



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 12:28 AM EST

PDB ID : 5KAI
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 2.80 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)

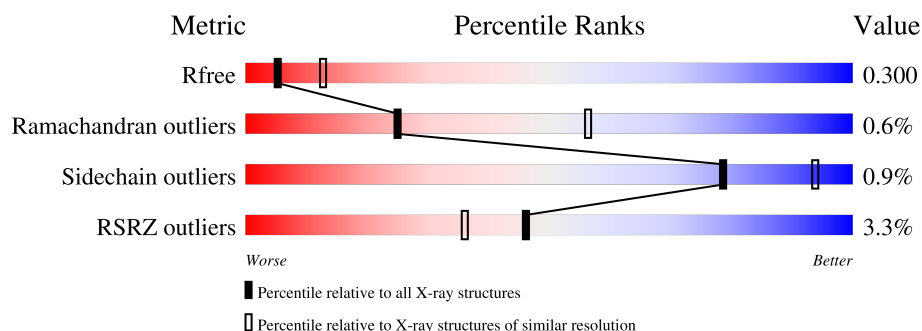
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3140 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RSRZ outliers | 127900 | 3078 (2.80-2.80) |

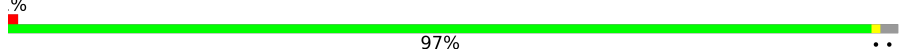
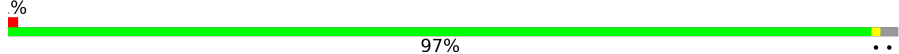
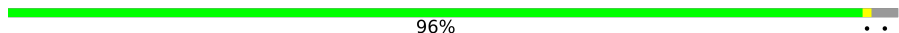
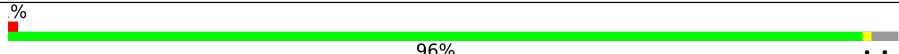
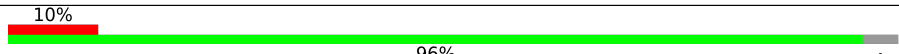
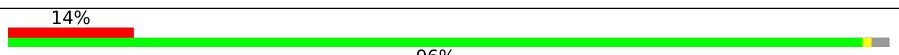
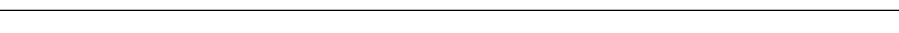



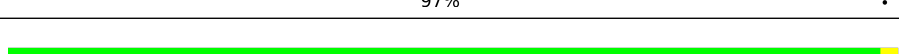
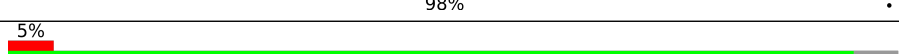
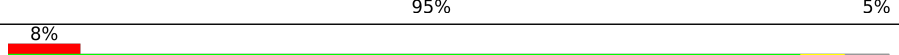
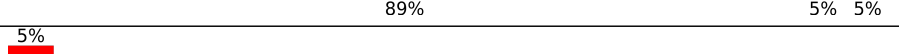
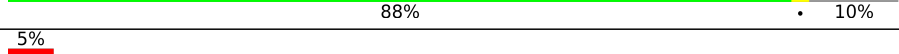


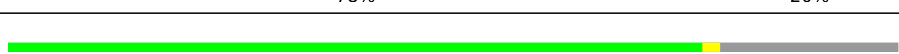

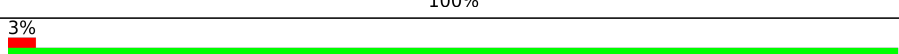
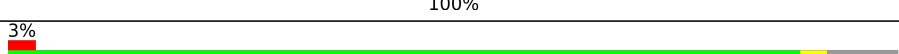
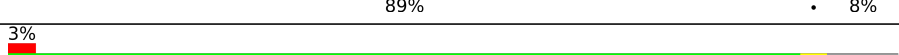
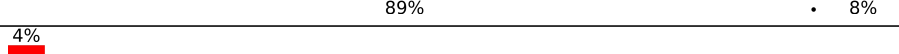


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 | 344 | |
| 1 | a | 344 | |
| 2 | B | 510 | |
| 2 | b | 510 | |

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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 | 461 | %  97% .. |
| 3 | c | 461 | %  97% .. |
| 4 | D | 352 |  96% .. |
| 4 | d | 352 | %  96% .. |
| 5 | E | 84 | 10%  96% . |
| 5 | e | 84 | 14%  96% .. |
| 6 | F | 45 |  76% 24% |
| 6 | f | 45 |  76% 24% |
| 7 | H | 63 | 3%  97% . |
| 7 | h | 63 |  98% . |
| 8 | I | 38 | 5%  95% 5% |
| 8 | i | 38 | 8%  89% 5% 5% |
| 9 | J | 40 | 5%  88% . 10% |
| 9 | j | 40 | 5%  88% . 10% |
| 10 | K | 46 | 9%  78% . 20% |
| 10 | k | 46 |  78% . 20% |
| 11 | L | 37 |  100% |
| 11 | l | 37 | 3%  100% |
| 12 | M | 36 | 3%  89% . 8% |
| 12 | m | 36 | 3%  89% . 8% |
| 13 | O | 272 | 4%  89% . 10% |
| 13 | o | 272 | 3%  86% . 10% |
| 14 | T | 32 | 3%  94% 6% |
| 14 | t | 32 |  94% 6% |
| 15 | U | 134 | 2%  72% 28% |

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

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25 | CLA | A | 606 | X | - | - | - |
| 25 | CLA | A | 607 | X | - | - | - |
| 25 | CLA | A | 609 | X | - | - | - |
| 25 | CLA | B | 602 | X | - | - | - |
| 25 | CLA | B | 603 | X | - | - | - |
| 25 | CLA | B | 604 | X | - | - | - |
| 25 | CLA | B | 605 | X | - | - | - |
| 25 | CLA | B | 606 | X | - | - | - |
| 25 | CLA | B | 607 | X | - | - | - |
| 25 | CLA | B | 608 | X | - | - | - |
| 25 | CLA | B | 609 | X | - | - | - |
| 25 | CLA | B | 610 | X | - | - | - |
| 25 | CLA | B | 611 | X | - | - | - |
| 25 | CLA | B | 612 | X | - | - | - |
| 25 | CLA | B | 613 | X | - | - | - |
| 25 | CLA | B | 614 | X | - | - | - |
| 25 | CLA | B | 615 | X | - | - | - |
| 25 | CLA | B | 616 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25 | CLA | B | 617 | X | - | - | - |
| 25 | CLA | C | 502 | X | - | - | - |
| 25 | CLA | C | 503 | X | - | - | - |
| 25 | CLA | C | 504 | X | - | - | - |
| 25 | CLA | C | 505 | X | - | - | - |
| 25 | CLA | C | 506 | X | - | - | - |
| 25 | CLA | C | 507 | X | - | - | - |
| 25 | CLA | C | 508 | X | - | - | - |
| 25 | CLA | C | 509 | X | - | - | - |
| 25 | CLA | C | 510 | X | - | - | - |
| 25 | CLA | C | 511 | X | - | - | - |
| 25 | CLA | C | 512 | X | - | - | - |
| 25 | CLA | C | 513 | X | - | - | - |
| 25 | CLA | C | 514 | X | - | - | - |
| 25 | CLA | D | 402 | X | - | - | - |
| 25 | CLA | D | 403 | X | - | - | - |
| 25 | CLA | D | 404 | X | - | - | - |
| 25 | CLA | a | 707 | X | - | - | - |
| 25 | CLA | a | 708 | X | - | - | - |
| 25 | CLA | a | 711 | X | - | - | - |
| 25 | CLA | a | 719 | X | - | - | - |
| 25 | CLA | b | 607 | X | - | - | - |
| 25 | CLA | b | 608 | X | - | - | - |
| 25 | CLA | b | 609 | X | - | - | - |
| 25 | CLA | b | 610 | X | - | - | - |
| 25 | CLA | b | 611 | X | - | - | - |
| 25 | CLA | b | 612 | X | - | - | - |
| 25 | CLA | b | 613 | X | - | - | - |
| 25 | CLA | b | 614 | X | - | - | - |
| 25 | CLA | b | 615 | X | - | - | - |
| 25 | CLA | b | 616 | X | - | - | - |
| 25 | CLA | b | 617 | X | - | - | - |
| 25 | CLA | b | 618 | X | - | - | - |
| 25 | CLA | b | 619 | X | - | - | - |
| 25 | CLA | b | 620 | X | - | - | - |
| 25 | CLA | b | 621 | X | - | - | - |
| 25 | CLA | b | 622 | X | - | - | - |
| 25 | CLA | c | 501 | X | - | - | - |
| 25 | CLA | c | 502 | X | - | - | - |
| 25 | CLA | c | 503 | X | - | - | - |
| 25 | CLA | c | 504 | X | - | - | - |
| 25 | CLA | c | 505 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25 | CLA | c | 506 | X | - | - | - |
| 25 | CLA | c | 507 | X | - | - | - |
| 25 | CLA | c | 508 | X | - | - | - |
| 25 | CLA | c | 509 | X | - | - | - |
| 25 | CLA | c | 510 | X | - | - | - |
| 25 | CLA | c | 511 | X | - | - | - |
| 25 | CLA | c | 512 | X | - | - | - |
| 25 | CLA | c | 513 | X | - | - | - |
| 25 | CLA | d | 402 | X | - | - | - |
| 25 | CLA | d | 403 | X | - | - | - |
| 29 | SQD | I | 102 | - | - | - | X |

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50284 atoms, of which 0 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 | N | O | S | 0 | 0 | 0 |
| | | | 2622 | 1717 | 431 | 459 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2622 | 1717 | 431 | 459 | 15 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3969 | 2605 | 661 | 690 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3968 | 2605 | 661 | 689 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 13 | | | |
| 3 | c | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2716 | 1800 | 444 | 460 | 12 | | | |
| 4 | d | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2716 | 1800 | 444 | 460 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5 | E | 81 | Total | C | N | O | 0 | 0 | 0 |
| | | | 661 | 432 | 107 | 122 | | | |
| 5 | e | 82 | Total | C | N | O | 0 | 0 | 0 |
| | | | 665 | 434 | 108 | 123 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6 | F | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |
| 6 | f | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | H | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 498 | 333 | 80 | 83 | 2 | | | |
| 7 | h | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 498 | 333 | 80 | 83 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | I | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 296 | 200 | 46 | 49 | 1 | | | |
| 8 | i | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 296 | 200 | 46 | 49 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| I | 1 | FME | - | expression tag | UNP Q8DJZ6 |
| i | 1 | FME | - | expression tag | UNP Q8DJZ6 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | J | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 257 | 174 | 40 | 42 | 1 | | | |
| 9 | j | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 257 | 174 | 40 | 42 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | K | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |
| 10 | k | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 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 | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |
| 11 | l | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | M | 33 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 260 | 173 | 38 | 48 | 1 | | | |
| 12 | m | 33 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 260 | 173 | 38 | 48 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | 1 | FME | - | expression tag | UNP Q8DHA7 |
| m | 1 | FME | - | expression tag | UNP Q8DHA7 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | O | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1874 | 1170 | 317 | 383 | 4 | | | |
| 13 | o | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1874 | 1170 | 317 | 383 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | T | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 258 | 181 | 36 | 39 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | t | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 258 | 181 | 36 | 39 | 2 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| T | 1 | FME | - | expression tag | UNP Q8DIQ0 |
| t | 1 | FME | - | expression tag | UNP Q8DIQ0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15 | U | 97 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | | |
| 15 | u | 97 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | V | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 177 | 208 | 4 | | | |
| 16 | v | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 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 | N | O | S | 0 | 0 | 0 |
| | | | 200 | 131 | 35 | 31 | 3 | | | |
| 17 | y | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 224 | 147 | 38 | 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 | N | O | | 0 | 0 | 0 |
| | | | 281 | 188 | 45 | 48 | | | | |
| 18 | x | 38 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 279 | 187 | 45 | 47 | | | | |

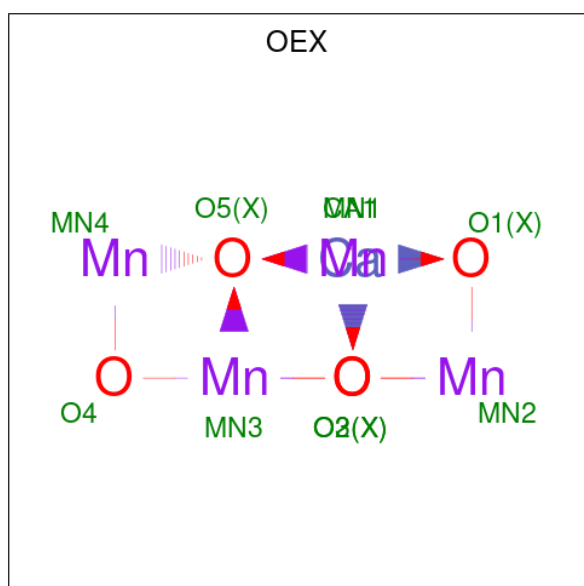
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 19 | Z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |
| 19 | z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 478 | 328 | 72 | 76 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 20 | R | 34 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 273 | 186 | 47 | 40 | | | | |
| 20 | r | 34 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 270 | 183 | 47 | 40 | | | | |

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|--|---------|---------|
| 21 | A | 1 | Total | Ca | Mn | O | | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | | |
| 21 | a | 1 | Total | Ca | Mn | O | | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | | |

