 | b | 613 | CLA | O2A-CGA-O1A | -2.23 | 117.97 | 123.59 |
| 23 | B | 615 | CLA | CHB-C4A-NA | 2.23 | 127.59 | 124.51 |
| 23 | c | 503 | CLA | O1D-CGD-CBD | 2.22 | 129.03 | 124.48 |
| 23 | D | 404 | CLA | O2A-CGA-O1A | -2.22 | 117.98 | 123.59 |
| 23 | b | 615 | CLA | C6-C5-C3 | -2.22 | 107.63 | 113.45 |
| 23 | B | 615 | CLA | CMB-C2B-C3B | 2.22 | 128.83 | 124.68 |
| 23 | C | 505 | CLA | C6-C5-C3 | 2.22 | 119.28 | 113.45 |
| 23 | C | 506 | CLA | OBD-CAD-C3D | 2.22 | 131.67 | 127.98 |
| 23 | C | 504 | CLA | C2C-C1C-NC | 2.22 | 112.05 | 109.97 |
| 25 | t | 101 | BCR | C11-C10-C9 | -2.22 | 124.14 | 127.31 |
| 23 | C | 502 | CLA | CMD-C2D-C3D | 2.22 | 128.83 | 124.68 |
| 24 | d | 401 | PHO | C3A-C4A-CHB | -2.22 | 118.00 | 121.83 |
| 23 | d | 402 | CLA | C3B-C4B-NB | -2.22 | 106.34 | 109.21 |
| 25 | D | 405 | BCR | C7-C8-C9 | -2.22 | 122.89 | 126.23 |
| 33 | M | 101 | LMG | O8-C28-O10 | -2.22 | 118.00 | 123.59 |
| 23 | c | 507 | CLA | CMD-C2D-C3D | 2.21 | 128.82 | 124.68 |
| 28 | c | 516 | DGD | C4B-C3B-C2B | -2.21 | 105.23 | 113.19 |
| 28 | a | 413 | DGD | C1G-O1G-C1A | 2.21 | 125.32 | 117.12 |
| 23 | B | 609 | CLA | CHD-C4C-NC | 2.21 | 127.69 | 124.20 |
| 23 | B | 607 | CLA | CMC-C2C-C1C | 2.21 | 128.41 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 601 | CLA | CHB-C4A-NA | 2.21 | 127.57 | 124.51 |
| 23 | b | 611 | CLA | CHA-C1A-NA | -2.21 | 121.33 | 126.40 |
| 23 | b | 607 | CLA | C4-C3-C5 | 2.21 | 118.99 | 115.27 |
| 25 | A | 408 | BCR | C8-C7-C6 | -2.21 | 120.99 | 127.20 |
| 27 | A | 410 | SQD | C3-C4-C5 | 2.21 | 114.18 | 110.24 |
| 23 | B | 612 | CLA | C2A-C3A-C4A | 2.21 | 105.44 | 101.87 |
| 23 | A | 404 | CLA | CMD-C2D-C3D | 2.21 | 128.81 | 124.68 |
| 23 | b | 605 | CLA | O2D-CGD-CBD | 2.21 | 115.19 | 111.27 |
| 25 | d | 405 | BCR | C29-C30-C25 | 2.21 | 113.88 | 110.48 |
| 25 | B | 619 | BCR | C40-C30-C25 | 2.21 | 113.88 | 110.30 |
| 28 | H | 102 | DGD | C6D-C5D-C4D | 2.21 | 116.70 | 112.09 |
| 25 | x | 102 | BCR | C35-C13-C12 | 2.21 | 121.55 | 118.08 |
| 27 | F | 101 | SQD | O48-C23-O10 | -2.21 | 118.03 | 123.59 |
| 23 | B | 602 | CLA | C1D-CHD-C4C | 2.20 | 125.47 | 122.56 |
| 23 | b | 605 | CLA | C1B-CHB-C4A | -2.20 | 125.75 | 130.12 |
| 23 | B | 612 | CLA | CHC-C1C-NC | 2.20 | 127.55 | 124.20 |
| 23 | C | 508 | CLA | CHA-C1A-NA | -2.20 | 121.35 | 126.40 |
| 23 | c | 507 | CLA | O2D-CGD-CBD | 2.20 | 115.18 | 111.27 |
| 25 | C | 520 | BCR | C15-C14-C13 | -2.20 | 124.17 | 127.31 |
| 23 | C | 502 | CLA | C4-C3-C5 | 2.20 | 118.97 | 115.27 |
| 24 | d | 401 | PHO | C2B-C1B-NB | -2.20 | 106.47 | 109.79 |
| 23 | b | 610 | CLA | OBD-CAD-CBD | -2.20 | 122.75 | 125.89 |
| 23 | C | 514 | CLA | C6-C7-C8 | -2.20 | 108.81 | 115.92 |
| 27 | A | 410 | SQD | O48-C46-C45 | 2.20 | 114.83 | 108.43 |
| 23 | C | 509 | CLA | C2A-C1A-CHA | 2.20 | 127.70 | 123.86 |
| 23 | B | 608 | CLA | OBD-CAD-C3D | 2.20 | 131.63 | 127.98 |
| 23 | c | 511 | CLA | OBD-CAD-C3D | 2.19 | 131.62 | 127.98 |
| 27 | f | 101 | SQD | O5-C1-O6 | 2.19 | 115.17 | 109.97 |
| 23 | c | 507 | CLA | C2C-C1C-NC | 2.19 | 112.03 | 109.97 |
| 23 | B | 608 | CLA | C4D-C3D-CAD | -2.19 | 107.25 | 108.47 |
| 23 | c | 512 | CLA | O2D-CGD-O1D | -2.19 | 119.55 | 123.84 |
| 26 | d | 406 | PL9 | C32-C33-C34 | -2.19 | 122.39 | 127.66 |
| 33 | C | 501 | LMG | O7-C10-O9 | -2.19 | 118.41 | 123.70 |
| 23 | B | 613 | CLA | CHC-C1C-C2C | -2.19 | 120.67 | 126.72 |
| 23 | B | 612 | CLA | OBD-CAD-CBD | -2.19 | 122.77 | 125.89 |
| 25 | d | 405 | BCR | C1-C6-C5 | -2.19 | 119.53 | 122.61 |
| 23 | B | 611 | CLA | CHB-C4A-NA | 2.19 | 127.54 | 124.51 |
| 23 | B | 616 | CLA | OBD-CAD-CBD | -2.19 | 122.77 | 125.89 |
| 23 | b | 609 | CLA | C11-C10-C8 | -2.19 | 108.85 | 115.92 |
| 23 | B | 610 | CLA | O1D-CGD-CBD | 2.19 | 128.96 | 124.48 |
| 23 | b | 607 | CLA | CHA-C1A-NA | -2.19 | 121.39 | 126.40 |
| 25 | Z | 101 | BCR | C34-C9-C8 | -2.18 | 114.64 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | B | 608 | CLA | CHD-C4C-NC | 2.18 | 127.64 | 124.20 |
| 23 | b | 605 | CLA | C7-C6-C5 | -2.18 | 107.44 | 113.36 |
| 28 | h | 101 | DGD | O5D-C6D-C5D | -2.18 | 105.01 | 109.05 |
| 23 | A | 407 | CLA | C4A-NA-C1A | 2.18 | 107.69 | 106.71 |
| 24 | d | 401 | PHO | CMB-C2B-C1B | -2.18 | 121.71 | 125.06 |
| 29 | E | 101 | LHG | O8-C23-O10 | -2.18 | 118.10 | 123.59 |
| 28 | C | 518 | DGD | O5D-C6D-C5D | -2.18 | 105.02 | 109.05 |
| 23 | B | 616 | CLA | C1-C2-C3 | 2.18 | 129.81 | 126.04 |
| 23 | b | 607 | CLA | CHD-C4C-C3C | -2.17 | 121.64 | 124.84 |
| 23 | c | 508 | CLA | CHB-C4A-NA | 2.17 | 127.51 | 124.51 |
| 28 | c | 518 | DGD | O6E-C1E-O5D | -2.17 | 104.84 | 109.97 |
| 24 | a | 407 | PHO | O2A-CGA-O1A | -2.17 | 118.12 | 123.59 |
| 23 | b | 614 | CLA | OBD-CAD-C3D | 2.17 | 131.58 | 127.98 |
| 23 | b | 606 | CLA | CMD-C2D-C3D | 2.17 | 128.74 | 124.68 |
| 24 | D | 401 | PHO | CHB-C4A-NA | 2.17 | 128.67 | 124.94 |
| 33 | D | 407 | LMG | O8-C28-O10 | -2.17 | 118.12 | 123.59 |
| 27 | b | 601 | SQD | O8-S-O7 | -2.17 | 105.98 | 111.27 |
| 23 | c | 506 | CLA | C3C-C4C-NC | -2.16 | 108.14 | 110.57 |
| 23 | b | 602 | CLA | C3B-C4B-NB | -2.16 | 106.41 | 109.21 |
| 23 | b | 611 | CLA | C11-C12-C13 | -2.16 | 108.93 | 115.92 |
| 23 | B | 611 | CLA | CHD-C4C-NC | 2.16 | 127.61 | 124.20 |
| 23 | c | 507 | CLA | O2D-CGD-O1D | -2.16 | 119.61 | 123.84 |
| 23 | B | 611 | CLA | O1A-CGA-CBA | 2.16 | 132.16 | 123.73 |
| 23 | b | 604 | CLA | C4-C3-C5 | 2.16 | 118.91 | 115.27 |
| 23 | B | 612 | CLA | CMB-C2B-C1B | -2.16 | 125.14 | 128.46 |
| 23 | C | 513 | CLA | CMD-C2D-C3D | 2.16 | 128.72 | 124.68 |
| 23 | b | 609 | CLA | OBD-CAD-C3D | 2.16 | 131.57 | 127.98 |
| 23 | C | 503 | CLA | CHD-C4C-NC | 2.16 | 127.61 | 124.20 |
| 28 | C | 517 | DGD | O5E-C6E-C5E | -2.16 | 103.88 | 111.29 |
| 26 | a | 410 | PL9 | O1-C4-C3 | -2.16 | 118.34 | 120.72 |
| 23 | b | 606 | CLA | OBD-CAD-C3D | 2.16 | 131.56 | 127.98 |
| 23 | C | 504 | CLA | C4D-C3D-CAD | -2.16 | 107.27 | 108.47 |
| 29 | A | 413 | LHG | O4-P-O6 | -2.16 | 97.73 | 107.75 |
| 23 | B | 607 | CLA | C1B-CHB-C4A | -2.16 | 125.85 | 130.12 |
| 25 | d | 405 | BCR | C11-C10-C9 | -2.15 | 124.23 | 127.31 |
| 25 | a | 409 | BCR | C27-C26-C25 | 2.15 | 125.86 | 122.73 |
| 23 | b | 612 | CLA | CHA-C1A-NA | -2.15 | 121.46 | 126.40 |
| 23 | A | 405 | CLA | C11-C12-C13 | -2.15 | 108.96 | 115.92 |
| 25 | c | 514 | BCR | C38-C26-C27 | -2.15 | 109.48 | 113.62 |
| 23 | c | 501 | CLA | C2A-C1A-CHA | 2.15 | 127.62 | 123.86 |
| 23 | C | 502 | CLA | CMC-C2C-C1C | 2.15 | 128.32 | 125.04 |
| 25 | c | 521 | BCR | C30-C25-C26 | -2.15 | 119.58 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 504 | CLA | C1D-CHD-C4C | 2.15 | 125.40 | 122.56 |
| 33 | C | 519 | LMG | O3-C3-C2 | -2.15 | 105.38 | 110.35 |
| 23 | B | 606 | CLA | C1-C2-C3 | -2.15 | 122.33 | 126.04 |
| 23 | d | 403 | CLA | C4D-C3D-CAD | -2.15 | 107.27 | 108.47 |
| 23 | B | 612 | CLA | C16-C15-C13 | -2.15 | 108.98 | 115.92 |
| 23 | a | 406 | CLA | OBD-CAD-C3D | 2.15 | 131.54 | 127.98 |
| 26 | d | 406 | PL9 | C11-C9-C8 | -2.14 | 116.78 | 121.12 |
| 23 | a | 405 | CLA | O1D-CGD-CBD | 2.14 | 128.87 | 124.48 |
| 23 | b | 603 | CLA | C3C-C4C-NC | -2.14 | 108.17 | 110.57 |
| 27 | F | 101 | SQD | C1-C2-C3 | -2.14 | 105.53 | 110.00 |
| 25 | T | 101 | BCR | C1-C6-C5 | -2.14 | 119.60 | 122.61 |
| 23 | b | 607 | CLA | C2A-C1A-CHA | 2.14 | 127.60 | 123.86 |
| 25 | T | 101 | BCR | C33-C5-C6 | -2.14 | 122.12 | 124.53 |
| 25 | t | 101 | BCR | C3-C4-C5 | -2.14 | 110.26 | 114.08 |
| 29 | A | 413 | LHG | C5-O7-C7 | -2.14 | 112.53 | 117.79 |
| 23 | C | 502 | CLA | CGD-CBD-CAD | -2.14 | 103.81 | 110.73 |
| 33 | c | 519 | LMG | O8-C28-O10 | -2.14 | 118.20 | 123.59 |
| 23 | b | 612 | CLA | C11-C12-C13 | -2.14 | 109.01 | 115.92 |
| 23 | C | 514 | CLA | C1B-CHB-C4A | -2.14 | 125.89 | 130.12 |
| 25 | c | 515 | BCR | C15-C16-C17 | -2.14 | 119.10 | 123.47 |
| 23 | C | 507 | CLA | C1D-CHD-C4C | 2.13 | 125.38 | 122.56 |
| 23 | B | 611 | CLA | C11-C10-C8 | -2.13 | 109.02 | 115.92 |
| 28 | C | 516 | DGD | C3E-C4E-C5E | -2.13 | 106.43 | 110.24 |
| 33 | C | 501 | LMG | C36-C35-C34 | -2.13 | 103.60 | 114.42 |
| 23 | b | 616 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 23 | B | 614 | CLA | C3B-C4B-NB | -2.13 | 106.45 | 109.21 |
| 28 | c | 517 | DGD | C3D-C4D-C5D | -2.13 | 106.44 | 110.24 |
| 23 | B | 609 | CLA | O1D-CGD-CBD | 2.13 | 128.84 | 124.48 |
| 23 | B | 609 | CLA | CHD-C4C-C3C | -2.13 | 121.71 | 124.84 |
| 23 | c | 513 | CLA | C1B-CHB-C4A | -2.13 | 125.91 | 130.12 |
| 29 | L | 101 | LHG | C20-C19-C18 | -2.12 | 103.64 | 114.42 |
| 28 | C | 516 | DGD | O3D-C3D-C4D | -2.12 | 105.44 | 110.35 |
| 26 | a | 410 | PL9 | C7-C8-C9 | -2.12 | 123.26 | 126.79 |
| 25 | B | 617 | BCR | C3-C4-C5 | -2.12 | 110.28 | 114.08 |
| 29 | d | 407 | LHG | C18-C17-C16 | -2.12 | 103.64 | 114.42 |
| 25 | K | 101 | BCR | C24-C23-C22 | -2.12 | 123.03 | 126.23 |
| 23 | C | 513 | CLA | C11-C12-C13 | -2.12 | 109.06 | 115.92 |
| 29 | l | 101 | LHG | C27-C26-C25 | -2.12 | 103.66 | 114.42 |
| 23 | B | 605 | CLA | C1-O2A-CGA | -2.12 | 110.88 | 116.44 |
| 23 | C | 512 | CLA | C4-C3-C5 | 2.12 | 118.84 | 115.27 |
| 25 | c | 515 | BCR | C8-C9-C10 | 2.12 | 122.19 | 118.94 |
| 25 | C | 520 | BCR | C2-C1-C6 | 2.12 | 113.74 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 512 | CLA | O2D-CGD-CBD | 2.12 | 115.03 | 111.27 |
| 25 | x | 102 | BCR | C37-C22-C21 | -2.12 | 119.96 | 122.92 |
| 23 | b | 616 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |
| 23 | c | 509 | CLA | C2C-C1C-NC | -2.12 | 107.99 | 109.97 |
| 26 | d | 406 | PL9 | C31-C32-C33 | -2.11 | 104.94 | 111.88 |
| 23 | b | 617 | CLA | C4D-C3D-CAD | -2.11 | 107.29 | 108.47 |
| 25 | c | 515 | BCR | C38-C26-C27 | -2.11 | 109.56 | 113.62 |
| 23 | B | 602 | CLA | O2A-CGA-O1A | -2.11 | 118.26 | 123.59 |
| 25 | t | 101 | BCR | C31-C1-C6 | 2.11 | 113.72 | 110.30 |
| 23 | C | 504 | CLA | C1B-CHB-C4A | -2.11 | 125.93 | 130.12 |
| 28 | A | 412 | DGD | O5D-C6D-C5D | -2.11 | 105.14 | 109.05 |
| 28 | a | 413 | DGD | C2G-O2G-C1B | 2.11 | 122.99 | 117.79 |
| 28 | C | 517 | DGD | CBB-CAB-C9B | -2.11 | 103.71 | 114.42 |
| 23 | C | 508 | CLA | CHD-C4C-NC | 2.11 | 127.53 | 124.20 |
| 23 | b | 610 | CLA | O2A-CGA-O1A | -2.11 | 118.27 | 123.59 |
| 23 | b | 608 | CLA | CMB-C2B-C3B | 2.11 | 128.63 | 124.68 |
| 23 | c | 510 | CLA | C9-C8-C10 | 2.11 | 118.93 | 111.29 |
| 25 | b | 619 | BCR | C11-C10-C9 | -2.11 | 124.30 | 127.31 |
| 25 | x | 102 | BCR | C33-C5-C6 | -2.11 | 122.16 | 124.53 |
| 23 | c | 506 | CLA | CMC-C2C-C1C | 2.11 | 128.25 | 125.04 |
| 25 | c | 515 | BCR | C1-C6-C5 | -2.11 | 119.64 | 122.61 |
| 24 | d | 401 | PHO | C1-C2-C3 | -2.11 | 122.40 | 126.04 |
| 23 | A | 405 | CLA | CAC-C3C-C2C | -2.10 | 123.93 | 127.53 |
| 23 | C | 514 | CLA | OBD-CAD-CBD | -2.10 | 122.89 | 125.89 |
| 23 | b | 615 | CLA | OBD-CAD-C3D | 2.10 | 131.47 | 127.98 |
| 23 | C | 512 | CLA | OBD-CAD-C3D | 2.10 | 131.47 | 127.98 |
| 23 | B | 606 | CLA | CMA-C3A-C4A | -2.10 | 106.14 | 111.77 |
| 23 | B | 605 | CLA | C1B-CHB-C4A | -2.10 | 125.97 | 130.12 |
| 26 | D | 406 | PL9 | C42-C43-C44 | -2.09 | 122.62 | 127.66 |
| 26 | A | 409 | PL9 | C40-C39-C41 | 2.09 | 118.79 | 115.27 |
| 23 | B | 612 | CLA | CMB-C2B-C3B | 2.09 | 128.59 | 124.68 |
| 25 | B | 617 | BCR | C35-C13-C14 | -2.09 | 120.00 | 122.92 |
| 23 | c | 506 | CLA | CHA-C1A-NA | -2.09 | 121.61 | 126.40 |
| 33 | m | 101 | LMG | O8-C28-O10 | -2.09 | 118.32 | 123.59 |
| 27 | f | 101 | SQD | C46-C45-C44 | -2.09 | 106.85 | 111.79 |
| 23 | C | 511 | CLA | CMB-C2B-C3B | 2.09 | 128.58 | 124.68 |
| 25 | C | 515 | BCR | C38-C26-C27 | -2.09 | 109.61 | 113.62 |
| 33 | C | 501 | LMG | C9-C8-C7 | -2.09 | 106.85 | 111.79 |
| 33 | c | 522 | LMG | O8-C28-O10 | -2.09 | 118.33 | 123.59 |
| 23 | C | 504 | CLA | OBD-CAD-CBD | -2.09 | 122.92 | 125.89 |
| 25 | b | 618 | BCR | C38-C26-C25 | -2.08 | 122.19 | 124.53 |
| 23 | c | 501 | CLA | CMC-C2C-C1C | 2.08 | 128.21 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 505 | CLA | CMC-C2C-C1C | 2.08 | 128.21 | 125.04 |
| 29 | l | 101 | LHG | C11-C10-C9 | -2.08 | 103.86 | 114.42 |
| 28 | c | 516 | DGD | C1D-C2D-C3D | -2.08 | 105.66 | 110.00 |
| 28 | c | 518 | DGD | C7A-C6A-C5A | -2.08 | 103.87 | 114.42 |
| 23 | b | 606 | CLA | CHD-C4C-C3C | -2.08 | 121.78 | 124.84 |
| 25 | t | 101 | BCR | C15-C16-C17 | -2.08 | 119.22 | 123.47 |
| 33 | C | 519 | LMG | O6-C1-O1 | -2.08 | 105.05 | 109.97 |
| 33 | c | 519 | LMG | C4-C3-C2 | -2.08 | 107.19 | 110.82 |
| 28 | h | 101 | DGD | O6E-C5E-C4E | 2.08 | 113.47 | 109.69 |
| 27 | F | 101 | SQD | C46-C45-C44 | -2.08 | 106.79 | 113.70 |
| 26 | D | 406 | PL9 | C7-C8-C9 | -2.08 | 123.34 | 126.79 |
| 25 | t | 101 | BCR | C35-C13-C12 | 2.08 | 121.35 | 118.08 |
| 25 | x | 102 | BCR | C16-C15-C14 | -2.07 | 119.23 | 123.47 |
| 33 | m | 101 | LMG | C9-C8-C7 | -2.07 | 106.89 | 111.79 |
| 23 | B | 608 | CLA | CMD-C2D-C3D | 2.07 | 128.56 | 124.68 |
| 28 | C | 518 | DGD | C1D-C2D-C3D | -2.07 | 105.68 | 110.00 |
| 27 | B | 621 | SQD | O47-C45-C46 | 2.07 | 115.90 | 108.40 |
| 23 | C | 504 | CLA | CHC-C1C-C2C | -2.07 | 121.00 | 126.72 |
| 25 | C | 515 | BCR | C30-C25-C26 | -2.07 | 119.70 | 122.61 |
| 23 | C | 504 | CLA | C5-C3-C2 | -2.07 | 116.93 | 121.12 |
| 23 | b | 611 | CLA | CMB-C2B-C3B | 2.07 | 128.55 | 124.68 |
| 27 | B | 621 | SQD | O48-C23-C24 | 2.07 | 118.40 | 111.91 |
| 25 | c | 521 | BCR | C38-C26-C27 | -2.07 | 109.64 | 113.62 |
| 23 | b | 604 | CLA | O2A-C1-C2 | -2.07 | 103.20 | 108.64 |
| 23 | b | 614 | CLA | C5-C3-C2 | -2.07 | 116.94 | 121.12 |
| 23 | B | 603 | CLA | C4-C3-C2 | -2.07 | 118.38 | 123.68 |
| 23 | D | 402 | CLA | CMB-C2B-C1B | -2.07 | 125.29 | 128.46 |
| 25 | t | 101 | BCR | C30-C25-C26 | -2.07 | 119.70 | 122.61 |
| 23 | C | 513 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 29 | D | 408 | LHG | C11-C10-C9 | -2.06 | 103.95 | 114.42 |
| 23 | D | 404 | CLA | O2D-CGD-CBD | 2.06 | 114.93 | 111.27 |
| 23 | c | 509 | CLA | C3B-C4B-NB | -2.06 | 106.55 | 109.21 |
| 23 | B | 610 | CLA | CHD-C4C-NC | 2.06 | 127.45 | 124.20 |
| 23 | C | 510 | CLA | C1B-CHB-C4A | -2.06 | 126.03 | 130.12 |
| 23 | C | 504 | CLA | CMB-C2B-C3B | 2.06 | 128.53 | 124.68 |
| 23 | b | 608 | CLA | O2A-C1-C2 | -2.06 | 103.22 | 108.64 |
| 23 | b | 611 | CLA | O1D-CGD-CBD | 2.06 | 128.70 | 124.48 |
| 33 | M | 101 | LMG | O7-C10-O9 | -2.06 | 118.72 | 123.70 |
| 26 | A | 409 | PL9 | C31-C32-C33 | -2.06 | 105.11 | 111.88 |
| 23 | c | 511 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 27 | a | 412 | SQD | O6-C44-C45 | -2.06 | 106.32 | 111.78 |
| 28 | c | 518 | DGD | O6E-C5E-C6E | -2.06 | 101.32 | 106.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | c | 513 | CLA | C16-C15-C13 | -2.06 | 109.27 | 115.92 |
| 25 | D | 405 | BCR | C16-C15-C14 | -2.06 | 119.26 | 123.47 |
| 23 | B | 606 | CLA | C2C-C1C-NC | 2.06 | 111.90 | 109.97 |
| 23 | b | 612 | CLA | C5-C3-C2 | 2.06 | 125.28 | 121.12 |
| 23 | b | 612 | CLA | CMB-C2B-C3B | 2.06 | 128.52 | 124.68 |
| 25 | A | 408 | BCR | C11-C10-C9 | -2.05 | 124.38 | 127.31 |
| 29 | D | 409 | LHG | O8-C6-C5 | -2.05 | 102.46 | 108.43 |
| 28 | C | 518 | DGD | C5B-C4B-C3B | -2.05 | 104.01 | 114.42 |
| 23 | B | 601 | CLA | O2D-CGD-CBD | 2.05 | 114.91 | 111.27 |
| 23 | b | 616 | CLA | CHD-C4C-C3C | -2.05 | 121.83 | 124.84 |
| 23 | B | 607 | CLA | C2A-C1A-CHA | 2.05 | 127.44 | 123.86 |
| 23 | a | 408 | CLA | OBD-CAD-C3D | 2.05 | 131.38 | 127.98 |
| 23 | c | 504 | CLA | O2D-CGD-O1D | -2.05 | 119.83 | 123.84 |
| 25 | b | 618 | BCR | C32-C1-C6 | -2.05 | 106.98 | 110.30 |
| 29 | d | 407 | LHG | O8-C23-O10 | -2.05 | 118.42 | 123.59 |
| 23 | B | 609 | CLA | CHB-C4A-NA | 2.05 | 127.34 | 124.51 |
| 23 | B | 610 | CLA | CAA-CBA-CGA | -2.05 | 107.27 | 113.25 |
| 23 | B | 612 | CLA | CGD-CBD-CAD | 2.05 | 117.36 | 110.73 |
| 25 | d | 405 | BCR | C2-C1-C6 | 2.05 | 113.63 | 110.48 |
| 28 | C | 517 | DGD | O3D-C3D-C4D | -2.05 | 105.62 | 110.35 |
| 25 | B | 617 | BCR | C15-C14-C13 | -2.04 | 124.39 | 127.31 |
| 23 | c | 512 | CLA | CMB-C2B-C1B | -2.04 | 125.32 | 128.46 |
| 23 | D | 402 | CLA | C7-C6-C5 | -2.04 | 107.81 | 113.36 |
| 23 | b | 604 | CLA | CHB-C4A-NA | 2.04 | 127.34 | 124.51 |
| 23 | C | 513 | CLA | C4A-NA-C1A | 2.04 | 107.62 | 106.71 |
| 23 | b | 603 | CLA | C1D-CHD-C4C | 2.04 | 125.25 | 122.56 |
| 24 | d | 401 | PHO | CAA-C2A-C3A | -2.04 | 107.19 | 112.78 |
| 23 | b | 615 | CLA | CHC-C1C-NC | 2.04 | 127.30 | 124.20 |
| 23 | b | 610 | CLA | CHD-C4C-NC | 2.04 | 127.42 | 124.20 |
| 23 | B | 606 | CLA | O2A-CGA-O1A | -2.04 | 118.45 | 123.59 |
| 23 | b | 608 | CLA | O2D-CGD-O1D | -2.04 | 119.85 | 123.84 |
| 25 | B | 617 | BCR | C33-C5-C6 | -2.04 | 122.24 | 124.53 |
| 34 | E | 103 | HEM | CMB-C2B-C3B | 2.04 | 128.49 | 124.68 |
| 26 | a | 410 | PL9 | C36-C34-C33 | -2.04 | 117.00 | 121.12 |
| 25 | c | 515 | BCR | C4-C5-C6 | 2.04 | 125.69 | 122.73 |
| 23 | c | 509 | CLA | C3A-C2A-C1A | 2.03 | 104.39 | 101.34 |
| 29 | D | 409 | LHG | C6-C5-C4 | 2.03 | 116.60 | 111.79 |
| 23 | b | 611 | CLA | CAC-C3C-C4C | 2.03 | 127.45 | 124.81 |
| 28 | C | 518 | DGD | C8B-C7B-C6B | -2.03 | 104.10 | 114.42 |
| 23 | c | 511 | CLA | C3B-C4B-NB | -2.03 | 106.58 | 109.21 |
| 23 | b | 617 | CLA | O2D-CGD-CBD | 2.03 | 114.88 | 111.27 |
| 25 | b | 619 | BCR | C37-C22-C21 | -2.03 | 120.08 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | c | 513 | CLA | C1D-CHD-C4C | 2.03 | 125.24 | 122.56 |
| 23 | C | 509 | CLA | C1B-CHB-C4A | -2.03 | 126.09 | 130.12 |
| 23 | b | 615 | CLA | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 28 | C | 518 | DGD | C3G-C2G-C1G | -2.03 | 106.98 | 111.79 |
| 23 | B | 605 | CLA | CMB-C2B-C1B | -2.03 | 125.34 | 128.46 |
| 23 | c | 509 | CLA | O2A-CGA-CBA | 2.03 | 118.28 | 111.91 |
| 23 | b | 611 | CLA | CMB-C2B-C1B | -2.03 | 125.34 | 128.46 |
| 28 | C | 516 | DGD | CCB-CBB-CAB | -2.03 | 104.13 | 114.42 |
| 26 | d | 406 | PL9 | C41-C39-C38 | -2.03 | 117.02 | 121.12 |
| 23 | C | 508 | CLA | CHB-C4A-NA | 2.02 | 127.31 | 124.51 |
| 23 | C | 511 | CLA | O2D-CGD-CBD | 2.02 | 114.86 | 111.27 |
| 23 | B | 608 | CLA | C6-C7-C8 | -2.02 | 109.38 | 115.92 |
| 23 | C | 502 | CLA | C3D-CAD-CBD | -2.02 | 104.94 | 107.61 |
| 25 | K | 101 | BCR | C15-C16-C17 | -2.02 | 119.33 | 123.47 |
| 23 | B | 601 | CLA | OBD-CAD-C3D | 2.02 | 131.34 | 127.98 |
| 33 | C | 519 | LMG | O2-C2-C1 | -2.02 | 105.14 | 110.05 |
| 27 | b | 601 | SQD | O4-C4-C3 | -2.02 | 105.68 | 110.35 |
| 23 | b | 603 | CLA | CMC-C2C-C3C | 2.02 | 131.60 | 126.12 |
| 28 | c | 516 | DGD | O3G-C1D-C2D | -2.02 | 105.15 | 108.30 |
| 25 | x | 102 | BCR | C7-C8-C9 | -2.02 | 123.19 | 126.23 |
| 24 | A | 406 | PHO | C2B-C1B-NB | -2.02 | 106.75 | 109.79 |
| 33 | C | 519 | LMG | C38-C37-C36 | -2.02 | 104.18 | 114.42 |
| 25 | x | 102 | BCR | C38-C26-C27 | -2.02 | 109.74 | 113.62 |
| 23 | C | 507 | CLA | CMA-C3A-C4A | -2.02 | 106.35 | 111.77 |
| 23 | c | 506 | CLA | CMB-C2B-C1B | -2.02 | 125.36 | 128.46 |
| 29 | A | 413 | LHG | C11-C10-C9 | -2.02 | 104.19 | 114.42 |
| 23 | B | 613 | CLA | C16-C15-C13 | -2.02 | 109.41 | 115.92 |
| 23 | c | 513 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 23 | C | 509 | CLA | CMC-C2C-C3C | 2.01 | 131.58 | 126.12 |
| 23 | C | 502 | CLA | CMB-C2B-C1B | -2.01 | 125.37 | 128.46 |
| 23 | a | 408 | CLA | CHA-C1A-NA | -2.01 | 121.79 | 126.40 |
| 23 | c | 508 | CLA | O2D-CGD-CBD | 2.01 | 114.84 | 111.27 |
| 28 | c | 516 | DGD | O1G-C1A-C2A | -2.01 | 105.59 | 111.91 |
| 25 | Z | 101 | BCR | C8-C9-C10 | 2.01 | 122.03 | 118.94 |
| 26 | d | 406 | PL9 | C30-C29-C28 | -2.01 | 118.52 | 123.68 |
| 23 | c | 503 | CLA | C3C-C4C-NC | -2.01 | 108.32 | 110.57 |
| 29 | D | 408 | LHG | C27-C26-C25 | -2.01 | 104.23 | 114.42 |
| 26 | D | 406 | PL9 | C31-C29-C28 | 2.01 | 125.18 | 121.12 |
| 23 | A | 404 | CLA | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 29 | e | 101 | LHG | O10-C23-C24 | -2.01 | 115.90 | 123.73 |
| 23 | c | 502 | CLA | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 28 | H | 102 | DGD | C5B-C4B-C3B | -2.01 | 104.24 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28 | c | 518 | DGD | CBB-CAB-C9B | -2.00 | 104.25 | 114.42 |
| 25 | D | 405 | BCR | C2-C1-C6 | 2.00 | 113.56 | 110.48 |
| 25 | K | 101 | BCR | C32-C1-C6 | -2.00 | 107.05 | 110.30 |
| 23 | B | 614 | CLA | CHB-C4A-NA | 2.00 | 127.28 | 124.51 |
| 23 | C | 514 | CLA | CAC-C3C-C4C | 2.00 | 127.41 | 124.81 |
| 29 | e | 101 | LHG | C18-C17-C16 | -2.00 | 104.26 | 114.42 |
| 33 | c | 519 | LMG | C31-C30-C29 | -2.00 | 105.99 | 113.19 |
| 33 | D | 410 | LMG | C35-C34-C33 | -2.00 | 104.26 | 114.42 |
| 33 | C | 519 | LMG | C33-C32-C31 | -2.00 | 104.27 | 114.42 |
| 23 | b | 609 | CLA | O2D-CGD-CBD | 2.00 | 114.82 | 111.27 |

All (188) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | A | 404 | CLA | NC |
| 23 | A | 404 | CLA | NA |
| 23 | A | 404 | CLA | ND |
| 23 | A | 405 | CLA | NC |
| 23 | A | 405 | CLA | NA |
| 23 | A | 405 | CLA | ND |
| 23 | A | 407 | CLA | NC |
| 23 | A | 407 | CLA | NA |
| 23 | A | 407 | CLA | ND |
| 23 | B | 601 | CLA | NC |
| 23 | B | 601 | CLA | NA |
| 23 | B | 601 | CLA | ND |
| 23 | B | 602 | CLA | NC |
| 23 | B | 602 | CLA | NA |
| 23 | B | 602 | CLA | ND |
| 23 | B | 603 | CLA | NC |
| 23 | B | 603 | CLA | NA |
| 23 | B | 603 | CLA | ND |
| 23 | B | 604 | CLA | NC |
| 23 | B | 604 | CLA | ND |
| 23 | B | 605 | CLA | NC |
| 23 | B | 605 | CLA | NA |
| 23 | B | 605 | CLA | ND |
| 23 | B | 606 | CLA | NC |
| 23 | B | 606 | CLA | NA |
| 23 | B | 606 | CLA | ND |
| 23 | B | 607 | CLA | NC |
| 23 | B | 607 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | B | 607 | CLA | ND |
| 23 | B | 608 | CLA | NC |
| 23 | B | 608 | CLA | NA |
| 23 | B | 609 | CLA | NC |
| 23 | B | 609 | CLA | NA |
| 23 | B | 610 | CLA | NC |
| 23 | B | 610 | CLA | NA |
| 23 | B | 610 | CLA | ND |
| 23 | B | 611 | CLA | NC |
| 23 | B | 611 | CLA | NA |
| 23 | B | 611 | CLA | ND |
| 23 | B | 612 | CLA | NC |
| 23 | B | 612 | CLA | NA |
| 23 | B | 612 | CLA | ND |
| 23 | B | 613 | CLA | NC |
| 23 | B | 613 | CLA | NA |
| 23 | B | 613 | CLA | ND |
| 23 | B | 614 | CLA | NC |
| 23 | B | 614 | CLA | NA |
| 23 | B | 614 | CLA | ND |
| 23 | B | 615 | CLA | NC |
| 23 | B | 615 | CLA | NA |
| 23 | B | 615 | CLA | ND |
| 23 | B | 616 | CLA | NC |
| 23 | B | 616 | CLA | NA |
| 23 | B | 616 | CLA | ND |
| 23 | C | 502 | CLA | NC |
| 23 | C | 502 | CLA | NA |
| 23 | C | 502 | CLA | ND |
| 23 | C | 503 | CLA | NC |
| 23 | C | 503 | CLA | NA |
| 23 | C | 503 | CLA | ND |
| 23 | C | 504 | CLA | NC |
| 23 | C | 505 | CLA | NC |
| 23 | C | 505 | CLA | NA |
| 23 | C | 505 | CLA | ND |
| 23 | C | 506 | CLA | NC |
| 23 | C | 506 | CLA | NA |
| 23 | C | 506 | CLA | ND |
| 23 | C | 507 | CLA | NC |
| 23 | C | 508 | CLA | NC |
| 23 | C | 508 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | C | 508 | CLA | ND |
| 23 | C | 509 | CLA | NC |
| 23 | C | 509 | CLA | NA |
| 23 | C | 509 | CLA | ND |
| 23 | C | 510 | CLA | NC |
| 23 | C | 510 | CLA | NA |
| 23 | C | 510 | CLA | ND |
| 23 | C | 511 | CLA | NC |
| 23 | C | 511 | CLA | NA |
| 23 | C | 511 | CLA | ND |
| 23 | C | 512 | CLA | NC |
| 23 | C | 512 | CLA | NA |
| 23 | C | 512 | CLA | ND |
| 23 | C | 513 | CLA | NC |
| 23 | C | 513 | CLA | NA |
| 23 | C | 513 | CLA | ND |
| 23 | C | 514 | CLA | NC |
| 23 | C | 514 | CLA | NA |
| 23 | C | 514 | CLA | ND |
| 23 | D | 402 | CLA | NA |
| 23 | D | 402 | CLA | ND |
| 23 | D | 403 | CLA | NA |
| 23 | D | 404 | CLA | NC |
| 23 | D | 404 | CLA | NA |
| 23 | a | 405 | CLA | NA |
| 23 | a | 405 | CLA | ND |
| 23 | a | 406 | CLA | NC |
| 23 | a | 406 | CLA | NA |
| 23 | a | 406 | CLA | ND |
| 23 | a | 408 | CLA | NC |
| 23 | a | 408 | CLA | NA |
| 23 | a | 408 | CLA | ND |
| 23 | b | 602 | CLA | NA |
| 23 | b | 602 | CLA | ND |
| 23 | b | 603 | CLA | NC |
| 23 | b | 603 | CLA | NA |
| 23 | b | 603 | CLA | ND |
| 23 | b | 604 | CLA | NC |
| 23 | b | 604 | CLA | NA |
| 23 | b | 604 | CLA | ND |
| 23 | b | 605 | CLA | NC |
| 23 | b | 605 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | b | 605 | CLA | ND |
| 23 | b | 606 | CLA | NC |
| 23 | b | 606 | CLA | NA |
| 23 | b | 606 | CLA | ND |
| 23 | b | 607 | CLA | NC |
| 23 | b | 607 | CLA | NA |
| 23 | b | 607 | CLA | ND |
| 23 | b | 608 | CLA | NC |
| 23 | b | 608 | CLA | NA |
| 23 | b | 608 | CLA | ND |
| 23 | b | 609 | CLA | NA |
| 23 | b | 609 | CLA | ND |
| 23 | b | 610 | CLA | NC |
| 23 | b | 610 | CLA | ND |
| 23 | b | 611 | CLA | NC |
| 23 | b | 611 | CLA | NA |
| 23 | b | 611 | CLA | ND |
| 23 | b | 612 | CLA | NC |
| 23 | b | 612 | CLA | NA |
| 23 | b | 612 | CLA | ND |
| 23 | b | 613 | CLA | NC |
| 23 | b | 613 | CLA | NA |
| 23 | b | 613 | CLA | ND |
| 23 | b | 614 | CLA | NC |
| 23 | b | 614 | CLA | NA |
| 23 | b | 614 | CLA | ND |
| 23 | b | 615 | CLA | NC |
| 23 | b | 615 | CLA | NA |
| 23 | b | 615 | CLA | ND |
| 23 | b | 616 | CLA | NC |
| 23 | b | 616 | CLA | NA |
| 23 | b | 616 | CLA | ND |
| 23 | b | 617 | CLA | NC |
| 23 | b | 617 | CLA | NA |
| 23 | b | 617 | CLA | ND |
| 23 | c | 501 | CLA | NC |
| 23 | c | 501 | CLA | NA |
| 23 | c | 501 | CLA | ND |
| 23 | c | 502 | CLA | NC |
| 23 | c | 502 | CLA | NA |
| 23 | c | 503 | CLA | NC |
| 23 | c | 503 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | c | 503 | CLA | ND |
| 23 | c | 504 | CLA | NC |
| 23 | c | 504 | CLA | NA |
| 23 | c | 504 | CLA | ND |
| 23 | c | 505 | CLA | NA |
| 23 | c | 505 | CLA | ND |
| 23 | c | 506 | CLA | NA |
| 23 | c | 506 | CLA | ND |
| 23 | c | 507 | CLA | NC |
| 23 | c | 507 | CLA | NA |
| 23 | c | 507 | CLA | ND |
| 23 | c | 508 | CLA | NA |
| 23 | c | 509 | CLA | NC |
| 23 | c | 509 | CLA | NA |
| 23 | c | 509 | CLA | ND |
| 23 | c | 510 | CLA | NC |
| 23 | c | 510 | CLA | NA |
| 23 | c | 510 | CLA | ND |
| 23 | c | 511 | CLA | NC |
| 23 | c | 511 | CLA | NA |
| 23 | c | 511 | CLA | ND |
| 23 | c | 512 | CLA | NC |
| 23 | c | 512 | CLA | NA |
| 23 | c | 512 | CLA | ND |
| 23 | c | 513 | CLA | NC |
| 23 | c | 513 | CLA | NA |
| 23 | c | 513 | CLA | ND |
| 23 | d | 402 | CLA | NC |
| 23 | d | 402 | CLA | NA |
| 23 | d | 402 | CLA | ND |
| 23 | d | 403 | CLA | NA |
| 23 | d | 404 | CLA | NC |
| 23 | d | 404 | CLA | NA |
| 23 | d | 404 | CLA | ND |