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

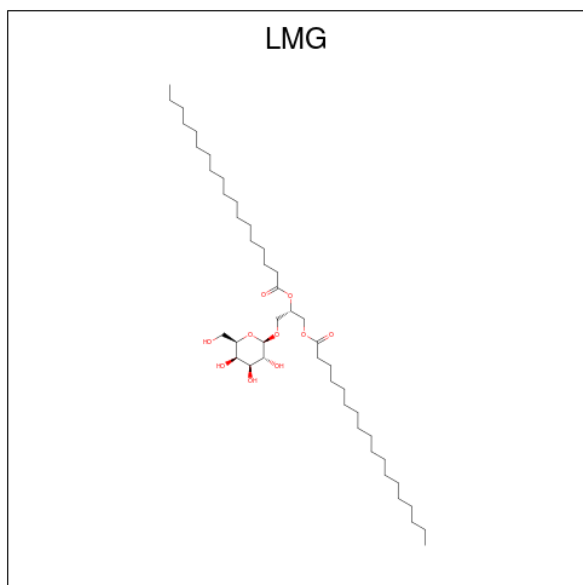
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | A | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | a | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23 | A | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | B | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | D | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | M | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | a | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | a | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | b | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |

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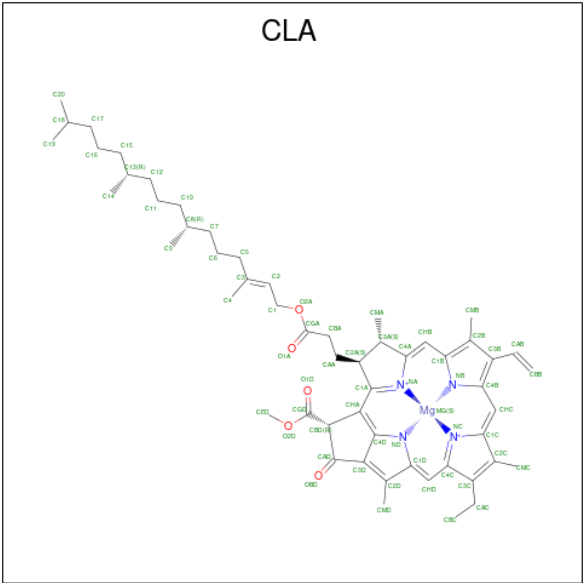
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23 | b | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | b | 1 | Total | C | | 0 | 0 |
| | | | 9 | 9 | | | |
| 23 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 23 | d | 1 | Total | C | O | 0 | 0 |
| | | | 40 | 35 | 5 | | |
| 23 | f | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 24 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 24 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 25 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | A | 1 | Total 54 | C 44 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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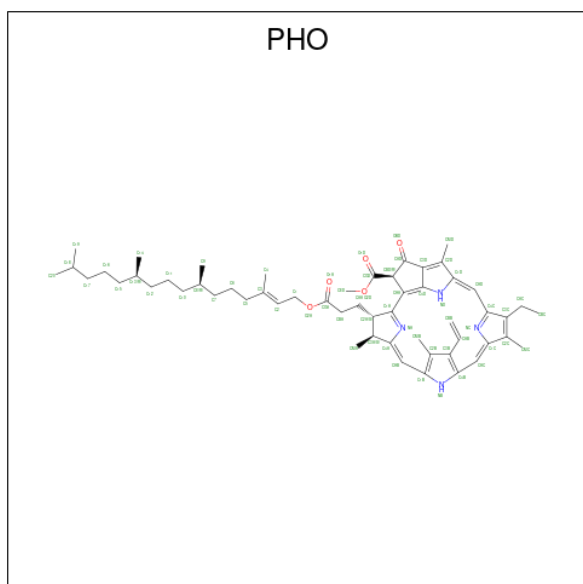
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | b | 1 | Total 47 | C 37 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 58 | C 48 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 25 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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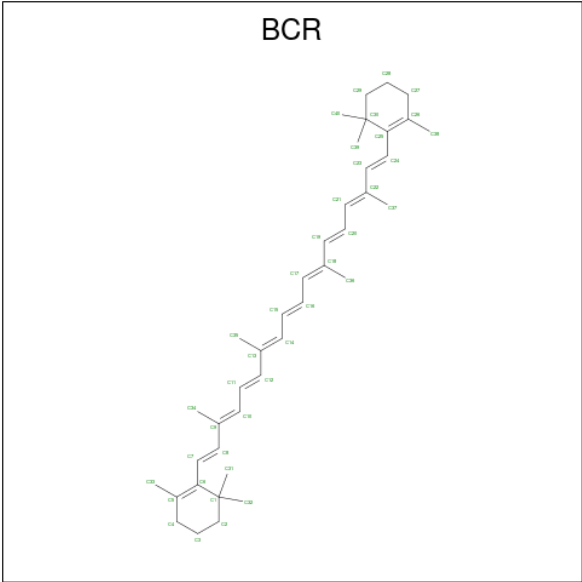
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 25 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 25 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 25 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 25 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 25 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 25 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 26 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 26 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 26 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 26 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



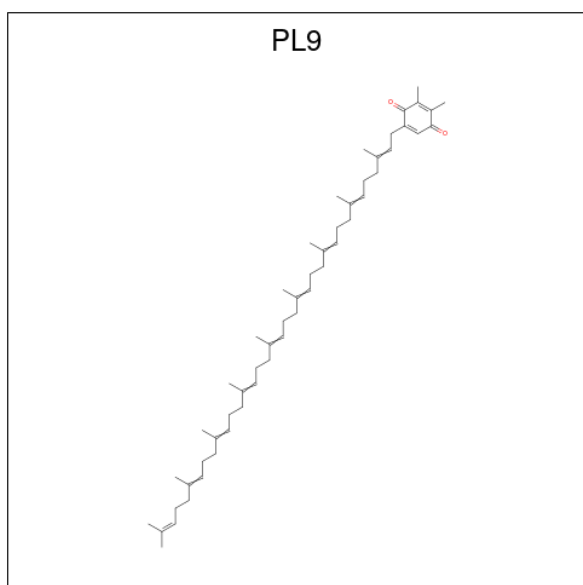
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 27 | A | 1 | Total C 40 40 | 0 | 0 |
| 27 | B | 1 | Total C 40 40 | 0 | 0 |
| 27 | B | 1 | Total C 40 40 | 0 | 0 |
| 27 | B | 1 | Total C 40 40 | 0 | 0 |
| 27 | C | 1 | Total C 40 40 | 0 | 0 |
| 27 | C | 1 | Total C 40 40 | 0 | 0 |
| 27 | D | 1 | Total C 40 40 | 0 | 0 |
| 27 | H | 1 | Total C 40 40 | 0 | 0 |
| 27 | K | 1 | Total C 40 40 | 0 | 0 |
| 27 | Y | 1 | Total C 40 40 | 0 | 0 |
| 27 | a | 1 | Total C 40 40 | 0 | 0 |
| 27 | b | 1 | Total C 40 40 | 0 | 0 |
| 27 | b | 1 | Total C 40 40 | 0 | 0 |
| 27 | b | 1 | Total C 40 40 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 27 | b | 1 | Total C 40 40 | 0 | 0 |
| 27 | c | 1 | Total C 40 40 | 0 | 0 |
| 27 | c | 1 | Total C 40 40 | 0 | 0 |
| 27 | d | 1 | Total C 40 40 | 0 | 0 |
| 27 | h | 1 | Total C 40 40 | 0 | 0 |
| 27 | k | 1 | Total C 40 40 | 0 | 0 |
| 27 | k | 1 | Total C 40 40 | 0 | 0 |
| 27 | t | 1 | Total C 40 40 | 0 | 0 |

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



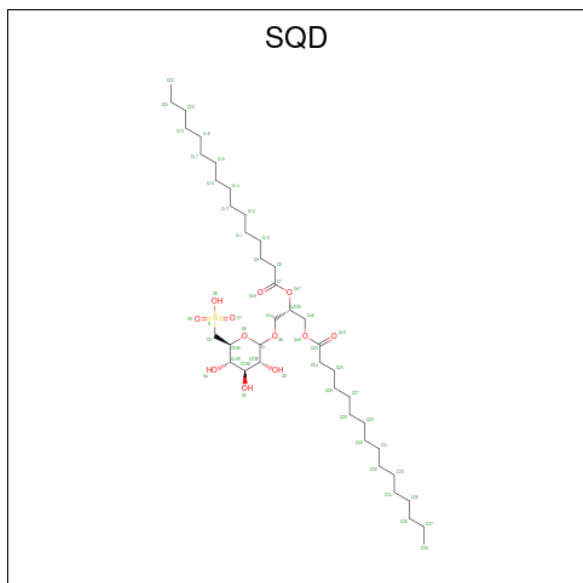
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 28 | A | 1 | Total C O 55 53 2 | 0 | 0 |
| 28 | D | 1 | Total C O 55 53 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | d | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).

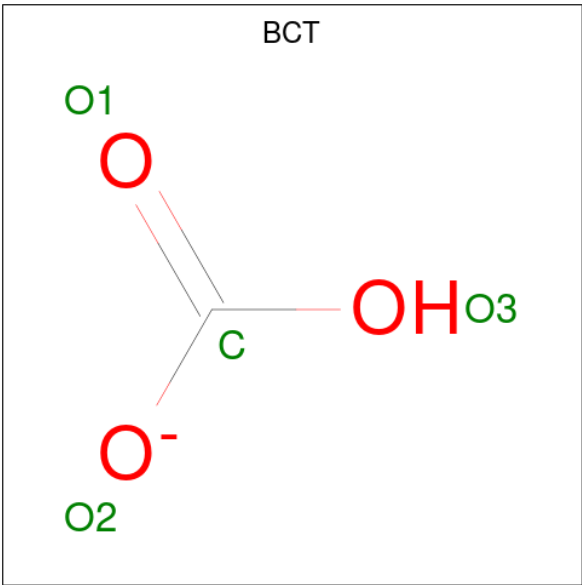


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 29 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 52 | 39 | 12 | 1 | | |
| 29 | A | 1 | Total | C | O | | 0 | 0 |
| | | | 40 | 35 | 5 | | | |
| 29 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 47 | 34 | 12 | 1 | | |
| 29 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 29 | D | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 29 | I | 1 | Total | C | O | | 0 | 0 |
| | | | 40 | 35 | 5 | | | |
| 29 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 29 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 29 | f | 1 | Total | C | O | S | 0 | 0 |
| | | | 41 | 28 | 12 | 1 | | |

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

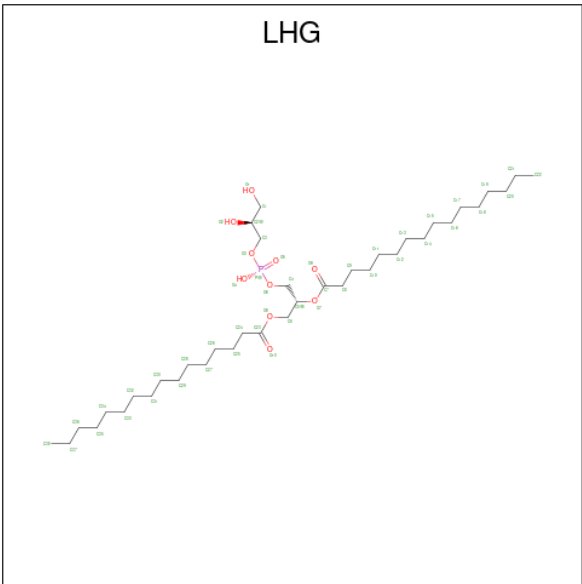
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 30 | A | 1 | Total C 7 7 | 0 | 0 |
| 30 | B | 3 | Total C 29 29 | 0 | 0 |
| 30 | H | 1 | Total C 8 8 | 0 | 0 |
| 30 | I | 1 | Total C 9 9 | 0 | 0 |
| 30 | M | 2 | Total C 22 22 | 0 | 0 |
| 30 | a | 3 | Total C 24 24 | 0 | 0 |
| 30 | b | 4 | Total C 48 48 | 0 | 0 |
| 30 | d | 1 | Total C 22 22 | 0 | 0 |
| 30 | i | 1 | Total C 22 22 | 0 | 0 |
| 30 | j | 1 | Total C 9 9 | 0 | 0 |
| 30 | m | 2 | Total C 17 17 | 0 | 0 |
| 30 | t | 2 | Total C 15 15 | 0 | 0 |
| 30 | z | 1 | Total C 11 11 | 0 | 0 |

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



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 31 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 31 | a | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



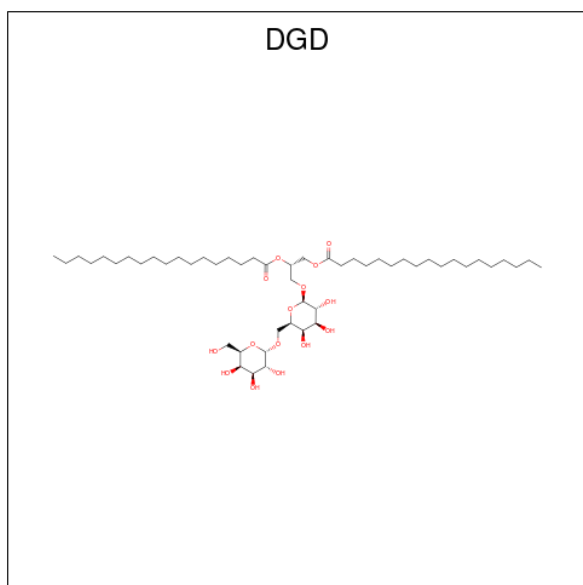
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 32 | B | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | a | 1 | Total | C | O | P | 0 | 0 |
| | | | 39 | 28 | 10 | 1 | | |
| 32 | b | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | e | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