All (1732) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | A | 405 | CLA | CHA-CBD-CGD-O1D |
| 23 | A | 405 | CLA | CHA-CBD-CGD-O2D |
| 23 | A | 407 | CLA | C2-C3-C5-C6 |
| 23 | A | 407 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 601 | CLA | CBD-CGD-O2D-CED |
| 23 | B | 605 | CLA | C2-C3-C5-C6 |
| 23 | B | 605 | CLA | C4-C3-C5-C6 |
| 23 | B | 606 | CLA | CHA-CBD-CGD-O1D |
| 23 | B | 606 | CLA | CHA-CBD-CGD-O2D |
| 23 | B | 614 | CLA | CAD-CBD-CGD-O1D |
| 23 | B | 614 | CLA | CAD-CBD-CGD-O2D |
| 23 | C | 503 | CLA | CHA-CBD-CGD-O1D |
| 23 | C | 505 | CLA | C4-C3-C5-C6 |
| 23 | C | 509 | CLA | CHA-CBD-CGD-O1D |
| 23 | C | 509 | CLA | CHA-CBD-CGD-O2D |
| 23 | D | 402 | CLA | CHA-CBD-CGD-O1D |
| 23 | D | 402 | CLA | CHA-CBD-CGD-O2D |
| 23 | D | 403 | CLA | C12-C13-C15-C16 |
| 23 | b | 602 | CLA | C1A-C2A-CAA-CBA |
| 23 | b | 602 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 607 | CLA | C2A-CAA-CBA-CGA |
| 23 | b | 607 | CLA | CHA-CBD-CGD-O1D |
| 23 | b | 607 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 607 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 608 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 615 | CLA | CAD-CBD-CGD-O1D |
| 23 | b | 615 | CLA | CAD-CBD-CGD-O2D |
| 23 | c | 502 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 503 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 506 | CLA | C2-C3-C5-C6 |
| 23 | c | 506 | CLA | C4-C3-C5-C6 |
| 23 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 23 | c | 510 | CLA | C11-C10-C8-C9 |
| 23 | c | 512 | CLA | C1A-C2A-CAA-CBA |
| 23 | c | 512 | CLA | C6-C7-C8-C9 |
| 24 | a | 407 | PHO | O2A-C1-C2-C3 |
| 25 | A | 408 | BCR | C7-C8-C9-C34 |
| 25 | A | 408 | BCR | C20-C21-C22-C37 |
| 25 | B | 617 | BCR | C16-C17-C18-C36 |
| 25 | B | 618 | BCR | C35-C13-C14-C15 |
| 25 | B | 618 | BCR | C16-C17-C18-C36 |
| 25 | B | 619 | BCR | C11-C10-C9-C8 |
| 25 | C | 515 | BCR | C11-C10-C9-C34 |
| 25 | C | 515 | BCR | C11-C12-C13-C14 |
| 25 | C | 515 | BCR | C11-C12-C13-C35 |
| 25 | C | 520 | BCR | C16-C17-C18-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | C | 520 | BCR | C18-C19-C20-C21 |
| 25 | C | 520 | BCR | C20-C21-C22-C37 |
| 25 | D | 405 | BCR | C37-C22-C23-C24 |
| 25 | D | 405 | BCR | C23-C24-C25-C26 |
| 25 | H | 101 | BCR | C11-C12-C13-C35 |
| 25 | K | 101 | BCR | C7-C8-C9-C34 |
| 25 | K | 101 | BCR | C11-C12-C13-C35 |
| 25 | K | 101 | BCR | C17-C18-C19-C20 |
| 25 | K | 101 | BCR | C21-C22-C23-C24 |
| 25 | T | 101 | BCR | C20-C21-C22-C23 |
| 25 | T | 101 | BCR | C20-C21-C22-C37 |
| 25 | Z | 101 | BCR | C7-C8-C9-C34 |
| 25 | Z | 101 | BCR | C10-C11-C12-C13 |
| 25 | Z | 101 | BCR | C11-C12-C13-C35 |
| 25 | Z | 101 | BCR | C16-C17-C18-C19 |
| 25 | Z | 101 | BCR | C16-C17-C18-C36 |
| 25 | b | 619 | BCR | C7-C8-C9-C34 |
| 25 | b | 619 | BCR | C11-C10-C9-C8 |
| 25 | b | 619 | BCR | C11-C12-C13-C14 |
| 25 | b | 619 | BCR | C11-C12-C13-C35 |
| 25 | b | 619 | BCR | C20-C21-C22-C37 |
| 25 | b | 619 | BCR | C23-C24-C25-C30 |
| 25 | b | 620 | BCR | C11-C12-C13-C14 |
| 25 | b | 620 | BCR | C11-C12-C13-C35 |
| 25 | b | 620 | BCR | C37-C22-C23-C24 |
| 25 | c | 514 | BCR | C7-C8-C9-C34 |
| 25 | c | 514 | BCR | C11-C12-C13-C35 |
| 25 | c | 514 | BCR | C35-C13-C14-C15 |
| 25 | c | 514 | BCR | C18-C19-C20-C21 |
| 25 | c | 514 | BCR | C20-C21-C22-C37 |
| 25 | c | 515 | BCR | C35-C13-C14-C15 |
| 25 | c | 515 | BCR | C20-C21-C22-C37 |
| 25 | c | 521 | BCR | C11-C12-C13-C35 |
| 25 | c | 521 | BCR | C17-C18-C19-C20 |
| 25 | c | 521 | BCR | C36-C18-C19-C20 |
| 25 | d | 405 | BCR | C6-C7-C8-C9 |
| 25 | d | 405 | BCR | C7-C8-C9-C34 |
| 25 | d | 405 | BCR | C11-C12-C13-C35 |
| 25 | d | 405 | BCR | C20-C21-C22-C37 |
| 25 | d | 405 | BCR | C37-C22-C23-C24 |
| 25 | d | 405 | BCR | C22-C23-C24-C25 |
| 25 | k | 101 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | k | 101 | BCR | C11-C10-C9-C8 |
| 25 | k | 101 | BCR | C11-C12-C13-C35 |
| 25 | t | 101 | BCR | C12-C13-C14-C15 |
| 25 | t | 101 | BCR | C35-C13-C14-C15 |
| 25 | t | 101 | BCR | C14-C15-C16-C17 |
| 25 | t | 101 | BCR | C20-C21-C22-C37 |
| 25 | x | 102 | BCR | C7-C8-C9-C34 |
| 25 | x | 102 | BCR | C11-C12-C13-C35 |
| 25 | x | 102 | BCR | C37-C22-C23-C24 |
| 25 | x | 102 | BCR | C23-C24-C25-C26 |
| 26 | A | 409 | PL9 | C9-C11-C12-C13 |
| 26 | A | 409 | PL9 | C12-C13-C14-C16 |
| 26 | A | 409 | PL9 | C18-C19-C21-C22 |
| 26 | A | 409 | PL9 | C22-C23-C24-C25 |
| 26 | A | 409 | PL9 | C22-C23-C24-C26 |
| 26 | A | 409 | PL9 | C32-C33-C34-C36 |
| 26 | A | 409 | PL9 | C37-C38-C39-C40 |
| 26 | A | 409 | PL9 | C37-C38-C39-C41 |
| 26 | D | 406 | PL9 | C32-C33-C34-C35 |
| 26 | D | 406 | PL9 | C32-C33-C34-C36 |
| 26 | D | 406 | PL9 | C47-C48-C49-C50 |
| 26 | a | 410 | PL9 | C22-C23-C24-C25 |
| 26 | a | 410 | PL9 | C22-C23-C24-C26 |
| 26 | a | 410 | PL9 | C24-C26-C27-C28 |
| 26 | a | 410 | PL9 | C32-C33-C34-C36 |
| 26 | a | 410 | PL9 | C33-C34-C36-C37 |
| 26 | a | 410 | PL9 | C34-C36-C37-C38 |
| 26 | a | 410 | PL9 | C42-C43-C44-C46 |
| 26 | d | 406 | PL9 | C32-C33-C34-C35 |
| 26 | d | 406 | PL9 | C37-C38-C39-C40 |
| 26 | d | 406 | PL9 | C38-C39-C41-C42 |
| 26 | d | 406 | PL9 | C42-C43-C44-C45 |
| 26 | d | 406 | PL9 | C44-C46-C47-C48 |
| 27 | A | 410 | SQD | C5-C6-S-O7 |
| 27 | B | 621 | SQD | O5-C1-O6-C44 |
| 27 | B | 621 | SQD | O6-C44-C45-O47 |
| 27 | B | 621 | SQD | O49-C7-O47-C45 |
| 27 | B | 621 | SQD | C8-C7-O47-C45 |
| 27 | a | 411 | SQD | O47-C45-C46-O48 |
| 27 | a | 412 | SQD | O49-C7-O47-C45 |
| 27 | a | 412 | SQD | O10-C23-O48-C46 |
| 27 | f | 101 | SQD | O5-C1-O6-C44 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | A | 412 | DGD | C2B-C1B-O2G-C2G |
| 28 | A | 412 | DGD | O1B-C1B-O2G-C2G |
| 28 | A | 412 | DGD | O2G-C2G-C3G-O3G |
| 28 | a | 413 | DGD | O1A-C1A-O1G-C1G |
| 28 | a | 413 | DGD | O2G-C2G-C3G-O3G |
| 29 | A | 413 | LHG | O1-C1-C2-C3 |
| 29 | A | 413 | LHG | C3-O3-P-O5 |
| 29 | A | 413 | LHG | C3-O3-P-O6 |
| 29 | D | 408 | LHG | O1-C1-C2-C3 |
| 29 | D | 408 | LHG | O2-C2-C3-O3 |
| 29 | D | 408 | LHG | C3-O3-P-O5 |
| 29 | D | 408 | LHG | C4-O6-P-O4 |
| 29 | D | 409 | LHG | C3-O3-P-O5 |
| 29 | D | 409 | LHG | C3-O3-P-O6 |
| 29 | E | 101 | LHG | O1-C1-C2-C3 |
| 29 | E | 101 | LHG | C4-O6-P-O4 |
| 29 | E | 101 | LHG | O10-C23-O8-C6 |
| 29 | L | 101 | LHG | C4-O6-P-O4 |
| 29 | L | 101 | LHG | C4-O6-P-O5 |
| 29 | d | 407 | LHG | O1-C1-C2-C3 |
| 29 | d | 407 | LHG | C3-O3-P-O4 |
| 29 | d | 407 | LHG | C3-O3-P-O5 |
| 29 | d | 407 | LHG | C3-O3-P-O6 |
| 29 | d | 408 | LHG | C4-O6-P-O4 |
| 29 | d | 408 | LHG | C4-O6-P-O5 |
| 29 | e | 101 | LHG | O1-C1-C2-C3 |
| 29 | e | 101 | LHG | C3-O3-P-O5 |
| 29 | e | 101 | LHG | C4-O6-P-O3 |
| 29 | e | 101 | LHG | C4-O6-P-O4 |
| 29 | e | 101 | LHG | C4-O6-P-O5 |
| 29 | e | 101 | LHG | O10-C23-O8-C6 |
| 29 | l | 101 | LHG | C4-O6-P-O3 |
| 29 | l | 101 | LHG | C4-O6-P-O5 |
| 33 | C | 501 | LMG | O6-C1-O1-C7 |
| 33 | C | 501 | LMG | O9-C10-O7-C8 |
| 33 | C | 519 | LMG | C11-C10-O7-C8 |
| 33 | D | 410 | LMG | O1-C7-C8-C9 |
| 33 | D | 410 | LMG | O1-C7-C8-O7 |
| 33 | D | 410 | LMG | C11-C10-O7-C8 |
| 33 | D | 411 | LMG | C28-C29-C30-C31 |
| 33 | b | 622 | LMG | O9-C10-O7-C8 |
| 33 | b | 622 | LMG | C11-C10-O7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | c | 524 | LMG | O6-C1-O1-C7 |
| 33 | c | 524 | LMG | O10-C28-O8-C9 |
| 33 | c | 524 | LMG | C29-C28-O8-C9 |
| 23 | C | 504 | CLA | O1D-CGD-O2D-CED |
| 23 | b | 602 | CLA | O1D-CGD-O2D-CED |
| 23 | C | 504 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 617 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 508 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 24 | d | 401 | PHO | CBD-CGD-O2D-CED |
| 23 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 23 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 27 | a | 412 | SQD | C24-C23-O48-C46 |
| 29 | E | 101 | LHG | C24-C23-O8-C6 |
| 29 | e | 101 | LHG | C24-C23-O8-C6 |
| 23 | B | 606 | CLA | CBD-CGD-O2D-CED |
| 23 | C | 502 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 613 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 511 | CLA | CBD-CGD-O2D-CED |
| 27 | F | 101 | SQD | O10-C23-O48-C46 |
| 33 | c | 522 | LMG | O10-C28-O8-C9 |
| 23 | B | 601 | CLA | O1D-CGD-O2D-CED |
| 23 | c | 503 | CLA | O1D-CGD-O2D-CED |
| 23 | b | 604 | CLA | CBD-CGD-O2D-CED |
| 28 | a | 413 | DGD | O1B-C1B-O2G-C2G |
| 33 | C | 519 | LMG | O9-C10-O7-C8 |
| 33 | D | 410 | LMG | O9-C10-O7-C8 |
| 33 | c | 522 | LMG | O9-C10-O7-C8 |
| 27 | b | 601 | SQD | O10-C23-O48-C46 |
| 23 | b | 602 | CLA | C3-C5-C6-C7 |
| 23 | b | 605 | CLA | C3-C5-C6-C7 |
| 27 | b | 601 | SQD | C24-C23-O48-C46 |
| 28 | a | 413 | DGD | C2A-C1A-O1G-C1G |
| 33 | c | 522 | LMG | C29-C28-O8-C9 |
| 27 | a | 412 | SQD | C8-C7-O47-C45 |
| 33 | C | 501 | LMG | C11-C10-O7-C8 |
| 23 | b | 607 | CLA | O1D-CGD-O2D-CED |
| 23 | b | 608 | CLA | O1D-CGD-O2D-CED |
| 23 | B | 615 | CLA | CBD-CGD-O2D-CED |
| 26 | a | 410 | PL9 | C30-C29-C31-C32 |
| 26 | d | 406 | PL9 | C40-C39-C41-C42 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 505 | CLA | C2-C3-C5-C6 |
| 23 | b | 612 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 512 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 602 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 616 | CLA | C3-C5-C6-C7 |
| 27 | F | 101 | SQD | C24-C23-O48-C46 |
| 26 | d | 406 | PL9 | C47-C48-C49-C51 |
| 26 | A | 409 | PL9 | C12-C13-C14-C15 |
| 26 | a | 410 | PL9 | C42-C43-C44-C45 |
| 23 | b | 603 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 508 | CLA | O1D-CGD-O2D-CED |
| 26 | A | 409 | PL9 | C17-C18-C19-C21 |
| 26 | d | 406 | PL9 | C32-C33-C34-C36 |
| 26 | d | 406 | PL9 | C42-C43-C44-C46 |
| 25 | c | 514 | BCR | C9-C10-C11-C12 |
| 27 | F | 101 | SQD | C44-C45-C46-O48 |
| 23 | C | 512 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 616 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 505 | CLA | CBD-CGD-O2D-CED |
| 29 | D | 409 | LHG | O2-C2-C3-O3 |
| 28 | c | 518 | DGD | O1A-C1A-O1G-C1G |
| 24 | d | 401 | PHO | O1D-CGD-O2D-CED |
| 33 | C | 501 | LMG | C28-C29-C30-C31 |
| 23 | B | 612 | CLA | C3-C5-C6-C7 |
| 23 | b | 615 | CLA | C3-C5-C6-C7 |
| 28 | h | 101 | DGD | O6E-C5E-C6E-O5E |
| 33 | C | 501 | LMG | O10-C28-O8-C9 |
| 26 | A | 409 | PL9 | C47-C48-C49-C50 |
| 26 | a | 410 | PL9 | C47-C48-C49-C50 |
| 33 | c | 524 | LMG | O6-C5-C6-O5 |
| 23 | c | 507 | CLA | C4-C3-C5-C6 |
| 23 | c | 507 | CLA | C2-C3-C5-C6 |
| 23 | B | 606 | CLA | C2A-CAA-CBA-CGA |
| 23 | b | 617 | CLA | O1D-CGD-O2D-CED |
| 33 | c | 519 | LMG | C11-C10-O7-C8 |
| 33 | C | 501 | LMG | O6-C5-C6-O5 |
| 33 | c | 522 | LMG | C4-C5-C6-O5 |
| 26 | A | 409 | PL9 | C34-C36-C37-C38 |
| 26 | A | 409 | PL9 | C44-C46-C47-C48 |
| 26 | a | 410 | PL9 | C19-C21-C22-C23 |
| 26 | d | 406 | PL9 | C34-C36-C37-C38 |
| 23 | b | 613 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | C | 519 | LMG | C4-C5-C6-O5 |
| 23 | c | 511 | CLA | O1D-CGD-O2D-CED |
| 29 | D | 408 | LHG | C1-C2-C3-O3 |
| 23 | B | 601 | CLA | CBA-CGA-O2A-C1 |
| 27 | A | 411 | SQD | C24-C23-O48-C46 |
| 27 | f | 101 | SQD | C24-C23-O48-C46 |
| 33 | c | 519 | LMG | C29-C28-O8-C9 |
| 33 | c | 524 | LMG | C4-C5-C6-O5 |
| 29 | d | 407 | LHG | C7-C8-C9-C10 |
| 23 | c | 509 | CLA | C10-C11-C12-C13 |
| 23 | b | 607 | CLA | C15-C16-C17-C18 |
| 23 | c | 503 | CLA | C5-C6-C7-C8 |
| 27 | B | 621 | SQD | C2-C1-O6-C44 |
| 27 | f | 101 | SQD | C2-C1-O6-C44 |
| 33 | c | 524 | LMG | C2-C1-O1-C7 |
| 27 | a | 411 | SQD | C12-C13-C14-C15 |
| 29 | D | 409 | LHG | C29-C30-C31-C32 |
| 33 | C | 501 | LMG | C4-C5-C6-O5 |
| 23 | B | 605 | CLA | C11-C10-C8-C9 |
| 23 | B | 611 | CLA | C11-C12-C13-C14 |
| 23 | B | 614 | CLA | C11-C12-C13-C14 |
| 23 | B | 614 | CLA | C14-C13-C15-C16 |
| 23 | C | 503 | CLA | C6-C7-C8-C9 |
| 23 | C | 508 | CLA | C11-C10-C8-C9 |
| 23 | C | 510 | CLA | C11-C10-C8-C9 |
| 23 | D | 403 | CLA | C11-C10-C8-C9 |
| 23 | D | 404 | CLA | C11-C12-C13-C14 |
| 23 | b | 602 | CLA | C11-C10-C8-C9 |
| 23 | b | 605 | CLA | C6-C7-C8-C9 |
| 23 | b | 607 | CLA | C14-C13-C15-C16 |
| 23 | c | 502 | CLA | C6-C7-C8-C9 |
| 23 | c | 506 | CLA | C6-C7-C8-C9 |
| 23 | c | 509 | CLA | C6-C7-C8-C9 |
| 23 | c | 509 | CLA | C11-C12-C13-C14 |
| 23 | d | 404 | CLA | C11-C12-C13-C14 |
| 24 | A | 406 | PHO | C14-C13-C15-C16 |
| 23 | c | 507 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 101 | BCR | C37-C22-C23-C24 |
| 25 | b | 620 | BCR | C36-C18-C19-C20 |
| 25 | c | 515 | BCR | C37-C22-C23-C24 |
| 25 | k | 101 | BCR | C7-C8-C9-C34 |
| 25 | d | 405 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | k | 101 | BCR | C7-C8-C9-C10 |
| 33 | m | 101 | LMG | C10-C11-C12-C13 |
| 23 | B | 601 | CLA | O1A-CGA-O2A-C1 |
| 23 | b | 615 | CLA | C8-C10-C11-C12 |
| 23 | c | 512 | CLA | C13-C15-C16-C17 |
| 23 | B | 606 | CLA | O1D-CGD-O2D-CED |
| 29 | E | 101 | LHG | C32-C33-C34-C35 |
| 23 | C | 507 | CLA | C3-C5-C6-C7 |
| 23 | b | 604 | CLA | C5-C6-C7-C8 |
| 27 | F | 101 | SQD | C23-C24-C25-C26 |
| 28 | c | 517 | DGD | C1B-C2B-C3B-C4B |
| 29 | e | 101 | LHG | C23-C24-C25-C26 |
| 27 | a | 411 | SQD | O10-C23-O48-C46 |
| 25 | B | 618 | BCR | C14-C15-C16-C17 |
| 23 | B | 606 | CLA | C15-C16-C17-C18 |
| 23 | B | 607 | CLA | C8-C10-C11-C12 |
| 23 | C | 510 | CLA | C10-C11-C12-C13 |
| 23 | C | 513 | CLA | C10-C11-C12-C13 |
| 23 | b | 606 | CLA | C5-C6-C7-C8 |
| 23 | b | 606 | CLA | C15-C16-C17-C18 |
| 23 | b | 608 | CLA | C10-C11-C12-C13 |
| 23 | b | 612 | CLA | C10-C11-C12-C13 |
| 23 | b | 612 | CLA | C13-C15-C16-C17 |
| 23 | b | 612 | CLA | C15-C16-C17-C18 |
| 23 | b | 615 | CLA | C5-C6-C7-C8 |
| 23 | c | 510 | CLA | C15-C16-C17-C18 |
| 28 | h | 101 | DGD | C4E-C5E-C6E-O5E |
| 29 | A | 413 | LHG | O1-C1-C2-O2 |
| 27 | A | 410 | SQD | C7-C8-C9-C10 |
| 28 | c | 518 | DGD | C1A-C2A-C3A-C4A |
| 29 | E | 101 | LHG | C7-C8-C9-C10 |
| 33 | c | 519 | LMG | O6-C5-C6-O5 |
| 23 | C | 502 | CLA | O1D-CGD-O2D-CED |
| 23 | c | 508 | CLA | C13-C15-C16-C17 |
| 27 | b | 601 | SQD | C11-C10-C9-C8 |
| 28 | c | 516 | DGD | O6E-C5E-C6E-O5E |
| 23 | c | 506 | CLA | C2-C1-O2A-CGA |
| 26 | d | 406 | PL9 | C37-C38-C39-C41 |
| 23 | b | 602 | CLA | C15-C16-C17-C18 |
| 23 | b | 607 | CLA | C10-C11-C12-C13 |
| 23 | c | 511 | CLA | C13-C15-C16-C17 |
| 27 | A | 411 | SQD | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | d | 403 | CLA | CBD-CGD-O2D-CED |
| 27 | b | 601 | SQD | C8-C7-O47-C45 |
| 23 | B | 604 | CLA | C10-C11-C12-C13 |
| 23 | B | 605 | CLA | C5-C6-C7-C8 |
| 23 | b | 602 | CLA | C8-C10-C11-C12 |
| 23 | b | 603 | CLA | C13-C15-C16-C17 |
| 23 | B | 612 | CLA | C6-C7-C8-C10 |
| 23 | C | 507 | CLA | C12-C13-C15-C16 |
| 23 | b | 613 | CLA | C6-C7-C8-C10 |
| 23 | c | 502 | CLA | C11-C12-C13-C15 |
| 23 | c | 512 | CLA | C11-C12-C13-C15 |
| 25 | B | 619 | BCR | C13-C14-C15-C16 |
| 23 | c | 512 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 615 | CLA | O1D-CGD-O2D-CED |
| 23 | B | 609 | CLA | C13-C15-C16-C17 |
| 23 | B | 615 | CLA | C10-C11-C12-C13 |
| 23 | C | 508 | CLA | C10-C11-C12-C13 |
| 23 | b | 610 | CLA | C15-C16-C17-C18 |
| 23 | c | 505 | CLA | C15-C16-C17-C18 |
| 33 | C | 519 | LMG | O6-C5-C6-O5 |
| 23 | c | 510 | CLA | C8-C10-C11-C12 |
| 33 | c | 522 | LMG | C10-C11-C12-C13 |
| 25 | B | 617 | BCR | C18-C19-C20-C21 |
| 25 | C | 515 | BCR | C10-C11-C12-C13 |
| 25 | Z | 101 | BCR | C18-C19-C20-C21 |
| 25 | b | 619 | BCR | C10-C11-C12-C13 |
| 25 | b | 619 | BCR | C18-C19-C20-C21 |
| 25 | x | 102 | BCR | C18-C19-C20-C21 |
| 29 | A | 413 | LHG | O2-C2-C3-O3 |
| 29 | d | 407 | LHG | O2-C2-C3-O3 |
| 29 | e | 101 | LHG | O2-C2-C3-O3 |
| 23 | A | 404 | CLA | C15-C16-C17-C18 |
| 23 | a | 406 | CLA | C10-C11-C12-C13 |
| 23 | c | 503 | CLA | C8-C10-C11-C12 |
| 28 | c | 518 | DGD | C2A-C1A-O1G-C1G |
| 23 | a | 408 | CLA | C10-C11-C12-C13 |
| 33 | M | 101 | LMG | O10-C28-O8-C9 |
| 23 | B | 607 | CLA | C13-C15-C16-C17 |
| 23 | B | 611 | CLA | C13-C15-C16-C17 |
| 23 | C | 510 | CLA | C13-C15-C16-C17 |
| 23 | C | 511 | CLA | C15-C16-C17-C18 |
| 23 | c | 509 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | D | 408 | LHG | C3-O3-P-O6 |
| 29 | L | 101 | LHG | C4-O6-P-O3 |
| 29 | d | 408 | LHG | C4-O6-P-O3 |
| 27 | A | 410 | SQD | C23-C24-C25-C26 |
| 23 | C | 503 | CLA | C3-C5-C6-C7 |
| 23 | B | 613 | CLA | C8-C10-C11-C12 |
| 23 | C | 506 | CLA | C5-C6-C7-C8 |
| 23 | c | 508 | CLA | C10-C11-C12-C13 |
| 23 | c | 512 | CLA | O1D-CGD-O2D-CED |
| 28 | A | 412 | DGD | O6D-C5D-C6D-O5D |
| 28 | c | 516 | DGD | C1A-C2A-C3A-C4A |
| 33 | M | 101 | LMG | C10-C11-C12-C13 |
| 33 | d | 411 | LMG | C28-C29-C30-C31 |
| 29 | A | 413 | LHG | C1-C2-C3-O3 |
| 29 | d | 407 | LHG | C1-C2-C3-O3 |
| 29 | e | 101 | LHG | C1-C2-C3-O3 |
| 23 | C | 508 | CLA | C13-C15-C16-C17 |
| 23 | B | 616 | CLA | C11-C12-C13-C14 |
| 23 | c | 506 | CLA | C16-C17-C18-C20 |
| 23 | c | 510 | CLA | C16-C17-C18-C20 |
| 26 | d | 406 | PL9 | C47-C48-C49-C50 |
| 23 | b | 608 | CLA | CBA-CGA-O2A-C1 |
| 33 | C | 501 | LMG | C29-C28-O8-C9 |
| 33 | C | 519 | LMG | C29-C28-O8-C9 |
| 23 | B | 602 | CLA | C13-C15-C16-C17 |
| 33 | d | 410 | LMG | C35-C36-C37-C38 |
| 23 | b | 616 | CLA | O1D-CGD-O2D-CED |
| 28 | a | 413 | DGD | C2B-C1B-O2G-C2G |
| 25 | A | 408 | BCR | C35-C13-C14-C15 |
| 25 | B | 617 | BCR | C35-C13-C14-C15 |
| 25 | B | 617 | BCR | C20-C21-C22-C37 |
| 25 | C | 515 | BCR | C16-C17-C18-C36 |
| 25 | C | 520 | BCR | C11-C10-C9-C34 |
| 25 | H | 101 | BCR | C20-C21-C22-C37 |
| 25 | K | 101 | BCR | C20-C21-C22-C37 |
| 25 | Z | 101 | BCR | C20-C21-C22-C37 |
| 25 | a | 409 | BCR | C20-C21-C22-C37 |
| 25 | b | 618 | BCR | C20-C21-C22-C37 |
| 25 | b | 620 | BCR | C20-C21-C22-C37 |
| 25 | c | 514 | BCR | C16-C17-C18-C36 |
| 25 | c | 515 | BCR | C16-C17-C18-C36 |
| 25 | c | 521 | BCR | C16-C17-C18-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | d | 405 | BCR | C16-C17-C18-C36 |
| 25 | k | 101 | BCR | C11-C10-C9-C34 |
| 25 | k | 101 | BCR | C16-C17-C18-C36 |
| 25 | k | 101 | BCR | C20-C21-C22-C37 |
| 25 | x | 102 | BCR | C16-C17-C18-C36 |
| 27 | A | 410 | SQD | C11-C12-C13-C14 |
| 27 | A | 410 | SQD | C33-C34-C35-C36 |
| 27 | a | 411 | SQD | C34-C35-C36-C37 |
| 27 | a | 412 | SQD | C15-C16-C17-C18 |
| 28 | A | 412 | DGD | C5B-C6B-C7B-C8B |
| 28 | C | 518 | DGD | CAA-CBA-CCA-CDA |
| 28 | a | 413 | DGD | C5A-C6A-C7A-C8A |
| 28 | a | 413 | DGD | C8B-C9B-CAB-CBB |
| 28 | c | 516 | DGD | C3B-C4B-C5B-C6B |
| 29 | L | 101 | LHG | C32-C33-C34-C35 |
| 29 | d | 408 | LHG | C11-C12-C13-C14 |
| 29 | e | 101 | LHG | C11-C10-C9-C8 |
| 29 | e | 101 | LHG | C17-C18-C19-C20 |
| 29 | e | 101 | LHG | C26-C27-C28-C29 |
| 33 | M | 101 | LMG | C39-C40-C41-C42 |
| 33 | d | 411 | LMG | C34-C35-C36-C37 |
| 23 | b | 604 | CLA | O1D-CGD-O2D-CED |
| 23 | C | 503 | CLA | C16-C17-C18-C19 |
| 27 | a | 411 | SQD | C26-C27-C28-C29 |
| 28 | A | 412 | DGD | C4A-C5A-C6A-C7A |
| 28 | C | 517 | DGD | C8B-C9B-CAB-CBB |
| 28 | C | 517 | DGD | CCB-CDB-CEB-CFB |
| 28 | h | 101 | DGD | CBA-CCA-CDA-CEA |
| 33 | D | 407 | LMG | C39-C40-C41-C42 |
| 33 | c | 522 | LMG | C16-C17-C18-C19 |
| 23 | B | 614 | CLA | C5-C6-C7-C8 |
| 28 | A | 412 | DGD | CAA-CBA-CCA-CDA |
| 28 | C | 518 | DGD | C5A-C6A-C7A-C8A |
| 28 | H | 102 | DGD | C4B-C5B-C6B-C7B |
| 33 | D | 407 | LMG | C35-C36-C37-C38 |
| 27 | A | 411 | SQD | C14-C15-C16-C17 |
| 27 | F | 101 | SQD | C33-C34-C35-C36 |
| 29 | D | 409 | LHG | C32-C33-C34-C35 |
| 29 | d | 409 | LHG | C30-C31-C32-C33 |
| 33 | c | 524 | LMG | C12-C13-C14-C15 |
| 27 | b | 601 | SQD | C18-C19-C20-C21 |
| 28 | A | 412 | DGD | C6B-C7B-C8B-C9B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | C | 517 | DGD | C6A-C7A-C8A-C9A |
| 28 | H | 102 | DGD | CCA-CDA-CEA-CFA |
| 23 | b | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 617 | BCR | C12-C13-C14-C15 |
| 25 | B | 617 | BCR | C20-C21-C22-C23 |
| 25 | C | 515 | BCR | C11-C10-C9-C8 |
| 25 | C | 520 | BCR | C16-C17-C18-C19 |
| 25 | C | 520 | BCR | C20-C21-C22-C23 |
| 25 | H | 101 | BCR | C11-C10-C9-C8 |
| 25 | H | 101 | BCR | C20-C21-C22-C23 |
| 25 | c | 514 | BCR | C12-C13-C14-C15 |
| 25 | c | 514 | BCR | C20-C21-C22-C23 |
| 25 | c | 521 | BCR | C16-C17-C18-C19 |
| 25 | d | 405 | BCR | C11-C10-C9-C8 |
| 25 | k | 101 | BCR | C20-C21-C22-C23 |
| 25 | t | 101 | BCR | C16-C17-C18-C19 |
| 28 | A | 412 | DGD | C2E-C1E-O5D-C6D |
| 28 | C | 517 | DGD | C2E-C1E-O5D-C6D |
| 28 | c | 517 | DGD | C2E-C1E-O5D-C6D |
| 27 | B | 621 | SQD | C24-C23-O48-C46 |
| 27 | a | 411 | SQD | C11-C12-C13-C14 |
| 28 | c | 517 | DGD | C8B-C9B-CAB-CBB |
| 28 | h | 101 | DGD | C2B-C3B-C4B-C5B |
| 29 | A | 413 | LHG | C14-C15-C16-C17 |
| 29 | D | 409 | LHG | C27-C28-C29-C30 |
| 29 | d | 408 | LHG | C14-C15-C16-C17 |
| 29 | d | 409 | LHG | C27-C28-C29-C30 |
| 33 | b | 622 | LMG | C11-C12-C13-C14 |
| 33 | c | 522 | LMG | C34-C35-C36-C37 |
| 33 | d | 411 | LMG | C39-C40-C41-C42 |
| 33 | m | 101 | LMG | C11-C12-C13-C14 |
| 23 | A | 405 | CLA | C16-C17-C18-C20 |
| 23 | D | 404 | CLA | C16-C17-C18-C19 |
| 23 | d | 403 | CLA | C16-C17-C18-C19 |
| 23 | b | 612 | CLA | O1D-CGD-O2D-CED |
| 28 | C | 517 | DGD | C9A-CAA-CBA-CCA |
| 33 | C | 501 | LMG | C16-C17-C18-C19 |
| 33 | D | 407 | LMG | C20-C21-C22-C23 |
| 33 | M | 101 | LMG | C38-C39-C40-C41 |
| 33 | d | 410 | LMG | C37-C38-C39-C40 |
| 23 | C | 504 | CLA | C6-C7-C8-C9 |
| 23 | C | 513 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | b | 612 | CLA | C11-C10-C8-C9 |
| 23 | b | 616 | CLA | C14-C13-C15-C16 |
| 23 | b | 617 | CLA | C11-C10-C8-C9 |
| 23 | c | 504 | CLA | C11-C10-C8-C9 |
| 23 | c | 505 | CLA | C11-C10-C8-C9 |
| 23 | c | 506 | CLA | C14-C13-C15-C16 |
| 27 | B | 621 | SQD | C9-C10-C11-C12 |
| 27 | B | 621 | SQD | C11-C12-C13-C14 |
| 27 | a | 412 | SQD | C10-C11-C12-C13 |
| 27 | a | 412 | SQD | C12-C13-C14-C15 |
| 28 | C | 516 | DGD | C4A-C5A-C6A-C7A |
| 28 | C | 517 | DGD | C5B-C6B-C7B-C8B |
| 28 | a | 413 | DGD | C5B-C6B-C7B-C8B |
| 29 | E | 101 | LHG | C11-C10-C9-C8 |
| 29 | d | 408 | LHG | C29-C30-C31-C32 |
| 33 | c | 519 | LMG | C31-C32-C33-C34 |
| 33 | d | 410 | LMG | C38-C39-C40-C41 |
| 23 | B | 604 | CLA | C13-C15-C16-C17 |
| 27 | b | 601 | SQD | C16-C17-C18-C19 |
| 33 | c | 524 | LMG | C38-C39-C40-C41 |
| 29 | d | 408 | LHG | O1-C1-C2-C3 |
| 29 | d | 409 | LHG | O1-C1-C2-C3 |
| 25 | B | 617 | BCR | C17-C18-C19-C20 |
| 33 | c | 522 | LMG | C11-C10-O7-C8 |
| 27 | B | 621 | SQD | C17-C18-C19-C20 |
| 28 | A | 412 | DGD | CEA-CFA-CGA-CHA |
| 28 | h | 101 | DGD | C5B-C6B-C7B-C8B |
| 29 | D | 409 | LHG | C25-C26-C27-C28 |
| 33 | D | 407 | LMG | C34-C35-C36-C37 |
| 33 | b | 622 | LMG | C18-C19-C20-C21 |
| 28 | c | 517 | DGD | C1A-C2A-C3A-C4A |
| 27 | a | 411 | SQD | C30-C31-C32-C33 |
| 28 | A | 412 | DGD | CCA-CDA-CEA-CFA |
| 28 | A | 412 | DGD | C2B-C3B-C4B-C5B |
| 28 | a | 413 | DGD | C4A-C5A-C6A-C7A |
| 28 | h | 101 | DGD | CCB-CDB-CEB-CFB |
| 29 | D | 409 | LHG | C11-C12-C13-C14 |
| 29 | L | 101 | LHG | C27-C28-C29-C30 |
| 29 | d | 407 | LHG | C17-C18-C19-C20 |
| 29 | d | 408 | LHG | C32-C33-C34-C35 |
| 29 | e | 101 | LHG | C12-C13-C14-C15 |
| 29 | e | 101 | LHG | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | l | 101 | LHG | C13-C14-C15-C16 |
| 33 | D | 407 | LMG | C14-C15-C16-C17 |
| 33 | D | 411 | LMG | C33-C34-C35-C36 |
| 33 | b | 622 | LMG | C15-C16-C17-C18 |
| 33 | b | 622 | LMG | C19-C20-C21-C22 |
| 33 | c | 524 | LMG | C34-C35-C36-C37 |
| 28 | C | 516 | DGD | O6E-C5E-C6E-O5E |
| 23 | B | 611 | CLA | C16-C17-C18-C20 |
| 23 | c | 506 | CLA | C16-C17-C18-C19 |
| 28 | C | 517 | DGD | O6E-C1E-O5D-C6D |
| 28 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 23 | B | 611 | CLA | C15-C16-C17-C18 |
| 23 | B | 612 | CLA | C13-C15-C16-C17 |
| 27 | F | 101 | SQD | C25-C26-C27-C28 |
| 28 | A | 412 | DGD | CEB-CFB-CGB-CHB |
| 28 | c | 518 | DGD | CBB-CCB-CDB-CEB |
| 28 | h | 101 | DGD | C3A-C4A-C5A-C6A |
| 28 | h | 101 | DGD | CAB-CBB-CCB-CDB |
| 29 | D | 409 | LHG | C9-C10-C11-C12 |
| 29 | D | 409 | LHG | C34-C35-C36-C37 |
| 29 | E | 101 | LHG | C15-C16-C17-C18 |
| 29 | l | 101 | LHG | C29-C30-C31-C32 |
| 33 | D | 407 | LMG | C11-C12-C13-C14 |
| 33 | D | 407 | LMG | C19-C20-C21-C22 |
| 33 | M | 101 | LMG | C36-C37-C38-C39 |
| 28 | A | 412 | DGD | C4D-C5D-C6D-O5D |
| 27 | f | 101 | SQD | C29-C30-C31-C32 |
| 27 | f | 101 | SQD | C31-C32-C33-C34 |
| 28 | c | 518 | DGD | C4B-C5B-C6B-C7B |
| 29 | D | 408 | LHG | C10-C11-C12-C13 |
| 33 | D | 411 | LMG | C11-C12-C13-C14 |
| 29 | d | 408 | LHG | C7-C8-C9-C10 |
| 23 | b | 615 | CLA | C13-C15-C16-C17 |
| 27 | A | 411 | SQD | C12-C13-C14-C15 |
| 27 | a | 412 | SQD | C18-C19-C20-C21 |
| 28 | c | 516 | DGD | C9A-CAA-CBA-CCA |
| 29 | D | 408 | LHG | C15-C16-C17-C18 |
| 29 | L | 101 | LHG | C30-C31-C32-C33 |
| 33 | m | 101 | LMG | C17-C18-C19-C20 |
| 23 | c | 512 | CLA | CBA-CGA-O2A-C1 |
| 27 | a | 411 | SQD | C24-C23-O48-C46 |
| 28 | c | 516 | DGD | O6D-C5D-C6D-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | l | 101 | LHG | C16-C17-C18-C19 |
| 33 | d | 410 | LMG | C33-C34-C35-C36 |
| 23 | b | 602 | CLA | C3A-C2A-CAA-CBA |
| 23 | c | 512 | CLA | C3A-C2A-CAA-CBA |
| 25 | c | 514 | BCR | C13-C14-C15-C16 |
| 27 | f | 101 | SQD | C28-C29-C30-C31 |
| 28 | a | 413 | DGD | C3B-C4B-C5B-C6B |
| 33 | D | 411 | LMG | C32-C33-C34-C35 |
| 23 | b | 608 | CLA | O1A-CGA-O2A-C1 |
| 23 | A | 405 | CLA | C16-C17-C18-C19 |
| 23 | C | 503 | CLA | C16-C17-C18-C20 |
| 23 | a | 405 | CLA | C16-C17-C18-C20 |
| 23 | d | 403 | CLA | C16-C17-C18-C20 |
| 27 | B | 621 | SQD | C13-C14-C15-C16 |
| 27 | b | 601 | SQD | C10-C11-C12-C13 |
| 29 | d | 407 | LHG | C30-C31-C32-C33 |
| 29 | d | 409 | LHG | C26-C27-C28-C29 |
| 29 | l | 101 | LHG | C9-C10-C11-C12 |
| 33 | b | 622 | LMG | C31-C32-C33-C34 |
| 23 | C | 512 | CLA | O1D-CGD-O2D-CED |
| 33 | c | 522 | LMG | O6-C5-C6-O5 |
| 29 | d | 407 | LHG | C28-C29-C30-C31 |
| 29 | l | 101 | LHG | C27-C28-C29-C30 |
| 25 | b | 619 | BCR | C14-C15-C16-C17 |
| 23 | C | 513 | CLA | C3-C5-C6-C7 |
| 27 | a | 412 | SQD | C11-C12-C13-C14 |
| 33 | c | 524 | LMG | C16-C17-C18-C19 |
| 23 | C | 511 | CLA | C4-C3-C5-C6 |
| 24 | A | 406 | PHO | C4-C3-C5-C6 |
| 26 | D | 406 | PL9 | C30-C29-C31-C32 |
| 24 | A | 406 | PHO | C2-C3-C5-C6 |
| 26 | d | 406 | PL9 | C28-C29-C31-C32 |
| 23 | c | 505 | CLA | O1D-CGD-O2D-CED |
| 28 | A | 412 | DGD | CBA-CCA-CDA-CEA |
| 33 | D | 407 | LMG | C30-C31-C32-C33 |
| 33 | m | 101 | LMG | C31-C32-C33-C34 |
| 26 | D | 406 | PL9 | C47-C48-C49-C51 |
| 29 | D | 408 | LHG | O1-C1-C2-O2 |
| 29 | d | 407 | LHG | O1-C1-C2-O2 |
| 29 | e | 101 | LHG | O1-C1-C2-O2 |
| 28 | C | 518 | DGD | C3A-C4A-C5A-C6A |
| 28 | c | 516 | DGD | C4B-C5B-C6B-C7B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | D | 408 | LHG | C11-C10-C9-C8 |
| 29 | d | 407 | LHG | C32-C33-C34-C35 |
| 29 | d | 408 | LHG | C30-C31-C32-C33 |
| 23 | B | 616 | CLA | C11-C12-C13-C15 |
| 23 | c | 507 | CLA | C16-C17-C18-C20 |
| 29 | D | 408 | LHG | C11-C12-C13-C14 |
| 29 | e | 101 | LHG | C10-C11-C12-C13 |
| 33 | C | 501 | LMG | C14-C15-C16-C17 |
| 27 | B | 621 | SQD | C29-C30-C31-C32 |
| 28 | A | 412 | DGD | CDB-CEB-CFB-CGB |
| 28 | c | 517 | DGD | C6A-C7A-C8A-C9A |
| 29 | A | 413 | LHG | C27-C28-C29-C30 |
| 29 | e | 101 | LHG | C14-C15-C16-C17 |
| 33 | M | 101 | LMG | C12-C13-C14-C15 |
| 33 | c | 522 | LMG | C36-C37-C38-C39 |
| 33 | d | 410 | LMG | C31-C32-C33-C34 |
| 26 | a | 410 | PL9 | C47-C48-C49-C51 |
| 29 | A | 413 | LHG | C12-C13-C14-C15 |
| 29 | D | 408 | LHG | C30-C31-C32-C33 |
| 29 | d | 409 | LHG | C29-C30-C31-C32 |
| 33 | c | 519 | LMG | C39-C40-C41-C42 |
| 23 | a | 408 | CLA | C13-C15-C16-C17 |
| 23 | b | 602 | CLA | C10-C11-C12-C13 |
| 28 | c | 516 | DGD | C4D-C5D-C6D-O5D |
| 23 | c | 512 | CLA | O1A-CGA-O2A-C1 |
| 27 | A | 411 | SQD | C10-C11-C12-C13 |
| 23 | b | 607 | CLA | C3-C5-C6-C7 |
| 25 | A | 408 | BCR | C1-C6-C7-C8 |
| 25 | A | 408 | BCR | C5-C6-C7-C8 |
| 25 | B | 617 | BCR | C1-C6-C7-C8 |
| 25 | B | 617 | BCR | C5-C6-C7-C8 |
| 25 | C | 520 | BCR | C1-C6-C7-C8 |
| 25 | C | 520 | BCR | C5-C6-C7-C8 |
| 25 | D | 405 | BCR | C23-C24-C25-C30 |
| 25 | K | 101 | BCR | C1-C6-C7-C8 |
| 25 | K | 101 | BCR | C5-C6-C7-C8 |
| 25 | b | 619 | BCR | C23-C24-C25-C26 |
| 25 | x | 102 | BCR | C23-C24-C25-C30 |
| 28 | A | 412 | DGD | C9B-CAB-CBB-CCB |
| 28 | c | 517 | DGD | CAA-CBA-CCA-CDA |
| 33 | c | 519 | LMG | C36-C37-C38-C39 |
| 23 | B | 605 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 611 | CLA | C8-C10-C11-C12 |
| 23 | B | 612 | CLA | C10-C11-C12-C13 |
| 23 | C | 504 | CLA | C8-C10-C11-C12 |
| 23 | c | 504 | CLA | C5-C6-C7-C8 |
| 28 | c | 516 | DGD | C8B-C9B-CAB-CBB |
| 33 | c | 524 | LMG | C13-C14-C15-C16 |
| 33 | c | 522 | LMG | C32-C33-C34-C35 |
| 26 | A | 409 | PL9 | C47-C48-C49-C51 |
| 27 | F | 101 | SQD | C26-C27-C28-C29 |
| 29 | D | 408 | LHG | C32-C33-C34-C35 |
| 29 | D | 409 | LHG | C30-C31-C32-C33 |
| 23 | B | 614 | CLA | C4-C3-C5-C6 |
| 23 | B | 605 | CLA | C11-C10-C8-C7 |
| 23 | B | 615 | CLA | C11-C12-C13-C15 |
| 23 | C | 506 | CLA | C11-C12-C13-C15 |
| 23 | C | 507 | CLA | C11-C12-C13-C15 |
| 23 | C | 509 | CLA | C12-C13-C15-C16 |
| 23 | C | 511 | CLA | C2-C3-C5-C6 |
| 23 | C | 512 | CLA | C6-C7-C8-C10 |
| 23 | C | 514 | CLA | C11-C10-C8-C7 |
| 23 | D | 402 | CLA | C11-C12-C13-C15 |
| 23 | a | 406 | CLA | C6-C7-C8-C10 |
| 23 | b | 605 | CLA | C6-C7-C8-C10 |
| 23 | b | 607 | CLA | C12-C13-C15-C16 |
| 23 | b | 616 | CLA | C12-C13-C15-C16 |
| 23 | b | 617 | CLA | C11-C10-C8-C7 |
| 23 | c | 504 | CLA | C11-C10-C8-C7 |
| 23 | c | 506 | CLA | C6-C7-C8-C10 |
| 23 | c | 506 | CLA | C12-C13-C15-C16 |
| 23 | c | 509 | CLA | C12-C13-C15-C16 |
| 23 | c | 511 | CLA | C12-C13-C15-C16 |
| 26 | D | 406 | PL9 | C13-C14-C16-C17 |
| 26 | D | 406 | PL9 | C28-C29-C31-C32 |
| 27 | a | 411 | SQD | C14-C15-C16-C17 |
| 29 | E | 101 | LHG | O9-C7-O7-C5 |
| 29 | L | 101 | LHG | C23-C24-C25-C26 |
| 23 | c | 503 | CLA | CBA-CGA-O2A-C1 |
| 33 | m | 101 | LMG | C29-C28-O8-C9 |
| 29 | D | 408 | LHG | C29-C30-C31-C32 |
| 23 | b | 611 | CLA | C2A-CAA-CBA-CGA |
| 23 | D | 404 | CLA | C5-C6-C7-C8 |
| 28 | H | 102 | DGD | C8B-C9B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | c | 522 | LMG | C38-C39-C40-C41 |
| 28 | C | 518 | DGD | CCA-CDA-CEA-CFA |
| 28 | c | 518 | DGD | C8A-C9A-CAA-CBA |
| 29 | D | 409 | LHG | C24-C25-C26-C27 |
| 33 | b | 622 | LMG | C16-C17-C18-C19 |
| 33 | c | 522 | LMG | C11-C12-C13-C14 |
| 29 | A | 413 | LHG | C7-C8-C9-C10 |
| 33 | c | 524 | LMG | C28-C29-C30-C31 |
| 23 | D | 403 | CLA | C15-C16-C17-C18 |
| 28 | A | 412 | DGD | C4B-C5B-C6B-C7B |
| 29 | D | 408 | LHG | C34-C35-C36-C37 |
| 29 | L | 101 | LHG | C18-C19-C20-C21 |
| 33 | D | 407 | LMG | C13-C14-C15-C16 |
| 26 | D | 406 | PL9 | C7-C8-C9-C10 |
| 28 | C | 517 | DGD | C5A-C6A-C7A-C8A |
| 33 | D | 410 | LMG | C33-C34-C35-C36 |
| 28 | C | 518 | DGD | O1A-C1A-O1G-C1G |
| 28 | A | 412 | DGD | C2A-C1A-O1G-C1G |
| 28 | A | 412 | DGD | O6E-C1E-O5D-C6D |
| 23 | b | 615 | CLA | C15-C16-C17-C18 |
| 23 | c | 506 | CLA | C5-C6-C7-C8 |
| 23 | c | 507 | CLA | O1D-CGD-O2D-CED |
| 26 | D | 406 | PL9 | C44-C46-C47-C48 |
| 27 | F | 101 | SQD | C31-C32-C33-C34 |
| 28 | a | 413 | DGD | C7B-C8B-C9B-CAB |
| 29 | D | 408 | LHG | C25-C26-C27-C28 |
| 29 | d | 408 | LHG | C34-C35-C36-C37 |
| 29 | l | 101 | LHG | C32-C33-C34-C35 |
| 33 | b | 622 | LMG | C23-C24-C25-C26 |
| 33 | d | 410 | LMG | C32-C33-C34-C35 |
| 33 | d | 411 | LMG | C14-C15-C16-C17 |
| 33 | c | 519 | LMG | C35-C36-C37-C38 |
| 23 | C | 506 | CLA | CBD-CGD-O2D-CED |
| 29 | d | 407 | LHG | C33-C34-C35-C36 |
| 27 | B | 621 | SQD | C10-C11-C12-C13 |
| 33 | b | 622 | LMG | O6-C5-C6-O5 |
| 28 | C | 517 | DGD | C3A-C4A-C5A-C6A |
| 33 | M | 101 | LMG | C17-C18-C19-C20 |
| 23 | B | 607 | CLA | C16-C17-C18-C20 |
| 29 | e | 101 | LHG | C27-C28-C29-C30 |
| 33 | D | 411 | LMG | C31-C32-C33-C34 |
| 33 | b | 622 | LMG | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 612 | CLA | C5-C6-C7-C8 |
| 26 | a | 410 | PL9 | C40-C39-C41-C42 |
| 26 | d | 406 | PL9 | C15-C14-C16-C17 |
| 26 | d | 406 | PL9 | C4-C3-C7-C8 |
| 27 | B | 621 | SQD | C34-C35-C36-C37 |
| 23 | B | 615 | CLA | C11-C12-C13-C14 |
| 23 | C | 506 | CLA | C11-C12-C13-C14 |
| 23 | C | 507 | CLA | C6-C7-C8-C9 |
| 23 | C | 507 | CLA | C11-C12-C13-C14 |
| 23 | C | 507 | CLA | C14-C13-C15-C16 |
| 23 | C | 512 | CLA | C6-C7-C8-C9 |
| 23 | C | 514 | CLA | C11-C10-C8-C9 |
| 23 | a | 406 | CLA | C6-C7-C8-C9 |
| 23 | a | 408 | CLA | C11-C10-C8-C9 |
| 23 | b | 613 | CLA | C6-C7-C8-C9 |
| 23 | c | 502 | CLA | C11-C12-C13-C14 |
| 23 | c | 509 | CLA | C14-C13-C15-C16 |
| 23 | c | 511 | CLA | C14-C13-C15-C16 |
| 23 | c | 512 | CLA | C11-C12-C13-C14 |
| 33 | d | 411 | LMG | O6-C5-C6-O5 |
| 28 | c | 516 | DGD | C4A-C5A-C6A-C7A |
| 33 | C | 501 | LMG | C38-C39-C40-C41 |
| 23 | b | 609 | CLA | C5-C6-C7-C8 |
| 23 | B | 607 | CLA | C1A-C2A-CAA-CBA |
| 23 | a | 408 | CLA | C1A-C2A-CAA-CBA |
| 23 | c | 508 | CLA | C1A-C2A-CAA-CBA |
| 23 | a | 405 | CLA | C16-C17-C18-C19 |
| 23 | b | 608 | CLA | C16-C17-C18-C20 |
| 23 | c | 510 | CLA | C16-C17-C18-C19 |
| 27 | a | 411 | SQD | C8-C7-O47-C45 |
| 29 | E | 101 | LHG | C8-C7-O7-C5 |
| 33 | M | 101 | LMG | C11-C10-O7-C8 |
| 27 | A | 410 | SQD | C31-C32-C33-C34 |
| 27 | b | 601 | SQD | C13-C14-C15-C16 |
| 28 | C | 518 | DGD | C7A-C8A-C9A-CAA |
| 29 | L | 101 | LHG | C33-C34-C35-C36 |
| 29 | e | 101 | LHG | C16-C17-C18-C19 |
| 33 | D | 411 | LMG | C16-C17-C18-C19 |
| 33 | d | 410 | LMG | C34-C35-C36-C37 |
| 25 | B | 619 | BCR | C15-C16-C17-C18 |
| 23 | C | 513 | CLA | C8-C10-C11-C12 |
| 23 | b | 604 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | D | 408 | LHG | C4-O6-P-O3 |
| 29 | e | 101 | LHG | C3-O3-P-O6 |
| 28 | a | 413 | DGD | C2A-C3A-C4A-C5A |
| 23 | a | 408 | CLA | C5-C6-C7-C8 |
| 29 | E | 101 | LHG | O6-C4-C5-C6 |
| 29 | l | 101 | LHG | O6-C4-C5-C6 |
| 28 | a | 413 | DGD | CBA-CCA-CDA-CEA |
| 33 | D | 411 | LMG | C34-C35-C36-C37 |
| 29 | d | 409 | LHG | C23-C24-C25-C26 |
| 23 | c | 511 | CLA | C16-C17-C18-C20 |
| 28 | h | 101 | DGD | C7A-C8A-C9A-CAA |
| 29 | d | 407 | LHG | C16-C17-C18-C19 |
| 27 | A | 410 | SQD | C24-C25-C26-C27 |
| 28 | C | 516 | DGD | C2B-C3B-C4B-C5B |
| 28 | C | 517 | DGD | C2B-C3B-C4B-C5B |
| 28 | c | 518 | DGD | CCA-CDA-CEA-CFA |
| 33 | m | 101 | LMG | C37-C38-C39-C40 |
| 23 | B | 601 | CLA | C10-C11-C12-C13 |
| 23 | c | 507 | CLA | C5-C6-C7-C8 |
| 29 | E | 101 | LHG | C24-C25-C26-C27 |
| 33 | c | 522 | LMG | C40-C41-C42-C43 |
| 27 | a | 411 | SQD | C10-C11-C12-C13 |
| 28 | C | 516 | DGD | C4B-C5B-C6B-C7B |
| 29 | d | 407 | LHG | C25-C26-C27-C28 |
| 23 | B | 603 | CLA | C16-C17-C18-C20 |
| 23 | c | 511 | CLA | C16-C17-C18-C19 |
| 23 | A | 407 | CLA | C6-C7-C8-C9 |
| 27 | B | 621 | SQD | O6-C44-C45-C46 |
| 27 | a | 411 | SQD | C44-C45-C46-O48 |
| 27 | a | 412 | SQD | C44-C45-C46-O48 |
| 27 | b | 601 | SQD | C44-C45-C46-O48 |
| 28 | C | 516 | DGD | O1G-C1G-C2G-C3G |
| 28 | C | 517 | DGD | O6E-C5E-C6E-O5E |
| 28 | c | 518 | DGD | C6B-C7B-C8B-C9B |
| 23 | c | 503 | CLA | O1A-CGA-O2A-C1 |
| 27 | B | 621 | SQD | C45-C44-O6-C1 |
| 28 | C | 517 | DGD | C2G-C3G-O3G-C1D |
| 28 | C | 517 | DGD | C5D-C6D-O5D-C1E |
| 28 | c | 517 | DGD | C5D-C6D-O5D-C1E |
| 29 | L | 101 | LHG | C12-C13-C14-C15 |
| 28 | h | 101 | DGD | C6A-C7A-C8A-C9A |
| 33 | M | 101 | LMG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | D | 410 | LMG | C10-C11-C12-C13 |
| 26 | A | 409 | PL9 | C24-C26-C27-C28 |
| 29 | e | 101 | LHG | C28-C29-C30-C31 |
| 33 | C | 519 | LMG | C11-C12-C13-C14 |
| 27 | a | 411 | SQD | C18-C19-C20-C21 |
| 33 | b | 622 | LMG | C38-C39-C40-C41 |
| 23 | d | 404 | CLA | C8-C10-C11-C12 |
| 23 | B | 609 | CLA | C4-C3-C5-C6 |
| 23 | b | 612 | CLA | C4-C3-C5-C6 |
| 27 | A | 410 | SQD | C15-C16-C17-C18 |
| 28 | a | 413 | DGD | CFA-CGA-CHA-CIA |
| 28 | c | 517 | DGD | C4A-C5A-C6A-C7A |
| 29 | E | 101 | LHG | C13-C14-C15-C16 |
| 23 | C | 507 | CLA | C2-C3-C5-C6 |
| 33 | D | 410 | LMG | C28-C29-C30-C31 |
| 23 | B | 603 | CLA | C16-C17-C18-C19 |
| 23 | b | 612 | CLA | C8-C10-C11-C12 |
| 23 | c | 506 | CLA | C8-C10-C11-C12 |
| 27 | A | 411 | SQD | C27-C28-C29-C30 |
| 29 | D | 409 | LHG | C17-C18-C19-C20 |
| 33 | C | 519 | LMG | C40-C41-C42-C43 |
| 33 | d | 410 | LMG | C28-C29-C30-C31 |
| 27 | b | 601 | SQD | C46-C45-O47-C7 |
| 27 | F | 101 | SQD | C30-C31-C32-C33 |
| 28 | c | 518 | DGD | C2A-C3A-C4A-C5A |
| 29 | e | 101 | LHG | C11-C12-C13-C14 |
| 33 | D | 407 | LMG | O6-C5-C6-O5 |
| 29 | A | 413 | LHG | C25-C26-C27-C28 |
| 28 | c | 518 | DGD | CDB-CEB-CFB-CGB |
| 33 | D | 407 | LMG | C38-C39-C40-C41 |
| 33 | D | 411 | LMG | C37-C38-C39-C40 |
| 28 | C | 518 | DGD | C6B-C7B-C8B-C9B |
| 23 | C | 507 | CLA | C13-C15-C16-C17 |
| 33 | m | 101 | LMG | C19-C20-C21-C22 |
| 23 | B | 616 | CLA | C5-C6-C7-C8 |
| 23 | C | 507 | CLA | C8-C10-C11-C12 |
| 23 | a | 405 | CLA | C15-C16-C17-C18 |
| 25 | c | 514 | BCR | C16-C17-C18-C19 |
| 25 | d | 405 | BCR | C20-C21-C22-C23 |
| 29 | A | 413 | LHG | C18-C19-C20-C21 |
| 27 | A | 410 | SQD | O6-C44-C45-O47 |
| 33 | C | 501 | LMG | O1-C7-C8-O7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 505 | CLA | C11-C12-C13-C14 |
| 28 | C | 517 | DGD | CCA-CDA-CEA-CFA |
| 28 | c | 518 | DGD | C5B-C6B-C7B-C8B |
| 33 | D | 410 | LMG | C37-C38-C39-C40 |
| 29 | e | 101 | LHG | O9-C7-O7-C5 |
| 23 | b | 614 | CLA | C8-C10-C11-C12 |
| 23 | b | 616 | CLA | C5-C6-C7-C8 |
| 28 | H | 102 | DGD | O1A-C1A-O1G-C1G |
| 23 | D | 404 | CLA | C16-C17-C18-C20 |
| 23 | b | 608 | CLA | C16-C17-C18-C19 |
| 28 | C | 518 | DGD | CBA-CCA-CDA-CEA |
| 33 | m | 101 | LMG | C29-C30-C31-C32 |
| 23 | C | 507 | CLA | C4-C3-C5-C6 |
| 26 | d | 406 | PL9 | C45-C44-C46-C47 |
| 27 | f | 101 | SQD | C25-C26-C27-C28 |
| 23 | B | 605 | CLA | C12-C13-C15-C16 |
| 23 | B | 609 | CLA | C2-C3-C5-C6 |
| 23 | B | 614 | CLA | C11-C12-C13-C15 |
| 23 | B | 614 | CLA | C12-C13-C15-C16 |
| 23 | C | 505 | CLA | C11-C10-C8-C7 |
| 23 | C | 507 | CLA | C6-C7-C8-C10 |
| 23 | D | 404 | CLA | C11-C12-C13-C15 |
| 23 | a | 406 | CLA | C12-C13-C15-C16 |
| 23 | a | 408 | CLA | C11-C10-C8-C7 |
| 23 | b | 602 | CLA | C11-C10-C8-C7 |
| 23 | b | 606 | CLA | C11-C12-C13-C15 |
| 23 | b | 608 | CLA | C6-C7-C8-C10 |
| 23 | b | 613 | CLA | C12-C13-C15-C16 |
| 23 | b | 615 | CLA | C12-C13-C15-C16 |
| 23 | c | 508 | CLA | C12-C13-C15-C16 |
| 23 | c | 513 | CLA | C12-C13-C15-C16 |
| 24 | a | 407 | PHO | C6-C7-C8-C10 |
| 23 | B | 604 | CLA | C11-C10-C8-C9 |
| 23 | B | 605 | CLA | C11-C12-C13-C14 |
| 23 | B | 612 | CLA | C6-C7-C8-C9 |
| 23 | C | 509 | CLA | C11-C10-C8-C9 |
| 23 | D | 402 | CLA | C11-C12-C13-C14 |
| 23 | D | 404 | CLA | C11-C10-C8-C9 |
| 23 | a | 406 | CLA | C14-C13-C15-C16 |
| 23 | b | 604 | CLA | C11-C12-C13-C14 |
| 23 | b | 605 | CLA | C11-C12-C13-C14 |
| 23 | b | 605 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | b | 608 | CLA | C6-C7-C8-C9 |
| 23 | b | 609 | CLA | C11-C12-C13-C14 |
| 23 | b | 610 | CLA | C14-C13-C15-C16 |
| 23 | b | 613 | CLA | C14-C13-C15-C16 |
| 23 | c | 501 | CLA | C11-C12-C13-C14 |
| 23 | c | 505 | CLA | C6-C7-C8-C9 |
| 23 | c | 508 | CLA | C14-C13-C15-C16 |
| 23 | c | 511 | CLA | C6-C7-C8-C9 |
| 33 | C | 501 | LMG | C30-C31-C32-C33 |
| 33 | D | 411 | LMG | C14-C15-C16-C17 |
| 27 | a | 412 | SQD | C26-C27-C28-C29 |
| 33 | C | 519 | LMG | C18-C19-C20-C21 |
| 25 | C | 520 | BCR | C37-C22-C23-C24 |
| 23 | c | 504 | CLA | C11-C12-C13-C14 |
| 27 | a | 412 | SQD | C31-C32-C33-C34 |
| 29 | d | 407 | LHG | C19-C20-C21-C22 |
| 33 | M | 101 | LMG | C19-C20-C21-C22 |
| 28 | H | 102 | DGD | C3B-C4B-C5B-C6B |
| 33 | m | 101 | LMG | C32-C33-C34-C35 |
| 29 | l | 101 | LHG | C35-C36-C37-C38 |
| 23 | C | 514 | CLA | C10-C11-C12-C13 |
| 23 | b | 608 | CLA | C8-C10-C11-C12 |
| 23 | c | 513 | CLA | C5-C6-C7-C8 |
| 27 | a | 412 | SQD | C17-C18-C19-C20 |
| 27 | a | 412 | SQD | C29-C30-C31-C32 |
| 33 | C | 519 | LMG | C31-C32-C33-C34 |
| 28 | C | 516 | DGD | O6D-C5D-C6D-O5D |
| 28 | c | 517 | DGD | CAB-CBB-CCB-CDB |
| 27 | B | 621 | SQD | C23-C24-C25-C26 |
| 28 | H | 102 | DGD | C1A-C2A-C3A-C4A |
| 27 | A | 410 | SQD | C32-C33-C34-C35 |
| 29 | d | 407 | LHG | C10-C11-C12-C13 |
| 26 | A | 409 | PL9 | C25-C24-C26-C27 |
| 23 | b | 612 | CLA | C2-C3-C5-C6 |
| 29 | d | 409 | LHG | C7-C8-C9-C10 |
| 23 | B | 604 | CLA | C2C-C3C-CAC-CBC |
| 27 | b | 601 | SQD | C25-C26-C27-C28 |
| 29 | D | 408 | LHG | C16-C17-C18-C19 |
| 28 | C | 518 | DGD | CDB-CEB-CFB-CGB |
| 23 | A | 404 | CLA | C4C-C3C-CAC-CBC |
| 28 | c | 518 | DGD | C3A-C4A-C5A-C6A |
| 29 | d | 409 | LHG | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | F | 101 | SQD | C45-C44-O6-C1 |
| 27 | a | 412 | SQD | C11-C10-C9-C8 |
| 28 | C | 517 | DGD | C8A-C9A-CAA-CBA |
| 29 | l | 101 | LHG | C24-C25-C26-C27 |
| 33 | D | 407 | LMG | C40-C41-C42-C43 |
| 33 | c | 522 | LMG | C12-C13-C14-C15 |
| 23 | C | 506 | CLA | C16-C17-C18-C19 |
| 29 | l | 101 | LHG | C24-C23-O8-C6 |
| 29 | L | 101 | LHG | C25-C26-C27-C28 |
| 23 | B | 614 | CLA | C8-C10-C11-C12 |
| 27 | A | 410 | SQD | O6-C44-C45-C46 |
| 33 | b | 622 | LMG | C7-C8-C9-O8 |
| 33 | c | 522 | LMG | O1-C7-C8-C9 |
| 27 | A | 410 | SQD | C26-C27-C28-C29 |
| 27 | b | 601 | SQD | C15-C16-C17-C18 |
| 33 | D | 407 | LMG | C16-C17-C18-C19 |
| 33 | d | 411 | LMG | C35-C36-C37-C38 |
| 23 | C | 513 | CLA | O2A-C1-C2-C3 |
| 33 | C | 501 | LMG | C33-C34-C35-C36 |
| 27 | b | 601 | SQD | C26-C27-C28-C29 |
| 27 | b | 601 | SQD | C30-C31-C32-C33 |
| 24 | a | 407 | PHO | C4-C3-C5-C6 |
| 33 | D | 410 | LMG | C12-C13-C14-C15 |
| 27 | A | 411 | SQD | C28-C29-C30-C31 |
| 33 | c | 524 | LMG | C29-C30-C31-C32 |
| 33 | m | 101 | LMG | C14-C15-C16-C17 |
| 29 | d | 409 | LHG | O1-C1-C2-O2 |
| 23 | C | 511 | CLA | C10-C11-C12-C13 |
| 23 | C | 514 | CLA | C13-C15-C16-C17 |
| 23 | D | 403 | CLA | C10-C11-C12-C13 |
| 29 | D | 408 | LHG | C12-C13-C14-C15 |
| 29 | l | 101 | LHG | O6-C4-C5-O7 |
| 27 | A | 411 | SQD | C24-C25-C26-C27 |
| 26 | a | 410 | PL9 | C32-C33-C34-C35 |
| 29 | D | 409 | LHG | C23-C24-C25-C26 |
| 23 | B | 611 | CLA | C16-C17-C18-C19 |
| 23 | c | 509 | CLA | C2C-C3C-CAC-CBC |
| 28 | C | 516 | DGD | C6B-C7B-C8B-C9B |
| 23 | A | 404 | CLA | C2C-C3C-CAC-CBC |
| 27 | A | 411 | SQD | C19-C20-C21-C22 |
| 29 | d | 409 | LHG | C25-C26-C27-C28 |
| 33 | d | 411 | LMG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | D | 408 | LHG | C33-C34-C35-C36 |
| 29 | E | 101 | LHG | C9-C10-C11-C12 |
| 28 | A | 412 | DGD | CFA-CGA-CHA-CIA |
| 28 | A | 412 | DGD | C8B-C9B-CAB-CBB |
| 27 | a | 411 | SQD | O6-C44-C45-O47 |
| 27 | a | 412 | SQD | O47-C45-C46-O48 |
| 33 | M | 101 | LMG | O7-C8-C9-O8 |
| 23 | B | 603 | CLA | CBA-CGA-O2A-C1 |
| 29 | d | 408 | LHG | C15-C16-C17-C18 |
| 23 | B | 607 | CLA | C16-C17-C18-C19 |
| 28 | c | 517 | DGD | C8A-C9A-CAA-CBA |
| 23 | B | 613 | CLA | C5-C6-C7-C8 |
| 23 | c | 513 | CLA | C13-C15-C16-C17 |
| 28 | a | 413 | DGD | C1G-C2G-C3G-O3G |
| 29 | E | 101 | LHG | C16-C17-C18-C19 |
| 28 | c | 516 | DGD | O1B-C1B-O2G-C2G |
| 23 | B | 604 | CLA | C14-C13-C15-C16 |
| 23 | C | 505 | CLA | C11-C10-C8-C9 |
| 23 | C | 511 | CLA | C14-C13-C15-C16 |
| 23 | c | 510 | CLA | C11-C12-C13-C14 |
| 24 | A | 406 | PHO | C2C-C3C-CAC-CBC |
| 27 | F | 101 | SQD | C27-C28-C29-C30 |
| 28 | a | 413 | DGD | CAB-CBB-CCB-CDB |
| 28 | c | 516 | DGD | C2A-C3A-C4A-C5A |
| 29 | D | 408 | LHG | C28-C29-C30-C31 |
| 27 | a | 411 | SQD | C28-C29-C30-C31 |
| 29 | E | 101 | LHG | C33-C34-C35-C36 |
| 33 | D | 410 | LMG | C34-C35-C36-C37 |
| 23 | c | 507 | CLA | C16-C17-C18-C19 |
| 25 | H | 101 | BCR | C23-C24-C25-C26 |
| 25 | k | 101 | BCR | C5-C6-C7-C8 |
| 23 | c | 501 | CLA | C8-C10-C11-C12 |
| 29 | D | 408 | LHG | C18-C19-C20-C21 |
| 33 | m | 101 | LMG | C40-C41-C42-C43 |
| 25 | K | 101 | BCR | C7-C8-C9-C10 |
| 25 | x | 102 | BCR | C11-C12-C13-C14 |
| 25 | x | 102 | BCR | C17-C18-C19-C20 |
| 23 | d | 403 | CLA | O1D-CGD-O2D-CED |
| 25 | k | 101 | BCR | C14-C15-C16-C17 |
| 23 | b | 616 | CLA | C8-C10-C11-C12 |
| 29 | E | 101 | LHG | C29-C30-C31-C32 |
| 29 | L | 101 | LHG | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 506 | CLA | C16-C17-C18-C20 |
| 23 | c | 508 | CLA | C16-C17-C18-C19 |
| 33 | D | 410 | LMG | C15-C16-C17-C18 |
| 33 | c | 519 | LMG | O10-C28-O8-C9 |
| 28 | c | 516 | DGD | C2B-C3B-C4B-C5B |
| 23 | B | 605 | CLA | C15-C16-C17-C18 |
| 23 | C | 512 | CLA | C8-C10-C11-C12 |
| 29 | D | 409 | LHG | O6-C4-C5-C6 |
| 33 | C | 501 | LMG | C17-C18-C19-C20 |
| 23 | B | 604 | CLA | C11-C10-C8-C7 |
| 23 | B | 604 | CLA | C12-C13-C15-C16 |
| 23 | B | 605 | CLA | C11-C12-C13-C15 |
| 23 | B | 614 | CLA | C2-C3-C5-C6 |
| 23 | C | 506 | CLA | C12-C13-C15-C16 |
| 23 | C | 508 | CLA | C11-C10-C8-C7 |
| 23 | C | 509 | CLA | C11-C10-C8-C7 |
| 23 | C | 510 | CLA | C12-C13-C15-C16 |
| 23 | C | 511 | CLA | C12-C13-C15-C16 |
| 23 | C | 514 | CLA | C12-C13-C15-C16 |
| 23 | D | 404 | CLA | C11-C10-C8-C7 |
| 23 | D | 404 | CLA | C12-C13-C15-C16 |
| 23 | b | 604 | CLA | C11-C12-C13-C15 |
| 23 | b | 605 | CLA | C11-C10-C8-C7 |
| 23 | b | 605 | CLA | C11-C12-C13-C15 |
| 23 | b | 605 | CLA | C12-C13-C15-C16 |
| 23 | b | 609 | CLA | C11-C10-C8-C7 |
| 23 | b | 609 | CLA | C11-C12-C13-C15 |
| 23 | b | 610 | CLA | C12-C13-C15-C16 |
| 23 | b | 612 | CLA | C11-C10-C8-C7 |
| 23 | c | 501 | CLA | C11-C12-C13-C15 |
| 23 | c | 505 | CLA | C6-C7-C8-C10 |
| 23 | c | 505 | CLA | C11-C10-C8-C7 |
| 23 | c | 509 | CLA | C6-C7-C8-C10 |
| 23 | c | 510 | CLA | C11-C10-C8-C7 |
| 23 | d | 404 | CLA | C11-C12-C13-C15 |
| 27 | F | 101 | SQD | C32-C33-C34-C35 |
| 27 | a | 412 | SQD | O6-C44-C45-O47 |
| 23 | B | 601 | CLA | C15-C16-C17-C18 |
| 23 | c | 504 | CLA | C8-C10-C11-C12 |
| 23 | B | 615 | CLA | C16-C17-C18-C20 |
| 23 | c | 504 | CLA | C11-C12-C13-C15 |
| 33 | c | 519 | LMG | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 612 | CLA | C15-C16-C17-C18 |
| 28 | C | 516 | DGD | CBA-CCA-CDA-CEA |
| 25 | H | 101 | BCR | C11-C10-C9-C34 |
| 25 | H | 101 | BCR | C35-C13-C14-C15 |
| 25 | H | 101 | BCR | C16-C17-C18-C36 |
| 25 | K | 101 | BCR | C16-C17-C18-C36 |
| 25 | a | 409 | BCR | C11-C10-C9-C34 |
| 25 | b | 618 | BCR | C11-C10-C9-C34 |
| 25 | t | 101 | BCR | C16-C17-C18-C36 |
| 23 | C | 511 | CLA | C16-C17-C18-C20 |
| 28 | c | 518 | DGD | C2B-C3B-C4B-C5B |
| 33 | M | 101 | LMG | C33-C34-C35-C36 |
| 28 | C | 518 | DGD | CBB-CCB-CDB-CEB |
| 33 | c | 519 | LMG | C38-C39-C40-C41 |
| 23 | B | 604 | CLA | CAD-CBD-CGD-O2D |
| 23 | B | 610 | CLA | CAD-CBD-CGD-O2D |
| 23 | C | 506 | CLA | CAD-CBD-CGD-O2D |
| 23 | C | 511 | CLA | CAD-CBD-CGD-O2D |
| 23 | b | 604 | CLA | CAD-CBD-CGD-O2D |
| 23 | b | 608 | CLA | CAD-CBD-CGD-O2D |
| 23 | c | 509 | CLA | CAD-CBD-CGD-O2D |
| 24 | A | 406 | PHO | CAD-CBD-CGD-O2D |
| 29 | L | 101 | LHG | C10-C11-C12-C13 |
| 27 | a | 411 | SQD | C23-C24-C25-C26 |
| 33 | d | 410 | LMG | C36-C37-C38-C39 |
| 23 | B | 612 | CLA | CBA-CGA-O2A-C1 |
| 33 | C | 501 | LMG | C39-C40-C41-C42 |
| 33 | d | 410 | LMG | C39-C40-C41-C42 |
| 33 | c | 522 | LMG | C7-C8-C9-O8 |
| 27 | f | 101 | SQD | O10-C23-O48-C46 |
| 29 | D | 409 | LHG | O6-C4-C5-O7 |
| 23 | b | 608 | CLA | C5-C6-C7-C8 |
| 28 | H | 102 | DGD | CBA-CCA-CDA-CEA |
| 23 | c | 509 | CLA | CBA-CGA-O2A-C1 |
| 23 | B | 603 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 615 | CLA | C16-C17-C18-C19 |
| 28 | C | 516 | DGD | O1B-C1B-O2G-C2G |
| 23 | B | 607 | CLA | CHA-CBD-CGD-O1D |
| 23 | B | 612 | CLA | CHA-CBD-CGD-O1D |
| 23 | B | 614 | CLA | CHA-CBD-CGD-O1D |
| 23 | C | 503 | CLA | CHA-CBD-CGD-O2D |
| 23 | C | 505 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 505 | CLA | CHA-CBD-CGD-O2D |
| 23 | C | 508 | CLA | CHA-CBD-CGD-O1D |
| 23 | C | 508 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 606 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 502 | CLA | CHA-CBD-CGD-O2D |
| 23 | c | 504 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 504 | CLA | CHA-CBD-CGD-O2D |
| 23 | c | 506 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 506 | CLA | CHA-CBD-CGD-O2D |
| 23 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 508 | CLA | CHA-CBD-CGD-O1D |
| 23 | c | 512 | CLA | CHA-CBD-CGD-O1D |
| 23 | B | 612 | CLA | O1A-CGA-O2A-C1 |
| 28 | c | 517 | DGD | O1A-C1A-O1G-C1G |
| 33 | C | 519 | LMG | O10-C28-O8-C9 |
| 25 | B | 617 | BCR | C16-C17-C18-C19 |
| 25 | c | 515 | BCR | C12-C13-C14-C15 |
| 25 | x | 102 | BCR | C11-C10-C9-C8 |
| 27 | b | 601 | SQD | O6-C44-C45-O47 |
| 28 | C | 516 | DGD | O2G-C2G-C3G-O3G |
| 33 | c | 522 | LMG | O7-C8-C9-O8 |
| 23 | B | 610 | CLA | C8-C10-C11-C12 |
| 23 | C | 507 | CLA | C10-C11-C12-C13 |
| 29 | E | 101 | LHG | O1-C1-C2-O2 |
| 29 | d | 408 | LHG | O1-C1-C2-O2 |
| 29 | d | 408 | LHG | C26-C27-C28-C29 |
| 33 | M | 101 | LMG | C14-C15-C16-C17 |
| 23 | b | 610 | CLA | C3-C5-C6-C7 |
| 23 | C | 506 | CLA | C4-C3-C5-C6 |
| 23 | B | 603 | CLA | O1A-CGA-O2A-C1 |
| 29 | D | 408 | LHG | O10-C23-O8-C6 |
| 26 | A | 409 | PL9 | C13-C14-C16-C17 |
| 26 | A | 409 | PL9 | C4-C3-C7-C8 |
| 28 | C | 516 | DGD | O1G-C1A-C2A-C3A |
| 23 | C | 511 | CLA | C11-C10-C8-C9 |
| 23 | b | 609 | CLA | C11-C10-C8-C9 |
| 29 | L | 101 | LHG | C14-C15-C16-C17 |
| 23 | b | 603 | CLA | C8-C10-C11-C12 |
| 27 | A | 410 | SQD | C5-C6-S-O8 |
| 27 | b | 601 | SQD | C5-C6-S-O8 |
| 29 | D | 409 | LHG | C31-C32-C33-C34 |
| 33 | m | 101 | LMG | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | E | 101 | LHG | C10-C11-C12-C13 |
| 27 | f | 101 | SQD | C35-C36-C37-C38 |
| 25 | k | 101 | BCR | C17-C18-C19-C20 |
| 28 | H | 102 | DGD | C5A-C6A-C7A-C8A |
| 23 | c | 513 | CLA | C1A-C2A-CAA-CBA |
| 23 | b | 614 | CLA | C13-C15-C16-C17 |
| 28 | C | 516 | DGD | C4D-C5D-C6D-O5D |
| 28 | c | 518 | DGD | CCB-CDB-CEB-CFB |
| 29 | A | 413 | LHG | C24-C25-C26-C27 |
| 25 | K | 101 | BCR | C19-C20-C21-C22 |
| 23 | b | 614 | CLA | O1D-CGD-O2D-CED |
| 33 | D | 410 | LMG | C11-C12-C13-C14 |
| 33 | d | 411 | LMG | C38-C39-C40-C41 |
| 33 | C | 519 | LMG | C30-C31-C32-C33 |
| 33 | m | 101 | LMG | C36-C37-C38-C39 |
| 29 | D | 408 | LHG | C3-O3-P-O4 |
| 29 | D | 408 | LHG | C4-O6-P-O5 |
| 23 | B | 610 | CLA | C16-C17-C18-C19 |
| 28 | C | 517 | DGD | O6D-C1D-O3G-C3G |
| 23 | C | 512 | CLA | CBA-CGA-O2A-C1 |
| 28 | H | 102 | DGD | O2G-C1B-C2B-C3B |
| 28 | C | 518 | DGD | C3B-C4B-C5B-C6B |
| 33 | b | 622 | LMG | C42-C43-C44-C45 |
| 23 | c | 502 | CLA | C3-C5-C6-C7 |
| 23 | a | 406 | CLA | C15-C16-C17-C18 |
| 23 | C | 513 | CLA | C16-C17-C18-C19 |
| 23 | B | 601 | CLA | CAD-CBD-CGD-O1D |
| 23 | B | 612 | CLA | CAD-CBD-CGD-O1D |
| 23 | C | 503 | CLA | CAD-CBD-CGD-O1D |
| 23 | C | 505 | CLA | CAD-CBD-CGD-O1D |
| 23 | C | 514 | CLA | CAD-CBD-CGD-O1D |
| 23 | b | 606 | CLA | CAD-CBD-CGD-O1D |
| 23 | c | 502 | CLA | CAD-CBD-CGD-O1D |
| 23 | c | 504 | CLA | CAD-CBD-CGD-O1D |
| 23 | c | 506 | CLA | CAD-CBD-CGD-O1D |
| 23 | C | 503 | CLA | C10-C11-C12-C13 |
| 27 | A | 410 | SQD | C25-C26-C27-C28 |
| 28 | c | 518 | DGD | CAA-CBA-CCA-CDA |
| 29 | L | 101 | LHG | C19-C20-C21-C22 |
| 33 | d | 410 | LMG | C11-C12-C13-C14 |
| 23 | c | 507 | CLA | C8-C10-C11-C12 |
| 33 | b | 622 | LMG | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | E | 101 | LHG | C18-C19-C20-C21 |
| 23 | D | 404 | CLA | CBA-CGA-O2A-C1 |
| 23 | B | 606 | CLA | C11-C12-C13-C15 |
| 23 | B | 612 | CLA | C11-C10-C8-C7 |
| 23 | B | 616 | CLA | C6-C7-C8-C10 |
| 23 | C | 503 | CLA | C6-C7-C8-C10 |
| 23 | C | 504 | CLA | C6-C7-C8-C10 |
| 23 | C | 507 | CLA | C3A-C2A-CAA-CBA |
| 23 | C | 511 | CLA | C11-C10-C8-C7 |
| 23 | C | 513 | CLA | C12-C13-C15-C16 |
| 23 | b | 603 | CLA | C6-C7-C8-C10 |
| 23 | b | 608 | CLA | C11-C12-C13-C15 |
| 23 | b | 616 | CLA | C11-C10-C8-C7 |
| 23 | c | 503 | CLA | C11-C10-C8-C7 |
| 23 | c | 509 | CLA | C11-C12-C13-C15 |
| 23 | c | 512 | CLA | C11-C10-C8-C7 |
| 23 | d | 403 | CLA | C6-C7-C8-C10 |
| 24 | A | 406 | PHO | C12-C13-C15-C16 |
| 27 | f | 101 | SQD | C24-C25-C26-C27 |
| 28 | H | 102 | DGD | C9B-CAB-CBB-CCB |
| 27 | B | 621 | SQD | C25-C26-C27-C28 |
| 28 | c | 516 | DGD | C5B-C6B-C7B-C8B |
| 23 | B | 601 | CLA | C8-C10-C11-C12 |
| 27 | A | 411 | SQD | C32-C33-C34-C35 |
| 23 | D | 404 | CLA | O1A-CGA-O2A-C1 |
| 28 | c | 518 | DGD | C4A-C5A-C6A-C7A |
| 28 | A | 412 | DGD | C1G-C2G-C3G-O3G |
| 28 | C | 516 | DGD | C1G-C2G-C3G-O3G |
| 33 | M | 101 | LMG | C7-C8-C9-O8 |
| 29 | L | 101 | LHG | O9-C7-O7-C5 |
| 28 | C | 516 | DGD | O1G-C1G-C2G-O2G |
| 33 | c | 522 | LMG | O1-C7-C8-O7 |
| 28 | C | 518 | DGD | C4B-C5B-C6B-C7B |
| 28 | h | 101 | DGD | C5A-C6A-C7A-C8A |
| 29 | A | 413 | LHG | C29-C30-C31-C32 |
| 28 | c | 517 | DGD | C2G-C3G-O3G-C1D |
| 23 | B | 612 | CLA | C8-C10-C11-C12 |
| 23 | b | 614 | CLA | C5-C6-C7-C8 |
| 28 | C | 518 | DGD | C2A-C3A-C4A-C5A |
| 23 | c | 509 | CLA | O1A-CGA-O2A-C1 |
| 23 | b | 612 | CLA | C5-C6-C7-C8 |
| 23 | B | 601 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | c | 517 | DGD | C7B-C8B-C9B-CAB |
| 29 | L | 101 | LHG | C31-C32-C33-C34 |
| 29 | l | 101 | LHG | C19-C20-C21-C22 |
| 23 | D | 403 | CLA | C14-C13-C15-C16 |
| 23 | c | 513 | CLA | C14-C13-C15-C16 |
| 25 | b | 618 | BCR | C6-C7-C8-C9 |
| 25 | c | 514 | BCR | C22-C23-C24-C25 |
| 33 | C | 519 | LMG | C14-C15-C16-C17 |
| 23 | C | 513 | CLA | C16-C17-C18-C20 |
| 27 | A | 410 | SQD | C30-C31-C32-C33 |
| 29 | A | 413 | LHG | C19-C20-C21-C22 |
| 29 | d | 408 | LHG | C13-C14-C15-C16 |
| 23 | C | 512 | CLA | O1A-CGA-O2A-C1 |
| 23 | c | 506 | CLA | O1A-CGA-O2A-C1 |
| 29 | e | 101 | LHG | C7-C8-C9-C10 |
| 33 | D | 407 | LMG | C28-C29-C30-C31 |
| 23 | b | 610 | CLA | C16-C17-C18-C19 |
| 23 | d | 404 | CLA | C16-C17-C18-C19 |
| 29 | L | 101 | LHG | C29-C30-C31-C32 |
| 28 | H | 102 | DGD | CCB-CDB-CEB-CFB |
| 29 | d | 407 | LHG | C31-C32-C33-C34 |
| 23 | C | 506 | CLA | C2-C3-C5-C6 |
| 29 | d | 407 | LHG | C27-C28-C29-C30 |
| 27 | B | 621 | SQD | C11-C10-C9-C8 |
| 28 | c | 517 | DGD | CDA-CEA-CFA-CGA |
| 28 | c | 516 | DGD | C8A-C9A-CAA-CBA |
| 28 | a | 413 | DGD | C1G-C2G-O2G-C1B |
| 33 | C | 501 | LMG | C9-C8-O7-C10 |
| 33 | D | 410 | LMG | C9-C8-O7-C10 |
| 29 | D | 409 | LHG | C1-C2-C3-O3 |
| 23 | b | 615 | CLA | C2A-CAA-CBA-CGA |
| 23 | A | 404 | CLA | C2-C1-O2A-CGA |
| 23 | a | 405 | CLA | C2-C1-O2A-CGA |
| 23 | b | 613 | CLA | C2-C1-O2A-CGA |
| 23 | c | 512 | CLA | C2-C1-O2A-CGA |
| 33 | m | 101 | LMG | C15-C16-C17-C18 |
| 29 | D | 408 | LHG | C23-C24-C25-C26 |
| 28 | c | 518 | DGD | C5A-C6A-C7A-C8A |
| 33 | b | 622 | LMG | C30-C31-C32-C33 |
| 33 | c | 524 | LMG | C19-C20-C21-C22 |
| 33 | d | 410 | LMG | C29-C30-C31-C32 |
| 29 | E | 101 | LHG | O6-C4-C5-O7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | c | 511 | CLA | C15-C16-C17-C18 |
| 26 | A | 409 | PL9 | C20-C19-C21-C22 |
| 25 | b | 618 | BCR | C1-C6-C7-C8 |
| 27 | A | 411 | SQD | C30-C31-C32-C33 |
| 23 | C | 503 | CLA | C15-C16-C17-C18 |
| 28 | c | 516 | DGD | CAB-CBB-CCB-CDB |
| 23 | c | 512 | CLA | C16-C17-C18-C19 |
| 28 | C | 516 | DGD | O6E-C1E-O5D-C6D |
| 28 | c | 516 | DGD | O6E-C1E-O5D-C6D |
| 33 | C | 519 | LMG | O6-C1-O1-C7 |
| 27 | b | 601 | SQD | O47-C45-C46-O48 |
| 33 | c | 524 | LMG | C32-C33-C34-C35 |
| 29 | E | 101 | LHG | C4-O6-P-O3 |
| 29 | d | 408 | LHG | C3-O3-P-O6 |
| 28 | C | 516 | DGD | CAA-CBA-CCA-CDA |
| 33 | c | 522 | LMG | C37-C38-C39-C40 |
| 29 | D | 409 | LHG | C16-C17-C18-C19 |
| 23 | d | 403 | CLA | C3-C5-C6-C7 |
| 23 | c | 512 | CLA | C4-C3-C5-C6 |
| 28 | H | 102 | DGD | C6B-C7B-C8B-C9B |
| 33 | C | 501 | LMG | C11-C12-C13-C14 |
| 23 | B | 604 | CLA | C11-C12-C13-C15 |
| 23 | C | 510 | CLA | C11-C10-C8-C7 |
| 23 | C | 511 | CLA | C6-C7-C8-C10 |
| 23 | a | 405 | CLA | C11-C10-C8-C7 |
| 24 | a | 407 | PHO | C2-C3-C5-C6 |
| 29 | E | 101 | LHG | C30-C31-C32-C33 |
| 23 | B | 604 | CLA | C11-C12-C13-C14 |
| 23 | B | 605 | CLA | C14-C13-C15-C16 |
| 23 | B | 606 | CLA | C11-C12-C13-C14 |
| 23 | B | 612 | CLA | C11-C10-C8-C9 |
| 23 | C | 506 | CLA | C14-C13-C15-C16 |
| 23 | C | 510 | CLA | C14-C13-C15-C16 |
| 23 | D | 404 | CLA | C14-C13-C15-C16 |
| 23 | b | 605 | CLA | C11-C10-C8-C9 |
| 23 | b | 606 | CLA | C11-C12-C13-C14 |
| 23 | b | 608 | CLA | C11-C12-C13-C14 |
| 23 | b | 615 | CLA | C14-C13-C15-C16 |
| 23 | b | 616 | CLA | C11-C10-C8-C9 |
| 23 | c | 503 | CLA | C11-C10-C8-C9 |
| 23 | c | 513 | CLA | C6-C7-C8-C9 |
| 24 | a | 407 | PHO | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | b | 619 | BCR | C9-C10-C11-C12 |
| 25 | d | 405 | BCR | C9-C10-C11-C12 |
| 33 | D | 407 | LMG | C15-C16-C17-C18 |
| 33 | D | 407 | LMG | C21-C22-C23-C24 |
| 23 | C | 504 | CLA | C10-C11-C12-C13 |
| 29 | L | 101 | LHG | C24-C25-C26-C27 |
| 28 | H | 102 | DGD | C1B-C2B-C3B-C4B |
| 23 | b | 610 | CLA | C16-C17-C18-C20 |
| 29 | l | 101 | LHG | C14-C15-C16-C17 |
| 29 | E | 101 | LHG | C2-C3-O3-P |
| 29 | d | 409 | LHG | C2-C3-O3-P |
| 28 | c | 517 | DGD | C3A-C4A-C5A-C6A |
| 25 | k | 101 | BCR | C11-C12-C13-C14 |
| 28 | H | 102 | DGD | CAA-CBA-CCA-CDA |
| 28 | a | 413 | DGD | C1A-C2A-C3A-C4A |
| 33 | c | 522 | LMG | C28-C29-C30-C31 |
| 23 | B | 609 | CLA | C16-C17-C18-C19 |
| 23 | C | 511 | CLA | C16-C17-C18-C19 |
| 23 | A | 407 | CLA | CBA-CGA-O2A-C1 |
| 23 | b | 615 | CLA | CBA-CGA-O2A-C1 |
| 23 | c | 506 | CLA | CBA-CGA-O2A-C1 |
| 28 | c | 518 | DGD | C9A-CAA-CBA-CCA |
| 28 | c | 516 | DGD | C7B-C8B-C9B-CAB |
| 24 | A | 406 | PHO | CBA-CGA-O2A-C1 |
| 27 | a | 412 | SQD | C27-C28-C29-C30 |
| 23 | C | 502 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 602 | CLA | C16-C17-C18-C19 |
| 25 | K | 101 | BCR | C13-C14-C15-C16 |
| 25 | c | 514 | BCR | C15-C16-C17-C18 |
| 25 | c | 521 | BCR | C9-C10-C11-C12 |
| 33 | c | 519 | LMG | C4-C5-C6-O5 |
| 27 | a | 411 | SQD | C24-C25-C26-C27 |
| 25 | A | 408 | BCR | C18-C19-C20-C21 |
| 23 | a | 406 | CLA | C8-C10-C11-C12 |
| 23 | a | 406 | CLA | C13-C15-C16-C17 |
| 33 | M | 101 | LMG | C40-C41-C42-C43 |
| 23 | C | 503 | CLA | O1A-CGA-O2A-C1 |
| 28 | A | 412 | DGD | CCB-CDB-CEB-CFB |
| 23 | B | 609 | CLA | C5-C6-C7-C8 |
| 29 | l | 101 | LHG | C34-C35-C36-C37 |
| 23 | B | 613 | CLA | C2-C1-O2A-CGA |
| 23 | C | 514 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | b | 614 | CLA | C2-C1-O2A-CGA |
| 23 | B | 602 | CLA | C8-C10-C11-C12 |
| 28 | C | 516 | DGD | CAB-CBB-CCB-CDB |
| 28 | c | 517 | DGD | CCA-CDA-CEA-CFA |
| 28 | h | 101 | DGD | C7B-C8B-C9B-CAB |
| 28 | c | 517 | DGD | O1G-C1G-C2G-O2G |
| 33 | b | 622 | LMG | O7-C8-C9-O8 |
| 28 | C | 518 | DGD | CDA-CEA-CFA-CGA |
| 33 | M | 101 | LMG | C32-C33-C34-C35 |
| 27 | b | 601 | SQD | O49-C7-O47-C45 |
| 27 | A | 410 | SQD | C35-C36-C37-C38 |
| 26 | a | 410 | PL9 | C4-C3-C7-C8 |
| 27 | F | 101 | SQD | O48-C23-C24-C25 |
| 23 | b | 603 | CLA | C14-C13-C15-C16 |
| 23 | b | 615 | CLA | C6-C7-C8-C9 |
| 28 | A | 412 | DGD | C3B-C4B-C5B-C6B |
| 23 | C | 507 | CLA | CBA-CGA-O2A-C1 |
| 23 | c | 503 | CLA | C15-C16-C17-C18 |
| 25 | B | 619 | BCR | C20-C21-C22-C37 |
| 25 | C | 515 | BCR | C35-C13-C14-C15 |
| 23 | b | 615 | CLA | O1A-CGA-O2A-C1 |
| 27 | A | 410 | SQD | C17-C18-C19-C20 |
| 29 | e | 101 | LHG | C13-C14-C15-C16 |
| 23 | D | 404 | CLA | O2A-C1-C2-C3 |
| 23 | b | 602 | CLA | O2A-C1-C2-C3 |
| 33 | D | 410 | LMG | C29-C30-C31-C32 |
| 23 | c | 508 | CLA | C15-C16-C17-C18 |
| 27 | f | 101 | SQD | C44-C45-O47-C7 |
| 27 | f | 101 | SQD | C46-C45-O47-C7 |
| 28 | a | 413 | DGD | O2G-C1B-C2B-C3B |
| 23 | B | 606 | CLA | C6-C7-C8-C10 |
| 23 | a | 406 | CLA | C11-C10-C8-C7 |
| 23 | c | 502 | CLA | C6-C7-C8-C10 |
| 23 | c | 511 | CLA | C6-C7-C8-C10 |
| 23 | c | 512 | CLA | C6-C7-C8-C10 |
| 23 | c | 512 | CLA | C12-C13-C15-C16 |
| 26 | a | 410 | PL9 | C38-C39-C41-C42 |
| 23 | B | 610 | CLA | C2C-C3C-CAC-CBC |
| 23 | A | 407 | CLA | O1A-CGA-O2A-C1 |
| 25 | d | 405 | BCR | C19-C20-C21-C22 |
| 33 | M | 101 | LMG | O6-C5-C6-O5 |
| 27 | B | 621 | SQD | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | b | 622 | LMG | C12-C13-C14-C15 |
| 23 | B | 610 | CLA | C16-C17-C18-C20 |
| 23 | c | 501 | CLA | C2A-CAA-CBA-CGA |
| 33 | D | 410 | LMG | C31-C32-C33-C34 |
| 24 | A | 406 | PHO | O1A-CGA-O2A-C1 |
| 23 | C | 506 | CLA | C8-C10-C11-C12 |
| 28 | A | 412 | DGD | CBB-CCB-CDB-CEB |
| 23 | B | 602 | CLA | C16-C17-C18-C20 |
| 33 | D | 411 | LMG | C29-C30-C31-C32 |
| 23 | c | 510 | CLA | C4-C3-C5-C6 |
| 28 | c | 516 | DGD | CCA-CDA-CEA-CFA |
| 23 | B | 604 | CLA | C15-C16-C17-C18 |
| 23 | D | 402 | CLA | C13-C15-C16-C17 |
| 29 | d | 408 | LHG | C23-C24-C25-C26 |
| 25 | A | 408 | BCR | C20-C21-C22-C23 |
| 27 | A | 411 | SQD | O47-C45-C46-O48 |
| 28 | a | 413 | DGD | O1G-C1G-C2G-O2G |
| 29 | e | 101 | LHG | O7-C5-C6-O8 |
| 33 | m | 101 | LMG | C39-C40-C41-C42 |
| 33 | M | 101 | LMG | C29-C30-C31-C32 |
| 33 | b | 622 | LMG | O8-C28-C29-C30 |
| 29 | d | 407 | LHG | C24-C25-C26-C27 |
| 23 | b | 610 | CLA | O1D-CGD-O2D-CED |
| 26 | a | 410 | PL9 | C7-C8-C9-C10 |
| 23 | C | 507 | CLA | C2-C1-O2A-CGA |
| 23 | B | 601 | CLA | C2-C3-C5-C6 |
| 28 | A | 412 | DGD | CAB-CBB-CCB-CDB |
| 23 | B | 606 | CLA | C14-C13-C15-C16 |
| 23 | C | 507 | CLA | C11-C10-C8-C9 |
| 23 | C | 511 | CLA | C6-C7-C8-C9 |
| 23 | c | 510 | CLA | C14-C13-C15-C16 |
| 27 | A | 411 | SQD | C26-C27-C28-C29 |
| 23 | b | 610 | CLA | CBD-CGD-O2D-CED |
| 23 | C | 507 | CLA | O1A-CGA-O2A-C1 |
| 27 | a | 411 | SQD | C16-C17-C18-C19 |
| 29 | D | 409 | LHG | C15-C16-C17-C18 |
| 28 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 33 | c | 519 | LMG | C40-C41-C42-C43 |
| 23 | D | 403 | CLA | C16-C17-C18-C19 |
| 23 | b | 602 | CLA | C16-C17-C18-C20 |
| 23 | c | 509 | CLA | C4C-C3C-CAC-CBC |
| 24 | A | 406 | PHO | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | C | 517 | DGD | O1A-C1A-O1G-C1G |
| 25 | C | 520 | BCR | C23-C24-C25-C30 |
| 25 | H | 101 | BCR | C23-C24-C25-C30 |
| 25 | K | 101 | BCR | C23-C24-C25-C30 |
| 25 | b | 618 | BCR | C5-C6-C7-C8 |
| 25 | d | 405 | BCR | C23-C24-C25-C30 |
| 28 | h | 101 | DGD | O2G-C1B-C2B-C3B |
| 28 | c | 516 | DGD | O1G-C1G-C2G-C3G |
| 33 | C | 519 | LMG | O1-C7-C8-C9 |
| 23 | b | 609 | CLA | C13-C15-C16-C17 |
| 33 | d | 410 | LMG | C12-C13-C14-C15 |
| 27 | a | 412 | SQD | C19-C20-C21-C22 |
| 29 | E | 101 | LHG | C28-C29-C30-C31 |
| 23 | B | 613 | CLA | C4-C3-C5-C6 |
| 23 | c | 508 | CLA | C4-C3-C5-C6 |
| 23 | d | 404 | CLA | C13-C15-C16-C17 |
| 23 | c | 512 | CLA | C2-C3-C5-C6 |
| 28 | c | 516 | DGD | C5D-C6D-O5D-C1E |
| 33 | m | 101 | LMG | C8-C7-O1-C1 |
| 28 | c | 518 | DGD | C7A-C8A-C9A-CAA |
| 33 | m | 101 | LMG | C33-C34-C35-C36 |
| 23 | C | 502 | CLA | C16-C17-C18-C20 |
| 23 | c | 512 | CLA | C16-C17-C18-C20 |
| 23 | c | 508 | CLA | CBA-CGA-O2A-C1 |
| 28 | h | 101 | DGD | O6E-C1E-O5D-C6D |
| 26 | a | 410 | PL9 | C35-C34-C36-C37 |
| 23 | b | 603 | CLA | C12-C13-C15-C16 |
| 23 | b | 610 | CLA | C2-C3-C5-C6 |
| 27 | B | 621 | SQD | C33-C34-C35-C36 |
| 28 | c | 516 | DGD | CDB-CEB-CFB-CGB |
| 33 | D | 410 | LMG | C14-C15-C16-C17 |
| 23 | C | 514 | CLA | C4C-C3C-CAC-CBC |
| 28 | C | 516 | DGD | C5A-C6A-C7A-C8A |
| 28 | C | 516 | DGD | C2E-C1E-O5D-C6D |
| 28 | C | 517 | DGD | C2D-C1D-O3G-C3G |
| 23 | b | 614 | CLA | CAA-CBA-CGA-O2A |
| 26 | d | 406 | PL9 | C2-C3-C7-C8 |
| 23 | C | 503 | CLA | CBA-CGA-O2A-C1 |
| 23 | d | 402 | CLA | CBA-CGA-O2A-C1 |
| 33 | D | 411 | LMG | C30-C31-C32-C33 |
| 23 | b | 606 | CLA | C8-C10-C11-C12 |
| 26 | d | 406 | PL9 | C33-C34-C36-C37 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 604 | CLA | C4C-C3C-CAC-CBC |
| 33 | c | 524 | LMG | O8-C28-C29-C30 |
| 23 | B | 610 | CLA | C4C-C3C-CAC-CBC |
| 23 | B | 603 | CLA | C11-C10-C8-C9 |
| 23 | B | 610 | CLA | C14-C13-C15-C16 |
| 23 | C | 513 | CLA | C14-C13-C15-C16 |
| 23 | C | 514 | CLA | C14-C13-C15-C16 |
| 23 | b | 610 | CLA | C11-C10-C8-C9 |
| 23 | c | 512 | CLA | C11-C10-C8-C9 |
| 23 | B | 616 | CLA | O1D-CGD-O2D-CED |
| 23 | B | 612 | CLA | CAA-CBA-CGA-O2A |
| 23 | A | 407 | CLA | CAD-CBD-CGD-O2D |
| 23 | B | 603 | CLA | CAD-CBD-CGD-O2D |
| 23 | B | 605 | CLA | CAD-CBD-CGD-O2D |
| 23 | B | 609 | CLA | CAD-CBD-CGD-O2D |
| 23 | B | 616 | CLA | CAD-CBD-CGD-O2D |
| 23 | C | 510 | CLA | CAD-CBD-CGD-O2D |
| 23 | C | 513 | CLA | CAD-CBD-CGD-O2D |
| 23 | b | 602 | CLA | CAD-CBD-CGD-O2D |
| 23 | b | 605 | CLA | CAD-CBD-CGD-O2D |
| 23 | c | 508 | CLA | CAD-CBD-CGD-O2D |
| 23 | c | 510 | CLA | CAD-CBD-CGD-O2D |
| 23 | c | 512 | CLA | CAD-CBD-CGD-O2D |
| 24 | a | 407 | PHO | CAD-CBD-CGD-O2D |
| 26 | a | 410 | PL9 | C37-C38-C39-C40 |
| 29 | L | 101 | LHG | C13-C14-C15-C16 |
| 23 | C | 510 | CLA | C5-C6-C7-C8 |
| 23 | b | 613 | CLA | CAA-CBA-CGA-O2A |
| 27 | A | 410 | SQD | O47-C7-C8-C9 |
| 28 | C | 516 | DGD | CDA-CEA-CFA-CGA |
| 25 | b | 619 | BCR | C22-C23-C24-C25 |
| 23 | B | 602 | CLA | C15-C16-C17-C18 |
| 28 | H | 102 | DGD | C5B-C6B-C7B-C8B |
| 23 | c | 510 | CLA | C2-C3-C5-C6 |
| 23 | c | 509 | CLA | CAA-CBA-CGA-O2A |
| 27 | B | 621 | SQD | O47-C7-C8-C9 |
| 25 | B | 619 | BCR | C11-C12-C13-C14 |
| 25 | Z | 101 | BCR | C7-C8-C9-C10 |
| 25 | Z | 101 | BCR | C11-C12-C13-C14 |
| 25 | t | 101 | BCR | C17-C18-C19-C20 |
| 29 | e | 101 | LHG | C25-C26-C27-C28 |
| 27 | b | 601 | SQD | O6-C44-C45-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | e | 101 | LHG | C4-C5-C6-O8 |
| 33 | C | 501 | LMG | O1-C7-C8-C9 |
| 23 | C | 504 | CLA | C15-C16-C17-C18 |
| 23 | b | 617 | CLA | C10-C11-C12-C13 |
| 33 | m | 101 | LMG | O8-C28-C29-C30 |
| 23 | B | 603 | CLA | C15-C16-C17-C18 |
| 23 | B | 604 | CLA | O2A-C1-C2-C3 |
| 23 | D | 403 | CLA | O2A-C1-C2-C3 |
| 23 | B | 614 | CLA | C2A-CAA-CBA-CGA |
| 23 | b | 610 | CLA | C13-C15-C16-C17 |
| 33 | C | 519 | LMG | C32-C33-C34-C35 |
| 29 | d | 407 | LHG | C11-C10-C9-C8 |
| 23 | B | 607 | CLA | CHA-CBD-CGD-O2D |
| 23 | B | 610 | CLA | CHA-CBD-CGD-O2D |
| 23 | B | 612 | CLA | CHA-CBD-CGD-O2D |
| 23 | B | 614 | CLA | CHA-CBD-CGD-O2D |
| 23 | C | 511 | CLA | CHA-CBD-CGD-O2D |
| 23 | a | 406 | CLA | CHA-CBD-CGD-O1D |
| 23 | a | 406 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 604 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 606 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 608 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 612 | CLA | CHA-CBD-CGD-O1D |
| 23 | b | 612 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 615 | CLA | CHA-CBD-CGD-O1D |
| 23 | b | 615 | CLA | CHA-CBD-CGD-O2D |
| 23 | b | 617 | CLA | CHA-CBD-CGD-O2D |
| 23 | c | 508 | CLA | CHA-CBD-CGD-O2D |
| 23 | d | 402 | CLA | CHA-CBD-CGD-O1D |
| 23 | d | 402 | CLA | CHA-CBD-CGD-O2D |
| 24 | D | 401 | PHO | CHA-CBD-CGD-O1D |
| 24 | D | 401 | PHO | CHA-CBD-CGD-O2D |
| 24 | d | 401 | PHO | CHA-CBD-CGD-O2D |
| 25 | c | 521 | BCR | C13-C14-C15-C16 |
| 27 | a | 411 | SQD | O47-C7-C8-C9 |
| 28 | c | 516 | DGD | CBB-CCB-CDB-CEB |
| 33 | D | 407 | LMG | C31-C32-C33-C34 |
| 25 | B | 617 | BCR | C11-C10-C9-C8 |
| 29 | L | 101 | LHG | O7-C7-C8-C9 |
| 23 | B | 613 | CLA | CAA-CBA-CGA-O2A |
| 23 | c | 501 | CLA | CAA-CBA-CGA-O2A |
| 27 | a | 411 | SQD | O48-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 602 | CLA | C2A-CAA-CBA-CGA |
| 23 | C | 509 | CLA | C16-C17-C18-C19 |
| 23 | C | 514 | CLA | CBA-CGA-O2A-C1 |
| 23 | d | 404 | CLA | CBA-CGA-O2A-C1 |
| 23 | B | 612 | CLA | C11-C12-C13-C15 |
| 23 | b | 603 | CLA | C11-C12-C13-C15 |
| 27 | a | 411 | SQD | C25-C26-C27-C28 |
| 29 | d | 408 | LHG | C31-C32-C33-C34 |
| 33 | C | 501 | LMG | C34-C35-C36-C37 |
| 23 | B | 616 | CLA | C6-C7-C8-C9 |
| 23 | a | 406 | CLA | C11-C10-C8-C9 |
| 23 | a | 408 | CLA | C6-C7-C8-C9 |
| 23 | b | 603 | CLA | C6-C7-C8-C9 |
| 23 | c | 512 | CLA | C14-C13-C15-C16 |
| 23 | d | 403 | CLA | C6-C7-C8-C9 |
| 27 | B | 621 | SQD | C7-C8-C9-C10 |
| 29 | D | 409 | LHG | C28-C29-C30-C31 |
| 23 | B | 606 | CLA | C16-C17-C18-C19 |
| 23 | b | 602 | CLA | C16-C17-C18-C19 |
| 23 | c | 513 | CLA | C3-C5-C6-C7 |
| 23 | c | 508 | CLA | O1A-CGA-O2A-C1 |
| 28 | H | 102 | DGD | CDB-CEB-CFB-CGB |
| 26 | D | 406 | PL9 | C21-C22-C23-C24 |
| 23 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 23 | b | 604 | CLA | C4-C3-C5-C6 |
| 23 | B | 610 | CLA | CBD-CGD-O2D-CED |
| 29 | e | 101 | LHG | O10-C23-C24-C25 |
| 25 | H | 101 | BCR | C17-C18-C19-C20 |
| 25 | c | 514 | BCR | C7-C8-C9-C10 |
| 29 | D | 409 | LHG | C24-C23-O8-C6 |
| 28 | C | 516 | DGD | C3B-C4B-C5B-C6B |
| 33 | m | 101 | LMG | C21-C22-C23-C24 |
| 23 | B | 602 | CLA | C1A-C2A-CAA-CBA |
| 23 | C | 507 | CLA | C1A-C2A-CAA-CBA |
| 23 | C | 514 | CLA | C1A-C2A-CAA-CBA |
| 27 | a | 411 | SQD | C29-C30-C31-C32 |
| 28 | c | 518 | DGD | C9B-CAB-CBB-CCB |
| 23 | c | 506 | CLA | C10-C11-C12-C13 |
| 23 | D | 403 | CLA | C2-C1-O2A-CGA |
| 23 | B | 607 | CLA | C15-C16-C17-C18 |
| 23 | B | 612 | CLA | CAA-CBA-CGA-O1A |
| 28 | c | 518 | DGD | O1B-C1B-C2B-C3B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | h | 101 | DGD | C3B-C4B-C5B-C6B |
| 27 | f | 101 | SQD | C44-C45-C46-O48 |
| 28 | h | 101 | DGD | C1G-C2G-C3G-O3G |
| 23 | C | 510 | CLA | C8-C10-C11-C12 |
| 23 | b | 602 | CLA | C13-C15-C16-C17 |
| 23 | B | 610 | CLA | C2A-CAA-CBA-CGA |
| 23 | b | 614 | CLA | CBD-CGD-O2D-CED |
| 27 | B | 621 | SQD | O49-C7-C8-C9 |
| 23 | b | 613 | CLA | C8-C10-C11-C12 |
| 23 | b | 610 | CLA | C4-C3-C5-C6 |
| 23 | b | 613 | CLA | CAA-CBA-CGA-O1A |
| 23 | b | 614 | CLA | CAA-CBA-CGA-O1A |
| 29 | D | 409 | LHG | O10-C23-C24-C25 |
| 23 | b | 604 | CLA | C2-C3-C5-C6 |
| 25 | Z | 101 | BCR | C6-C7-C8-C9 |
| 27 | A | 411 | SQD | C16-C17-C18-C19 |
| 29 | E | 101 | LHG | C4-O6-P-O5 |
| 29 | d | 408 | LHG | C3-O3-P-O5 |
| 28 | a | 413 | DGD | C7A-C8A-C9A-CAA |
| 23 | c | 501 | CLA | CAA-CBA-CGA-O1A |
| 28 | c | 517 | DGD | C9A-CAA-CBA-CCA |
| 29 | E | 101 | LHG | C14-C15-C16-C17 |
| 23 | b | 614 | CLA | C15-C16-C17-C18 |
| 23 | C | 514 | CLA | C2C-C3C-CAC-CBC |
| 27 | b | 601 | SQD | C14-C15-C16-C17 |
| 23 | C | 514 | CLA | O1A-CGA-O2A-C1 |
| 23 | C | 506 | CLA | CAA-CBA-CGA-O2A |
| 28 | A | 412 | DGD | C7A-C8A-C9A-CAA |
| 27 | f | 101 | SQD | C27-C28-C29-C30 |
| 23 | B | 603 | CLA | C10-C11-C12-C13 |
| 23 | c | 509 | CLA | C8-C10-C11-C12 |
| 23 | C | 513 | CLA | O1D-CGD-O2D-CED |
| 23 | B | 603 | CLA | C4-C3-C5-C6 |
| 23 | B | 603 | CLA | C5-C6-C7-C8 |
| 23 | B | 607 | CLA | CAD-CBD-CGD-O1D |
| 23 | C | 507 | CLA | CAD-CBD-CGD-O1D |
| 23 | b | 610 | CLA | CAD-CBD-CGD-O1D |
| 28 | C | 516 | DGD | O1B-C1B-C2B-C3B |
| 28 | h | 101 | DGD | C6B-C7B-C8B-C9B |
| 29 | L | 101 | LHG | C11-C12-C13-C14 |
| 33 | D | 407 | LMG | O7-C10-C11-C12 |
| 23 | a | 405 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | b | 603 | CLA | C11-C12-C13-C14 |
| 23 | b | 614 | CLA | C14-C13-C15-C16 |
| 33 | C | 519 | LMG | C39-C40-C41-C42 |
| 23 | B | 601 | CLA | CAA-CBA-CGA-O2A |
| 27 | b | 601 | SQD | O47-C7-C8-C9 |
| 33 | m | 101 | LMG | O7-C10-C11-C12 |
| 28 | C | 516 | DGD | C6A-C7A-C8A-C9A |
| 27 | f | 101 | SQD | C30-C31-C32-C33 |
| 28 | c | 516 | DGD | O2G-C1B-C2B-C3B |
| 26 | a | 410 | PL9 | C21-C22-C23-C24 |
| 23 | b | 605 | CLA | C13-C15-C16-C17 |
| 23 | d | 402 | CLA | C2C-C3C-CAC-CBC |
| 27 | f | 101 | SQD | C26-C27-C28-C29 |
| 33 | C | 501 | LMG | C37-C38-C39-C40 |
| 23 | c | 505 | CLA | C4-C3-C5-C6 |
| 23 | C | 508 | CLA | C5-C6-C7-C8 |
| 33 | D | 410 | LMG | C16-C17-C18-C19 |
| 23 | B | 606 | CLA | C12-C13-C15-C16 |
| 23 | D | 403 | CLA | C6-C7-C8-C10 |
| 23 | D | 403 | CLA | C11-C10-C8-C7 |
| 23 | b | 607 | CLA | C11-C10-C8-C7 |
| 23 | b | 612 | CLA | C6-C7-C8-C10 |
| 23 | c | 505 | CLA | C2-C3-C5-C6 |
| 23 | c | 513 | CLA | C6-C7-C8-C10 |
| 23 | d | 403 | CLA | C11-C12-C13-C15 |
| 24 | d | 401 | PHO | C2C-C3C-CAC-CBC |
| 23 | a | 408 | CLA | CAA-CBA-CGA-O2A |
| 28 | C | 517 | DGD | O1G-C1A-C2A-C3A |
| 28 | c | 518 | DGD | O1G-C1A-C2A-C3A |
| 25 | b | 619 | BCR | C21-C22-C23-C24 |
| 25 | c | 514 | BCR | C11-C12-C13-C14 |
| 25 | x | 102 | BCR | C7-C8-C9-C10 |
| 33 | M | 101 | LMG | O10-C28-C29-C30 |
| 25 | C | 520 | BCR | C19-C20-C21-C22 |
| 33 | b | 622 | LMG | O6-C1-O1-C7 |
| 23 | B | 612 | CLA | C2C-C3C-CAC-CBC |
| 23 | B | 601 | CLA | CAA-CBA-CGA-O1A |
| 23 | B | 613 | CLA | CAA-CBA-CGA-O1A |
| 23 | b | 613 | CLA | C3-C5-C6-C7 |
| 28 | C | 518 | DGD | C8A-C9A-CAA-CBA |
| 23 | c | 505 | CLA | C10-C11-C12-C13 |
| 26 | D | 406 | PL9 | C36-C37-C38-C39 |

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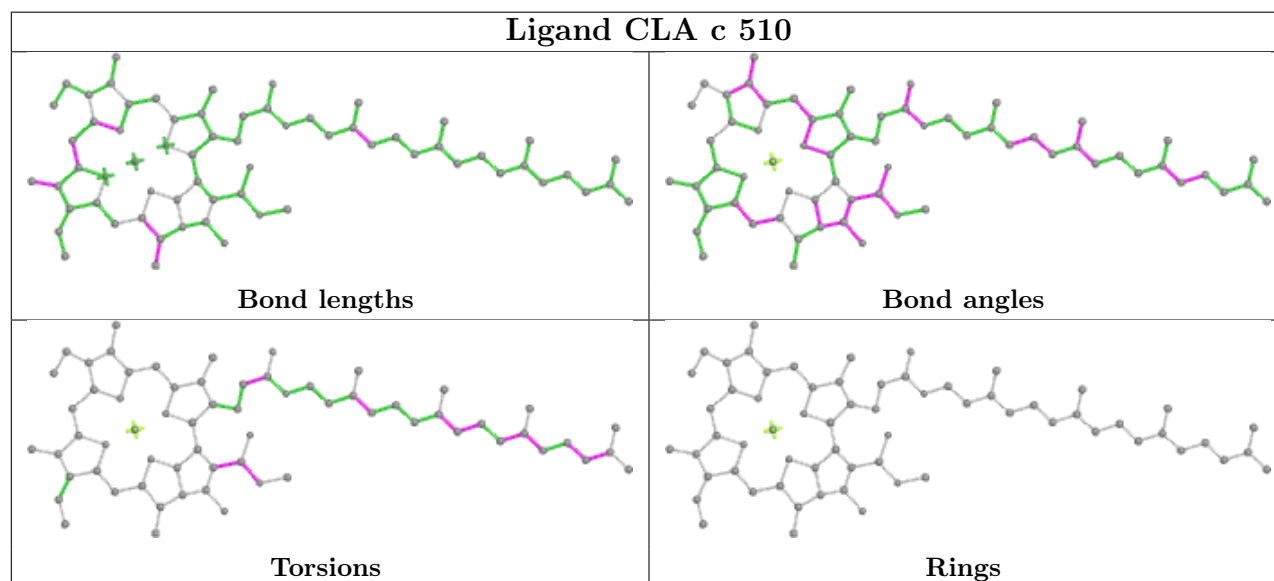
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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | d | 404 | CLA | O1A-CGA-O2A-C1 |
| 28 | C | 516 | DGD | O2G-C1B-C2B-C3B |
| 29 | L | 101 | LHG | C15-C16-C17-C18 |
| 23 | c | 510 | CLA | CAA-CBA-CGA-O1A |
| 33 | m | 101 | LMG | O9-C10-C11-C12 |
| 23 | B | 606 | CLA | C13-C15-C16-C17 |

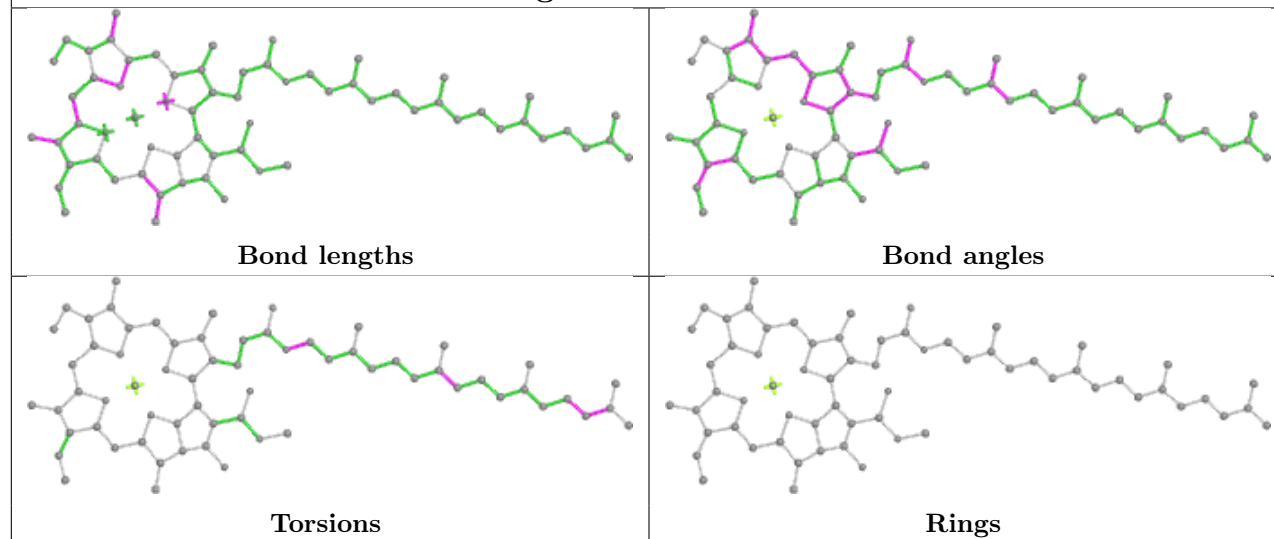
There are no ring outliers.

No monomer is involved in short contacts.

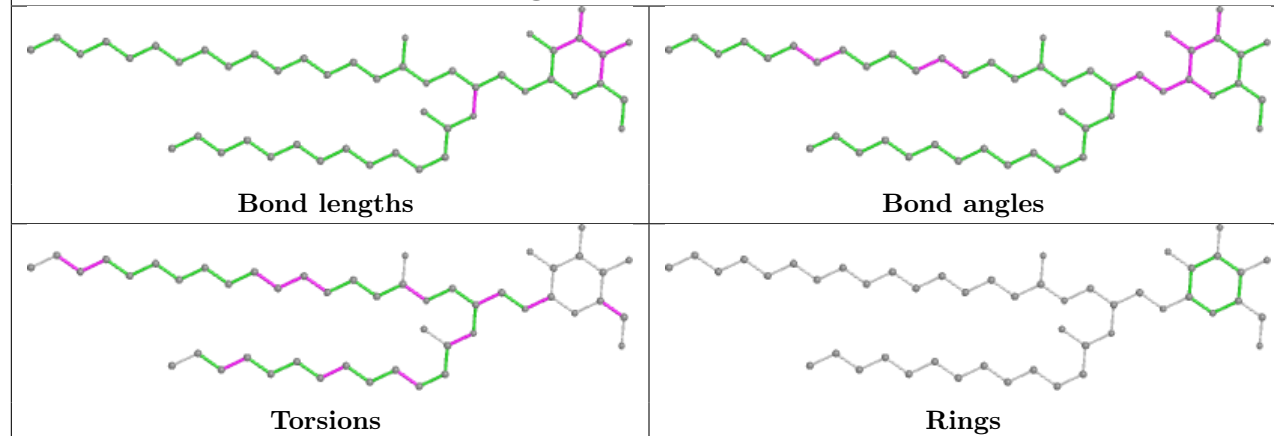
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



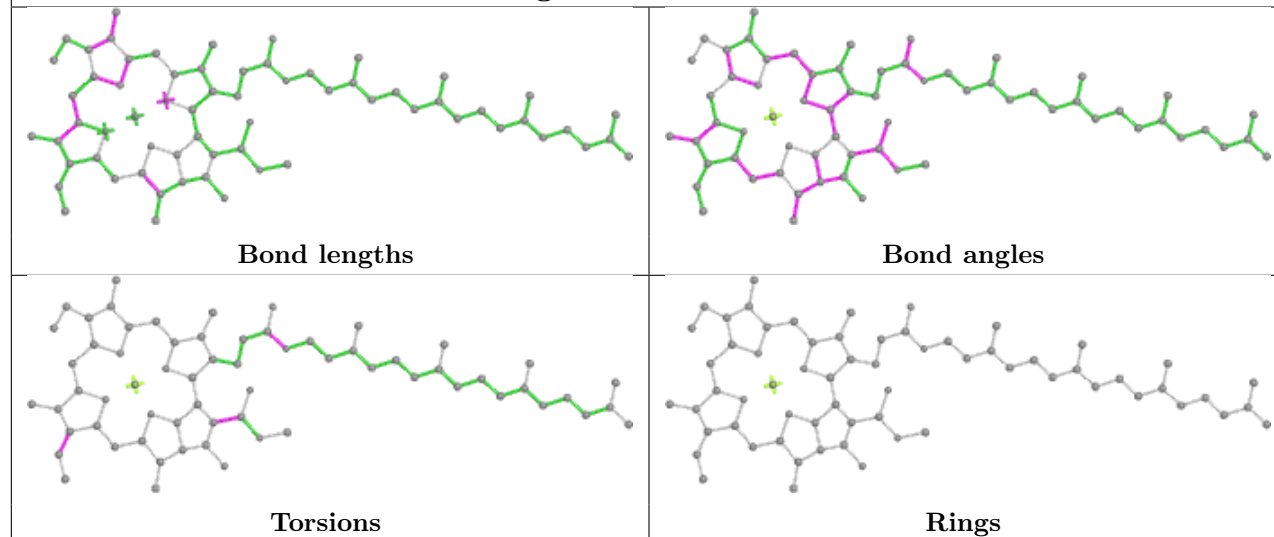
Ligand CLA a 405



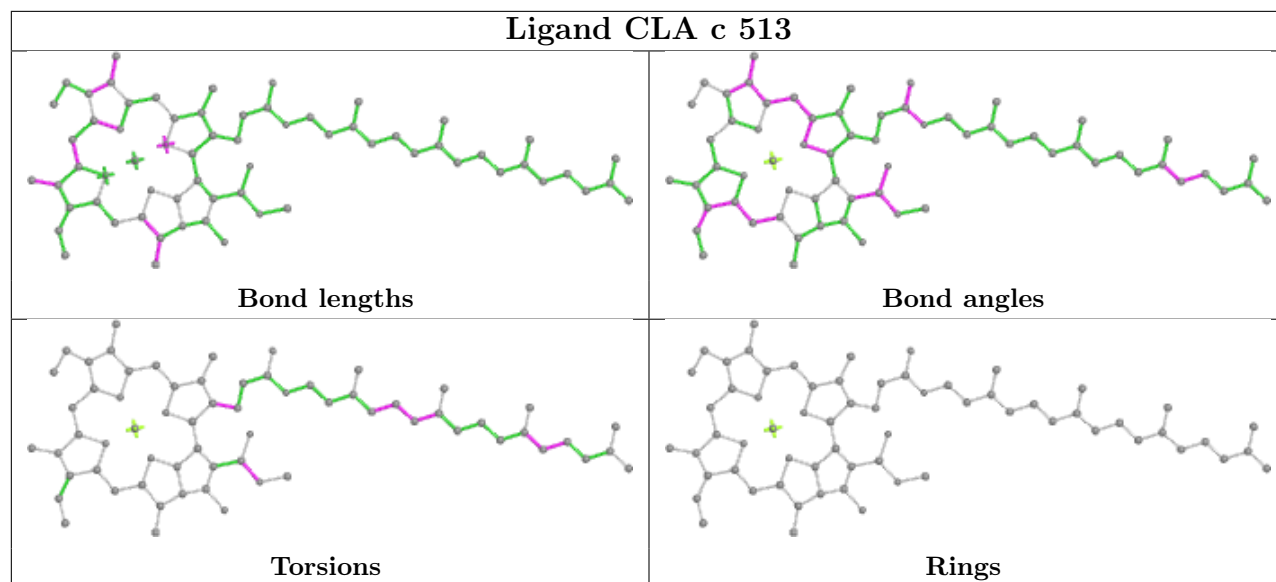
Ligand LMG C 519



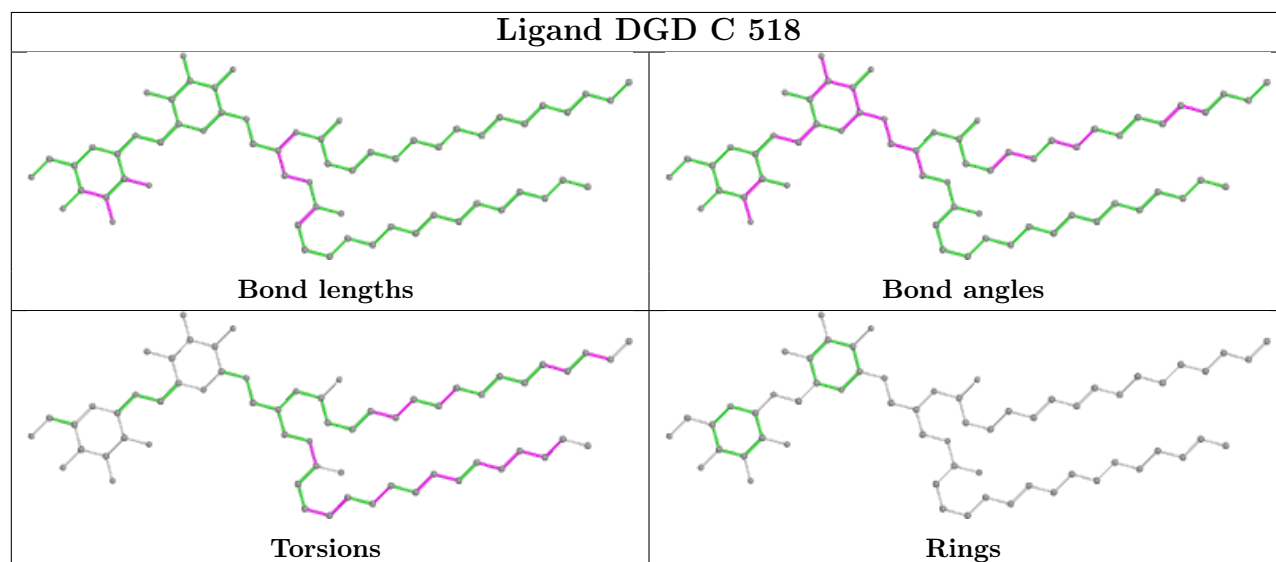
Ligand CLA d 402



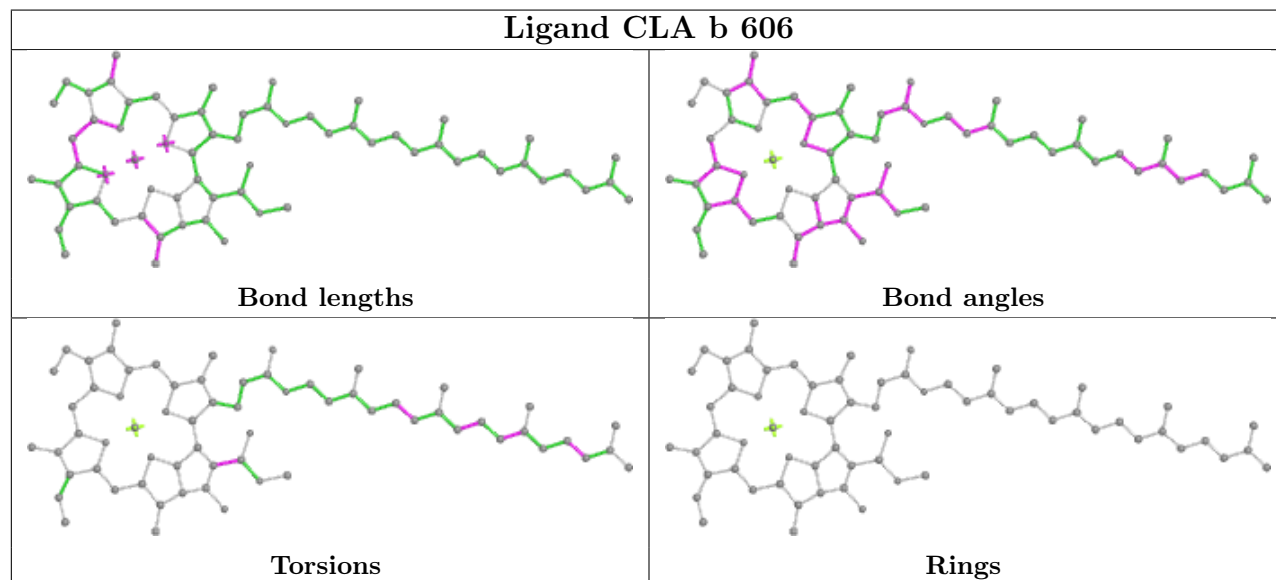
Ligand CLA c 513

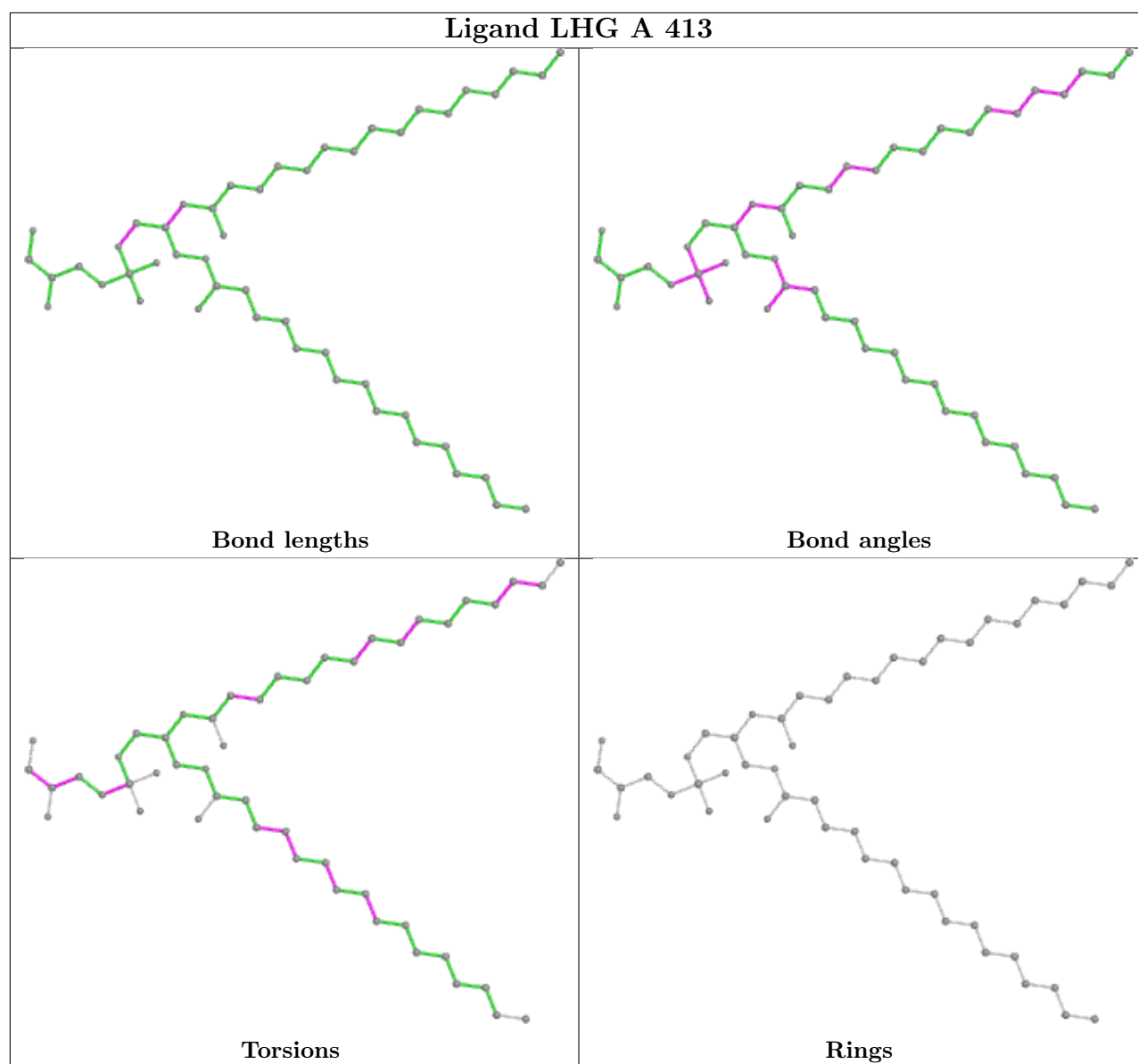


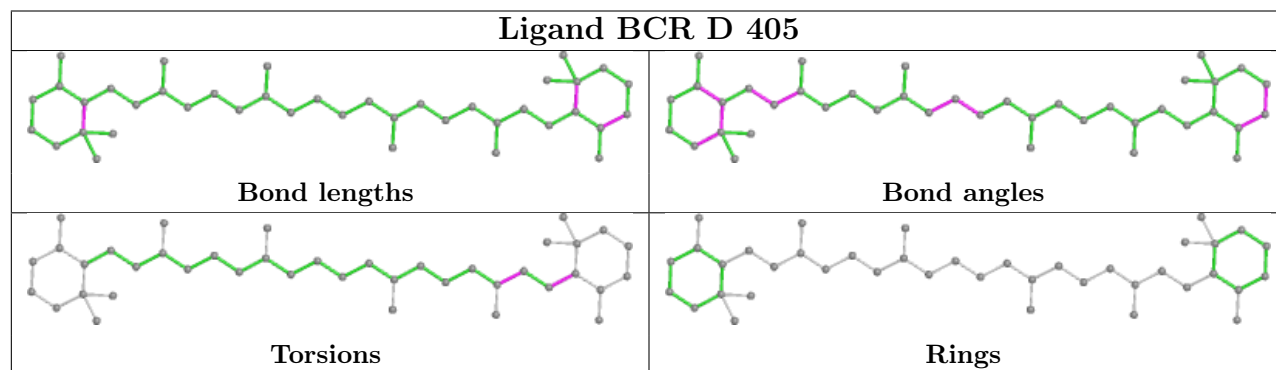
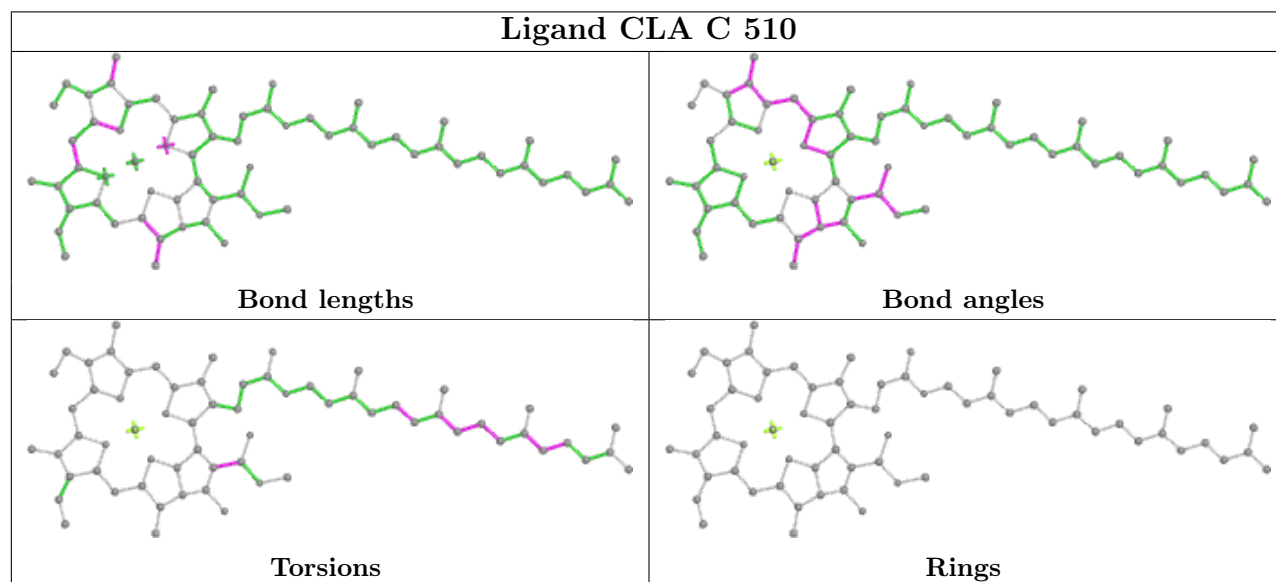
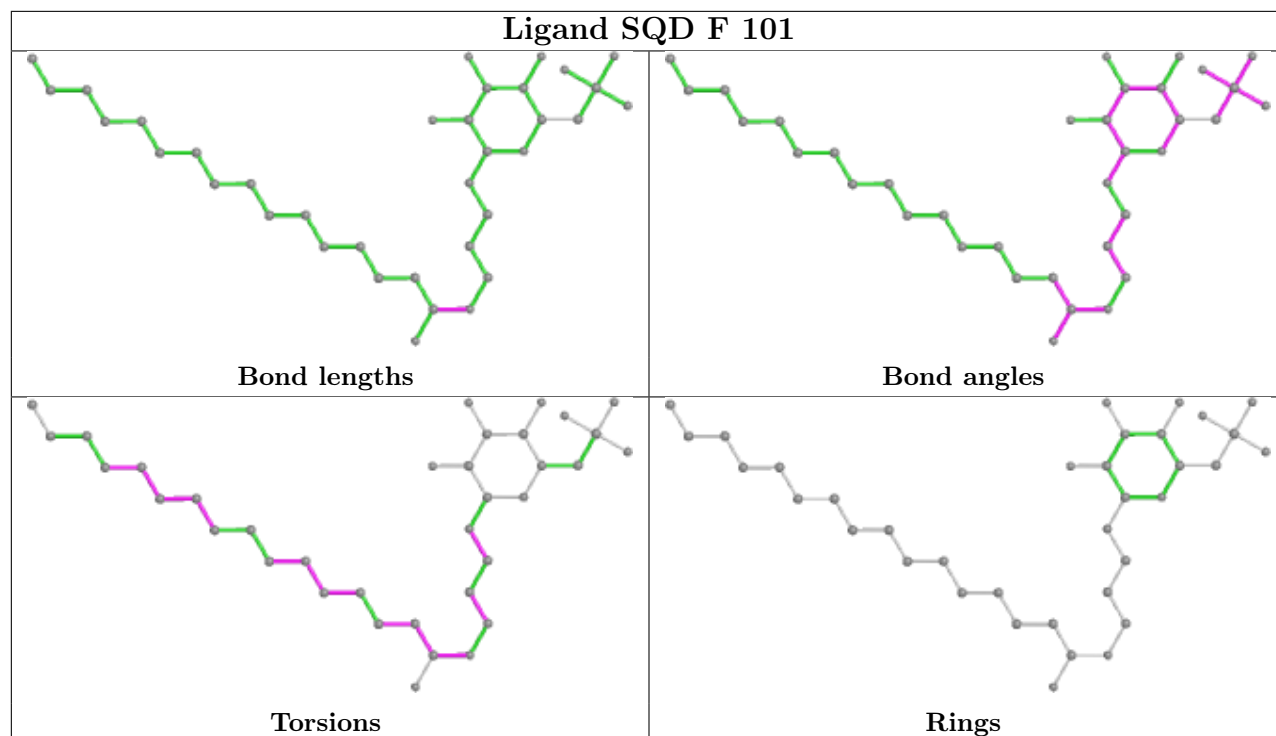
Ligand DGD C 518



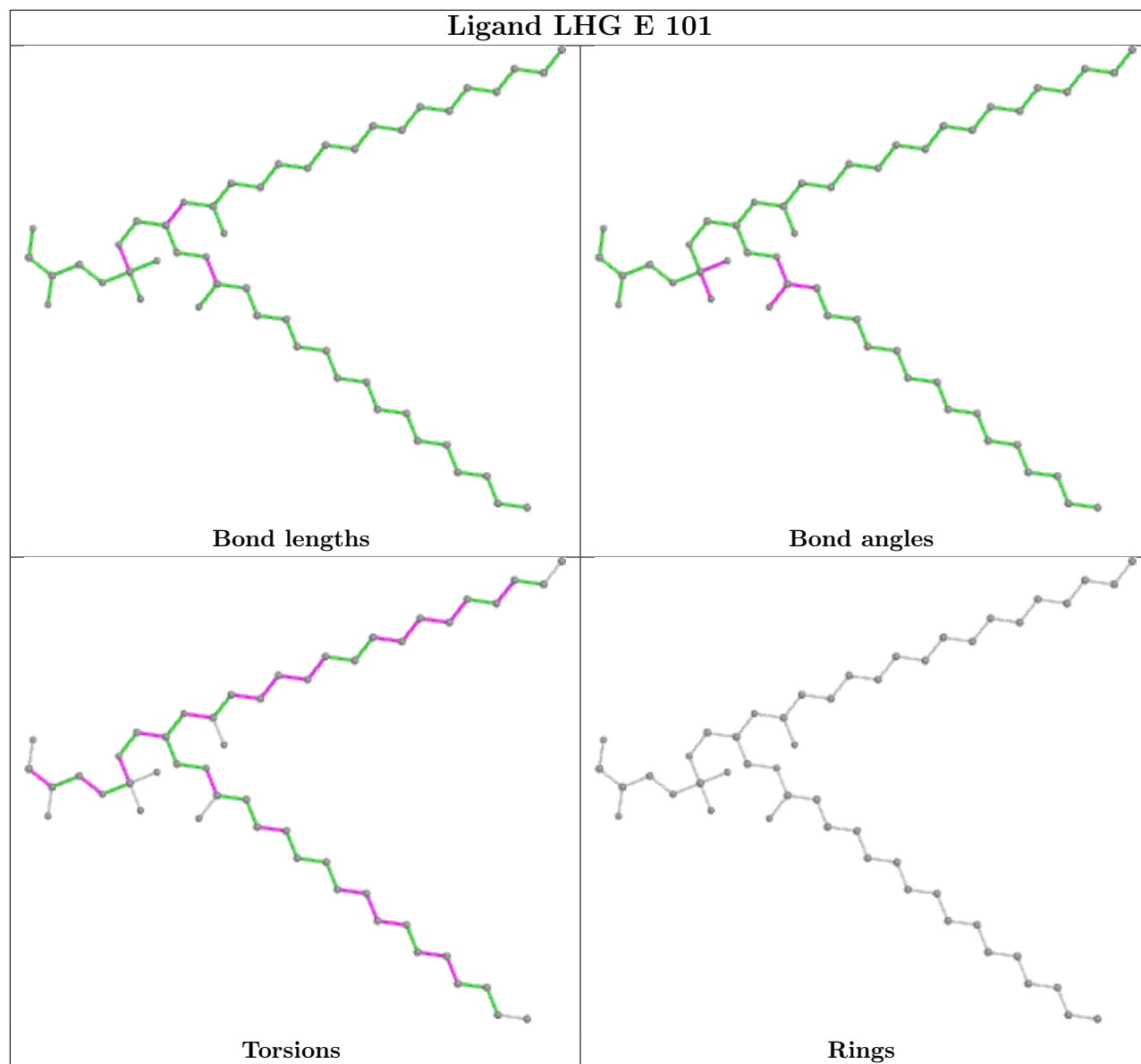
Ligand CLA b 606



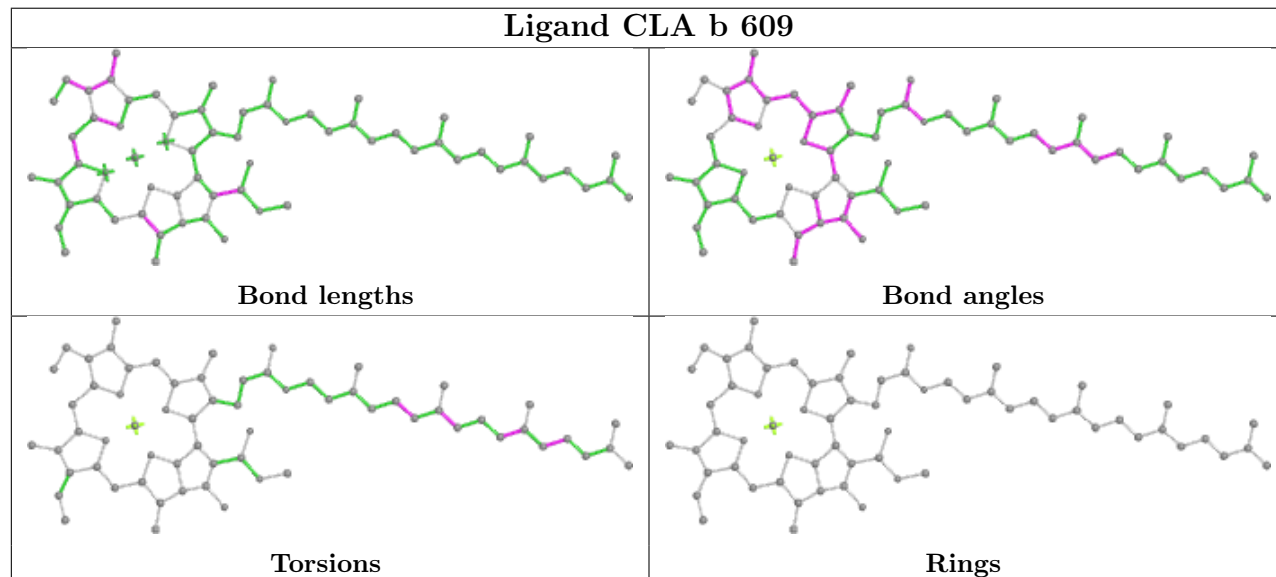


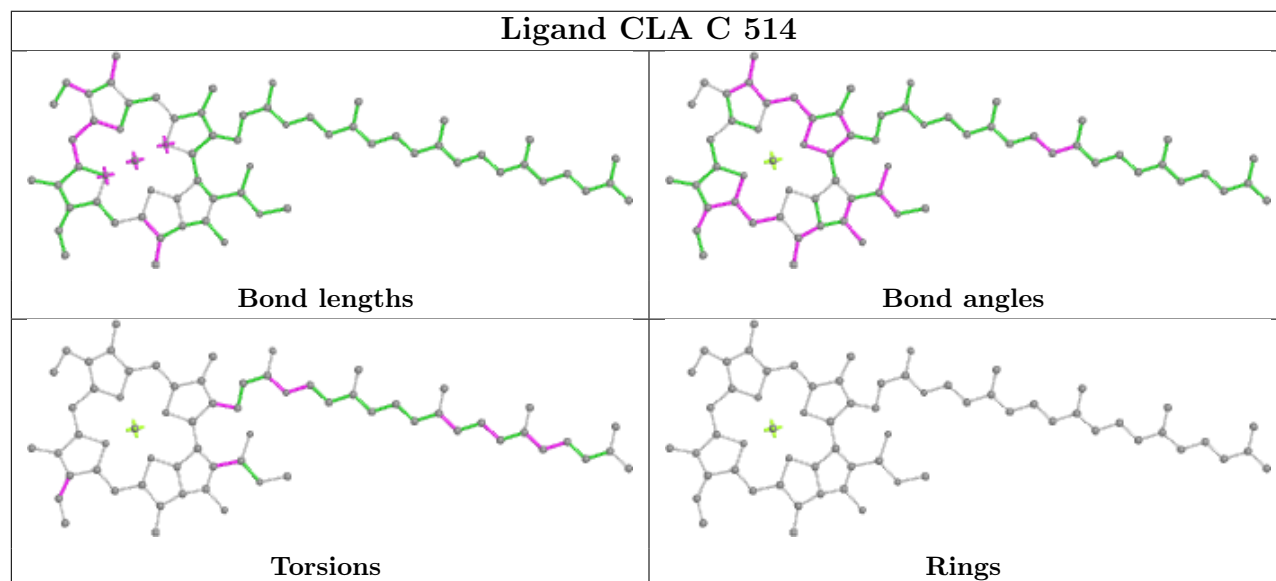
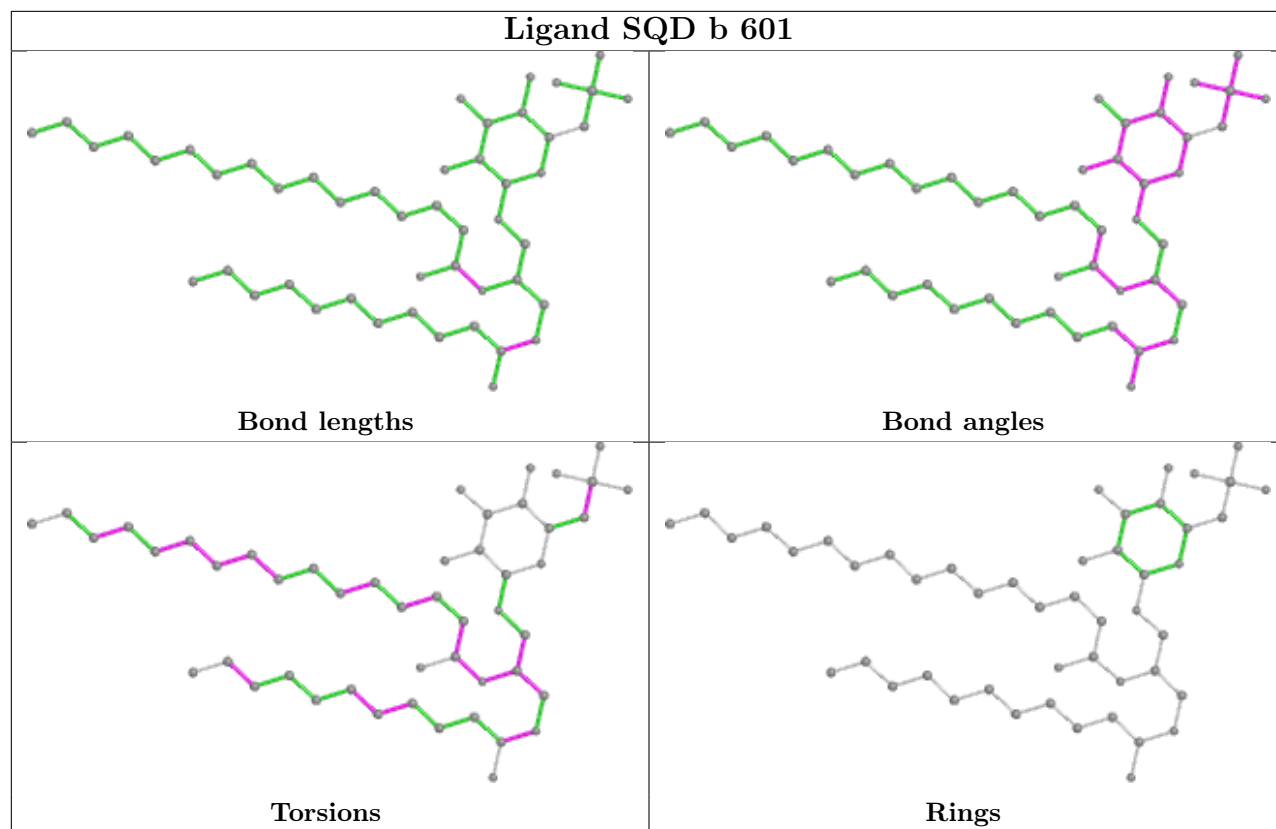


Ligand LHG E 101

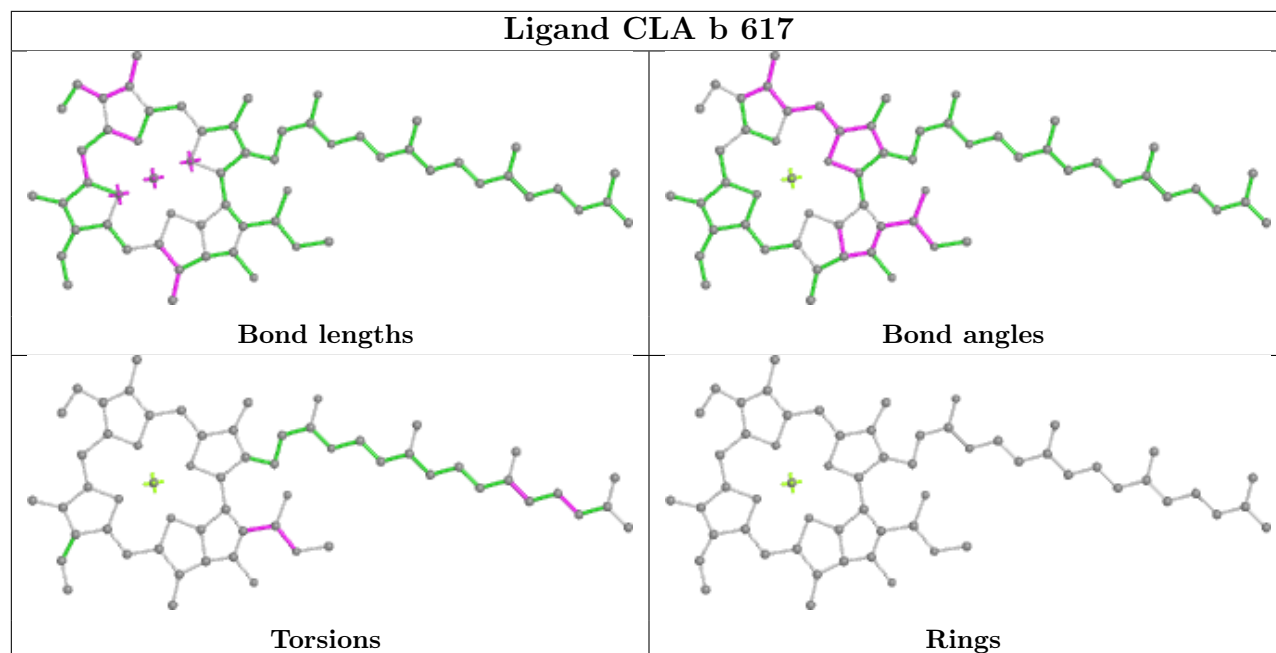


Ligand CLA b 609

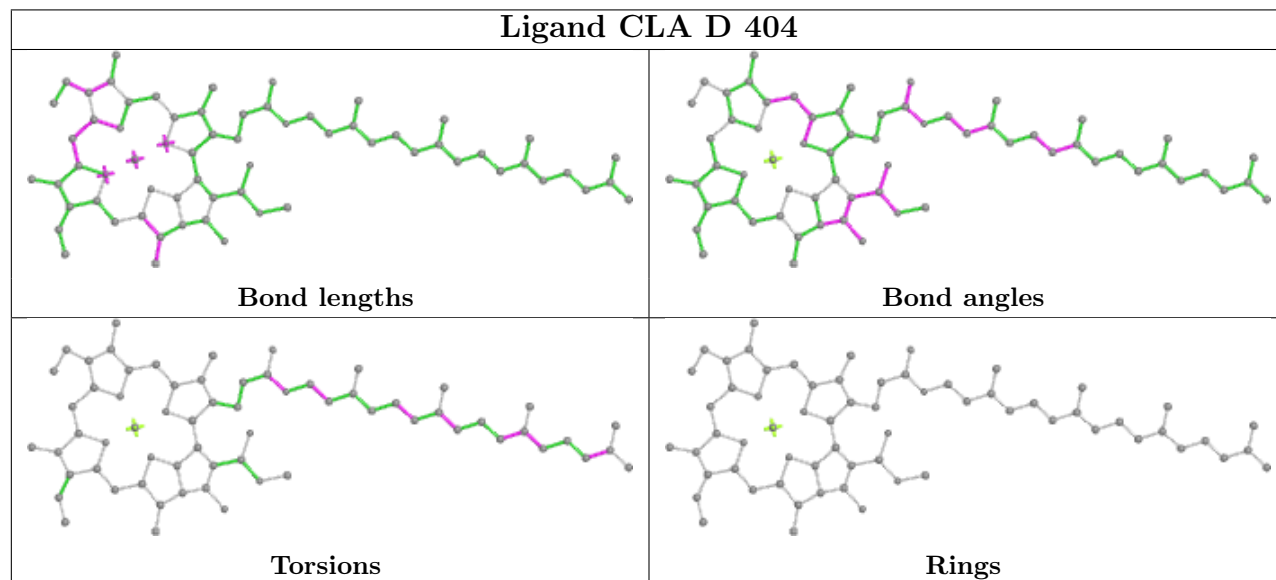




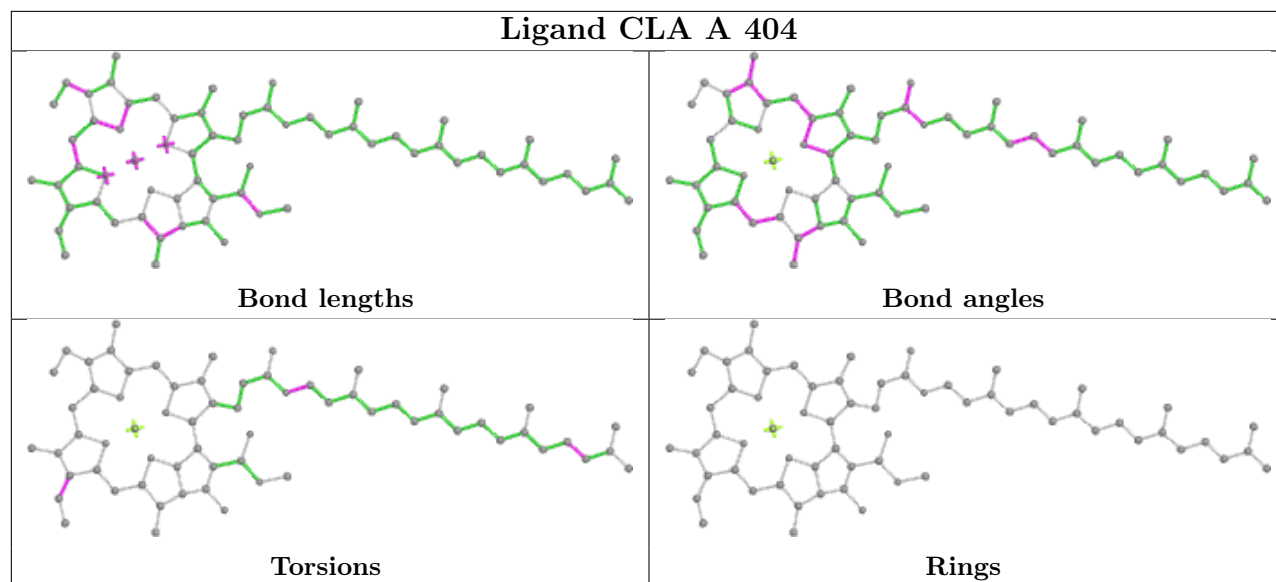
Ligand CLA b 617



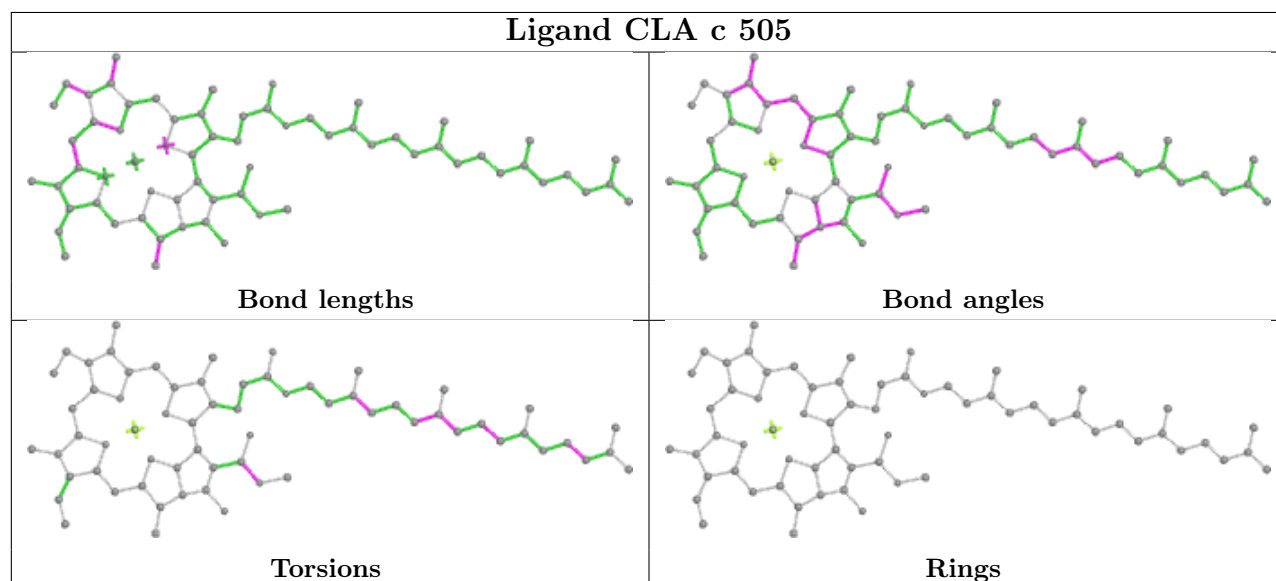
Ligand CLA D 404



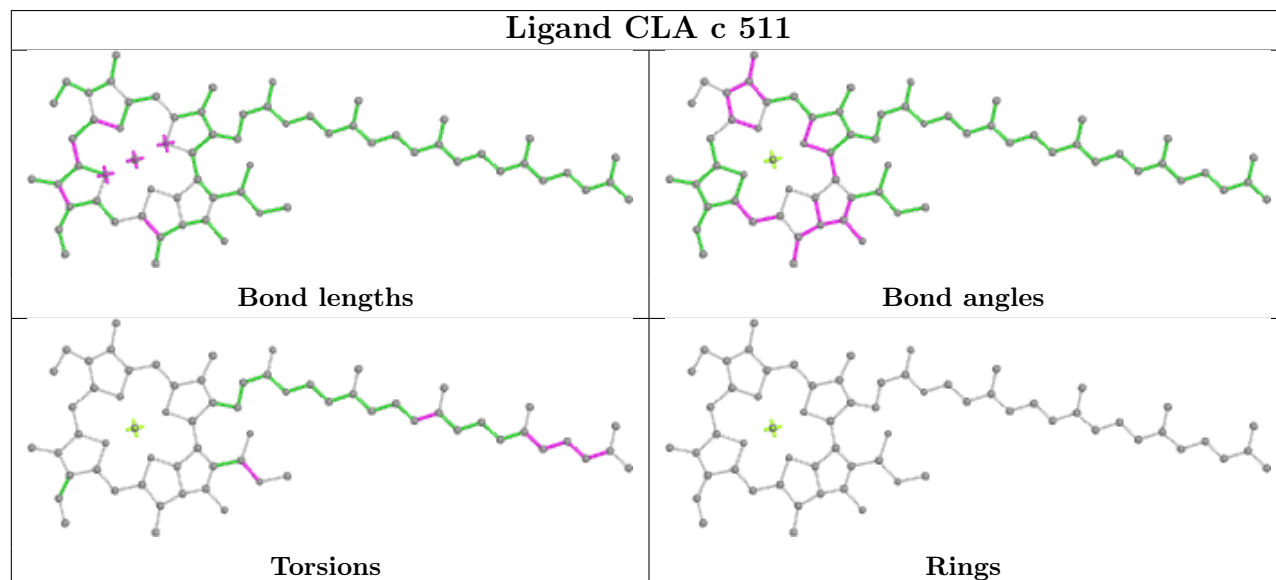
Ligand CLA A 404



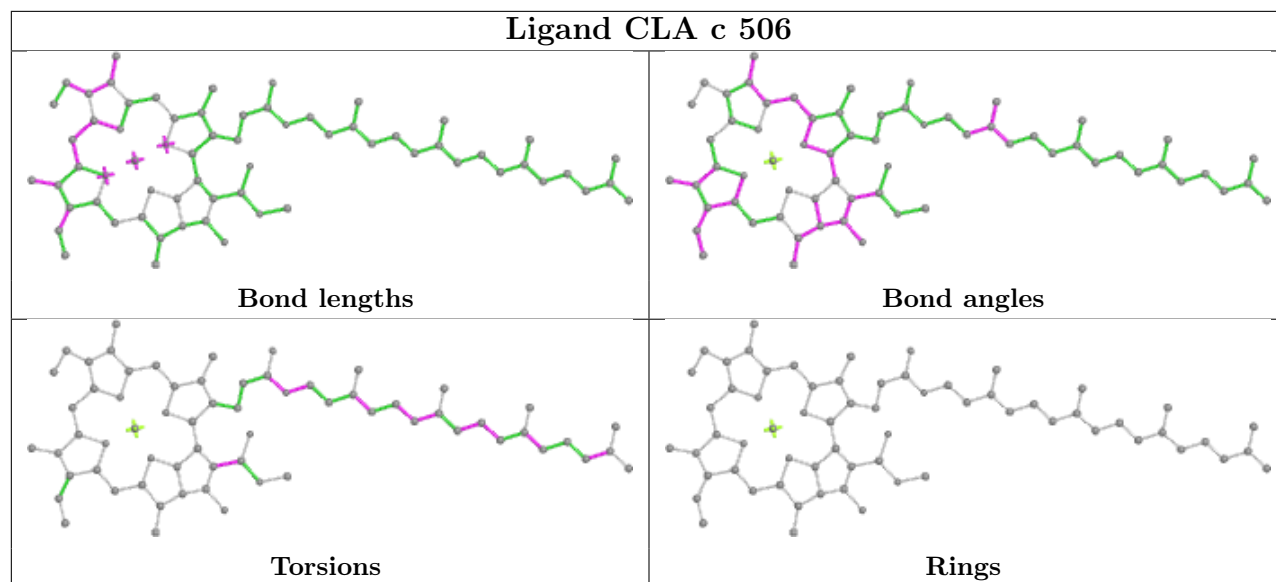
Ligand CLA c 505



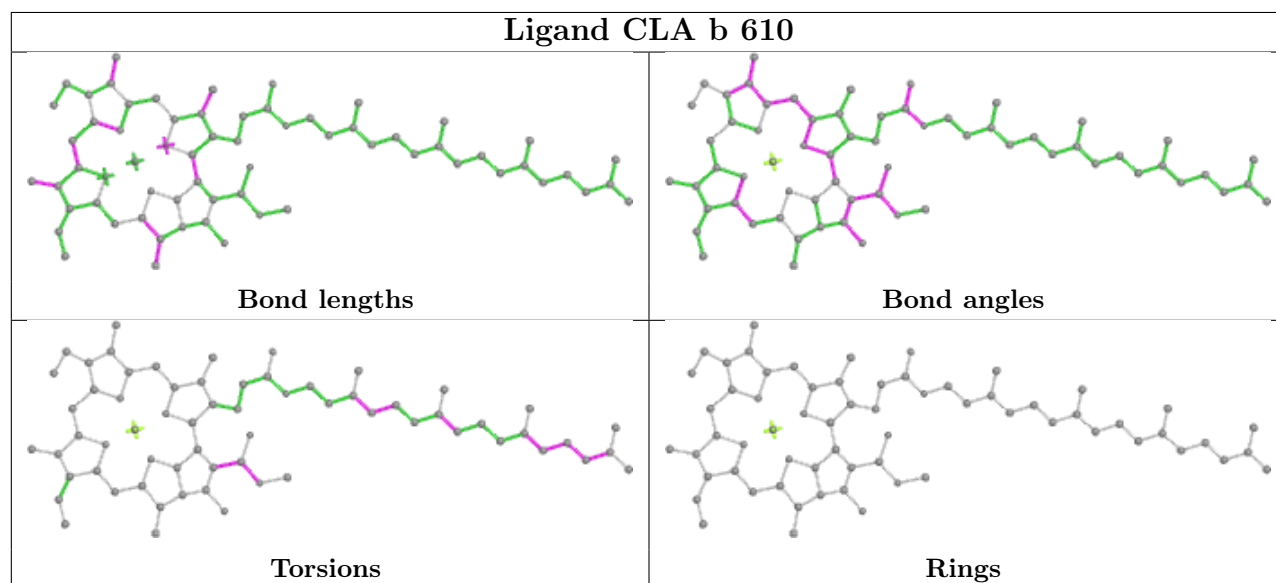
Ligand CLA c 511

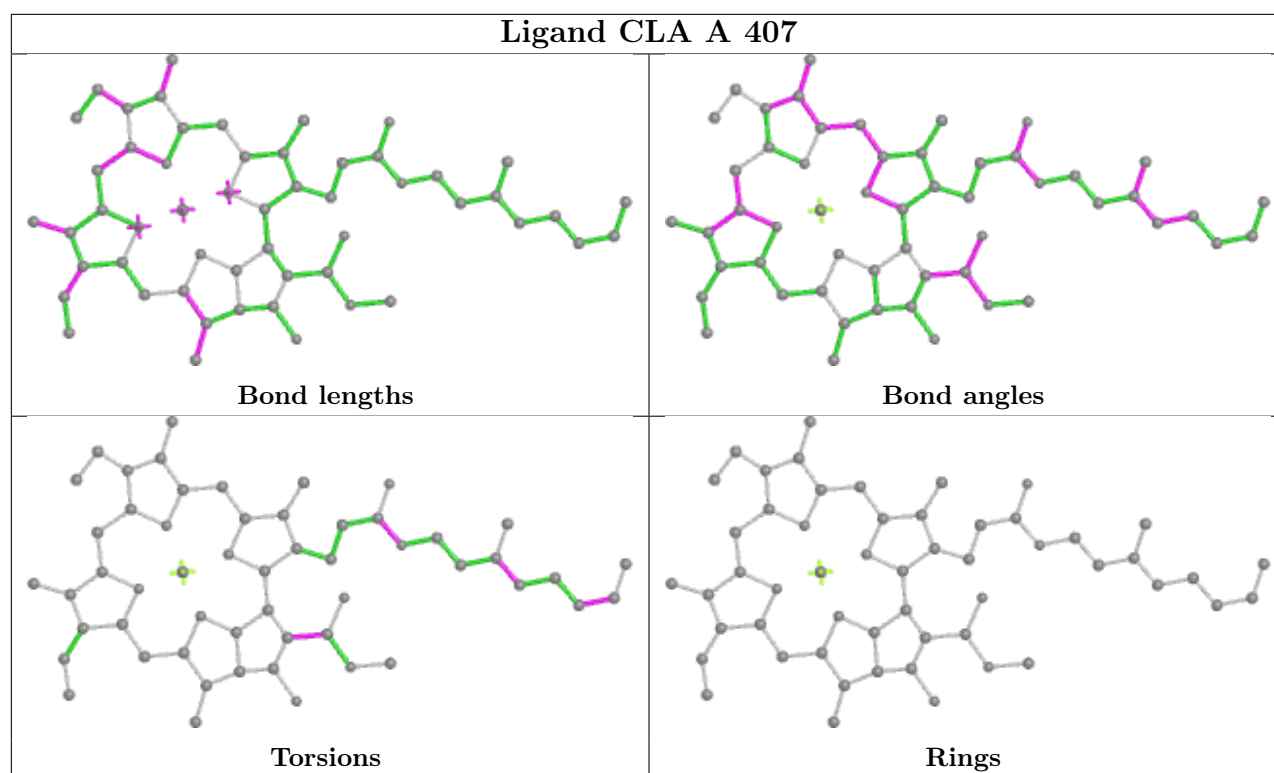


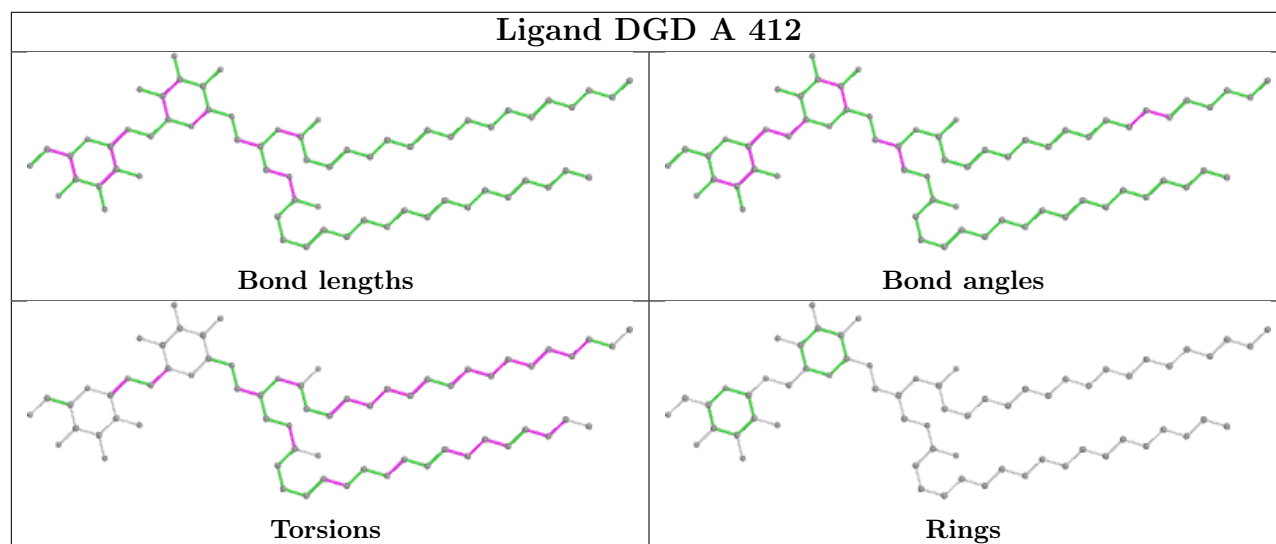
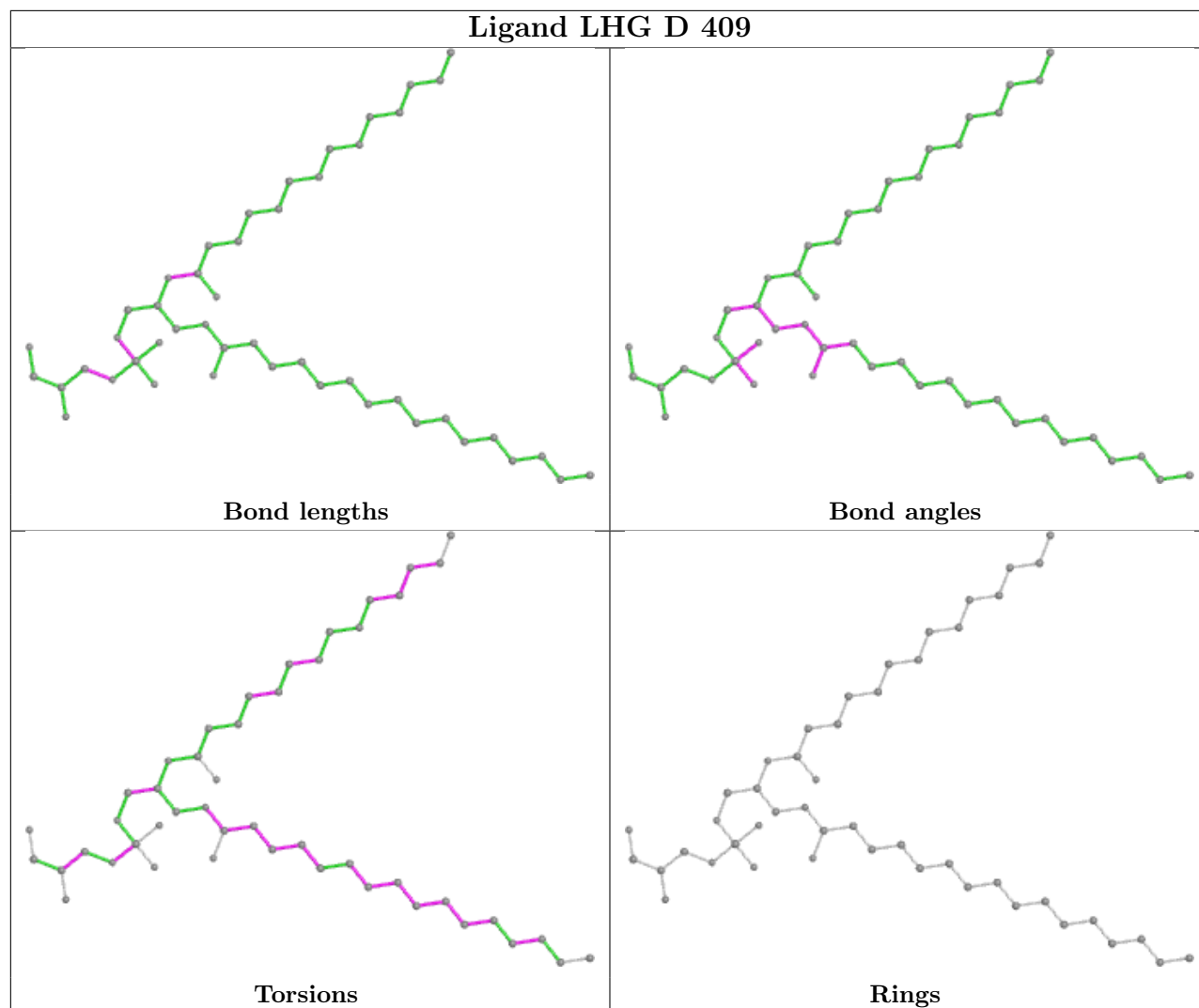
Ligand CLA c 506

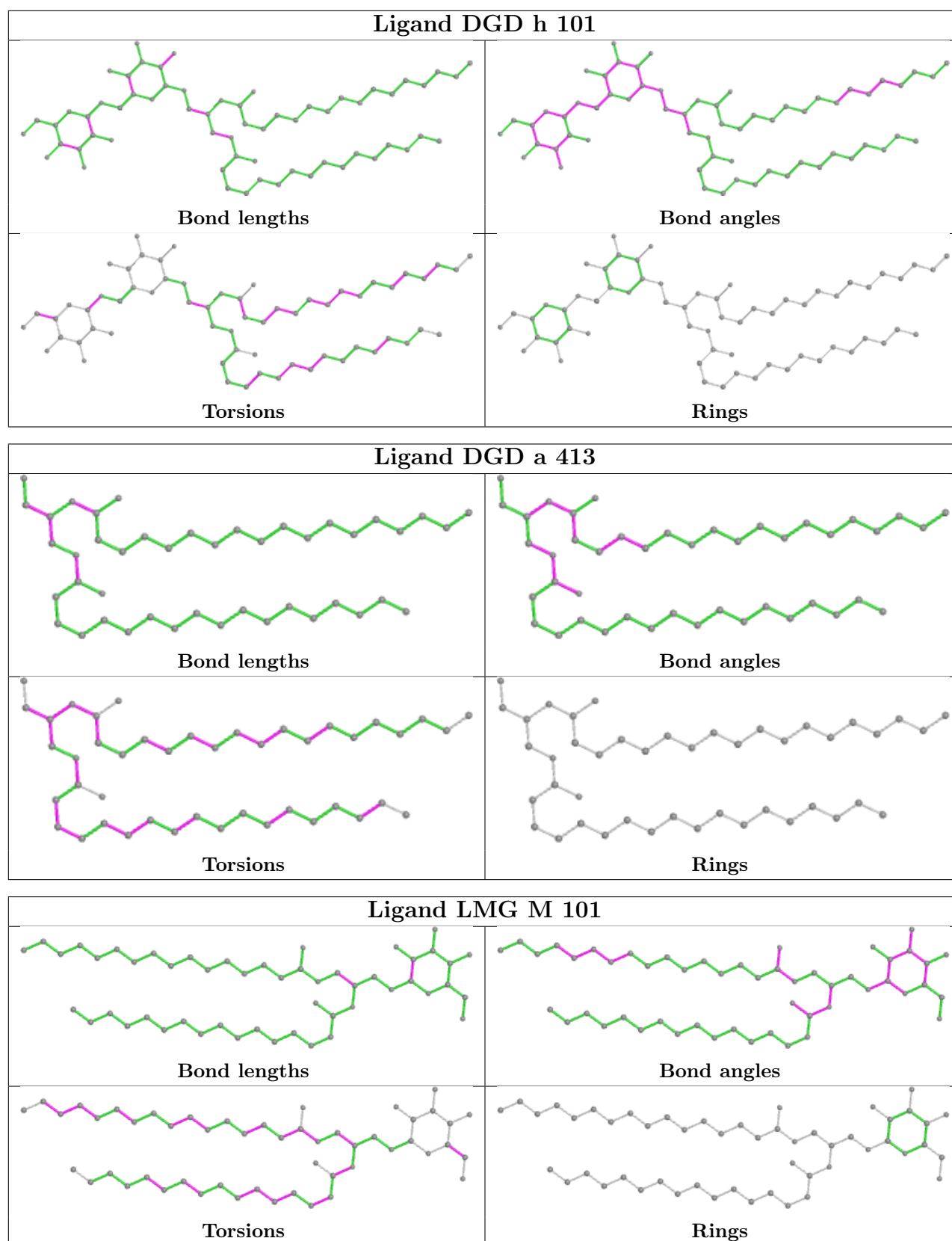


Ligand CLA b 610

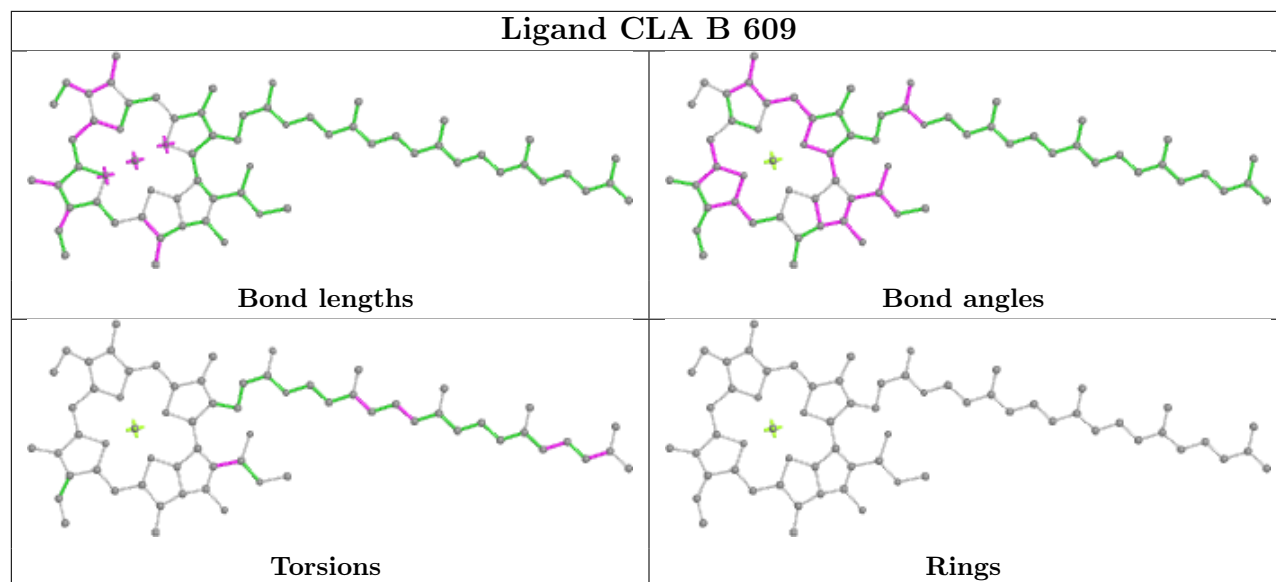




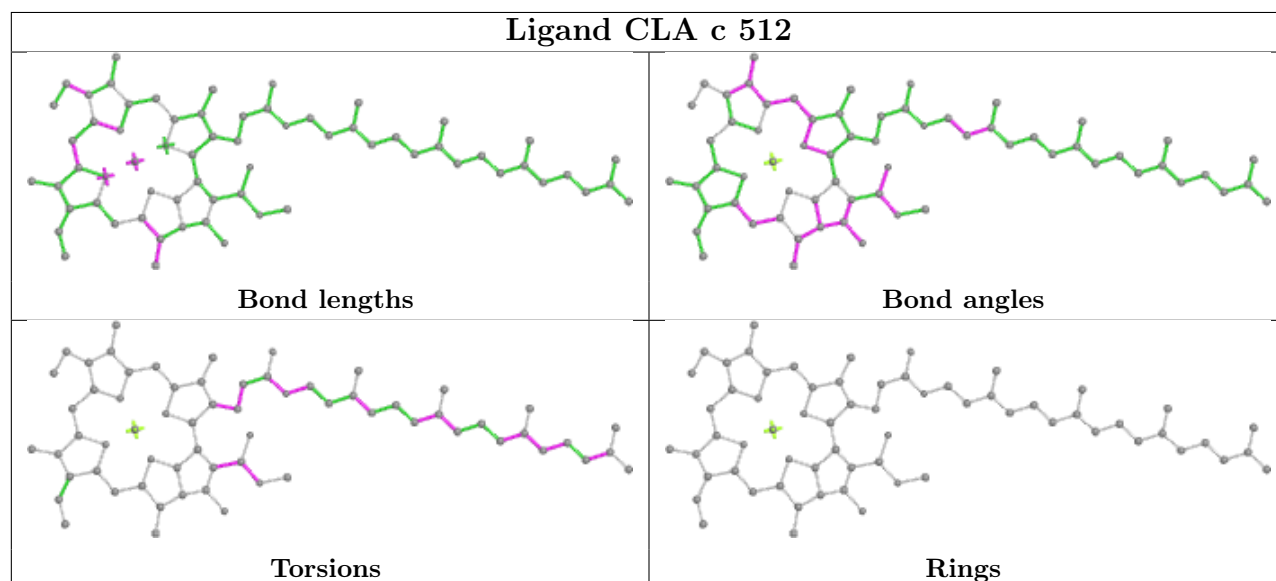




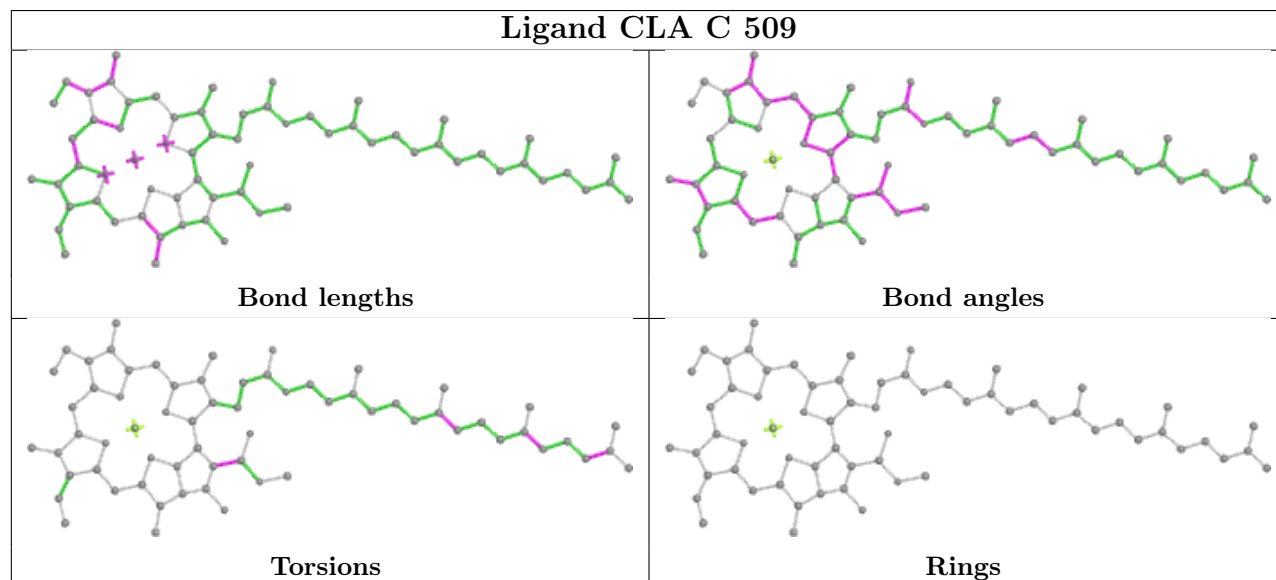
Ligand CLA B 609

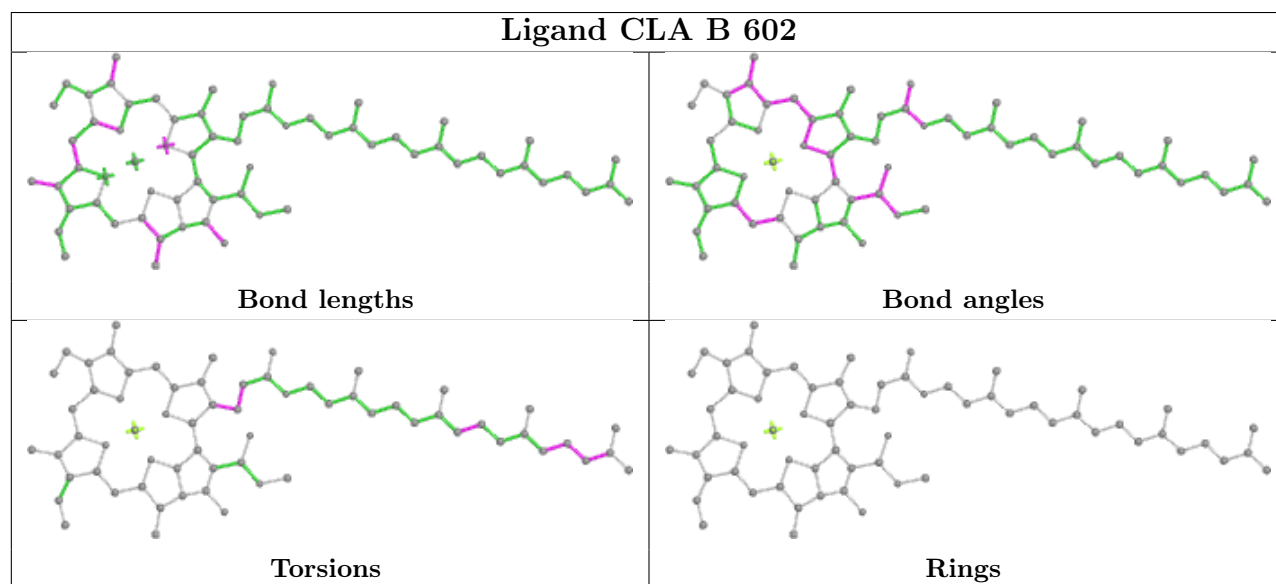
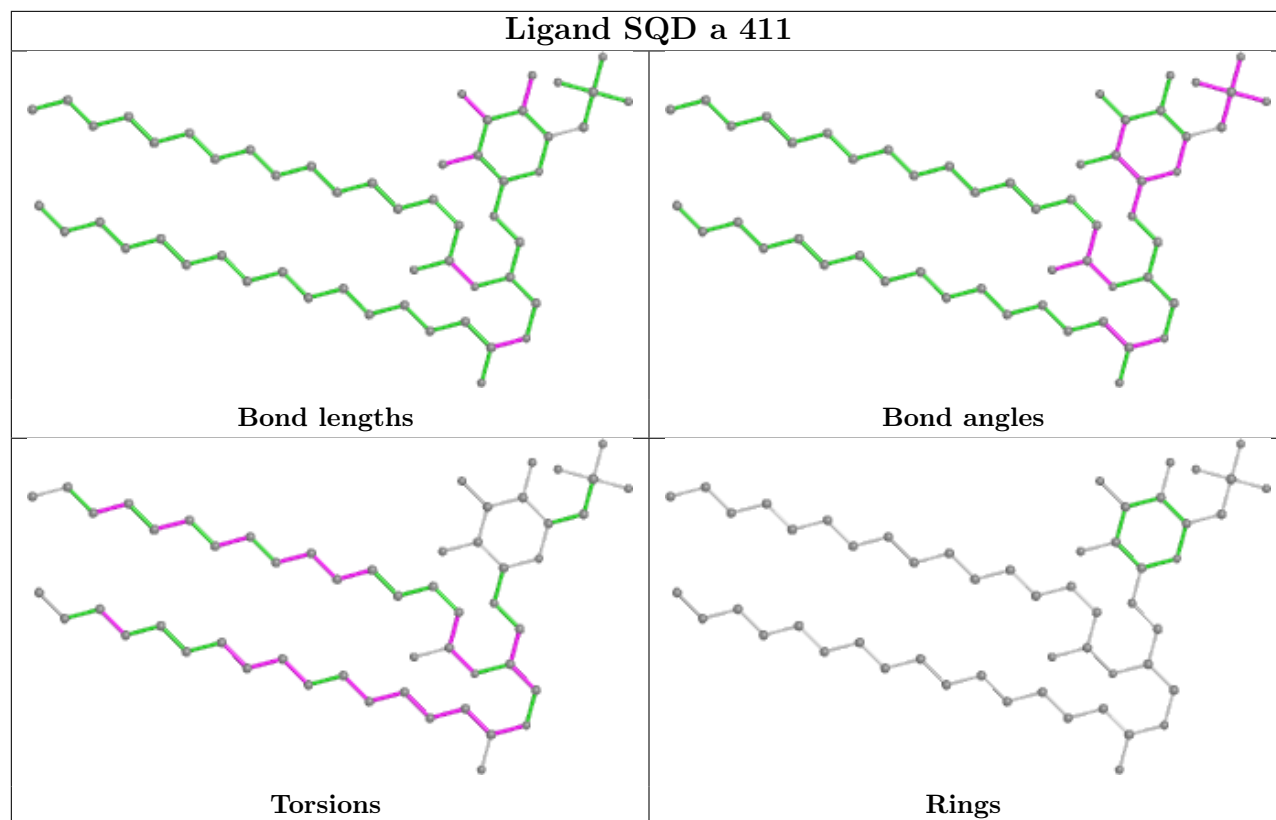


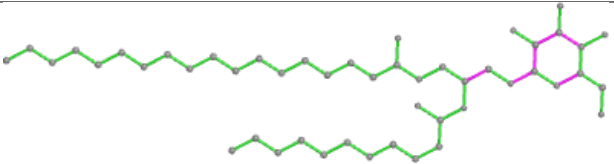
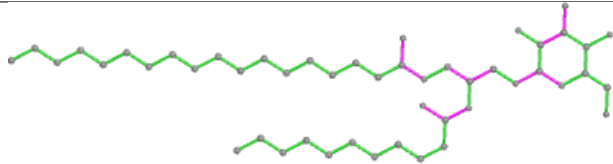
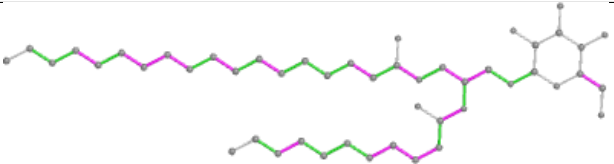

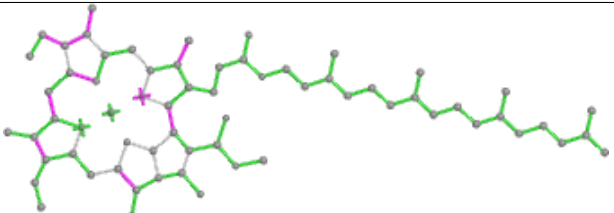
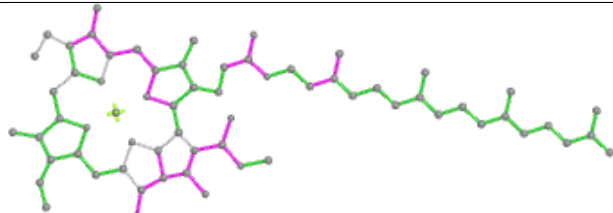
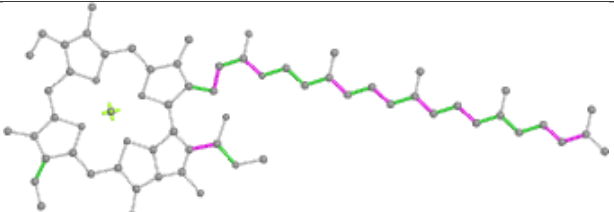
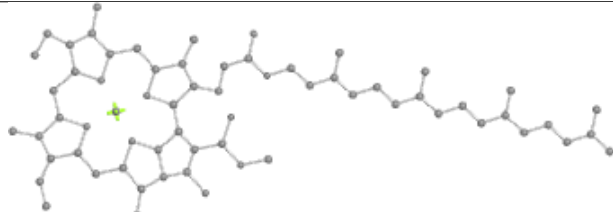
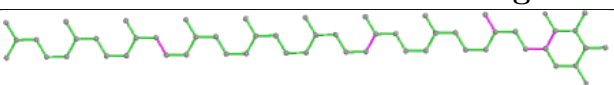
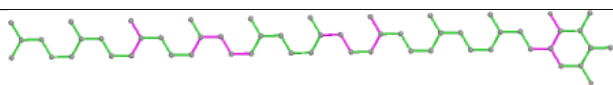
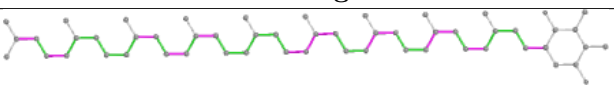
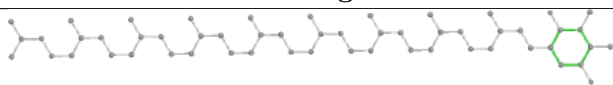
Ligand CLA c 512

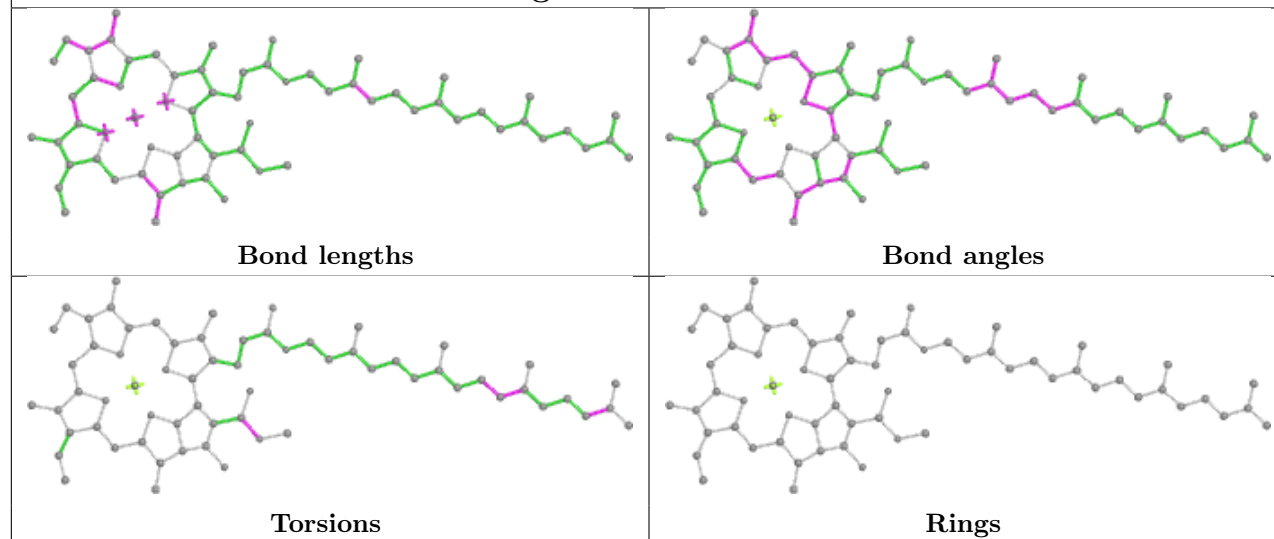
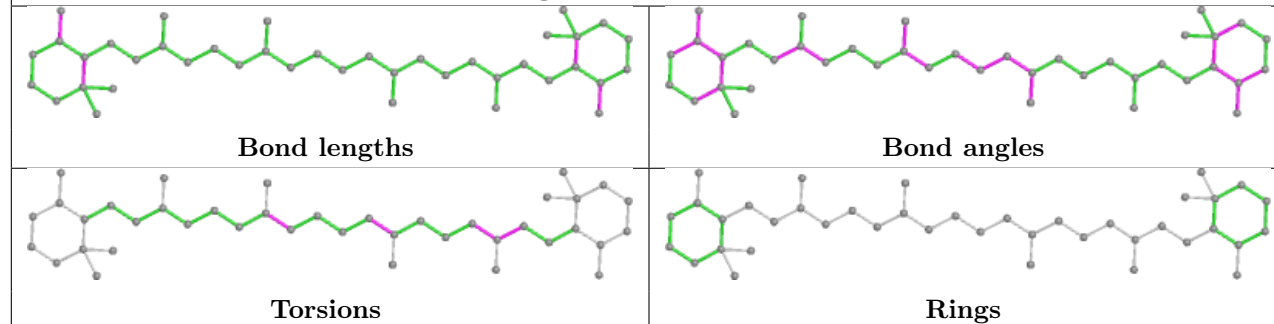
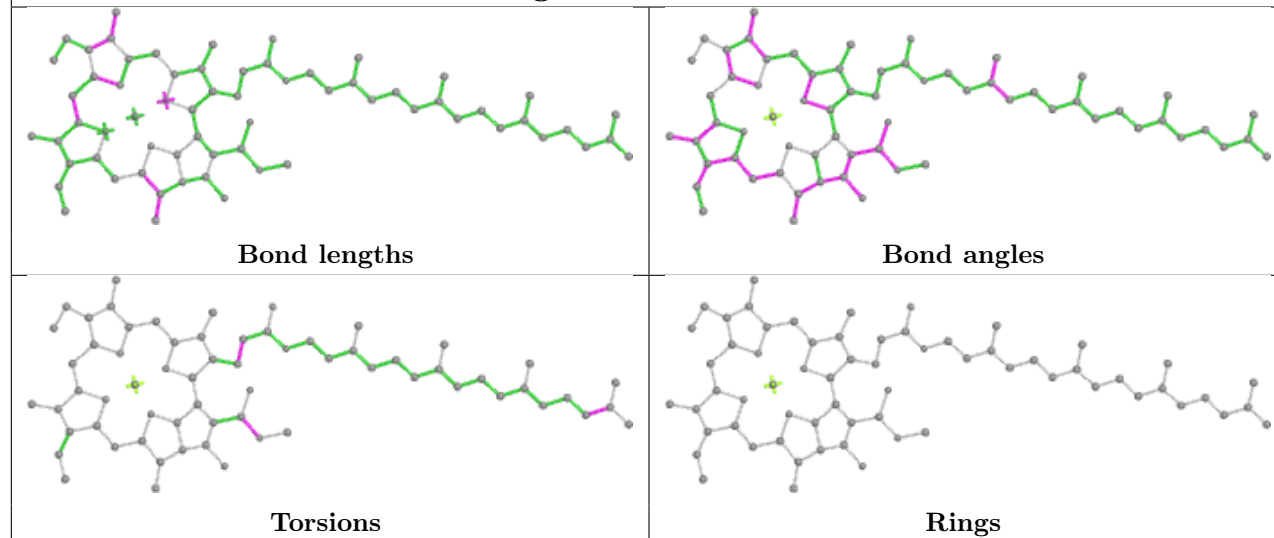


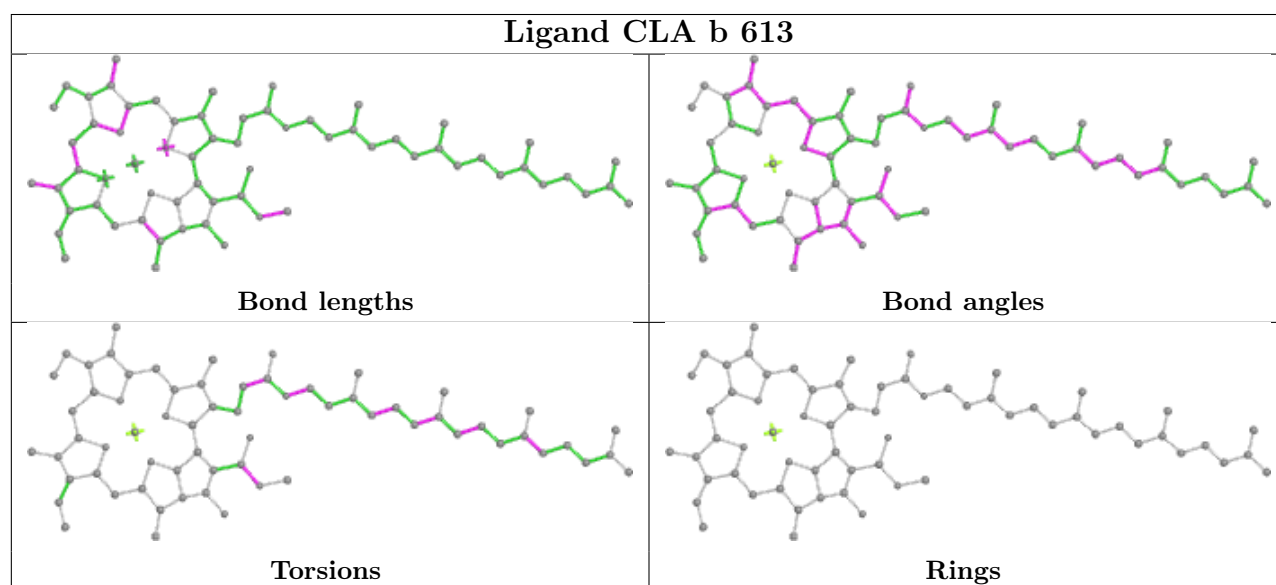
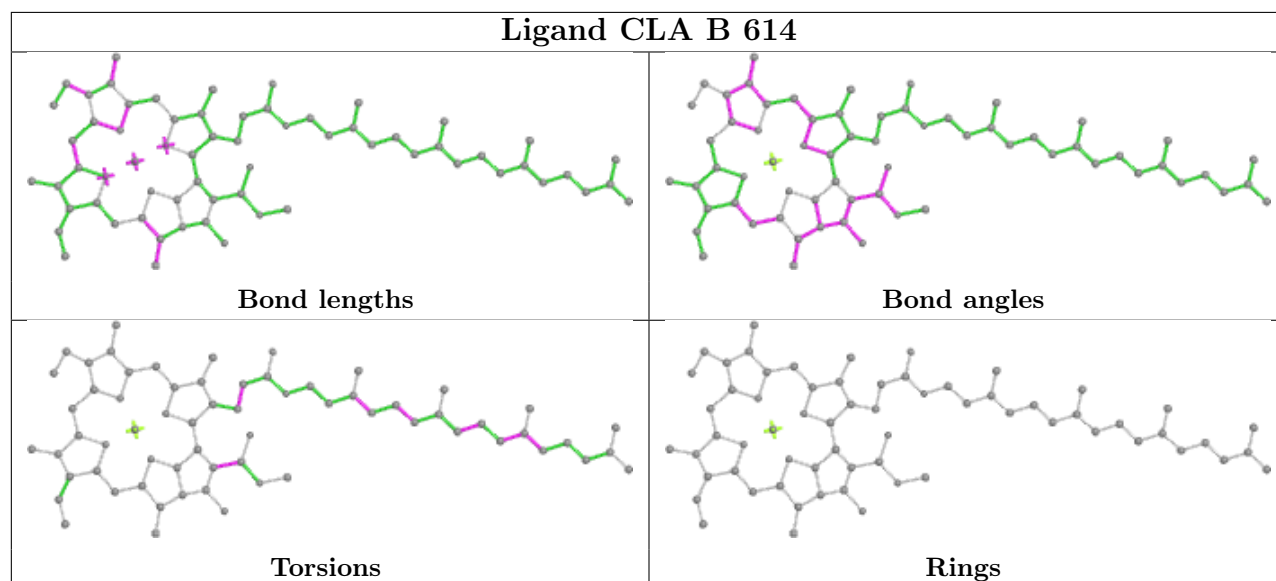
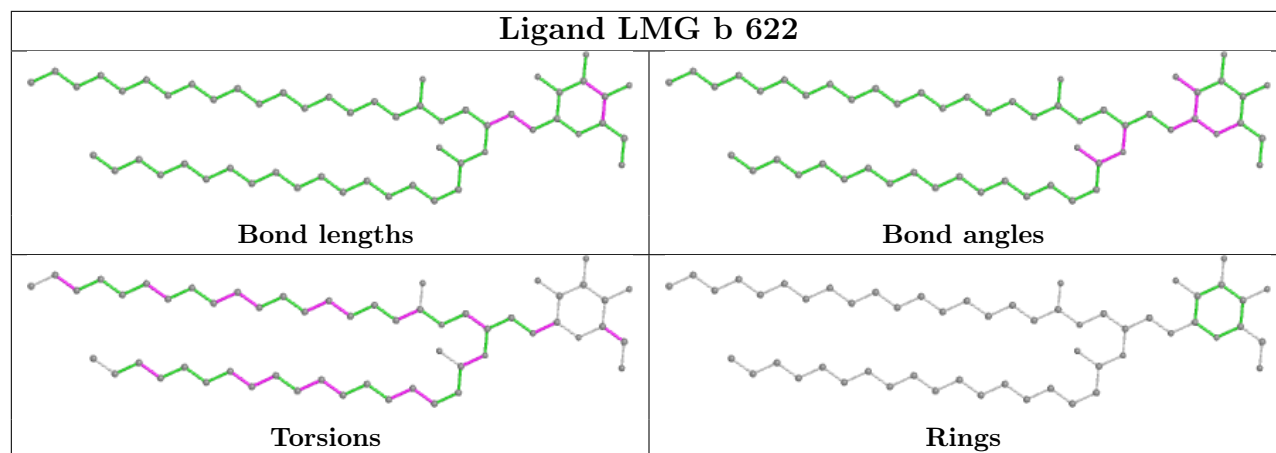
Ligand CLA C 509



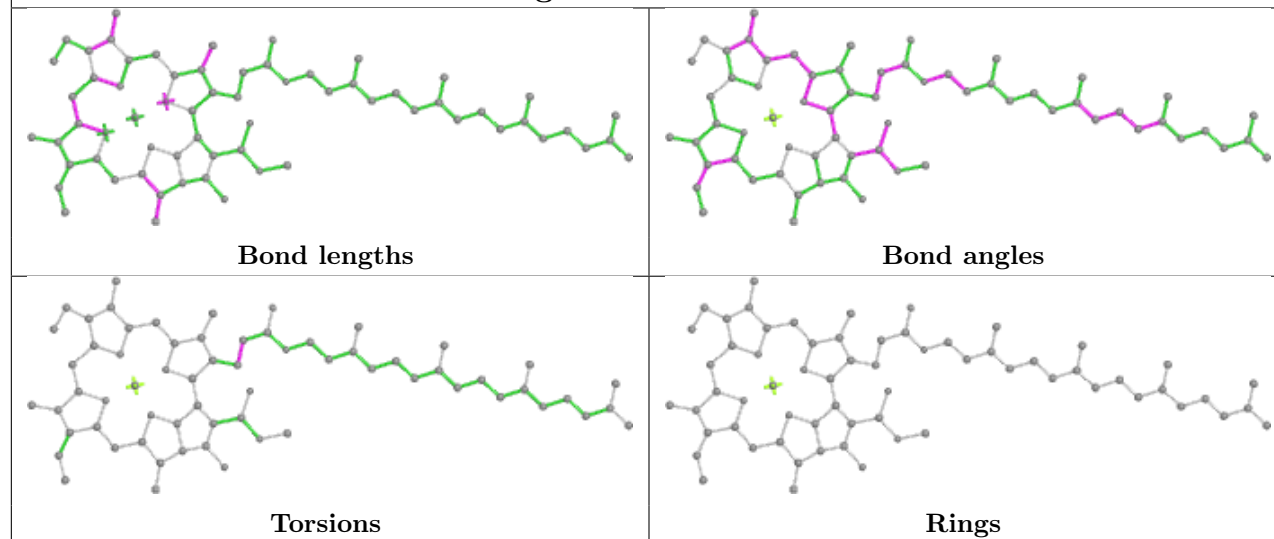


| Ligand LMG c 522 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CLA B 603 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand PL9 A 409 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |

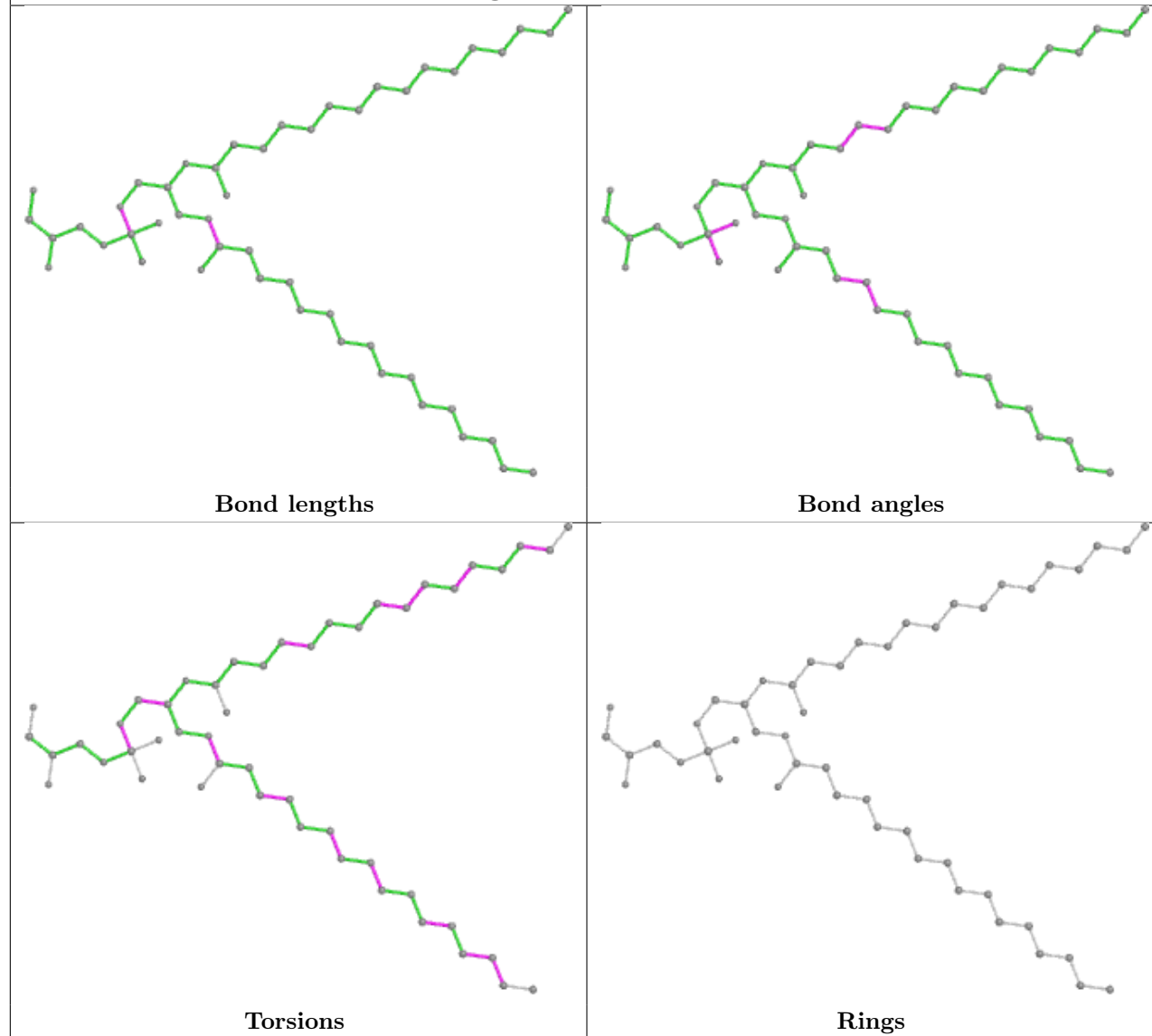
Ligand CLA B 615**Ligand BCR c 515****Ligand CLA C 502**

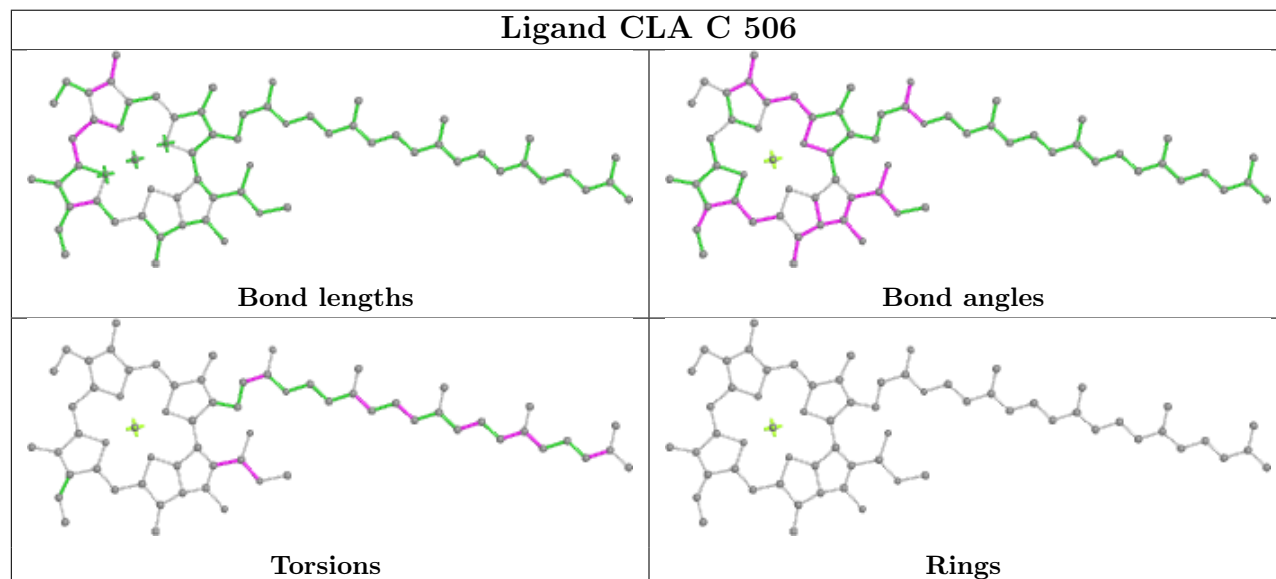
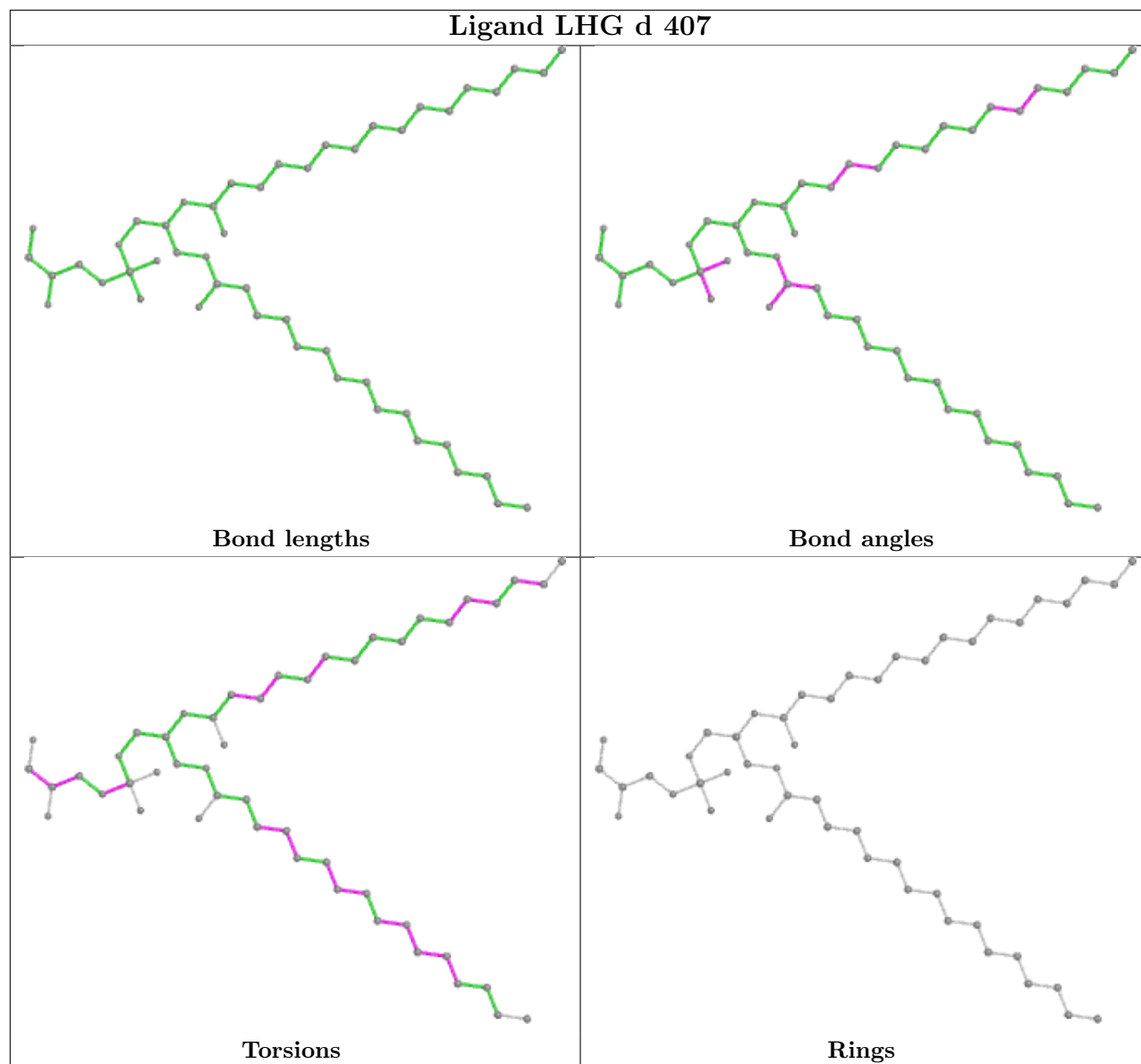