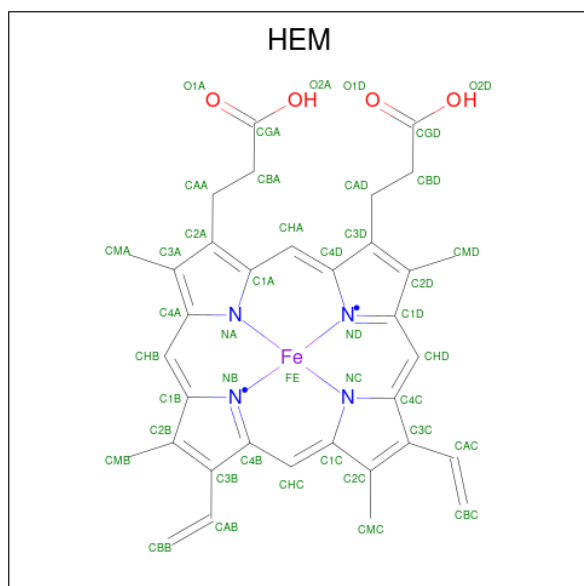
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 33 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

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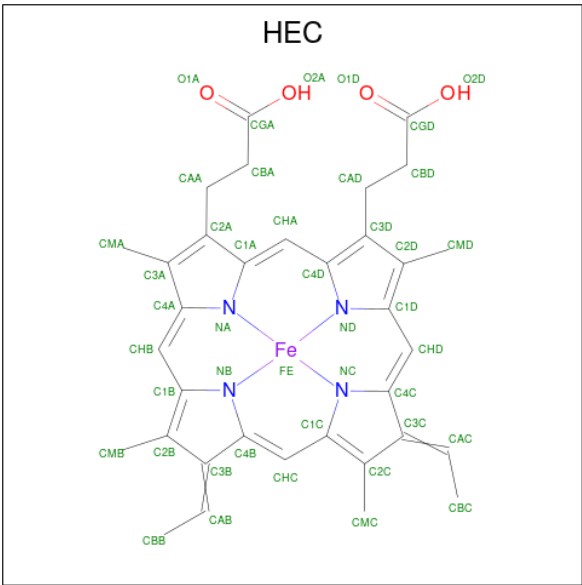
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 33 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | H | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 33 | h | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 34 | E | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 34 | e | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 35 | V | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 35 | v | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

- Molecule 36 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 36 | A | 14 | Total | O | 0 | 0 |
| | | | 14 | 14 | | |
| 36 | B | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 36 | C | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 36 | D | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 36 | H | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | K | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | L | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | M | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | O | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 36 | U | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

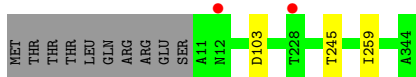
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 36 | V | 6 | Total 6 | O 6 | 0 | 0 |
| 36 | a | 13 | Total 13 | O 13 | 0 | 0 |
| 36 | b | 12 | Total 12 | O 12 | 0 | 0 |
| 36 | c | 8 | Total 8 | O 8 | 0 | 0 |
| 36 | d | 11 | Total 11 | O 11 | 0 | 0 |
| 36 | e | 1 | Total 1 | O 1 | 0 | 0 |
| 36 | h | 1 | Total 1 | O 1 | 0 | 0 |
| 36 | l | 1 | Total 1 | O 1 | 0 | 0 |
| 36 | o | 5 | Total 5 | O 5 | 0 | 0 |
| 36 | u | 5 | Total 5 | O 5 | 0 | 0 |
| 36 | v | 3 | Total 3 | O 3 | 0 | 0 |
| 36 | z | 1 | Total 1 | O 1 | 0 | 0 |

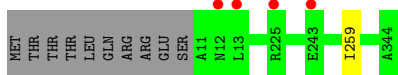
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

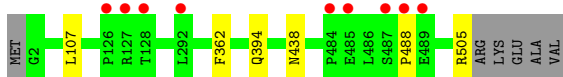
- Molecule 1: Photosystem II protein D1 1



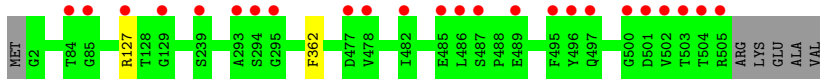
- Molecule 1: Photosystem II protein D1 1



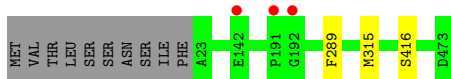
- Molecule 2: Photosystem II CP47 reaction center protein



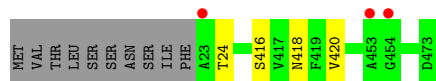
- Molecule 2: Photosystem II CP47 reaction center protein



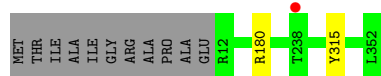
- Molecule 3: Photosystem II CP43 reaction center protein



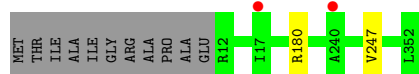
- Molecule 3: Photosystem II CP43 reaction center protein



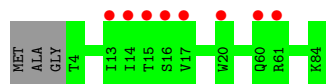
- Molecule 4: Photosystem II D2 protein



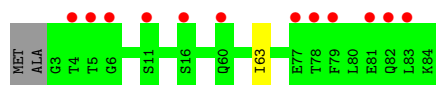
- Molecule 4: Photosystem II D2 protein



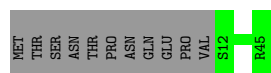
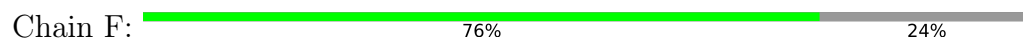
- Molecule 5: Cytochrome b559 subunit alpha



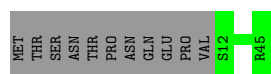
- Molecule 5: Cytochrome b559 subunit alpha



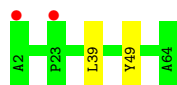
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



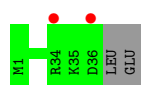
- Molecule 7: Photosystem II reaction center protein H



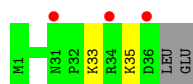
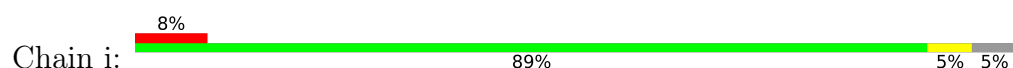
- Molecule 7: Photosystem II reaction center protein H



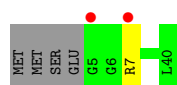
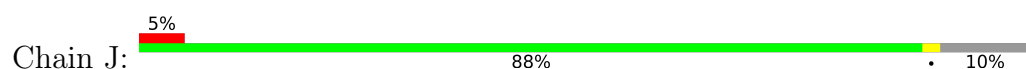
- Molecule 8: Photosystem II reaction center protein I



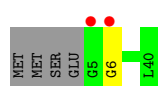
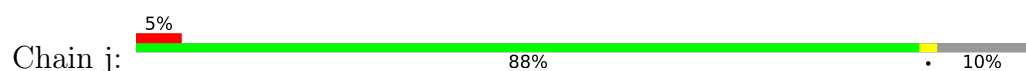
- Molecule 8: Photosystem II reaction center protein I



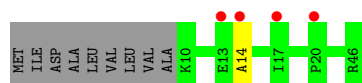
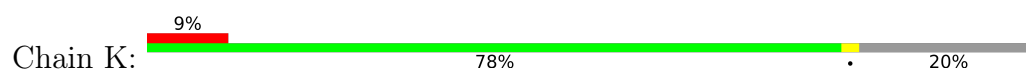
- Molecule 9: Photosystem II reaction center protein J




- Molecule 9: Photosystem II reaction center protein J

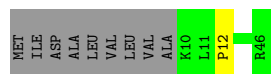


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

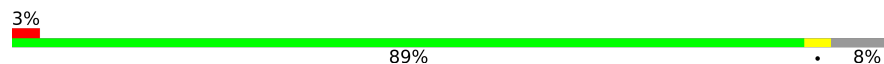
There are no outlier residues recorded for this chain.

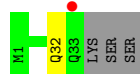
- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 100%

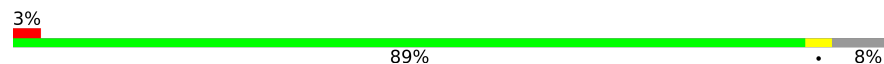


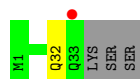
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 89% 8%

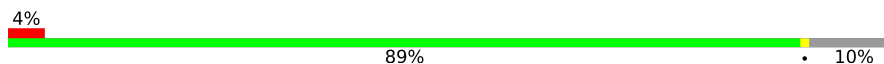


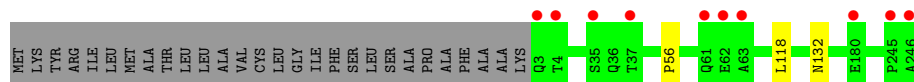
- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 89% 8%




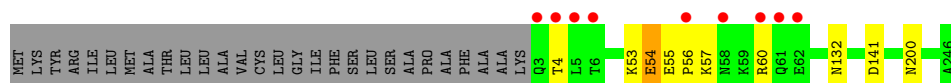
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  4% 89% 10%

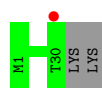


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

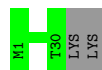
Chain o:  3% 86% 10%



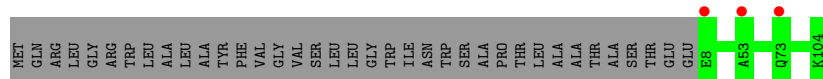
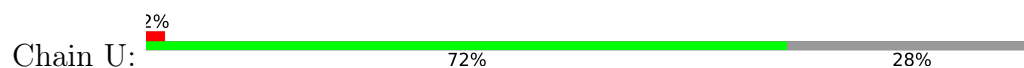
- Molecule 14: Photosystem II reaction center protein T



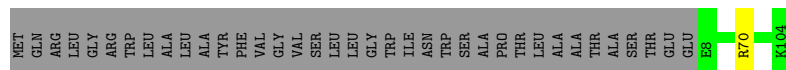
- Molecule 14: Photosystem II reaction center protein T



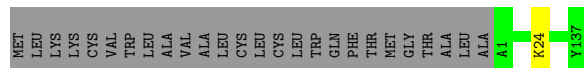
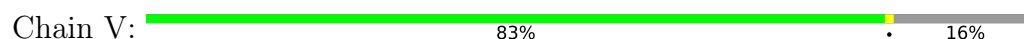
- Molecule 15: Photosystem II 12 kDa extrinsic protein



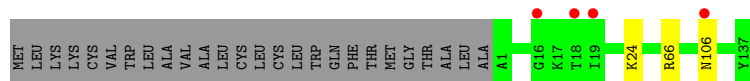
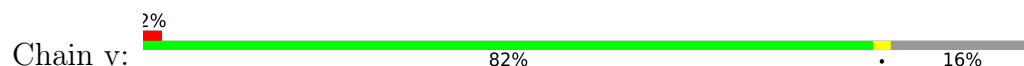
- Molecule 15: Photosystem II 12 kDa extrinsic protein



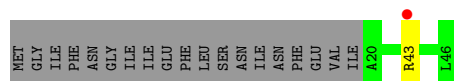
- Molecule 16: Cytochrome c-550



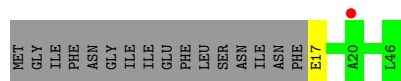
- Molecule 16: Cytochrome c-550



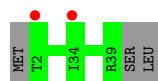
- Molecule 17: Photosystem II reaction center protein Ycf12



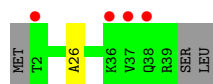
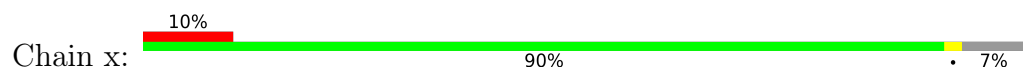
- Molecule 17: Photosystem II reaction center protein Ycf12



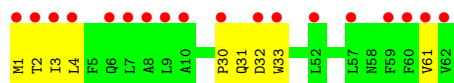
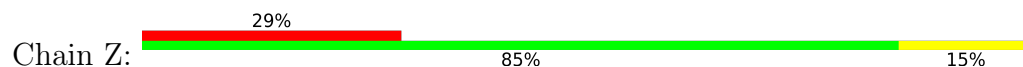
- Molecule 18: Photosystem II reaction center X protein



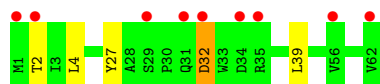
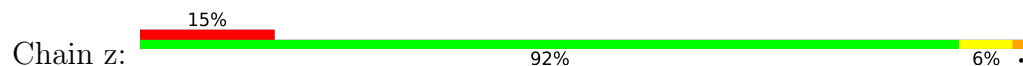
- Molecule 18: Photosystem II reaction center X protein



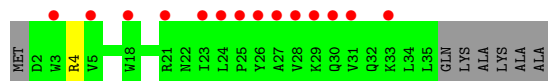
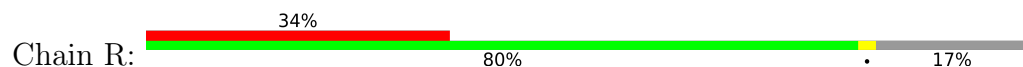
- Molecule 19: Photosystem II reaction center protein Z



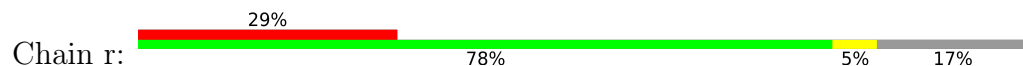
- Molecule 19: Photosystem II reaction center protein Z

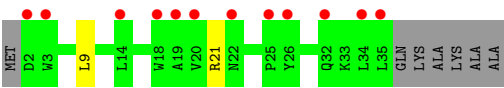


- Molecule 20: Photosystem II protein Y



- 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 | 117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 43.57 – 2.80 43.57 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 98.0 (43.57-2.80) 87.7 (43.57-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.11 (at 2.81Å) | Xtriage |
| Refinement program | PHENIX dev_2411 | Depositor |
| R, R_{free} | 0.250 , 0.300 0.250 , 0.300 | Depositor DCC |
| R_{free} test set | 1792 reflections (0.84%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 48.9 | Xtriage |
| Anisotropy | 0.225 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 50.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 50284 | wwPDB-VP |
| Average B, all atoms (Å ²) | 56.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|---------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.26 | 0/2707 | 0.42 | 0/3692 |
| 1 | a | 0.25 | 0/2707 | 0.40 | 0/3692 |
| 2 | B | 0.26 | 0/4109 | 0.41 | 0/5600 |
| 2 | b | 0.25 | 0/4111 | 0.41 | 0/5603 |
| 3 | C | 0.25 | 0/3599 | 0.40 | 0/4900 |
| 3 | c | 0.26 | 0/3599 | 0.43 | 0/4900 |
| 4 | D | 0.25 | 0/2811 | 0.40 | 0/3830 |
| 4 | d | 0.25 | 0/2811 | 0.40 | 0/3830 |
| 5 | E | 0.26 | 0/680 | 0.42 | 0/928 |
| 5 | e | 0.32 | 1/684 (0.1%) | 0.40 | 0/933 |
| 6 | F | 0.25 | 0/284 | 0.40 | 0/387 |
| 6 | f | 0.24 | 0/284 | 0.36 | 0/387 |
| 7 | H | 0.27 | 0/511 | 0.44 | 0/697 |
| 7 | h | 0.24 | 0/511 | 0.41 | 0/697 |
| 8 | I | 0.26 | 0/293 | 0.40 | 0/396 |
| 8 | i | 0.56 | 1/293 (0.3%) | 0.54 | 0/396 |
| 9 | J | 0.24 | 0/263 | 0.38 | 0/356 |
| 9 | j | 0.24 | 0/263 | 0.38 | 0/356 |
| 10 | K | 0.30 | 0/303 | 0.50 | 0/416 |
| 10 | k | 0.43 | 0/303 | 0.45 | 0/416 |
| 11 | L | 0.27 | 0/311 | 0.43 | 0/422 |
| 11 | l | 0.24 | 0/311 | 0.38 | 0/422 |
| 12 | M | 0.24 | 0/253 | 0.35 | 0/346 |
| 12 | m | 0.24 | 0/253 | 0.33 | 0/346 |
| 13 | O | 0.26 | 0/1905 | 0.46 | 0/2583 |
| 13 | o | 0.27 | 0/1905 | 0.52 | 1/2583 (0.0%) |
| 14 | T | 0.27 | 0/257 | 0.36 | 0/349 |
| 14 | t | 0.26 | 0/257 | 0.36 | 0/349 |
| 15 | U | 0.24 | 0/785 | 0.43 | 0/1064 |
| 15 | u | 0.26 | 0/785 | 0.48 | 0/1064 |
| 16 | V | 0.23 | 0/1085 | 0.43 | 0/1473 |
| 16 | v | 0.23 | 0/1085 | 0.44 | 0/1473 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | Y | 0.23 | 0/201 | 0.41 | 0/268 |
| 17 | y | 0.35 | 0/225 | 0.45 | 0/301 |
| 18 | X | 0.25 | 0/284 | 0.42 | 0/384 |
| 18 | x | 0.24 | 0/282 | 0.39 | 0/381 |
| 19 | Z | 0.30 | 0/490 | 0.51 | 0/669 |
| 19 | z | 0.35 | 0/489 | 0.52 | 0/669 |
| 20 | R | 0.27 | 0/279 | 0.52 | 0/383 |
| 20 | r | 0.25 | 0/276 | 0.51 | 0/379 |
| All | All | 0.26 | 2/42844 (0.0%) | 0.42 | 1/58320 (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 |
|-----|-------|---------------------|---------------------|
| 13 | o | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | i | 33 | LYS | CB-CG | -6.06 | 1.36 | 1.52 |
| 5 | e | 63 | ILE | C-N | 5.53 | 1.44 | 1.34 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 13 | o | 54 | GLU | C-N-CA | 5.75 | 136.08 | 121.70 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 13 | o | 4 | THR | 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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | A | 332/344 (96%) | 324 (98%) | 7 (2%) | 1 (0%) | 41 | 72 |
| 1 | a | 332/344 (96%) | 325 (98%) | 6 (2%) | 1 (0%) | 41 | 72 |
| 2 | B | 502/510 (98%) | 482 (96%) | 19 (4%) | 1 (0%) | 47 | 78 |
| 2 | b | 503/510 (99%) | 484 (96%) | 19 (4%) | 0 | 100 | 100 |
| 3 | C | 449/461 (97%) | 431 (96%) | 17 (4%) | 1 (0%) | 47 | 78 |
| 3 | c | 449/461 (97%) | 430 (96%) | 17 (4%) | 2 (0%) | 34 | 66 |
| 4 | D | 339/352 (96%) | 325 (96%) | 14 (4%) | 0 | 100 | 100 |
| 4 | d | 339/352 (96%) | 323 (95%) | 16 (5%) | 0 | 100 | 100 |
| 5 | E | 79/84 (94%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 5 | e | 80/84 (95%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 6 | F | 32/45 (71%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 6 | f | 32/45 (71%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 61/63 (97%) | 54 (88%) | 7 (12%) | 0 | 100 | 100 |
| 7 | h | 61/63 (97%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 8 | I | 34/38 (90%) | 29 (85%) | 5 (15%) | 0 | 100 | 100 |
| 8 | i | 34/38 (90%) | 31 (91%) | 3 (9%) | 0 | 100 | 100 |
| 9 | J | 34/40 (85%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | j | 34/40 (85%) | 32 (94%) | 1 (3%) | 1 (3%) | 4 | 15 |
| 10 | K | 35/46 (76%) | 33 (94%) | 1 (3%) | 1 (3%) | 4 | 15 |
| 10 | k | 35/46 (76%) | 32 (91%) | 2 (6%) | 1 (3%) | 4 | 15 |
| 11 | L | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 11 | l | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 12 | M | 31/36 (86%) | 29 (94%) | 1 (3%) | 1 (3%) | 4 | 13 |
| 12 | m | 31/36 (86%) | 29 (94%) | 1 (3%) | 1 (3%) | 4 | 13 |
| 13 | O | 242/272 (89%) | 230 (95%) | 10 (4%) | 2 (1%) | 19 | 49 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13 | o | 242/272 (89%) | 223 (92%) | 15 (6%) | 4 (2%) | 9 | 29 |
| 14 | T | 28/32 (88%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 28/32 (88%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 15 | U | 95/134 (71%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | u | 95/134 (71%) | 88 (93%) | 7 (7%) | 0 | 100 | 100 |
| 16 | V | 135/163 (83%) | 129 (96%) | 6 (4%) | 0 | 100 | 100 |
| 16 | v | 135/163 (83%) | 125 (93%) | 10 (7%) | 0 | 100 | 100 |
| 17 | Y | 25/46 (54%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 17 | y | 28/46 (61%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 18 | X | 36/41 (88%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 18 | x | 36/41 (88%) | 32 (89%) | 3 (8%) | 1 (3%) | 5 | 17 |
| 19 | Z | 60/62 (97%) | 51 (85%) | 1 (2%) | 8 (13%) | 0 | 0 |
| 19 | z | 60/62 (97%) | 53 (88%) | 4 (7%) | 3 (5%) | 2 | 6 |
| 20 | R | 32/41 (78%) | 29 (91%) | 3 (9%) | 0 | 100 | 100 |
| 20 | r | 32/41 (78%) | 30 (94%) | 1 (3%) | 1 (3%) | 4 | 14 |
| All | All | 5237/5694 (92%) | 4987 (95%) | 220 (4%) | 30 (1%) | 25 | 56 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | Z | 30 | PRO |
| 19 | Z | 31 | GLN |
| 19 | Z | 33 | TRP |
| 19 | Z | 61 | VAL |
| 3 | c | 24 | THR |
| 10 | k | 12 | PRO |
| 13 | o | 53 | LYS |
| 13 | o | 55 | GLU |
| 19 | z | 32 | ASP |
| 3 | C | 416 | SER |
| 10 | K | 14 | ALA |
| 12 | M | 32 | GLN |
| 19 | Z | 3 | ILE |
| 19 | Z | 32 | ASP |
| 3 | c | 416 | SER |
| 18 | x | 26 | ALA |
| 13 | O | 132 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | Z | 2 | THR |
| 13 | o | 54 | GLU |
| 1 | a | 259 | ILE |
| 19 | z | 2 | THR |
| 19 | z | 4 | LEU |
| 20 | r | 21 | ARG |
| 13 | O | 56 | PRO |
| 19 | Z | 4 | LEU |
| 12 | m | 32 | GLN |
| 2 | B | 488 | PRO |
| 9 | j | 6 | GLY |
| 1 | A | 259 | ILE |
| 13 | o | 56 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | A | 270/280 (96%) | 268 (99%) | 2 (1%) | 84 | 95 |
| 1 | a | 270/280 (96%) | 270 (100%) | 0 | 100 | 100 |
| 2 | B | 402/407 (99%) | 397 (99%) | 5 (1%) | 71 | 92 |
| 2 | b | 402/407 (99%) | 400 (100%) | 2 (0%) | 88 | 96 |
| 3 | C | 352/362 (97%) | 350 (99%) | 2 (1%) | 86 | 96 |
| 3 | c | 352/362 (97%) | 350 (99%) | 2 (1%) | 86 | 96 |
| 4 | D | 276/283 (98%) | 274 (99%) | 2 (1%) | 84 | 95 |
| 4 | d | 276/283 (98%) | 274 (99%) | 2 (1%) | 84 | 95 |
| 5 | E | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 5 | e | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 6 | F | 28/39 (72%) | 28 (100%) | 0 | 100 | 100 |
| 6 | f | 28/39 (72%) | 28 (100%) | 0 | 100 | 100 |
| 7 | H | 53/53 (100%) | 51 (96%) | 2 (4%) | 33 | 67 |
| 7 | h | 53/53 (100%) | 52 (98%) | 1 (2%) | 57 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8 | I | 32/34 (94%) | 32 (100%) | 0 | 100 | 100 |
| 8 | i | 32/34 (94%) | 31 (97%) | 1 (3%) | 40 | 74 |
| 9 | J | 24/28 (86%) | 23 (96%) | 1 (4%) | 30 | 63 |
| 9 | j | 24/28 (86%) | 24 (100%) | 0 | 100 | 100 |
| 10 | K | 30/37 (81%) | 30 (100%) | 0 | 100 | 100 |
| 10 | k | 30/37 (81%) | 30 (100%) | 0 | 100 | 100 |
| 11 | L | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 11 | l | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 12 | M | 29/32 (91%) | 29 (100%) | 0 | 100 | 100 |
| 12 | m | 29/32 (91%) | 29 (100%) | 0 | 100 | 100 |
| 13 | O | 207/228 (91%) | 206 (100%) | 1 (0%) | 88 | 96 |
| 13 | o | 207/228 (91%) | 202 (98%) | 5 (2%) | 49 | 81 |