Ligand CLA b 611

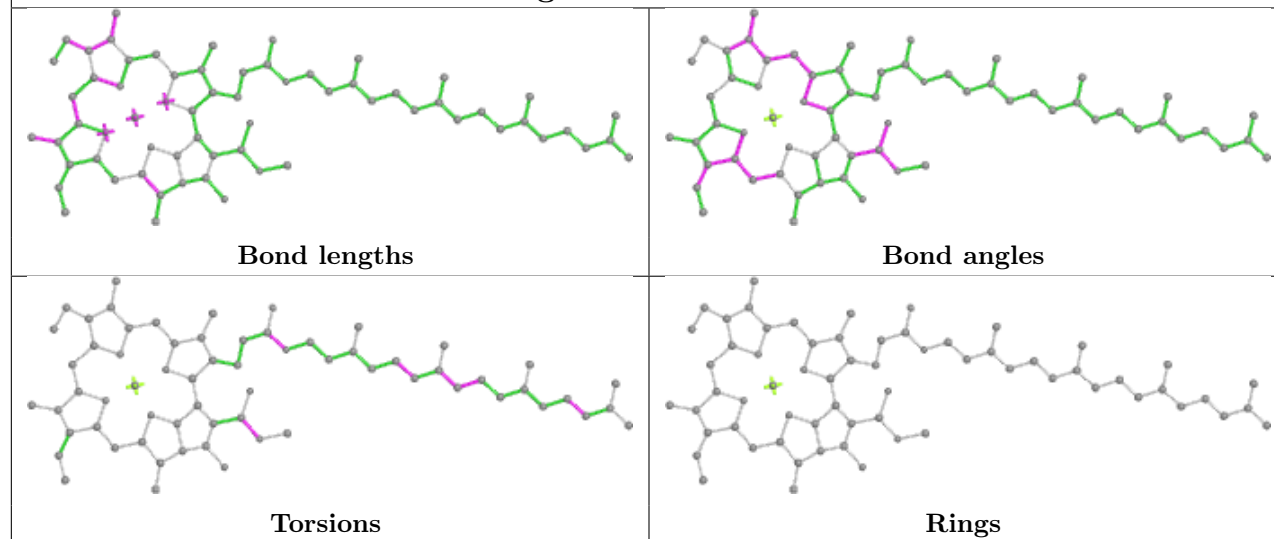


Ligand LHG l 101

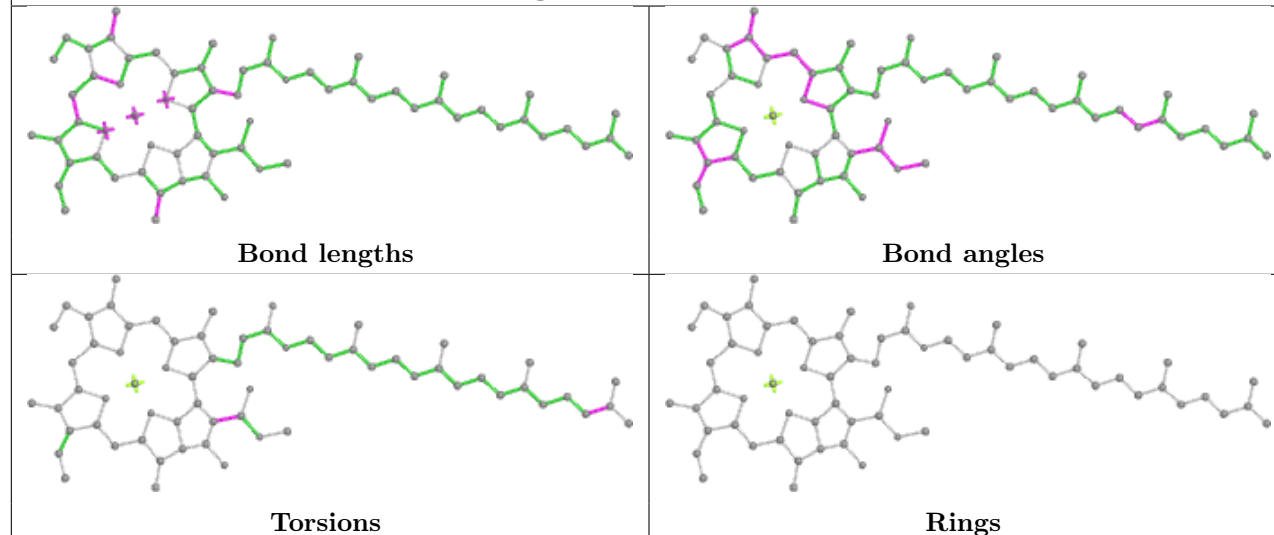




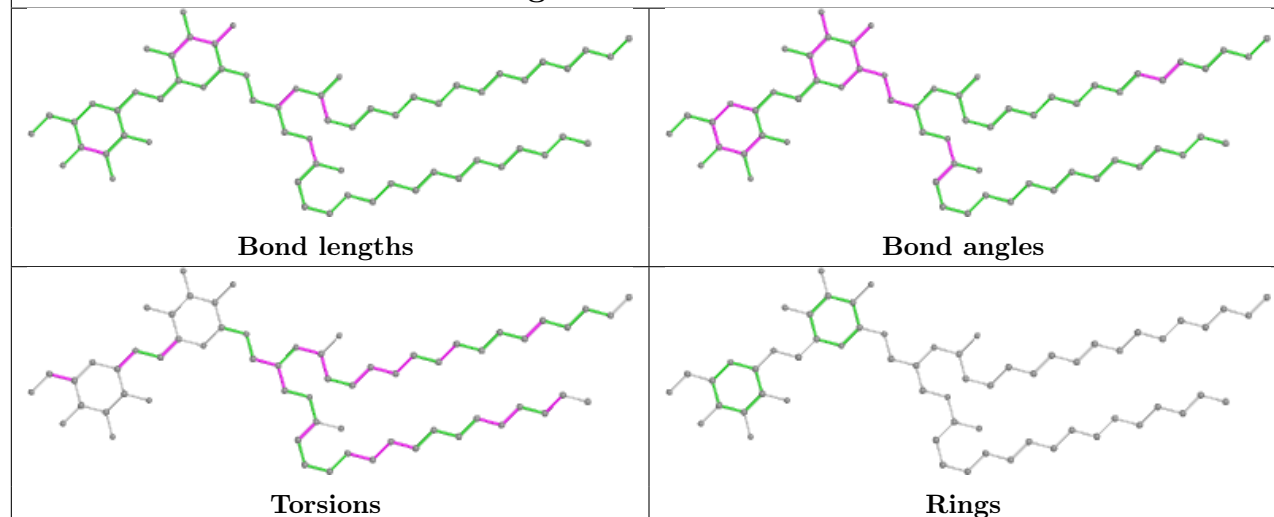
Ligand CLA c 503



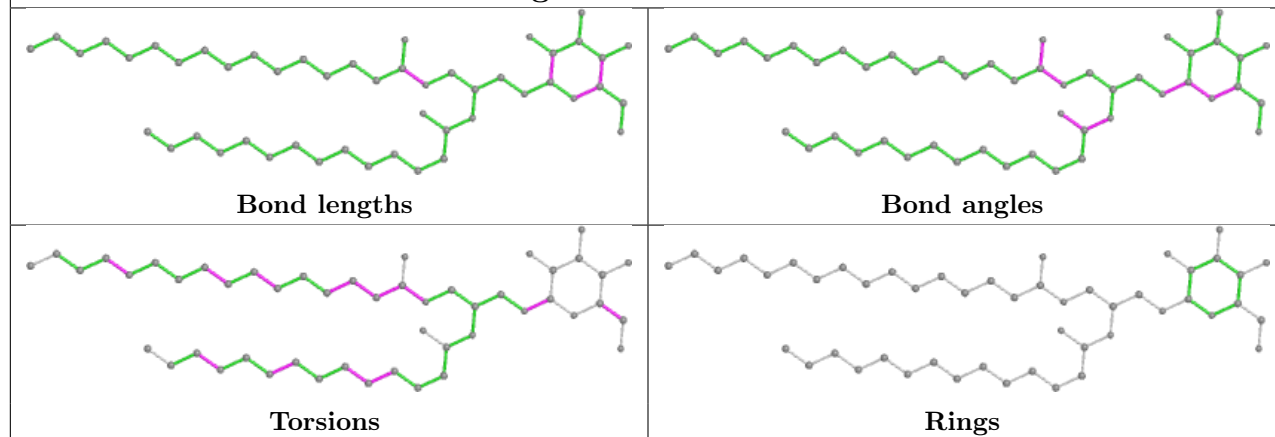
Ligand CLA A 405



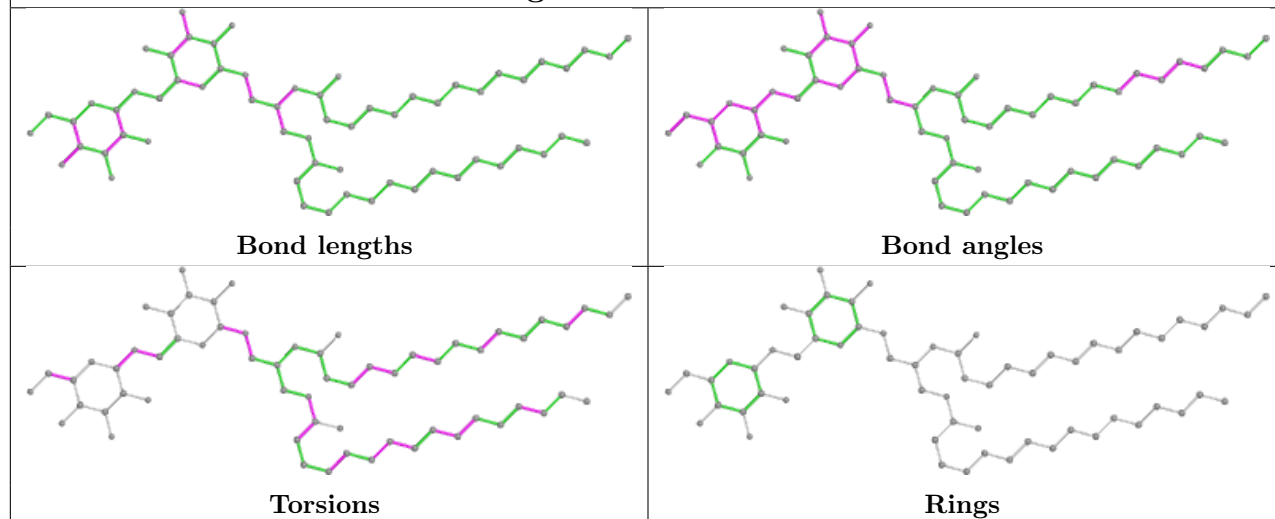
Ligand DGD C 516



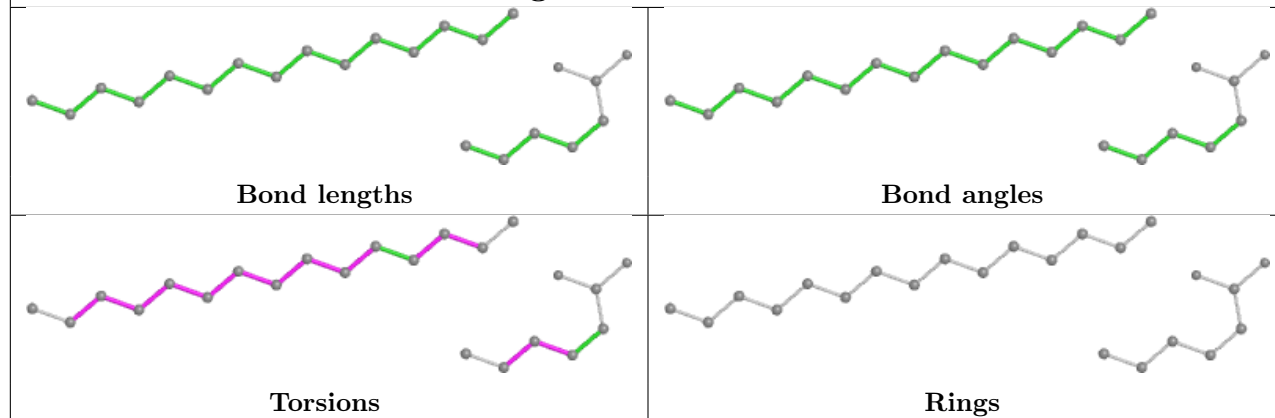
Ligand LMG c 524



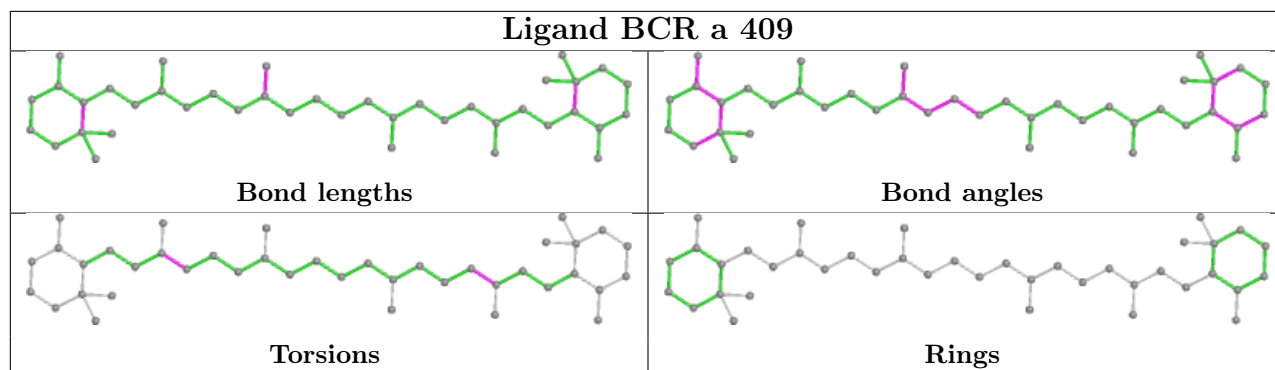
Ligand DGD C 517



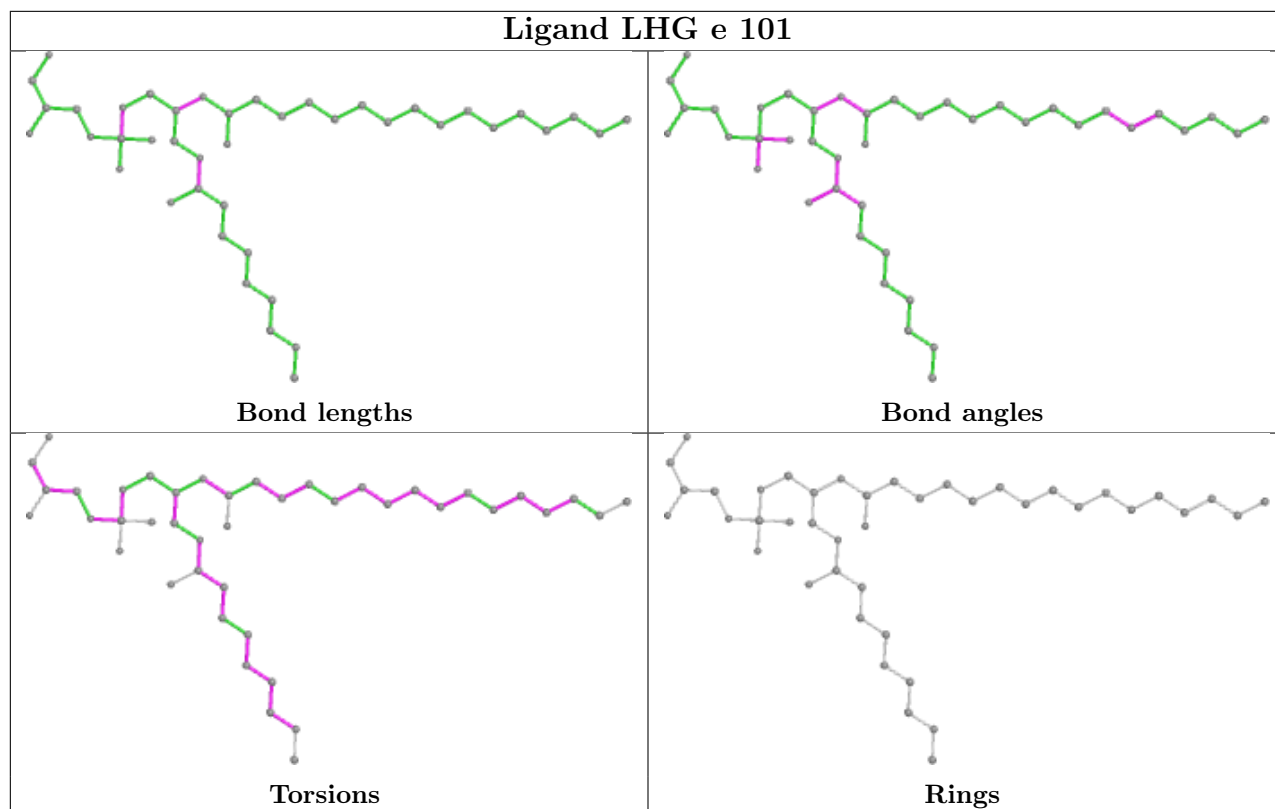
Ligand LMG d 410



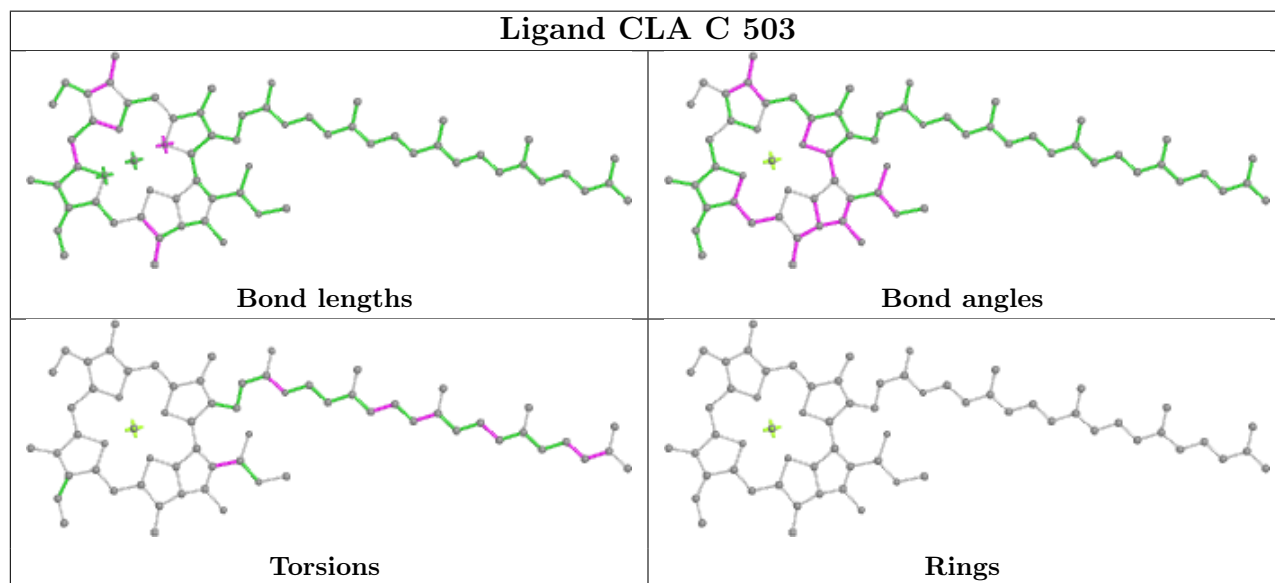
Ligand BCR a 409



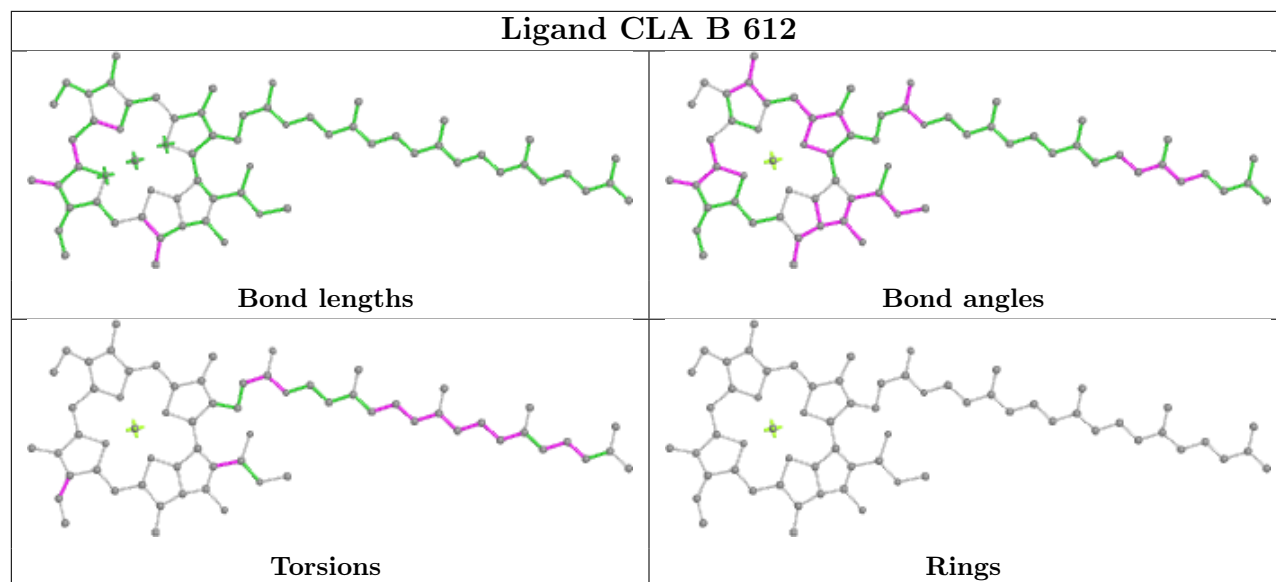
Ligand LHG e 101



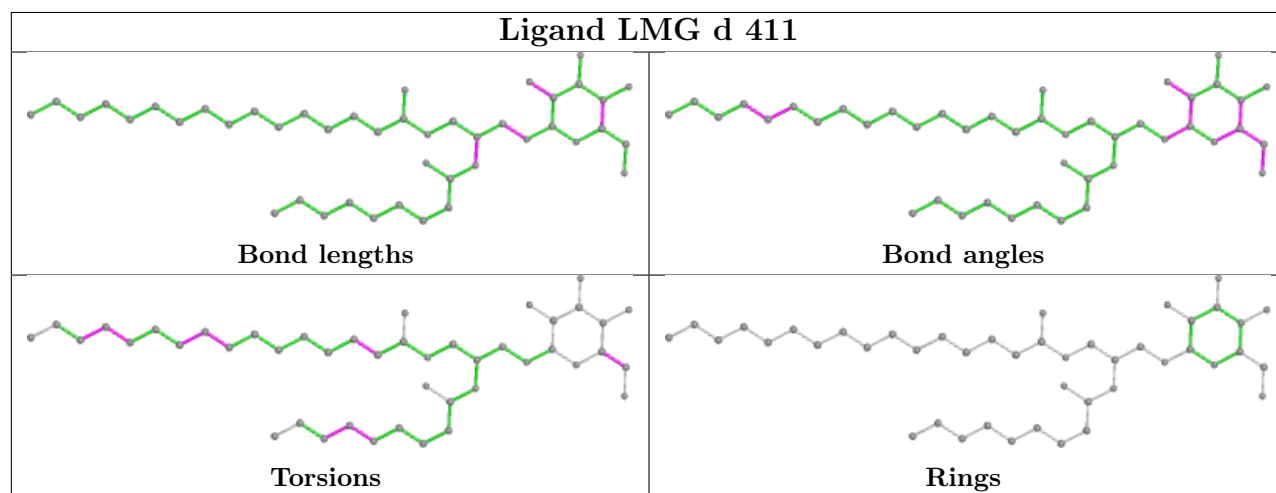
Ligand CLA C 503



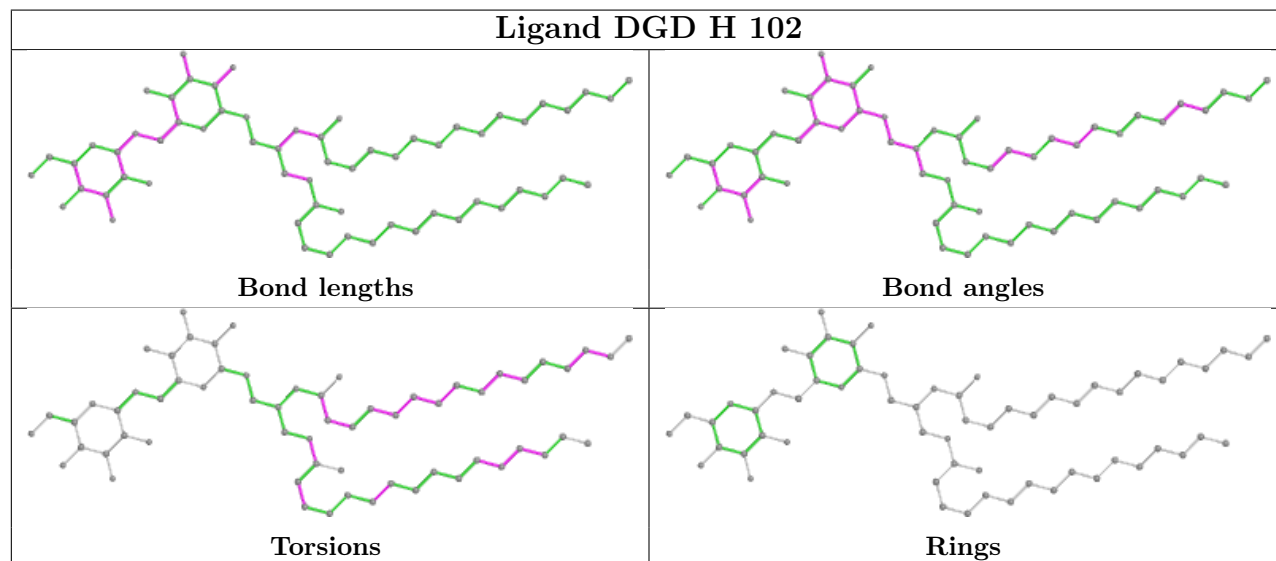
Ligand CLA B 612



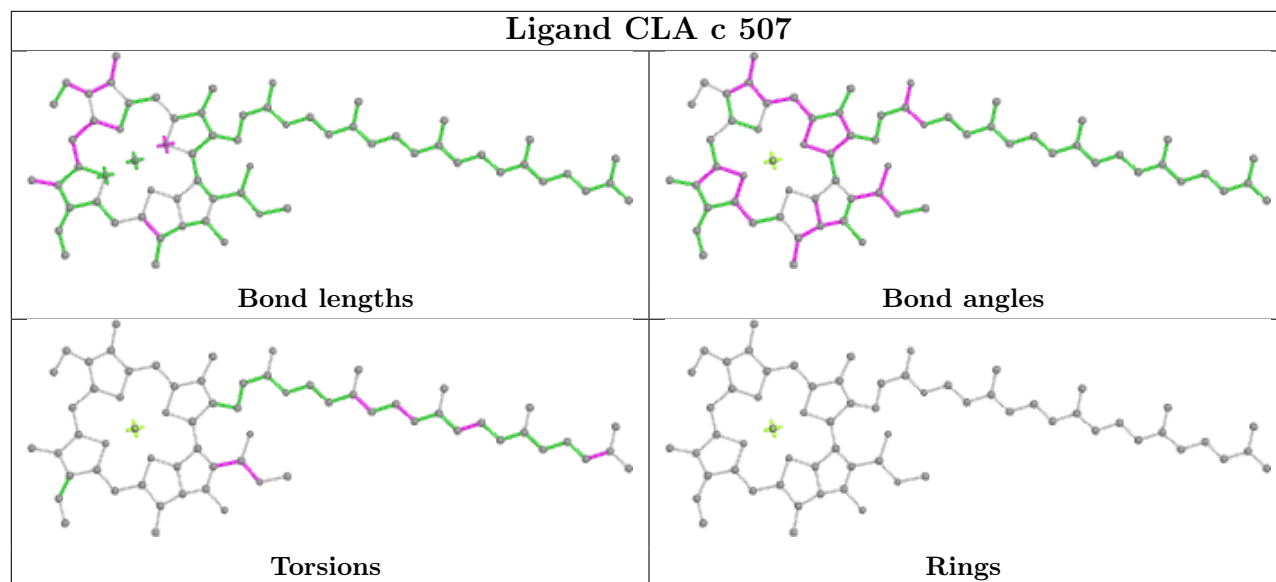
Ligand LMG d 411



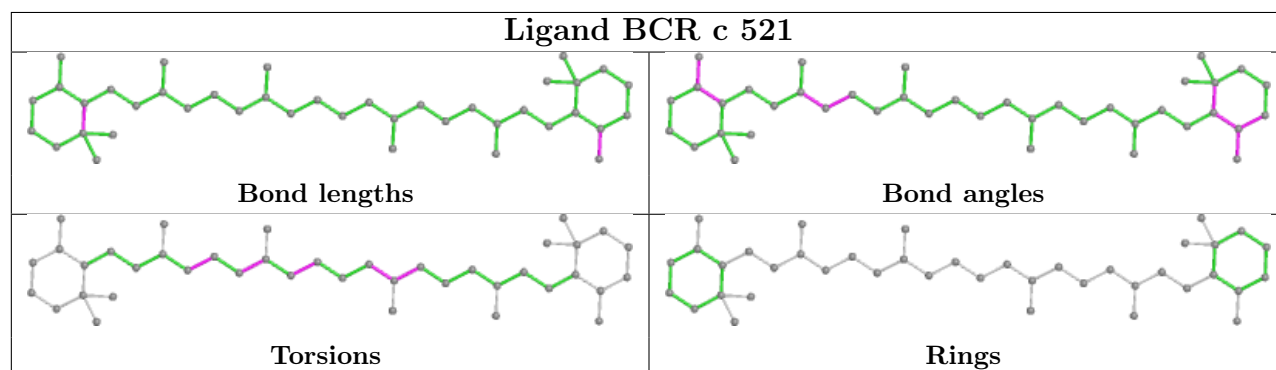
Ligand DGD H 102



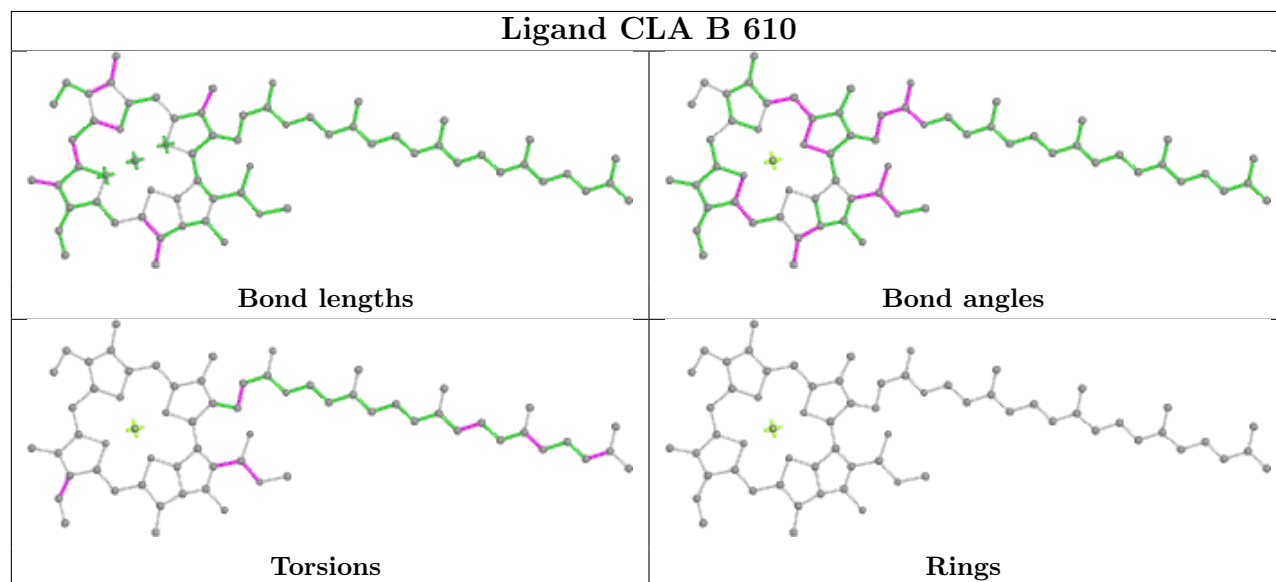
Ligand CLA c 507



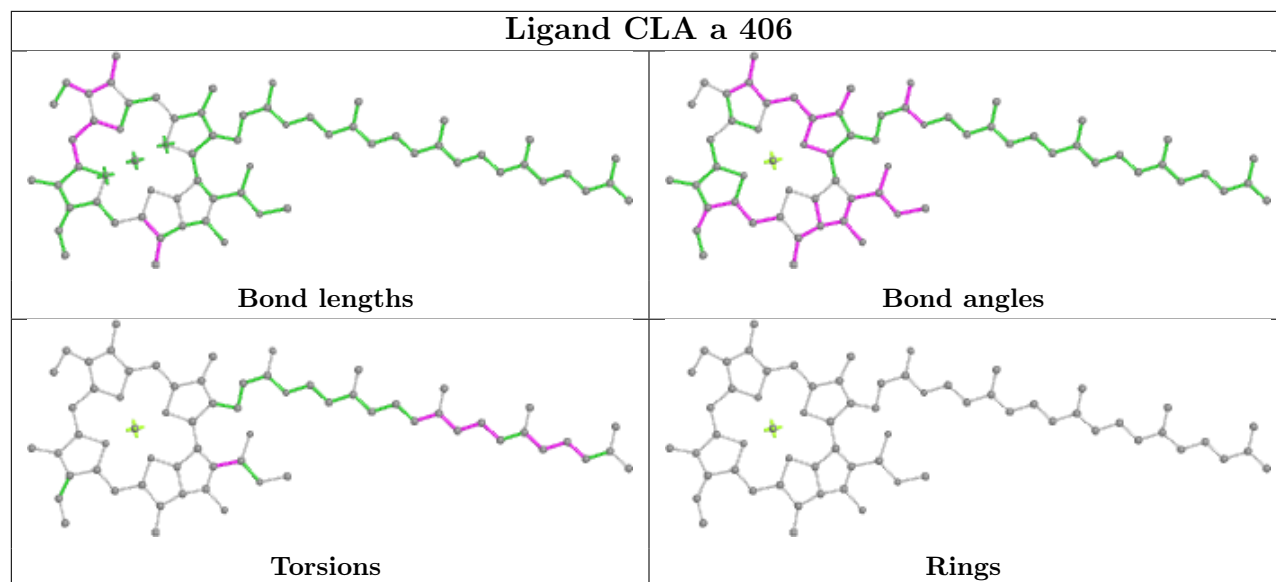
Ligand BCR c 521



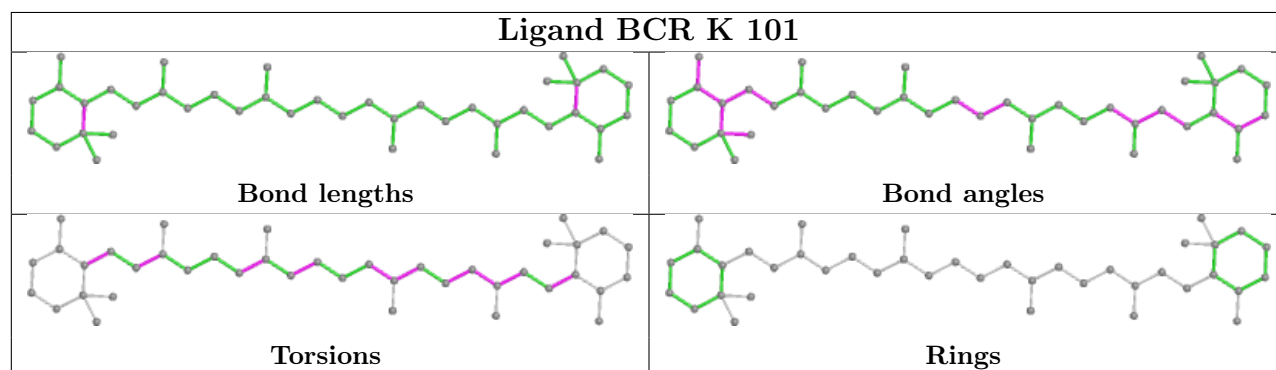
Ligand CLA B 610



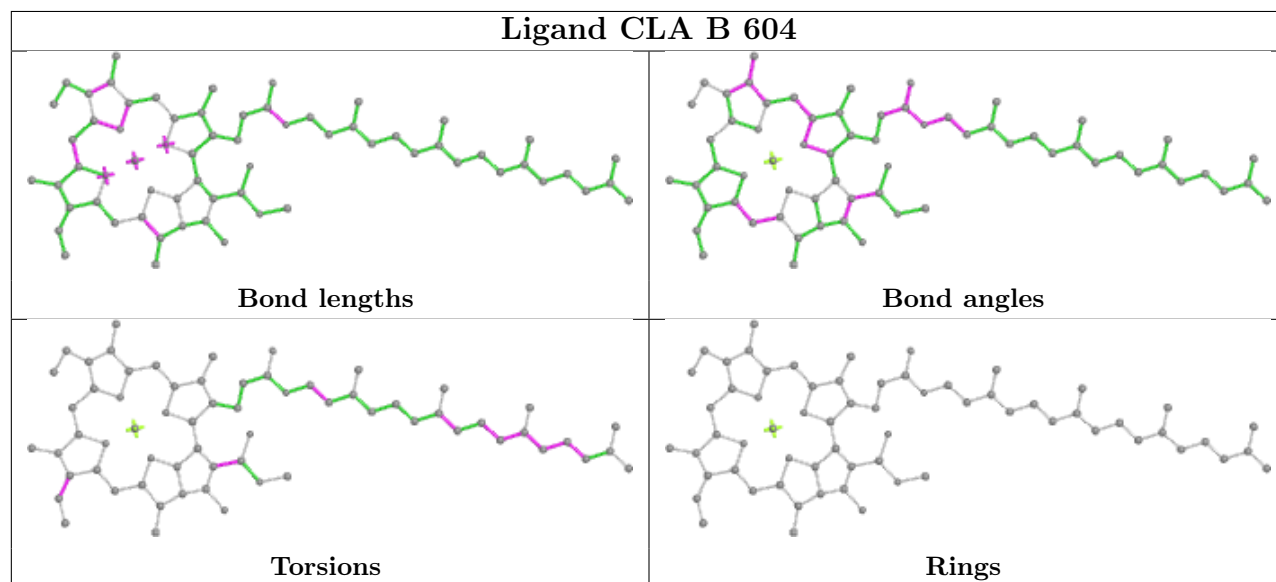
Ligand CLA a 406



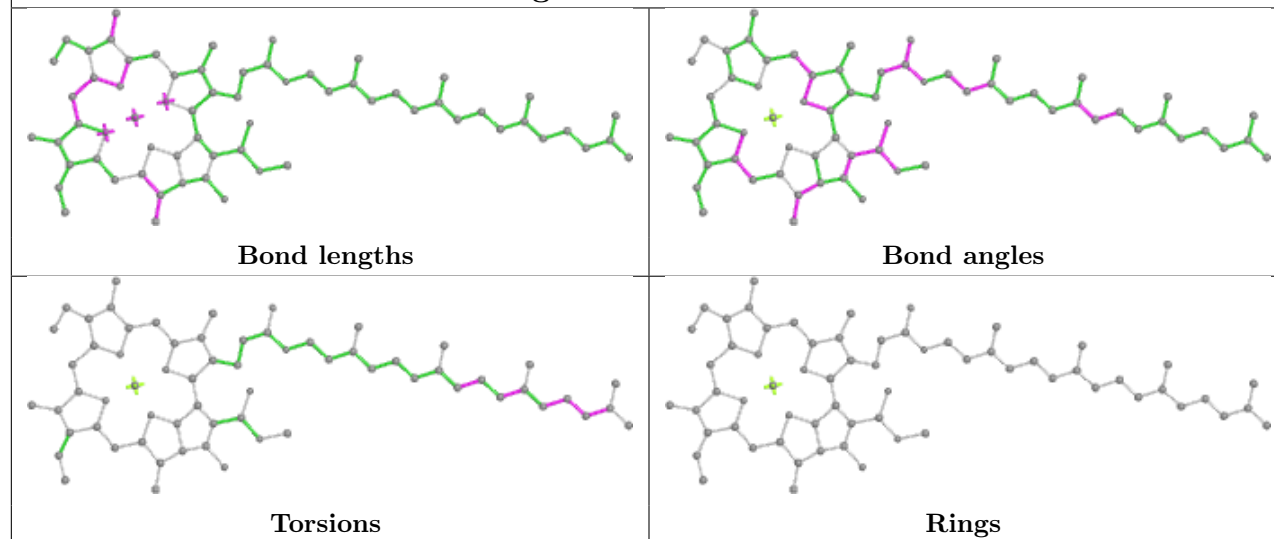
Ligand BCR K 101



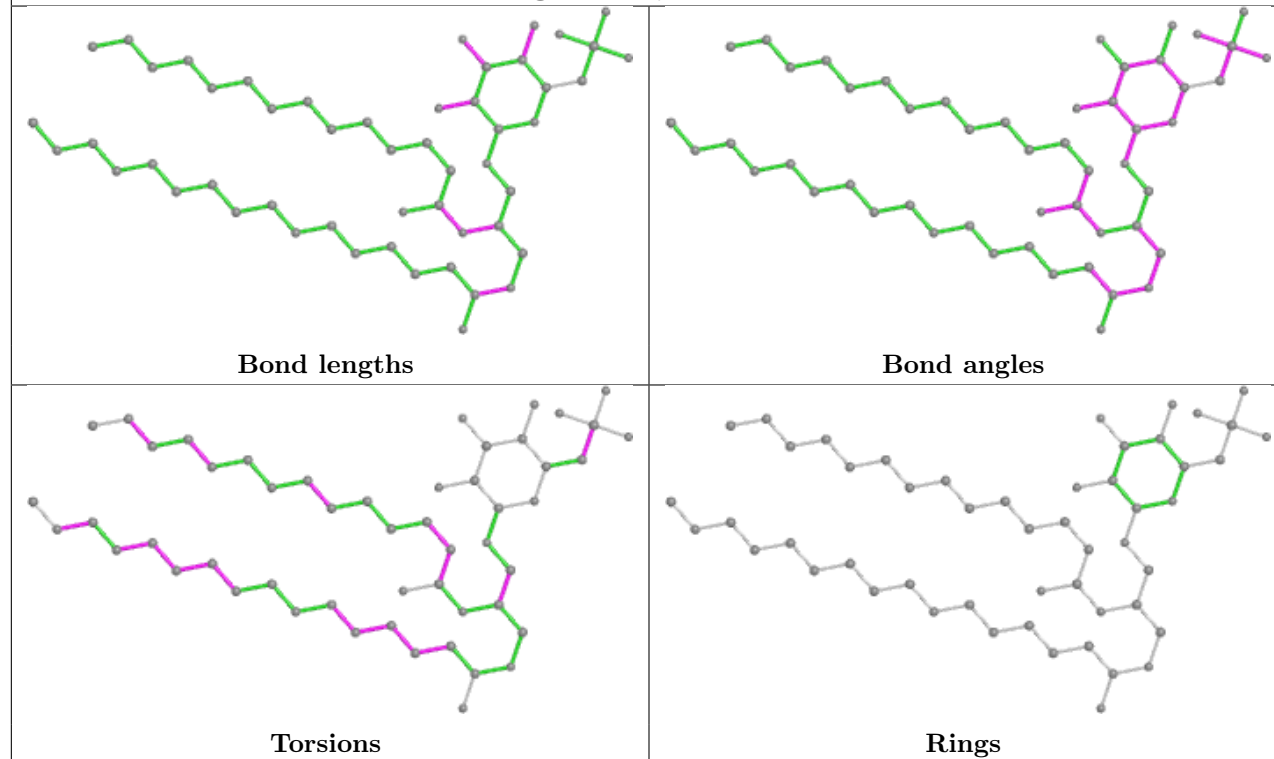
Ligand CLA B 604



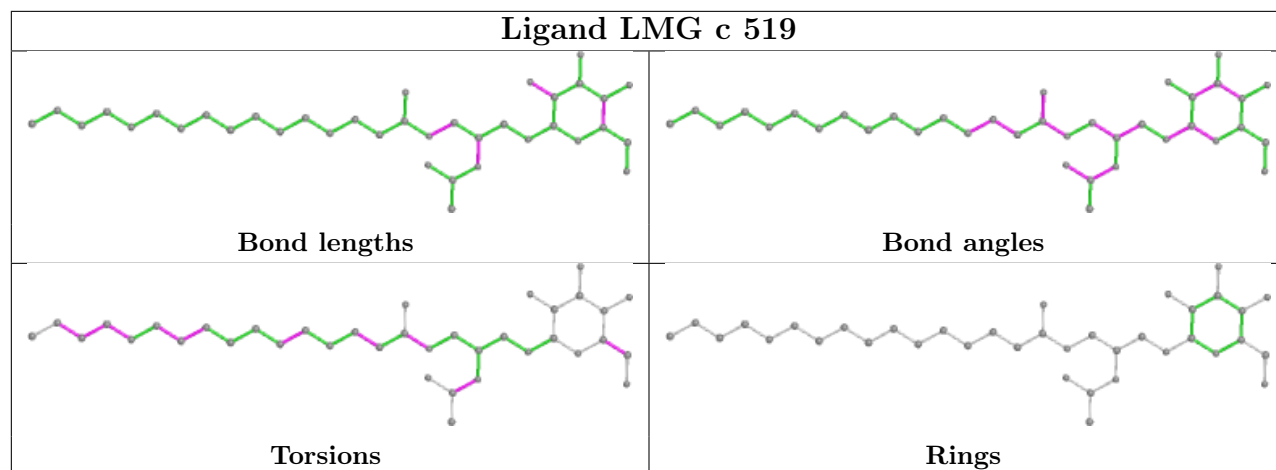
Ligand CLA B 611



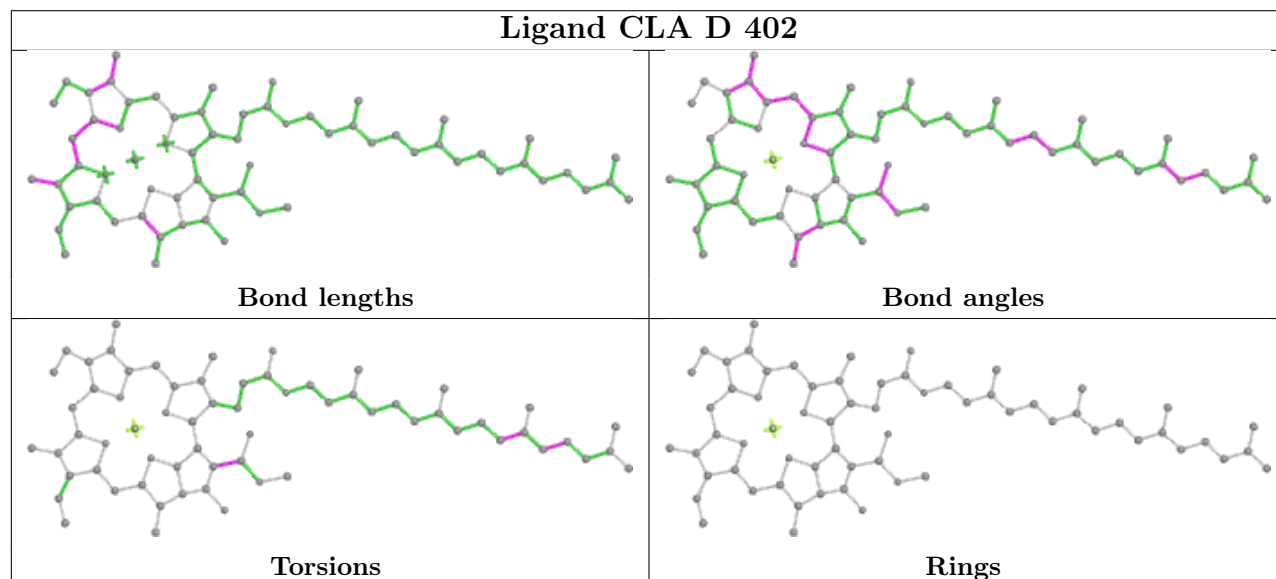
Ligand SQD A 410



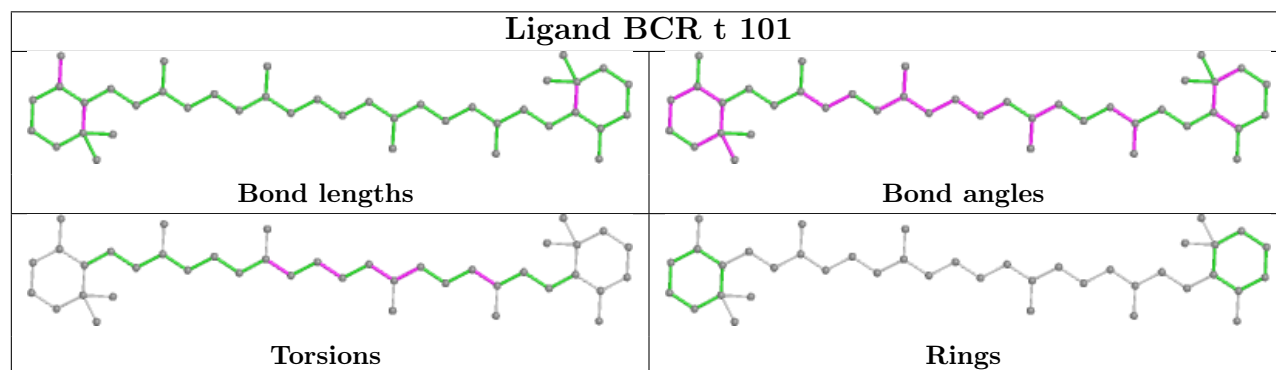
Ligand LMG c 519

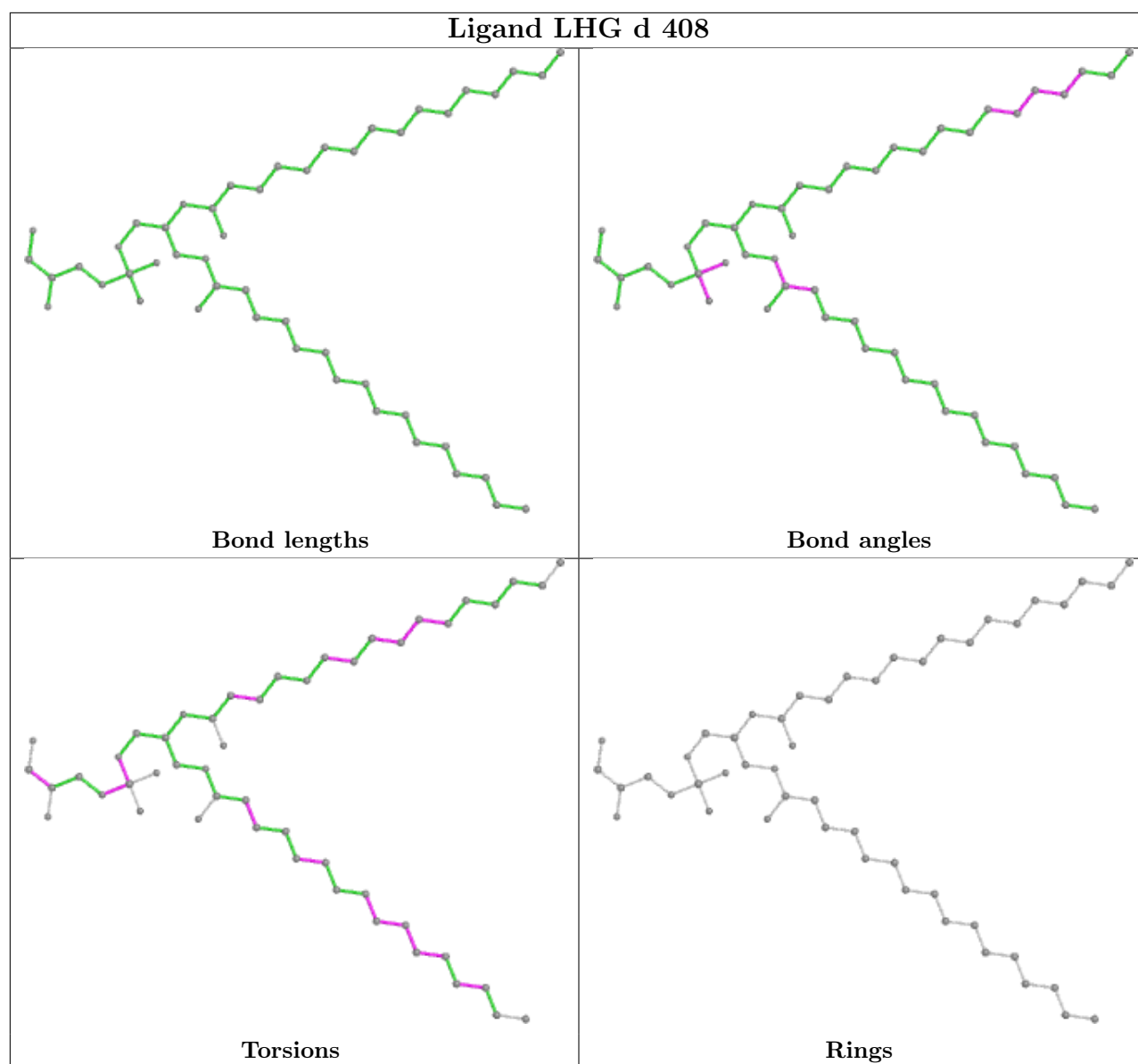


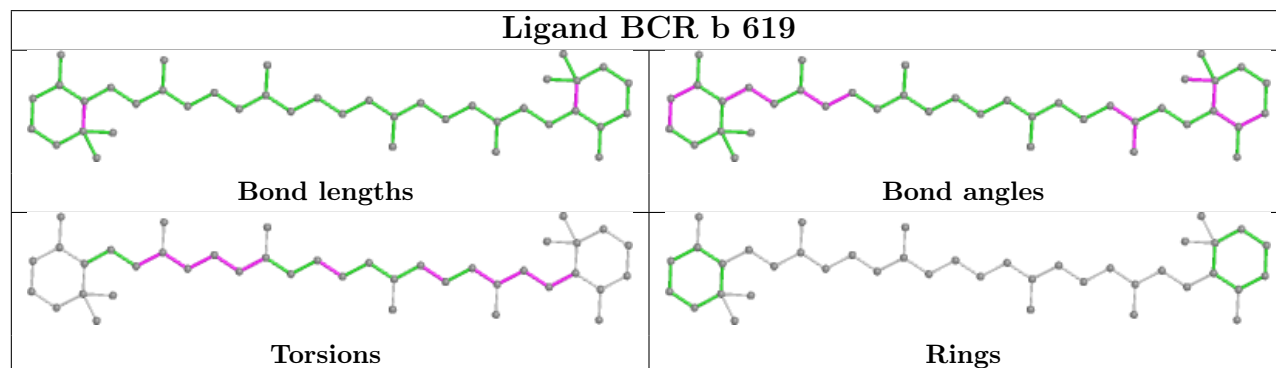
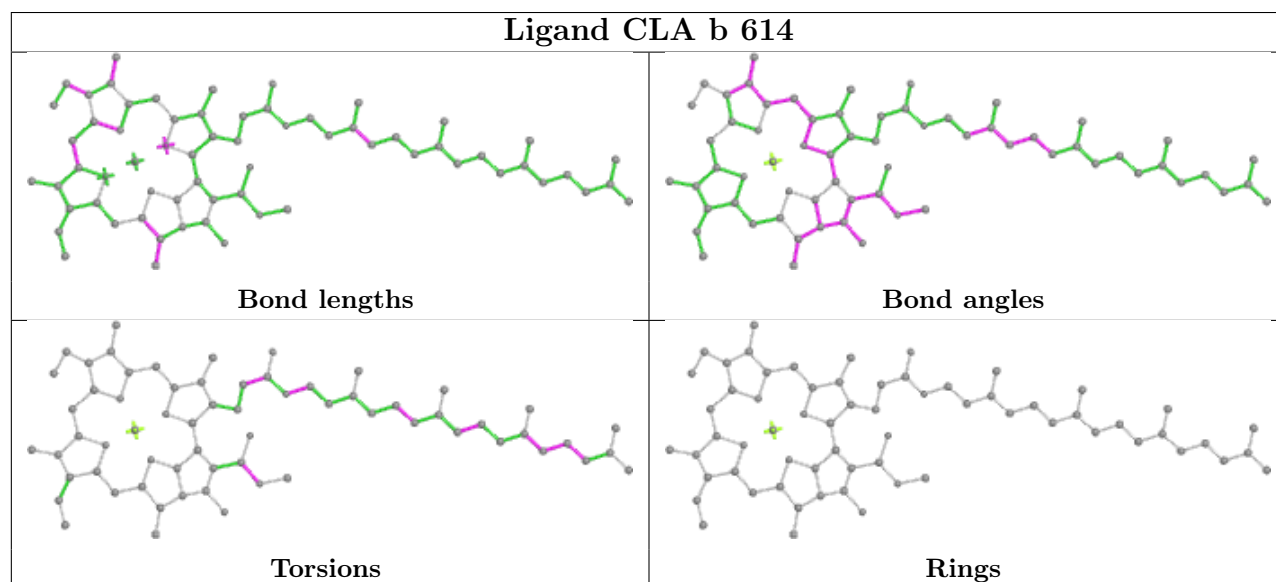
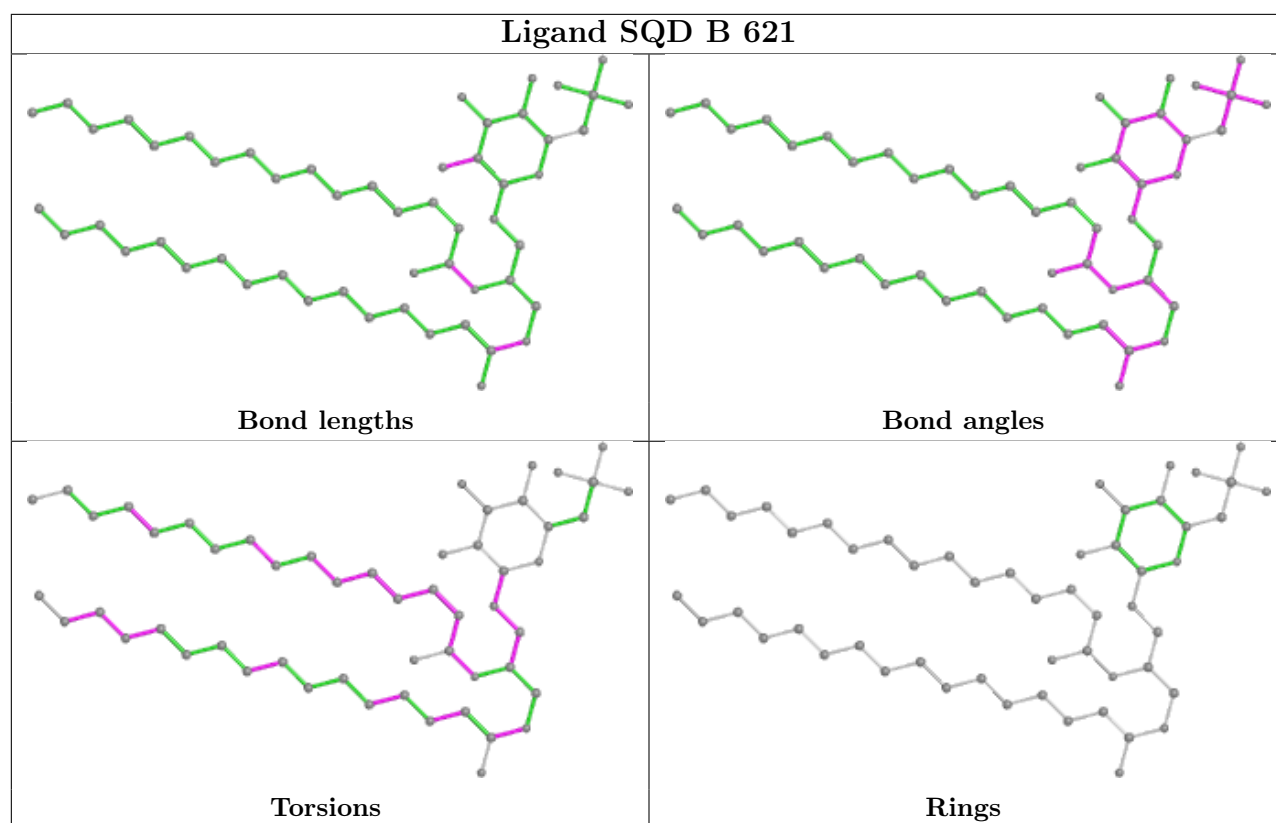
Ligand CLA D 402



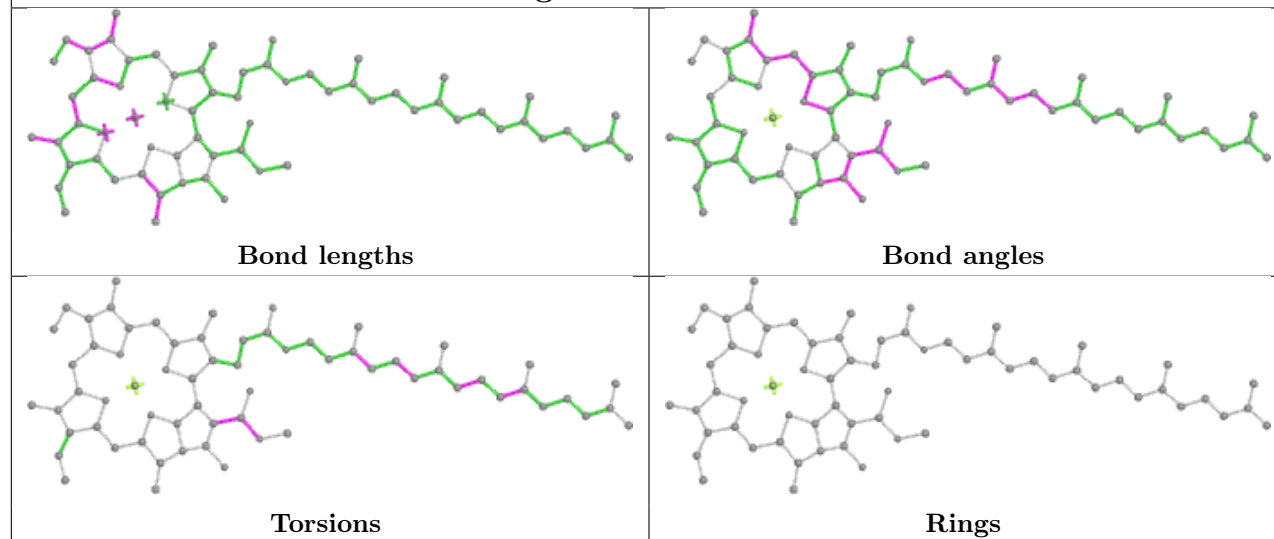
Ligand BCR t 101



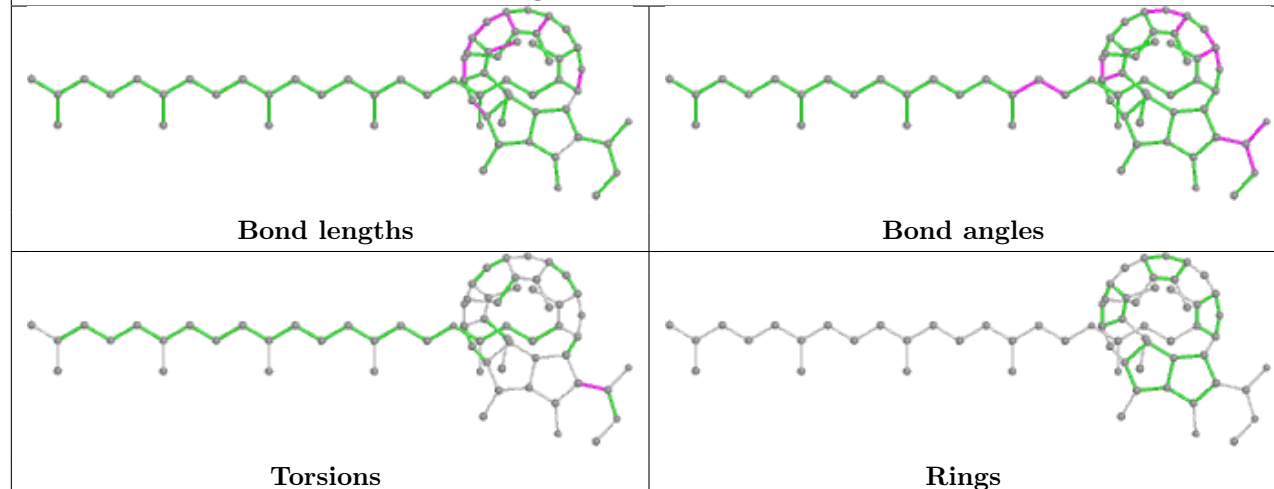




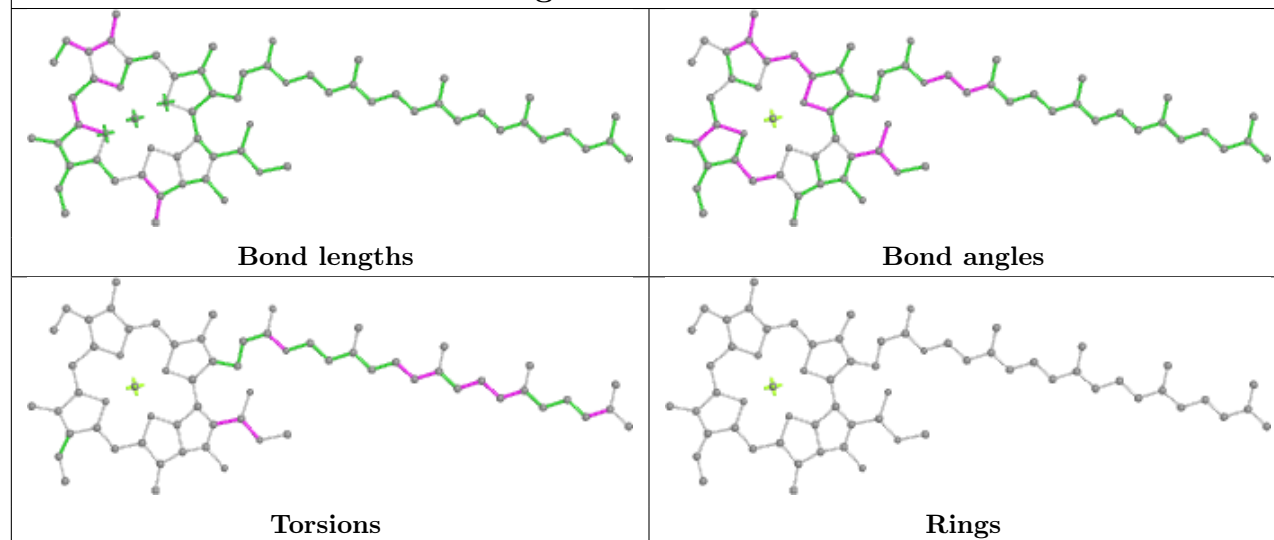
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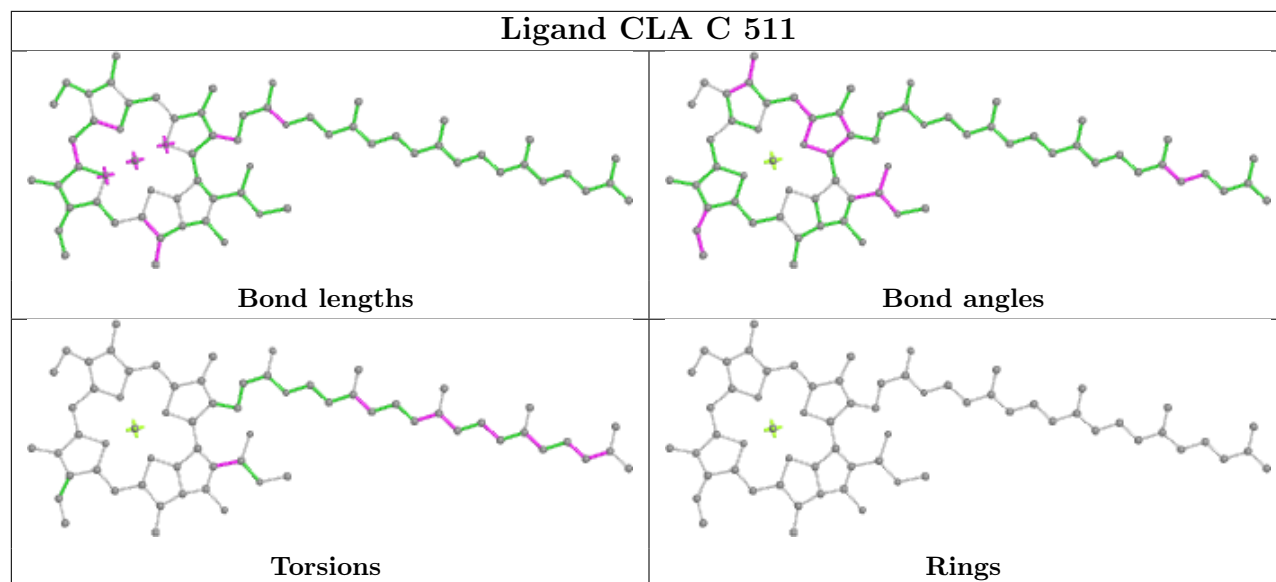
Ligand PHO D 401



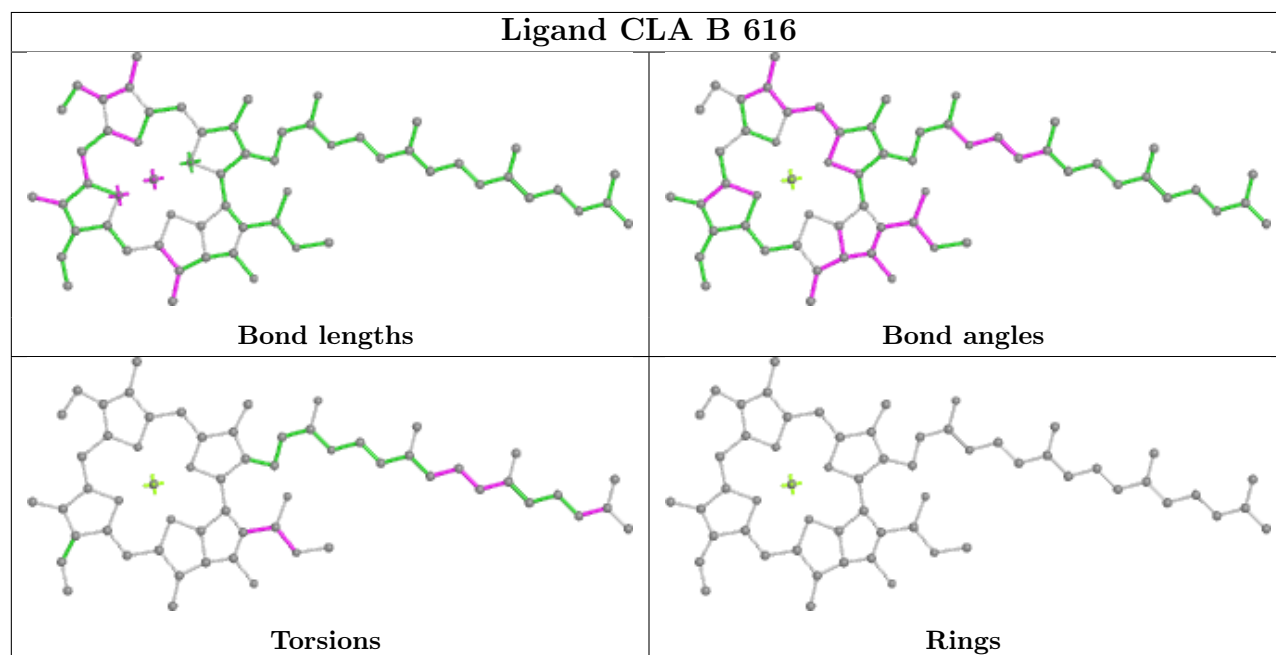
Ligand CLA b 608



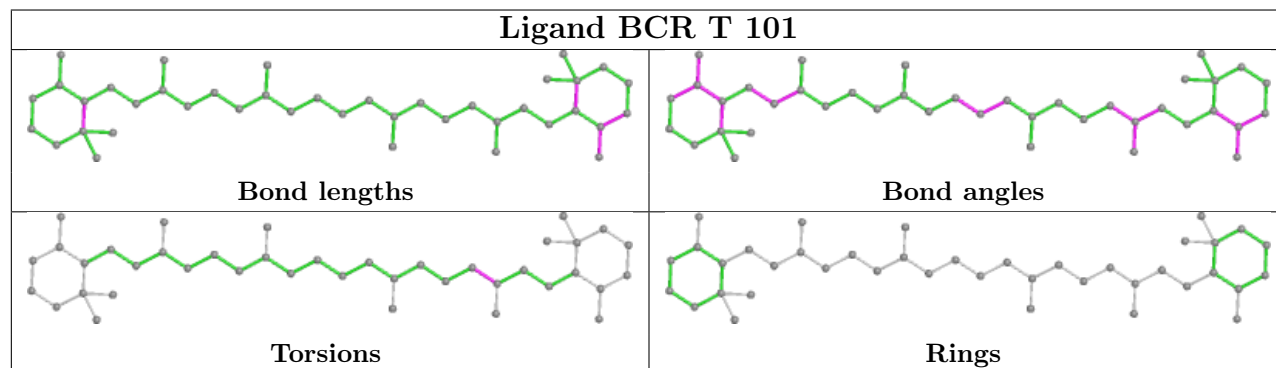
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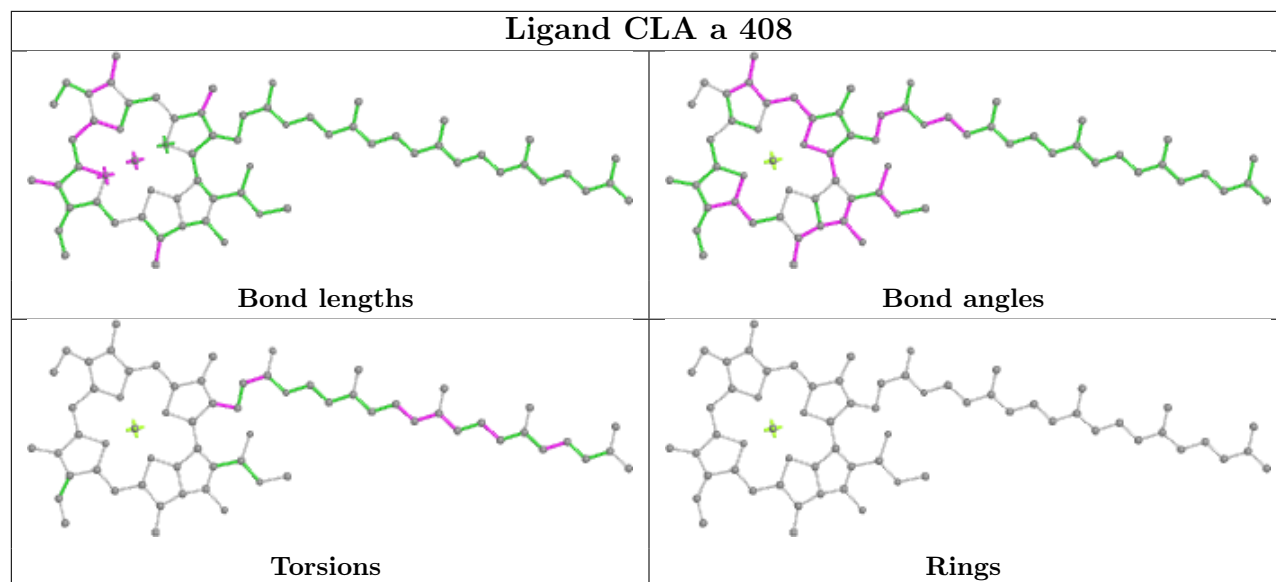
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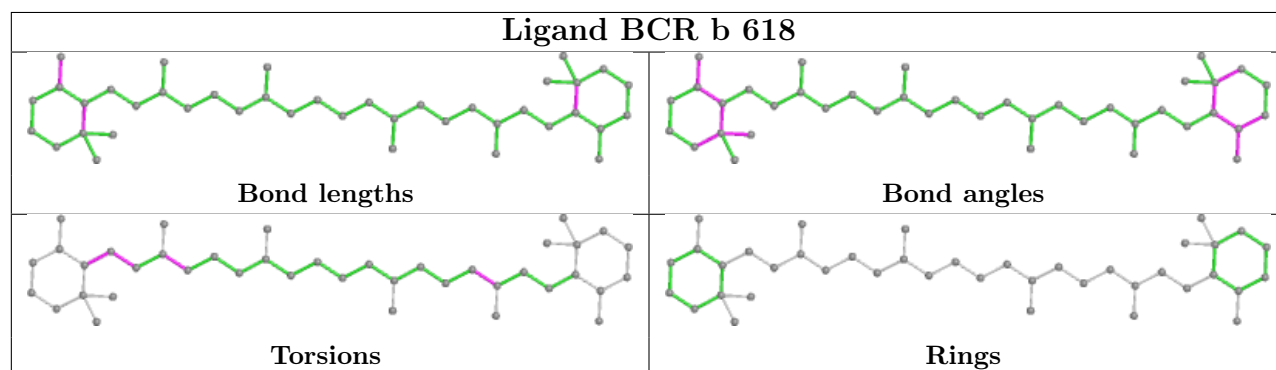
Ligand BCR T 101



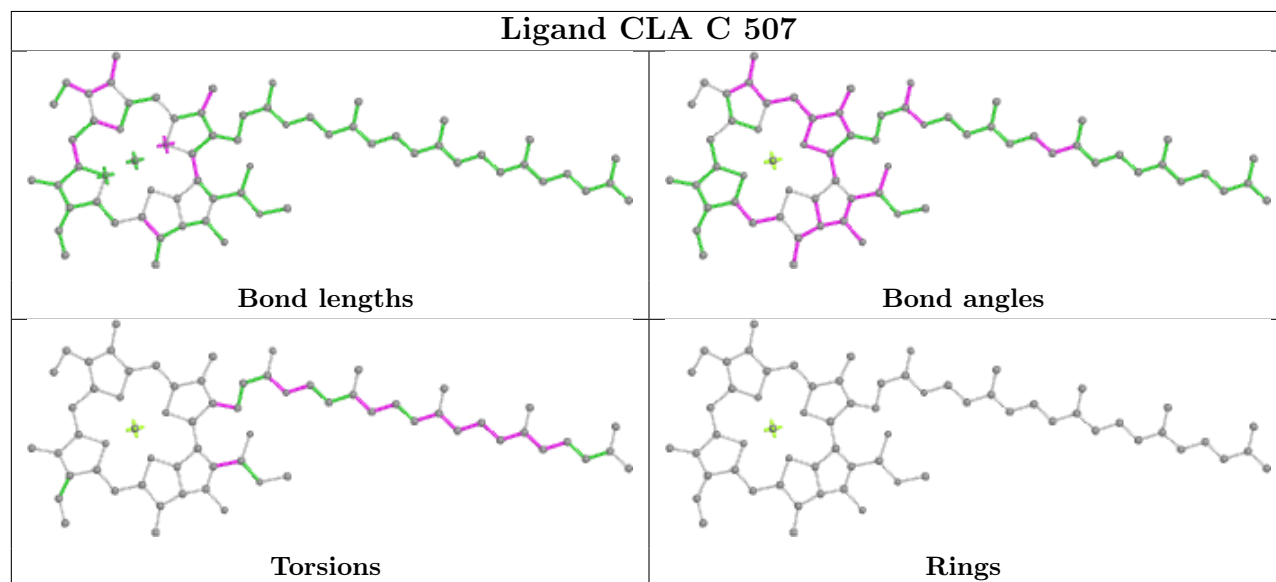
Ligand CLA a 408

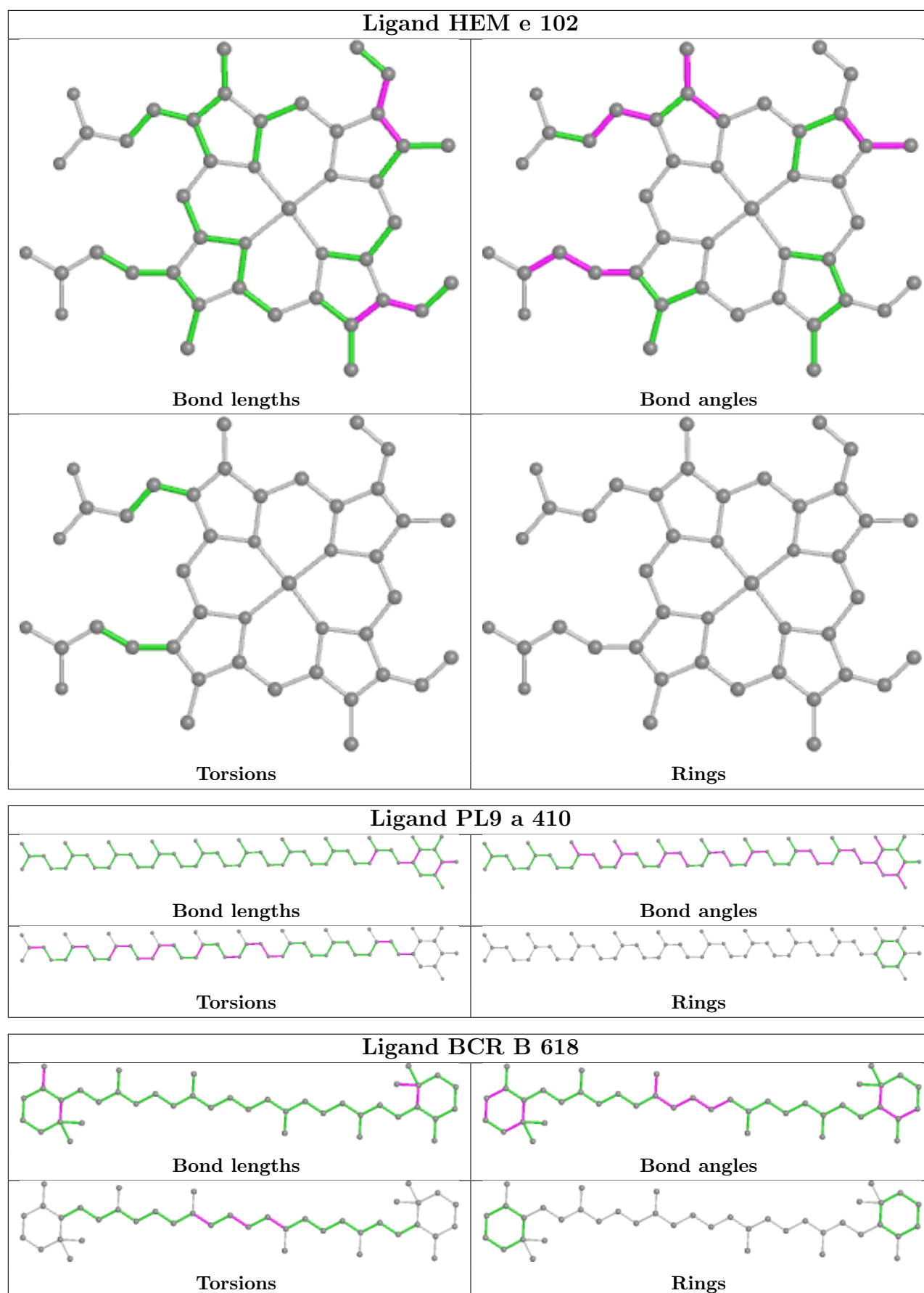


Ligand BCR b 618

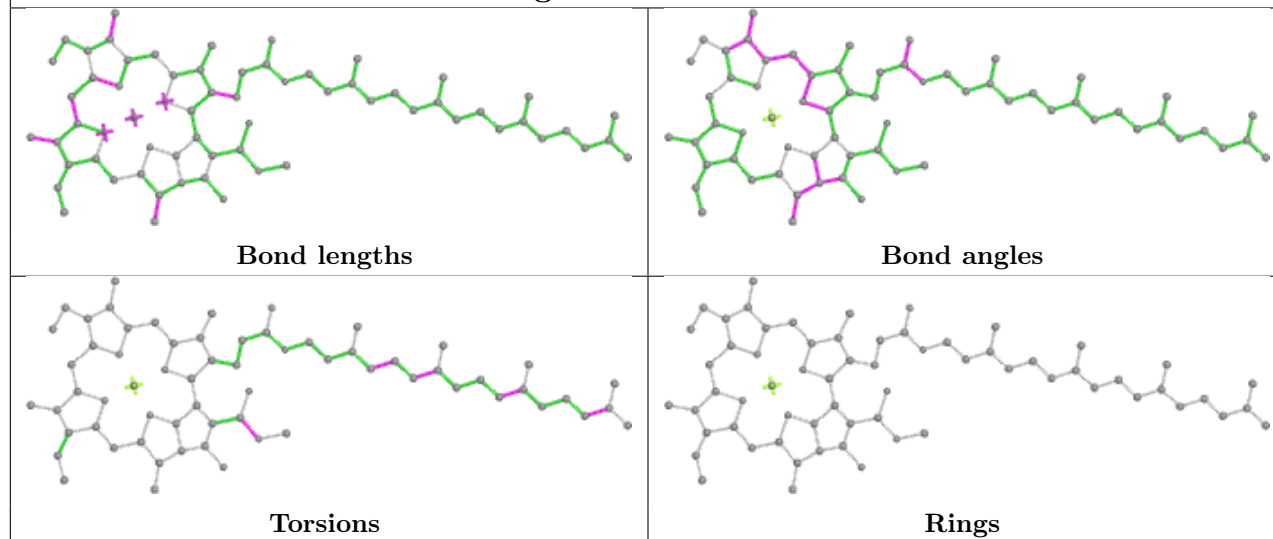


Ligand CLA C 507

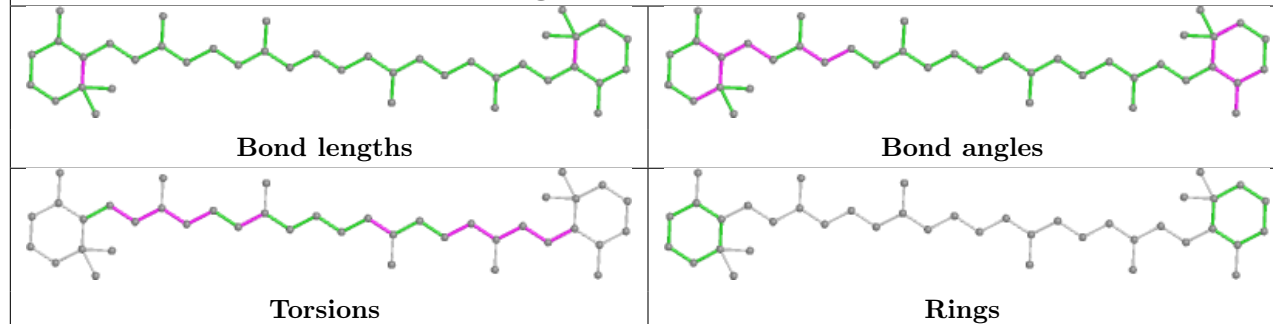


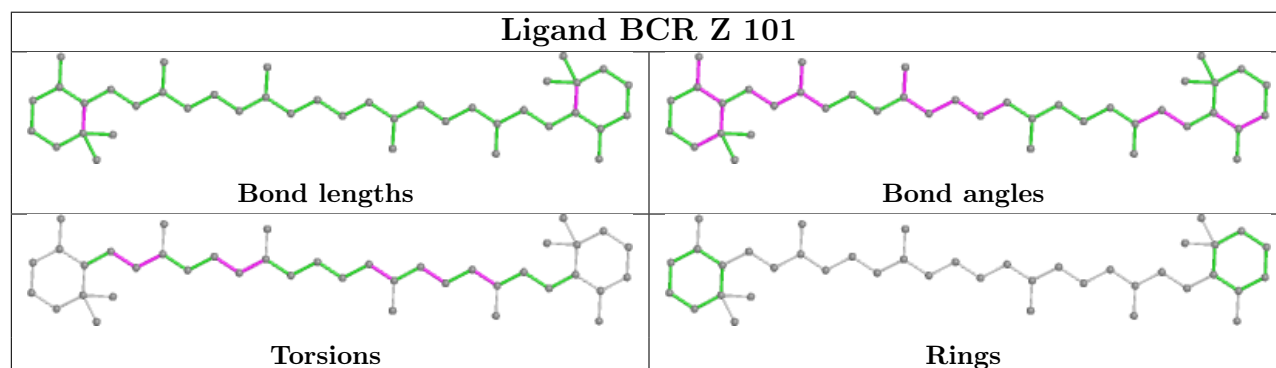
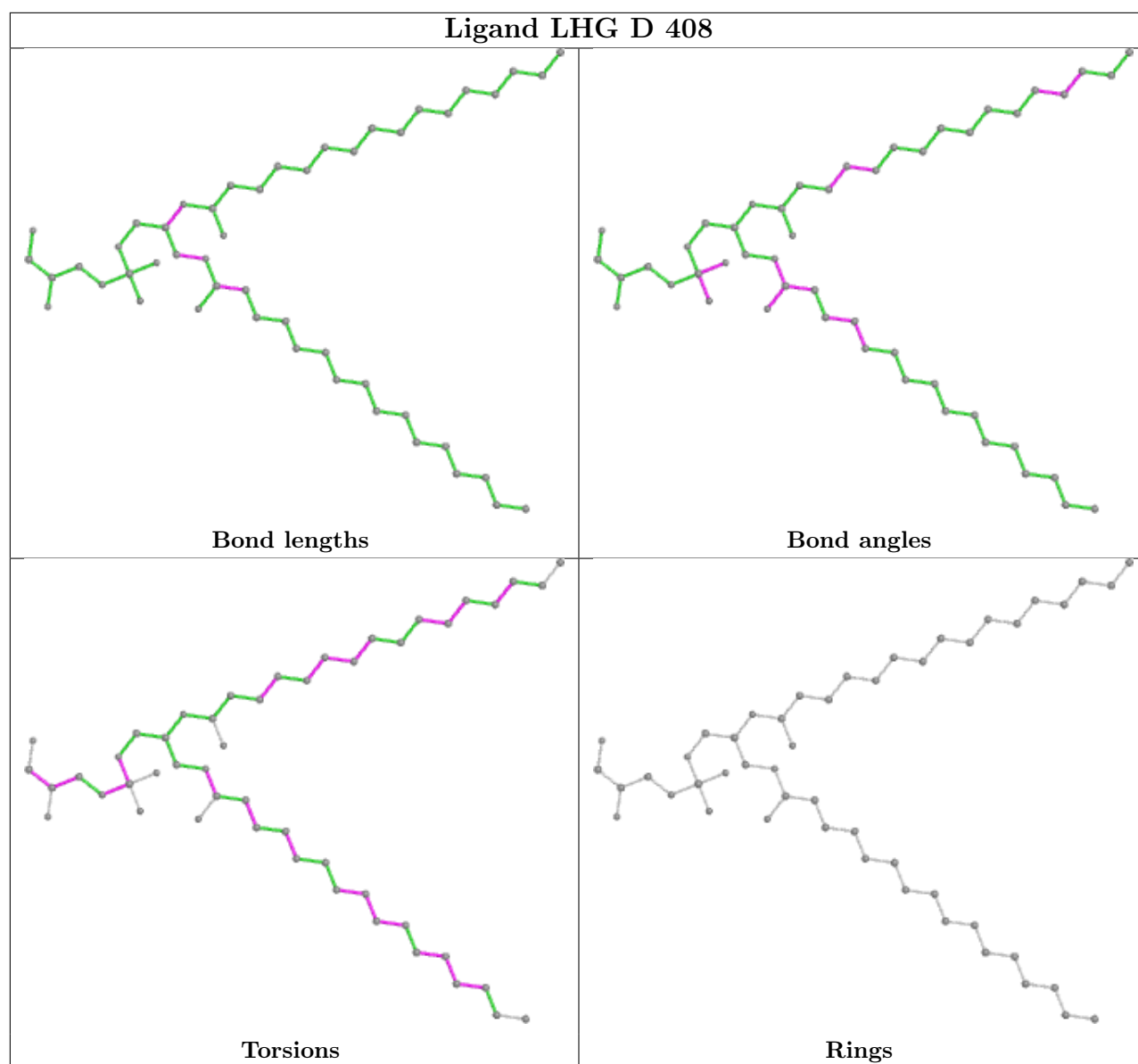


Ligand CLA d 403

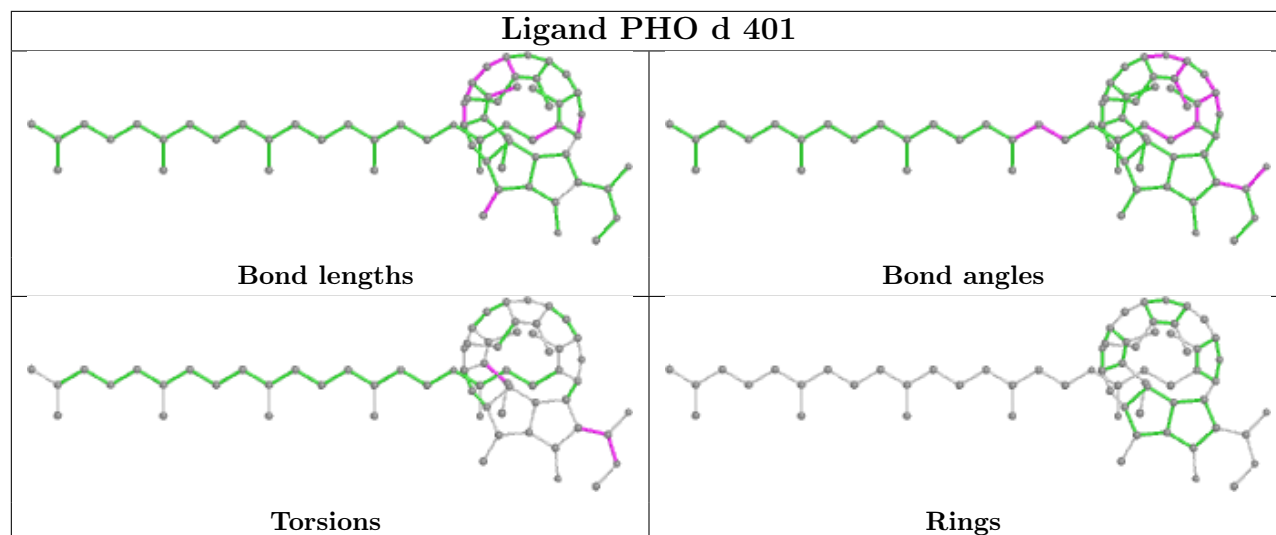


Ligand BCR d 405

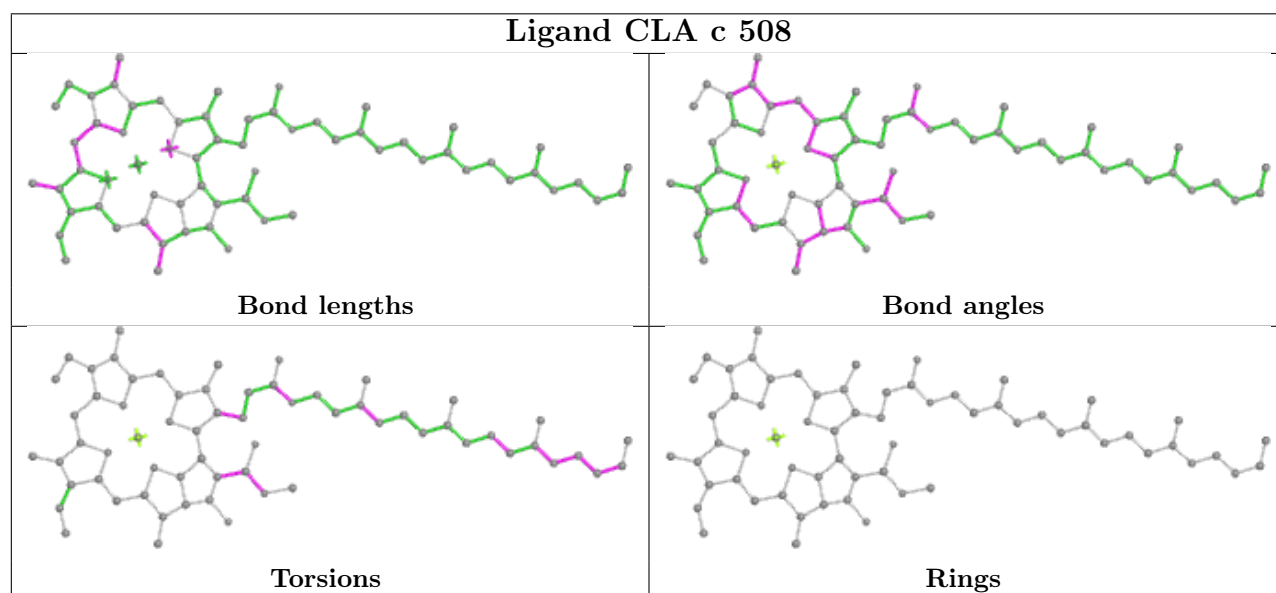




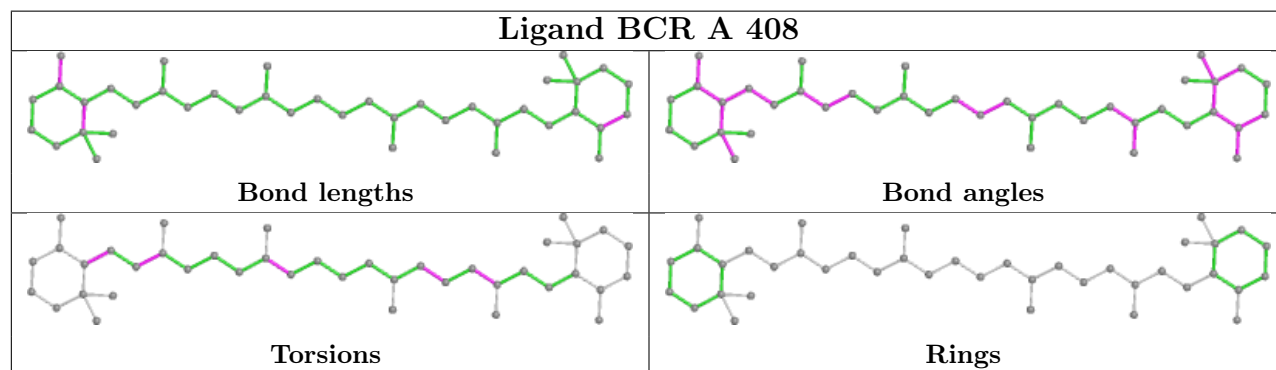
Ligand PHO d 401

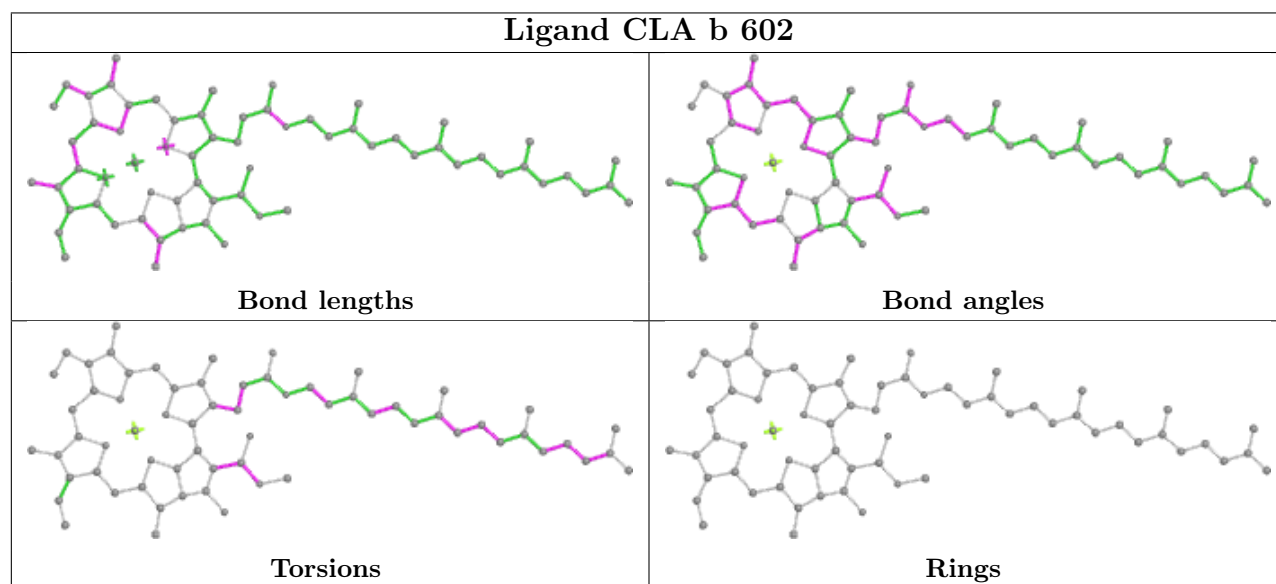
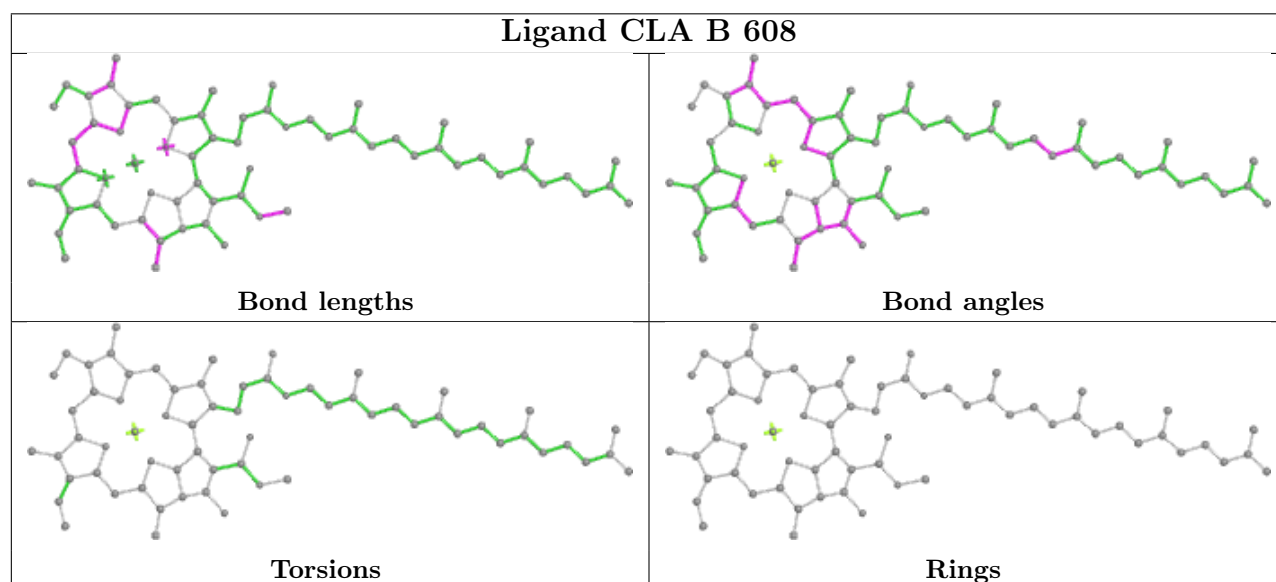
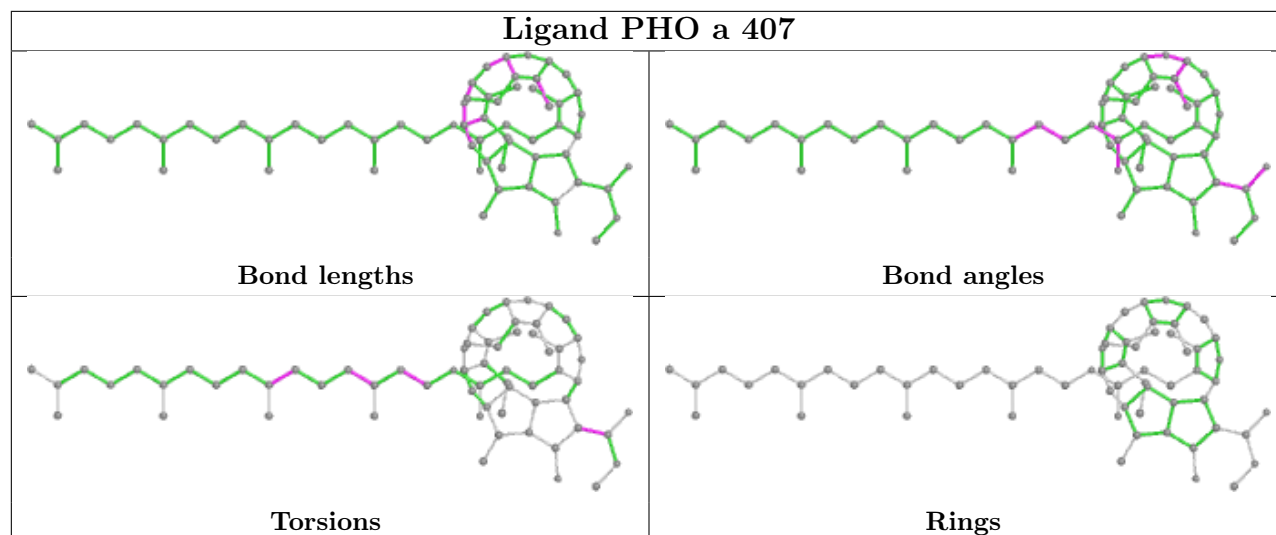


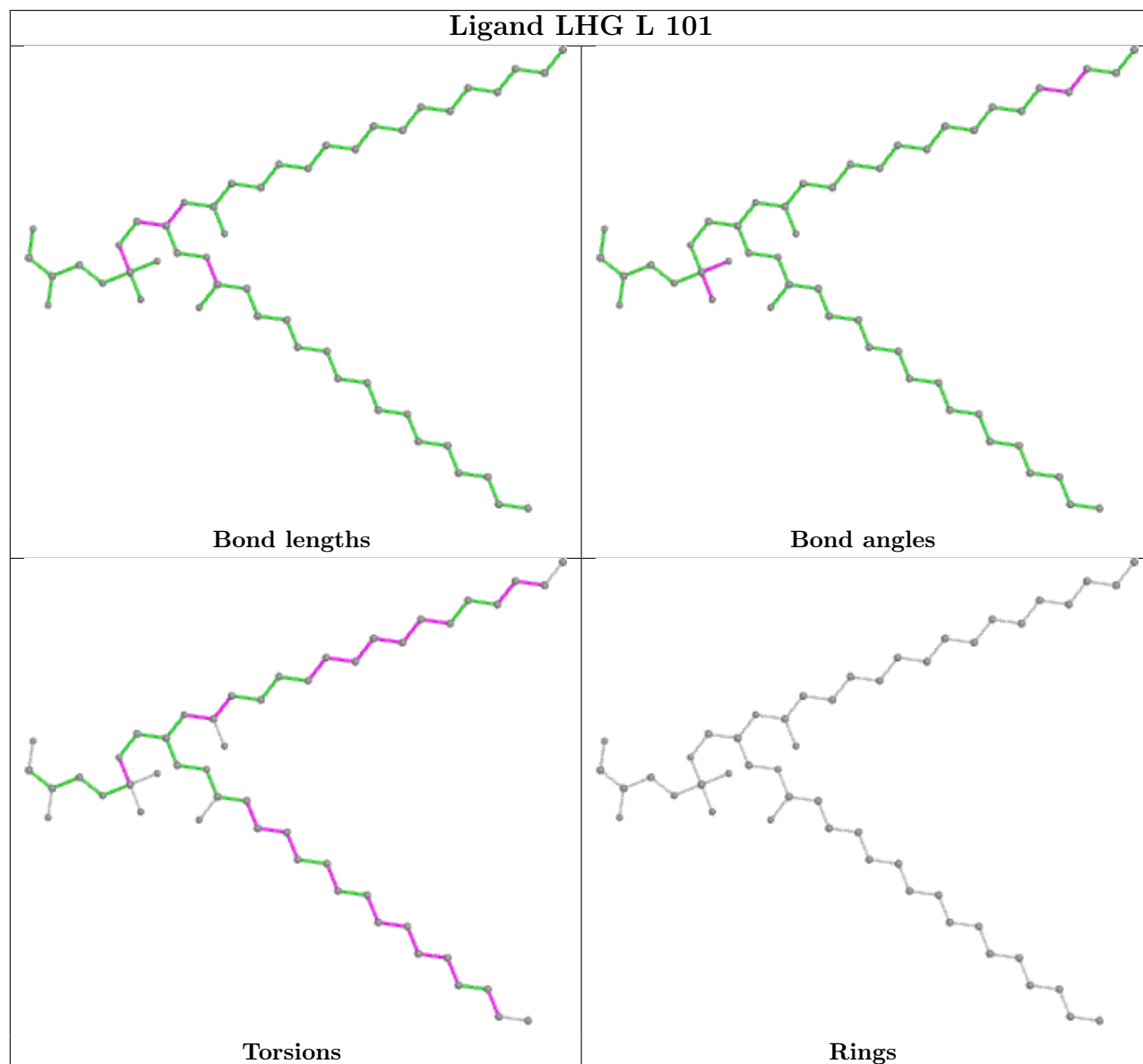
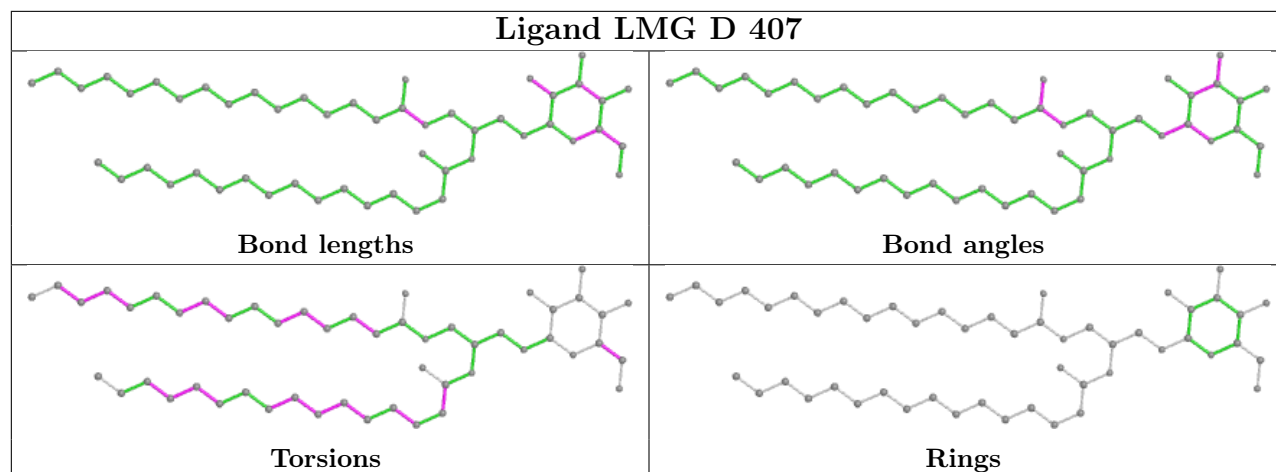
Ligand CLA c 508



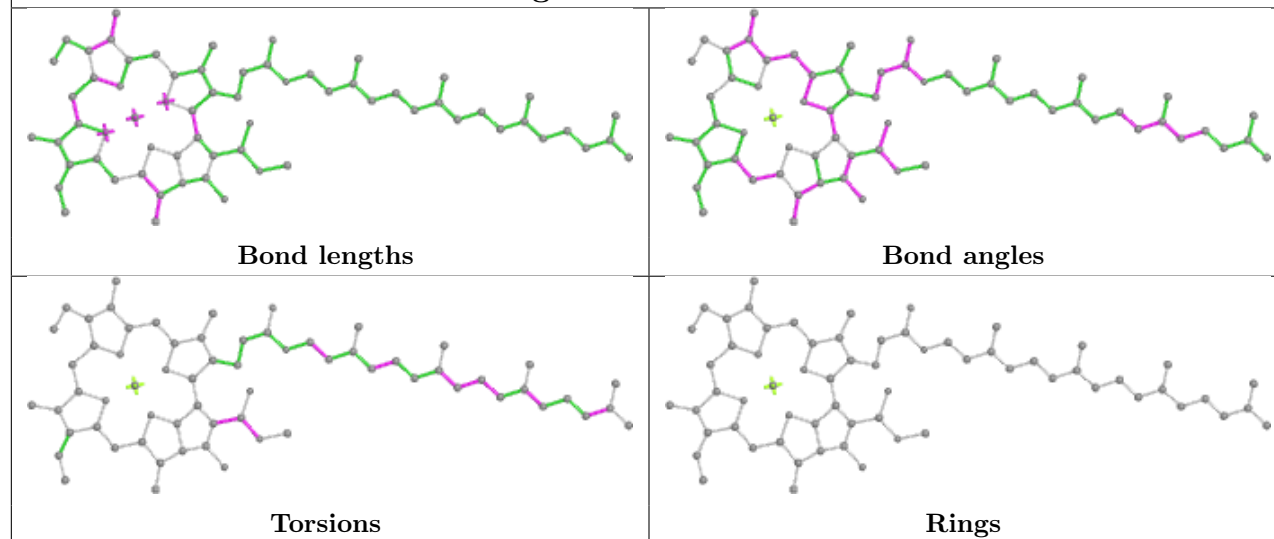
Ligand BCR A 408



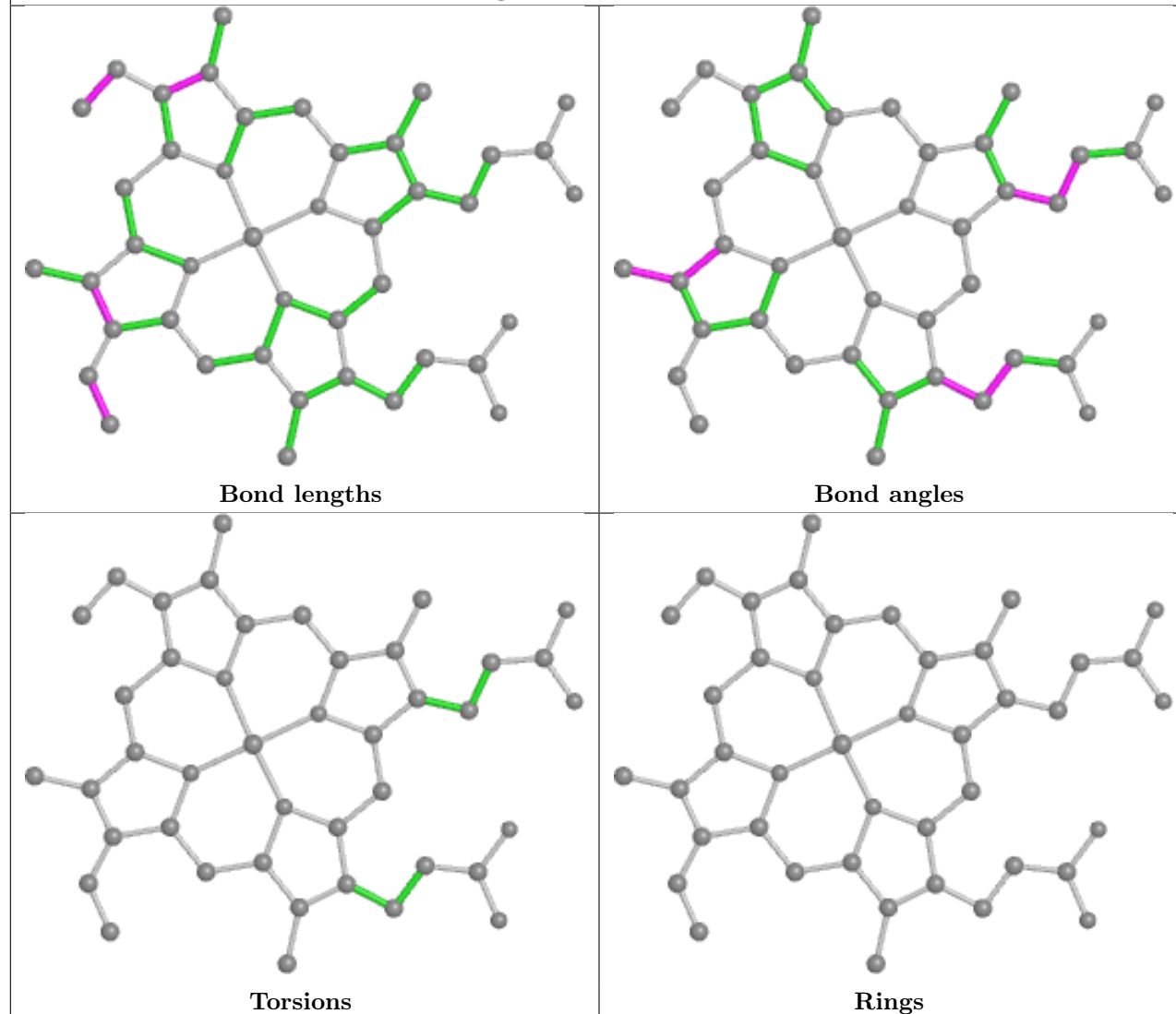




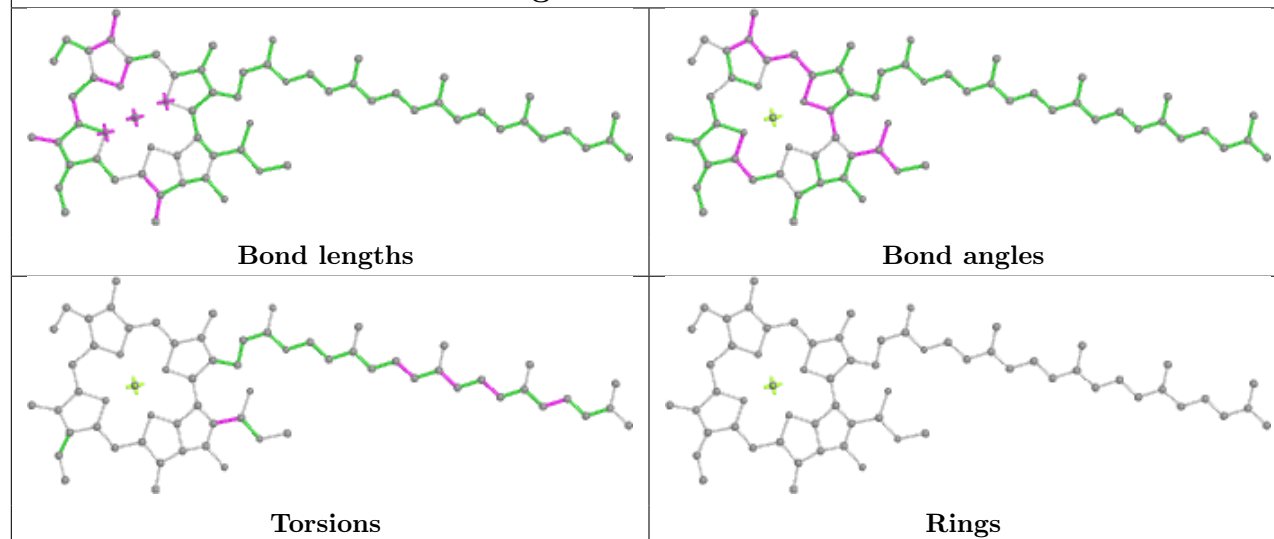
Ligand CLA C 513



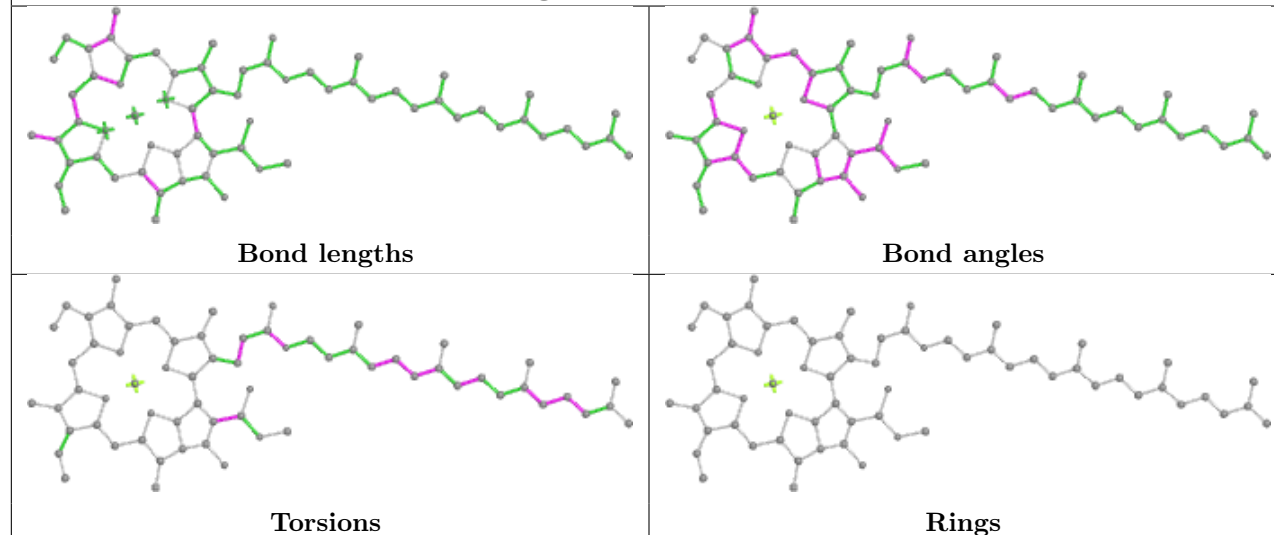
Ligand HEC v 201



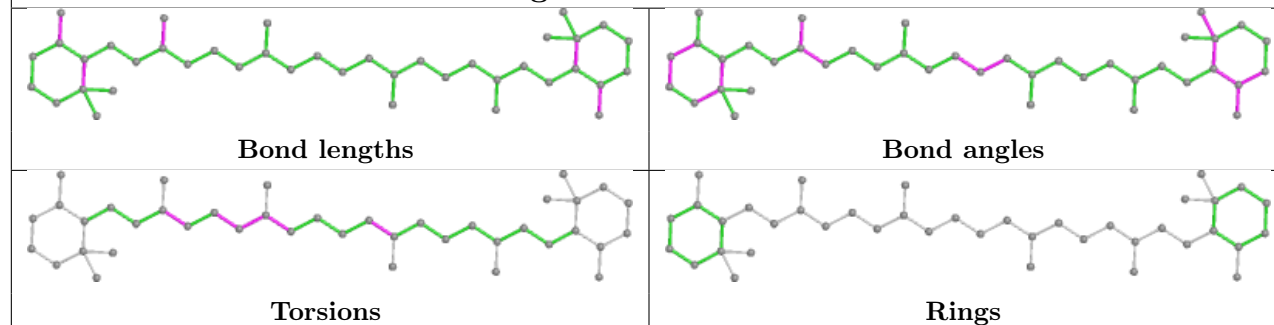
Ligand CLA C 508

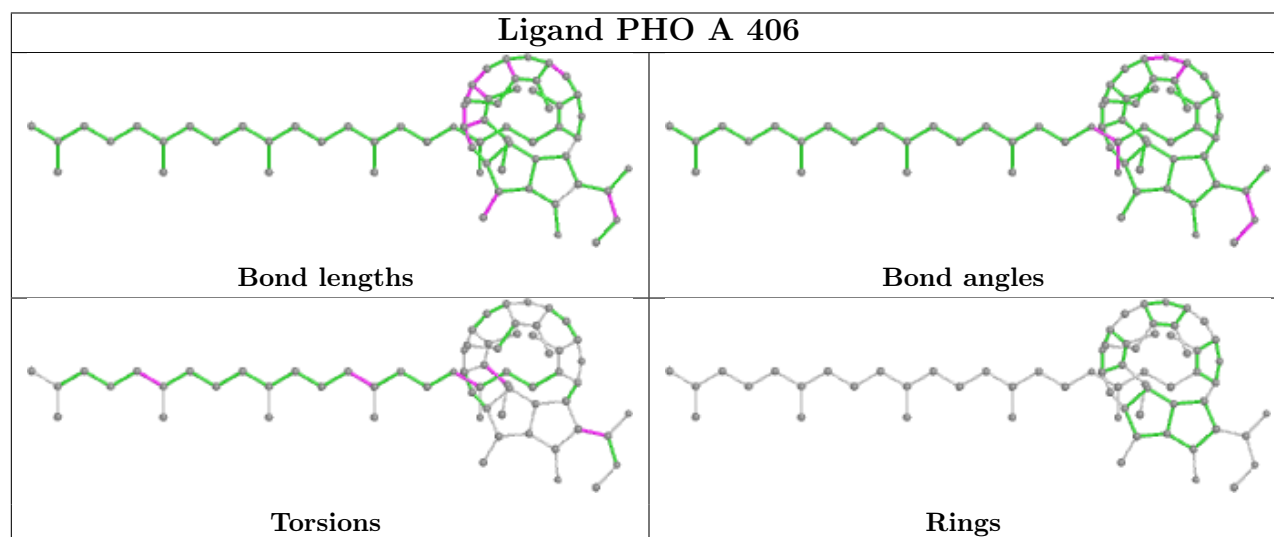
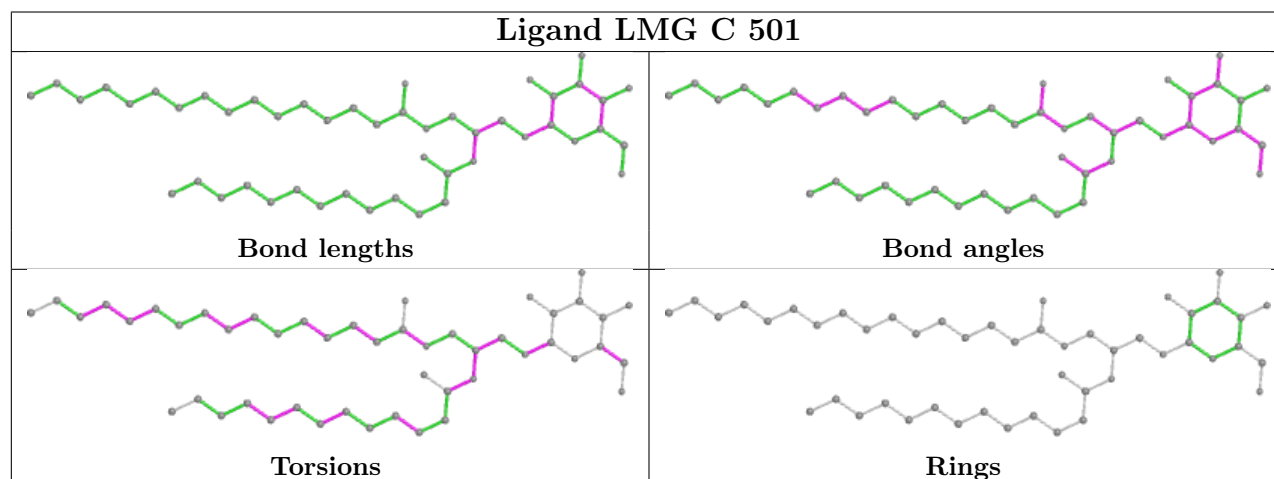
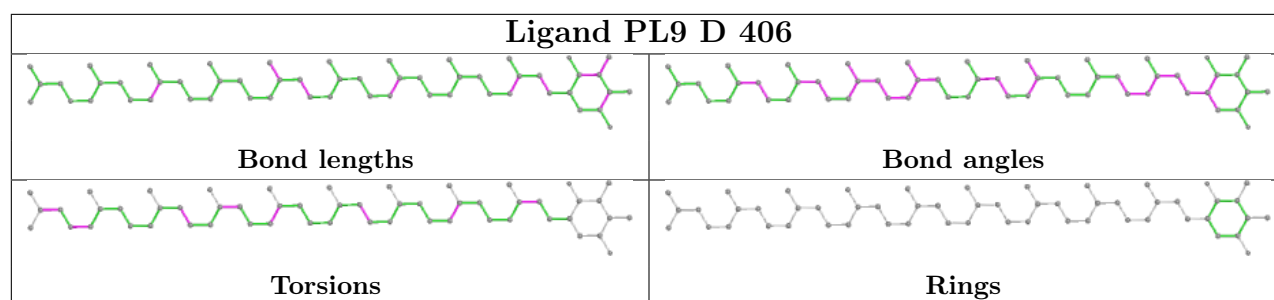