| 14 | T | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 14 | t | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 15 | U | 84/112 (75%) | 84 (100%) | 0 | 100 | 100 |
| 15 | u | 84/112 (75%) | 83 (99%) | 1 (1%) | 71 | 92 |
| 16 | V | 117/138 (85%) | 116 (99%) | 1 (1%) | 78 | 94 |
| 16 | v | 117/138 (85%) | 114 (97%) | 3 (3%) | 46 | 79 |
| 17 | Y | 20/37 (54%) | 19 (95%) | 1 (5%) | 24 | 56 |
| 17 | y | 23/37 (62%) | 22 (96%) | 1 (4%) | 29 | 62 |
| 18 | X | 31/34 (91%) | 31 (100%) | 0 | 100 | 100 |
| 18 | x | 30/34 (88%) | 30 (100%) | 0 | 100 | 100 |
| 19 | Z | 52/52 (100%) | 51 (98%) | 1 (2%) | 57 | 85 |
| 19 | z | 52/52 (100%) | 49 (94%) | 3 (6%) | 20 | 50 |
| 20 | R | 29/33 (88%) | 28 (97%) | 1 (3%) | 37 | 71 |
| 20 | r | 28/33 (85%) | 27 (96%) | 1 (4%) | 35 | 69 |
| All | All | 4339/4650 (93%) | 4298 (99%) | 41 (1%) | 78 | 94 |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 103 | ASP |
| 1 | A | 245 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 107 | LEU |
| 2 | B | 362 | PHE |
| 2 | B | 394 | GLN |
| 2 | B | 438 | ASN |
| 2 | B | 505 | ARG |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 4 | D | 180 | ARG |
| 4 | D | 315 | TYR |
| 7 | H | 39 | LEU |
| 7 | H | 49 | TYR |
| 9 | J | 7 | ARG |
| 13 | O | 118 | LEU |
| 16 | V | 24 | LYS |
| 17 | Y | 43 | ARG |
| 19 | Z | 1 | MET |
| 20 | R | 4 | ARG |
| 2 | b | 127 | ARG |
| 2 | b | 362 | PHE |
| 3 | c | 418 | ASN |
| 3 | c | 420 | VAL |
| 4 | d | 180 | ARG |
| 4 | d | 247 | VAL |
| 7 | h | 49 | TYR |
| 8 | i | 35 | LYS |
| 13 | o | 57 | LYS |
| 13 | o | 60 | ARG |
| 13 | o | 132 | ASN |
| 13 | o | 141 | ASP |
| 13 | o | 200 | ASN |
| 15 | u | 70 | ARG |
| 16 | v | 24 | LYS |
| 16 | v | 66 | ARG |
| 16 | v | 106 | ASN |
| 17 | y | 17 | GLU |
| 19 | z | 27 | TYR |
| 19 | z | 32 | ASP |
| 19 | z | 39 | LEU |
| 20 | r | 9 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 241 | GLN |
| 1 | A | 252 | HIS |
| 1 | A | 312 | ASN |
| 2 | B | 216 | HIS |
| 2 | B | 409 | GLN |
| 3 | C | 201 | ASN |
| 3 | C | 311 | GLN |
| 4 | D | 98 | GLN |
| 5 | E | 74 | GLN |
| 11 | L | 6 | ASN |
| 13 | O | 82 | GLN |
| 13 | O | 130 | GLN |
| 13 | O | 200 | ASN |
| 15 | U | 29 | ASN |
| 16 | V | 106 | ASN |
| 20 | R | 32 | GLN |
| 1 | a | 261 | GLN |
| 1 | a | 335 | ASN |
| 2 | b | 216 | HIS |
| 2 | b | 223 | GLN |
| 2 | b | 409 | GLN |
| 3 | c | 311 | GLN |
| 4 | d | 239 | GLN |
| 5 | e | 74 | GLN |
| 13 | o | 46 | GLN |
| 13 | o | 61 | GLN |
| 13 | o | 147 | ASN |
| 13 | o | 236 | GLN |
| 16 | v | 25 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 12 | FME | M | 1 | 12 | 8,9,10 | 0.90 | 0 | 7,9,11 | 0.86 | 0 |
| 14 | FME | t | 1 | 14 | 8,9,10 | 0.94 | 0 | 7,9,11 | 0.86 | 0 |
| 8 | FME | I | 1 | 8 | 8,9,10 | 0.95 | 0 | 7,9,11 | 1.08 | 0 |
| 12 | FME | m | 1 | 12 | 8,9,10 | 0.94 | 0 | 7,9,11 | 0.89 | 0 |
| 8 | FME | i | 1 | 8 | 8,9,10 | 0.94 | 0 | 7,9,11 | 0.92 | 0 |
| 14 | FME | T | 1 | 14 | 8,9,10 | 0.95 | 0 | 7,9,11 | 0.92 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 12 | FME | M | 1 | 12 | - | 3/7/9/11 | - |
| 14 | FME | t | 1 | 14 | - | 2/7/9/11 | - |
| 8 | FME | I | 1 | 8 | - | 1/7/9/11 | - |
| 12 | FME | m | 1 | 12 | - | 2/7/9/11 | - |
| 8 | FME | i | 1 | 8 | - | 2/7/9/11 | - |
| 14 | FME | T | 1 | 14 | - | 3/7/9/11 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 8 | I | 1 | FME | CB-CA-N-CN |
| 12 | m | 1 | FME | CB-CA-N-CN |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 6 are monoatomic and 23 are unknown - leaving 151 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 | $\# Z > 2$ |
| 27 | BCR | h | 101 | - | 41,41,41 | 1.06 | 2 (4%) | 56,56,56 | 1.24 | 6 (10%) |
| 25 | CLA | b | 618 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.43 | 9 (13%) |
| 25 | CLA | a | 719 | 36 | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.36 | 9 (13%) |
| 33 | DGD | c | 518 | - | 63,63,67 | 0.86 | 2 (3%) | 77,77,81 | 1.41 | 11 (14%) |
| 27 | BCR | B | 620 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.19 | 4 (7%) |
| 23 | LMG | D | 409 | - | 51,51,55 | 0.72 | 0 | 59,59,63 | 1.30 | 5 (8%) |
| 23 | LMG | C | 521 | - | 51,51,55 | 0.79 | 1 (1%) | 59,59,63 | 1.37 | 6 (10%) |
| 27 | BCR | Y | 101 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.16 | 5 (8%) |
| 25 | CLA | d | 403 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.45 | 10 (14%) |
| 25 | CLA | b | 616 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.36 | 9 (13%) |
| 27 | BCR | C | 516 | - | 41,41,41 | 1.12 | 2 (4%) | 56,56,56 | 1.21 | 5 (8%) |
| 23 | LMG | B | 621 | - | 51,51,55 | 0.73 | 0 | 59,59,63 | 1.37 | 7 (11%) |
| 27 | BCR | b | 602 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.22 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | CLA | c | 513 | - | 59,73,73 | 1.35 | 5 (8%) | 67,113,113 | 1.46 | 8 (11%) |
| 27 | BCR | t | 103 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.24 | 6 (10%) |
| 28 | PL9 | d | 405 | - | 55,55,55 | 0.94 | 3 (5%) | 68,69,69 | 1.51 | 11 (16%) |
| 25 | CLA | D | 404 | - | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.40 | 10 (14%) |
| 25 | CLA | b | 619 | - | 59,73,73 | 1.37 | 5 (8%) | 67,113,113 | 1.50 | 11 (16%) |
| 25 | CLA | c | 506 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.38 | 10 (14%) |
| 33 | DGD | c | 516 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 1.41 | 9 (11%) |
| 29 | SQD | A | 612 | - | 51,52,54 | 0.96 | 5 (9%) | 60,63,65 | 1.67 | 12 (20%) |
| 27 | BCR | c | 514 | - | 41,41,41 | 1.13 | 2 (4%) | 56,56,56 | 1.23 | 7 (12%) |
| 32 | LHG | D | 408 | - | 48,48,48 | 0.60 | 0 | 51,54,54 | 1.24 | 6 (11%) |
| 25 | CLA | B | 615 | - | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.40 | 10 (14%) |
| 28 | PL9 | D | 406 | - | 55,55,55 | 0.98 | 3 (5%) | 68,69,69 | 1.53 | 13 (19%) |
| 29 | SQD | B | 626 | - | 53,54,54 | 0.95 | 5 (9%) | 62,65,65 | 1.71 | 10 (16%) |
| 34 | HEM | E | 102 | 5,6 | 27,50,50 | 1.88 | 4 (14%) | 17,82,82 | 1.44 | 3 (17%) |
| 29 | SQD | f | 102 | - | 40,41,54 | 1.09 | 5 (12%) | 49,52,65 | 1.60 | 9 (18%) |
| 35 | HEC | V | 201 | 16 | 26,50,50 | 2.33 | 5 (19%) | 18,82,82 | 1.67 | 4 (22%) |
| 25 | CLA | B | 606 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.35 | 7 (10%) |
| 25 | CLA | c | 511 | 3 | 59,73,73 | 1.38 | 5 (8%) | 67,113,113 | 1.45 | 9 (13%) |
| 29 | SQD | b | 601 | - | 53,54,54 | 0.94 | 3 (5%) | 62,65,65 | 1.72 | 10 (16%) |
| 27 | BCR | b | 624 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.19 | 5 (8%) |
| 31 | BCT | A | 615 | 22 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 25 | CLA | b | 621 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.46 | 9 (13%) |
| 25 | CLA | B | 603 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.38 | 10 (14%) |
| 27 | BCR | B | 619 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.17 | 5 (8%) |
| 28 | PL9 | a | 713 | - | 55,55,55 | 0.98 | 3 (5%) | 68,69,69 | 1.51 | 12 (17%) |
| 25 | CLA | b | 622 | - | 41,55,73 | 1.64 | 5 (12%) | 45,91,113 | 1.72 | 8 (17%) |
| 25 | CLA | b | 609 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.33 | 8 (11%) |
| 25 | CLA | c | 502 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.41 | 10 (14%) |
| 25 | CLA | b | 607 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.44 | 10 (14%) |
| 25 | CLA | A | 609 | - | 48,62,73 | 1.57 | 5 (10%) | 53,99,113 | 1.52 | 10 (18%) |
| 25 | CLA | D | 402 | 36 | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.40 | 9 (13%) |
| 25 | CLA | B | 607 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.41 | 8 (11%) |
| 32 | LHG | b | 629 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.24 | 6 (11%) |
| 25 | CLA | b | 617 | - | 59,73,73 | 1.37 | 5 (8%) | 67,113,113 | 1.48 | 10 (14%) |
| 25 | CLA | B | 612 | - | 59,73,73 | 1.38 | 5 (8%) | 67,113,113 | 1.47 | 9 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | LMG | C | 501 | - | 51,51,55 | 0.73 | 0 | 59,59,63 | 1.31 | 5 (8%) |
| 27 | BCR | c | 515 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.21 | 5 (8%) |
| 25 | CLA | B | 602 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.42 | 9 (13%) |
| 23 | LMG | b | 626 | - | 51,51,55 | 0.81 | 2 (3%) | 59,59,63 | 1.53 | 9 (15%) |
| 33 | DGD | C | 519 | - | 63,63,67 | 0.88 | 1 (1%) | 77,77,81 | 1.41 | 9 (11%) |
| 35 | HEC | v | 201 | 16 | 26,50,50 | 2.31 | 5 (19%) | 18,82,82 | 1.65 | 3 (16%) |
| 25 | CLA | c | 508 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.42 | 10 (14%) |