Ligand CLA b 615

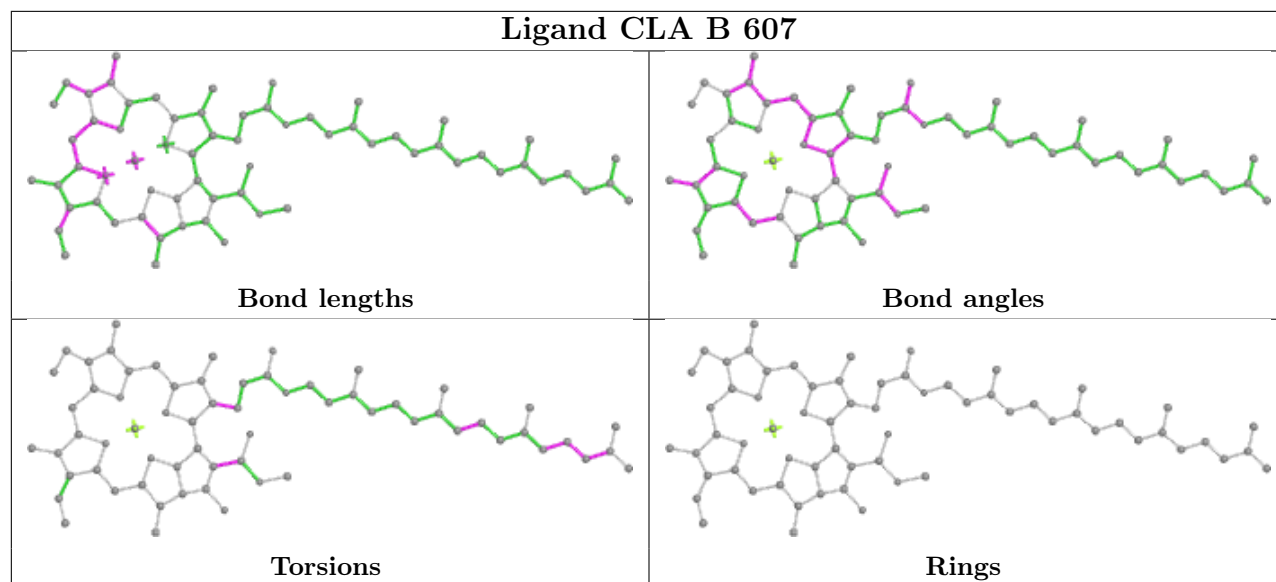


Ligand BCR C 515

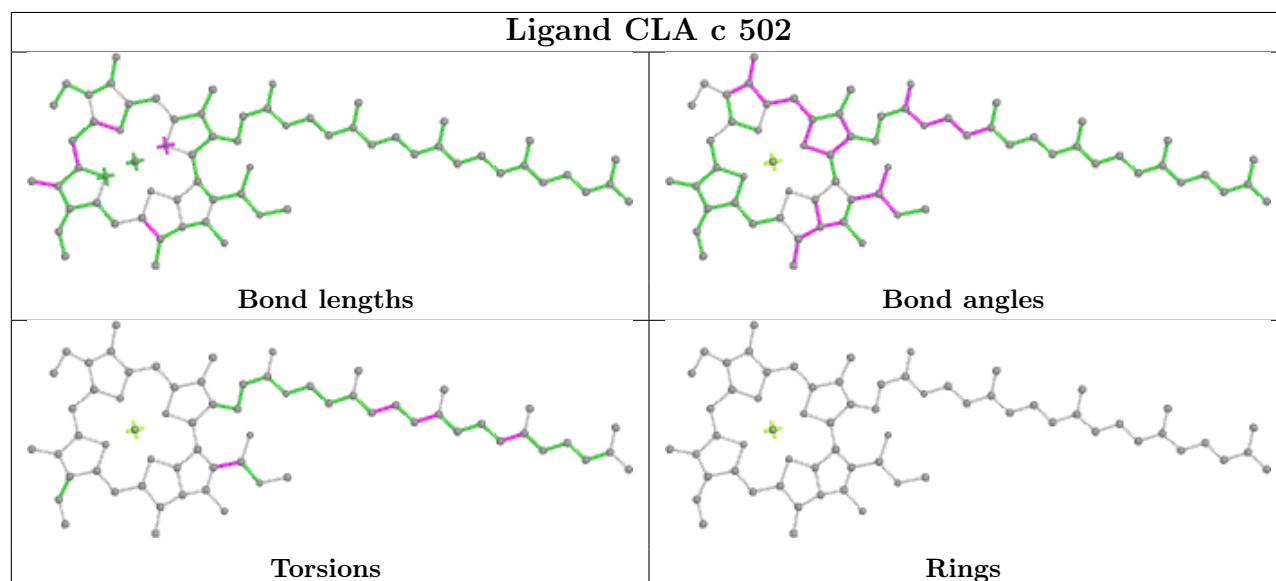




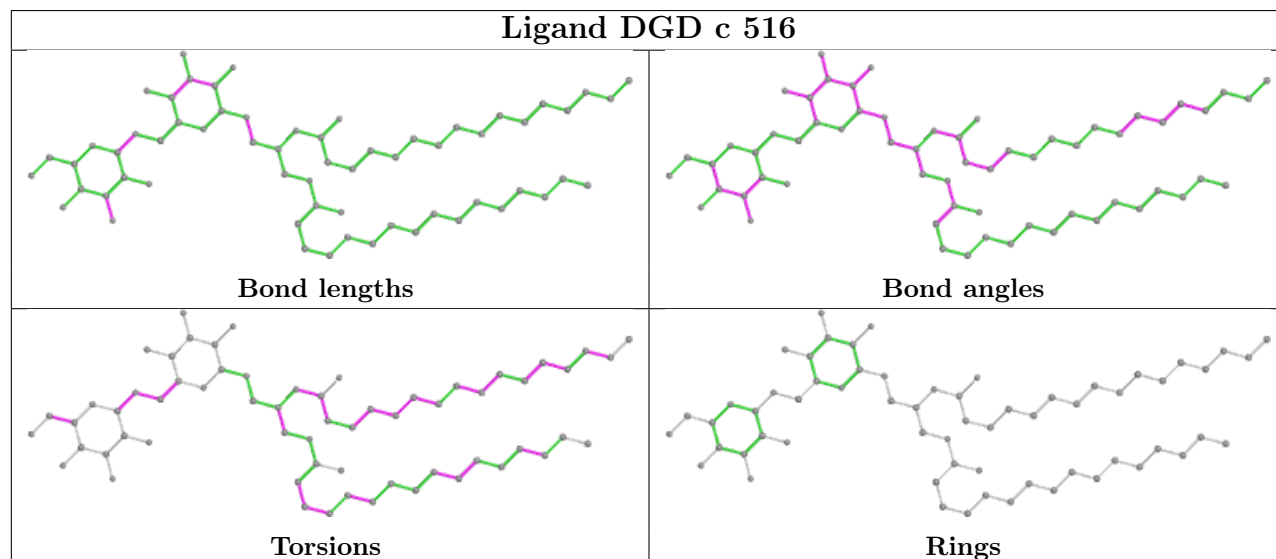
Ligand CLA B 607

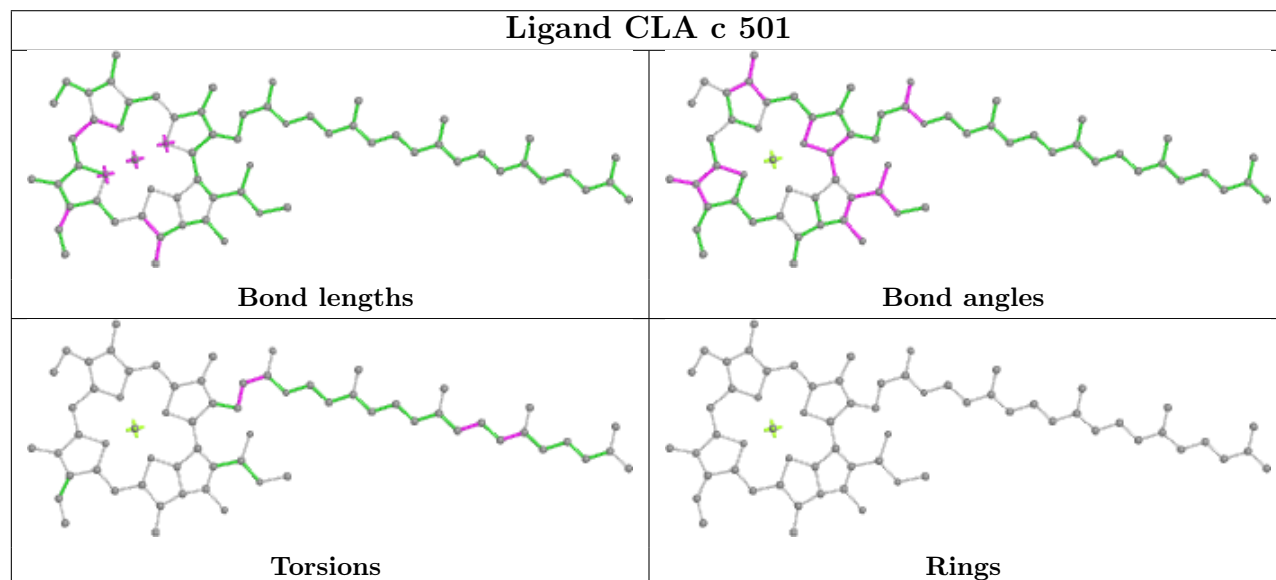
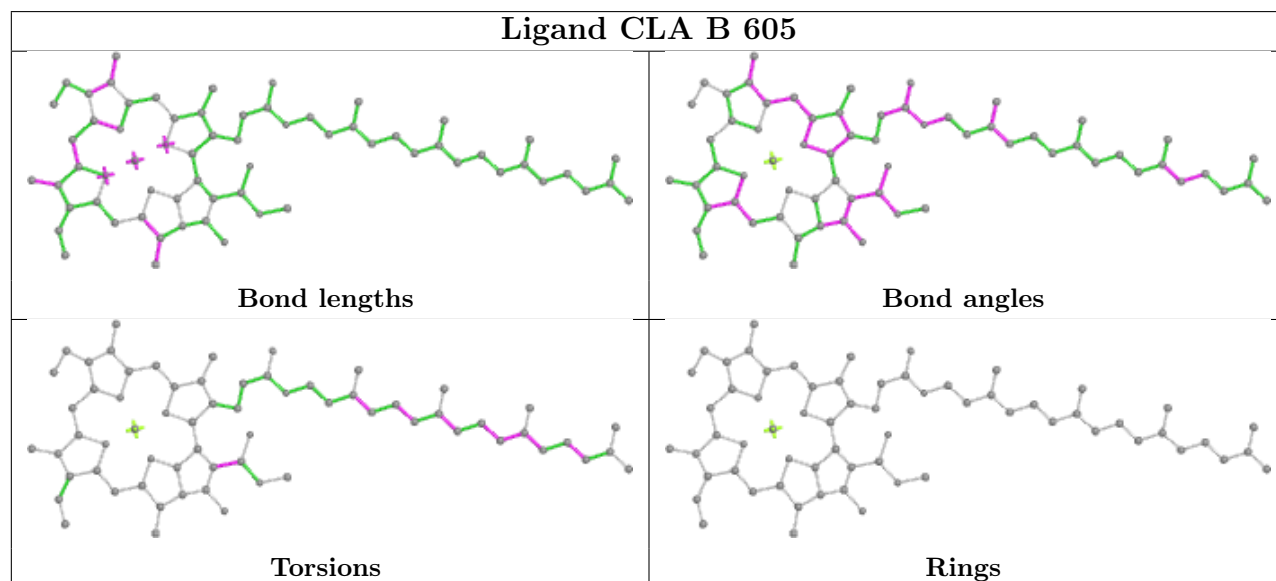
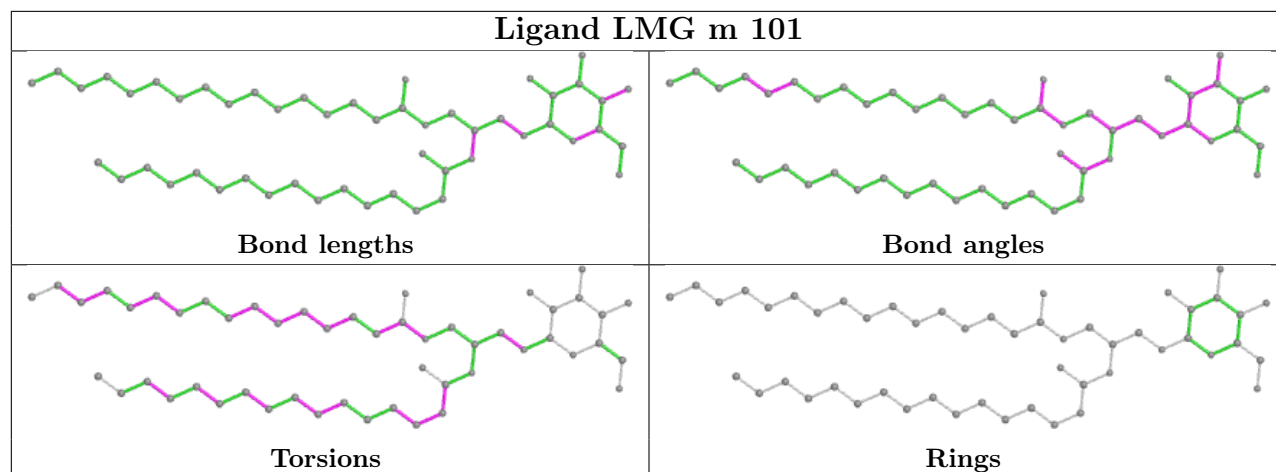


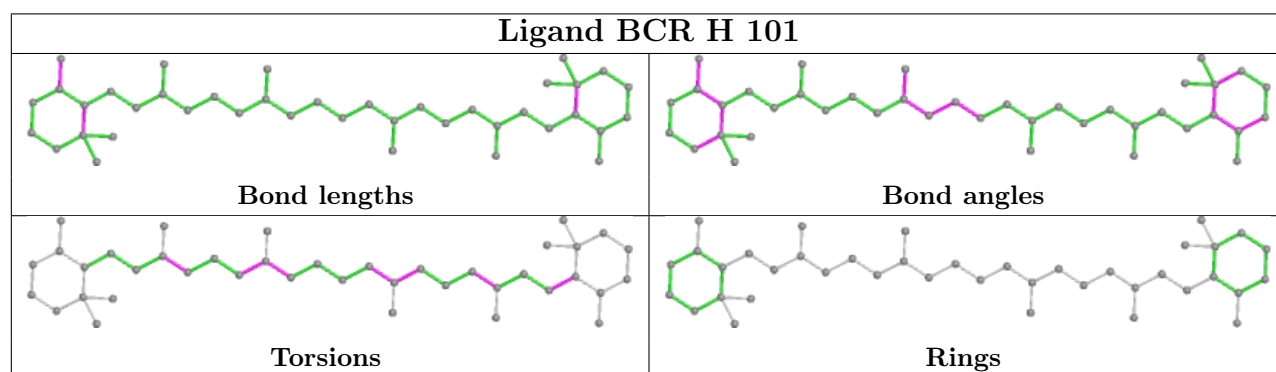
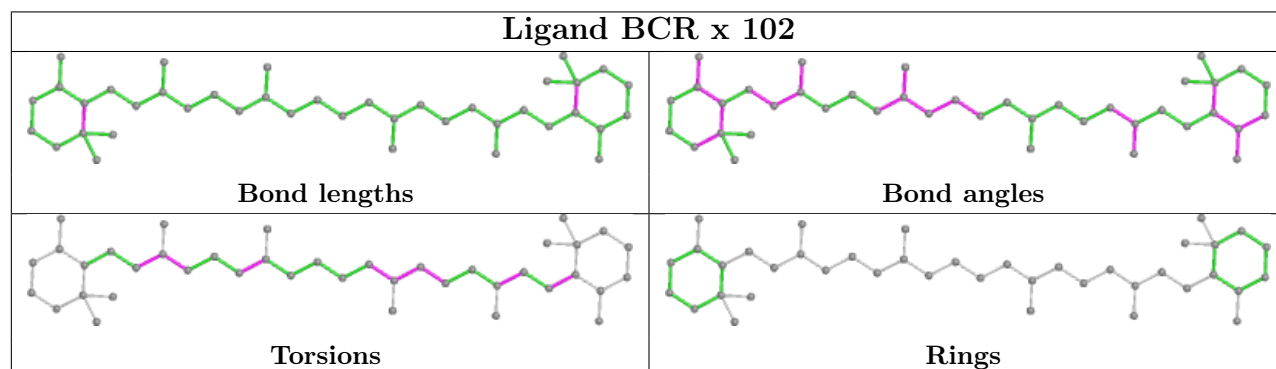
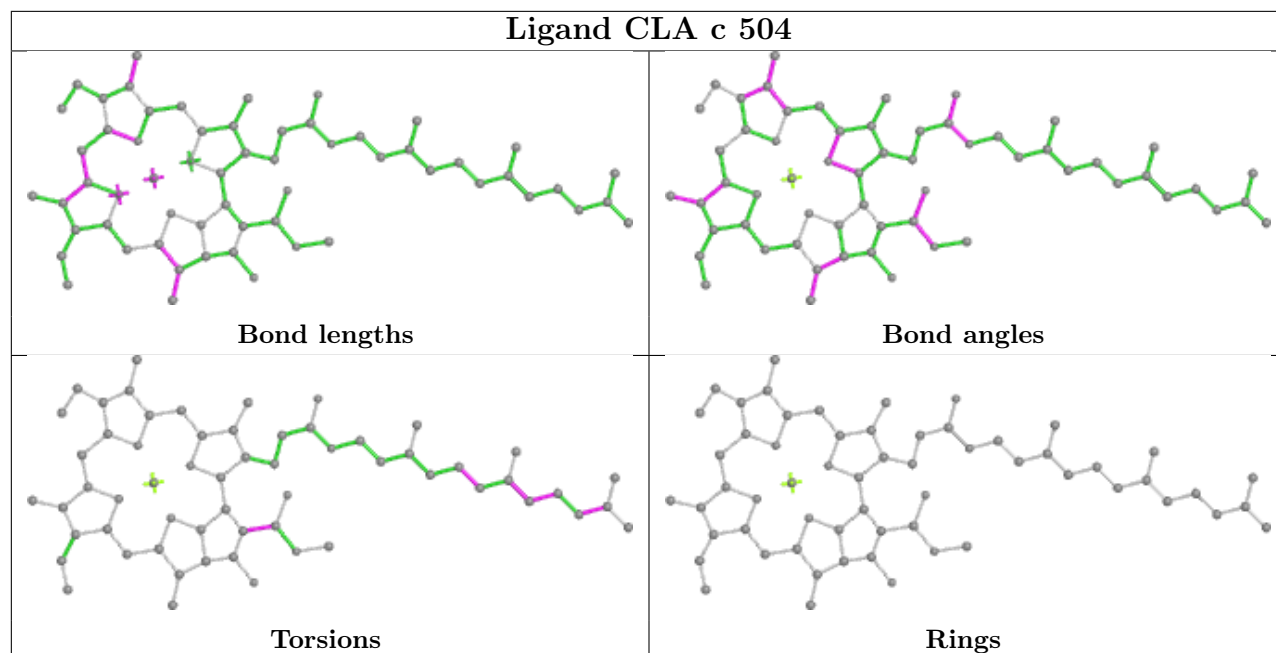
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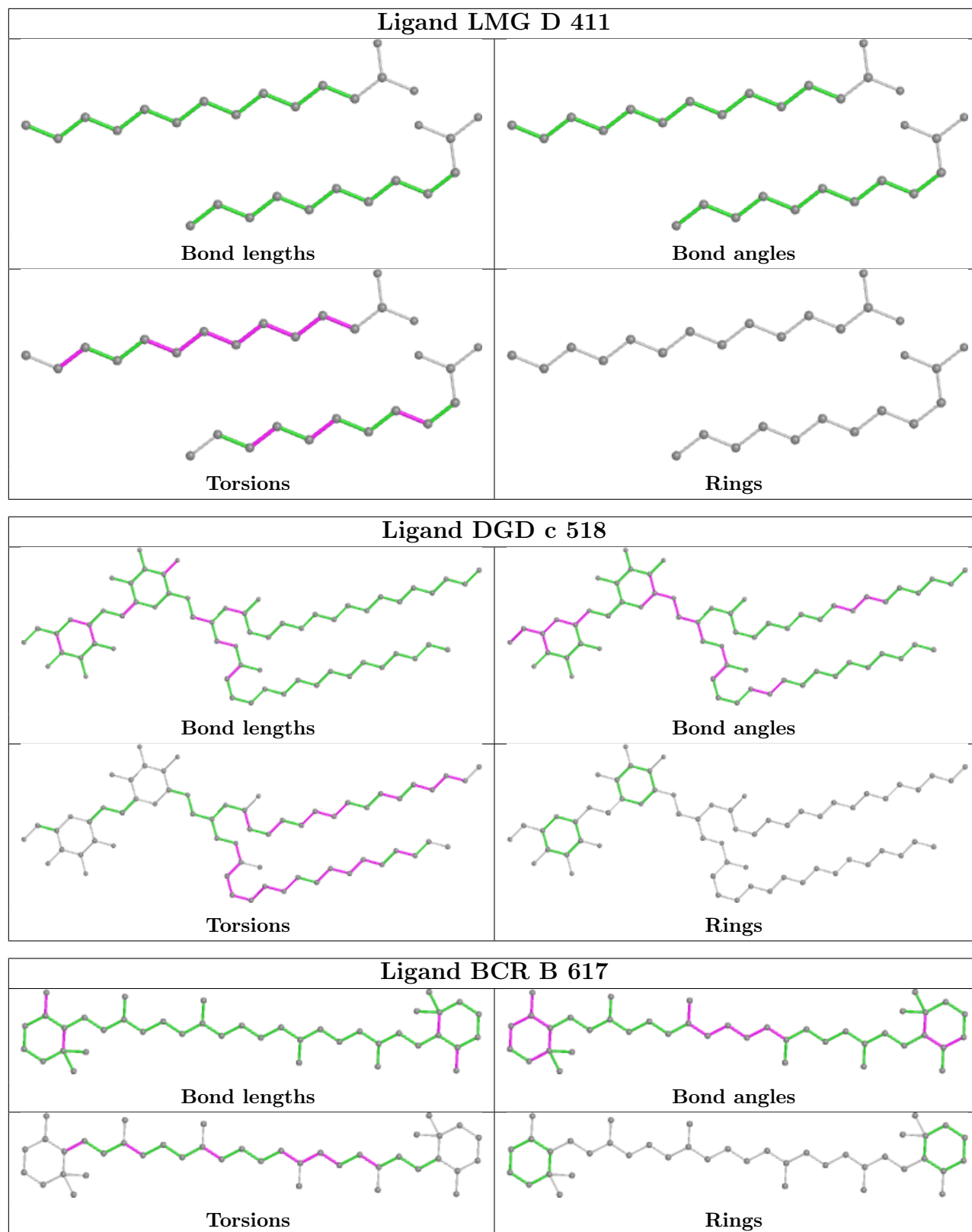


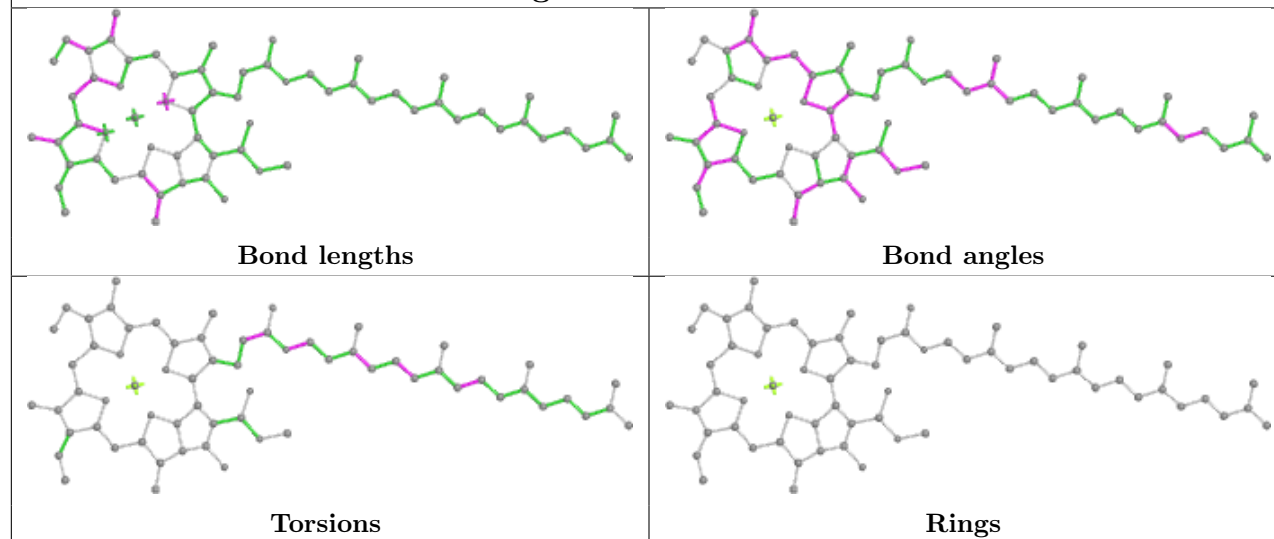
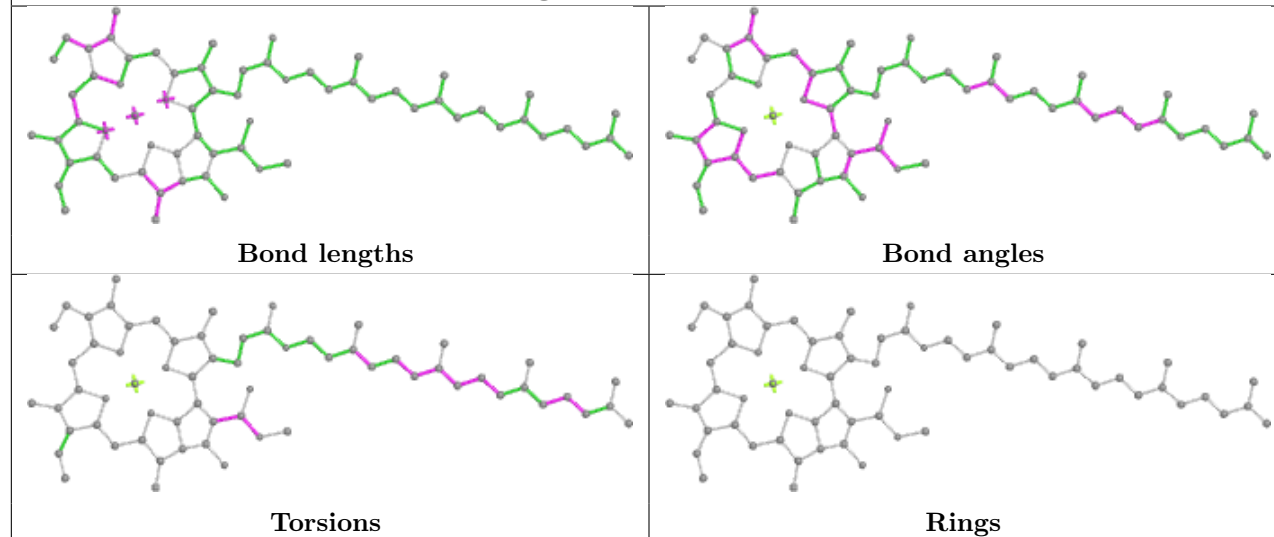
Ligand DGD c 516



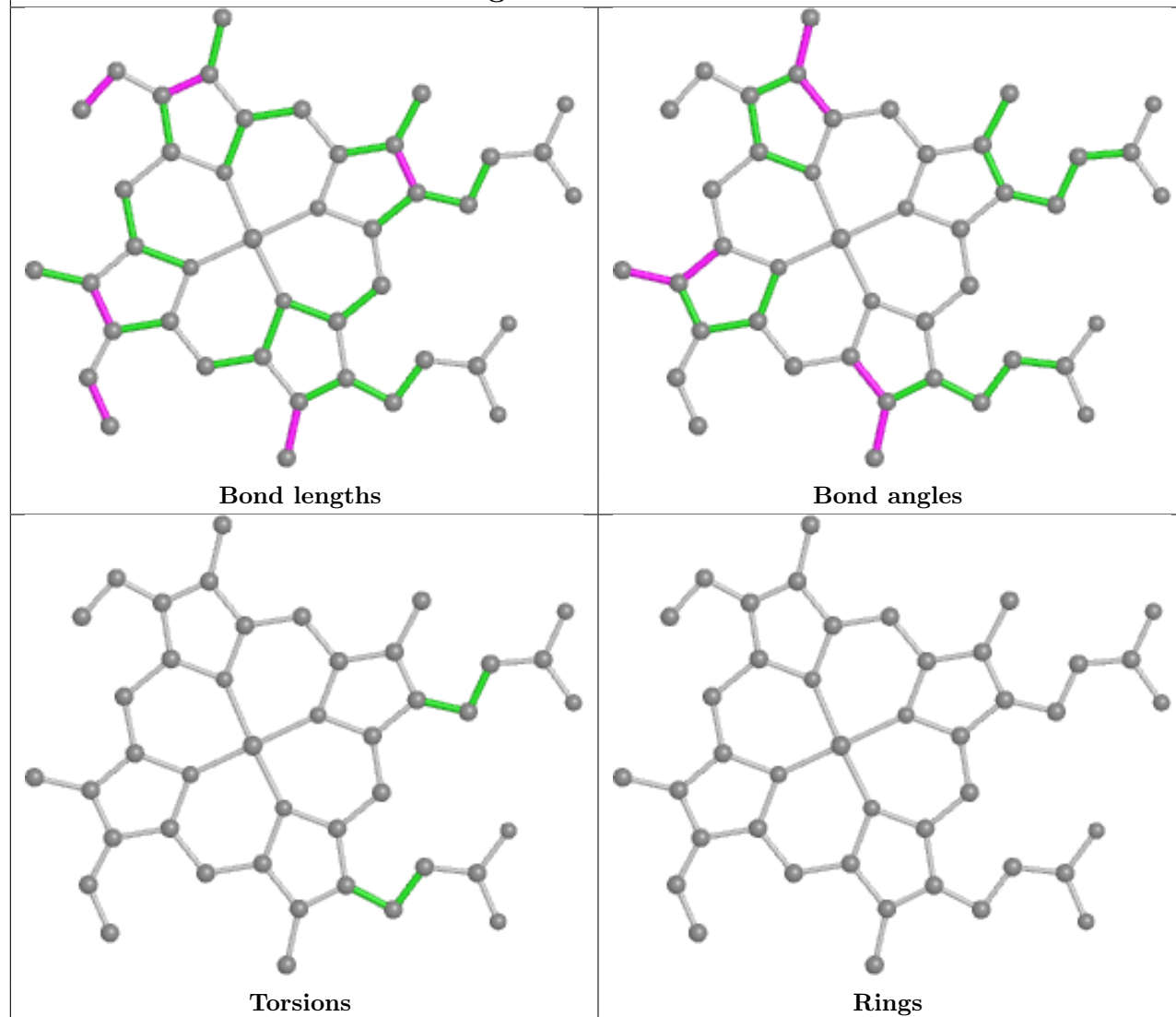




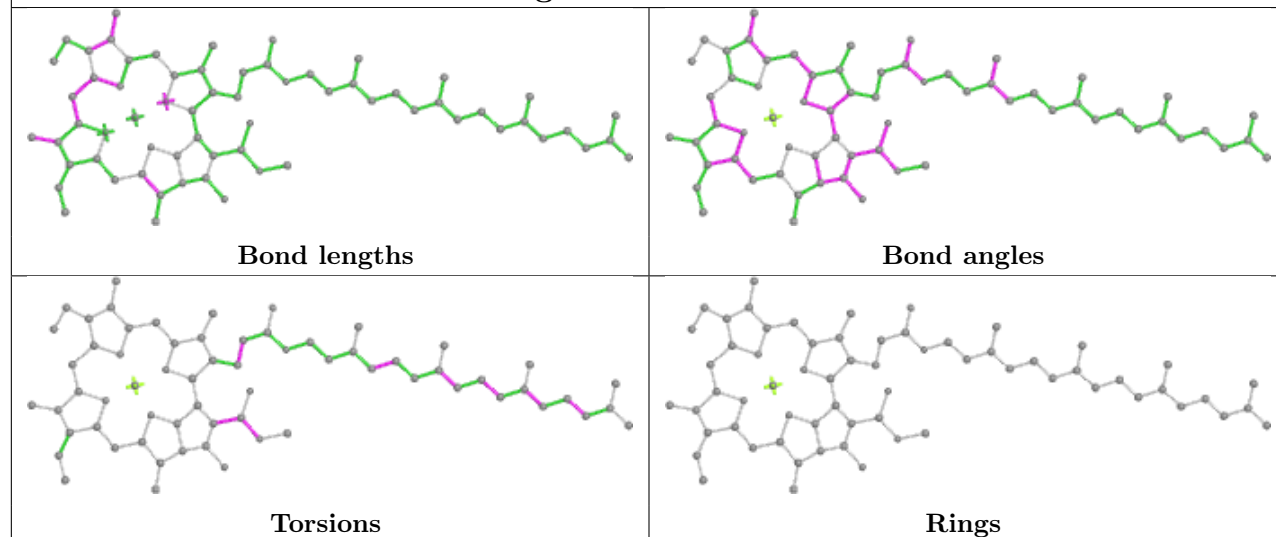


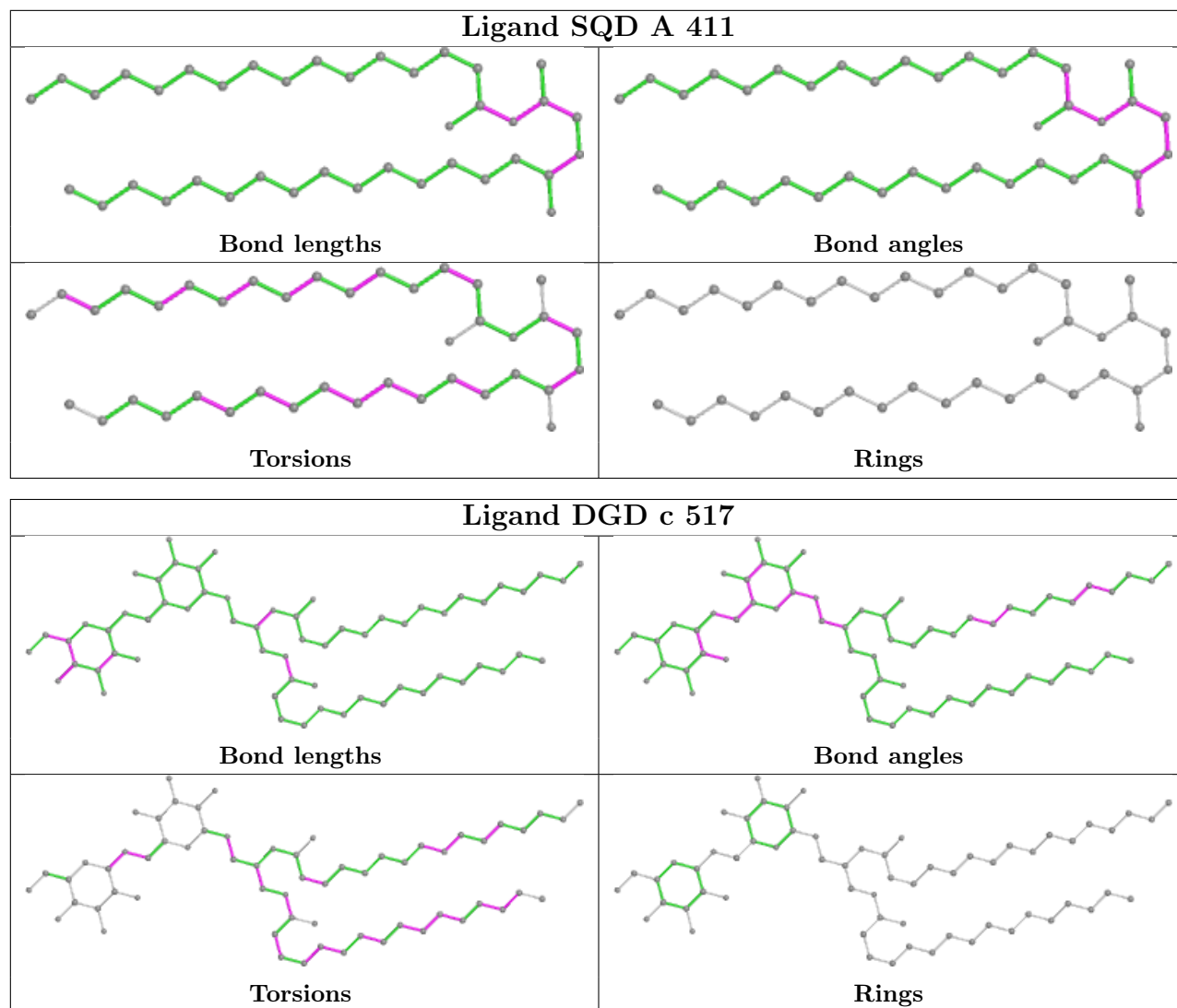
Ligand CLA B 613**Ligand CLA b 612**

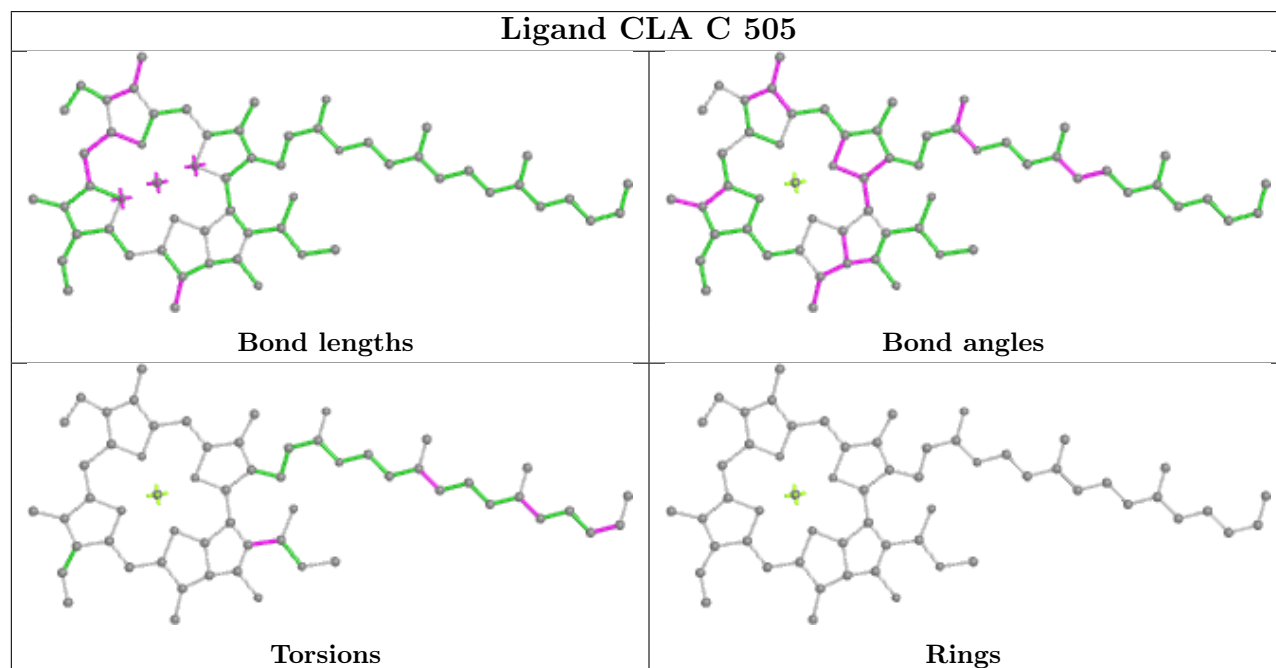
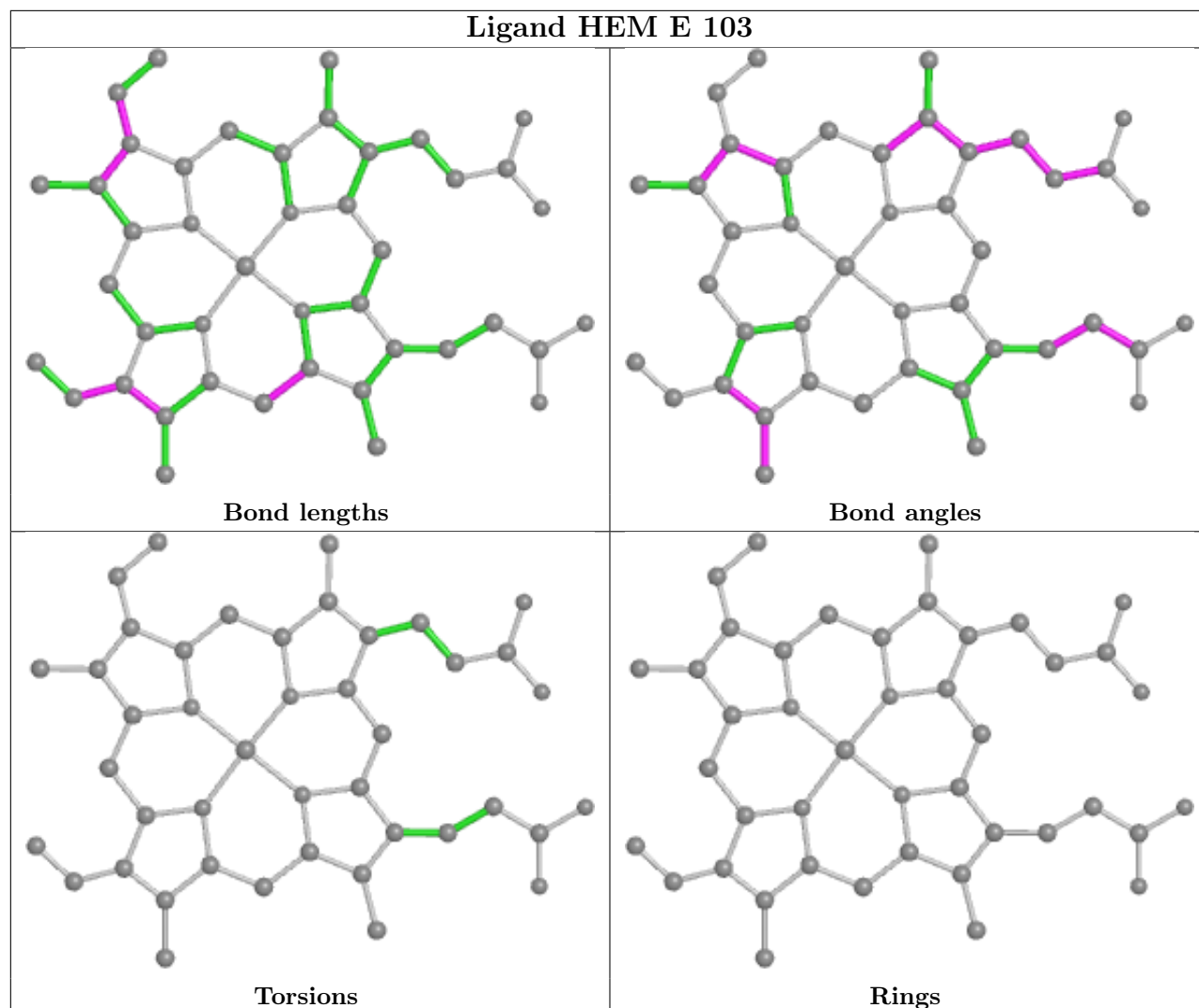
Ligand HEC V 201



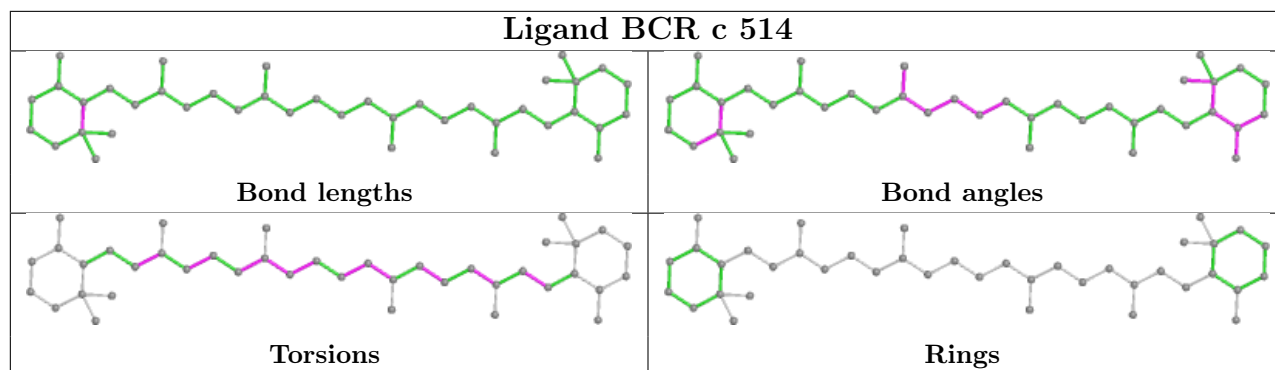
Ligand CLA b 607



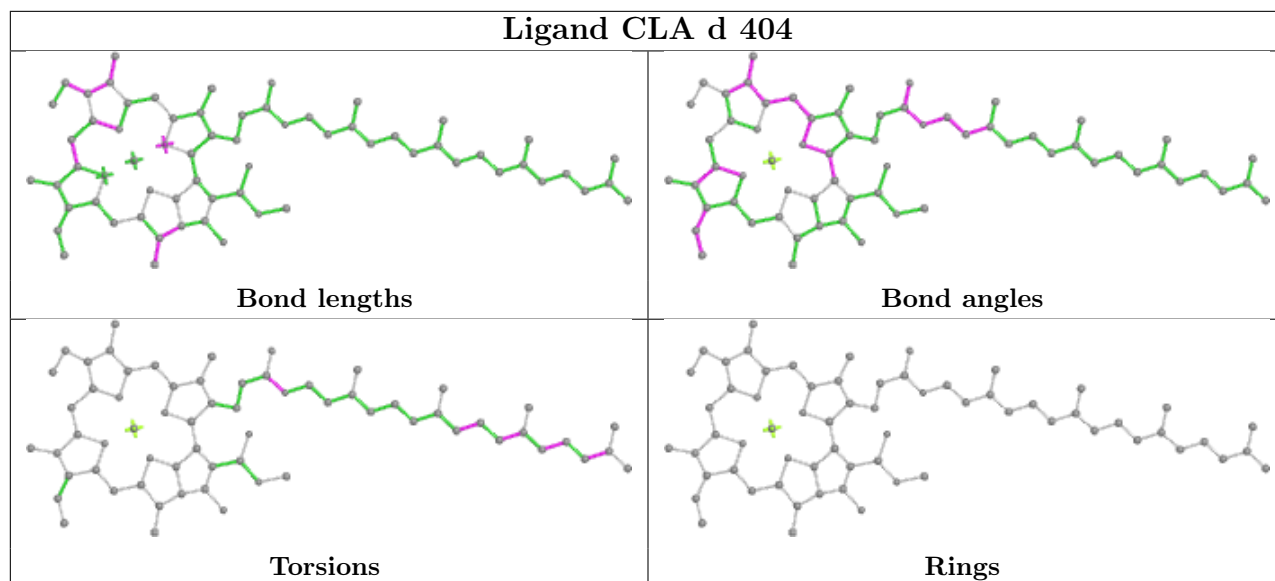




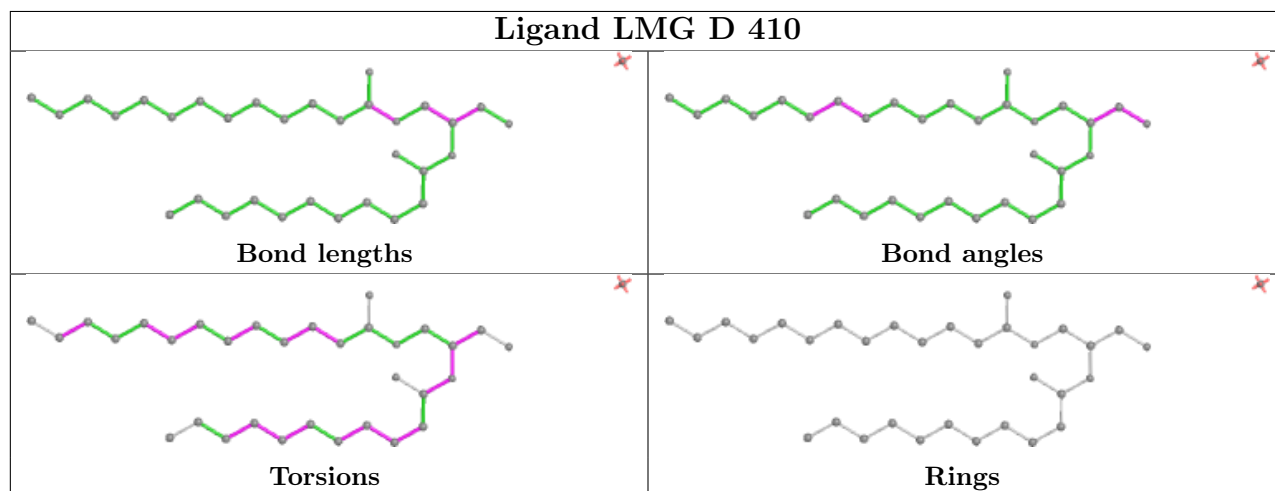
Ligand BCR c 514



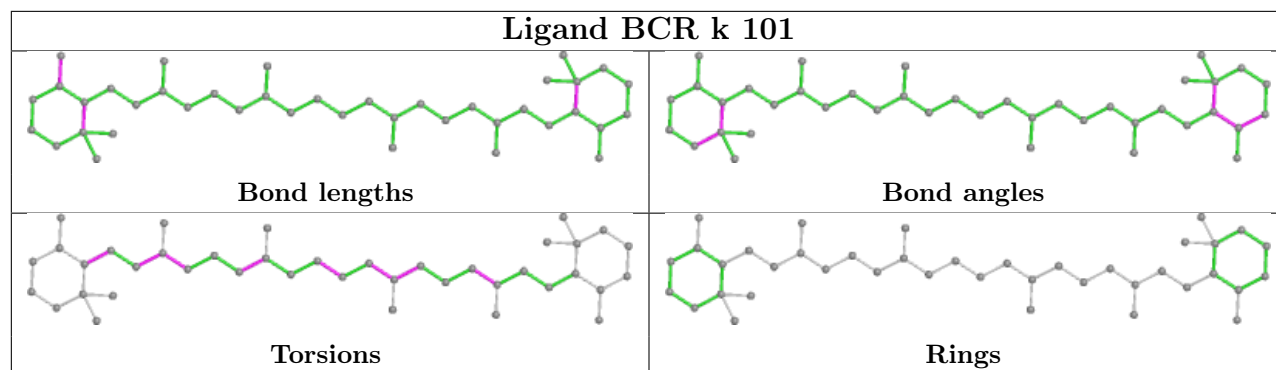
Ligand CLA d 404



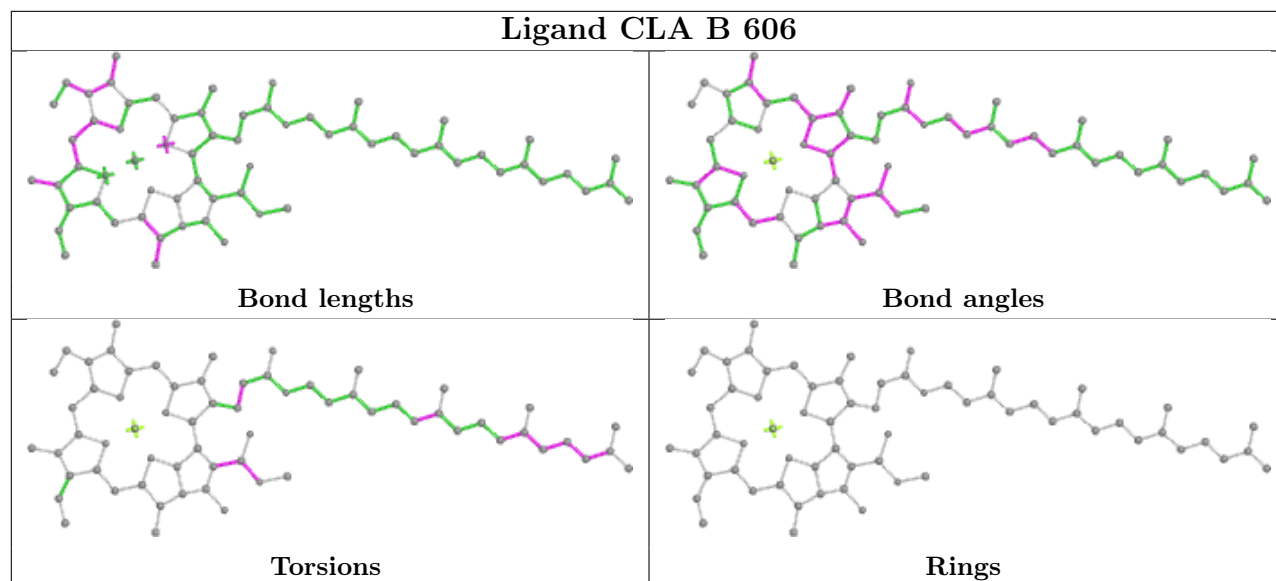
Ligand LMG D 410



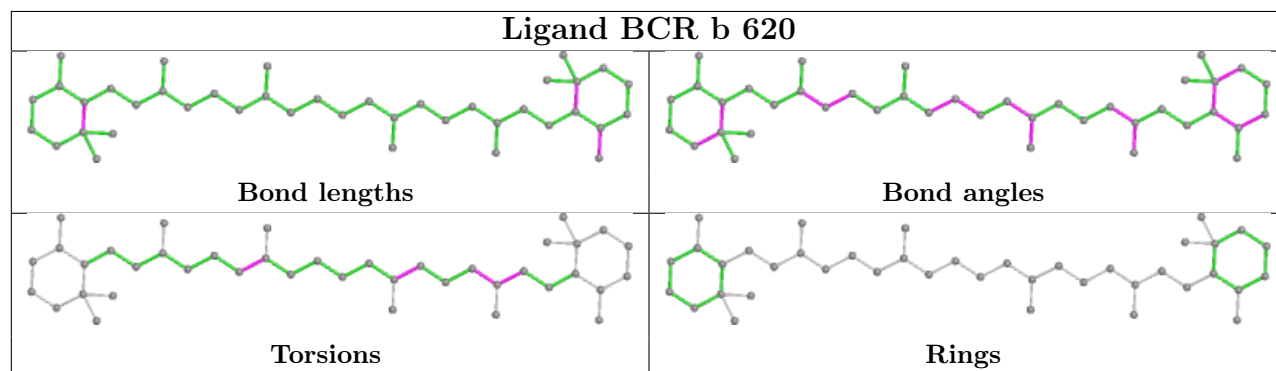
Ligand BCR k 101



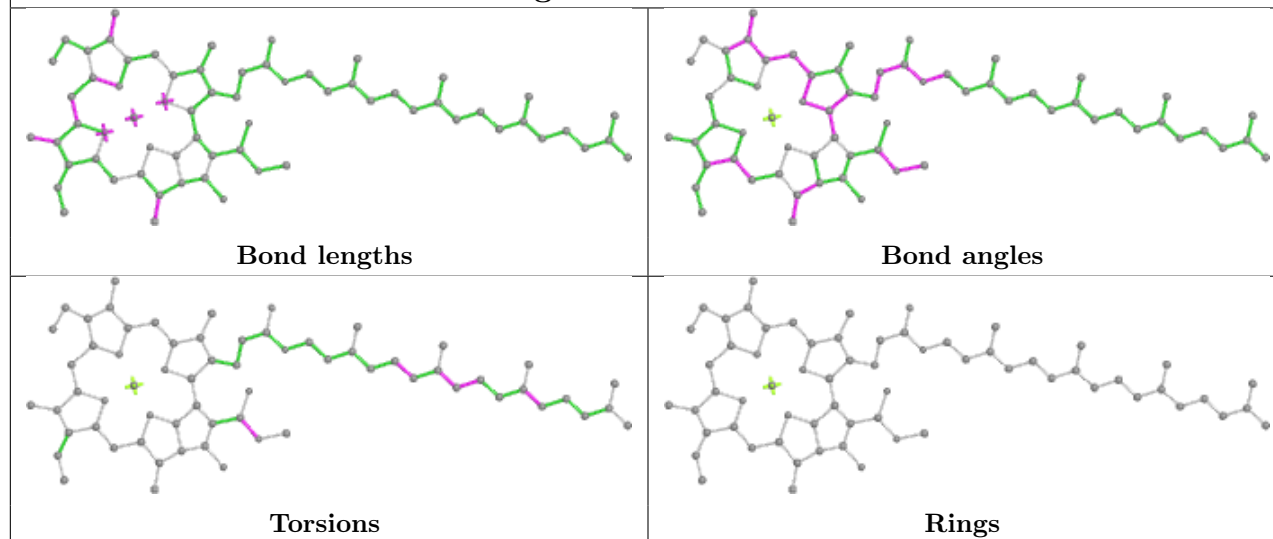
Ligand CLA B 606



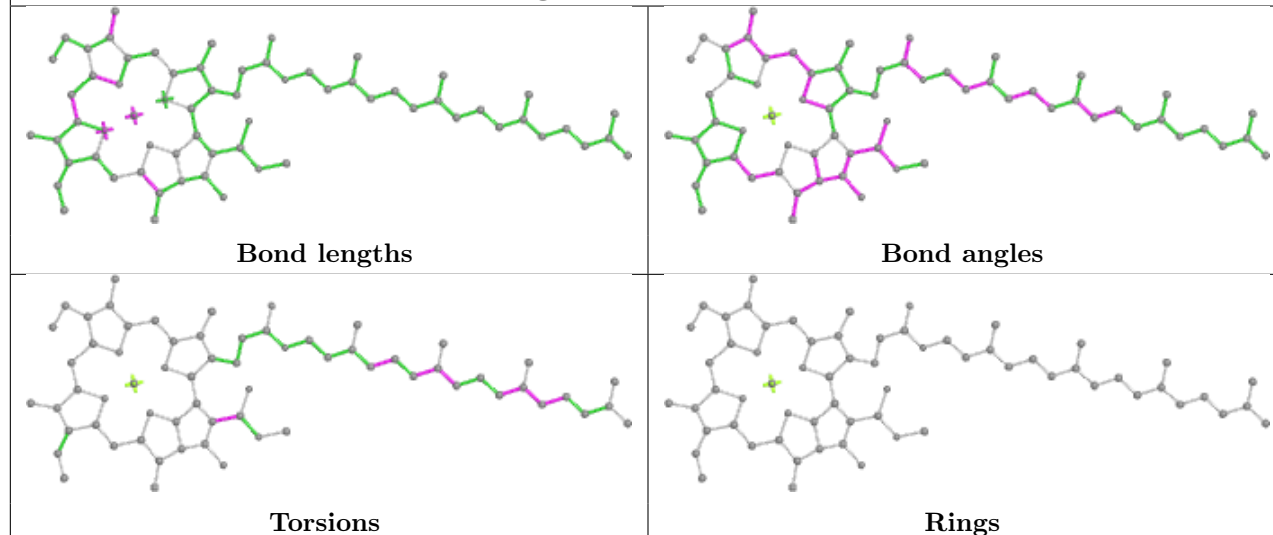
Ligand BCR b 620



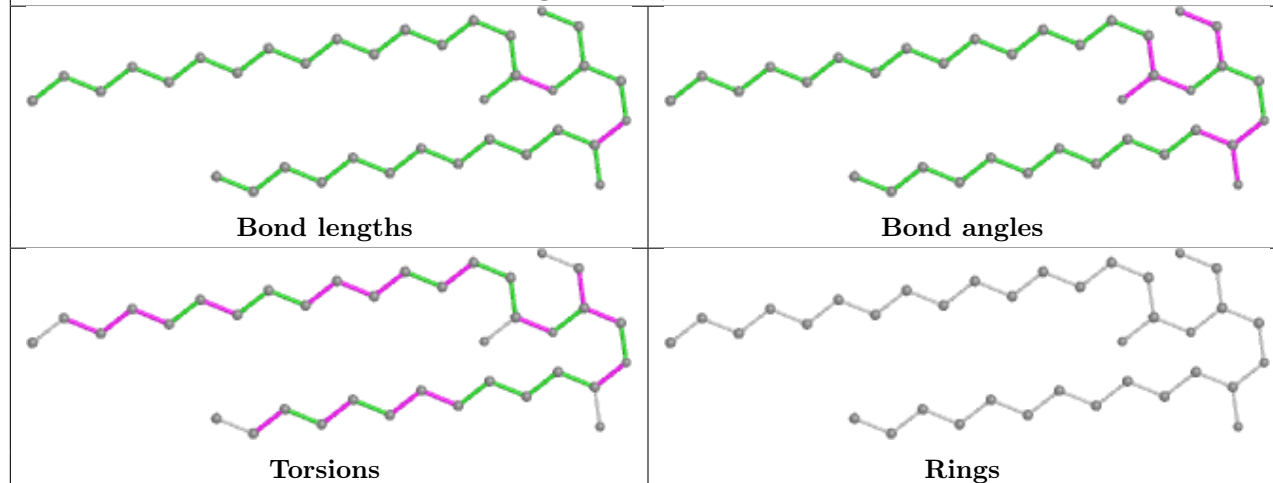
Ligand CLA b 616



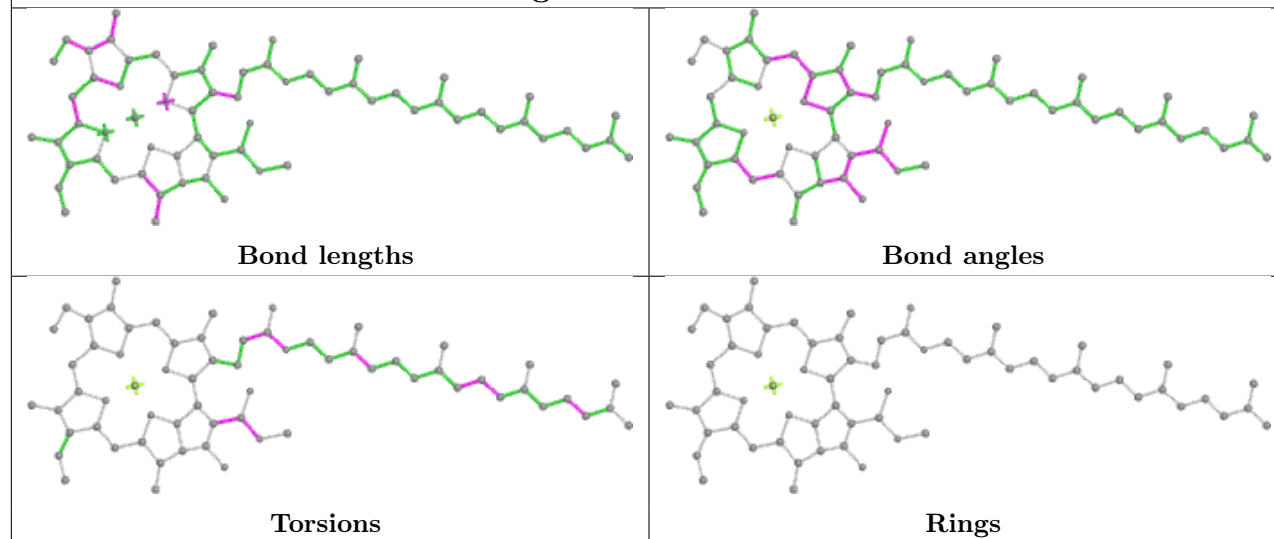
Ligand CLA b 605



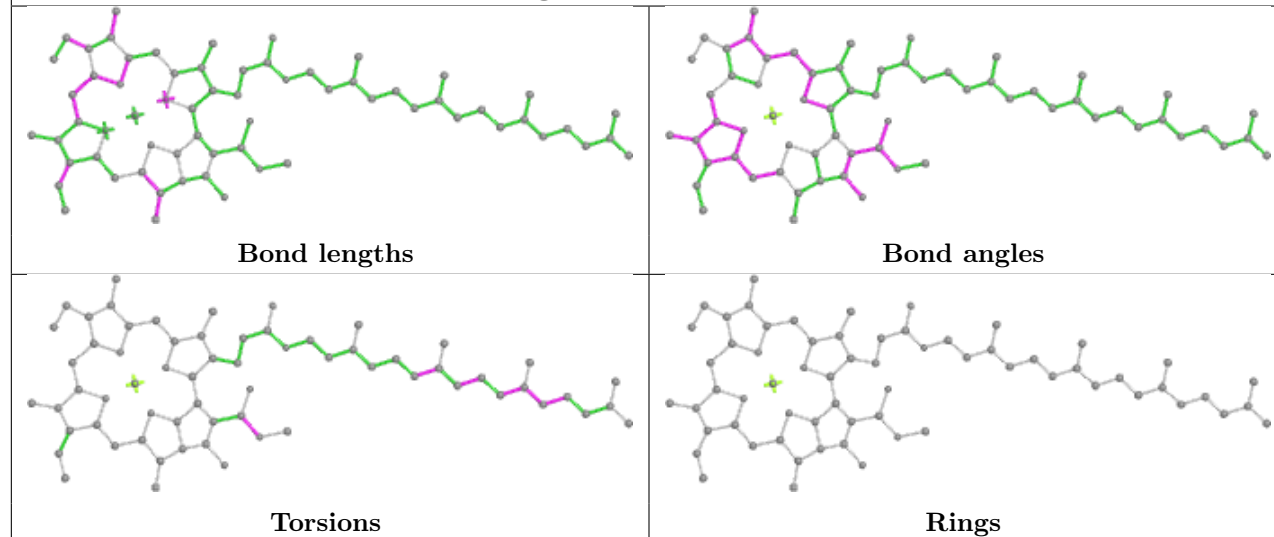
Ligand SQD a 412



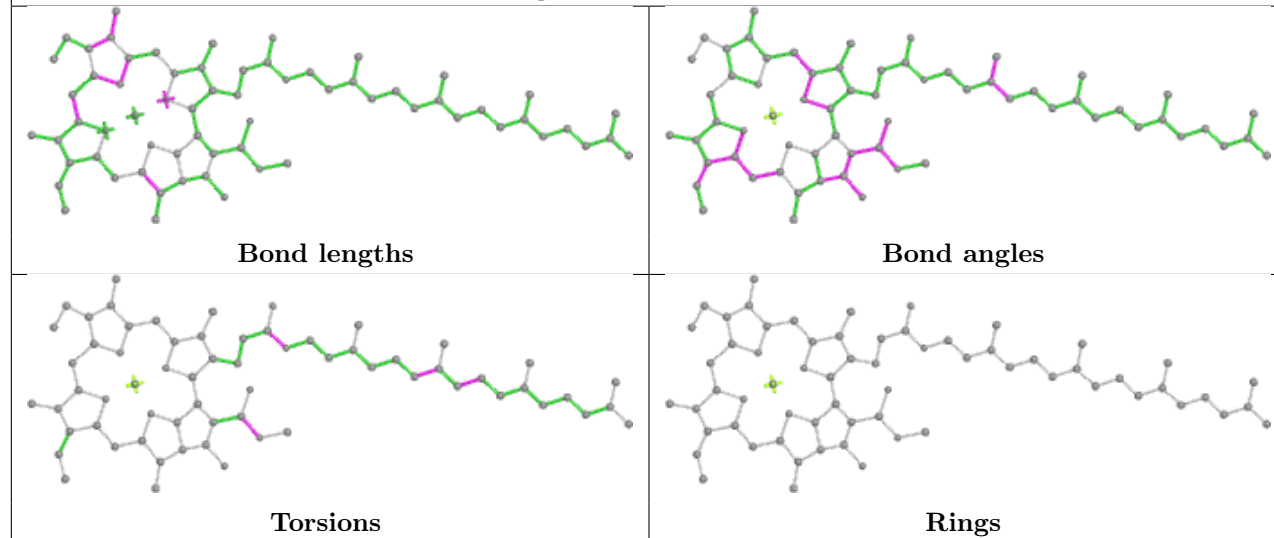
Ligand CLA B 601

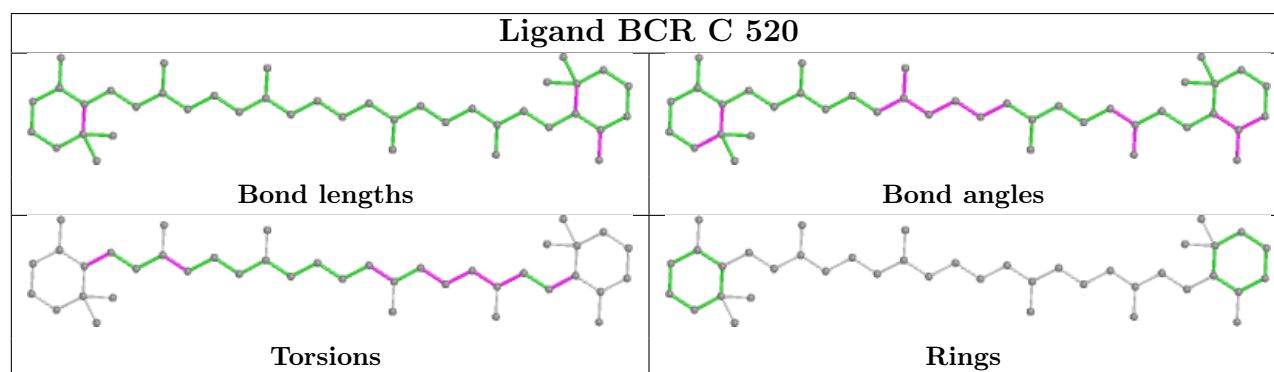
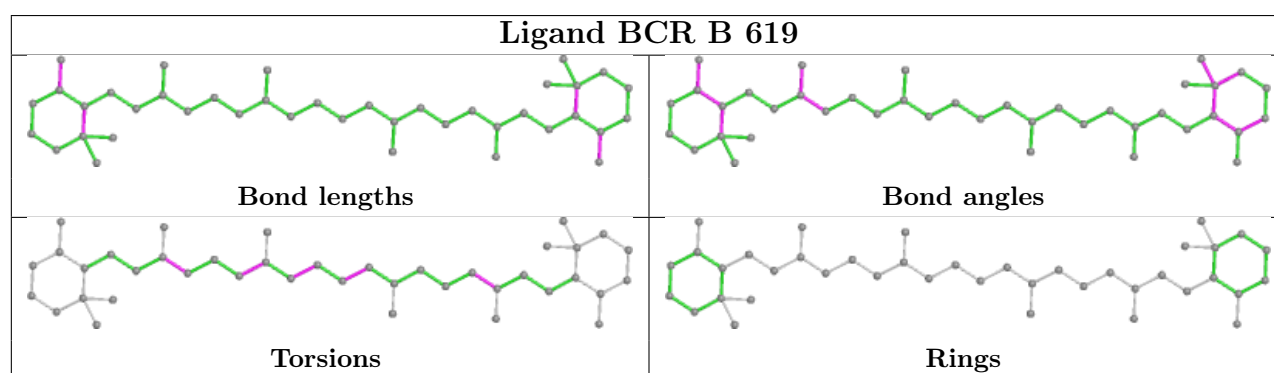
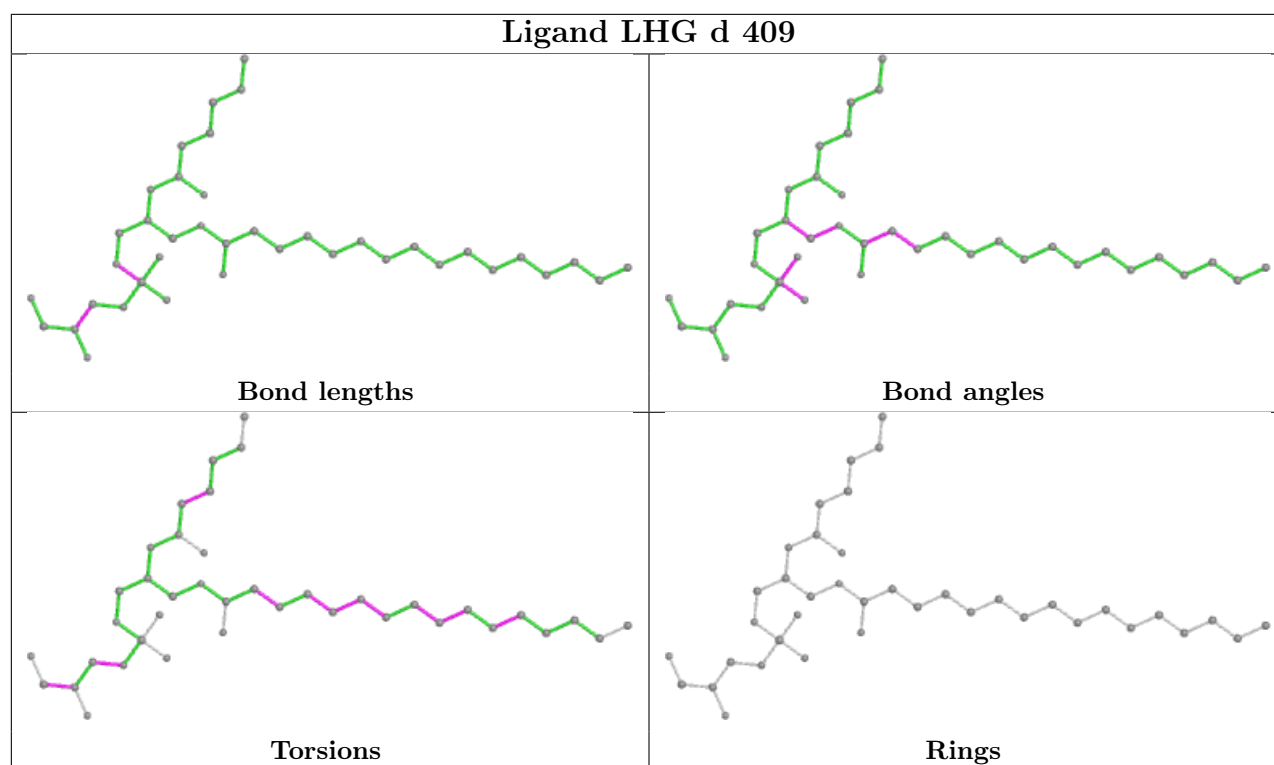


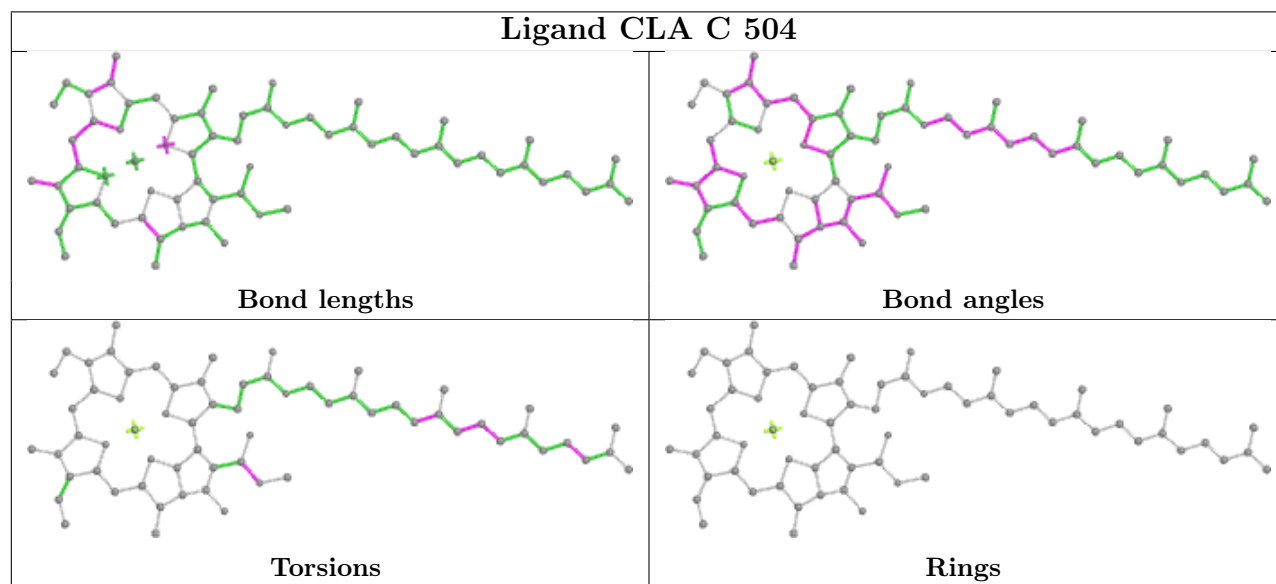
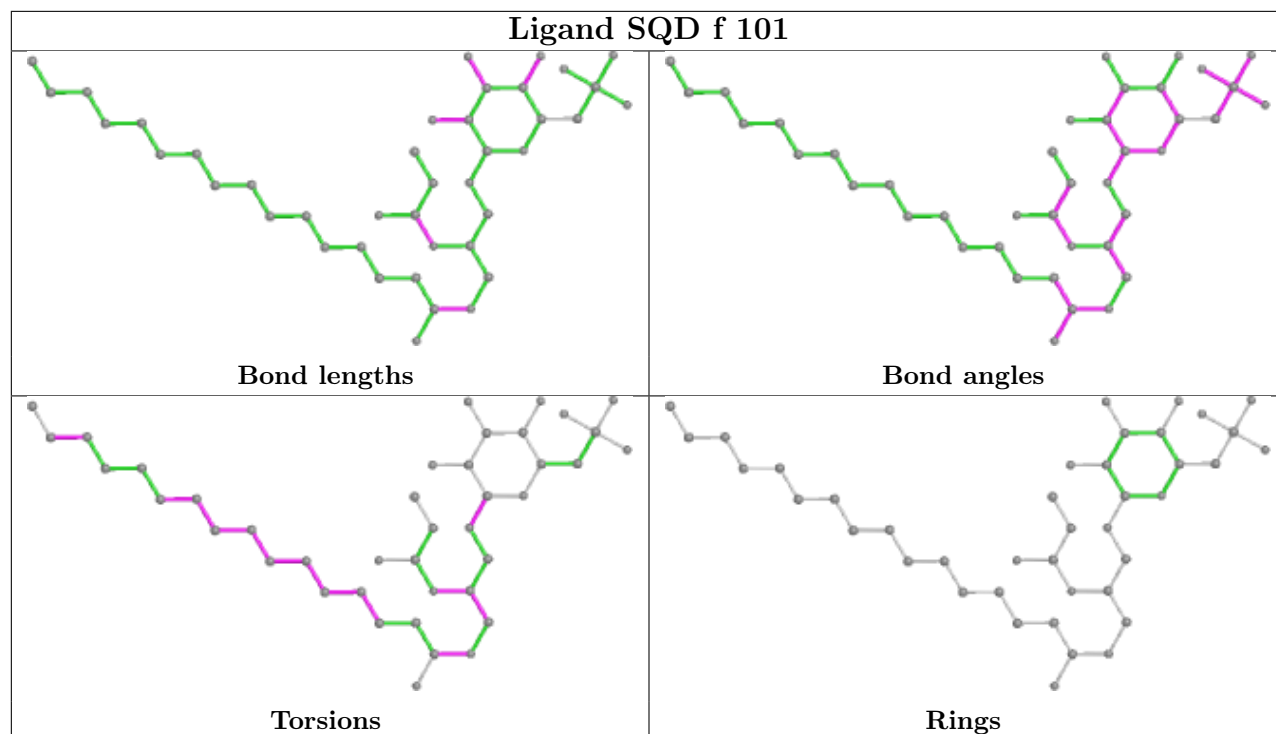
Ligand CLA b 603

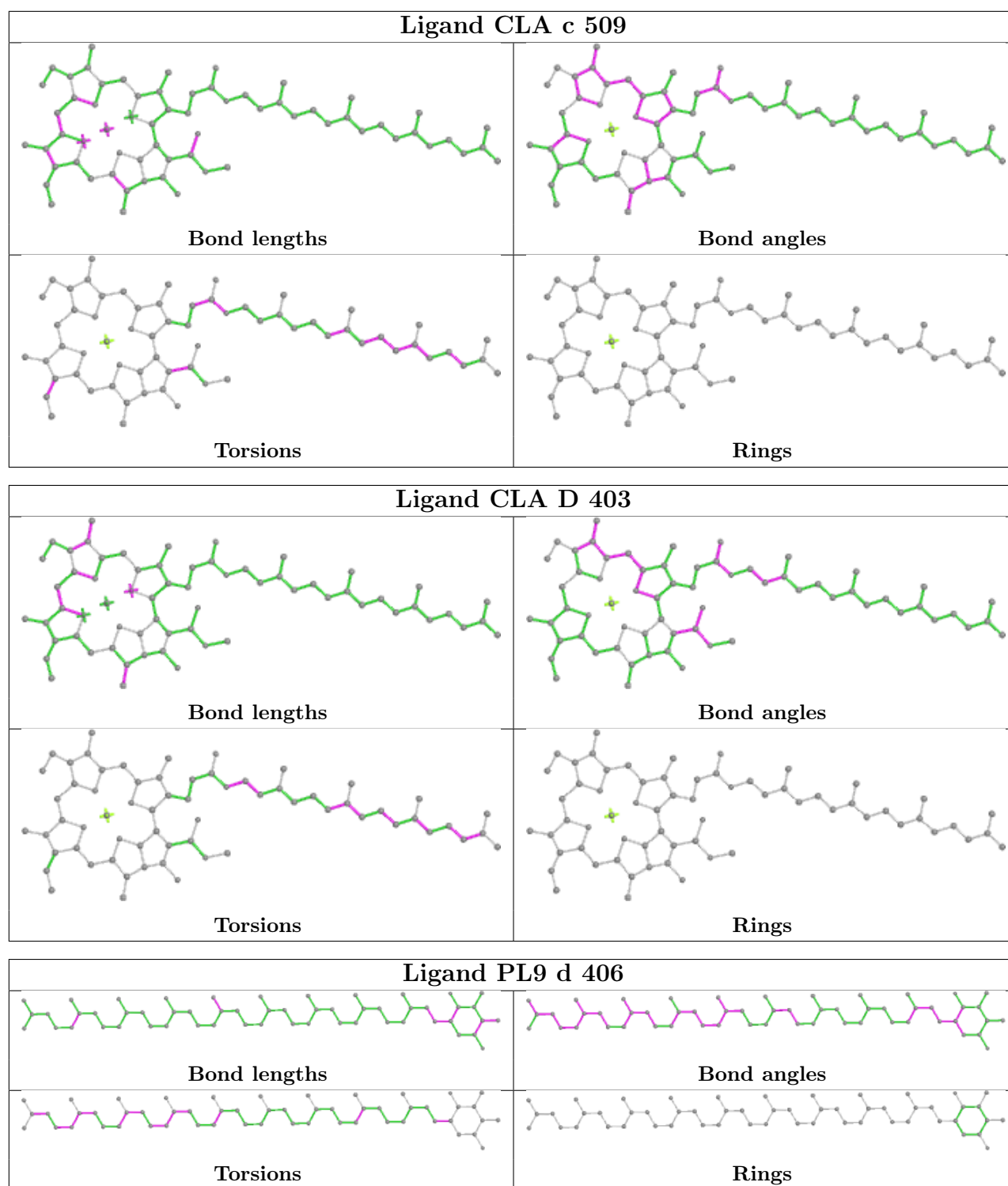


Ligand CLA C 512









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 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, 95th 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 ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 334/334 (100%) | -0.63 | 3 (0%) 84 86 | 27, 35, 53, 81 | 0 |
| 1 | a | 334/334 (100%) | -0.59 | 1 (0%) 94 94 | 26, 36, 63, 84 | 0 |
| 2 | B | 505/505 (100%) | -0.51 | 7 (1%) 75 77 | 27, 39, 67, 107 | 0 |
| 2 | b | 505/505 (100%) | -0.41 | 12 (2%) 59 62 | 27, 42, 78, 104 | 0 |
| 3 | C | 442/451 (98%) | -0.47 | 1 (0%) 95 95 | 29, 42, 59, 81 | 0 |
| 3 | c | 451/451 (100%) | -0.42 | 4 (0%) 84 86 | 31, 46, 68, 109 | 0 |
| 4 | D | 341/341 (100%) | -0.50 | 0 100 100 | 27, 36, 53, 90 | 0 |
| 4 | d | 341/341 (100%) | -0.46 | 3 (0%) 84 86 | 28, 40, 62, 92 | 0 |
| 5 | E | 81/82 (98%) | -0.11 | 3 (3%) 41 45 | 39, 56, 74, 91 | 0 |
| 5 | e | 82/82 (100%) | 0.23 | 5 (6%) 21 22 | 44, 63, 85, 94 | 0 |
| 6 | F | 34/34 (100%) | -0.58 | 2 (5%) 22 23 | 42, 48, 69, 86 | 0 |
| 6 | f | 34/34 (100%) | -0.46 | 0 100 100 | 49, 54, 83, 98 | 0 |
| 7 | H | 65/65 (100%) | -0.17 | 0 100 100 | 37, 45, 66, 87 | 0 |
| 7 | h | 63/65 (96%) | -0.12 | 2 (3%) 47 51 | 43, 54, 69, 78 | 0 |
| 8 | I | 35/36 (97%) | -0.49 | 0 100 100 | 32, 43, 73, 80 | 0 |
| 8 | i | 35/36 (97%) | -0.21 | 3 (8%) 10 10 | 33, 46, 83, 90 | 0 |
| 9 | J | 36/36 (100%) | 0.19 | 4 (11%) 5 5 | 43, 54, 80, 104 | 0 |
| 9 | j | 36/36 (100%) | 0.06 | 4 (11%) 5 5 | 42, 58, 93, 101 | 0 |
| 10 | K | 37/37 (100%) | -0.26 | 0 100 100 | 46, 60, 75, 77 | 0 |
| 10 | k | 37/37 (100%) | -0.05 | 1 (2%) 54 58 | 59, 67, 76, 82 | 0 |
| 11 | L | 37/37 (100%) | -0.46 | 0 100 100 | 29, 36, 75, 75 | 0 |
| 11 | l | 36/37 (97%) | -0.43 | 0 100 100 | 29, 37, 72, 83 | 0 |
| 12 | M | 32/33 (96%) | -0.36 | 1 (3%) 49 52 | 32, 38, 69, 75 | 0 |
| 12 | m | 31/33 (93%) | -0.42 | 0 100 100 | 32, 38, 57, 71 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | O | 244/244 (100%) | -0.13 | 12 (4%) 29 31 | 28, 48, 85, 150 | 0 |
| 13 | o | 244/244 (100%) | -0.26 | 12 (4%) 29 31 | 29, 46, 88, 133 | 0 |
| 14 | T | 29/30 (96%) | -0.77 | 1 (3%) 45 48 | 29, 37, 67, 74 | 0 |
| 14 | t | 29/30 (96%) | -0.60 | 2 (6%) 16 17 | 31, 37, 89, 92 | 0 |
| 15 | U | 97/97 (100%) | -0.34 | 2 (2%) 63 66 | 36, 49, 77, 103 | 0 |
| 15 | u | 97/97 (100%) | -0.50 | 1 (1%) 82 84 | 36, 46, 64, 91 | 0 |
| 16 | V | 137/137 (100%) | -0.63 | 0 100 100 | 34, 46, 62, 92 | 0 |
| 16 | v | 137/137 (100%) | -0.36 | 3 (2%) 62 65 | 36, 53, 76, 99 | 0 |
| 17 | Y | 27/30 (90%) | 1.63 | 11 (40%) 0 0 | 57, 79, 114, 120 | 0 |
| 17 | y | 30/30 (100%) | 0.39 | 1 (3%) 46 50 | 64, 78, 94, 111 | 0 |
| 18 | X | 38/38 (100%) | -0.13 | 3 (7%) 12 12 | 42, 53, 78, 83 | 0 |
| 18 | x | 38/38 (100%) | 0.14 | 1 (2%) 56 59 | 52, 63, 87, 96 | 0 |
| 19 | Z | 62/62 (100%) | 0.40 | 8 (12%) 3 3 | 55, 69, 115, 123 | 0 |
| 19 | z | 62/62 (100%) | 0.77 | 12 (19%) 1 1 | 62, 79, 121, 127 | 0 |
| 20 | R | 34/34 (100%) | 1.39 | 7 (20%) 1 0 | 66, 75, 95, 103 | 0 |
| 20 | r | 31/34 (91%) | 2.19 | 17 (54%) 0 0 | 79, 93, 106, 110 | 0 |
| All | All | 5300/5326 (99%) | -0.35 | 149 (2%) 53 56 | 26, 44, 80, 150 | 0 |