| 23 | LMG | M | 101 | - | 51,51,55 | 0.74 | 0 | 59,59,63 | 1.32 | 5 (8%) |
| 23 | LMG | b | 628 | - | 8,8,55 | 0.15 | 0 | 7,7,63 | 0.92 | 0 |
| 25 | CLA | B | 617 | - | 59,73,73 | 1.38 | 6 (10%) | 67,113,113 | 1.49 | 10 (14%) |
| 25 | CLA | c | 507 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.47 | 7 (10%) |
| 26 | PHO | a | 709 | - | 67,69,69 | 1.26 | 9 (13%) | 85,99,99 | 1.03 | 8 (9%) |
| 25 | CLA | d | 402 | - | 59,73,73 | 1.43 | 5 (8%) | 67,113,113 | 1.38 | 10 (14%) |
| 33 | DGD | C | 517 | - | 63,63,67 | 0.84 | 2 (3%) | 77,77,81 | 1.41 | 9 (11%) |
| 25 | CLA | b | 610 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.54 | 11 (16%) |
| 25 | CLA | b | 613 | 36 | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.32 | 10 (14%) |
| 25 | CLA | B | 604 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.39 | 8 (11%) |
| 25 | CLA | C | 509 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.46 | 9 (13%) |
| 21 | OEX | A | 601 | 36,1,3 | 0,15,15 | 0.00 | - | - | - | - |
| 25 | CLA | b | 611 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.36 | 8 (11%) |
| 25 | CLA | A | 607 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.36 | 10 (14%) |
| 25 | CLA | C | 506 | - | 59,73,73 | 1.43 | 5 (8%) | 67,113,113 | 1.42 | 8 (11%) |
| 32 | LHG | D | 407 | - | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.25 | 6 (11%) |
| 25 | CLA | b | 614 | - | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.39 | 10 (14%) |
| 32 | LHG | L | 101 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 27 | BCR | B | 618 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.26 | 8 (14%) |
| 29 | SQD | A | 614 | - | 39,39,54 | 0.88 | 2 (5%) | 41,41,65 | 1.19 | 3 (7%) |
| 25 | CLA | B | 610 | - | 59,73,73 | 1.45 | 5 (8%) | 67,113,113 | 1.42 | 10 (14%) |
| 27 | BCR | k | 101 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.13 | 2 (3%) |
| 25 | CLA | C | 512 | 3 | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.47 | 9 (13%) |
| 33 | DGD | h | 102 | - | 63,63,67 | 0.89 | 0 | 77,77,81 | 1.29 | 7 (9%) |
| 25 | CLA | b | 620 | - | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.34 | 9 (13%) |
| 33 | DGD | C | 518 | - | 63,63,67 | 0.92 | 4 (6%) | 77,77,81 | 1.44 | 9 (11%) |
| 25 | CLA | C | 507 | - | 59,73,73 | 1.44 | 5 (8%) | 67,113,113 | 1.37 | 9 (13%) |
| 25 | CLA | c | 509 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.47 | 9 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | SQD | a | 714 | - | 53,54,54 | 0.95 | 5 (9%) | 62,65,65 | 1.63 | 12 (19%) |
| 25 | CLA | c | 504 | 36 | 52,66,73 | 1.46 | 5 (9%) | 58,104,113 | 1.49 | 9 (15%) |
| 27 | BCR | D | 405 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.23 | 7 (12%) |
| 27 | BCR | K | 101 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.20 | 6 (10%) |
| 23 | LMG | c | 520 | - | 51,51,55 | 0.82 | 1 (1%) | 59,59,63 | 1.36 | 6 (10%) |
| 25 | CLA | b | 615 | - | 59,73,73 | 1.43 | 5 (8%) | 67,113,113 | 1.43 | 11 (16%) |
| 25 | CLA | D | 403 | - | 59,73,73 | 1.43 | 5 (8%) | 67,113,113 | 1.35 | 9 (13%) |
| 25 | CLA | C | 510 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.41 | 8 (11%) |
| 25 | CLA | b | 608 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.32 | 7 (10%) |
| 25 | CLA | C | 503 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.43 | 10 (14%) |
| 25 | CLA | C | 502 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.40 | 8 (11%) |
| 33 | DGD | H | 103 | - | 63,63,67 | 0.87 | 1 (1%) | 77,77,81 | 1.34 | 7 (9%) |
| 23 | LMG | c | 519 | - | 51,51,55 | 0.71 | 0 | 59,59,63 | 1.32 | 5 (8%) |
| 25 | CLA | a | 708 | 36 | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.38 | 9 (13%) |
| 29 | SQD | I | 102 | - | 39,39,54 | 0.86 | 2 (5%) | 41,41,65 | 1.22 | 2 (4%) |
| 32 | LHG | d | 406 | - | 48,48,48 | 0.61 | 0 | 51,54,54 | 1.28 | 6 (11%) |
| 33 | DGD | c | 517 | - | 63,63,67 | 0.95 | 4 (6%) | 77,77,81 | 1.41 | 9 (11%) |
| 27 | BCR | k | 102 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.19 | 6 (10%) |
| 25 | CLA | B | 616 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.44 | 7 (10%) |
| 27 | BCR | b | 623 | - | 41,41,41 | 1.14 | 2 (4%) | 56,56,56 | 1.23 | 7 (12%) |
| 25 | CLA | c | 510 | - | 59,73,73 | 1.37 | 5 (8%) | 67,113,113 | 1.42 | 7 (10%) |
| 23 | LMG | f | 101 | - | 51,51,55 | 0.71 | 0 | 59,59,63 | 1.35 | 7 (11%) |
| 27 | BCR | C | 515 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.22 | 8 (14%) |
| 25 | CLA | a | 707 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.36 | 8 (11%) |
| 25 | CLA | c | 505 | - | 59,73,73 | 1.43 | 5 (8%) | 67,113,113 | 1.35 | 8 (11%) |
| 25 | CLA | A | 606 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.32 | 9 (13%) |
| 26 | PHO | D | 401 | - | 67,69,69 | 1.26 | 8 (11%) | 85,99,99 | 1.04 | 6 (7%) |
| 32 | LHG | a | 720 | - | 38,38,48 | 0.68 | 0 | 41,44,54 | 1.17 | 3 (7%) |
| 23 | LMG | C | 520 | - | 51,51,55 | 0.75 | 1 (1%) | 59,59,63 | 1.31 | 5 (8%) |
| 28 | PL9 | A | 611 | - | 55,55,55 | 1.04 | 4 (7%) | 68,69,69 | 1.51 | 11 (16%) |
| 31 | BCT | a | 706 | 22 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 25 | CLA | B | 609 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.35 | 9 (13%) |
| 23 | LMG | a | 715 | - | 51,51,55 | 0.75 | 0 | 59,59,63 | 1.32 | 6 (10%) |
| 25 | CLA | B | 614 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.44 | 10 (14%) |
| 25 | CLA | C | 513 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.52 | 8 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 27 | BCR | a | 712 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.18 | 6 (10%) |
| 26 | PHO | A | 608 | - | 67,69,69 | 1.26 | 9 (13%) | 85,99,99 | 1.04 | 8 (9%) |
| 32 | LHG | d | 407 | - | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.25 | 6 (11%) |
| 27 | BCR | b | 625 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.21 | 8 (14%) |
| 29 | SQD | D | 410 | - | 42,43,54 | 1.06 | 5 (11%) | 51,54,65 | 1.63 | 10 (19%) |
| 23 | LMG | A | 603 | - | 51,51,55 | 0.95 | 2 (3%) | 59,59,63 | 1.40 | 7 (11%) |
| 27 | BCR | H | 102 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.31 | 7 (12%) |
| 26 | PHO | a | 710 | - | 67,69,69 | 1.25 | 8 (11%) | 85,99,99 | 1.05 | 5 (5%) |
| 25 | CLA | b | 612 | - | 59,73,73 | 1.41 | 5 (8%) | 67,113,113 | 1.39 | 9 (13%) |
| 25 | CLA | B | 613 | - | 59,73,73 | 1.38 | 5 (8%) | 67,113,113 | 1.47 | 9 (13%) |
| 32 | LHG | E | 101 | - | 48,48,48 | 0.67 | 1 (2%) | 51,54,54 | 1.22 | 6 (11%) |
| 25 | CLA | c | 501 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.40 | 10 (14%) |
| 23 | LMG | b | 627 | - | 51,51,55 | 0.78 | 0 | 59,59,63 | 1.27 | 4 (6%) |
| 25 | CLA | a | 711 | - | 59,73,73 | 1.42 | 5 (8%) | 67,113,113 | 1.39 | 10 (14%) |
| 23 | LMG | a | 701 | - | 51,51,55 | 0.80 | 0 | 59,59,63 | 1.32 | 7 (11%) |
| 25 | CLA | C | 511 | - | 59,73,73 | 1.38 | 5 (8%) | 67,113,113 | 1.44 | 10 (14%) |
| 21 | OEX | a | 702 | 36,1,3 | 0,15,15 | 0.00 | - | - | - | - |
| 32 | LHG | B | 625 | - | 48,48,48 | 0.62 | 2 (4%) | 51,54,54 | 1.27 | 6 (11%) |
| 25 | CLA | C | 505 | 36 | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.36 | 10 (14%) |
| 23 | LMG | d | 408 | - | 39,39,55 | 0.53 | 1 (2%) | 41,41,63 | 1.29 | 4 (9%) |
| 25 | CLA | c | 512 | - | 59,73,73 | 1.38 | 5 (8%) | 67,113,113 | 1.50 | 9 (13%) |
| 25 | CLA | C | 514 | - | 59,73,73 | 1.36 | 5 (8%) | 67,113,113 | 1.46 | 9 (13%) |
| 32 | LHG | e | 101 | - | 41,41,48 | 0.68 | 1 (2%) | 44,47,54 | 1.32 | 7 (15%) |
| 27 | BCR | A | 610 | - | 41,41,41 | 1.08 | 2 (4%) | 56,56,56 | 1.18 | 5 (8%) |
| 25 | CLA | C | 504 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.45 | 9 (13%) |
| 34 | HEM | e | 102 | 5,6 | 27,50,50 | 1.95 | 4 (14%) | 17,82,82 | 1.45 | 2 (11%) |
| 25 | CLA | B | 611 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.40 | 10 (14%) |
| 25 | CLA | C | 508 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.47 | 7 (10%) |
| 25 | CLA | B | 608 | 36 | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.33 | 9 (13%) |
| 25 | CLA | B | 605 | - | 59,73,73 | 1.39 | 5 (8%) | 67,113,113 | 1.53 | 10 (14%) |
| 25 | CLA | c | 503 | - | 59,73,73 | 1.40 | 5 (8%) | 67,113,113 | 1.45 | 8 (11%) |
| 29 | SQD | B | 623 | - | 46,47,54 | 1.01 | 3 (6%) | 55,58,65 | 1.82 | 12 (21%) |
| 27 | BCR | d | 404 | - | 41,41,41 | 1.13 | 2 (4%) | 56,56,56 | 1.22 | 8 (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 |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27 | BCR | h | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 25 | CLA | b | 618 | - | 3/3/20/25 | 12/37/135/135 | - |
| 25 | CLA | a | 719 | 36 | 3/3/20/25 | 9/37/135/135 | - |
| 33 | DGD | c | 518 | - | - | 11/51/91/95 | 0/2/2/2 |
| 27 | BCR | B | 620 | - | - | 6/29/63/63 | 0/2/2/2 |
| 23 | LMG | D | 409 | - | - | 19/46/66/70 | 0/1/1/1 |
| 23 | LMG | C | 521 | - | - | 18/46/66/70 | 0/1/1/1 |
| 27 | BCR | Y | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 25 | CLA | d | 403 | - | 2/2/20/25 | 9/37/135/135 | - |
| 25 | CLA | b | 616 | 36 | 3/3/20/25 | 5/37/135/135 | - |
| 27 | BCR | C | 516 | - | - | 6/29/63/63 | 0/2/2/2 |
| 23 | LMG | B | 621 | - | - | 19/46/66/70 | 0/1/1/1 |
| 27 | BCR | b | 602 | - | - | 6/29/63/63 | 0/2/2/2 |
| 25 | CLA | c | 513 | - | 3/3/20/25 | 17/37/135/135 | - |
| 27 | BCR | t | 103 | - | - | 8/29/63/63 | 0/2/2/2 |
| 28 | PL9 | d | 405 | - | - | 8/53/73/73 | 0/1/1/1 |
| 25 | CLA | D | 404 | - | 2/2/20/25 | 17/37/135/135 | - |
| 25 | CLA | b | 619 | - | 3/3/20/25 | 10/37/135/135 | - |
| 25 | CLA | c | 506 | - | 2/2/20/25 | 14/37/135/135 | - |
| 33 | DGD | c | 516 | - | - | 15/51/91/95 | 0/2/2/2 |
| 29 | SQD | A | 612 | - | - | 18/47/67/69 | 0/1/1/1 |
| 27 | BCR | c | 514 | - | - | 6/29/63/63 | 0/2/2/2 |
| 32 | LHG | D | 408 | - | - | 25/53/53/53 | - |
| 25 | CLA | B | 615 | - | 3/3/20/25 | 16/37/135/135 | - |
| 28 | PL9 | D | 406 | - | - | 9/53/73/73 | 0/1/1/1 |
| 29 | SQD | B | 626 | - | - | 23/49/69/69 | 0/1/1/1 |
| 34 | HEM | E | 102 | 5,6 | - | 0/6/54/54 | - |
| 29 | SQD | f | 102 | - | - | 11/36/56/69 | 0/1/1/1 |
| 35 | HEC | V | 201 | 16 | - | 0/6/54/54 | - |
| 25 | CLA | B | 606 | - | 3/3/20/25 | 15/37/135/135 | - |
| 25 | CLA | c | 511 | 3 | 3/3/20/25 | 10/37/135/135 | - |
| 29 | SQD | b | 601 | - | - | 25/49/69/69 | 0/1/1/1 |
| 27 | BCR | b | 624 | - | - | 7/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25 | CLA | b | 621 | - | 3/3/20/25 | 9/37/135/135 | - |
| 25 | CLA | B | 603 | - | 2/2/20/25 | 8/37/135/135 | - |
| 27 | BCR | B | 619 | - | - | 5/29/63/63 | 0/2/2/2 |
| 28 | PL9 | a | 713 | - | - | 13/53/73/73 | 0/1/1/1 |
| 25 | CLA | b | 622 | - | 3/3/16/25 | 2/16/114/135 | - |
| 25 | CLA | b | 609 | - | 3/3/20/25 | 17/37/135/135 | - |
| 25 | CLA | c | 502 | - | 3/3/20/25 | 13/37/135/135 | - |
| 25 | CLA | b | 607 | 36 | 3/3/20/25 | 16/37/135/135 | - |
| 25 | CLA | A | 609 | - | 3/3/17/25 | 0/24/122/135 | - |
| 25 | CLA | D | 402 | 36 | 2/2/20/25 | 6/37/135/135 | - |
| 25 | CLA | B | 607 | - | 3/3/20/25 | 16/37/135/135 | - |
| 25 | CLA | b | 617 | - | 3/3/20/25 | 16/37/135/135 | - |
| 25 | CLA | B | 612 | - | 3/3/20/25 | 5/37/135/135 | - |
| 23 | LMG | C | 501 | - | - | 22/46/66/70 | 0/1/1/1 |
| 27 | BCR | c | 515 | - | - | 6/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 602 | 36 | 3/3/20/25 | 15/37/135/135 | - |
| 23 | LMG | b | 626 | - | - | 16/46/66/70 | 0/1/1/1 |
| 33 | DGD | C | 519 | - | - | 16/51/91/95 | 0/2/2/2 |
| 35 | HEC | v | 201 | 16 | - | 0/6/54/54 | - |
| 25 | CLA | c | 508 | - | 2/2/20/25 | 14/37/135/135 | - |
| 23 | LMG | M | 101 | - | - | 13/46/66/70 | 0/1/1/1 |
| 25 | CLA | B | 617 | - | 3/3/20/25 | 11/37/135/135 | - |
| 25 | CLA | c | 507 | 36 | 3/3/20/25 | 8/37/135/135 | - |
| 23 | LMG | b | 628 | - | - | 3/6/6/70 | - |
| 26 | PHO | a | 709 | - | - | 6/53/103/103 | 0/5/6/6 |
| 25 | CLA | d | 402 | - | 2/2/20/25 | 9/37/135/135 | - |
| 33 | DGD | C | 517 | - | - | 17/51/91/95 | 0/2/2/2 |
| 25 | CLA | b | 610 | - | 3/3/20/25 | 11/37/135/135 | - |
| 25 | CLA | b | 613 | 36 | 3/3/20/25 | 9/37/135/135 | - |
| 25 | CLA | B | 604 | - | 3/3/20/25 | 18/37/135/135 | - |
| 25 | CLA | C | 509 | - | 3/3/20/25 | 7/37/135/135 | - |
| 25 | CLA | b | 611 | - | 2/2/20/25 | 11/37/135/135 | - |
| 25 | CLA | A | 607 | 36 | 3/3/20/25 | 7/37/135/135 | - |
| 25 | CLA | C | 506 | - | 2/2/20/25 | 7/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | LHG | D | 407 | - | - | 18/53/53/53 | - |
| 25 | CLA | b | 614 | - | 3/3/20/25 | 3/37/135/135 | - |
| 32 | LHG | L | 101 | - | - | 18/53/53/53 | - |
| 27 | BCR | B | 618 | - | - | 4/29/63/63 | 0/2/2/2 |
| 29 | SQD | A | 614 | - | - | 21/41/41/69 | - |
| 25 | CLA | B | 610 | - | 2/2/20/25 | 11/37/135/135 | - |
| 27 | BCR | k | 101 | - | - | 8/29/63/63 | 0/2/2/2 |
| 25 | CLA | C | 512 | 3 | 3/3/20/25 | 14/37/135/135 | - |
| 33 | DGD | h | 102 | - | - | 16/51/91/95 | 0/2/2/2 |
| 25 | CLA | b | 620 | - | 3/3/20/25 | 12/37/135/135 | - |
| 33 | DGD | C | 518 | - | - | 24/51/91/95 | 0/2/2/2 |
| 25 | CLA | C | 507 | - | 2/2/20/25 | 14/37/135/135 | - |
| 25 | CLA | c | 509 | - | 3/3/20/25 | 5/37/135/135 | - |
| 29 | SQD | a | 714 | - | - | 16/49/69/69 | 0/1/1/1 |
| 25 | CLA | c | 504 | 36 | 3/3/18/25 | 5/29/127/135 | - |
| 27 | BCR | D | 405 | - | - | 8/29/63/63 | 0/2/2/2 |
| 27 | BCR | K | 101 | - | - | 4/29/63/63 | 0/2/2/2 |
| 23 | LMG | c | 520 | - | - | 16/46/66/70 | 0/1/1/1 |
| 25 | CLA | b | 615 | - | 2/2/20/25 | 11/37/135/135 | - |
| 25 | CLA | D | 403 | - | 2/2/20/25 | 10/37/135/135 | - |
| 25 | CLA | C | 510 | - | 3/3/20/25 | 17/37/135/135 | - |
| 25 | CLA | b | 608 | - | 3/3/20/25 | 9/37/135/135 | - |
| 25 | CLA | C | 503 | - | 3/3/20/25 | 17/37/135/135 | - |
| 25 | CLA | C | 502 | - | 3/3/20/25 | 8/37/135/135 | - |
| 33 | DGD | H | 103 | - | - | 10/51/91/95 | 0/2/2/2 |
| 23 | LMG | c | 519 | - | - | 23/46/66/70 | 0/1/1/1 |
| 25 | CLA | a | 708 | 36 | 3/3/20/25 | 8/37/135/135 | - |
| 29 | SQD | I | 102 | - | - | 25/41/41/69 | - |
| 32 | LHG | d | 406 | - | - | 16/53/53/53 | - |
| 33 | DGD | c | 517 | - | - | 19/51/91/95 | 0/2/2/2 |
| 27 | BCR | k | 102 | - | - | 4/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 616 | - | 3/3/20/25 | 11/37/135/135 | - |
| 27 | BCR | b | 623 | - | - | 3/29/63/63 | 0/2/2/2 |
| 25 | CLA | c | 510 | - | 3/3/20/25 | 16/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | LMG | f | 101 | - | - | 16/46/66/70 | 0/1/1/1 |
| 27 | BCR | C | 515 | - | - | 4/29/63/63 | 0/2/2/2 |
| 25 | CLA | a | 707 | - | 3/3/20/25 | 6/37/135/135 | - |
| 25 | CLA | c | 505 | - | 2/2/20/25 | 7/37/135/135 | - |
| 25 | CLA | A | 606 | - | 3/3/20/25 | 2/37/135/135 | - |
| 26 | PHO | D | 401 | - | - | 6/53/103/103 | 0/5/6/6 |
| 32 | LHG | a | 720 | - | - | 18/43/43/53 | - |
| 23 | LMG | C | 520 | - | - | 25/46/66/70 | 0/1/1/1 |
| 28 | PL9 | A | 611 | - | - | 8/53/73/73 | 0/1/1/1 |
| 25 | CLA | B | 609 | - | 3/3/20/25 | 12/37/135/135 | - |
| 23 | LMG | a | 715 | - | - | 25/46/66/70 | 0/1/1/1 |
| 25 | CLA | B | 614 | - | 3/3/20/25 | 9/37/135/135 | - |
| 25 | CLA | C | 513 | - | 3/3/20/25 | 12/37/135/135 | - |
| 27 | BCR | a | 712 | - | - | 5/29/63/63 | 0/2/2/2 |
| 26 | PHO | A | 608 | - | - | 9/53/103/103 | 0/5/6/6 |
| 32 | LHG | d | 407 | - | - | 14/53/53/53 | - |
| 27 | BCR | b | 625 | - | - | 7/29/63/63 | 0/2/2/2 |
| 29 | SQD | D | 410 | - | - | 16/38/58/69 | 0/1/1/1 |
| 23 | LMG | A | 603 | - | - | 24/46/66/70 | 0/1/1/1 |
| 27 | BCR | H | 102 | - | - | 7/29/63/63 | 0/2/2/2 |
| 26 | PHO | a | 710 | - | - | 7/53/103/103 | 0/5/6/6 |
| 25 | CLA | b | 612 | - | 3/3/20/25 | 12/37/135/135 | - |
| 25 | CLA | B | 613 | - | 3/3/20/25 | 10/37/135/135 | - |
| 32 | LHG | E | 101 | - | - | 28/53/53/53 | - |
| 25 | CLA | c | 501 | - | 3/3/20/25 | 8/37/135/135 | - |
| 23 | LMG | b | 627 | - | - | 18/46/66/70 | 0/1/1/1 |
| 25 | CLA | a | 711 | - | 3/3/20/25 | 11/37/135/135 | - |
| 25 | CLA | C | 511 | - | 3/3/20/25 | 11/37/135/135 | - |
| 23 | LMG | a | 701 | - | - | 26/46/66/70 | 0/1/1/1 |
| 32 | LHG | B | 625 | - | - | 19/53/53/53 | - |
| 25 | CLA | C | 505 | 36 | 3/3/20/25 | 11/37/135/135 | - |
| 23 | LMG | d | 408 | - | - | 19/41/41/70 | - |
| 25 | CLA | c | 512 | - | 3/3/20/25 | 15/37/135/135 | - |
| 25 | CLA | C | 514 | - | 3/3/20/25 | 7/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | LHG | e | 101 | - | - | 22/46/46/53 | - |
| 27 | BCR | A | 610 | - | - | 4/29/63/63 | 0/2/2/2 |
| 25 | CLA | C | 504 | - | 3/3/20/25 | 13/37/135/135 | - |
| 34 | HEM | e | 102 | 5,6 | - | 1/6/54/54 | - |
| 25 | CLA | B | 611 | 36 | 3/3/20/25 | 10/37/135/135 | - |
| 25 | CLA | C | 508 | 36 | 3/3/20/25 | 9/37/135/135 | - |
| 25 | CLA | B | 608 | 36 | 3/3/20/25 | 11/37/135/135 | - |
| 25 | CLA | B | 605 | - | 3/3/20/25 | 10/37/135/135 | - |
| 25 | CLA | c | 503 | - | 3/3/20/25 | 9/37/135/135 | - |
| 29 | SQD | B | 623 | - | - | 23/42/62/69 | 0/1/1/1 |
| 27 | BCR | d | 404 | - | - | 7/29/63/63 | 0/2/2/2 |