All (149) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17 | Y | 20 | ALA | 8.4 |
| 13 | O | 60 | ARG | 7.9 |
| 19 | z | 33 | TRP | 7.2 |
| 13 | o | 3 | GLN | 7.0 |
| 13 | O | 3 | GLN | 6.3 |
| 9 | J | 5 | GLY | 6.0 |
| 13 | o | 58 | ASN | 5.7 |
| 13 | O | 61 | GLN | 5.5 |
| 13 | O | 59 | LYS | 5.2 |
| 1 | A | 13 | LEU | 5.2 |
| 9 | j | 7 | ARG | 5.1 |
| 13 | O | 62 | GLU | 5.0 |
| 20 | r | 26 | TYR | 4.8 |
| 5 | e | 79 | PHE | 4.7 |
| 2 | B | 502 | VAL | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | o | 56 | PRO | 4.5 |
| 9 | J | 7 | ARG | 4.5 |
| 9 | j | 8 | ILE | 4.3 |
| 17 | Y | 45 | ASN | 4.3 |
| 18 | x | 2 | THR | 4.3 |
| 3 | c | 23 | ALA | 4.3 |
| 17 | Y | 41 | VAL | 4.2 |
| 6 | F | 12 | SER | 4.2 |
| 17 | Y | 21 | GLN | 4.1 |
| 9 | J | 6 | GLY | 4.1 |
| 13 | o | 5 | LEU | 4.1 |
| 18 | X | 2 | THR | 4.1 |
| 17 | Y | 43 | ARG | 4.0 |
| 19 | z | 31 | GLN | 4.0 |
| 17 | Y | 42 | ARG | 3.9 |
| 20 | r | 3 | TRP | 3.8 |
| 13 | O | 5 | LEU | 3.8 |
| 13 | O | 56 | PRO | 3.8 |
| 19 | z | 62 | VAL | 3.7 |
| 20 | r | 2 | ASP | 3.6 |
| 17 | Y | 23 | THR | 3.5 |
| 20 | r | 6 | LEU | 3.5 |
| 8 | i | 36 | ASP | 3.5 |
| 19 | Z | 33 | TRP | 3.5 |
| 2 | b | 127 | ARG | 3.5 |
| 19 | z | 35 | ARG | 3.4 |
| 20 | R | 3 | TRP | 3.4 |
| 20 | R | 6 | LEU | 3.4 |
| 13 | O | 4 | THR | 3.3 |
| 9 | j | 5 | GLY | 3.3 |
| 2 | B | 506 | ARG | 3.3 |
| 18 | X | 3 | ILE | 3.3 |
| 20 | r | 25 | PRO | 3.3 |
| 20 | r | 4 | ARG | 3.3 |
| 20 | r | 28 | VAL | 3.3 |
| 13 | o | 4 | THR | 3.2 |
| 18 | X | 39 | ARG | 3.2 |
| 14 | t | 28 | ARG | 3.2 |
| 20 | R | 21 | ARG | 3.2 |
| 19 | Z | 1 | MET | 3.2 |
| 20 | r | 14 | LEU | 3.2 |
| 20 | r | 27 | ALA | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 2 | b | 495 | PHE | 3.1 |
| 2 | b | 486 | LEU | 3.1 |
| 20 | r | 24 | LEU | 3.1 |
| 13 | o | 61 | GLN | 3.1 |
| 19 | z | 30 | PRO | 3.0 |
| 1 | a | 11 | ALA | 3.0 |
| 3 | c | 143 | TYR | 3.0 |
| 20 | R | 29 | LYS | 3.0 |
| 9 | J | 8 | ILE | 3.0 |
| 20 | R | 32 | GLN | 3.0 |
| 5 | E | 79 | PHE | 2.9 |
| 20 | r | 9 | LEU | 2.9 |
| 20 | r | 10 | LEU | 2.9 |
| 13 | O | 63 | ALA | 2.9 |
| 20 | R | 31 | VAL | 2.9 |
| 17 | y | 19 | ILE | 2.8 |
| 20 | r | 13 | LEU | 2.8 |
| 19 | z | 41 | PHE | 2.8 |
| 9 | j | 6 | GLY | 2.8 |
| 2 | B | 505 | ARG | 2.8 |
| 2 | b | 506 | ARG | 2.8 |
| 20 | r | 5 | VAL | 2.7 |
| 19 | Z | 62 | VAL | 2.6 |
| 17 | Y | 37 | PHE | 2.6 |
| 19 | z | 60 | PHE | 2.6 |
| 6 | F | 13 | TYR | 2.6 |
| 13 | O | 23 | ASP | 2.6 |
| 19 | z | 61 | VAL | 2.6 |
| 19 | Z | 30 | PRO | 2.6 |
| 19 | Z | 3 | ILE | 2.6 |
| 15 | U | 8 | GLU | 2.6 |
| 15 | U | 67 | LEU | 2.6 |
| 14 | t | 29 | ILE | 2.6 |
| 16 | v | 15 | GLU | 2.6 |
| 8 | i | 34 | ARG | 2.6 |
| 1 | A | 12 | ASN | 2.5 |
| 19 | z | 32 | ASP | 2.5 |
| 13 | O | 57 | LYS | 2.5 |
| 2 | b | 502 | VAL | 2.5 |
| 2 | b | 128 | THR | 2.5 |
| 5 | E | 84 | LYS | 2.5 |
| 4 | d | 227[A] | GLU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 19 | Z | 35 | ARG | 2.5 |
| 1 | A | 11 | ALA | 2.5 |
| 16 | v | 16 | GLY | 2.5 |
| 2 | b | 487 | SER | 2.4 |
| 17 | Y | 25 | ILE | 2.4 |
| 2 | B | 296 | ALA | 2.4 |
| 2 | b | 489 | GLU | 2.4 |
| 2 | B | 294 | SER | 2.4 |
| 3 | c | 193 | GLY | 2.4 |
| 13 | o | 246 | ALA | 2.4 |
| 5 | e | 71 | GLU | 2.4 |
| 7 | h | 10 | ILE | 2.3 |
| 7 | h | 6 | TRP | 2.3 |
| 5 | e | 61 | ARG | 2.3 |
| 8 | i | 35 | LYS | 2.3 |
| 20 | r | 29 | LYS | 2.3 |
| 3 | C | 143 | TYR | 2.3 |
| 5 | e | 72 | ALA | 2.3 |
| 15 | u | 53 | ALA | 2.3 |
| 12 | M | 33 | GLN | 2.2 |
| 19 | z | 34 | ASP | 2.2 |
| 13 | O | 64 | GLU | 2.2 |
| 2 | b | 161 | LEU | 2.2 |
| 19 | z | 37 | LYS | 2.2 |
| 19 | Z | 38 | GLN | 2.2 |
| 13 | o | 62 | GLU | 2.2 |
| 2 | b | 126 | PRO | 2.2 |
| 13 | o | 54 | GLU | 2.2 |
| 20 | r | 7 | VAL | 2.2 |
| 20 | R | 2 | ASP | 2.2 |
| 5 | E | 15 | THR | 2.2 |
| 13 | o | 57 | LYS | 2.1 |
| 20 | r | 16 | ALA | 2.1 |
| 4 | d | 226 | GLY | 2.1 |
| 13 | o | 207 | ARG | 2.1 |
| 19 | Z | 4 | LEU | 2.1 |
| 4 | d | 236 | ASN | 2.1 |
| 17 | Y | 24 | MET | 2.1 |
| 2 | B | 504 | THR | 2.1 |
| 14 | T | 29 | ILE | 2.1 |
| 2 | b | 490 | GLN | 2.1 |
| 2 | b | 289 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 19 | z | 59 | PHE | 2.1 |
| 5 | e | 15 | THR | 2.0 |
| 10 | k | 17 | ILE | 2.0 |
| 3 | c | 146 | PHE | 2.0 |
| 16 | v | 22 | THR | 2.0 |
| 2 | B | 486 | LEU | 2.0 |
| 17 | Y | 39 | LEU | 2.0 |
| 13 | o | 55 | GLU | 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, 95th 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 ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 12 | FME | M | 1 | 10/11 | 0.96 | 0.16 | 41,55,69,80 | 0 |
| 14 | FME | T | 1 | 10/11 | 0.96 | 0.14 | 33,58,80,90 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.96 | 0.18 | 39,54,68,78 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.96 | 0.16 | 37,54,75,81 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.97 | 0.14 | 48,61,72,83 | 0 |
| 14 | FME | t | 1 | 10/11 | 0.97 | 0.10 | 36,55,82,88 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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, 95th 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 ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 32 | UNL | H | 103 | 53/- | 0.74 | 0.32 | 44,89,115,116 | 0 |
| 32 | UNL | c | 523 | 28/- | 0.75 | 0.22 | 55,80,93,95 | 0 |
| 32 | UNL | a | 414 | 28/- | 0.78 | 0.29 | 44,66,82,84 | 0 |
| 32 | UNL | x | 101 | 55/- | 0.78 | 0.31 | 43,71,92,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 33 | LMG | c | 522 | 48/55 | 0.80 | 0.26 | 42,89,123,138 | 0 |
| 28 | DGD | A | 412 | 66/66 | 0.82 | 0.23 | 41,75,100,124 | 0 |
| 32 | UNL | E | 102 | 28/- | 0.82 | 0.32 | 66,88,97,103 | 0 |
| 32 | UNL | c | 520 | 55/- | 0.82 | 0.23 | 48,72,94,101 | 0 |
| 33 | LMG | d | 410 | 23/55 | 0.82 | 0.27 | 43,73,104,105 | 0 |
| 32 | UNL | B | 624 | 46/- | 0.83 | 0.20 | 55,68,83,87 | 0 |
| 33 | LMG | b | 622 | 55/55 | 0.84 | 0.27 | 48,80,99,104 | 0 |
| 32 | UNL | b | 621 | 55/- | 0.84 | 0.23 | 42,68,96,118 | 0 |
| 32 | UNL | B | 625 | 28/- | 0.84 | 0.41 | 47,67,91,99 | 0 |
| 28 | DGD | a | 413 | 44/66 | 0.85 | 0.18 | 36,62,86,88 | 0 |
| 29 | LHG | E | 101 | 49/49 | 0.85 | 0.23 | 54,88,118,126 | 0 |
| 33 | LMG | D | 410 | 33/55 | 0.85 | 0.20 | 34,61,107,111 | 0 |
| 29 | LHG | e | 101 | 42/49 | 0.85 | 0.30 | 68,92,115,158 | 0 |
| 27 | SQD | a | 412 | 36/54 | 0.85 | 0.19 | 40,72,101,113 | 0 |
| 23 | CLA | c | 512 | 65/65 | 0.85 | 0.19 | 45,68,99,114 | 0 |
| 32 | UNL | b | 623 | 40/- | 0.86 | 0.21 | 52,68,91,100 | 0 |
| 32 | UNL | b | 625 | 55/- | 0.86 | 0.19 | 50,73,87,98 | 0 |
| 32 | UNL | b | 626 | 26/- | 0.86 | 0.28 | 52,65,76,78 | 0 |
| 23 | CLA | b | 602 | 65/65 | 0.86 | 0.21 | 55,76,104,110 | 0 |
| 32 | UNL | B | 626 | 47/- | 0.86 | 0.34 | 54,73,88,96 | 0 |
| 25 | BCR | x | 102 | 40/40 | 0.87 | 0.16 | 40,62,84,87 | 0 |
| 26 | PL9 | A | 409 | 55/55 | 0.87 | 0.26 | 35,70,101,113 | 0 |
| 32 | UNL | C | 522 | 28/- | 0.87 | 0.18 | 41,61,81,83 | 0 |
| 26 | PL9 | a | 410 | 55/55 | 0.87 | 0.23 | 42,77,101,112 | 0 |
| 32 | UNL | t | 102 | 26/- | 0.87 | 0.25 | 56,75,87,88 | 0 |
| 32 | UNL | j | 101 | 28/- | 0.88 | 0.16 | 53,67,81,85 | 0 |
| 23 | CLA | C | 514 | 65/65 | 0.88 | 0.22 | 48,77,110,115 | 0 |
| 25 | BCR | H | 101 | 40/40 | 0.88 | 0.15 | 35,51,65,69 | 0 |
| 25 | BCR | K | 101 | 40/40 | 0.88 | 0.16 | 38,60,75,91 | 0 |
| 25 | BCR | k | 101 | 40/40 | 0.88 | 0.17 | 45,71,86,89 | 0 |
| 32 | UNL | B | 620 | 43/- | 0.88 | 0.15 | 41,59,81,83 | 0 |
| 27 | SQD | b | 601 | 49/54 | 0.88 | 0.17 | 47,68,101,117 | 0 |
| 27 | SQD | f | 101 | 41/54 | 0.89 | 0.22 | 58,91,129,142 | 0 |
| 32 | UNL | m | 102 | 28/- | 0.89 | 0.18 | 38,58,78,78 | 0 |
| 23 | CLA | c | 513 | 65/65 | 0.89 | 0.23 | 47,74,109,113 | 0 |
| 32 | UNL | D | 412 | 55/- | 0.89 | 0.26 | 35,65,88,94 | 0 |
| 23 | CLA | B | 616 | 60/65 | 0.90 | 0.17 | 24,45,91,96 | 0 |
| 32 | UNL | b | 624 | 44/- | 0.90 | 0.20 | 48,68,88,89 | 0 |
| 33 | LMG | C | 501 | 48/55 | 0.90 | 0.17 | 40,67,86,111 | 0 |
| 33 | LMG | C | 519 | 48/55 | 0.90 | 0.20 | 53,85,105,121 | 0 |
| 32 | UNL | d | 412 | 43/- | 0.90 | 0.20 | 50,62,78,83 | 0 |
| 33 | LMG | D | 411 | 28/55 | 0.90 | 0.18 | 34,58,76,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23 | CLA | D | 404 | 65/65 | 0.90 | 0.17 | 26,47,133,138 | 0 |
| 32 | UNL | I | 102 | 53/- | 0.90 | 0.19 | 36,55,96,102 | 0 |
| 32 | UNL | C | 521 | 28/- | 0.90 | 0.14 | 35,50,62,67 | 0 |
| 32 | UNL | T | 102 | 47/- | 0.91 | 0.21 | 34,52,79,81 | 0 |
| 27 | SQD | A | 411 | 39/54 | 0.91 | 0.23 | 43,73,96,111 | 0 |
| 27 | SQD | B | 621 | 54/54 | 0.91 | 0.16 | 43,67,104,121 | 0 |
| 27 | SQD | F | 101 | 36/54 | 0.91 | 0.16 | 48,76,102,107 | 0 |
| 23 | CLA | B | 601 | 65/65 | 0.91 | 0.16 | 36,65,116,139 | 0 |
| 23 | CLA | C | 513 | 65/65 | 0.91 | 0.17 | 35,62,112,146 | 0 |
| 32 | UNL | B | 622 | 34/- | 0.91 | 0.16 | 38,55,71,72 | 0 |
| 23 | CLA | a | 408 | 65/65 | 0.91 | 0.16 | 22,41,107,114 | 0 |
| 32 | UNL | I | 101 | 41/- | 0.91 | 0.14 | 42,62,95,99 | 0 |
| 33 | LMG | c | 519 | 37/55 | 0.91 | 0.18 | 45,74,99,105 | 0 |
| 32 | UNL | J | 101 | 28/- | 0.91 | 0.23 | 48,62,74,75 | 0 |
| 33 | LMG | c | 524 | 49/55 | 0.91 | 0.15 | 31,60,96,125 | 0 |
| 32 | UNL | M | 103 | 26/- | 0.91 | 0.20 | 36,54,72,72 | 0 |
| 23 | CLA | c | 508 | 64/65 | 0.92 | 0.15 | 32,54,97,122 | 0 |
| 25 | BCR | d | 405 | 40/40 | 0.92 | 0.16 | 39,59,110,121 | 0 |
| 33 | LMG | D | 407 | 51/55 | 0.92 | 0.18 | 34,64,86,98 | 0 |
| 28 | DGD | c | 517 | 62/66 | 0.92 | 0.15 | 37,62,94,112 | 0 |
| 23 | CLA | d | 404 | 65/65 | 0.92 | 0.16 | 31,56,111,137 | 0 |
| 25 | BCR | C | 515 | 40/40 | 0.92 | 0.15 | 24,46,60,75 | 0 |
| 32 | UNL | C | 523 | 47/- | 0.92 | 0.15 | 47,60,78,78 | 0 |
| 25 | BCR | D | 405 | 40/40 | 0.92 | 0.15 | 34,50,95,115 | 0 |
| 23 | CLA | b | 617 | 60/65 | 0.92 | 0.14 | 33,50,94,105 | 0 |
| 32 | UNL | B | 623 | 28/- | 0.92 | 0.12 | 36,52,70,76 | 0 |
| 23 | CLA | c | 511 | 65/65 | 0.93 | 0.17 | 45,66,85,88 | 0 |
| 27 | SQD | a | 411 | 54/54 | 0.93 | 0.16 | 45,75,97,102 | 0 |
| 28 | DGD | c | 518 | 62/66 | 0.93 | 0.15 | 30,63,82,92 | 0 |
| 23 | CLA | c | 502 | 65/65 | 0.93 | 0.15 | 36,52,71,82 | 0 |
| 33 | LMG | M | 101 | 51/55 | 0.93 | 0.13 | 33,54,75,89 | 0 |
| 23 | CLA | c | 503 | 65/65 | 0.93 | 0.19 | 33,54,68,71 | 0 |
| 23 | CLA | c | 507 | 65/65 | 0.93 | 0.15 | 35,51,66,69 | 0 |
| 23 | CLA | C | 503 | 65/65 | 0.93 | 0.14 | 37,51,67,80 | 0 |
| 28 | DGD | C | 516 | 62/66 | 0.93 | 0.15 | 27,44,87,103 | 0 |
| 28 | DGD | C | 517 | 62/66 | 0.93 | 0.14 | 40,62,111,122 | 0 |
| 33 | LMG | d | 411 | 44/55 | 0.93 | 0.14 | 41,63,94,112 | 0 |
| 33 | LMG | m | 101 | 51/55 | 0.93 | 0.14 | 37,60,85,98 | 0 |
| 25 | BCR | T | 101 | 40/40 | 0.94 | 0.13 | 30,50,64,70 | 0 |
| 25 | BCR | Z | 101 | 40/40 | 0.94 | 0.17 | 41,63,81,84 | 0 |
| 25 | BCR | b | 618 | 40/40 | 0.94 | 0.13 | 31,50,67,67 | 0 |
| 28 | DGD | h | 101 | 62/66 | 0.94 | 0.13 | 35,55,69,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25 | BCR | b | 620 | 40/40 | 0.94 | 0.14 | 34,58,75,80 | 0 |
| 29 | LHG | d | 407 | 49/49 | 0.94 | 0.16 | 38,59,98,112 | 0 |
| 29 | LHG | d | 409 | 39/49 | 0.94 | 0.14 | 35,56,75,81 | 0 |
| 25 | BCR | c | 514 | 40/40 | 0.94 | 0.21 | 44,65,80,80 | 0 |
| 25 | BCR | c | 521 | 40/40 | 0.94 | 0.18 | 39,61,68,74 | 0 |
| 23 | CLA | b | 605 | 65/65 | 0.94 | 0.16 | 25,42,84,98 | 0 |
| 23 | CLA | b | 607 | 65/65 | 0.94 | 0.12 | 30,48,78,87 | 0 |
| 23 | CLA | c | 509 | 65/65 | 0.94 | 0.22 | 37,56,73,83 | 0 |
| 23 | CLA | c | 510 | 65/65 | 0.94 | 0.16 | 39,57,78,89 | 0 |
| 23 | CLA | b | 615 | 65/65 | 0.94 | 0.17 | 24,46,85,89 | 0 |
| 23 | CLA | b | 616 | 65/65 | 0.94 | 0.14 | 33,48,69,80 | 0 |
| 23 | CLA | C | 506 | 65/65 | 0.94 | 0.19 | 27,46,69,79 | 0 |
| 23 | CLA | B | 606 | 65/65 | 0.94 | 0.13 | 26,43,85,94 | 0 |
| 25 | BCR | B | 618 | 40/40 | 0.94 | 0.12 | 29,45,68,69 | 0 |
| 25 | BCR | B | 619 | 40/40 | 0.94 | 0.12 | 33,49,66,84 | 0 |
| 23 | CLA | B | 615 | 65/65 | 0.94 | 0.15 | 27,46,70,81 | 0 |
| 25 | BCR | C | 520 | 40/40 | 0.94 | 0.18 | 42,60,75,79 | 0 |
| 23 | CLA | c | 504 | 60/65 | 0.94 | 0.14 | 36,54,83,87 | 0 |
| 32 | UNL | M | 102 | 37/- | 0.94 | 0.13 | 37,51,63,73 | 0 |
| 23 | CLA | c | 505 | 65/65 | 0.94 | 0.17 | 31,48,70,79 | 0 |
| 23 | CLA | c | 506 | 65/65 | 0.94 | 0.16 | 35,60,114,126 | 0 |
| 28 | DGD | H | 102 | 62/66 | 0.94 | 0.13 | 32,52,68,76 | 0 |
| 26 | PL9 | D | 406 | 55/55 | 0.95 | 0.13 | 22,38,49,55 | 0 |
| 23 | CLA | C | 512 | 65/65 | 0.95 | 0.14 | 37,58,76,83 | 0 |
| 29 | LHG | D | 409 | 47/49 | 0.95 | 0.14 | 36,56,90,108 | 0 |
| 27 | SQD | A | 410 | 52/54 | 0.95 | 0.15 | 37,68,94,102 | 0 |
| 23 | CLA | A | 405 | 65/65 | 0.95 | 0.13 | 23,41,104,122 | 0 |
| 23 | CLA | B | 604 | 65/65 | 0.95 | 0.14 | 25,41,92,98 | 0 |
| 23 | CLA | c | 501 | 65/65 | 0.95 | 0.15 | 30,46,58,67 | 0 |
| 23 | CLA | A | 407 | 54/65 | 0.95 | 0.14 | 25,38,83,85 | 0 |
| 25 | BCR | b | 619 | 40/40 | 0.95 | 0.11 | 33,46,58,62 | 0 |
| 23 | CLA | a | 406 | 65/65 | 0.95 | 0.14 | 31,48,99,114 | 0 |
| 25 | BCR | B | 617 | 40/40 | 0.95 | 0.13 | 32,48,61,67 | 0 |
| 25 | BCR | c | 515 | 40/40 | 0.95 | 0.15 | 32,52,66,80 | 0 |
| 23 | CLA | B | 613 | 65/65 | 0.95 | 0.14 | 24,36,71,82 | 0 |
| 23 | CLA | C | 507 | 65/65 | 0.95 | 0.14 | 27,49,103,114 | 0 |
| 23 | CLA | C | 508 | 65/65 | 0.95 | 0.15 | 29,44,66,71 | 0 |
| 23 | CLA | C | 511 | 65/65 | 0.95 | 0.13 | 35,55,81,86 | 0 |
| 23 | CLA | b | 614 | 65/65 | 0.95 | 0.15 | 23,41,92,97 | 0 |
| 28 | DGD | C | 518 | 62/66 | 0.96 | 0.12 | 32,58,86,104 | 0 |
| 23 | CLA | C | 509 | 65/65 | 0.96 | 0.12 | 28,51,114,130 | 0 |
| 23 | CLA | b | 606 | 65/65 | 0.96 | 0.14 | 27,43,57,61 | 0 |

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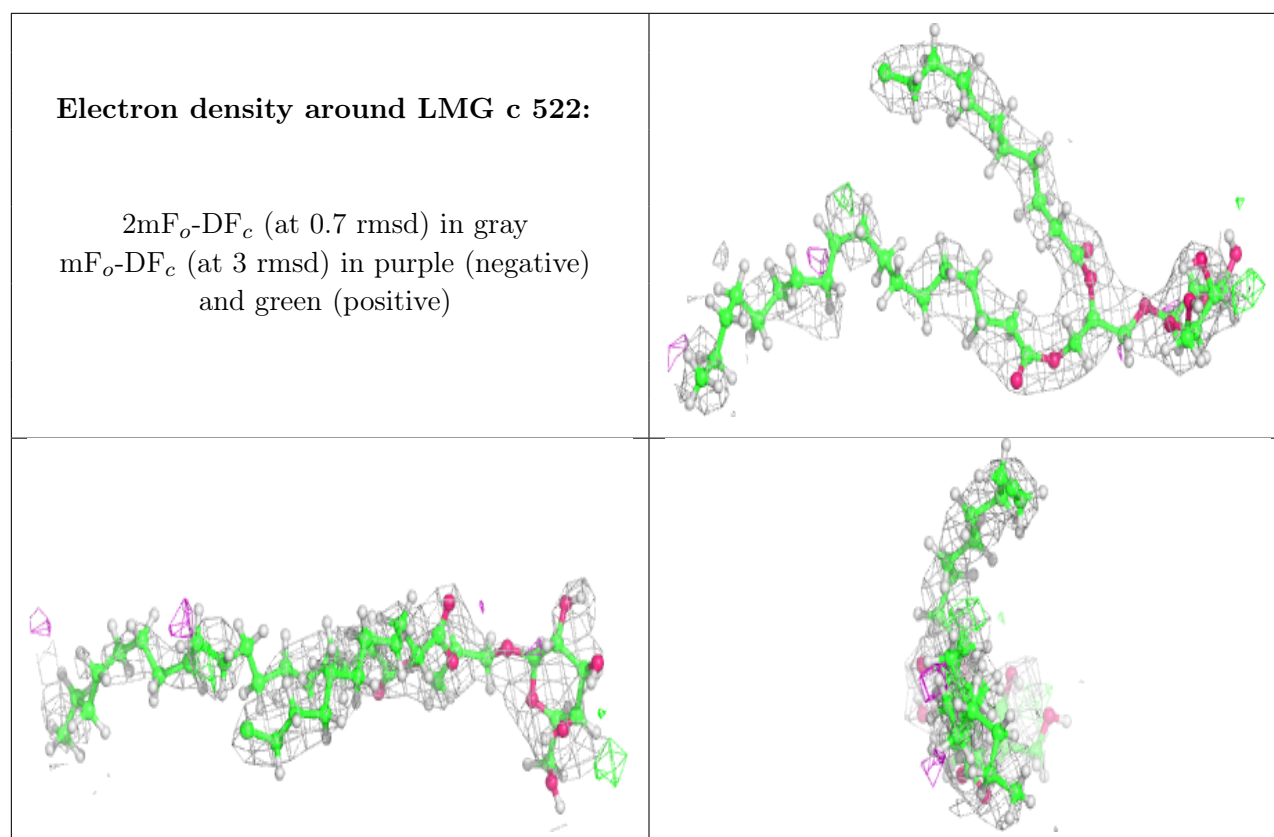
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28 | DGD | c | 516 | 62/66 | 0.96 | 0.12 | 25,46,78,94 | 0 |
| 23 | CLA | C | 510 | 65/65 | 0.96 | 0.14 | 35,51,71,72 | 0 |
| 23 | CLA | b | 608 | 65/65 | 0.96 | 0.12 | 23,42,73,81 | 0 |
| 23 | CLA | b | 610 | 65/65 | 0.96 | 0.12 | 27,48,67,93 | 0 |
| 29 | LHG | A | 413 | 49/49 | 0.96 | 0.13 | 31,53,82,87 | 0 |
| 23 | CLA | b | 613 | 65/65 | 0.96 | 0.16 | 24,40,56,65 | 0 |
| 23 | CLA | d | 402 | 65/65 | 0.96 | 0.12 | 26,39,50,54 | 0 |
| 23 | CLA | d | 403 | 65/65 | 0.96 | 0.12 | 24,41,75,83 | 0 |
| 25 | BCR | t | 101 | 40/40 | 0.96 | 0.10 | 31,45,57,65 | 0 |
| 23 | CLA | B | 605 | 65/65 | 0.96 | 0.17 | 23,39,55,60 | 0 |
| 29 | LHG | l | 101 | 49/49 | 0.96 | 0.12 | 38,51,63,81 | 0 |
| 24 | PHO | A | 406 | 64/64 | 0.96 | 0.12 | 20,35,49,55 | 0 |
| 24 | PHO | a | 407 | 64/64 | 0.96 | 0.14 | 24,36,48,50 | 0 |
| 25 | BCR | A | 408 | 40/40 | 0.96 | 0.10 | 25,37,50,51 | 0 |
| 26 | PL9 | d | 406 | 55/55 | 0.96 | 0.13 | 27,41,49,54 | 0 |
| 23 | CLA | B | 603 | 65/65 | 0.96 | 0.15 | 26,42,69,76 | 0 |
| 23 | CLA | B | 609 | 65/65 | 0.96 | 0.12 | 23,42,59,66 | 0 |
| 23 | CLA | C | 504 | 65/65 | 0.96 | 0.12 | 30,50,63,68 | 0 |
| 23 | CLA | D | 403 | 65/65 | 0.96 | 0.11 | 22,37,58,68 | 0 |
| 23 | CLA | C | 505 | 59/65 | 0.96 | 0.14 | 30,52,92,107 | 0 |
| 23 | CLA | B | 610 | 65/65 | 0.96 | 0.16 | 25,39,55,62 | 0 |
| 23 | CLA | B | 602 | 65/65 | 0.96 | 0.15 | 28,44,72,77 | 0 |
| 23 | CLA | B | 614 | 65/65 | 0.96 | 0.14 | 25,46,93,105 | 0 |
| 23 | CLA | b | 603 | 65/65 | 0.96 | 0.16 | 28,50,75,82 | 0 |
| 23 | CLA | b | 604 | 65/65 | 0.96 | 0.15 | 28,44,70,74 | 0 |
| 25 | BCR | a | 409 | 40/40 | 0.96 | 0.11 | 25,42,57,63 | 0 |
| 34 | HEM | E | 103 | 43/43 | 0.96 | 0.14 | 39,53,69,76 | 0 |
| 23 | CLA | b | 609 | 65/65 | 0.97 | 0.12 | 27,48,72,79 | 0 |
| 23 | CLA | B | 607 | 65/65 | 0.97 | 0.12 | 18,41,77,85 | 0 |
| 23 | CLA | b | 611 | 65/65 | 0.97 | 0.13 | 26,41,59,70 | 0 |
| 23 | CLA | b | 612 | 65/65 | 0.97 | 0.11 | 26,38,58,62 | 0 |
| 23 | CLA | D | 402 | 65/65 | 0.97 | 0.12 | 22,35,54,60 | 0 |
| 23 | CLA | B | 611 | 65/65 | 0.97 | 0.12 | 20,34,47,48 | 0 |
| 29 | LHG | D | 408 | 49/49 | 0.97 | 0.11 | 30,46,62,65 | 0 |
| 24 | PHO | D | 401 | 64/64 | 0.97 | 0.10 | 26,37,47,51 | 0 |
| 23 | CLA | B | 612 | 65/65 | 0.97 | 0.16 | 23,38,55,59 | 0 |
| 29 | LHG | L | 101 | 49/49 | 0.97 | 0.13 | 31,46,63,69 | 0 |
| 24 | PHO | d | 401 | 64/64 | 0.97 | 0.11 | 32,45,59,68 | 0 |
| 29 | LHG | d | 408 | 49/49 | 0.97 | 0.12 | 27,48,66,67 | 0 |
| 23 | CLA | a | 405 | 65/65 | 0.97 | 0.12 | 25,37,55,65 | 0 |
| 23 | CLA | C | 502 | 65/65 | 0.97 | 0.12 | 25,43,59,68 | 0 |
| 23 | CLA | A | 404 | 65/65 | 0.97 | 0.12 | 19,33,54,68 | 0 |

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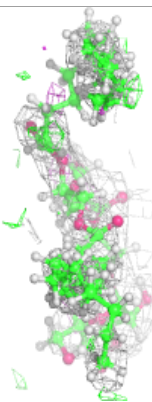
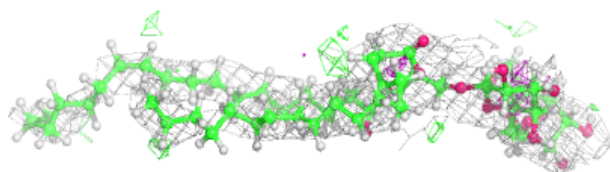
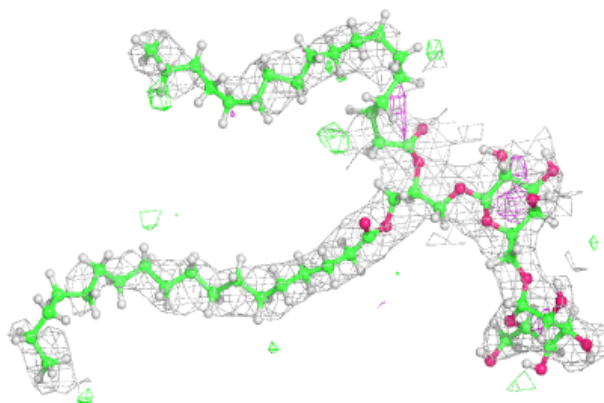
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 34 | HEM | e | 102 | 43/43 | 0.97 | 0.12 | 46,63,79,83 | 0 |
| 23 | CLA | B | 608 | 65/65 | 0.98 | 0.11 | 24,40,58,65 | 0 |
| 31 | BCT | a | 404 | 4/4 | 0.98 | 0.23 | 27,36,48,58 | 0 |
| 35 | HEC | V | 201 | 43/43 | 0.98 | 0.11 | 28,38,50,51 | 0 |
| 35 | HEC | v | 201 | 43/43 | 0.98 | 0.15 | 37,45,57,61 | 0 |
| 21 | FE2 | A | 401 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 21 | FE2 | a | 401 | 1/1 | 0.99 | 0.07 | 39,39,39,39 | 0 |
| 22 | CL | A | 402 | 1/1 | 0.99 | 0.06 | 36,36,36,36 | 0 |
| 22 | CL | A | 403 | 1/1 | 0.99 | 0.09 | 36,36,36,36 | 0 |
| 30 | OEX | A | 414 | 10/10 | 0.99 | 0.11 | 31,36,39,42 | 0 |
| 30 | OEX | a | 415 | 10/10 | 0.99 | 0.11 | 29,33,38,39 | 0 |
| 31 | BCT | A | 415 | 4/4 | 0.99 | 0.24 | 32,35,39,42 | 0 |
| 22 | CL | a | 402 | 1/1 | 1.00 | 0.08 | 34,34,34,34 | 0 |
| 22 | CL | a | 403 | 1/1 | 1.00 | 0.03 | 32,32,32,32 | 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.

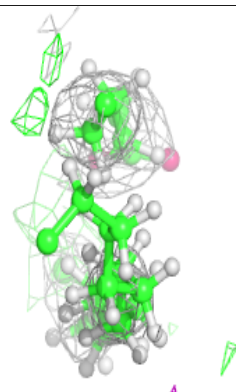
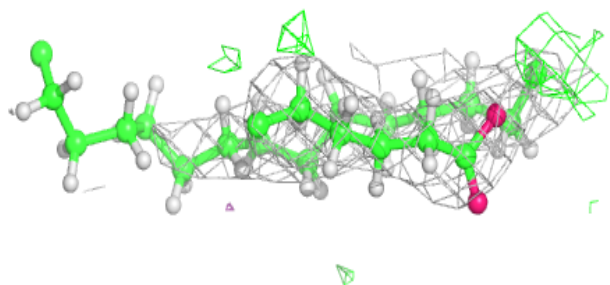
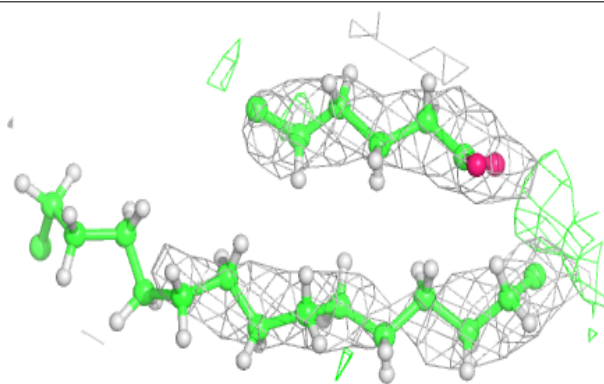


Electron density around DGD A 412:

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

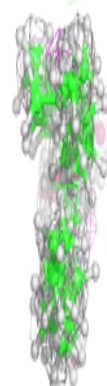
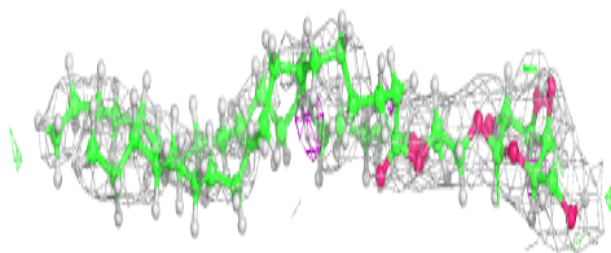
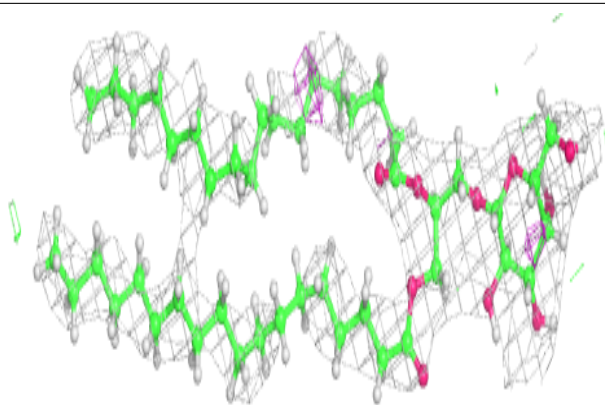
**Electron density around LMG d 410:**

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

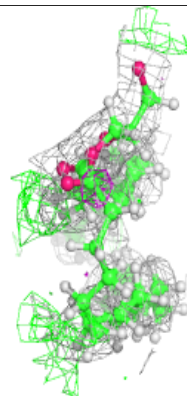
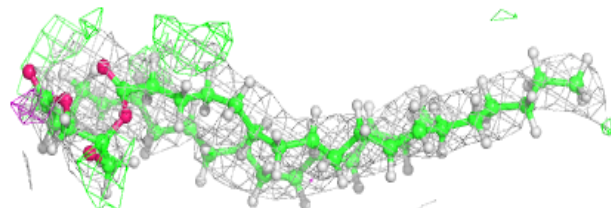
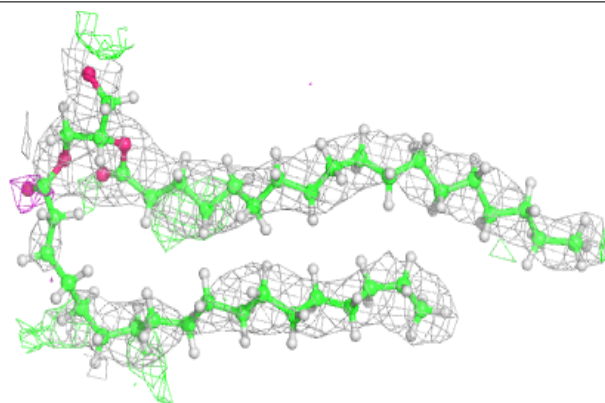


Electron density around LMG b 622:

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

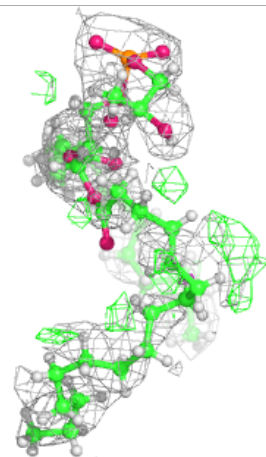
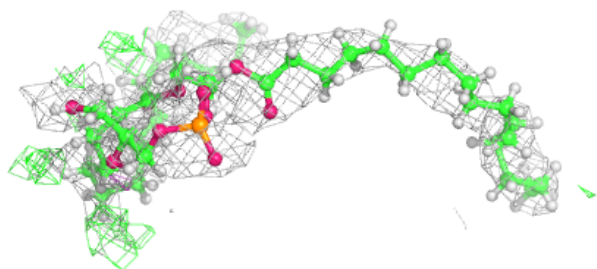
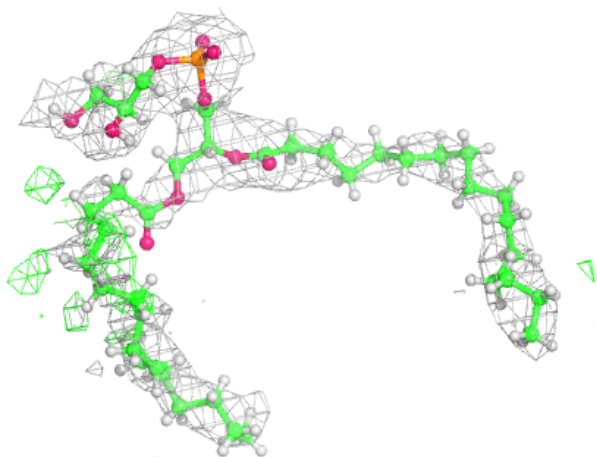
**Electron density around DGD a 413:**

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



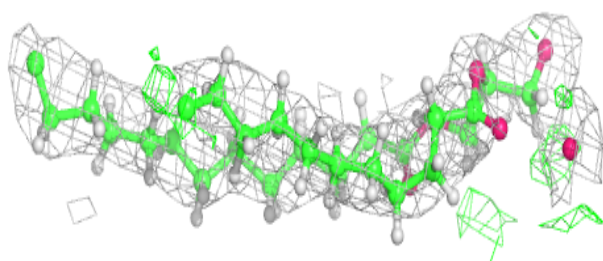
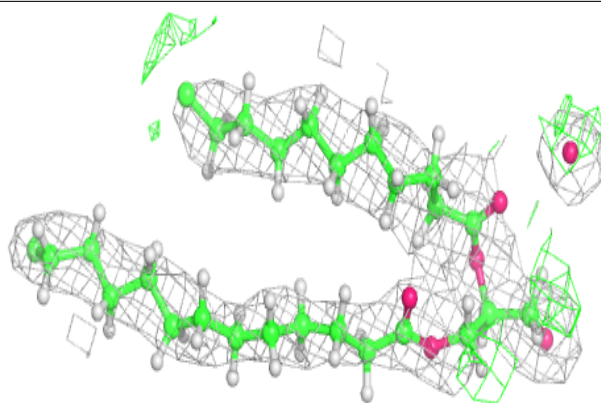
Electron density around LHG E 101:

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

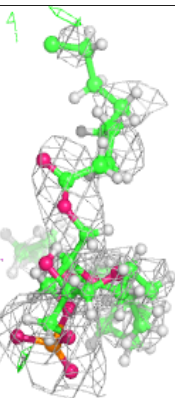
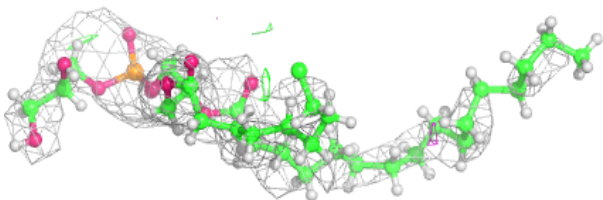
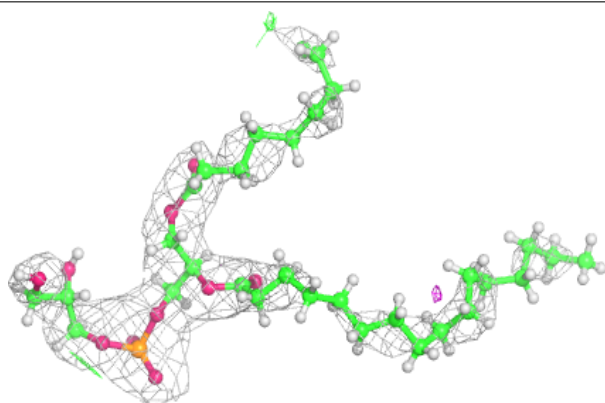


Electron density around LMG D 410:

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

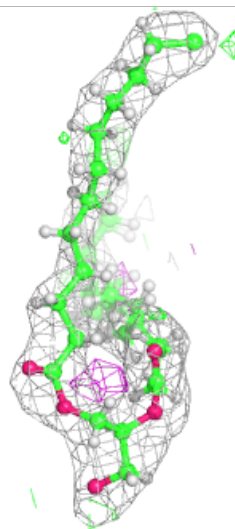
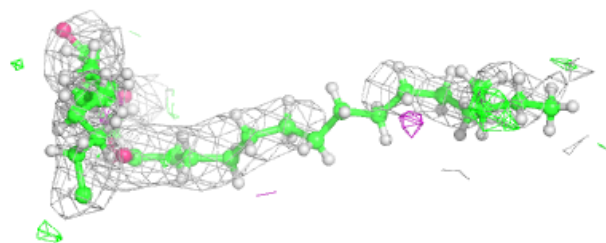
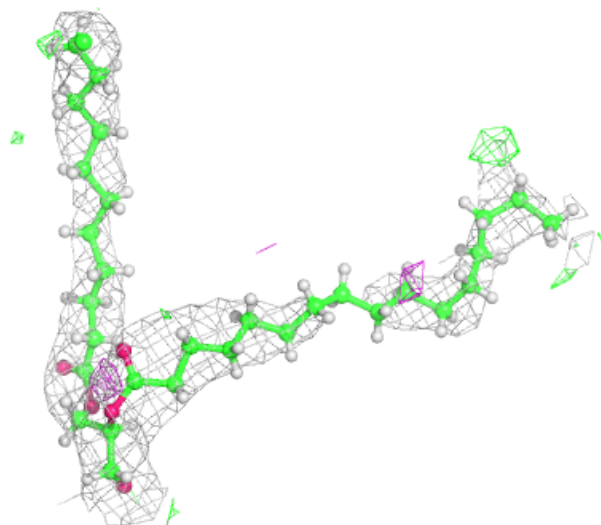
**Electron density around LHG e 101:**

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



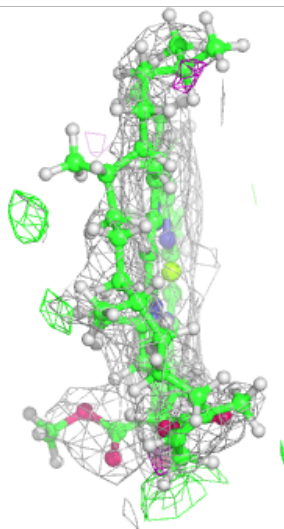
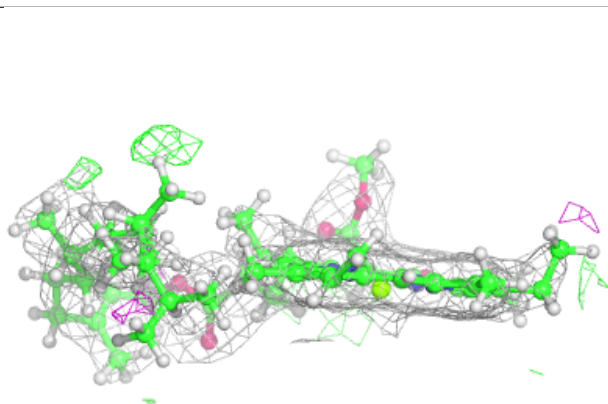
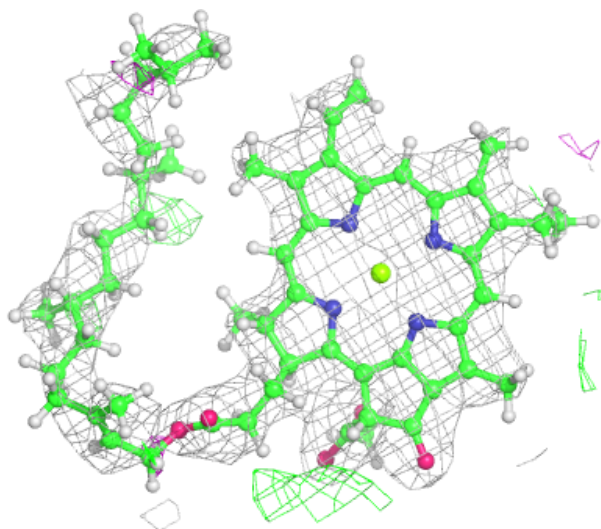
Electron density around SQD a 412:

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



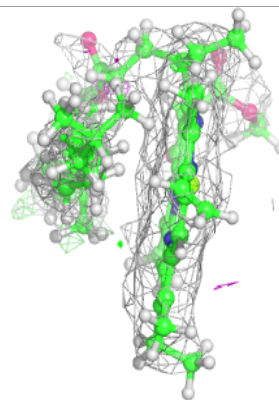
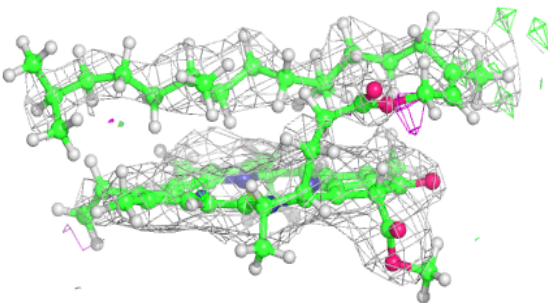
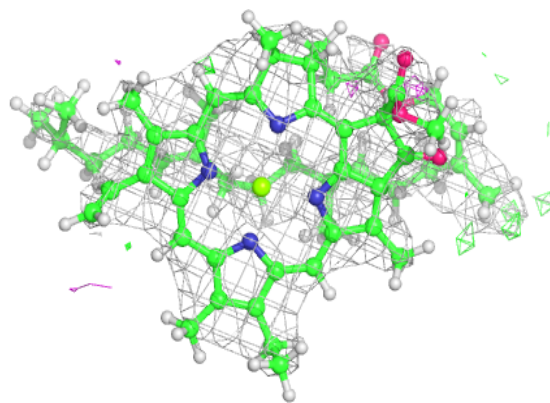
Electron density around CLA c 512:

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

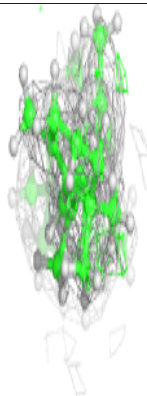
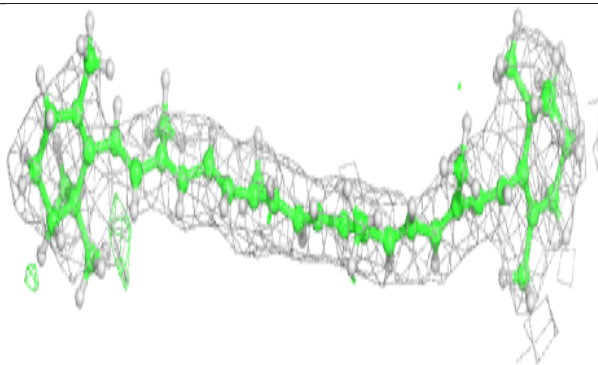
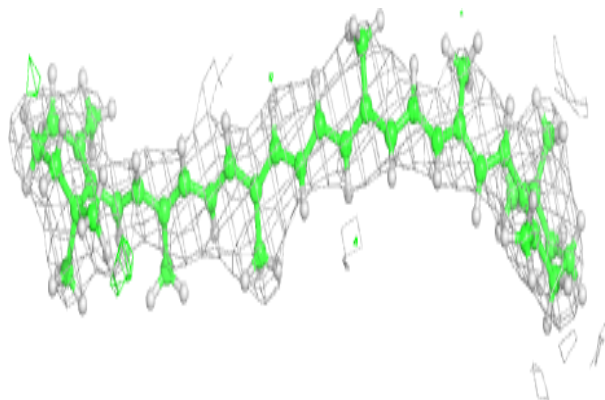


Electron density around CLA b 602:

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

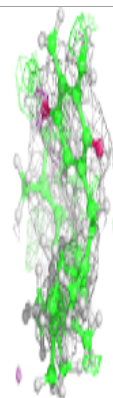
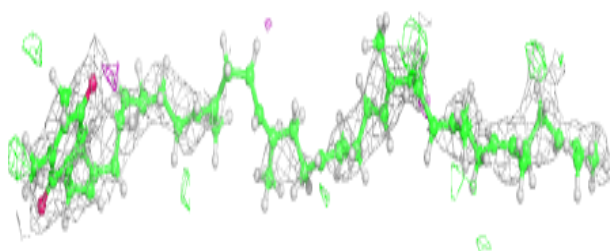
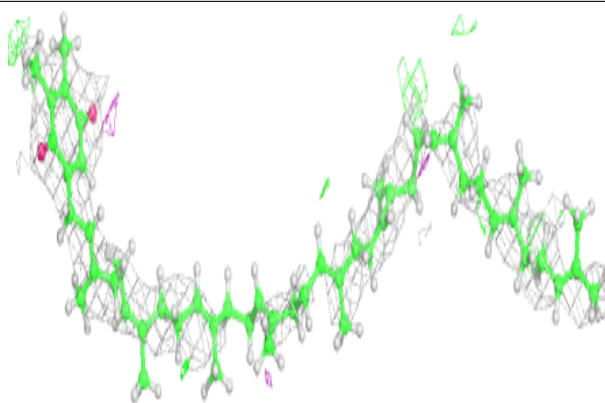
**Electron density around BCR x 102:**

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

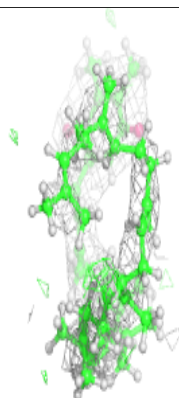
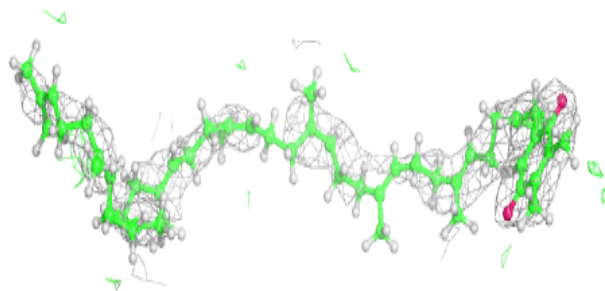
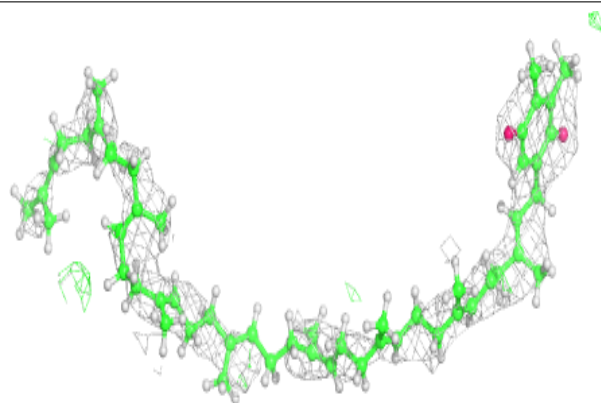


Electron density around PL9 A 409:

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

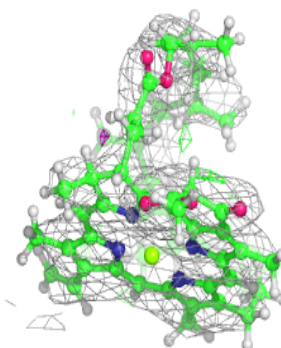
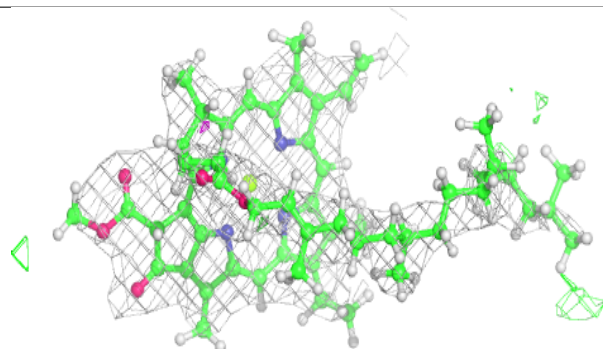
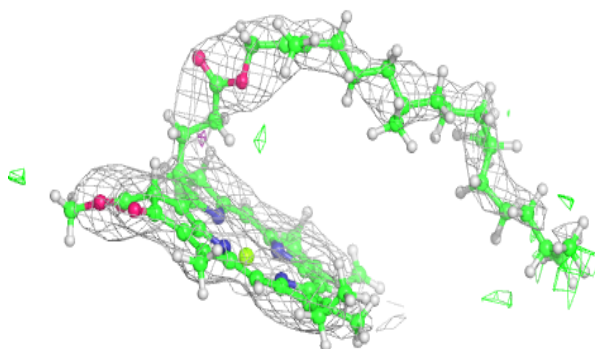
**Electron density around PL9 a 410:**

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

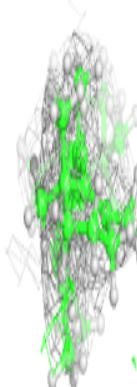
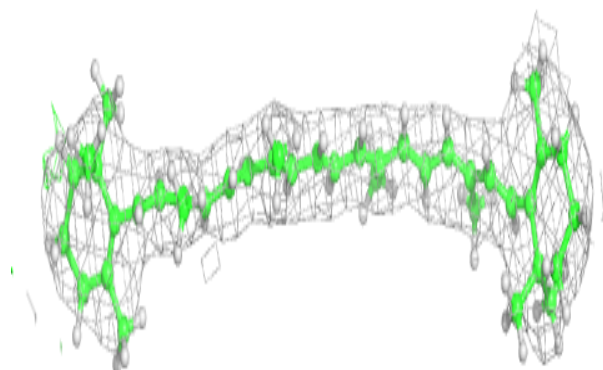
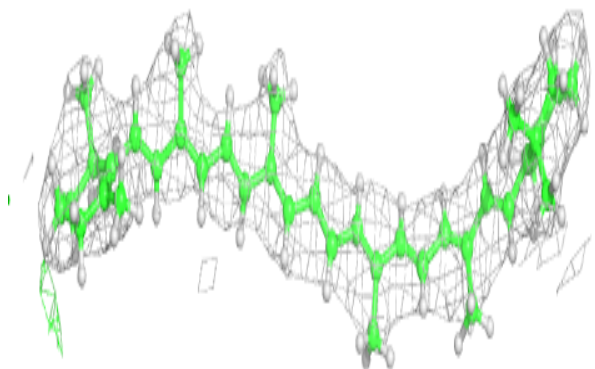


Electron density around CLA C 514:

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

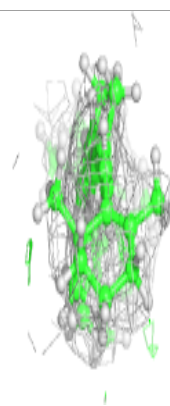
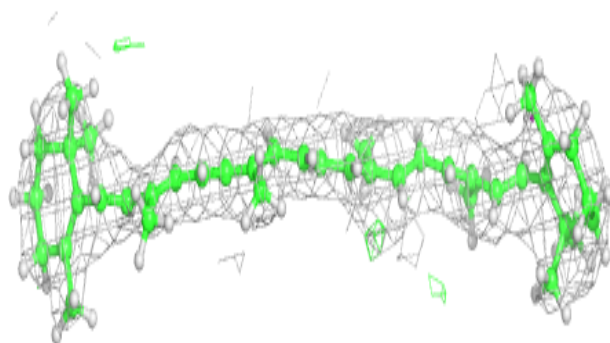
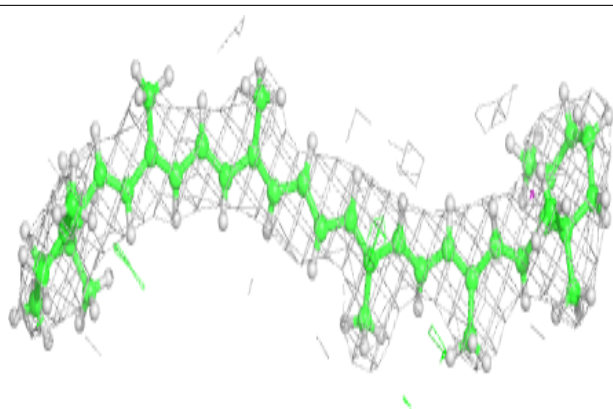
**Electron density around BCR H 101:**

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

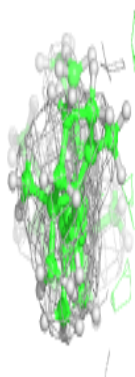
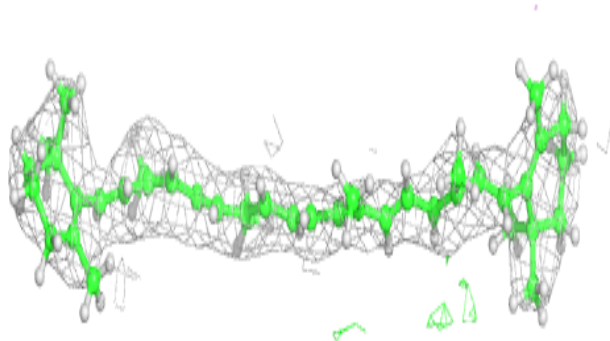
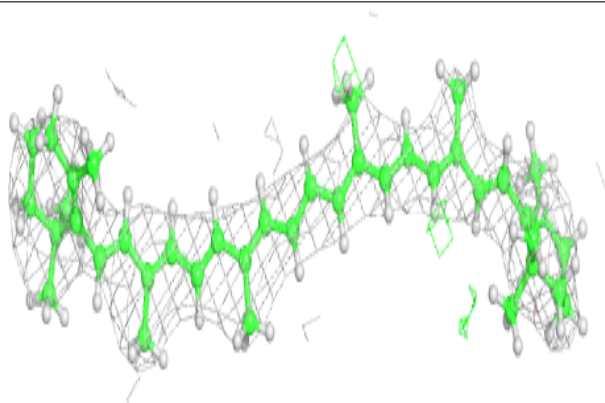


Electron density around BCR K 101:

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

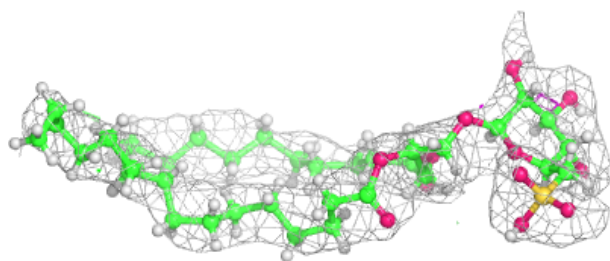
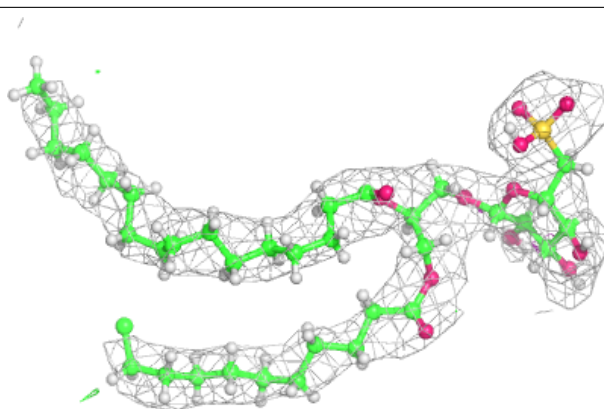
**Electron density around BCR k 101:**

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

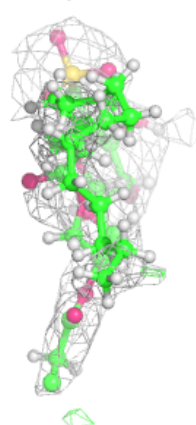
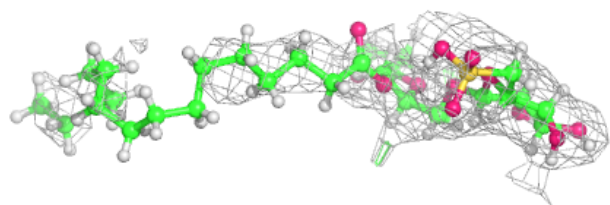
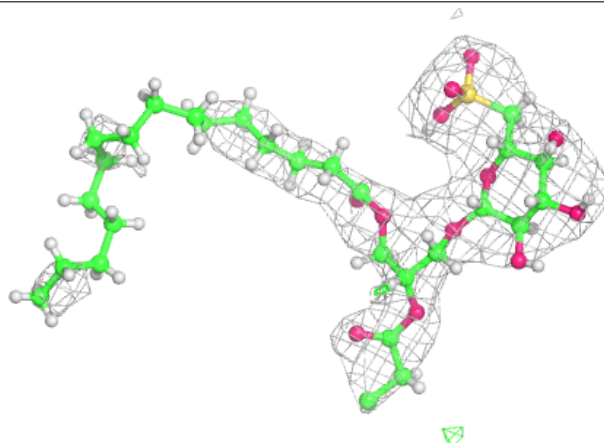


Electron density around SQD b 601:

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

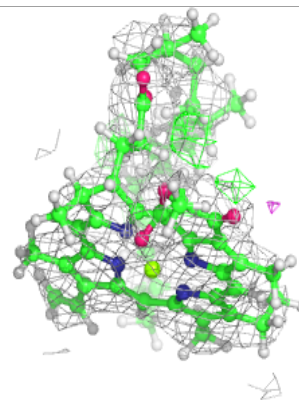
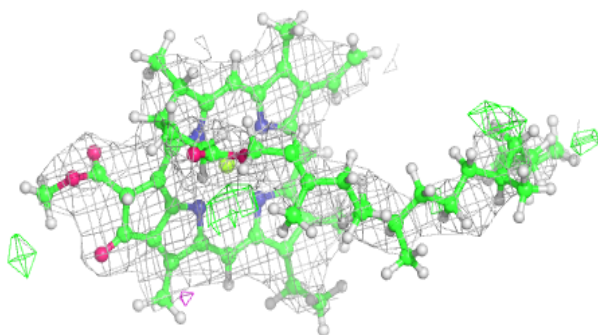
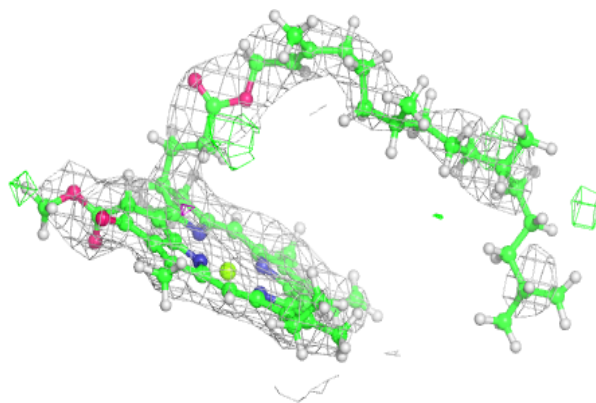
**Electron density around SQD f 101:**

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



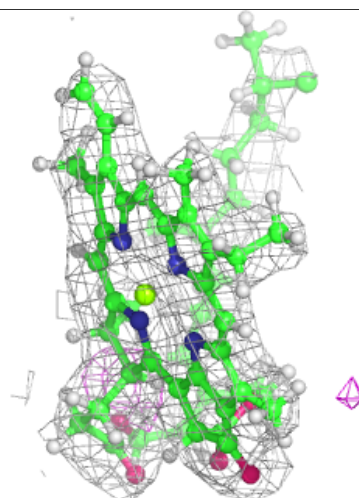
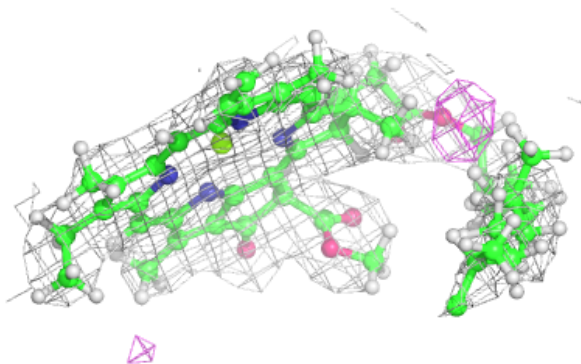
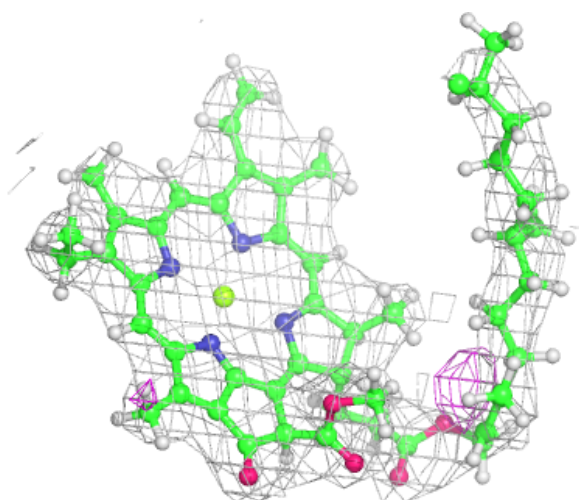
Electron density around CLA c 513:

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



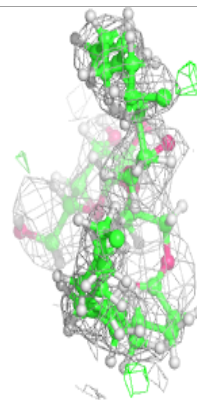
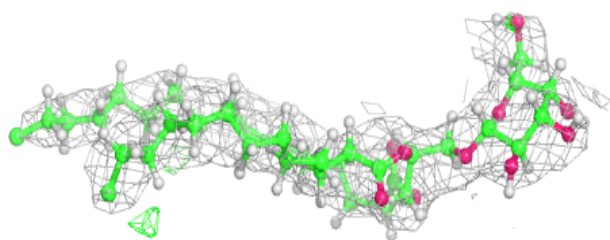
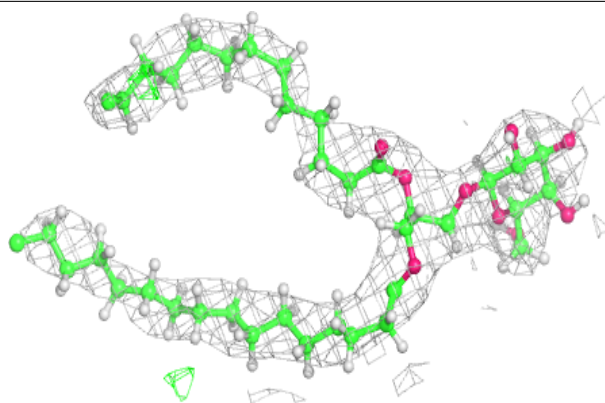
Electron density around CLA B 616:

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



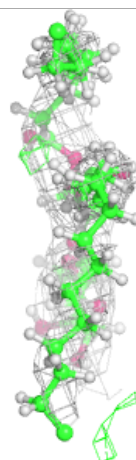
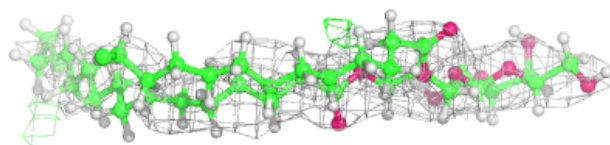
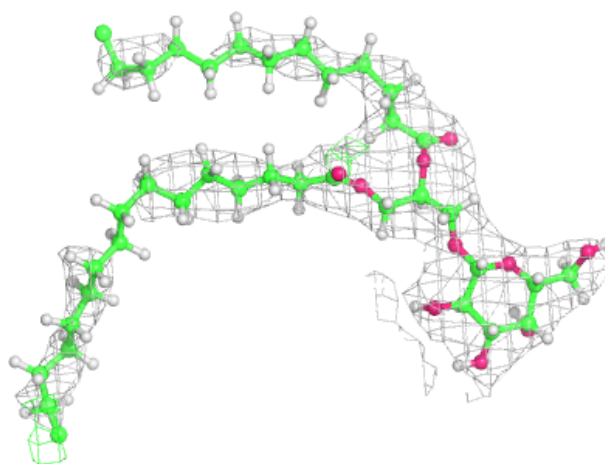
Electron density around LMG C 501:

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



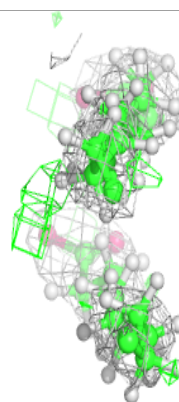
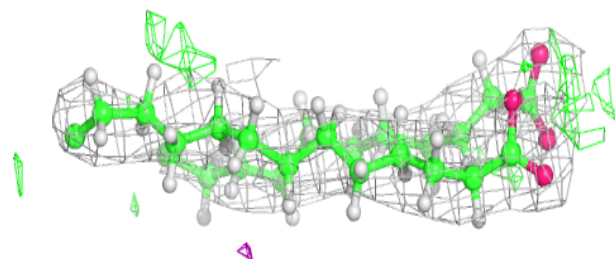
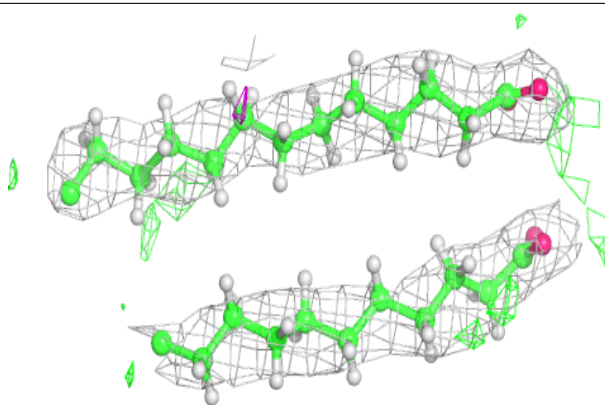
Electron density around LMG C 519:

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

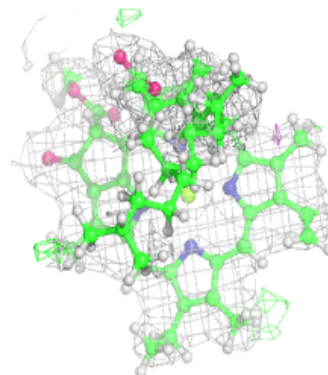
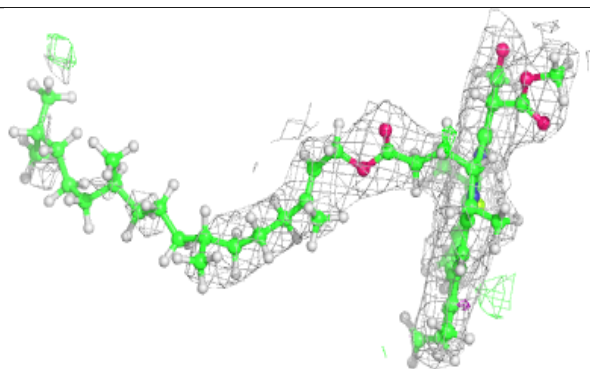
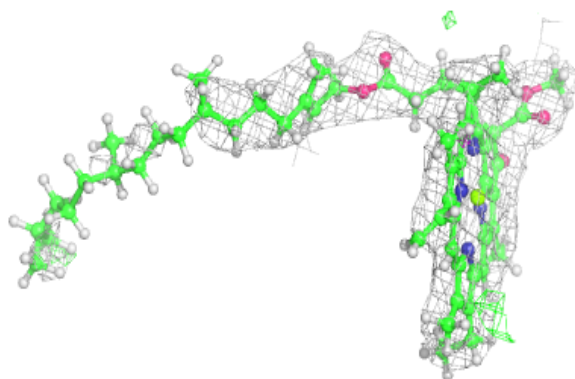


Electron density around LMG D 411:

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

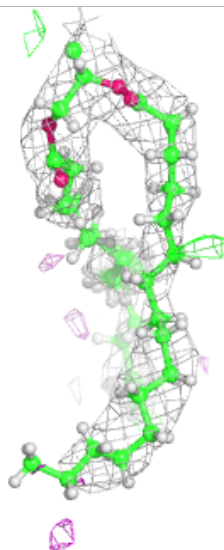
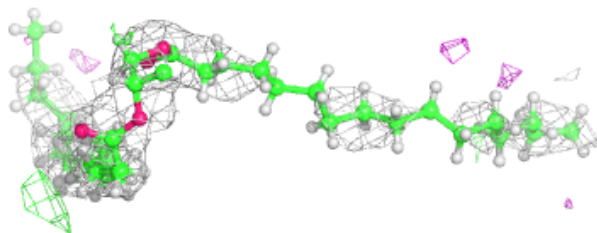
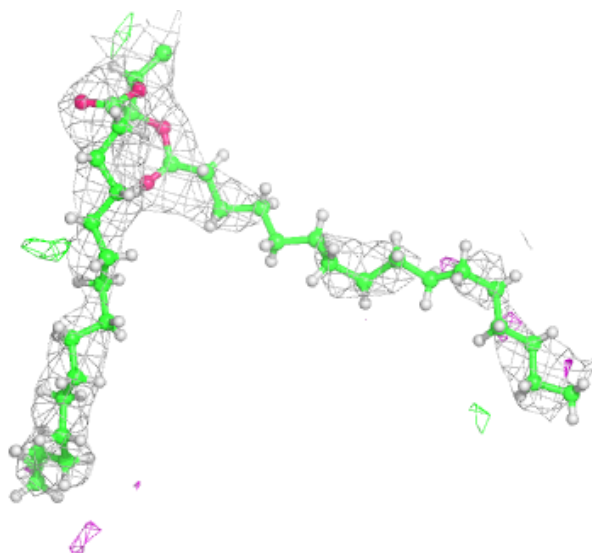
**Electron density around CLA D 404:**

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



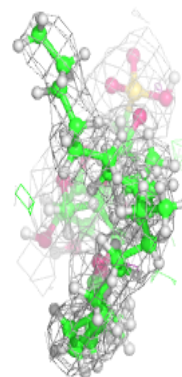
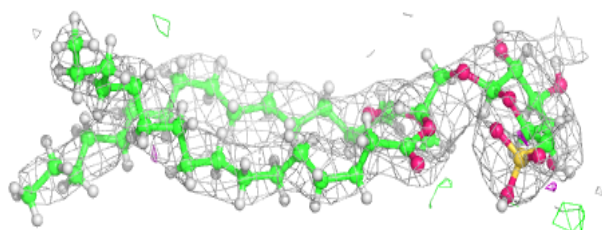
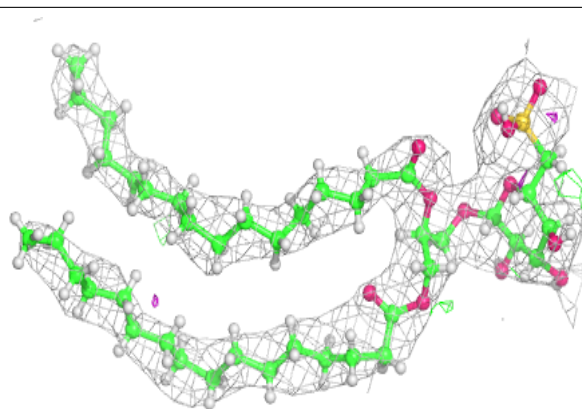
Electron density around SQD A 411:

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

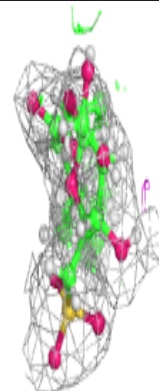
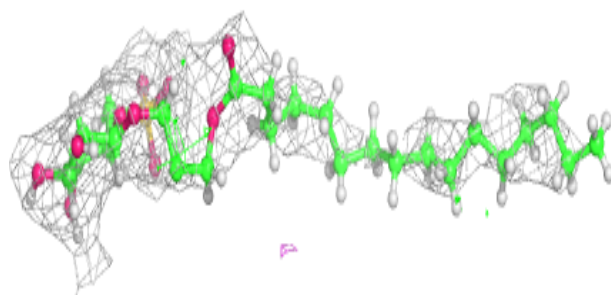
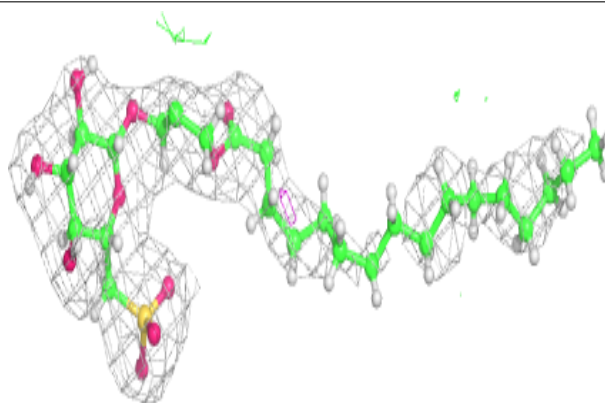


Electron density around SQD B 621:

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

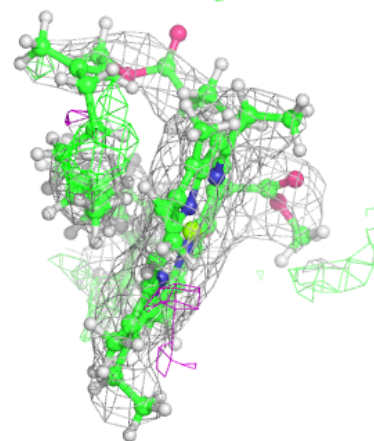
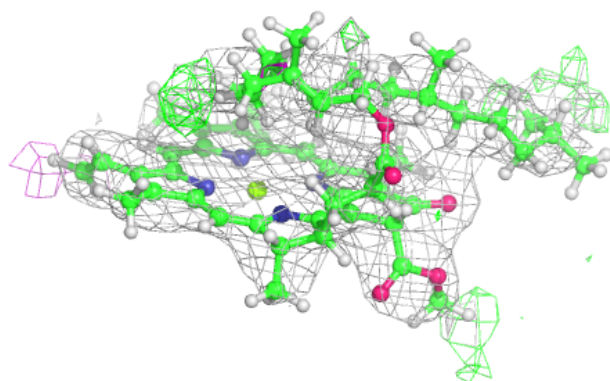
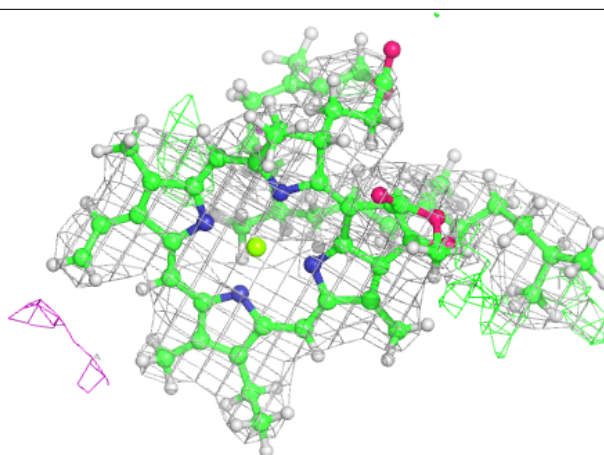
**Electron density around SQD F 101:**

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



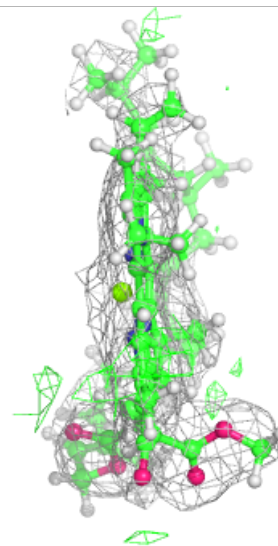
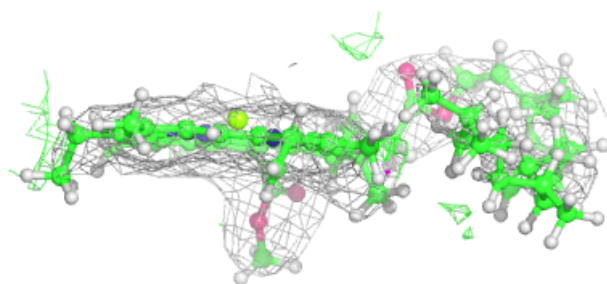
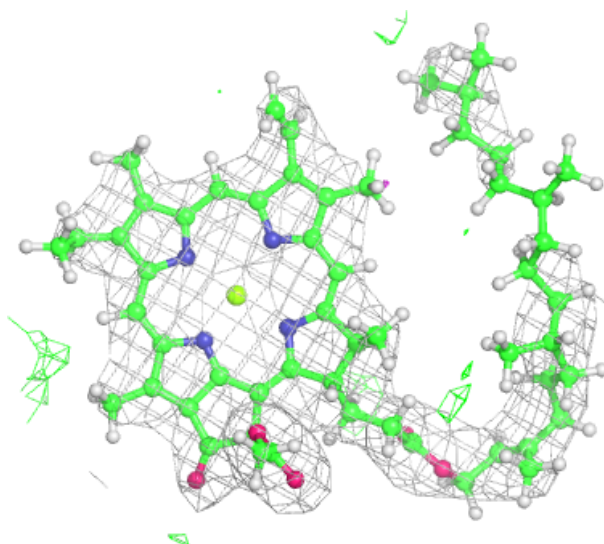
Electron density around CLA B 601:

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



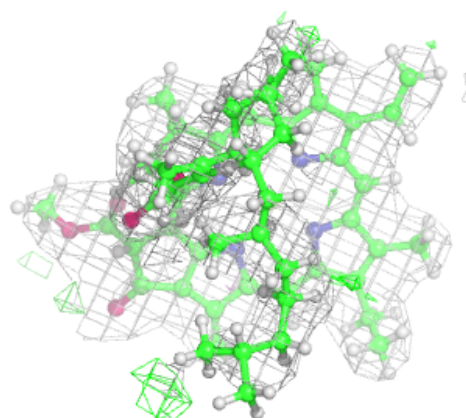
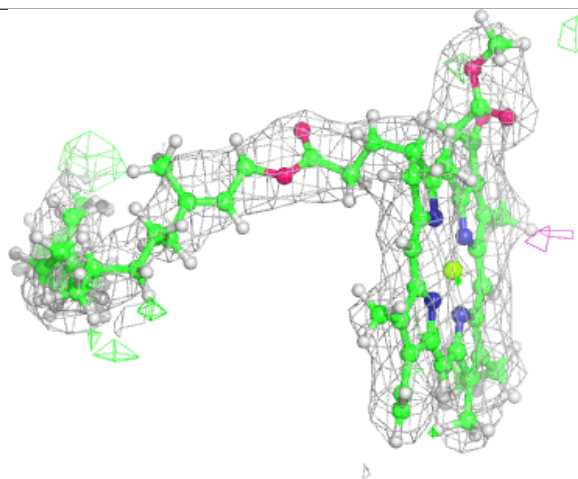
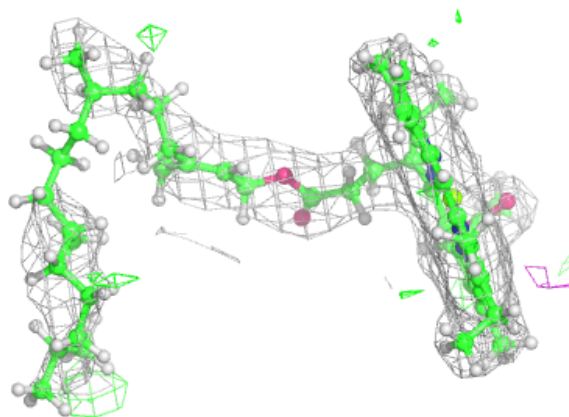
Electron density around CLA C 513:

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



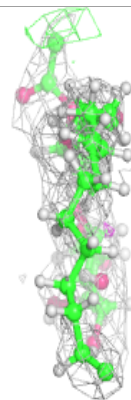
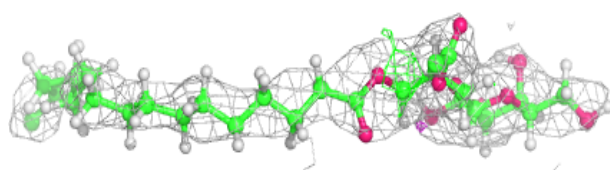
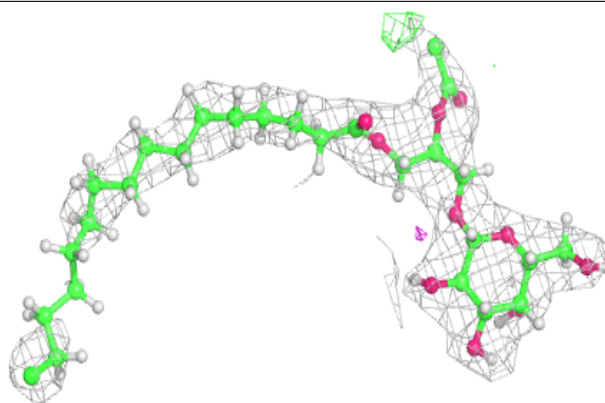
Electron density around CLA a 408:

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

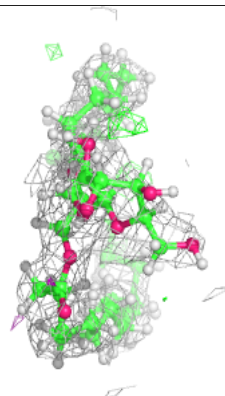
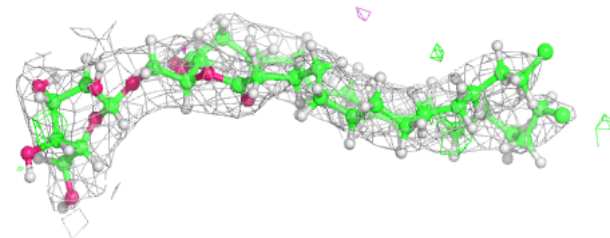
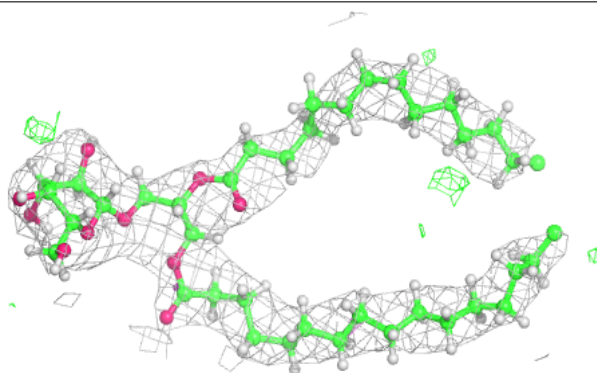


Electron density around LMG c 519:

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

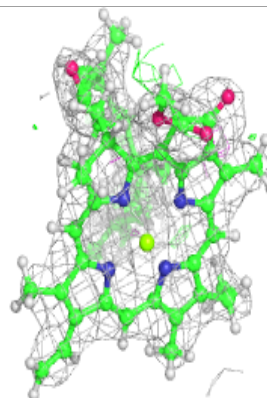
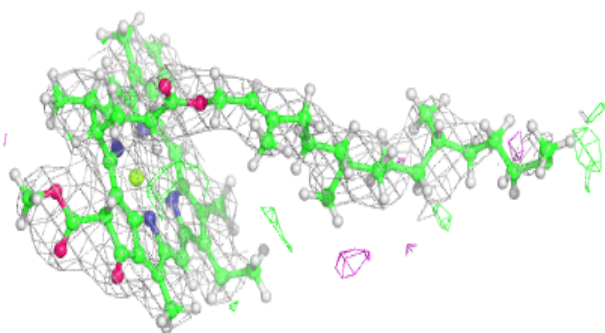
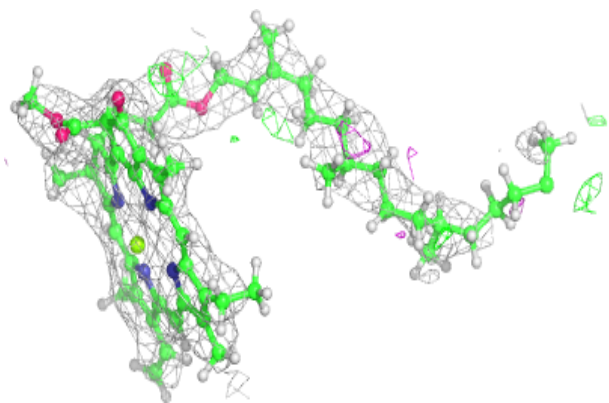
**Electron density around LMG c 524:**

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

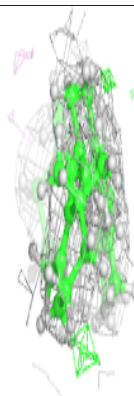
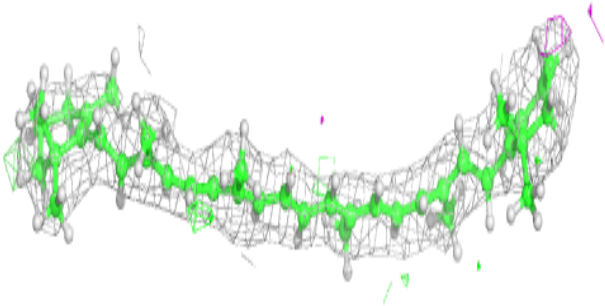
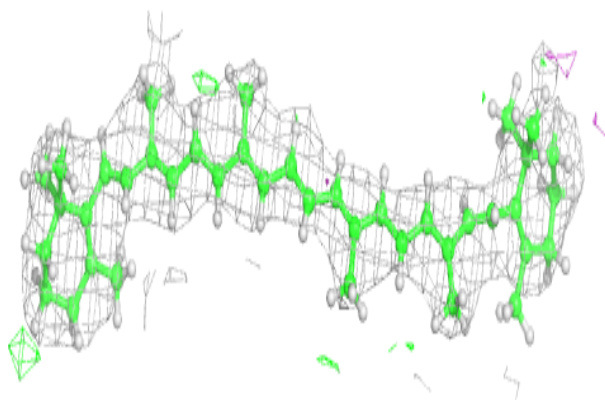


Electron density around CLA c 508:

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

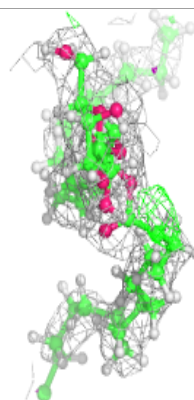
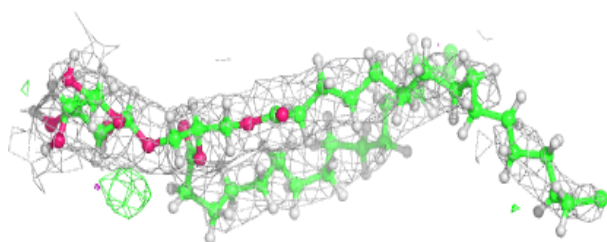
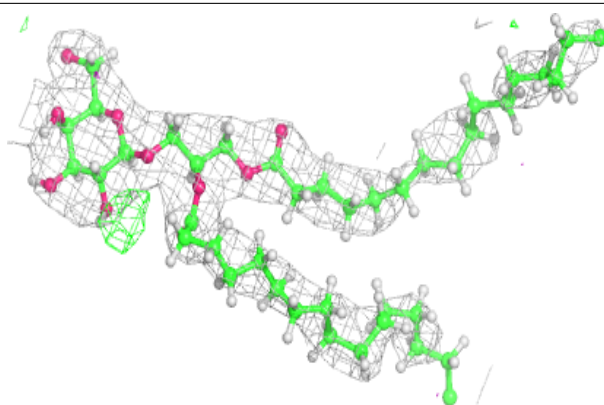
**Electron density around BCR d 405:**

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

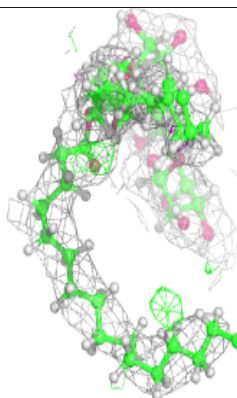
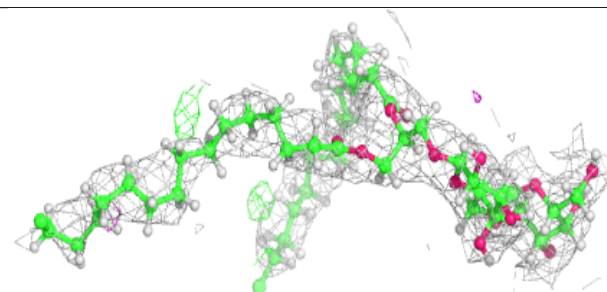
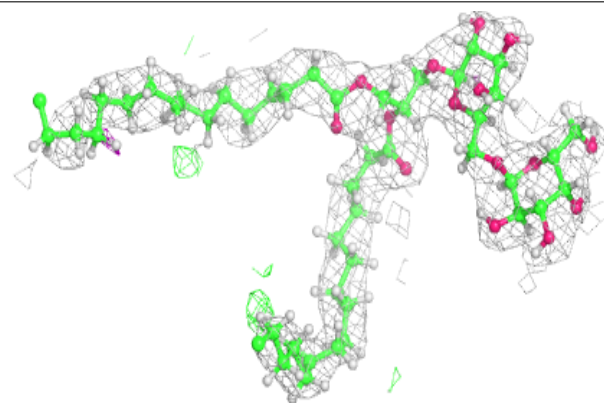


Electron density around LMG D 407:

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

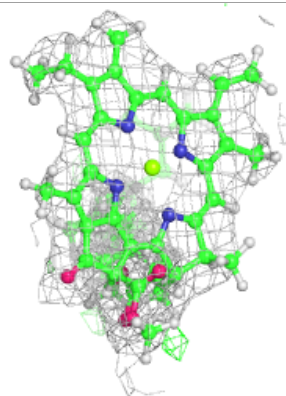
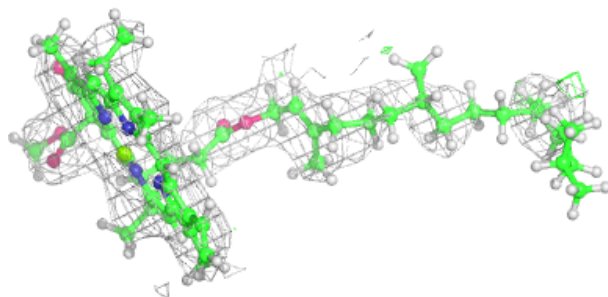
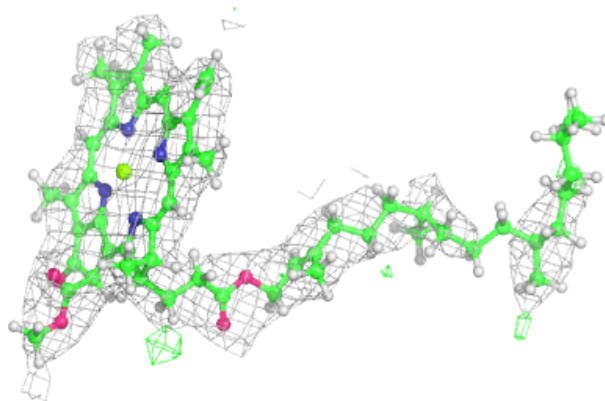
**Electron density around DGD c 517:**

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

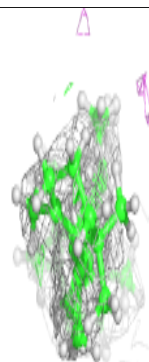
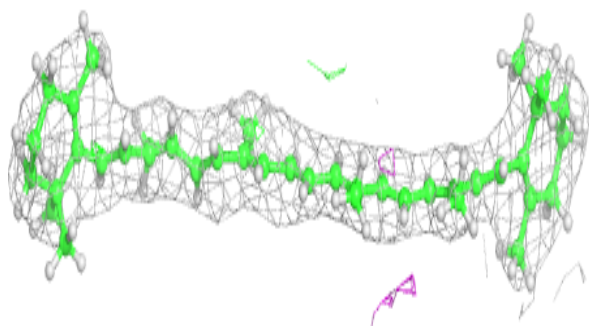
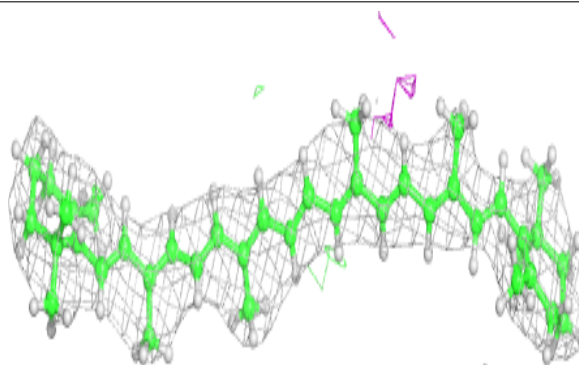


Electron density around CLA d 404:

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

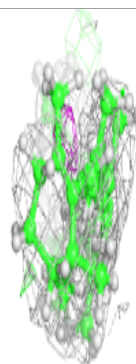
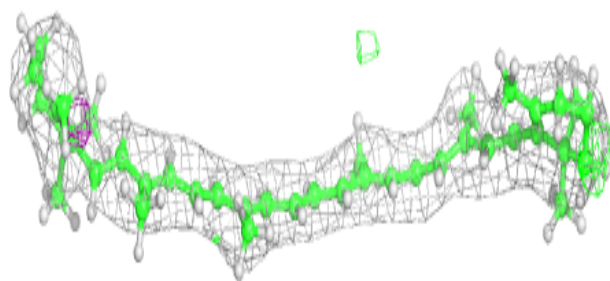
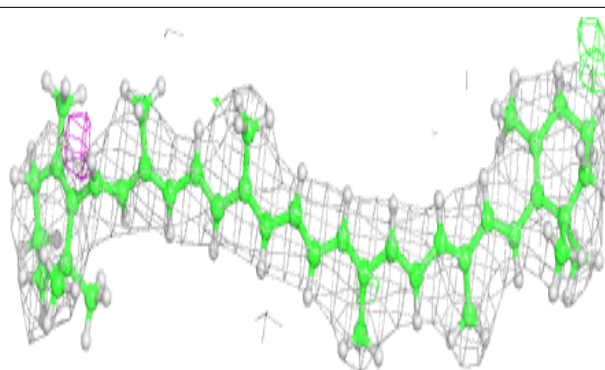
**Electron density around BCR C 515:**

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



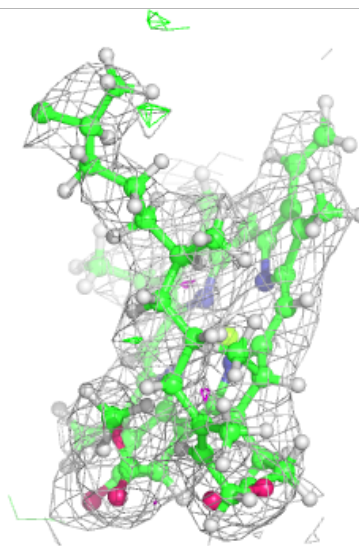
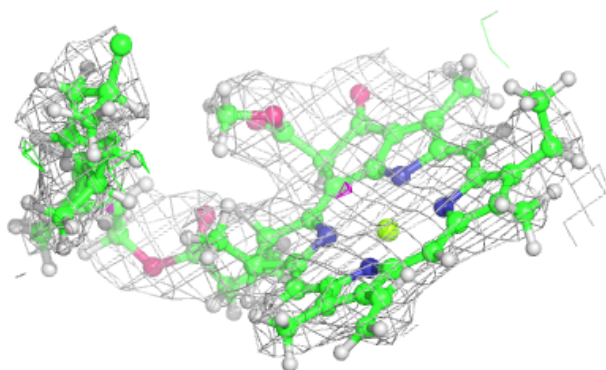
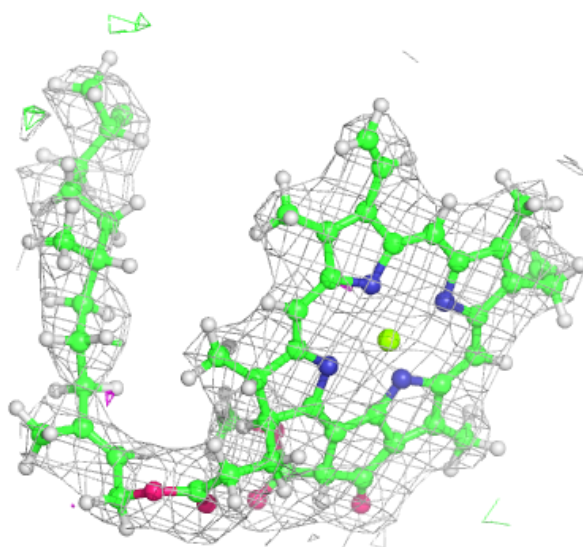
Electron density around BCR D 405:

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



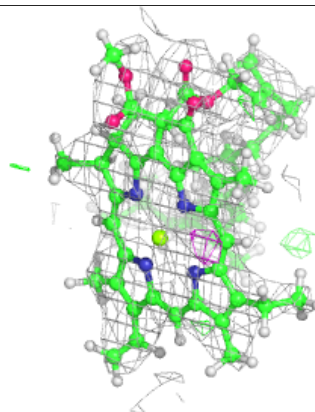
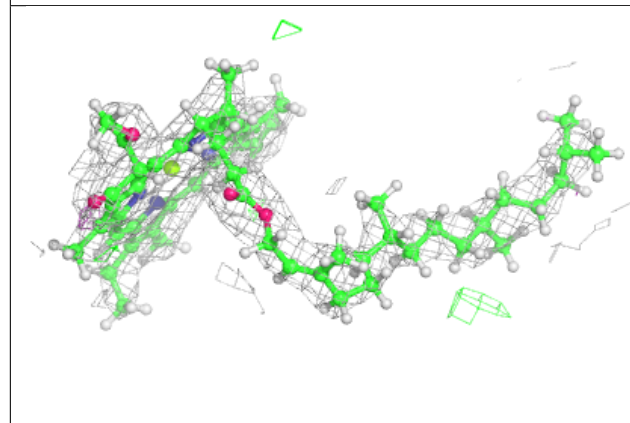
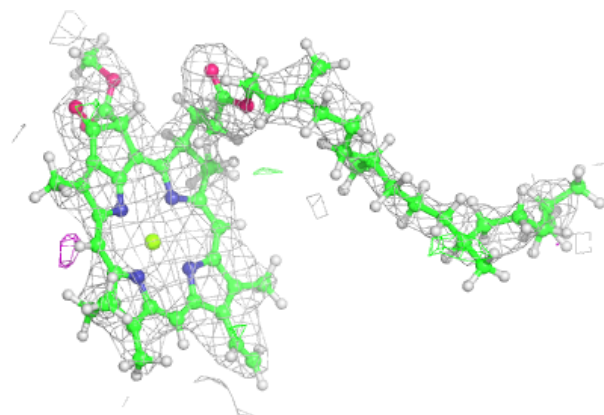
Electron density around CLA b 617:

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



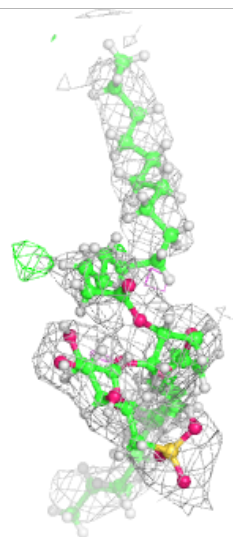
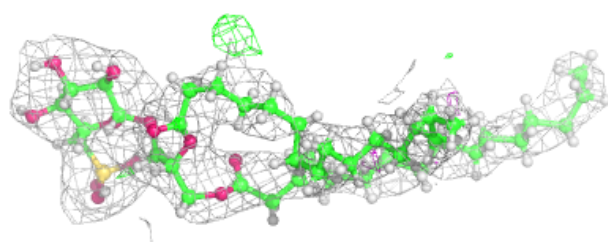
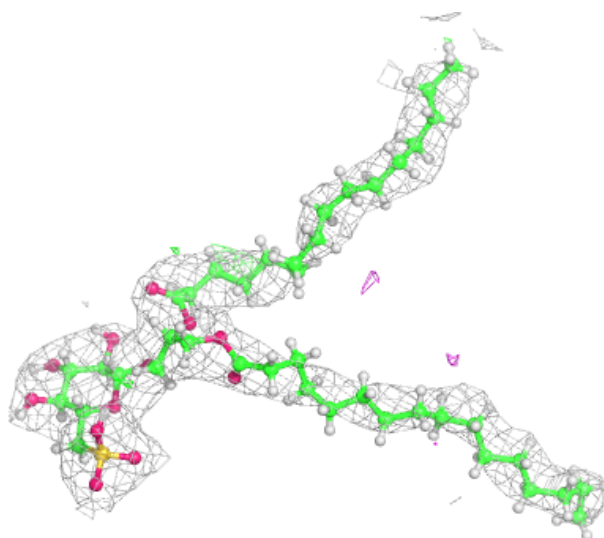
Electron density around CLA c 511:

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



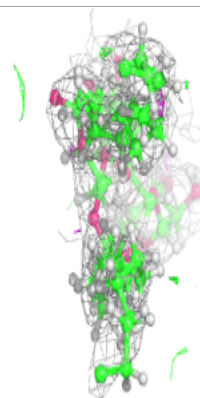
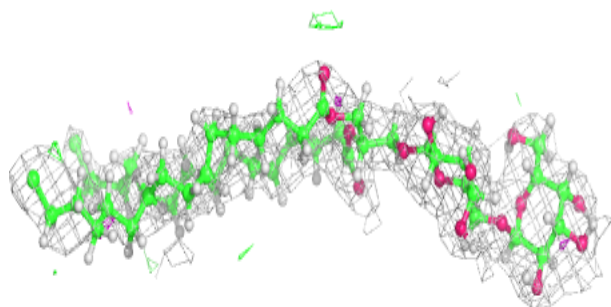
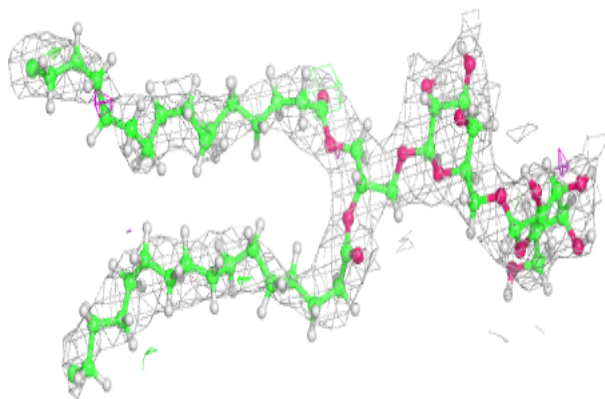
Electron density around SQD a 411:

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

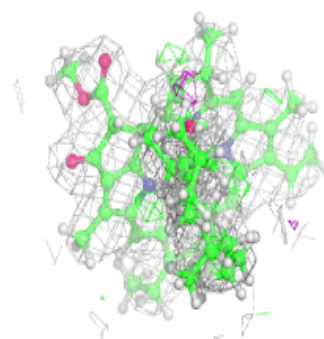
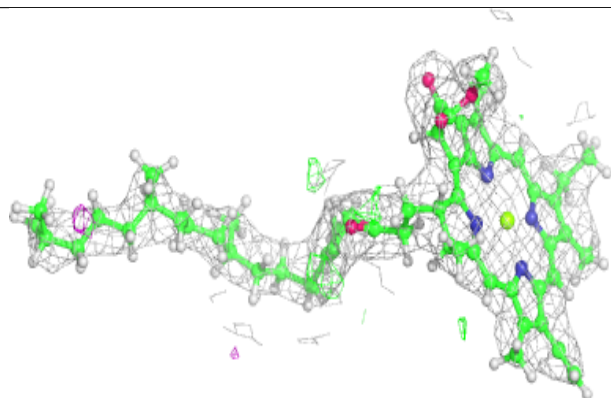
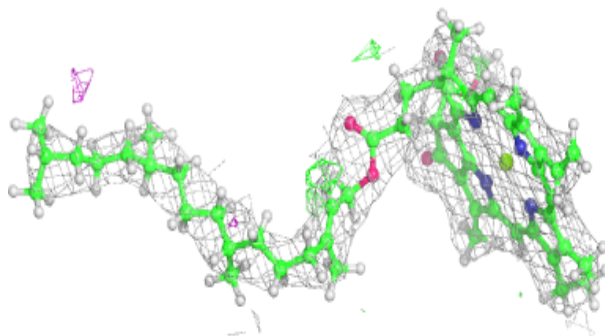


Electron density around DGD c 518:

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

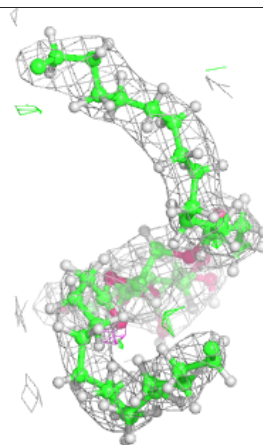
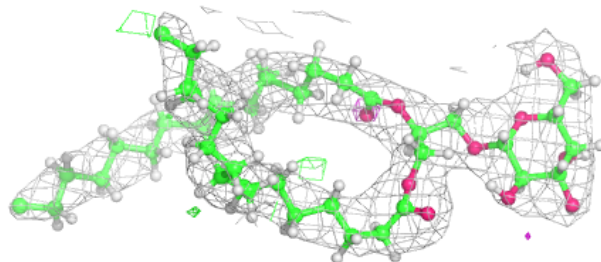
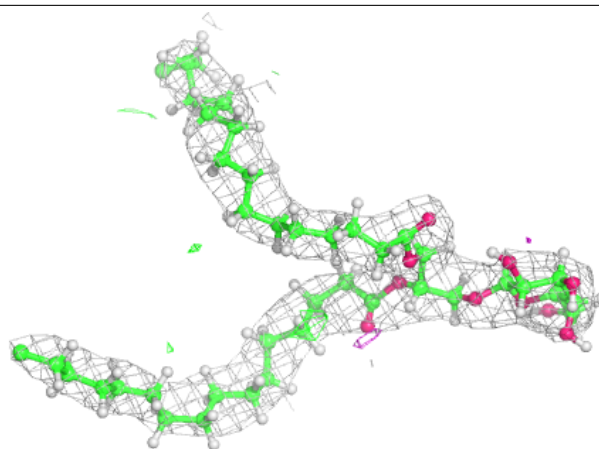
**Electron density around CLA c 502:**

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



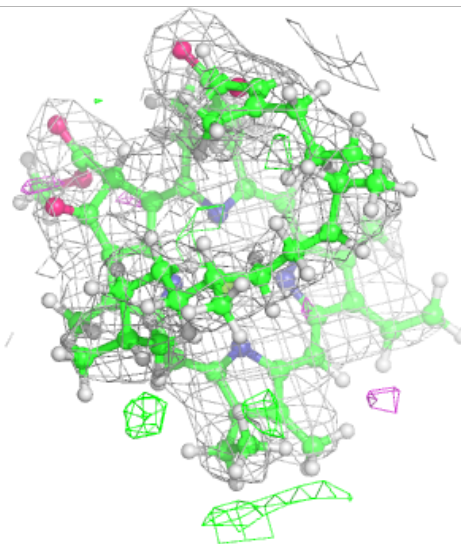
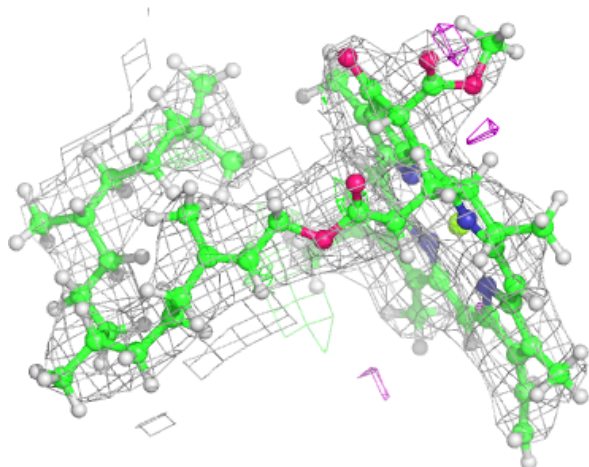
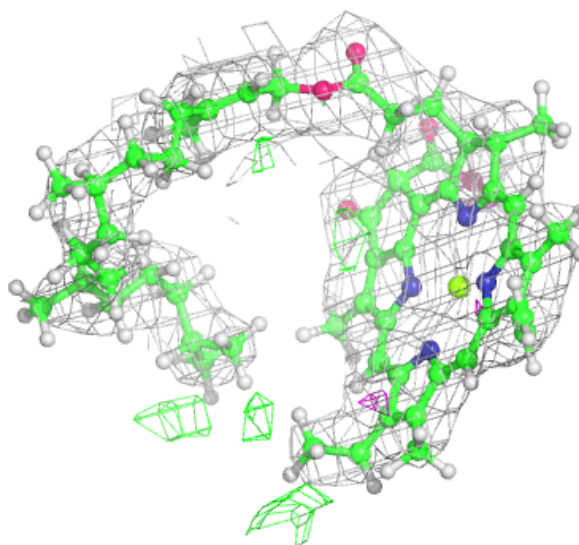
Electron density around LMG M 101:

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



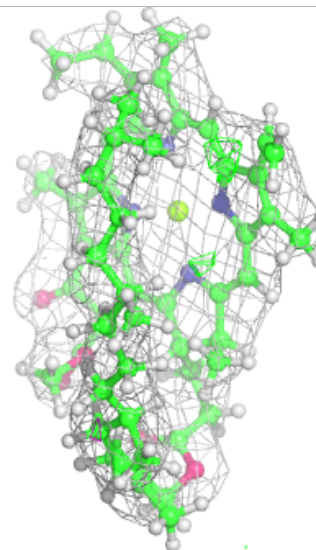
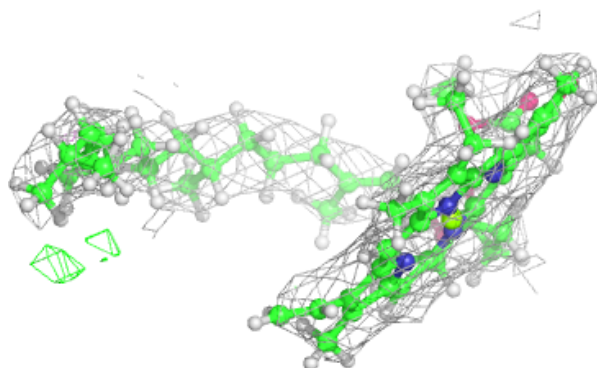
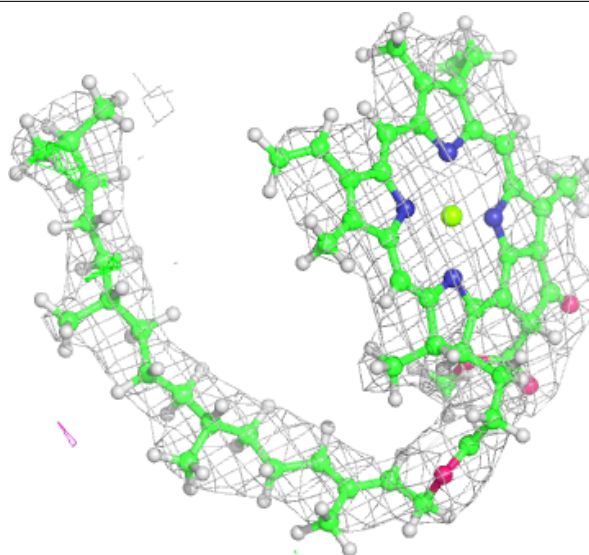
Electron density around CLA c 503:

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



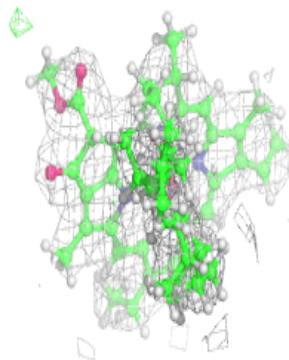
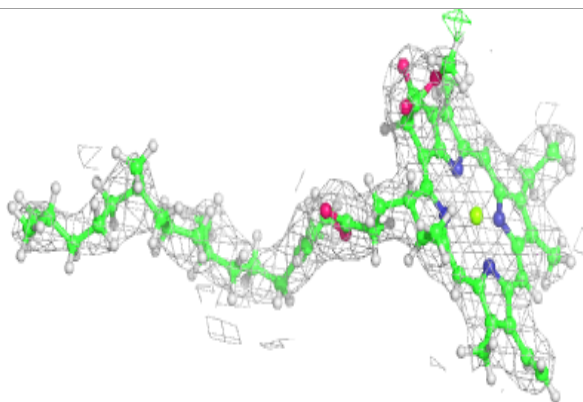
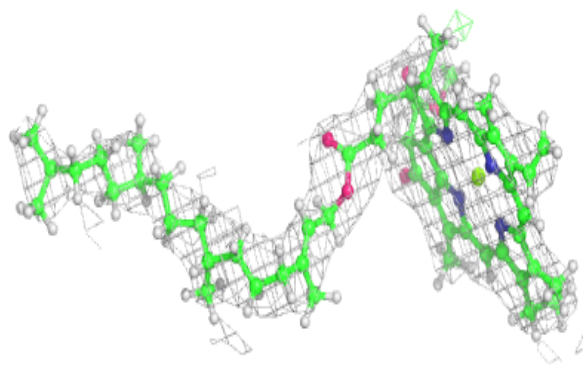
Electron density around CLA c 507:

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

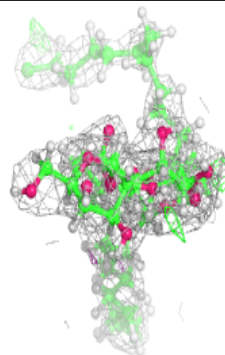
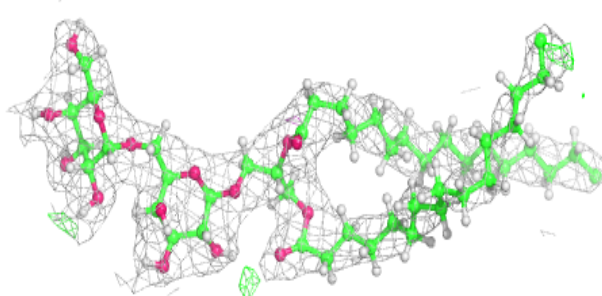
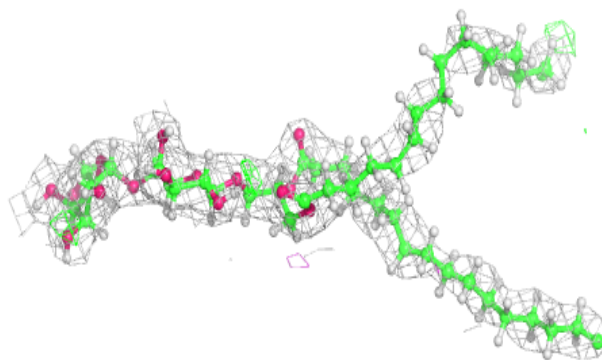


Electron density around CLA C 503:

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

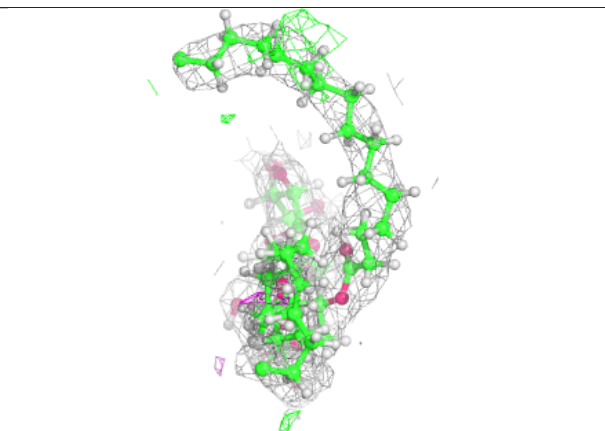
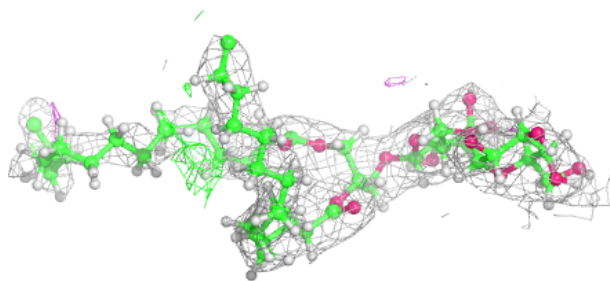
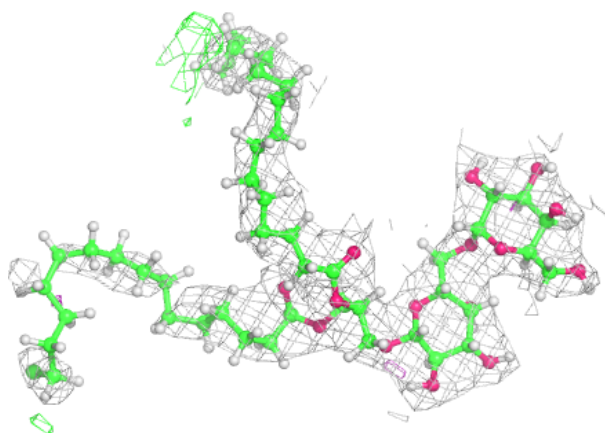
**Electron density around DGD C 516:**

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

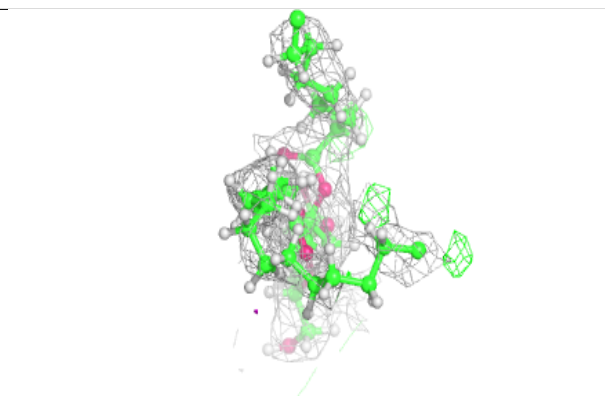
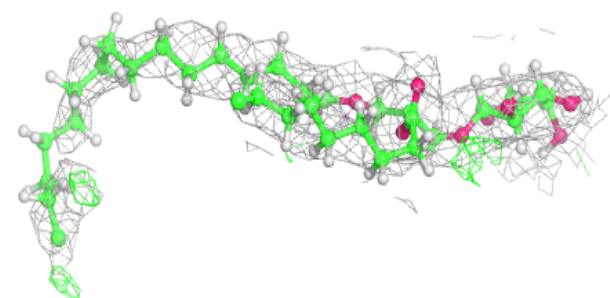
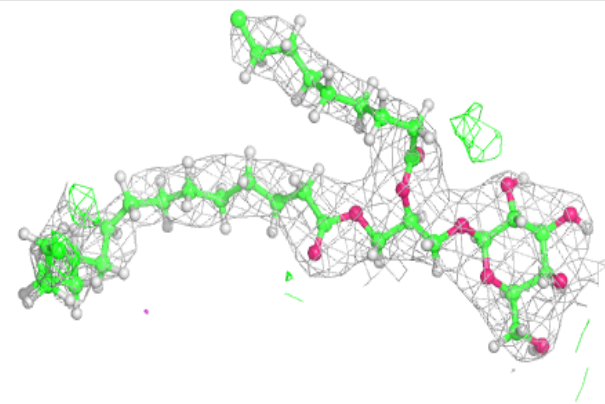


Electron density around DGD C 517:

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

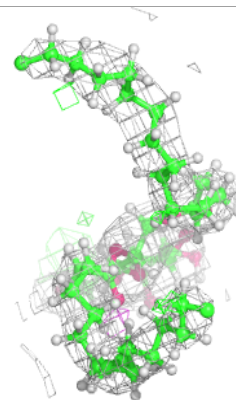
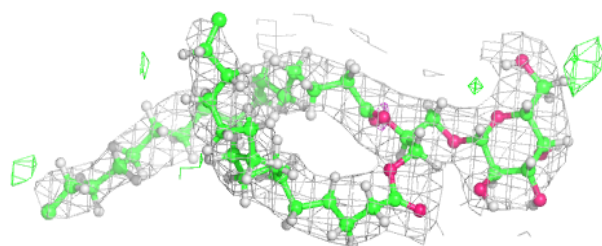
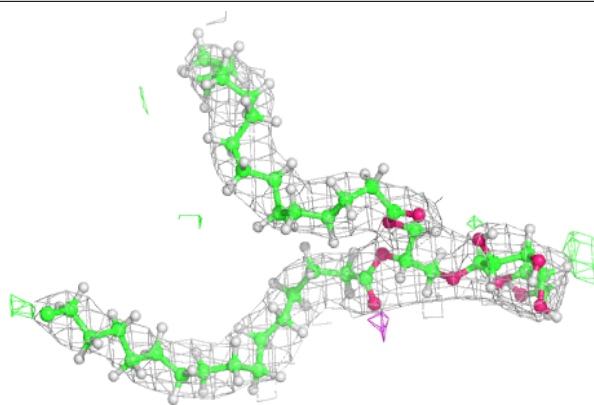
**Electron density around LMG d 411:**

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

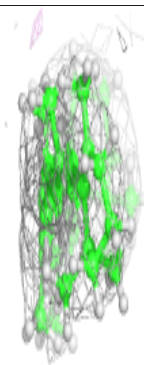
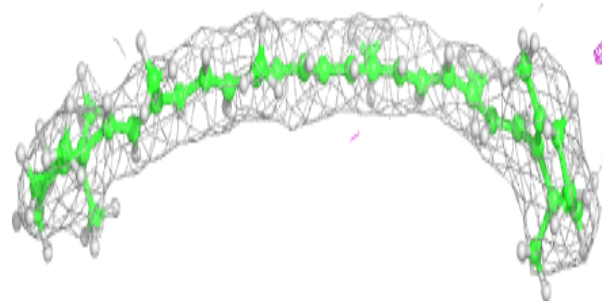
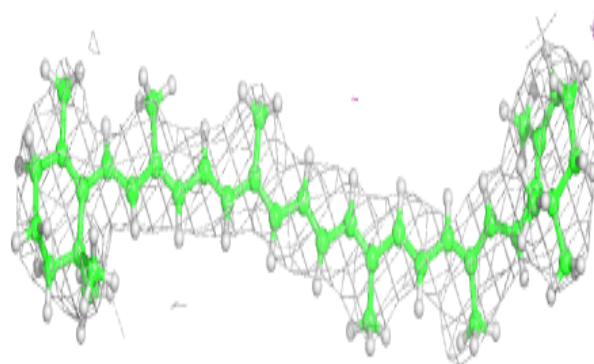


Electron density around LMG m 101:

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

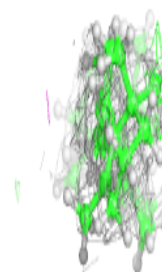
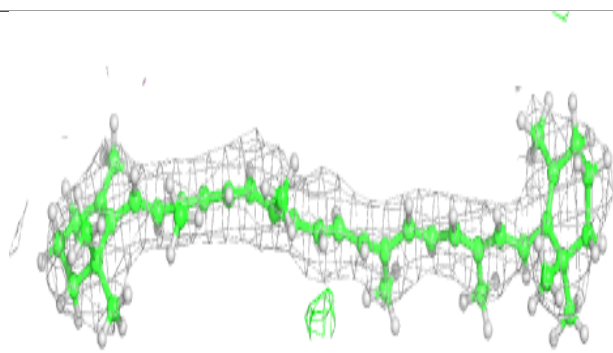
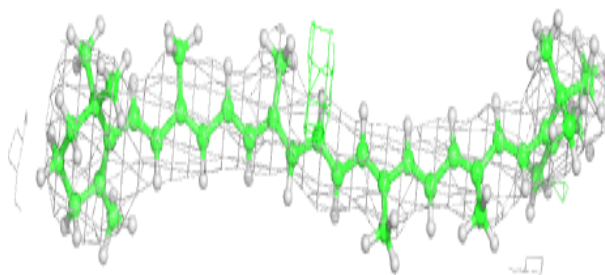
**Electron density around BCR T 101:**

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

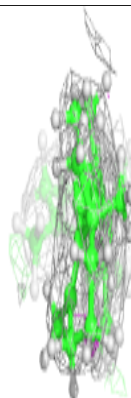
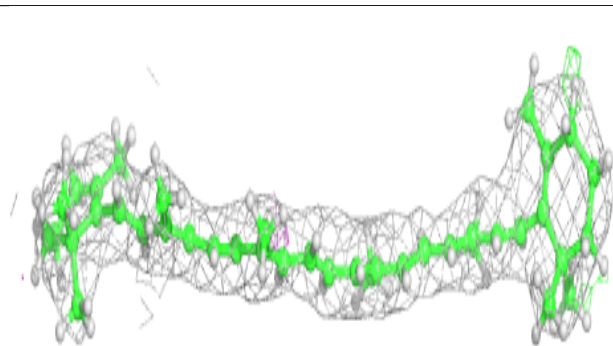
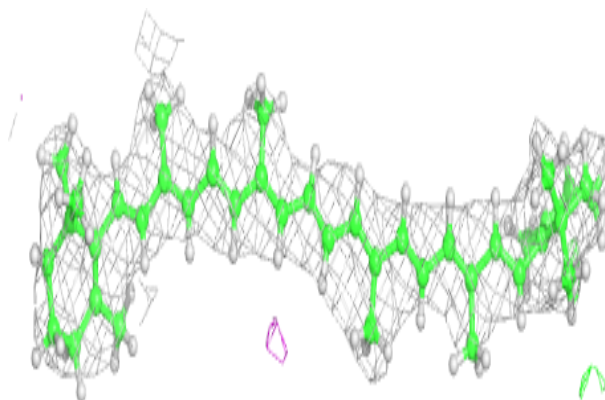


Electron density around BCR Z 101:

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

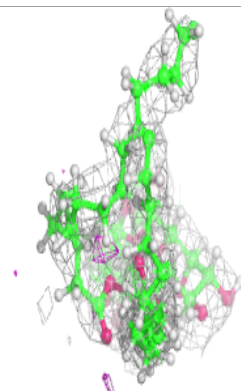
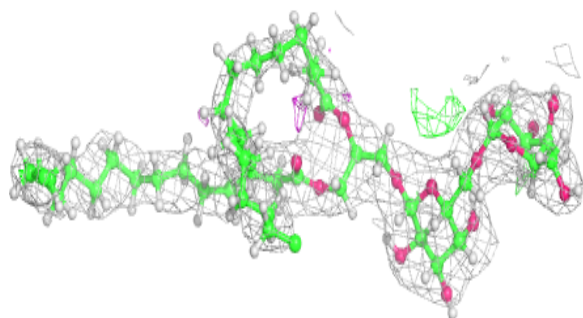
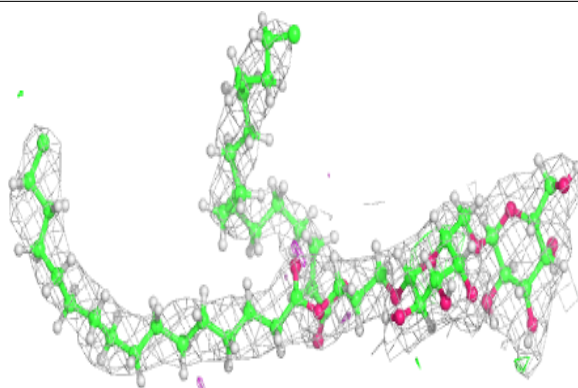
**Electron density around BCR b 618:**

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

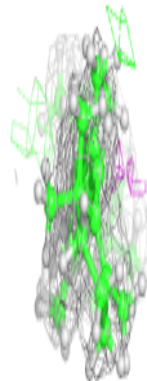
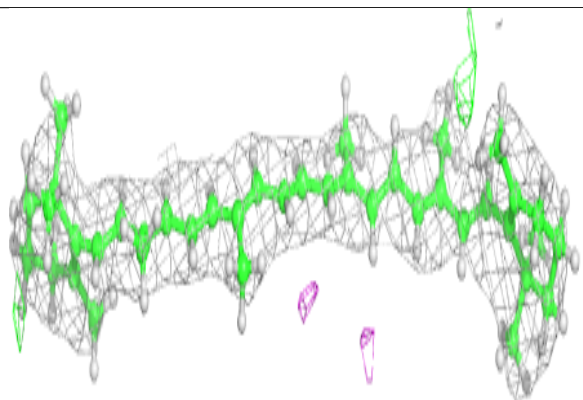
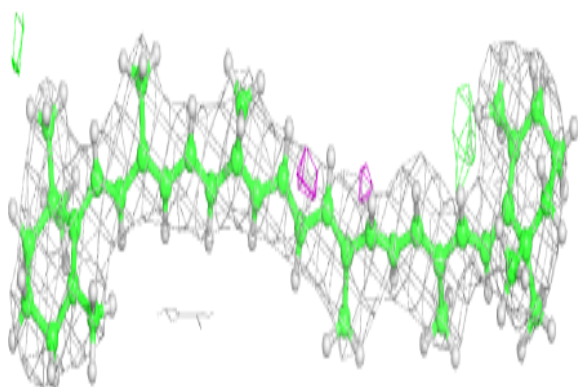


Electron density around DGD h 101:

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

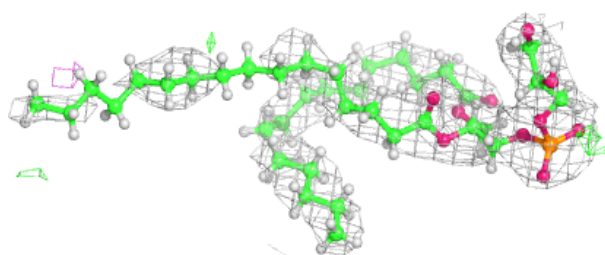
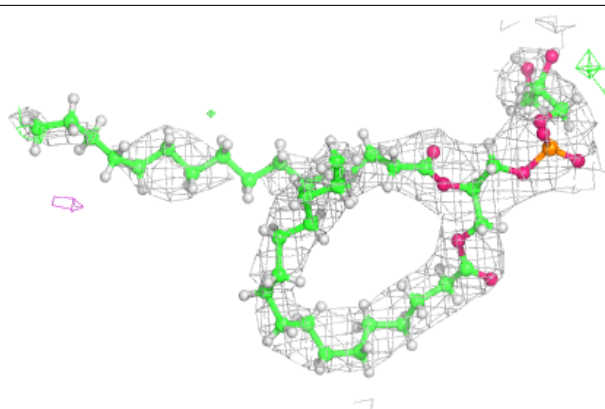
**Electron density around BCR b 620:**

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

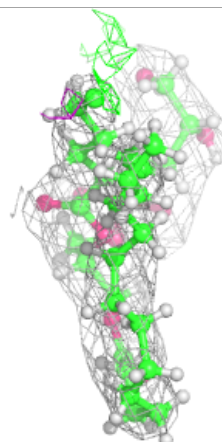
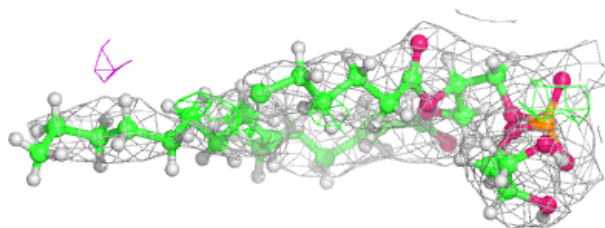
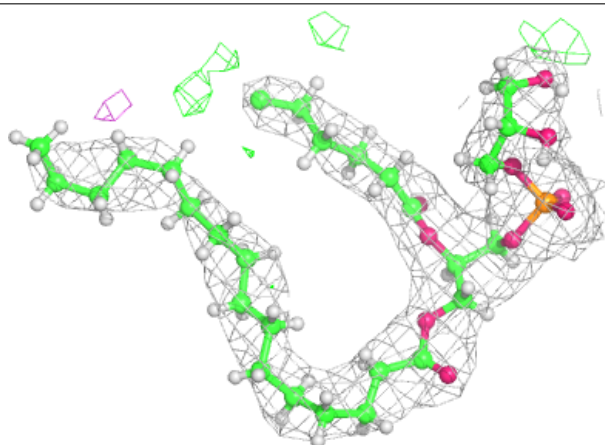


Electron density around LHG d 407:

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

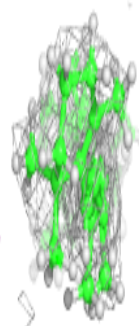
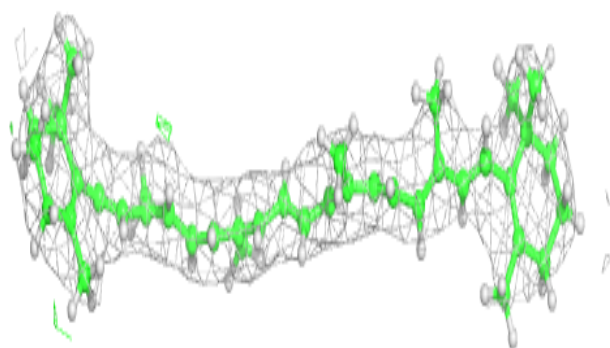
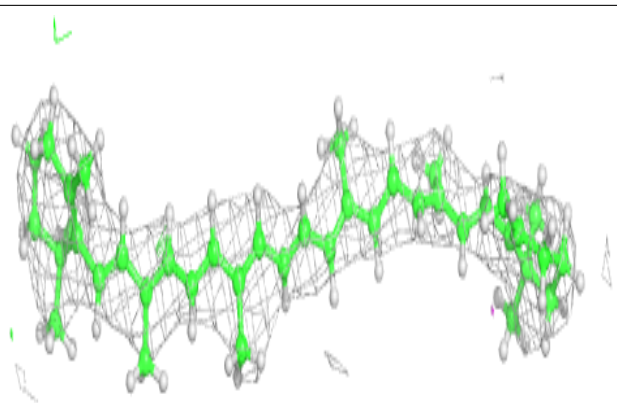
**Electron density around LHG d 409:**

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

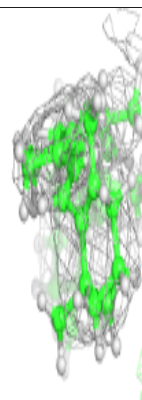
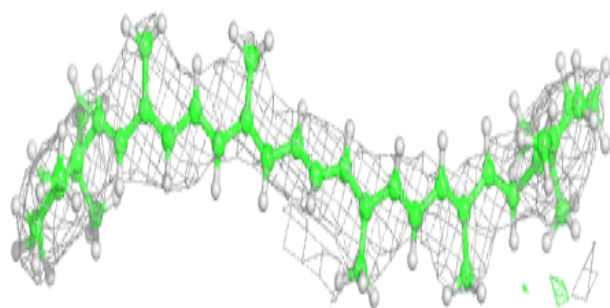
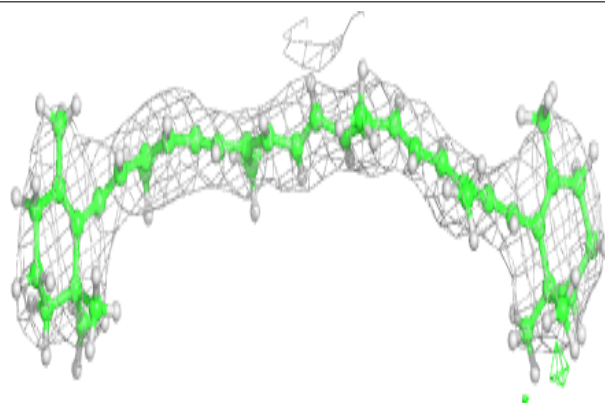


Electron density around BCR c 514:

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

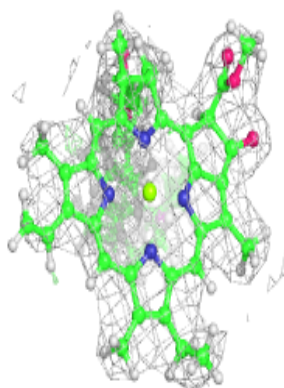
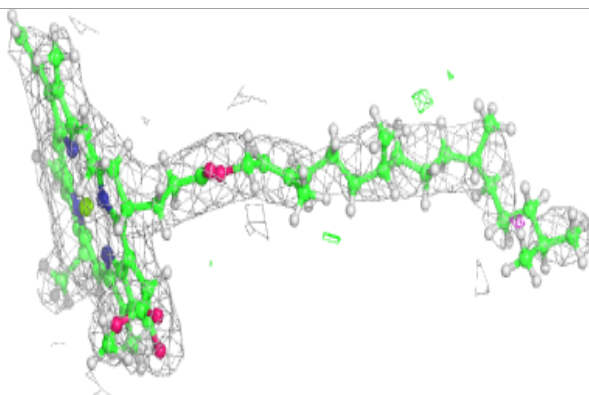
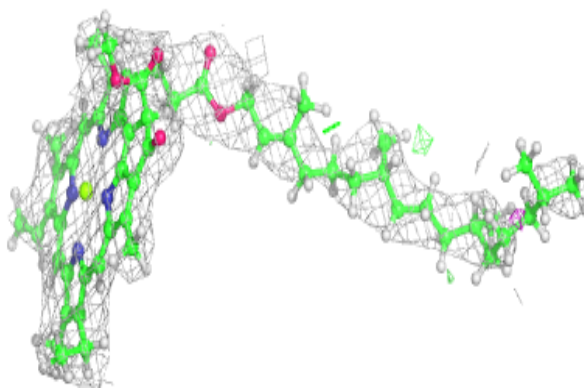
**Electron density around BCR c 521:**

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

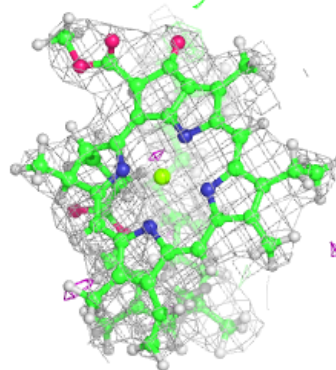
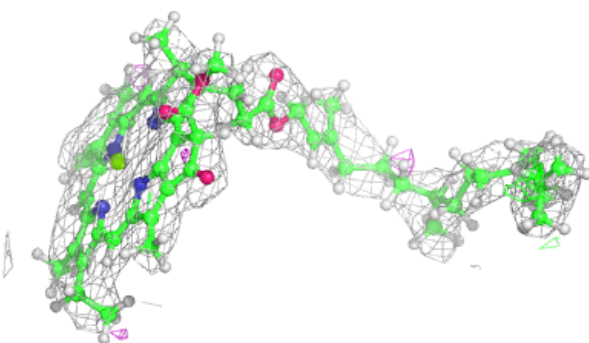
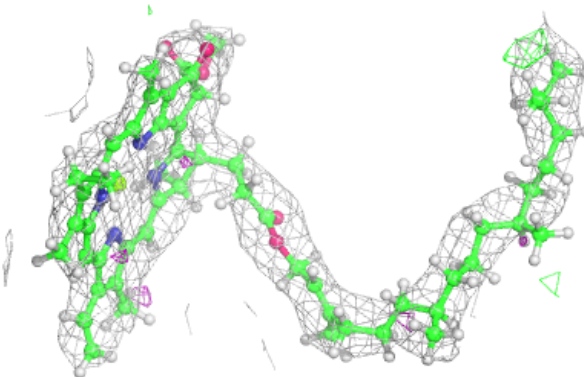


Electron density around CLA b 605:

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

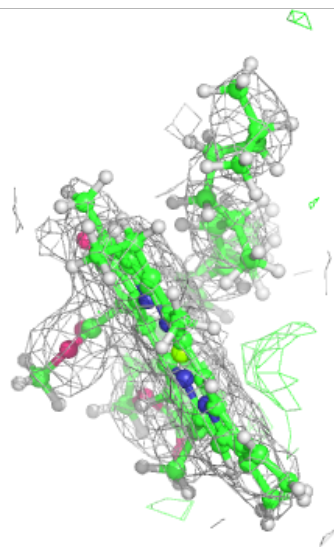
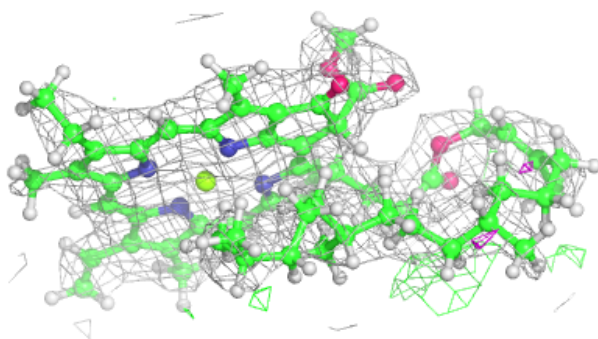
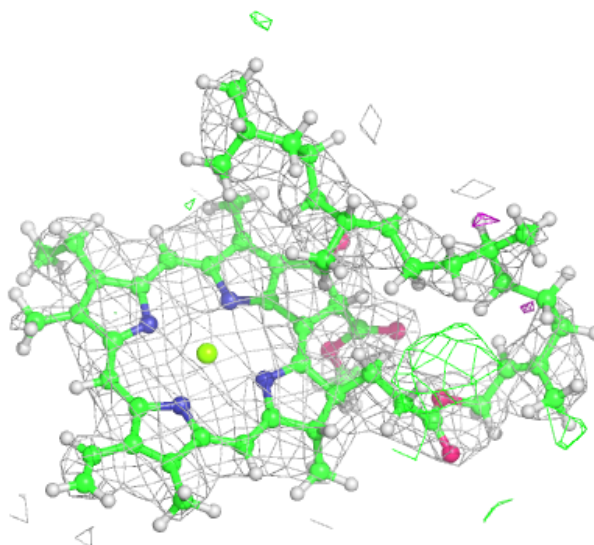
**Electron density around CLA b 607:**

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



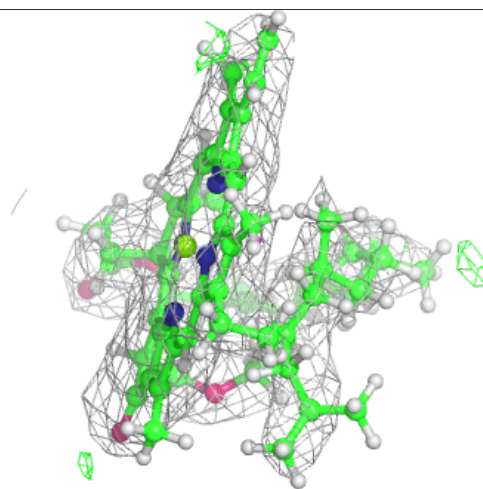
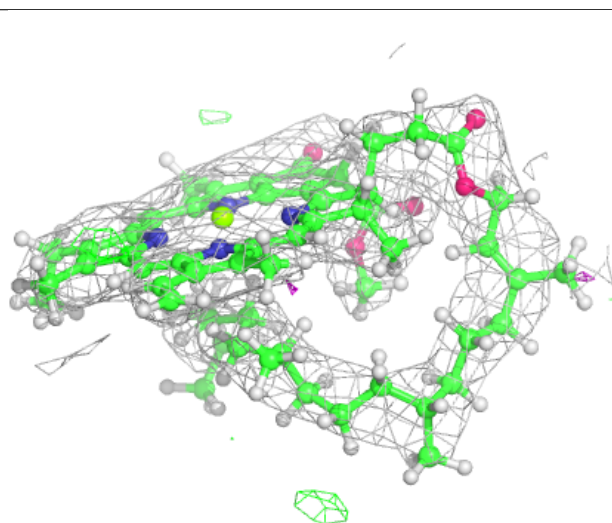
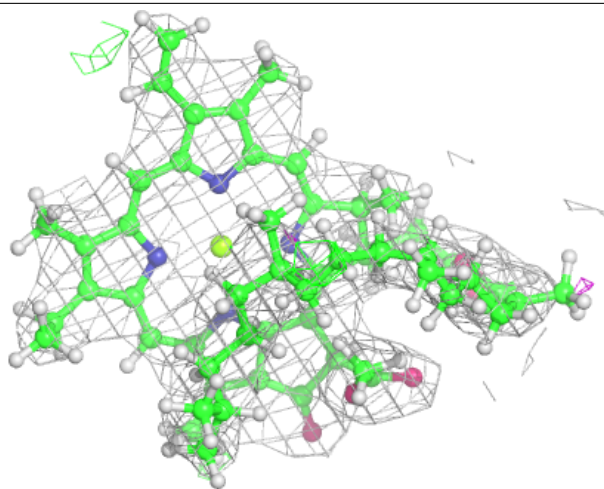
Electron density around CLA c 509:

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



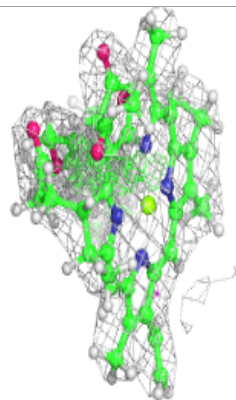
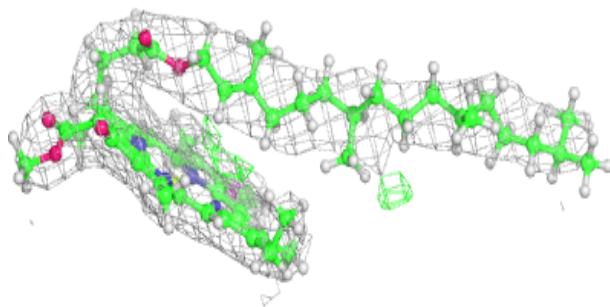
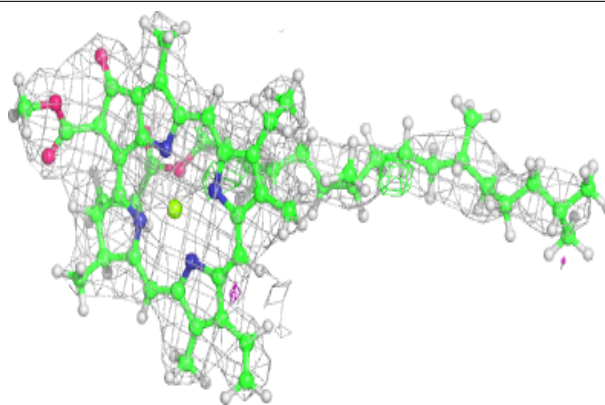
Electron density around CLA c 510:

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



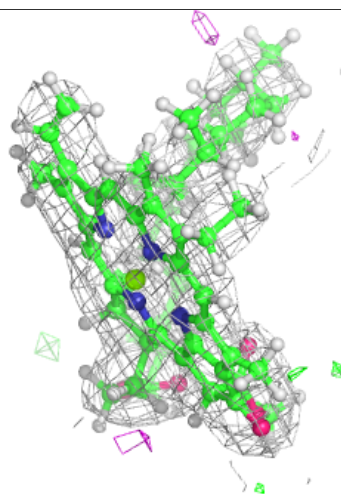
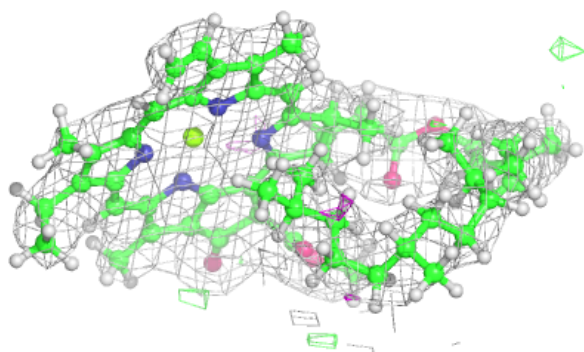
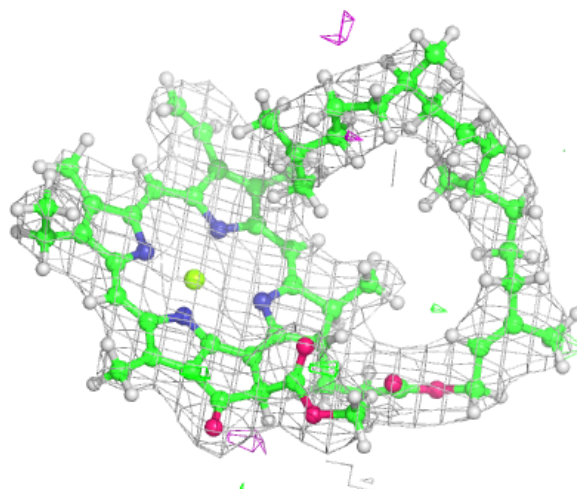
Electron density around CLA b 615:

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



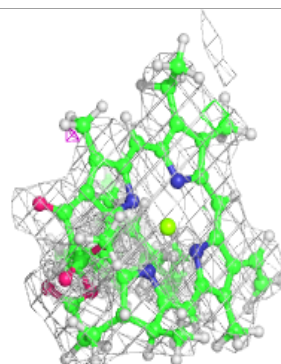
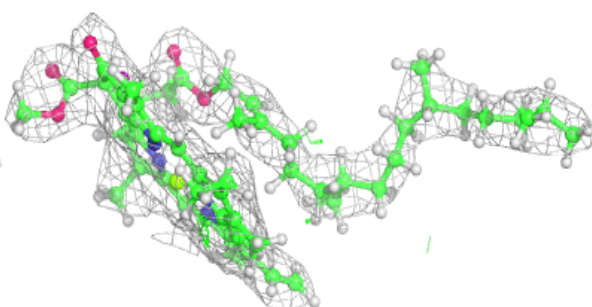
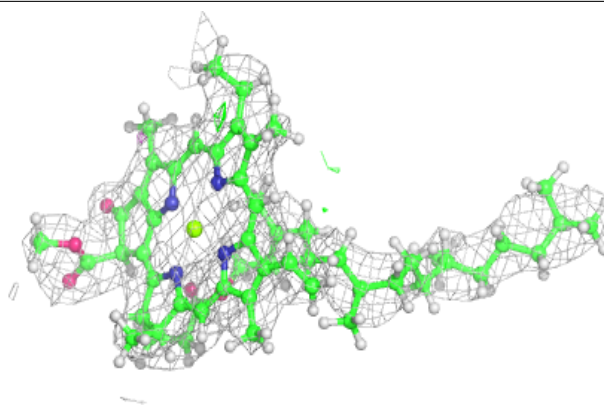
Electron density around CLA b 616:

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

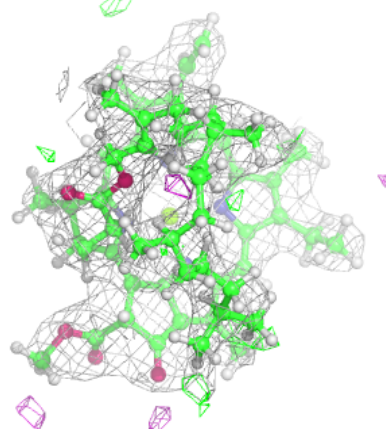
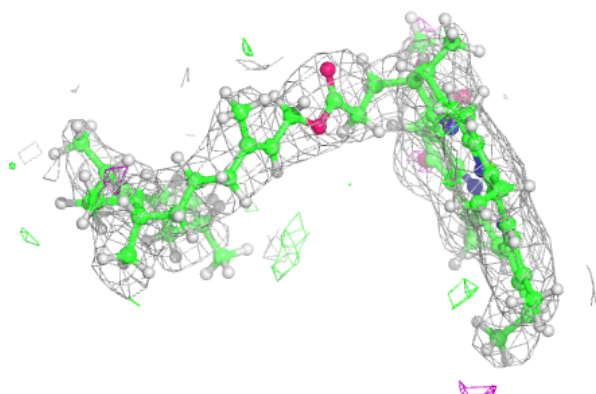
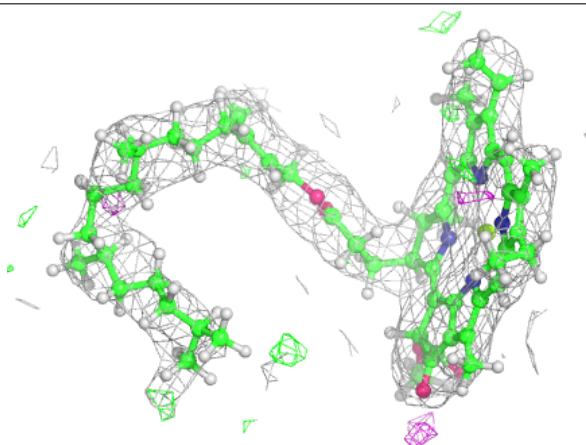


Electron density around CLA C 506:

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

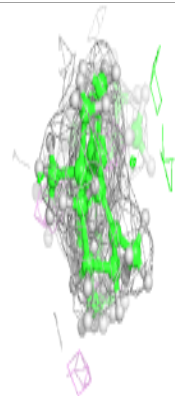
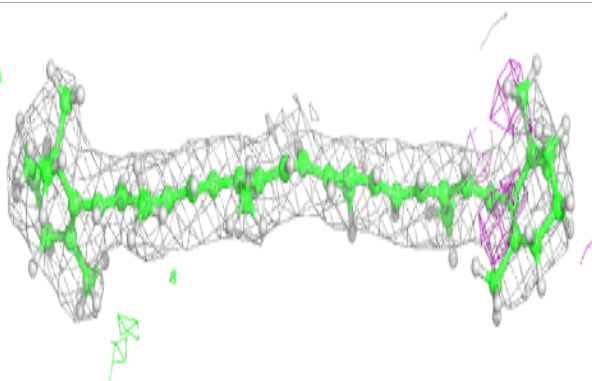
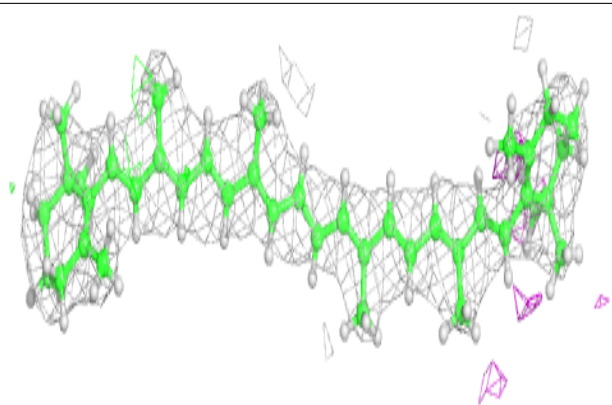
**Electron density around CLA B 606:**

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

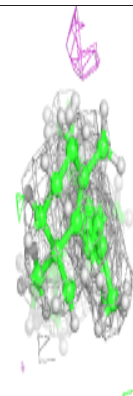
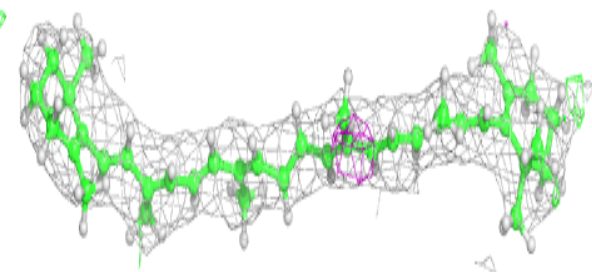
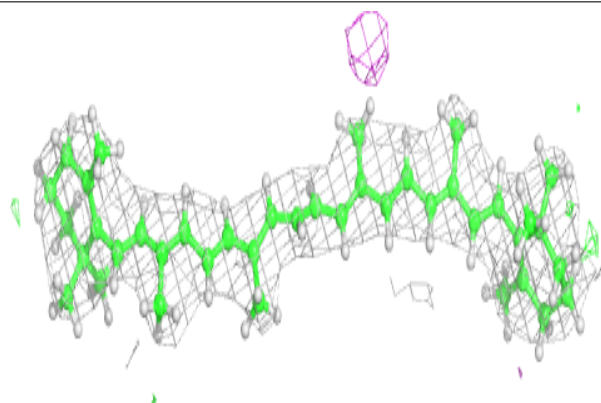


Electron density around BCR B 618:

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

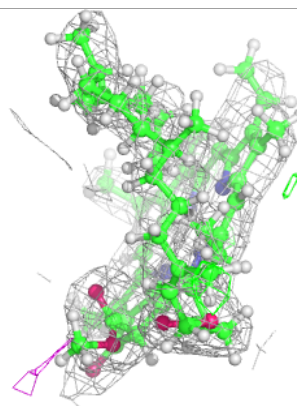
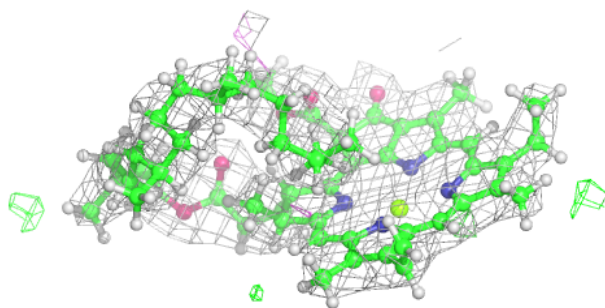
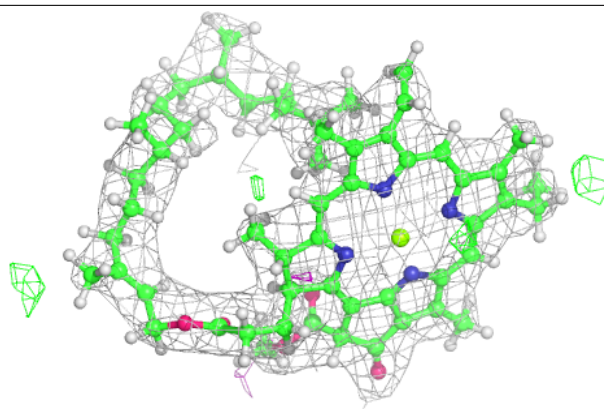
**Electron density around BCR B 619:**

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

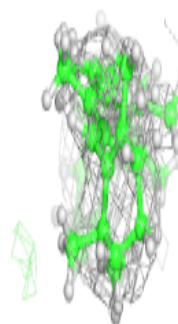
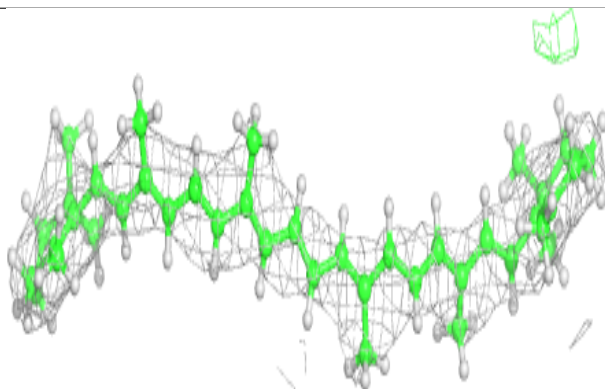
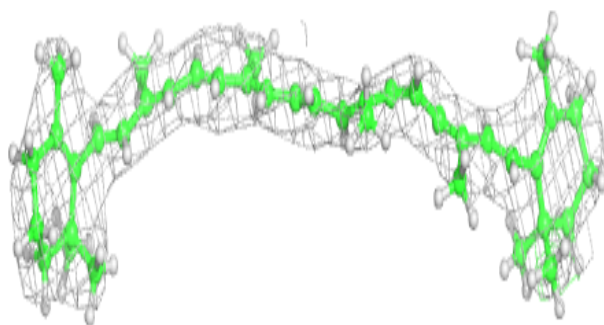


Electron density around CLA B 615:

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

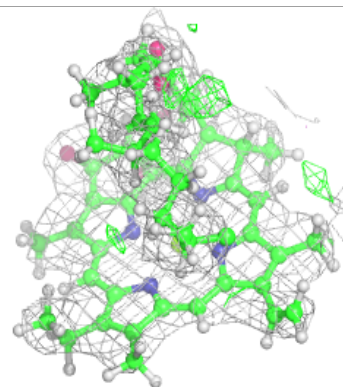
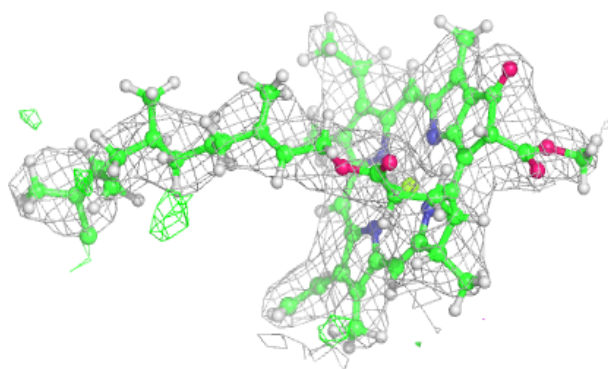
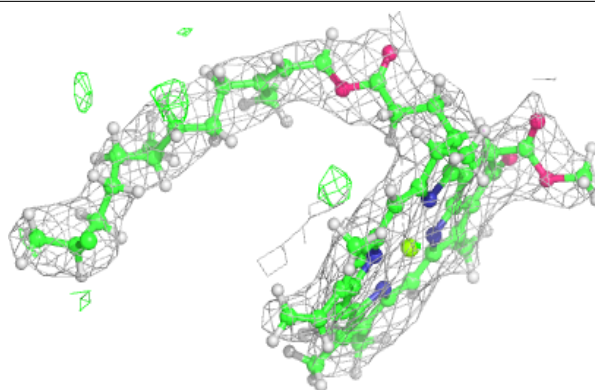
**Electron density around BCR C 520:**

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

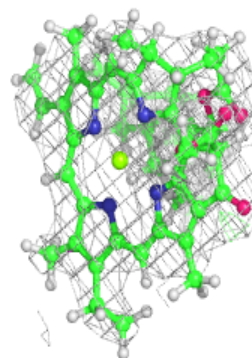
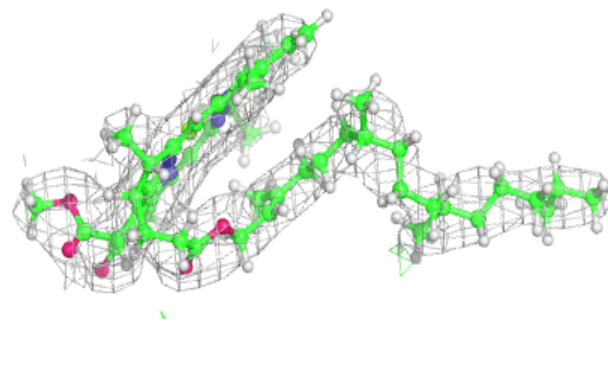
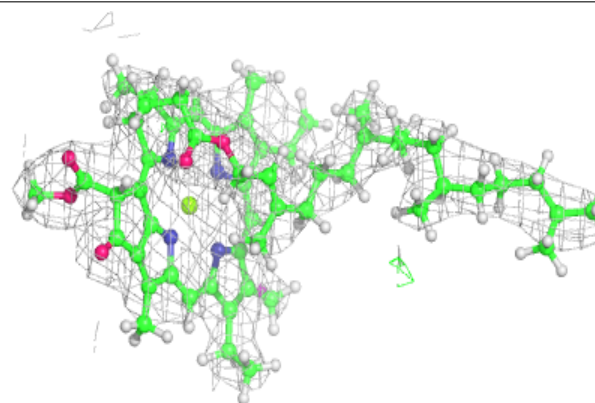


Electron density around CLA c 504:

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

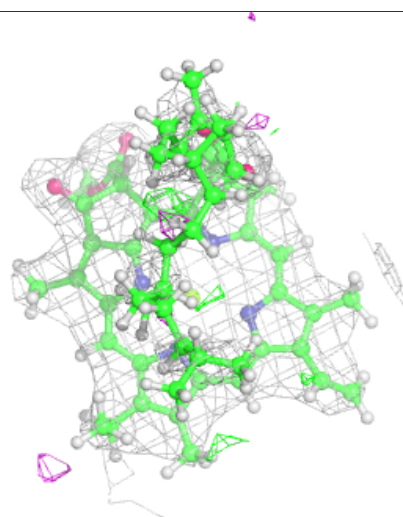
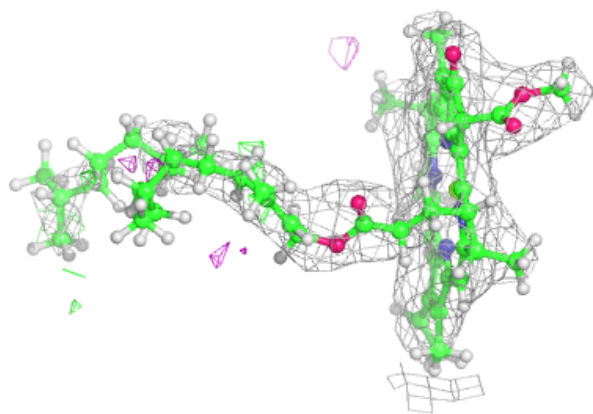
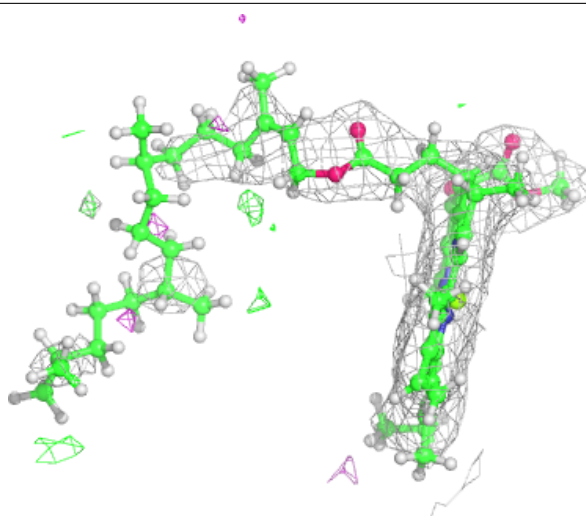
**Electron density around CLA c 505:**

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



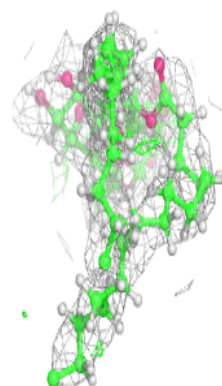
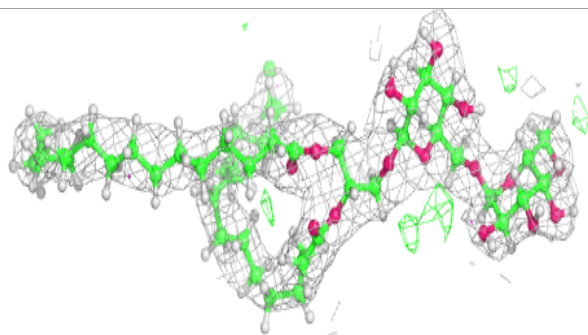
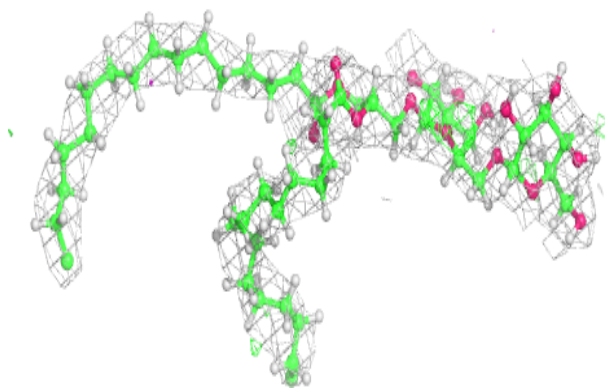
Electron density around CLA c 506:

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

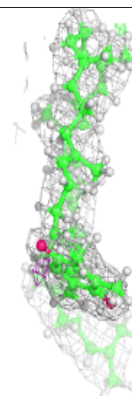
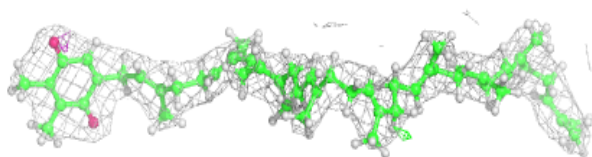
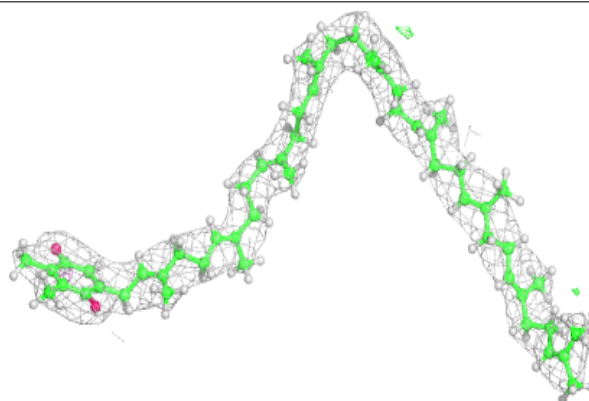


Electron density around DGD H 102:

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

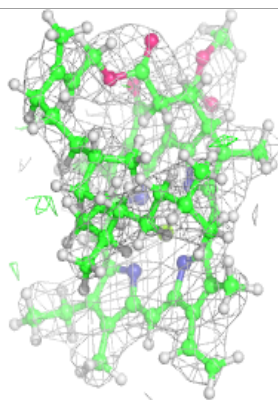
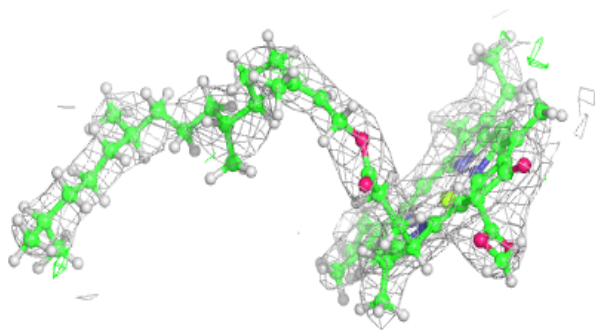
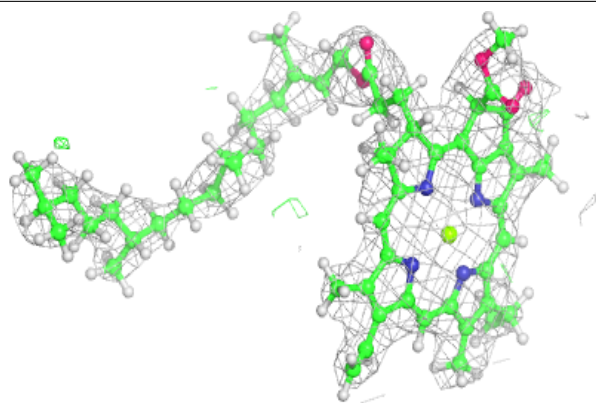
**Electron density around PL9 D 406:**

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

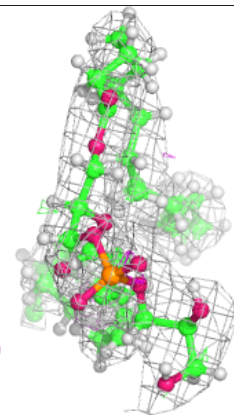
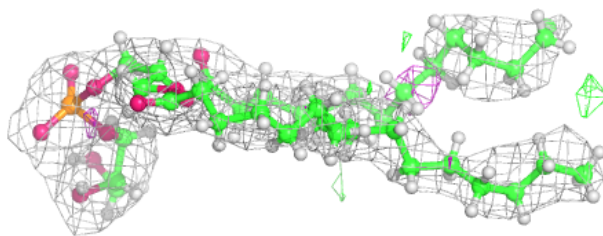
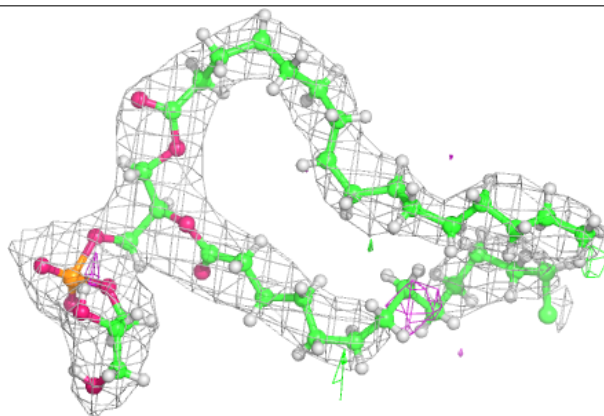


Electron density around CLA C 512:

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

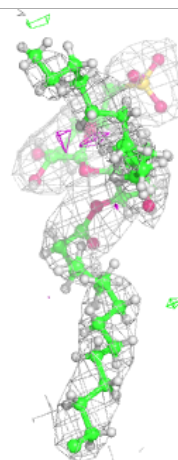
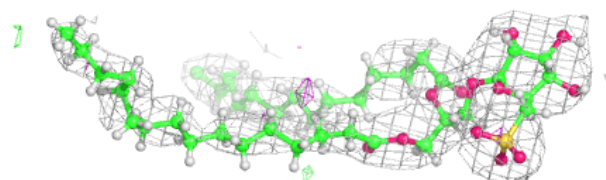
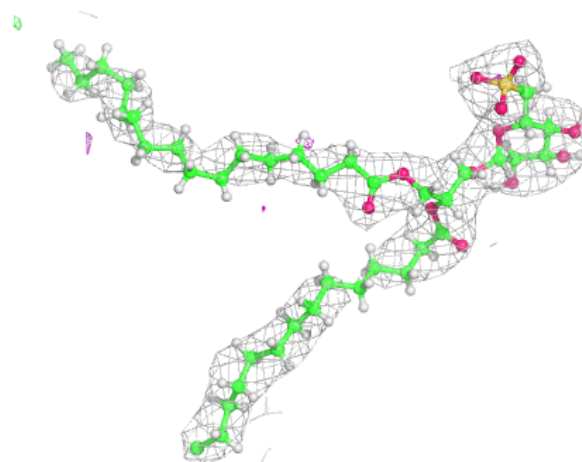
**Electron density around LHG D 409:**

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



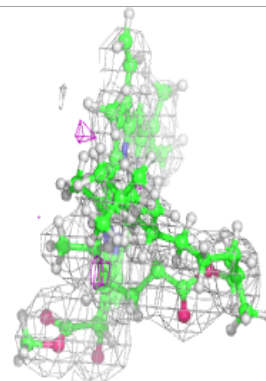
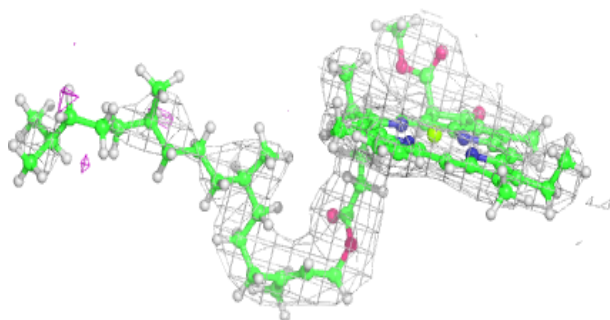
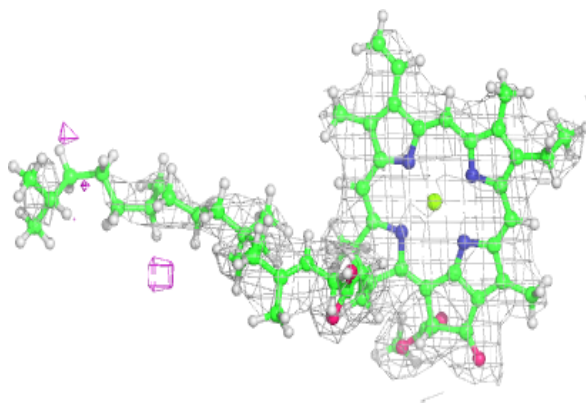
Electron density around SQD A 410:

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

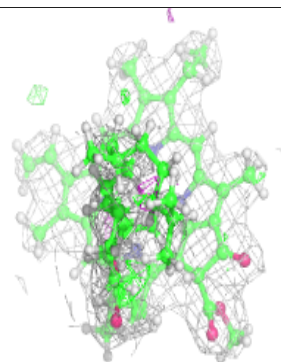
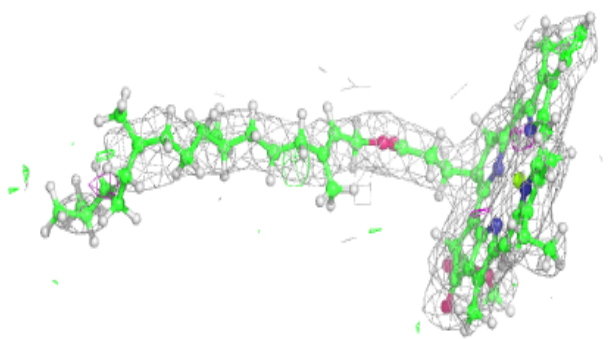
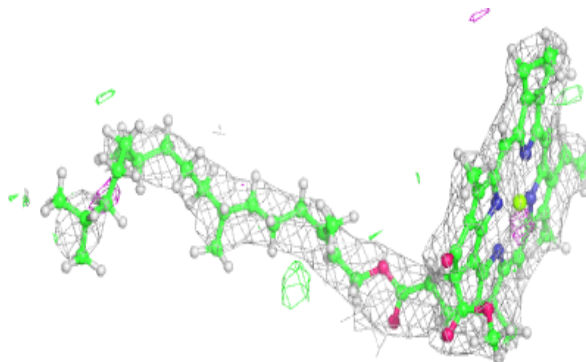


Electron density around CLA A 405:

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

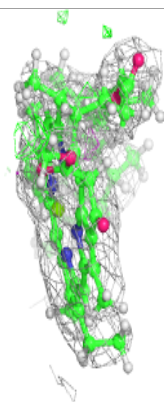
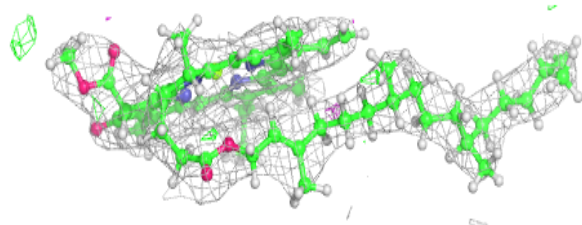
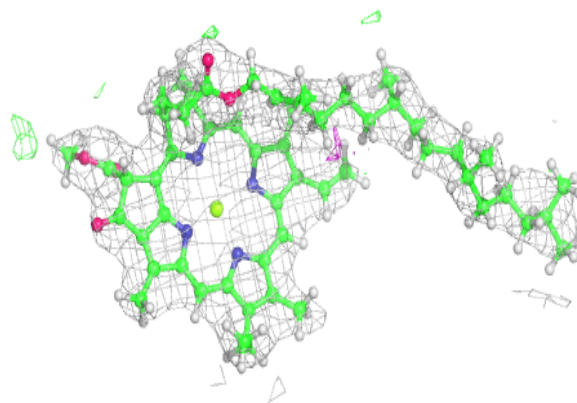
**Electron density around CLA B 604:**

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



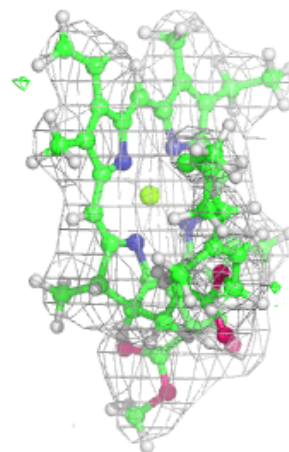
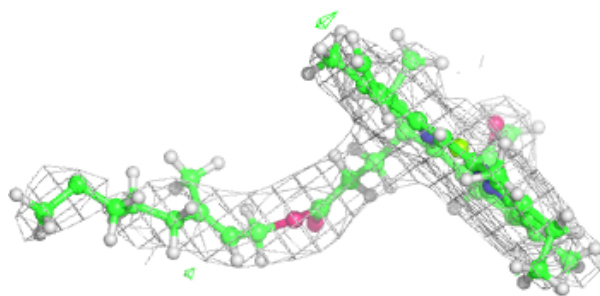
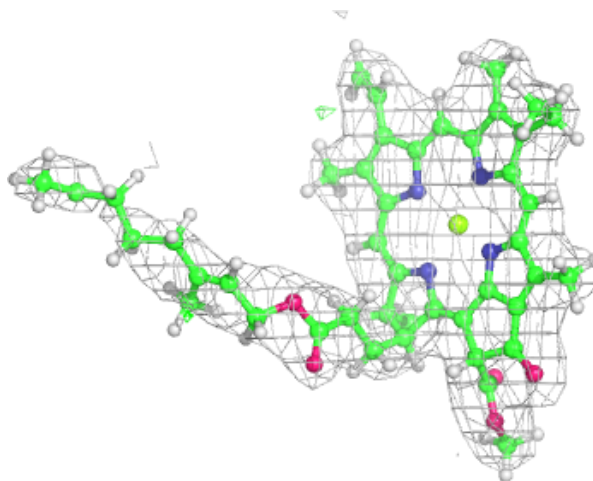
Electron density around CLA c 501:

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



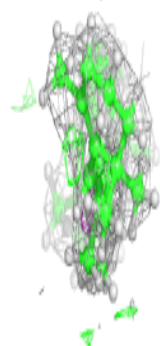
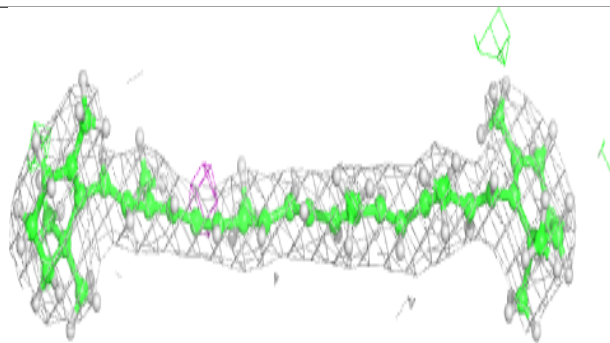
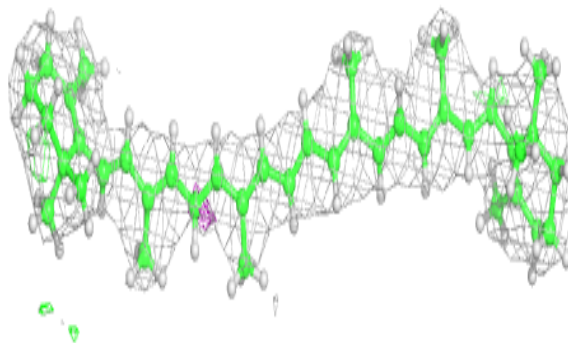
Electron density around CLA A 407:

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

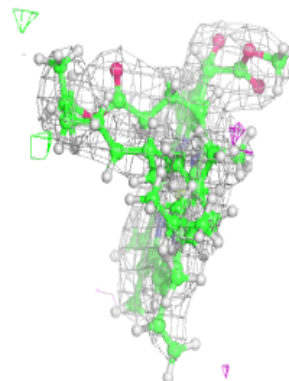
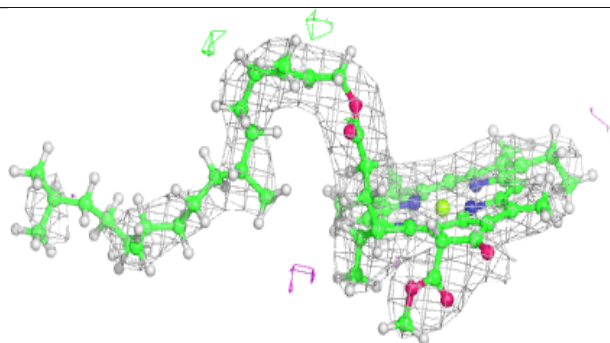
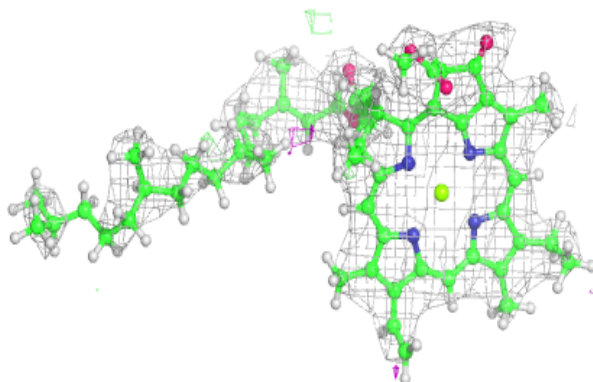


Electron density around BCR b 619:

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

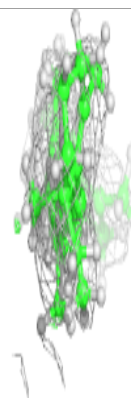
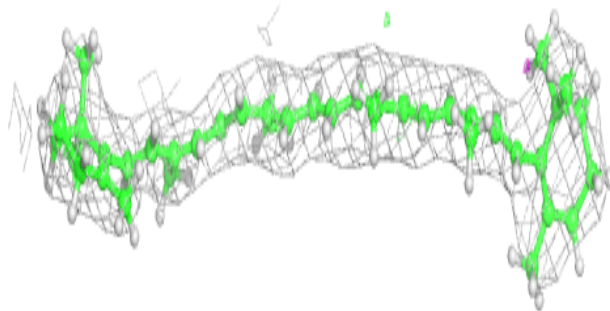
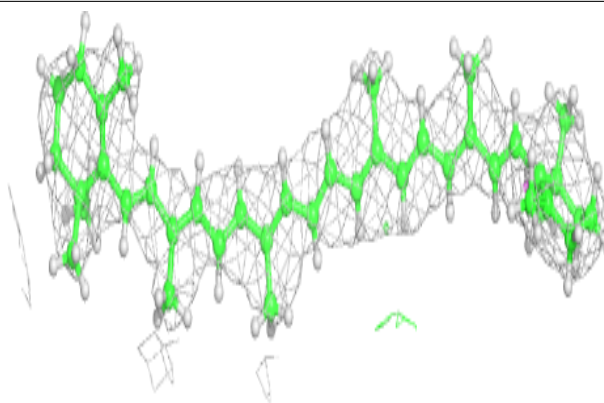
**Electron density around CLA a 406:**

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

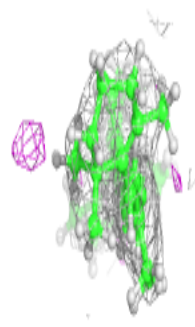
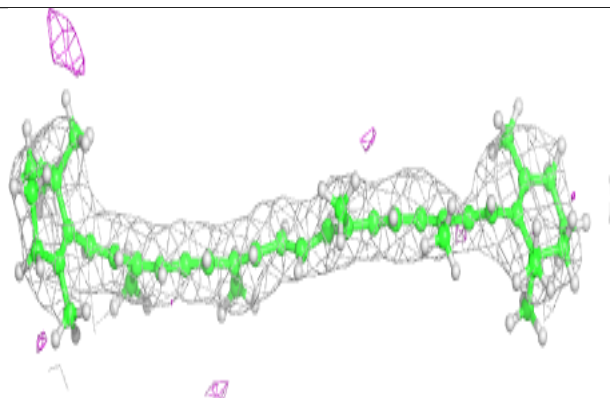
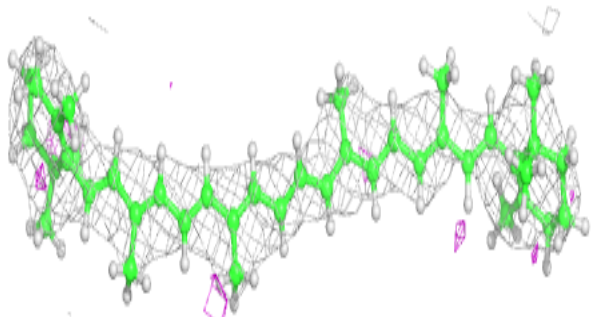


Electron density around BCR B 617:

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

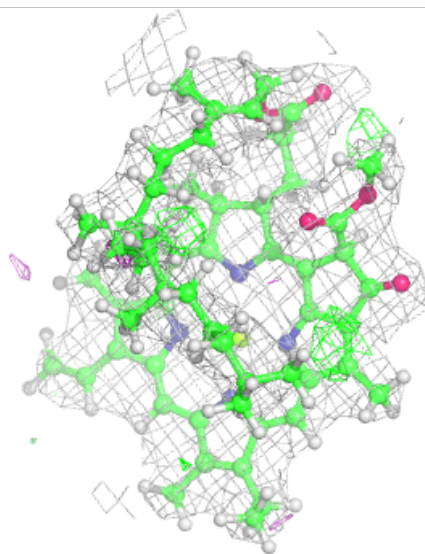
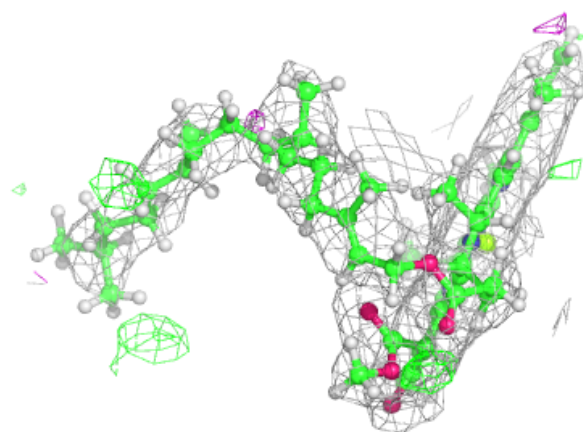
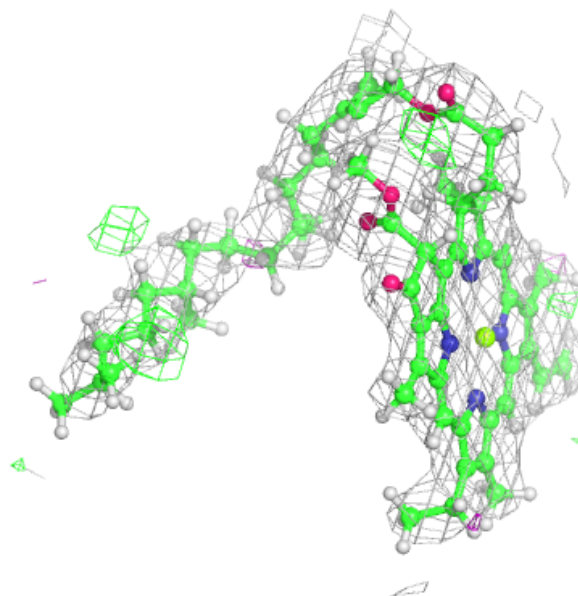
**Electron density around BCR c 515:**

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



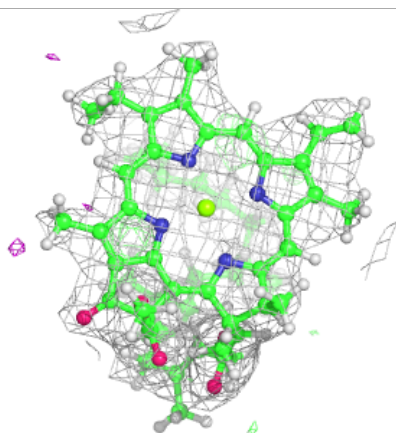
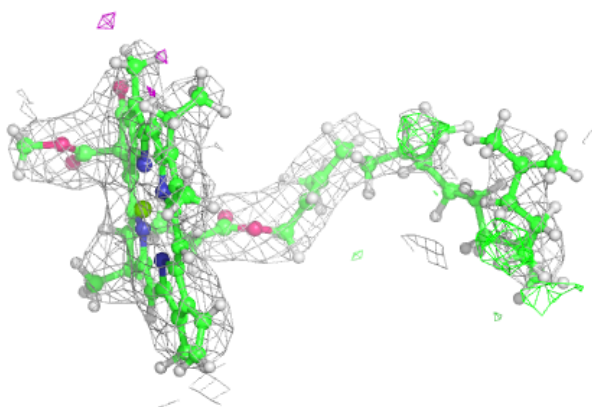
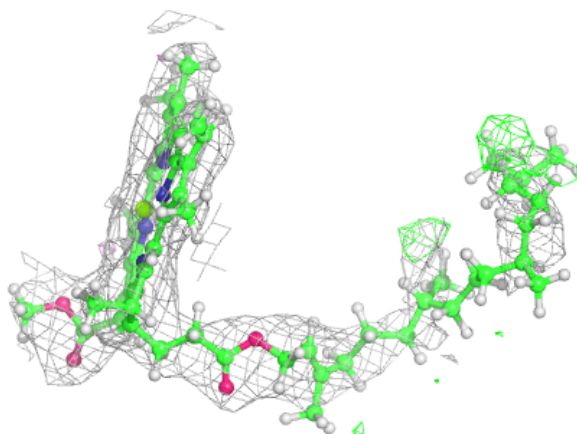
Electron density around CLA B 613:

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



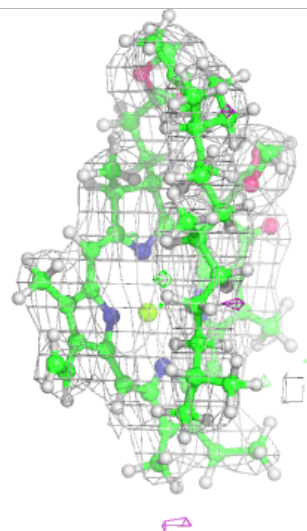
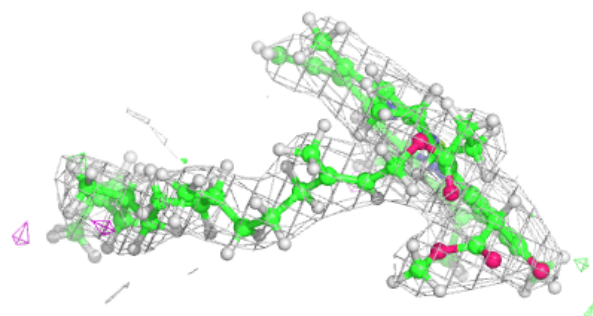
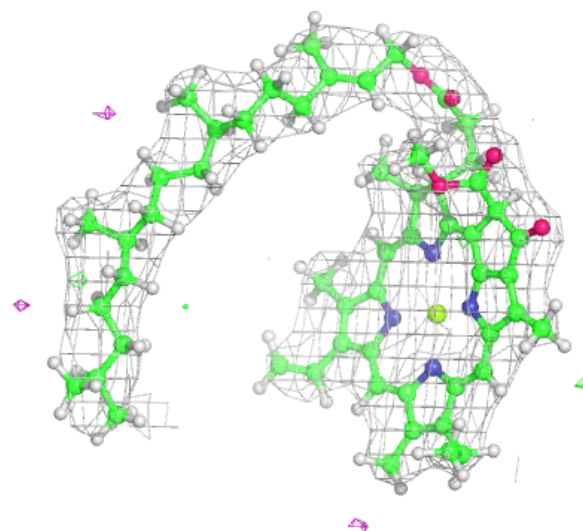
Electron density around CLA C 507:

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



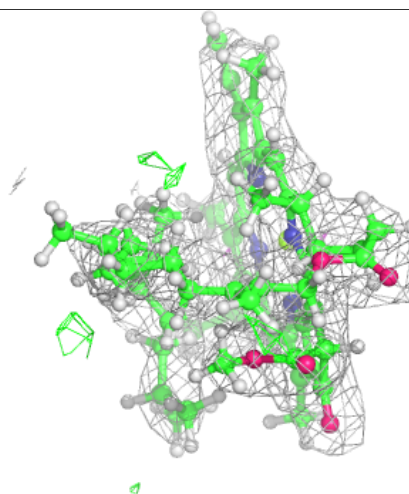
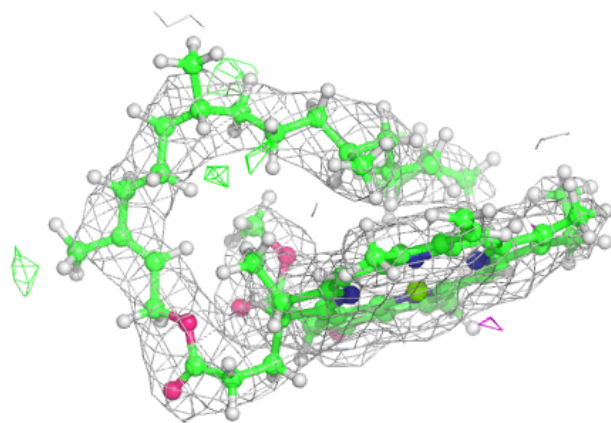
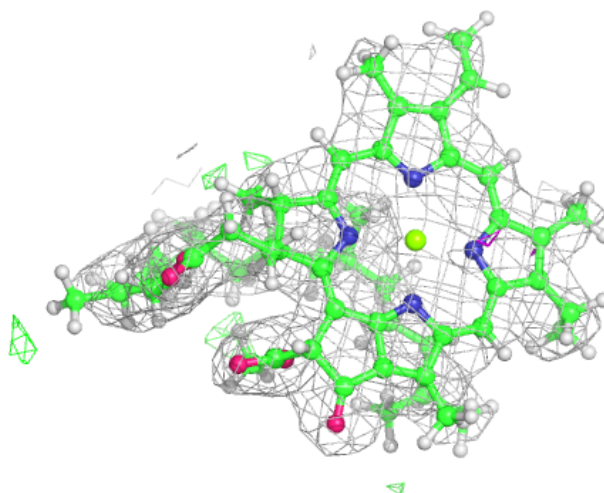
Electron density around CLA C 508:

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



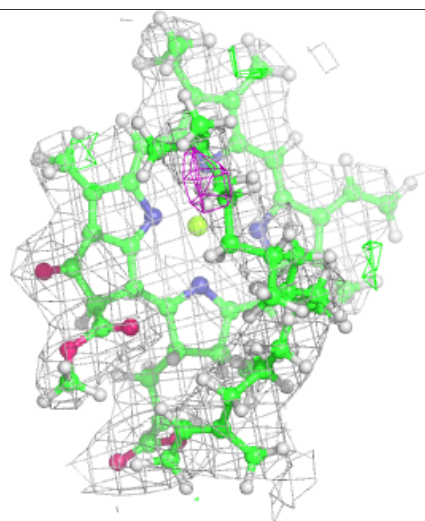
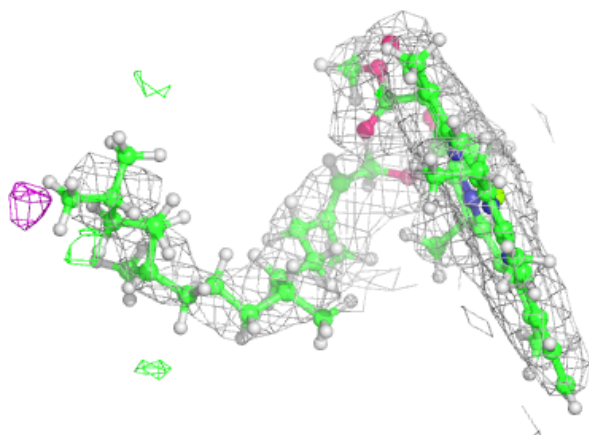
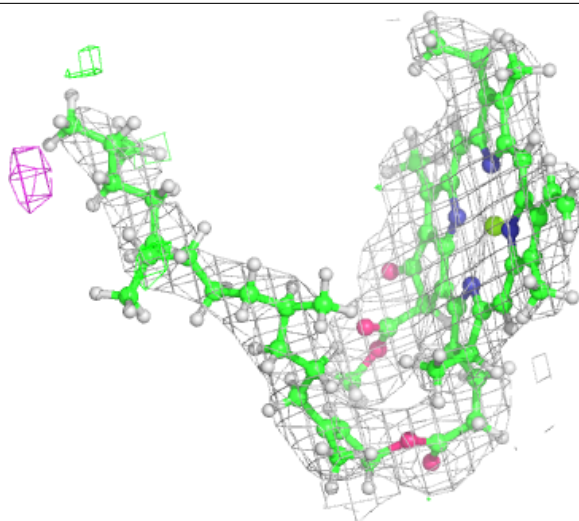
Electron density around CLA C 511:

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



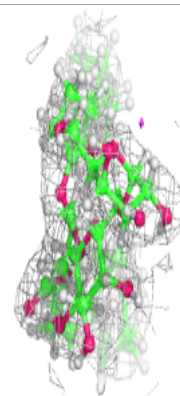
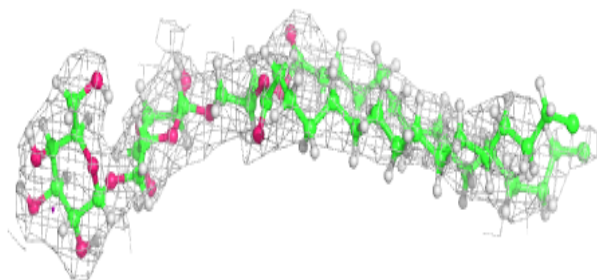
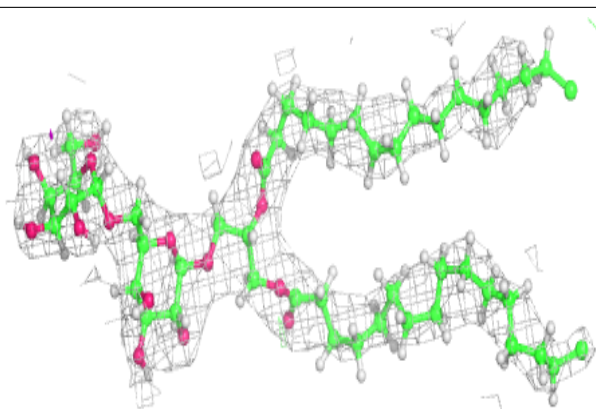
Electron density around CLA b 614:

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

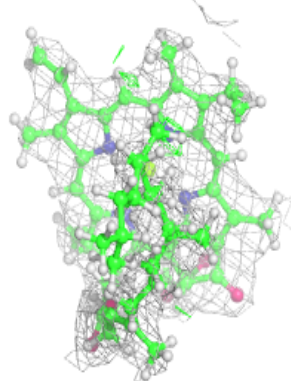
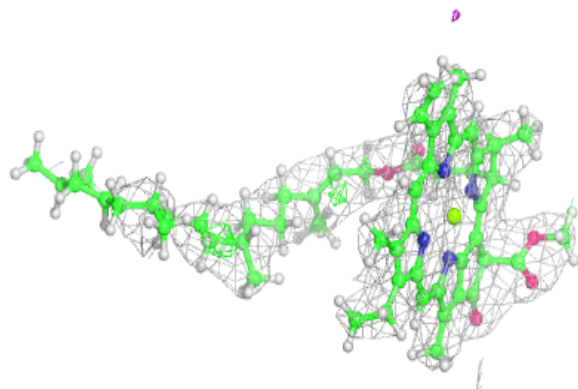
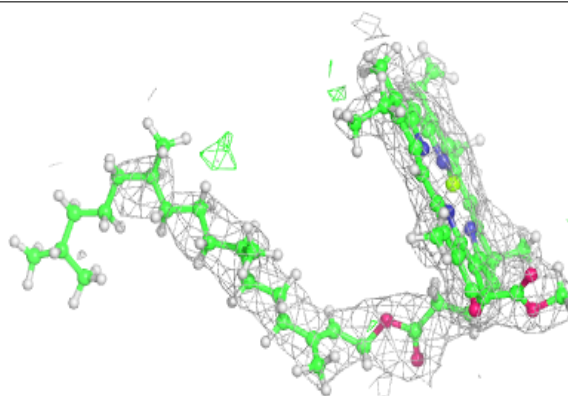


Electron density around DGD C 518:

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

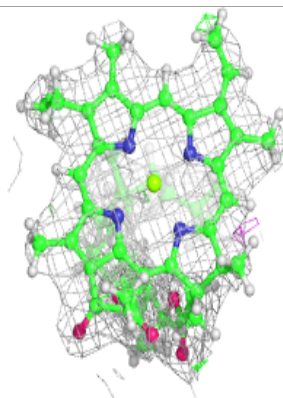
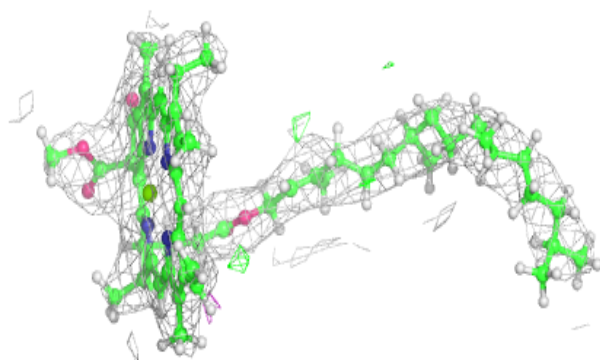
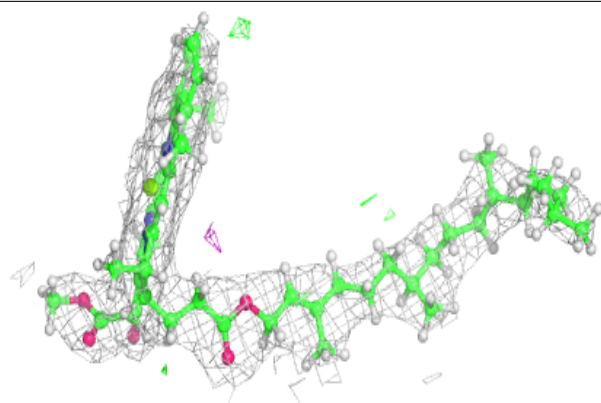
**Electron density around CLA C 509:**

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

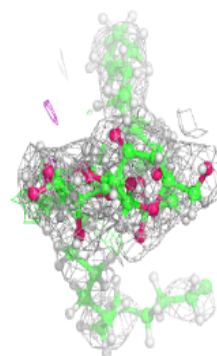
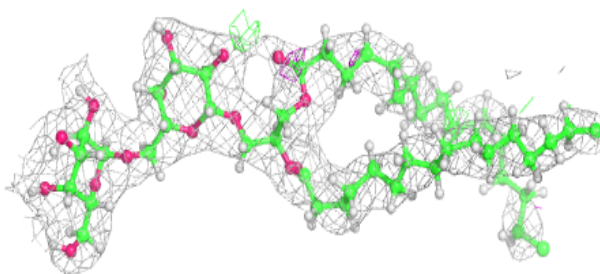
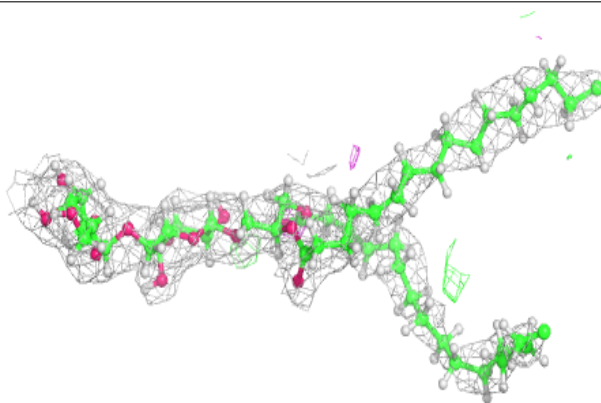


Electron density around CLA b 606:

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

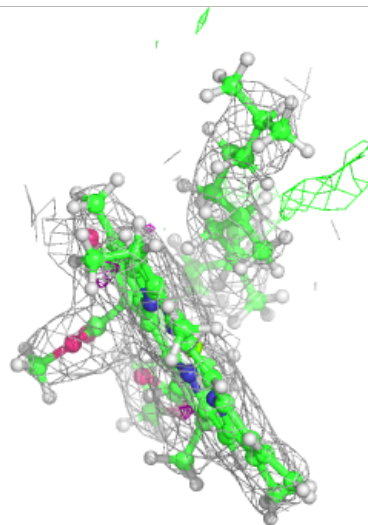
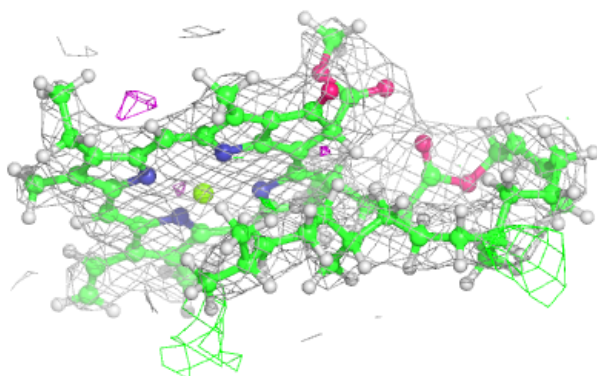
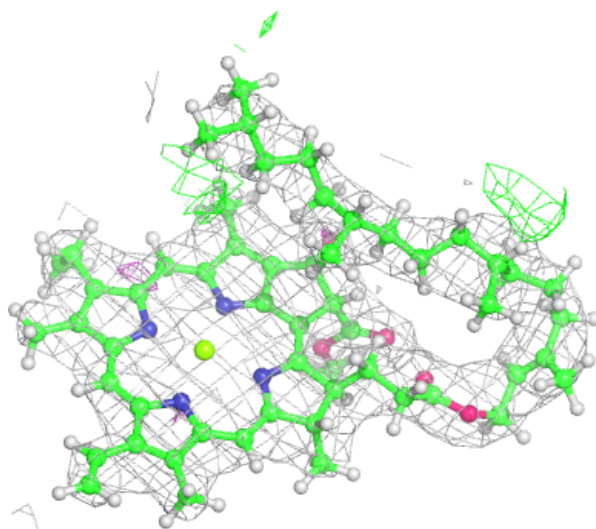
**Electron density around DGD c 516:**

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



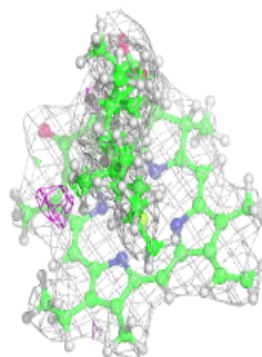
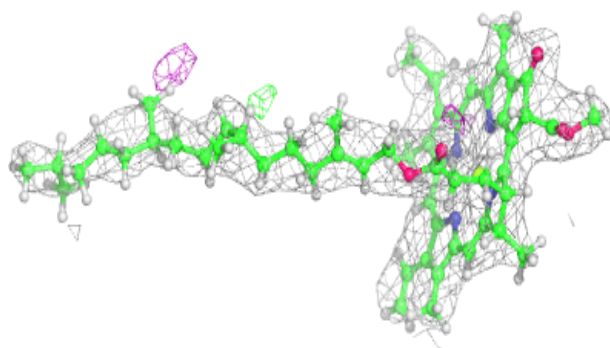
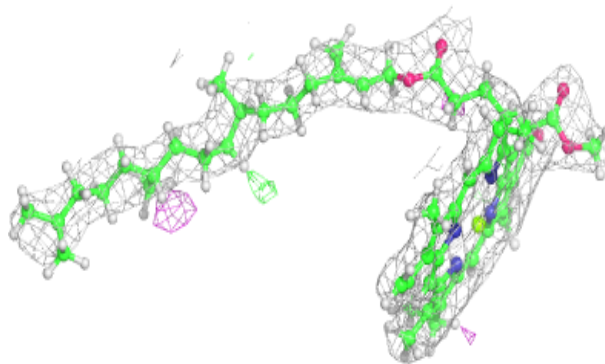
Electron density around CLA C 510:

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

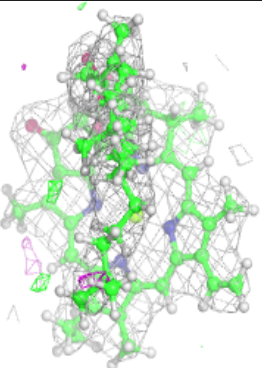
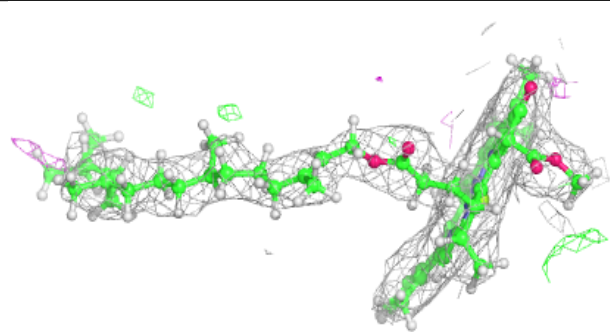
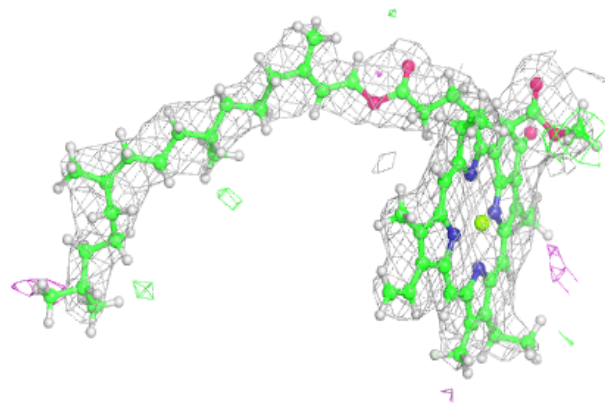


Electron density around CLA b 608:

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

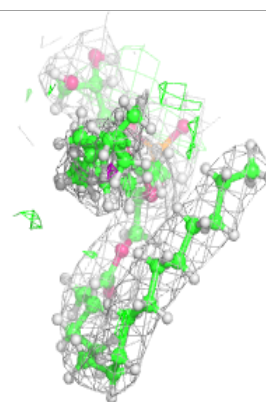
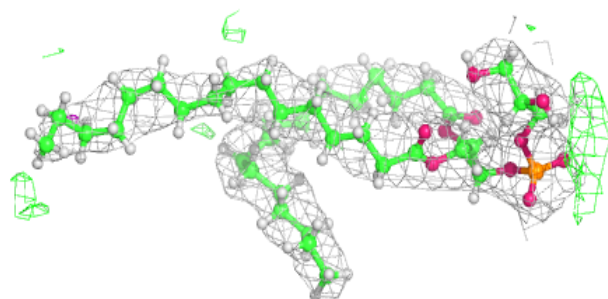
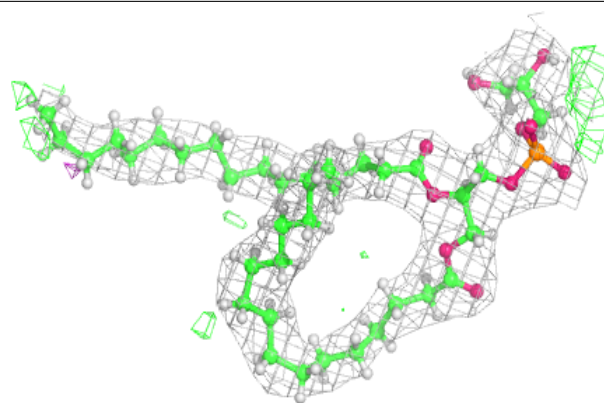
**Electron density around CLA b 610:**

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

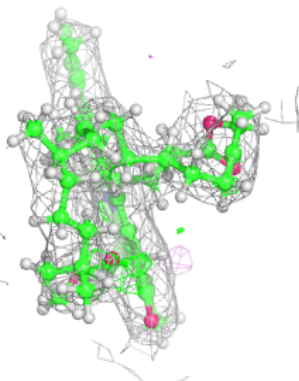
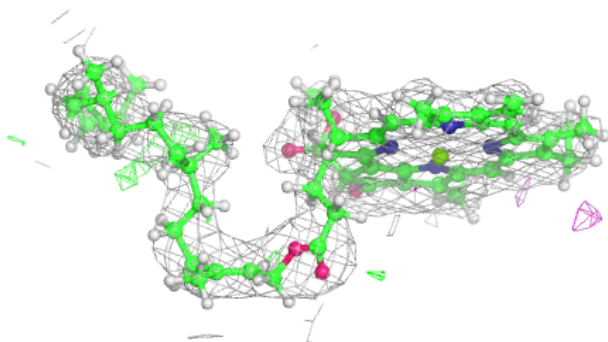
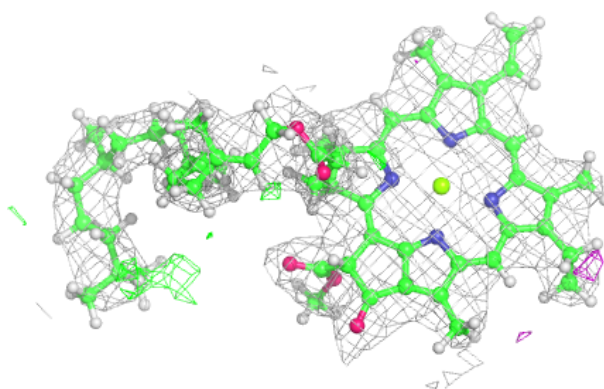


Electron density around LHG A 413:

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

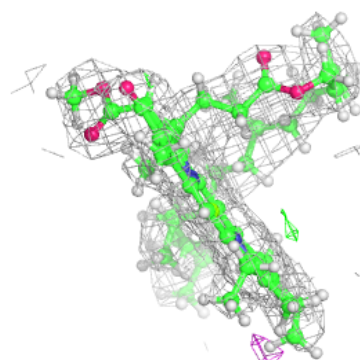
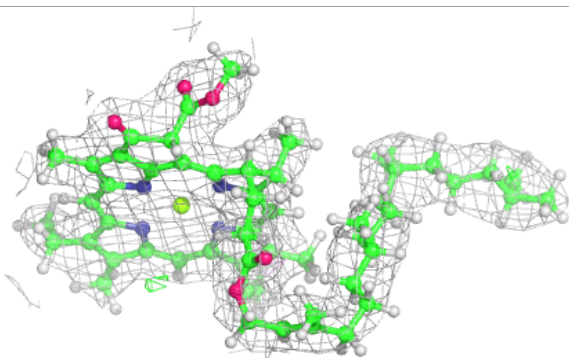
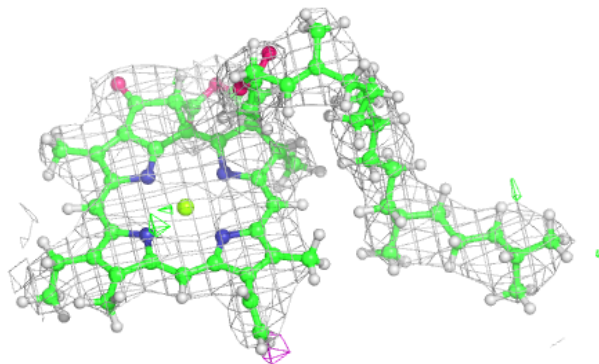
**Electron density around CLA b 613:**

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

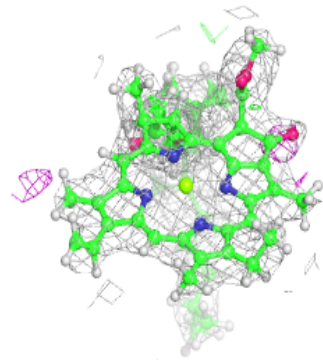
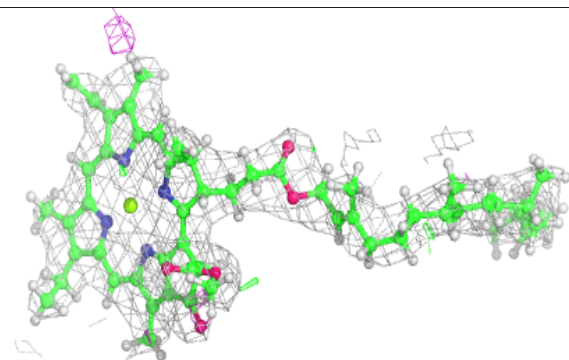
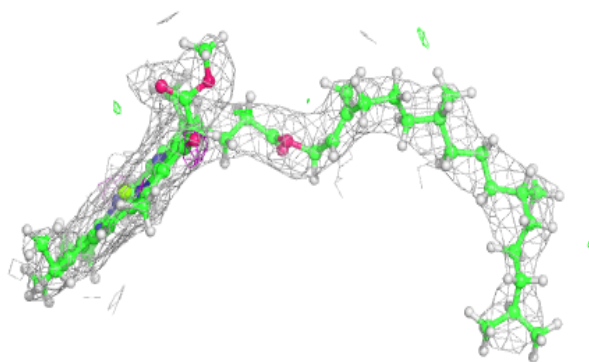


Electron density around CLA d 402:

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

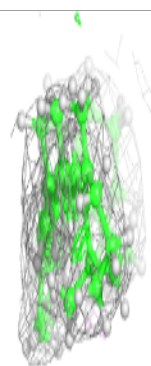
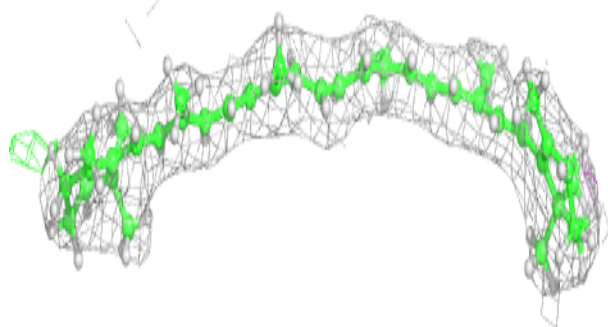
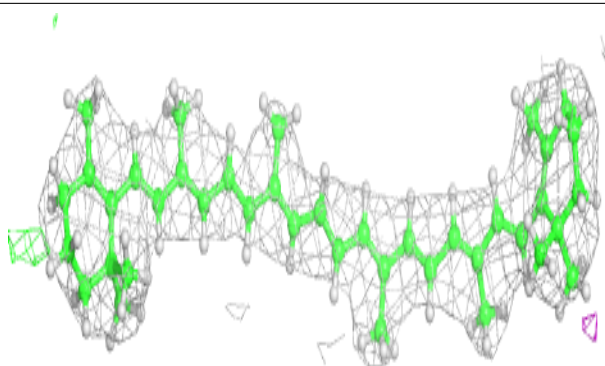
**Electron density around CLA d 403:**

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

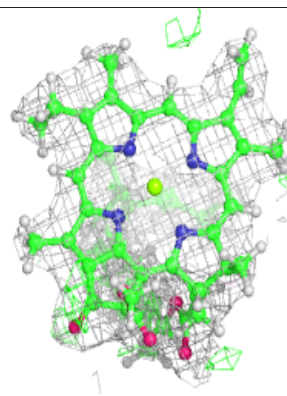
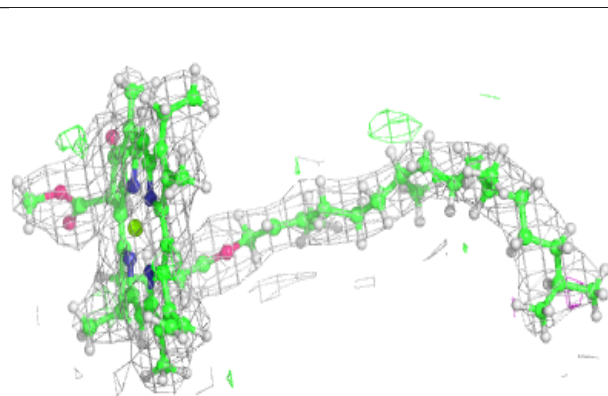
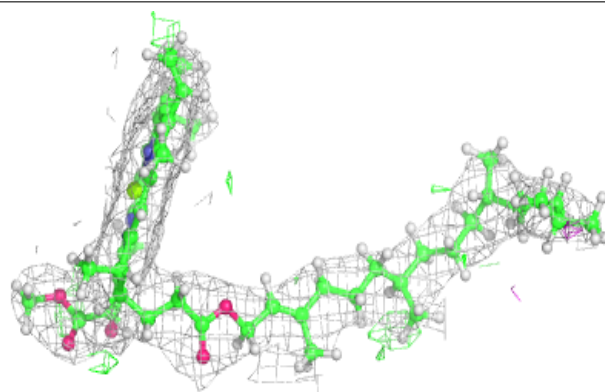


Electron density around BCR t 101:

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

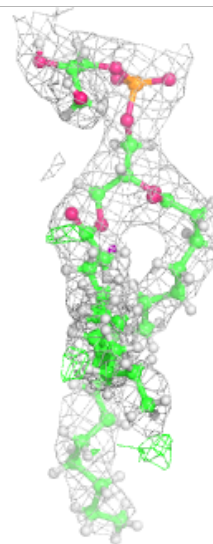
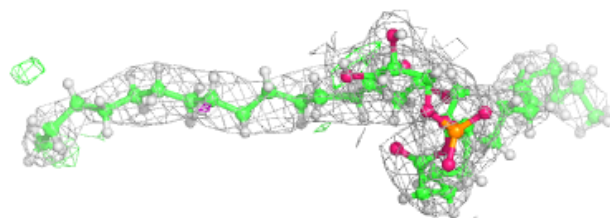
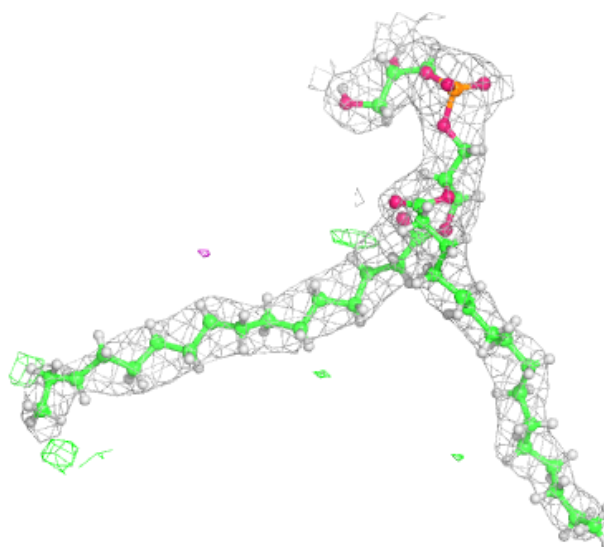
**Electron density around CLA B 605:**

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



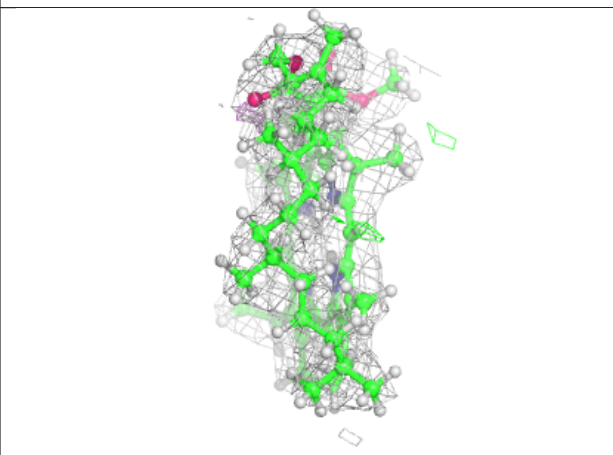
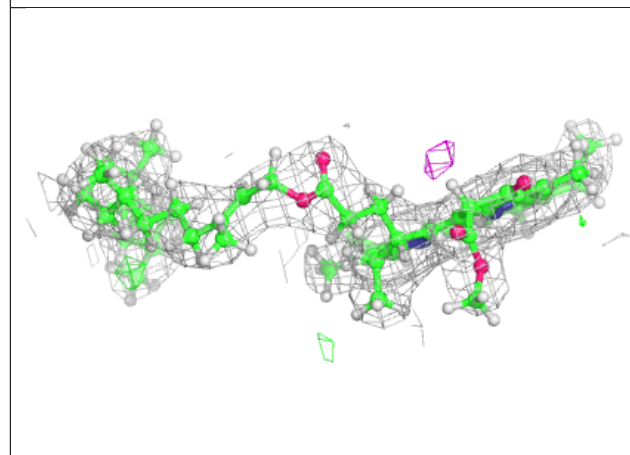
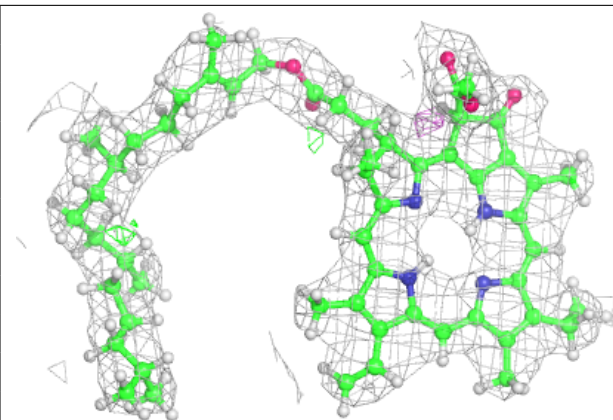
Electron density around LHG 1 101:

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



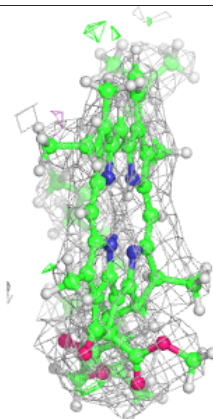
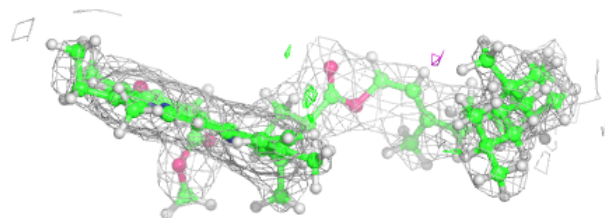
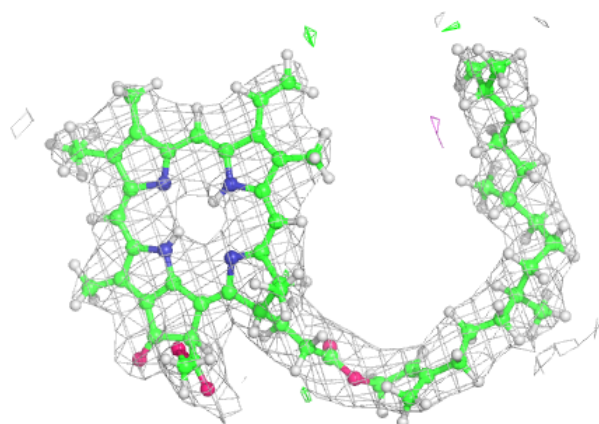
Electron density around PHO A 406:

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

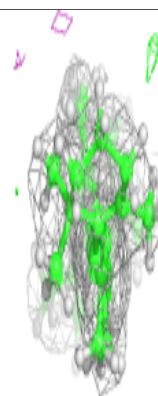
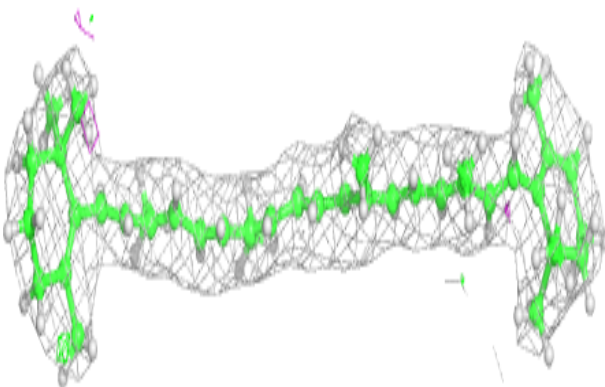
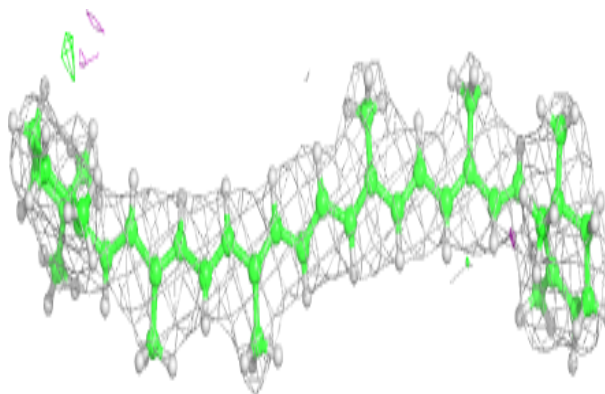


Electron density around PHO a 407:

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

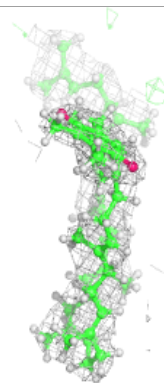
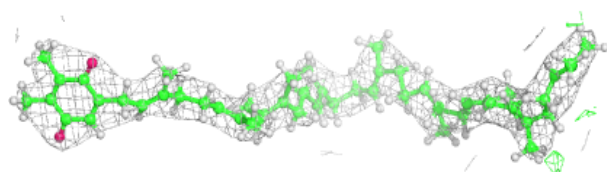
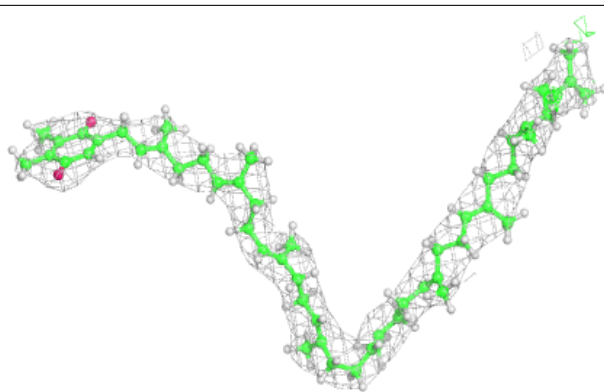
**Electron density around BCR A 408:**

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

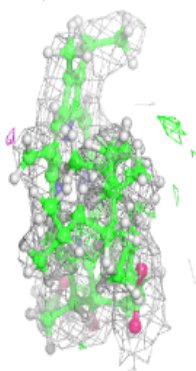
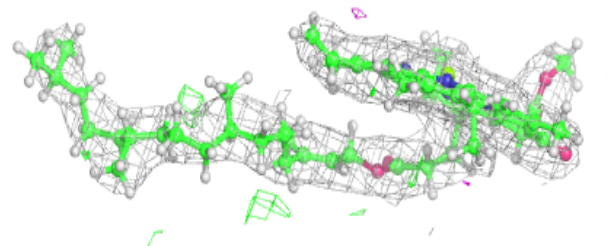
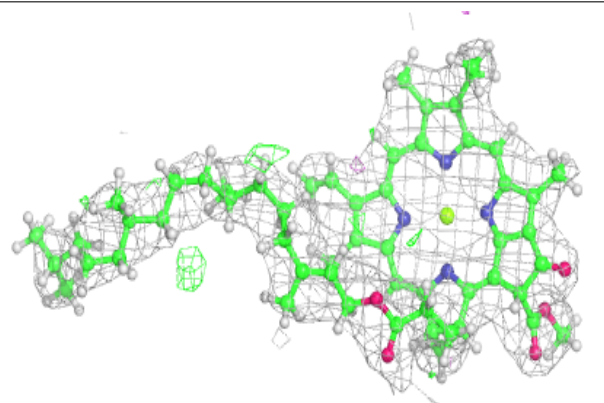


Electron density around PL9 d 406:

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

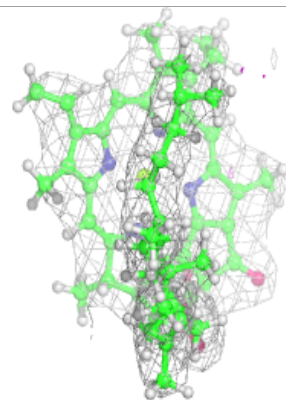
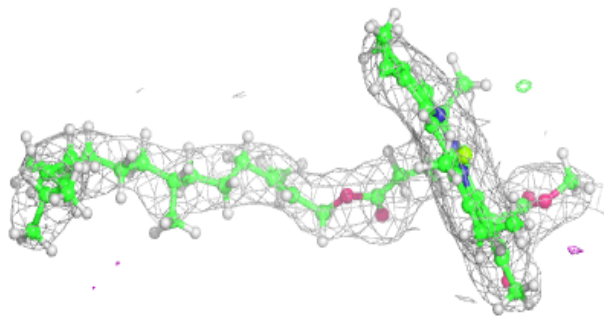
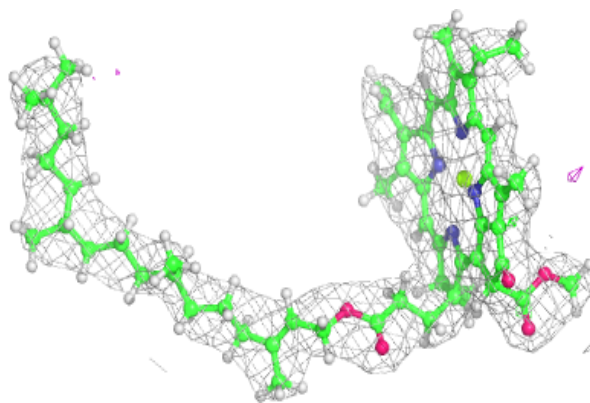
**Electron density around CLA B 603:**

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



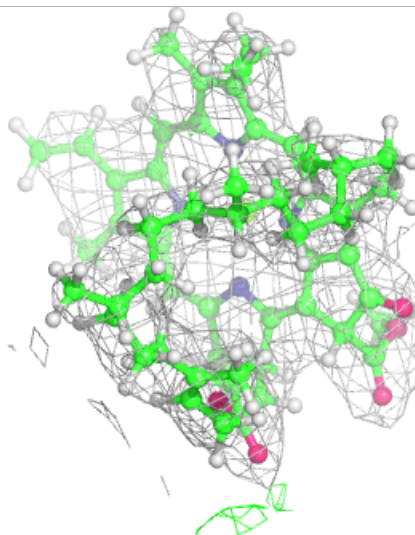
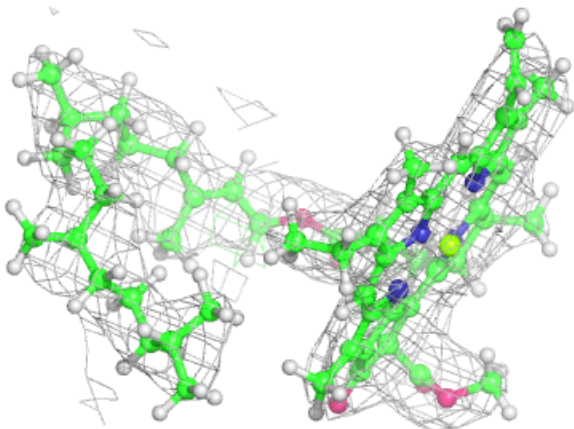
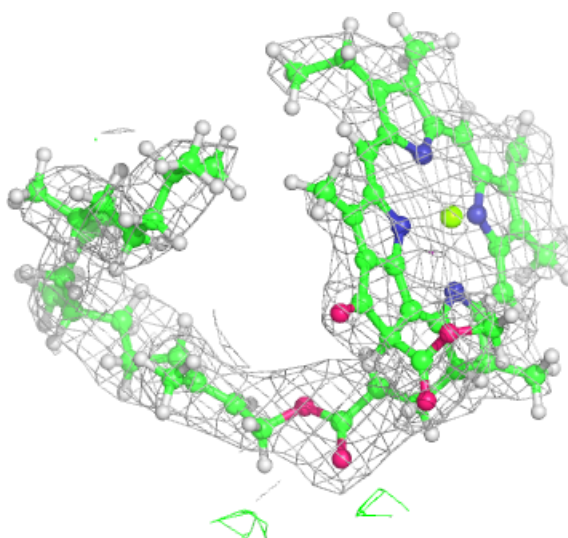
Electron density around CLA B 609:

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



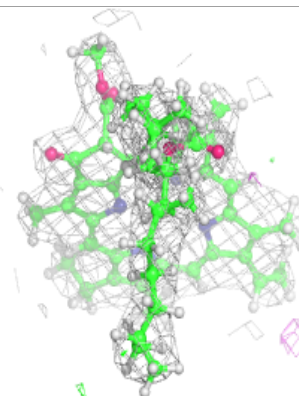
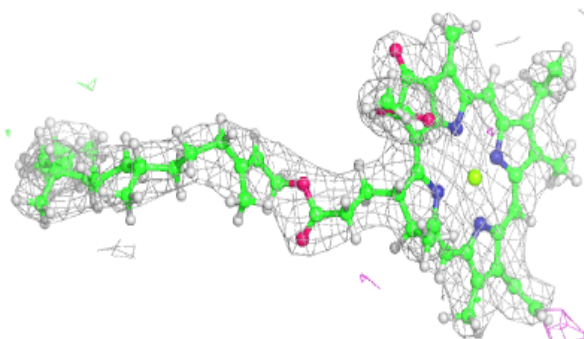
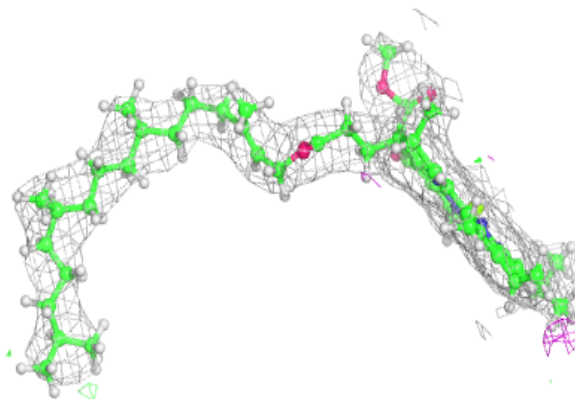
Electron density around CLA C 504:

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

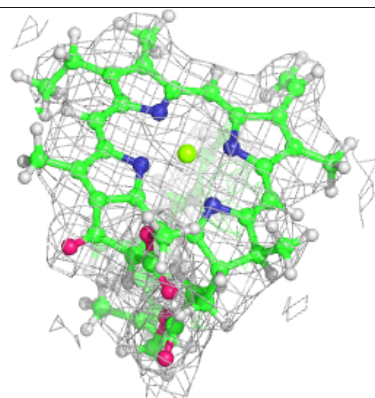
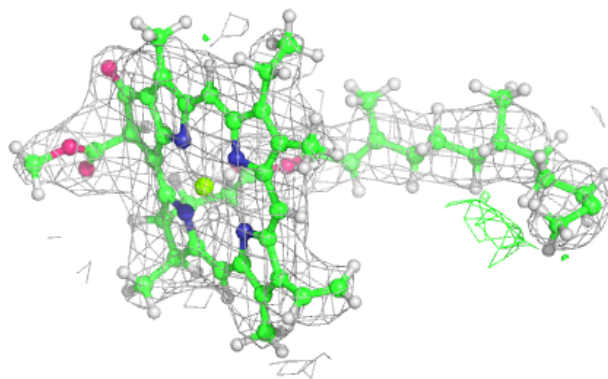
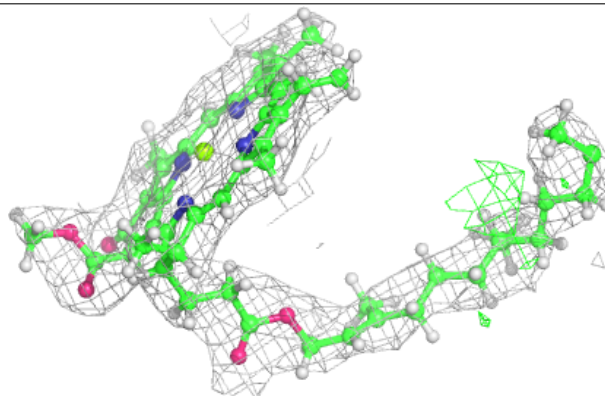


Electron density around CLA D 403:

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

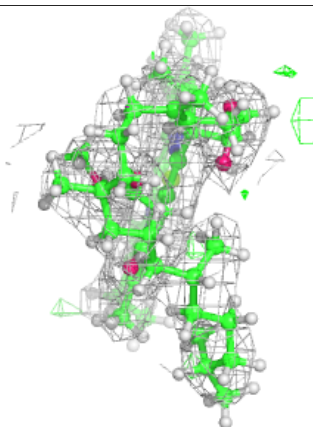
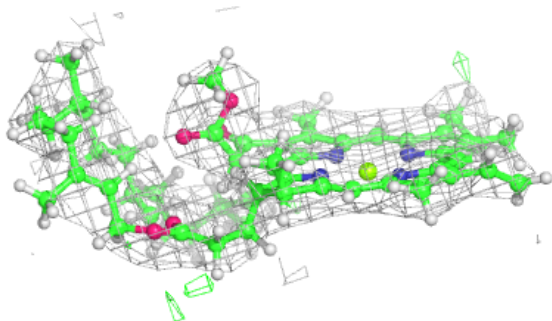
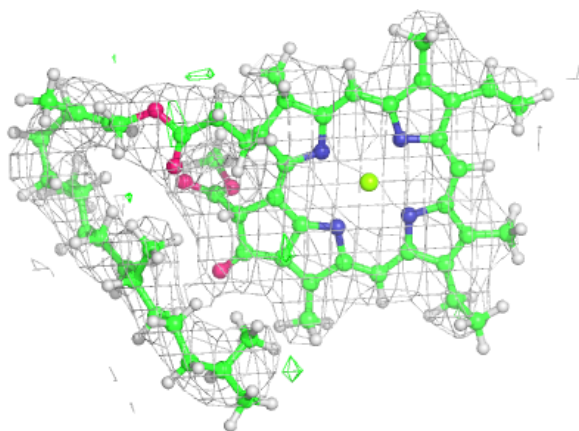
**Electron density around CLA C 505:**

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

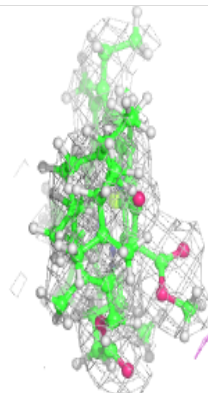
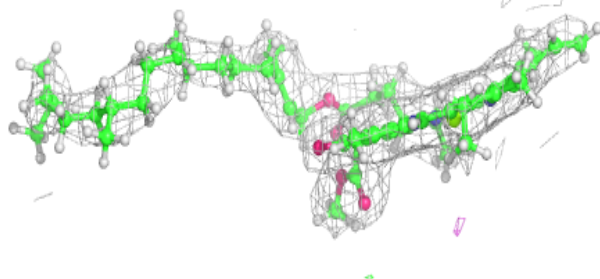
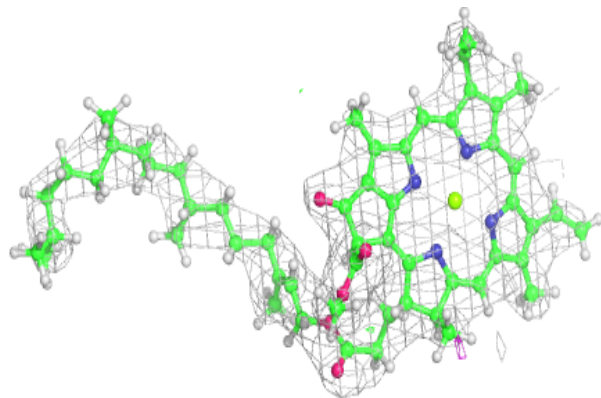


Electron density around CLA B 610:

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

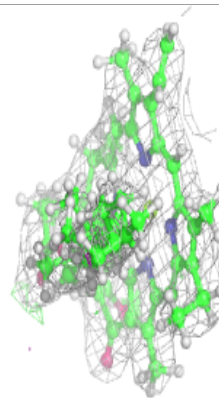
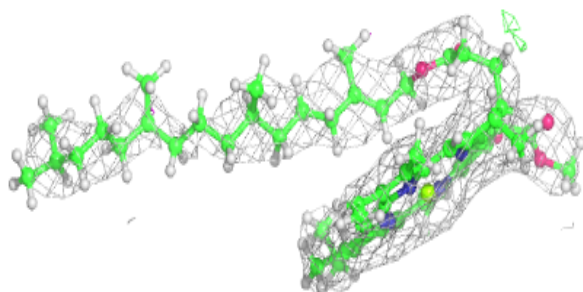
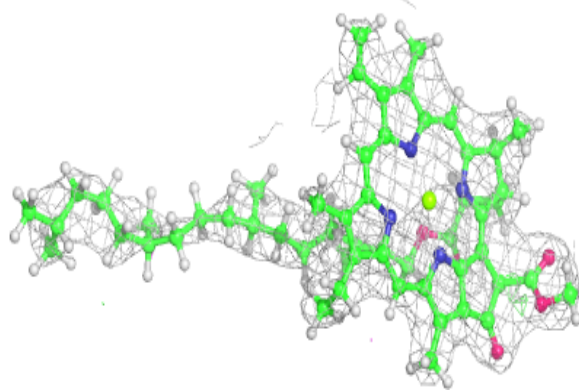
**Electron density around CLA B 602:**

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

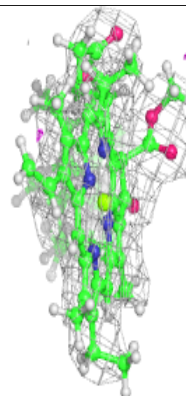
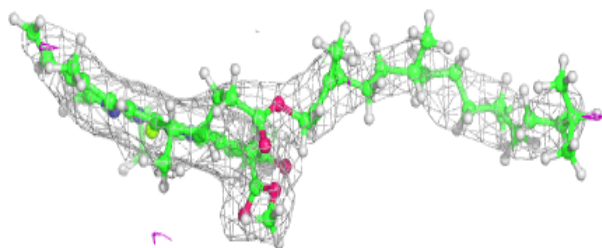
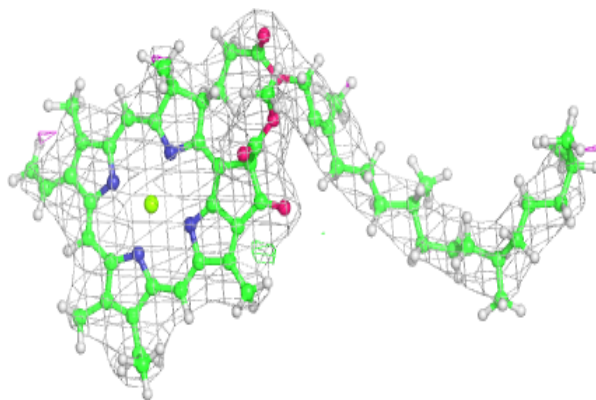


Electron density around CLA B 614:

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

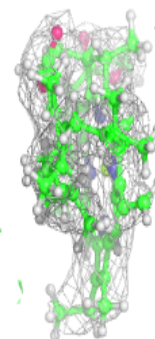
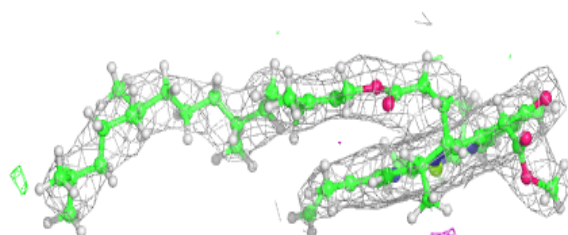
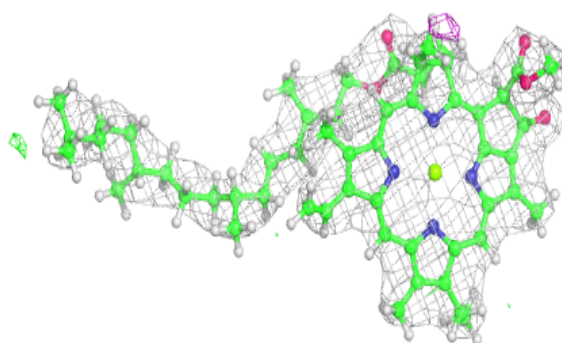
**Electron density around CLA b 603:**

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

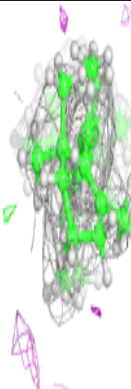
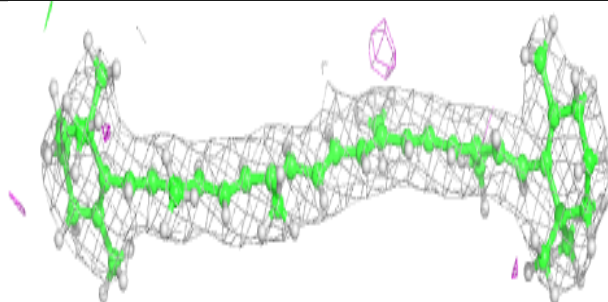
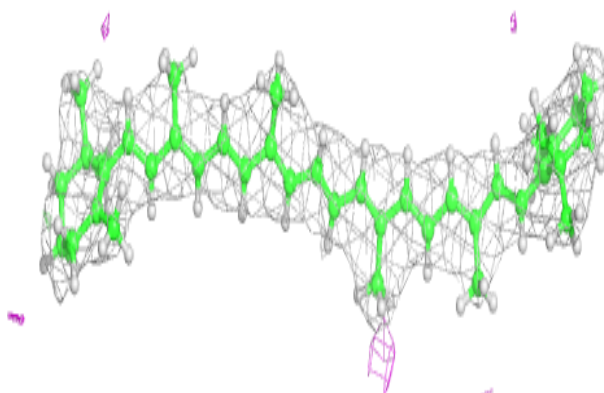


Electron density around CLA b 604:

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

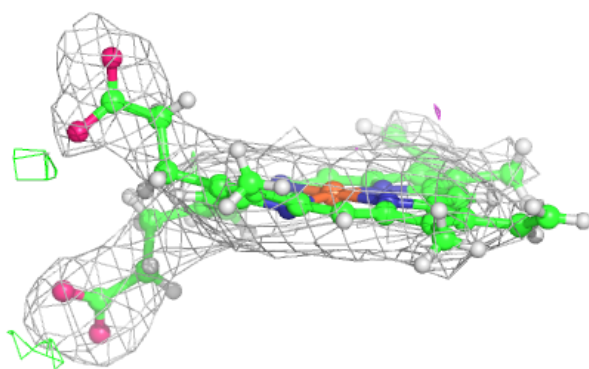
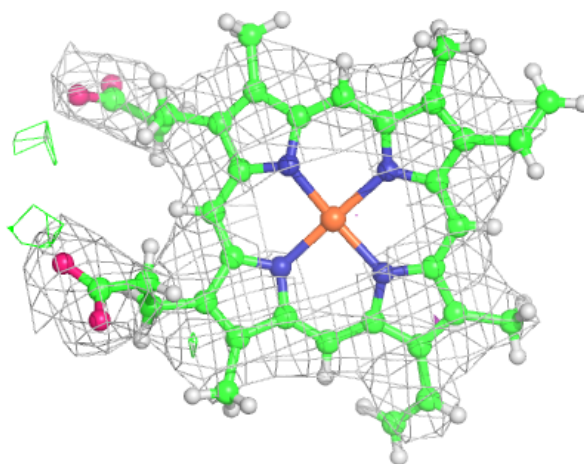
**Electron density around BCR a 409:**

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



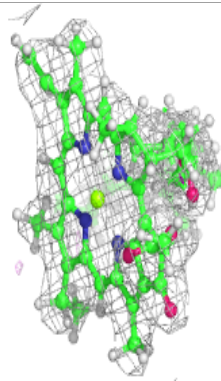
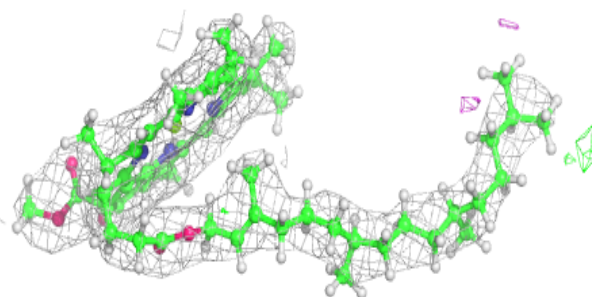
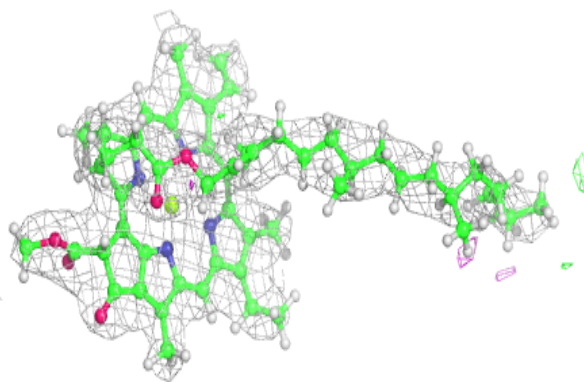
Electron density around HEM E 103:

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

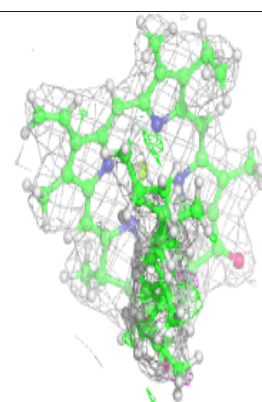
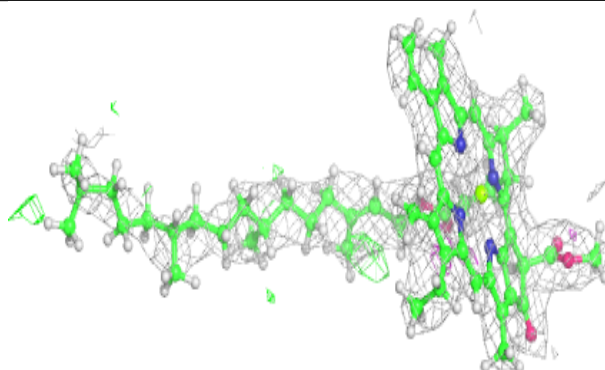
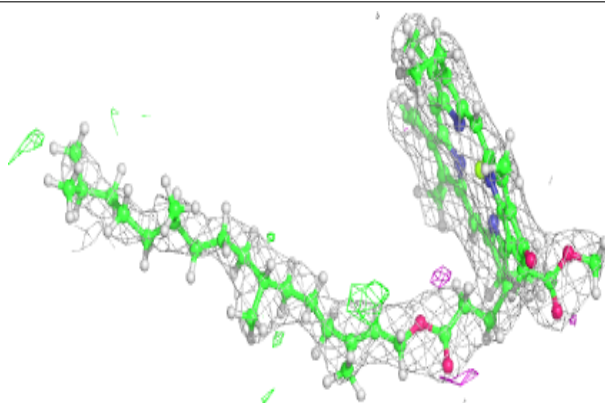


Electron density around CLA b 609:

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

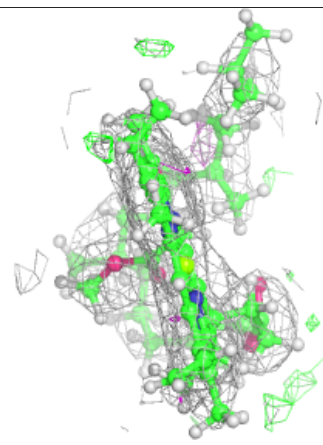
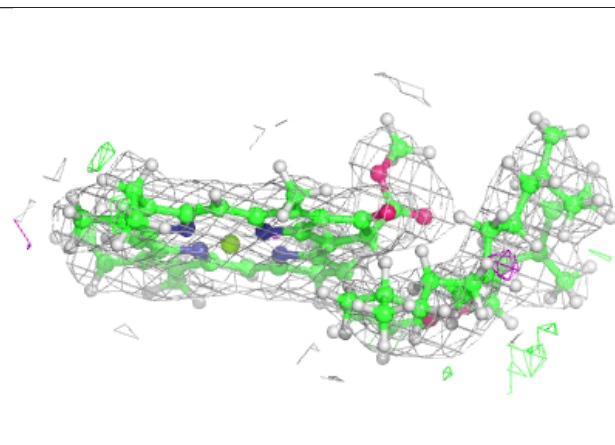
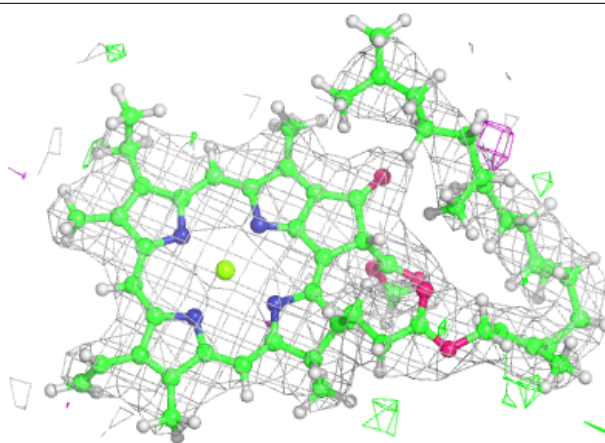
**Electron density around CLA B 607:**

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



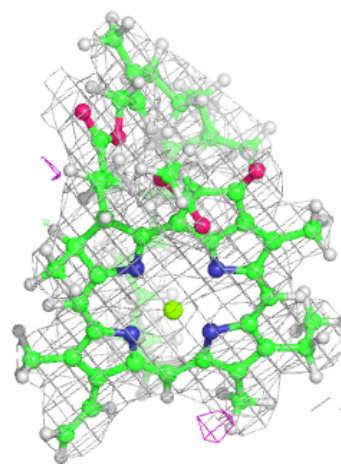
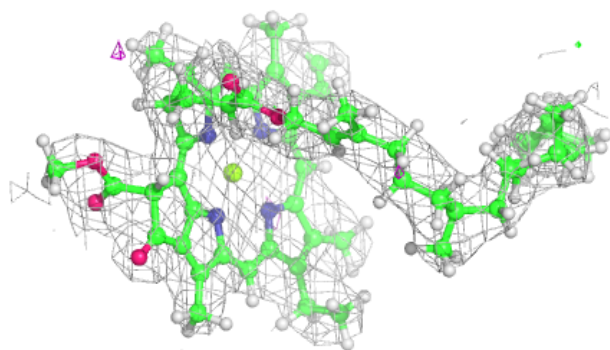
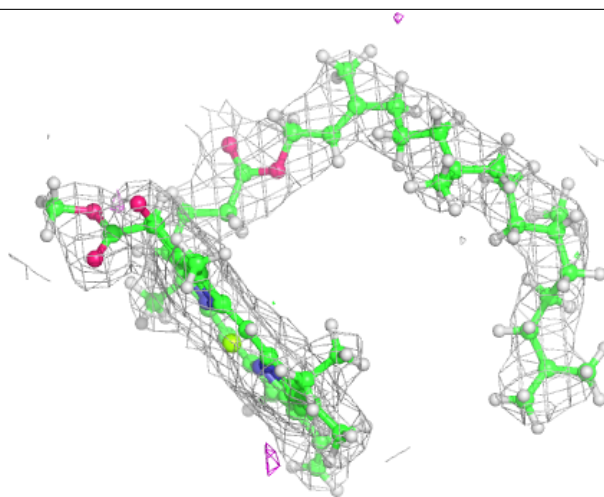
Electron density around CLA b 611:

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



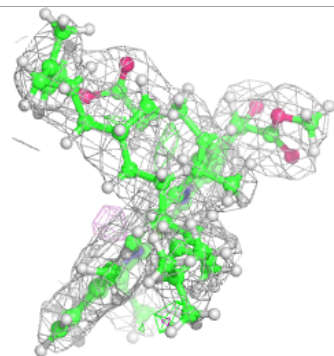
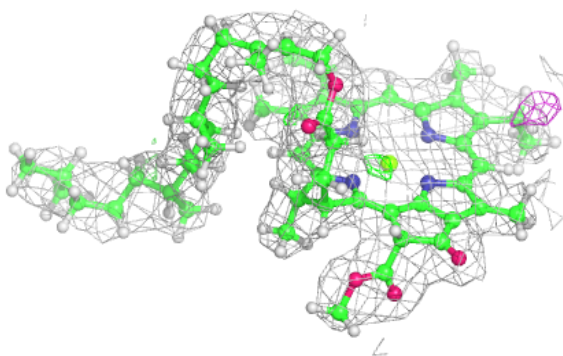
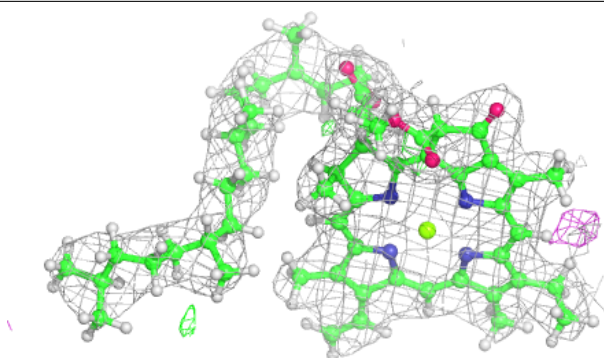
Electron density around CLA b 612:

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

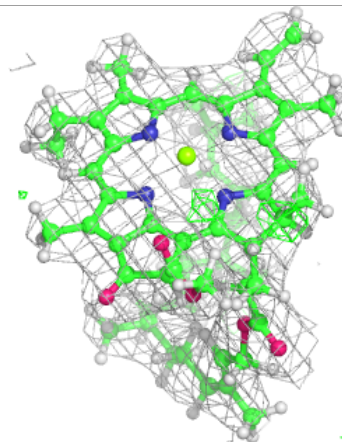
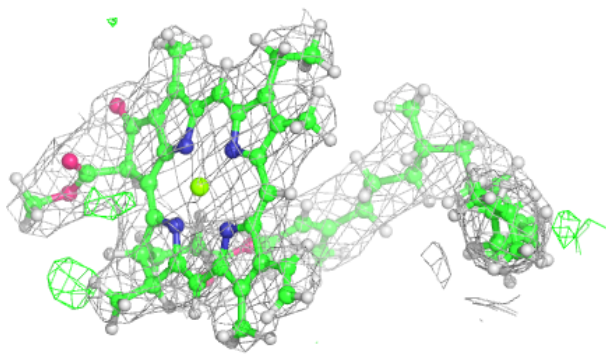
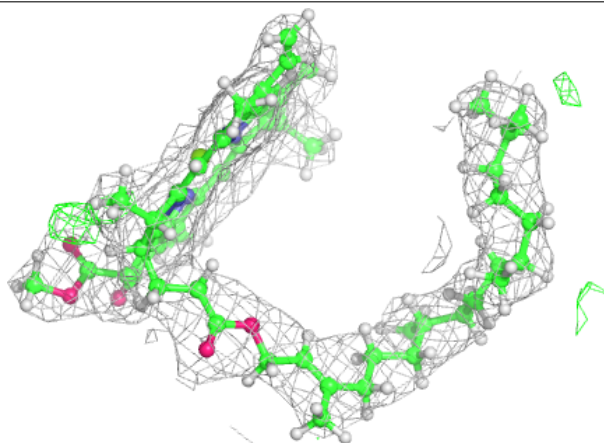


Electron density around CLA D 402:

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

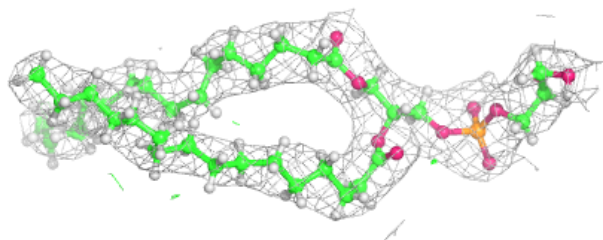
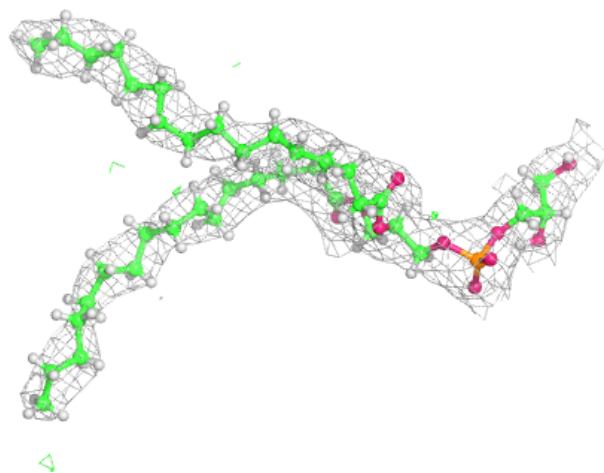
**Electron density around CLA B 611:**

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



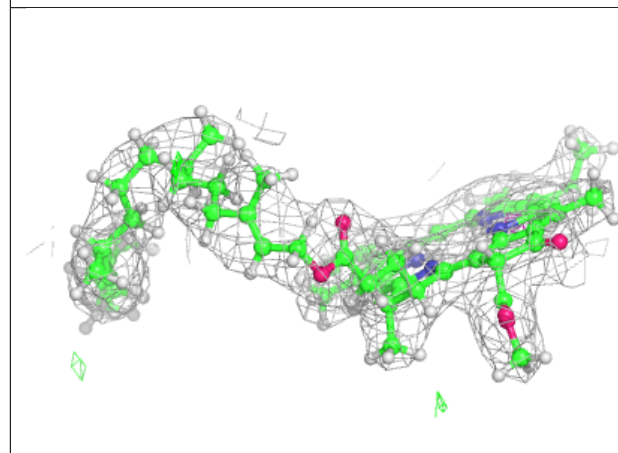
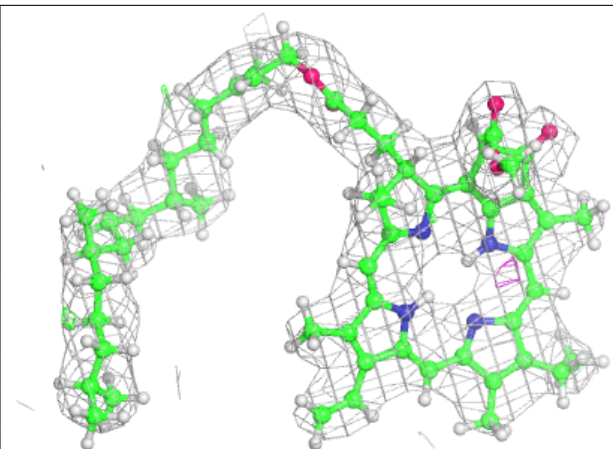
Electron density around LHG D 408:

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

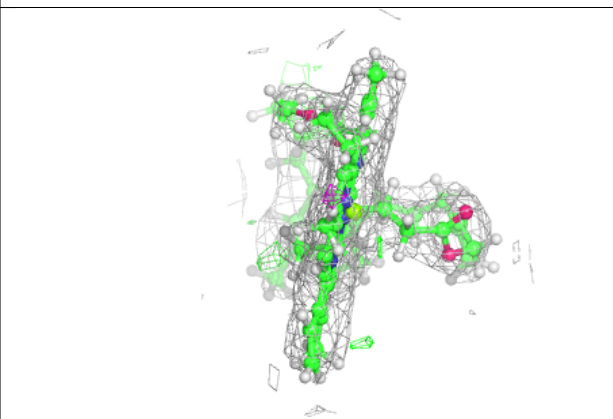
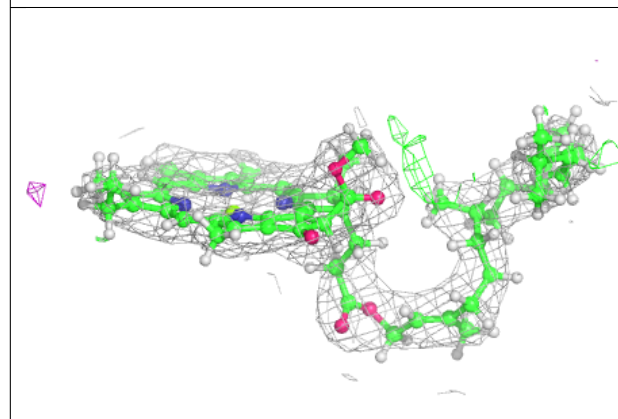
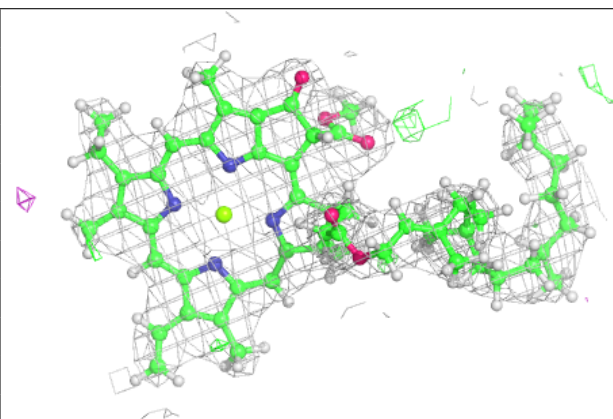


Electron density around PHO D 401:

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

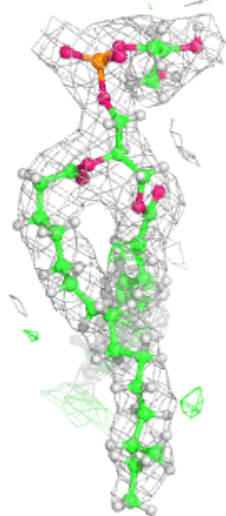
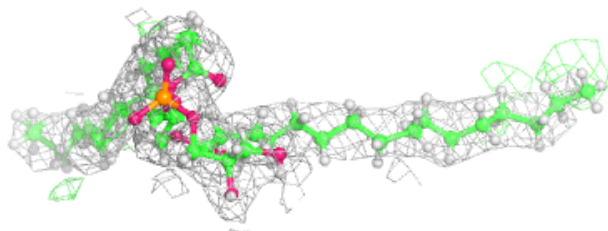
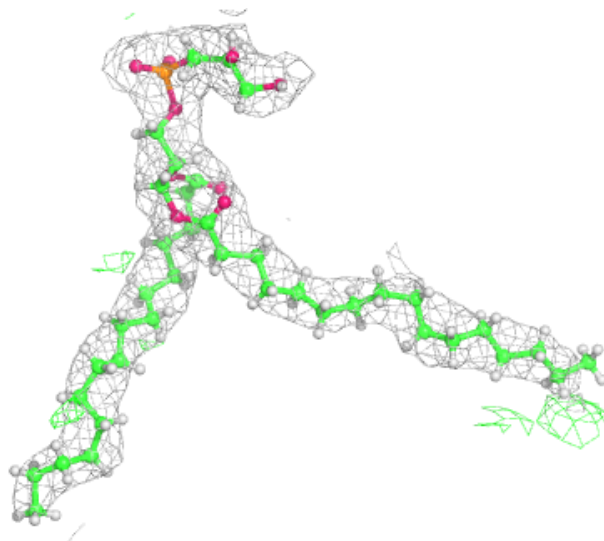
**Electron density around CLA B 612:**

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



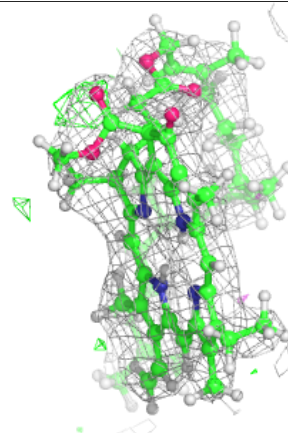
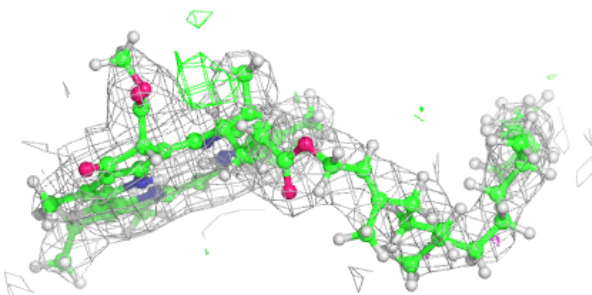
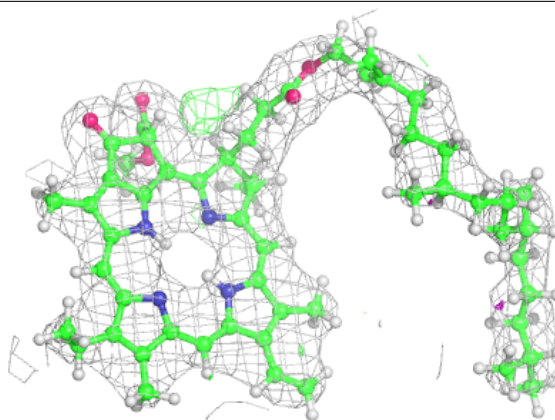
Electron density around LHG L 101:

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

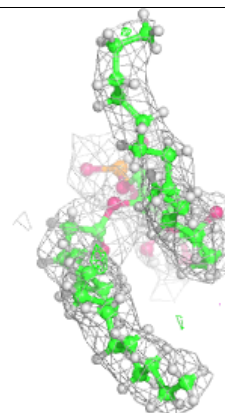
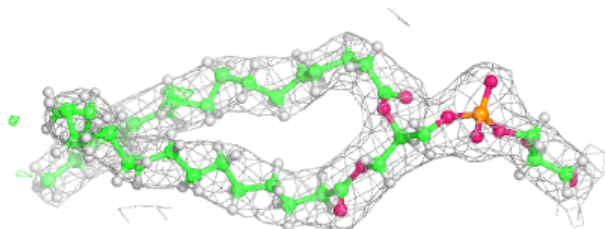
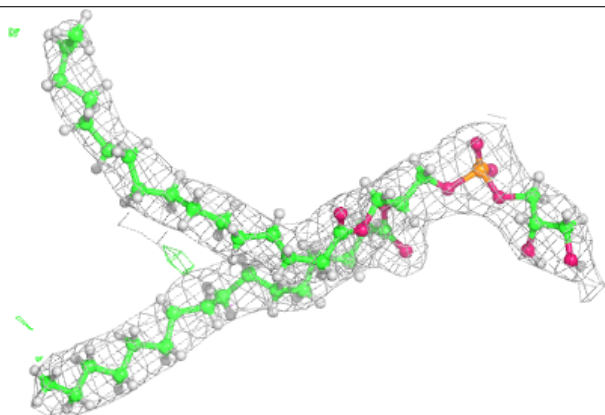


Electron density around PHO d 401:

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

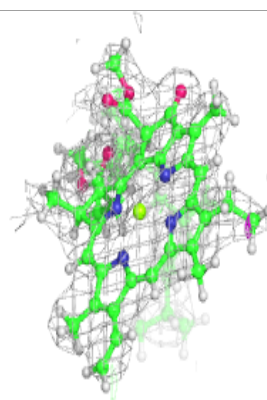
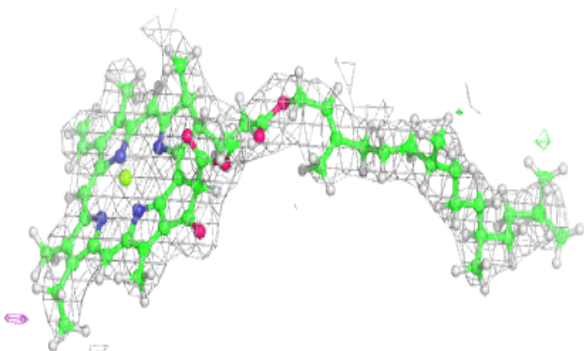
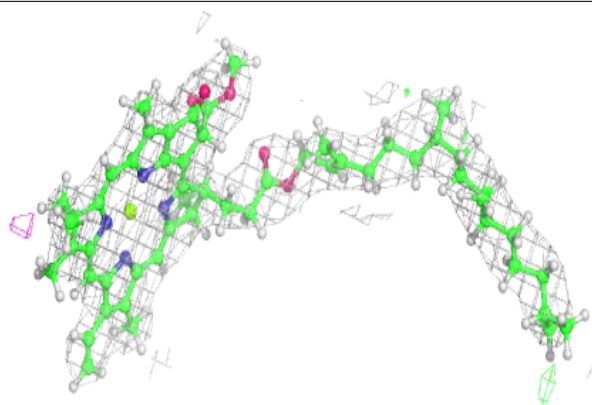
**Electron density around LHG d 408:**

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

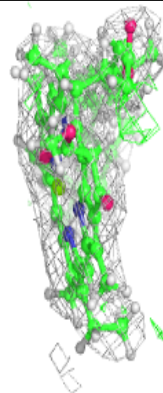
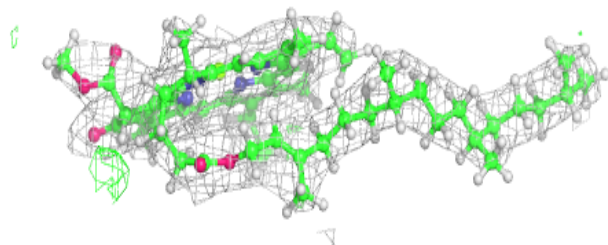
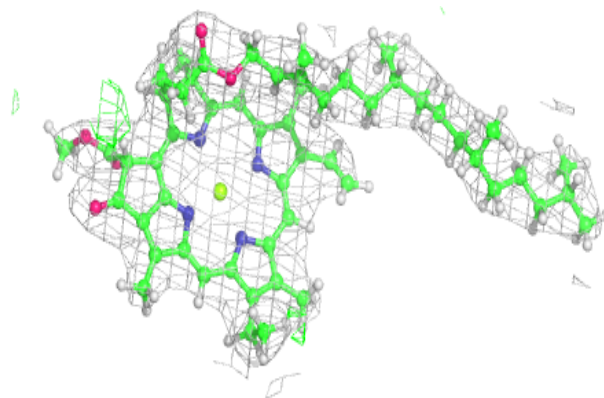


Electron density around CLA a 405:

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

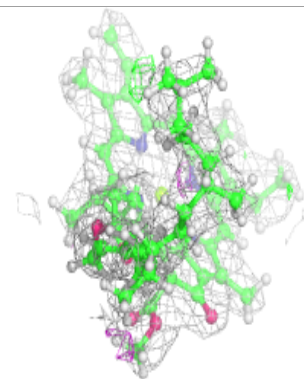
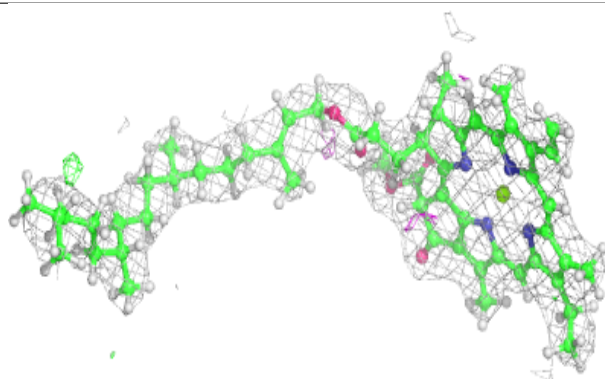
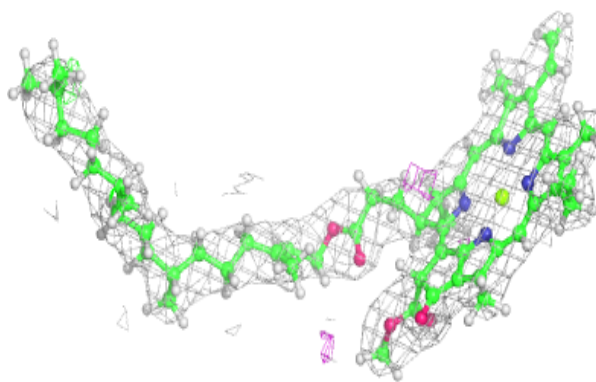
**Electron density around CLA C 502:**

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

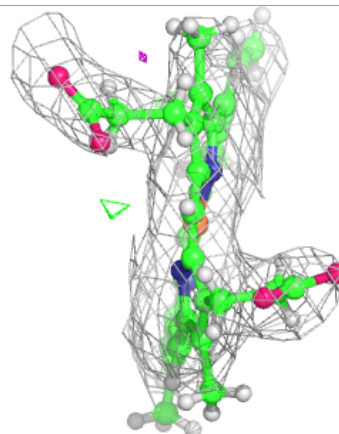
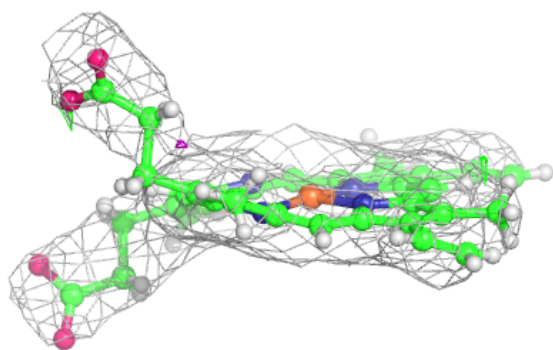
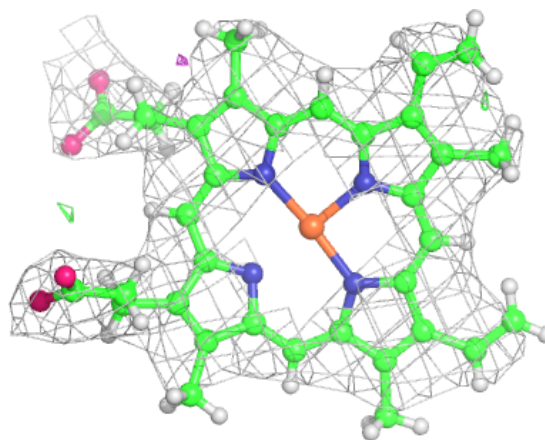


Electron density around CLA A 404:

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

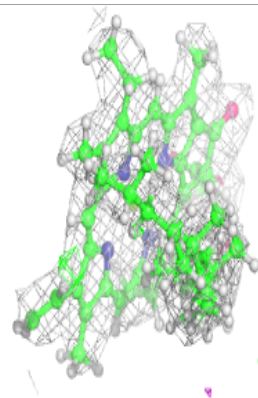
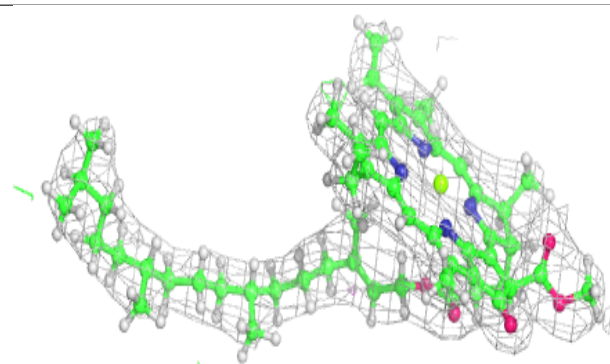
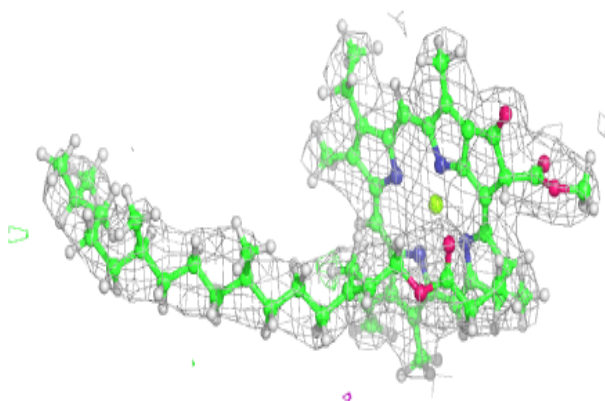
**Electron density around HEM e 102:**

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



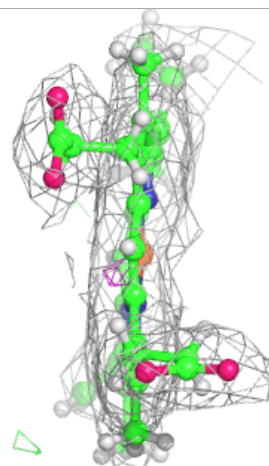
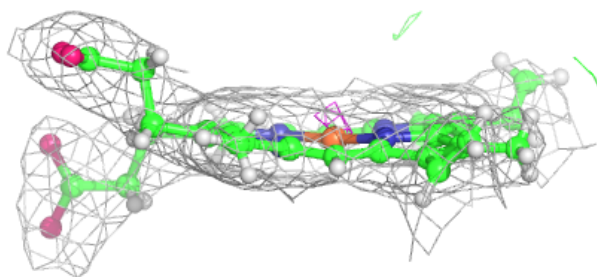
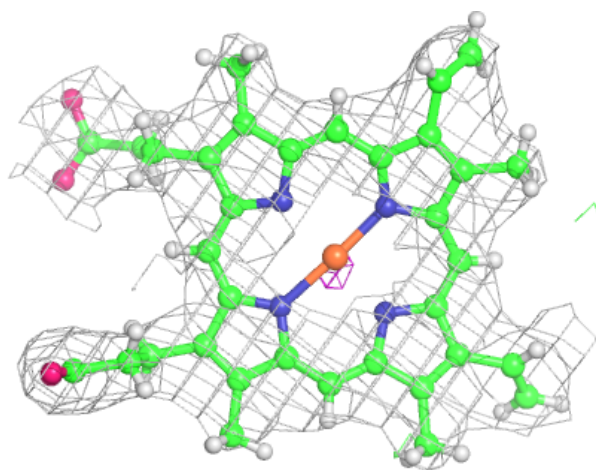
Electron density around CLA B 608:

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



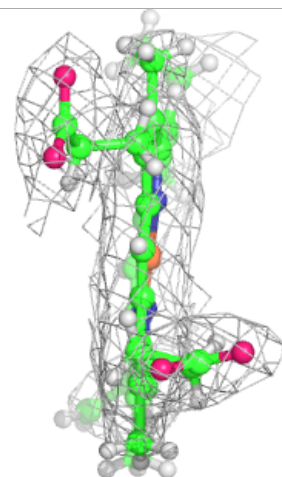
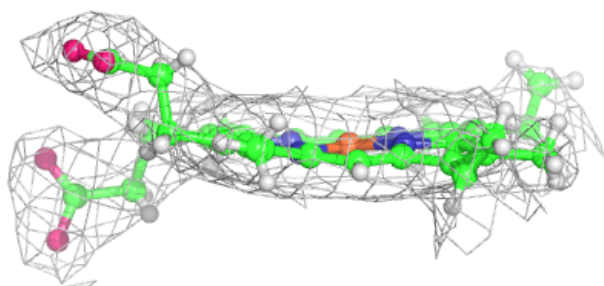
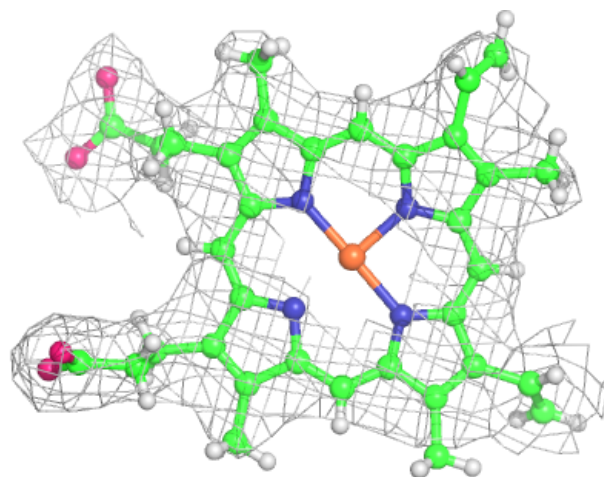
Electron density around HEC V 201:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.