All (527) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 25 | B | 610 | CLA | C4B-NB | 7.76 | 1.42 | 1.35 |
| 25 | C | 507 | CLA | C4B-NB | 7.73 | 1.42 | 1.35 |
| 25 | c | 505 | CLA | C4B-NB | 7.72 | 1.42 | 1.35 |
| 25 | D | 403 | CLA | C4B-NB | 7.70 | 1.42 | 1.35 |
| 25 | b | 615 | CLA | C4B-NB | 7.68 | 1.42 | 1.35 |
| 25 | C | 506 | CLA | C4B-NB | 7.66 | 1.42 | 1.35 |
| 25 | d | 402 | CLA | C4B-NB | 7.66 | 1.42 | 1.35 |
| 25 | b | 609 | CLA | C4B-NB | 7.64 | 1.42 | 1.35 |
| 25 | B | 607 | CLA | C4B-NB | 7.64 | 1.42 | 1.35 |
| 25 | A | 609 | CLA | C4B-NB | 7.60 | 1.42 | 1.35 |
| 25 | c | 506 | CLA | C4B-NB | 7.59 | 1.42 | 1.35 |
| 25 | b | 612 | CLA | C4B-NB | 7.58 | 1.42 | 1.35 |
| 25 | B | 616 | CLA | C4B-NB | 7.57 | 1.42 | 1.35 |
| 25 | B | 606 | CLA | C4B-NB | 7.55 | 1.41 | 1.35 |
| 25 | b | 608 | CLA | C4B-NB | 7.55 | 1.41 | 1.35 |
| 25 | a | 711 | CLA | C4B-NB | 7.54 | 1.41 | 1.35 |
| 25 | B | 615 | CLA | C4B-NB | 7.54 | 1.41 | 1.35 |
| 25 | B | 603 | CLA | C4B-NB | 7.52 | 1.41 | 1.35 |
| 25 | a | 719 | CLA | C4B-NB | 7.52 | 1.41 | 1.35 |
| 25 | D | 404 | CLA | C4B-NB | 7.52 | 1.41 | 1.35 |
| 25 | b | 611 | CLA | C4B-NB | 7.51 | 1.41 | 1.35 |
| 25 | B | 604 | CLA | C4B-NB | 7.50 | 1.41 | 1.35 |
| 25 | b | 620 | CLA | C4B-NB | 7.50 | 1.41 | 1.35 |
| 25 | c | 508 | CLA | C4B-NB | 7.50 | 1.41 | 1.35 |
| 25 | b | 614 | CLA | C4B-NB | 7.49 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 25 | a | 707 | CLA | C4B-NB | 7.48 | 1.41 | 1.35 |
| 25 | C | 504 | CLA | C4B-NB | 7.46 | 1.41 | 1.35 |
| 25 | b | 621 | CLA | C4B-NB | 7.45 | 1.41 | 1.35 |
| 25 | c | 507 | CLA | C4B-NB | 7.44 | 1.41 | 1.35 |
| 25 | b | 616 | CLA | C4B-NB | 7.44 | 1.41 | 1.35 |
| 25 | B | 602 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 25 | B | 611 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 25 | C | 509 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 25 | C | 508 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | C | 513 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | d | 403 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | C | 503 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | b | 607 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | b | 618 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 25 | b | 610 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 25 | B | 608 | CLA | C4B-NB | 7.39 | 1.41 | 1.35 |
| 25 | A | 606 | CLA | C4B-NB | 7.39 | 1.41 | 1.35 |
| 25 | B | 617 | CLA | C4B-NB | 7.37 | 1.41 | 1.35 |
| 25 | c | 512 | CLA | C4B-NB | 7.37 | 1.41 | 1.35 |
| 25 | c | 503 | CLA | C4B-NB | 7.37 | 1.41 | 1.35 |
| 25 | C | 505 | CLA | C4B-NB | 7.36 | 1.41 | 1.35 |
| 25 | b | 613 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 25 | B | 614 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 25 | C | 512 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 25 | c | 509 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 25 | B | 609 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 25 | B | 605 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 25 | C | 502 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 25 | c | 501 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 25 | B | 612 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 25 | b | 622 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 25 | A | 607 | CLA | C4B-NB | 7.30 | 1.41 | 1.35 |
| 25 | c | 511 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 25 | B | 613 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 25 | C | 511 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 25 | D | 402 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 25 | b | 619 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 25 | C | 510 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 25 | c | 502 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 25 | a | 708 | CLA | C4B-NB | 7.22 | 1.41 | 1.35 |
| 25 | c | 504 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 25 | b | 617 | CLA | C4B-NB | 7.17 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | c | 510 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 25 | C | 514 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 25 | c | 513 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 35 | V | 201 | HEC | C3C-C2C | -6.58 | 1.33 | 1.40 |
| 35 | v | 201 | HEC | C3C-C2C | -6.41 | 1.34 | 1.40 |
| 35 | v | 201 | HEC | C3B-C2B | -5.34 | 1.35 | 1.40 |
| 35 | V | 201 | HEC | C3B-C2B | -5.33 | 1.35 | 1.40 |
| 34 | e | 102 | HEM | C3B-C2B | -4.80 | 1.33 | 1.40 |
| 34 | E | 102 | HEM | C3C-C2C | -4.61 | 1.34 | 1.40 |
| 34 | e | 102 | HEM | C3C-C2C | -4.52 | 1.34 | 1.40 |
| 35 | V | 201 | HEC | CBC-CAC | -4.15 | 1.33 | 1.49 |
| 35 | v | 201 | HEC | CBC-CAC | -4.11 | 1.34 | 1.49 |
| 28 | A | 611 | PL9 | C7-C3 | -4.09 | 1.47 | 1.51 |
| 35 | V | 201 | HEC | CBB-CAB | -4.05 | 1.34 | 1.49 |
| 35 | v | 201 | HEC | CBB-CAB | -4.04 | 1.34 | 1.49 |
| 34 | E | 102 | HEM | C3B-CAB | 3.78 | 1.55 | 1.47 |
| 34 | E | 102 | HEM | C3B-C2B | -3.75 | 1.35 | 1.40 |
| 34 | e | 102 | HEM | C3C-CAC | 3.73 | 1.55 | 1.47 |
| 34 | E | 102 | HEM | C3C-CAC | 3.72 | 1.55 | 1.47 |
| 27 | d | 404 | BCR | C1-C6 | -3.71 | 1.48 | 1.53 |
| 27 | D | 405 | BCR | C30-C25 | -3.65 | 1.48 | 1.53 |
| 28 | a | 713 | PL9 | C7-C3 | -3.57 | 1.47 | 1.51 |
| 27 | D | 405 | BCR | C1-C6 | -3.56 | 1.48 | 1.53 |
| 23 | A | 603 | LMG | C4-C5 | 3.56 | 1.60 | 1.53 |
| 27 | b | 623 | BCR | C1-C6 | -3.55 | 1.48 | 1.53 |
| 34 | e | 102 | HEM | C3B-CAB | 3.53 | 1.55 | 1.47 |
| 27 | k | 101 | BCR | C1-C6 | -3.48 | 1.49 | 1.53 |
| 27 | c | 515 | BCR | C1-C6 | -3.47 | 1.49 | 1.53 |
| 27 | C | 516 | BCR | C1-C6 | -3.46 | 1.49 | 1.53 |
| 27 | Y | 101 | BCR | C1-C6 | -3.42 | 1.49 | 1.53 |
| 27 | t | 103 | BCR | C1-C6 | -3.42 | 1.49 | 1.53 |
| 27 | b | 602 | BCR | C1-C6 | -3.42 | 1.49 | 1.53 |
| 27 | B | 620 | BCR | C1-C6 | -3.42 | 1.49 | 1.53 |
| 26 | A | 608 | PHO | C3B-C4B | 3.39 | 1.50 | 1.43 |
| 26 | a | 710 | PHO | C3B-C4B | 3.39 | 1.50 | 1.43 |
| 27 | a | 712 | BCR | C1-C6 | -3.39 | 1.49 | 1.53 |
| 27 | c | 514 | BCR | C30-C25 | -3.37 | 1.49 | 1.53 |
| 27 | b | 624 | BCR | C1-C6 | -3.36 | 1.49 | 1.53 |
| 27 | B | 618 | BCR | C1-C6 | -3.36 | 1.49 | 1.53 |
| 27 | k | 102 | BCR | C1-C6 | -3.36 | 1.49 | 1.53 |
| 27 | K | 101 | BCR | C1-C6 | -3.35 | 1.49 | 1.53 |
| 26 | D | 401 | PHO | C3B-C4B | 3.34 | 1.50 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | b | 625 | BCR | C1-C6 | -3.34 | 1.49 | 1.53 |
| 27 | c | 514 | BCR | C1-C6 | -3.34 | 1.49 | 1.53 |
| 26 | a | 709 | PHO | C3B-C4B | 3.32 | 1.50 | 1.43 |
| 27 | B | 619 | BCR | C1-C6 | -3.31 | 1.49 | 1.53 |
| 27 | b | 623 | BCR | C30-C25 | -3.29 | 1.49 | 1.53 |
| 28 | D | 406 | PL9 | C7-C3 | -3.28 | 1.47 | 1.51 |
| 29 | A | 614 | SQD | O48-C23 | 3.28 | 1.42 | 1.33 |
| 25 | c | 503 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 25 | B | 609 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 25 | B | 613 | CLA | CHC-C1C | 3.25 | 1.43 | 1.35 |
| 25 | b | 620 | CLA | CHC-C1C | 3.25 | 1.43 | 1.35 |
| 25 | B | 615 | CLA | CHC-C1C | 3.25 | 1.43 | 1.35 |
| 27 | A | 610 | BCR | C1-C6 | -3.24 | 1.49 | 1.53 |
| 25 | A | 607 | CLA | CHC-C1C | 3.23 | 1.43 | 1.35 |
| 25 | C | 512 | CLA | CHC-C1C | 3.23 | 1.43 | 1.35 |
| 25 | C | 504 | CLA | CHC-C1C | 3.23 | 1.43 | 1.35 |
| 25 | C | 509 | CLA | CHC-C1C | 3.23 | 1.43 | 1.35 |
| 25 | b | 613 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 25 | b | 609 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 25 | d | 403 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 25 | C | 511 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 25 | c | 508 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 25 | b | 614 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 25 | B | 614 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 25 | c | 511 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 25 | b | 611 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 25 | B | 607 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 25 | B | 602 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | C | 507 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | b | 618 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | A | 609 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | B | 603 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | c | 509 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | b | 616 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 25 | C | 506 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | C | 514 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | C | 503 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | A | 606 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | D | 403 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | d | 402 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | c | 502 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 25 | c | 506 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | C | 505 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 25 | a | 708 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 25 | D | 402 | CLA | CHC-C1C | 3.18 | 1.43 | 1.35 |
| 25 | a | 711 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 25 | C | 513 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 25 | a | 719 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 25 | B | 610 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 25 | c | 510 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 25 | B | 606 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 27 | b | 625 | BCR | C30-C25 | -3.16 | 1.49 | 1.53 |
| 25 | B | 616 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 29 | D | 410 | SQD | O48-C23 | 3.16 | 1.42 | 1.33 |
| 25 | b | 622 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | c | 505 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | C | 502 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | a | 707 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | c | 504 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | C | 510 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 25 | b | 615 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 29 | a | 714 | SQD | O48-C23 | 3.16 | 1.42 | 1.33 |
| 25 | b | 607 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 25 | B | 612 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 25 | B | 617 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 29 | B | 623 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 25 | b | 617 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 25 | B | 611 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 25 | b | 608 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 29 | f | 102 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 25 | b | 610 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 25 | c | 501 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 25 | b | 619 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 25 | B | 608 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 27 | C | 515 | BCR | C30-C25 | -3.14 | 1.49 | 1.53 |
| 25 | c | 512 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 25 | c | 507 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 25 | B | 604 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 25 | c | 513 | CLA | CHC-C1C | 3.11 | 1.43 | 1.35 |
| 25 | D | 404 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 27 | C | 515 | BCR | C1-C6 | -3.11 | 1.49 | 1.53 |
| 25 | b | 612 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 29 | B | 626 | SQD | O48-C23 | 3.10 | 1.42 | 1.33 |
| 29 | I | 102 | SQD | O48-C23 | 3.09 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | C | 516 | BCR | C30-C25 | -3.09 | 1.49 | 1.53 |
| 29 | A | 612 | SQD | O48-C23 | 3.08 | 1.42 | 1.33 |
| 25 | C | 508 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 29 | b | 601 | SQD | O48-C23 | 3.08 | 1.42 | 1.33 |
| 27 | B | 620 | BCR | C30-C25 | -3.08 | 1.49 | 1.53 |
| 25 | b | 621 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 27 | c | 515 | BCR | C30-C25 | -3.06 | 1.49 | 1.53 |
| 27 | H | 102 | BCR | C1-C6 | -3.04 | 1.49 | 1.53 |
| 25 | B | 605 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 23 | A | 603 | LMG | C4-C3 | 3.04 | 1.60 | 1.52 |
| 27 | b | 624 | BCR | C30-C25 | -3.03 | 1.49 | 1.53 |
| 27 | a | 712 | BCR | C30-C25 | -3.03 | 1.49 | 1.53 |
| 27 | d | 404 | BCR | C30-C25 | -3.03 | 1.49 | 1.53 |
| 27 | Y | 101 | BCR | C30-C25 | -3.03 | 1.49 | 1.53 |
| 28 | d | 405 | PL9 | C7-C3 | -3.03 | 1.48 | 1.51 |
| 26 | a | 710 | PHO | CHC-C1C | 3.00 | 1.44 | 1.38 |
| 29 | A | 614 | SQD | O47-C7 | 3.00 | 1.42 | 1.34 |
| 26 | A | 608 | PHO | CHC-C1C | 2.99 | 1.44 | 1.38 |
| 29 | B | 623 | SQD | O47-C7 | 2.99 | 1.42 | 1.34 |
| 26 | D | 401 | PHO | CHC-C1C | 2.98 | 1.44 | 1.38 |
| 27 | B | 619 | BCR | C30-C25 | -2.96 | 1.49 | 1.53 |
| 27 | h | 101 | BCR | C1-C6 | -2.95 | 1.49 | 1.53 |
| 27 | k | 102 | BCR | C30-C25 | -2.94 | 1.49 | 1.53 |
| 27 | A | 610 | BCR | C30-C25 | -2.94 | 1.49 | 1.53 |
| 26 | a | 709 | PHO | CHC-C1C | 2.94 | 1.44 | 1.38 |
| 27 | b | 602 | BCR | C30-C25 | -2.93 | 1.49 | 1.53 |
| 27 | h | 101 | BCR | C30-C25 | -2.92 | 1.49 | 1.53 |
| 29 | I | 102 | SQD | O47-C7 | 2.90 | 1.42 | 1.34 |
| 27 | B | 618 | BCR | C30-C25 | -2.89 | 1.49 | 1.53 |
| 27 | k | 101 | BCR | C30-C25 | -2.89 | 1.49 | 1.53 |
| 29 | f | 102 | SQD | O47-C7 | 2.87 | 1.42 | 1.34 |
| 27 | K | 101 | BCR | C30-C25 | -2.87 | 1.49 | 1.53 |
| 29 | B | 626 | SQD | O47-C7 | 2.85 | 1.42 | 1.34 |
| 25 | A | 607 | CLA | C1D-C2D | 2.85 | 1.49 | 1.42 |
| 27 | H | 102 | BCR | C30-C25 | -2.85 | 1.49 | 1.53 |
| 27 | t | 103 | BCR | C30-C25 | -2.84 | 1.49 | 1.53 |
| 29 | D | 410 | SQD | O47-C7 | 2.84 | 1.42 | 1.34 |
| 29 | A | 612 | SQD | O47-C7 | 2.83 | 1.42 | 1.34 |
| 29 | a | 714 | SQD | O47-C7 | 2.81 | 1.42 | 1.34 |
| 25 | b | 611 | CLA | C1D-C2D | 2.81 | 1.48 | 1.42 |
| 25 | D | 402 | CLA | C1D-C2D | 2.80 | 1.48 | 1.42 |
| 25 | C | 505 | CLA | C1D-C2D | 2.80 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | b | 607 | CLA | C1D-C2D | 2.79 | 1.48 | 1.42 |
| 26 | a | 710 | PHO | C4C-NC | 2.79 | 1.43 | 1.36 |
| 25 | a | 719 | CLA | C1D-C2D | 2.78 | 1.48 | 1.42 |
| 29 | b | 601 | SQD | O47-C7 | 2.78 | 1.42 | 1.34 |
| 28 | D | 406 | PL9 | C3-C4 | -2.77 | 1.45 | 1.49 |
| 25 | a | 708 | CLA | C1D-C2D | 2.76 | 1.48 | 1.42 |
| 26 | D | 401 | PHO | C1A-NA | 2.76 | 1.43 | 1.37 |
| 25 | B | 602 | CLA | C1D-C2D | 2.76 | 1.48 | 1.42 |
| 25 | c | 504 | CLA | C1D-C2D | 2.76 | 1.48 | 1.42 |
| 25 | b | 620 | CLA | C1D-C2D | 2.76 | 1.48 | 1.42 |
| 26 | a | 709 | PHO | C1A-NA | 2.76 | 1.43 | 1.37 |
| 25 | b | 613 | CLA | C1D-C2D | 2.75 | 1.48 | 1.42 |
| 28 | A | 611 | PL9 | C3-C4 | -2.75 | 1.45 | 1.49 |
| 25 | B | 609 | CLA | C1D-C2D | 2.75 | 1.48 | 1.42 |
| 25 | C | 511 | CLA | C1D-C2D | 2.75 | 1.48 | 1.42 |
| 26 | D | 401 | PHO | C4C-NC | 2.75 | 1.42 | 1.36 |
| 26 | a | 709 | PHO | C4C-NC | 2.75 | 1.42 | 1.36 |
| 25 | B | 606 | CLA | C1D-C2D | 2.75 | 1.48 | 1.42 |
| 25 | B | 608 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 26 | A | 608 | PHO | C1A-NA | 2.74 | 1.42 | 1.37 |
| 25 | C | 514 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 25 | b | 614 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 25 | b | 617 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 25 | a | 711 | CLA | C1D-C2D | 2.74 | 1.48 | 1.42 |
| 25 | c | 506 | CLA | C1D-C2D | 2.73 | 1.48 | 1.42 |
| 25 | B | 603 | CLA | C1D-C2D | 2.73 | 1.48 | 1.42 |
| 25 | B | 615 | CLA | C1D-C2D | 2.73 | 1.48 | 1.42 |
| 25 | c | 509 | CLA | C1D-C2D | 2.72 | 1.48 | 1.42 |
| 25 | C | 502 | CLA | C1D-C2D | 2.72 | 1.48 | 1.42 |
| 25 | c | 501 | CLA | C1D-C2D | 2.72 | 1.48 | 1.42 |
| 25 | b | 610 | CLA | C1D-C2D | 2.71 | 1.48 | 1.42 |
| 25 | D | 404 | CLA | C1D-C2D | 2.71 | 1.48 | 1.42 |
| 25 | b | 612 | CLA | C1D-C2D | 2.70 | 1.48 | 1.42 |
| 25 | B | 613 | CLA | C1D-C2D | 2.70 | 1.48 | 1.42 |
| 25 | d | 403 | CLA | C1D-C2D | 2.70 | 1.48 | 1.42 |
| 25 | b | 609 | CLA | C1D-C2D | 2.70 | 1.48 | 1.42 |
| 25 | A | 606 | CLA | C1D-C2D | 2.70 | 1.48 | 1.42 |
| 26 | A | 608 | PHO | C4C-NC | 2.69 | 1.42 | 1.36 |
| 25 | C | 512 | CLA | C1D-C2D | 2.69 | 1.48 | 1.42 |
| 25 | A | 609 | CLA | C1D-C2D | 2.69 | 1.48 | 1.42 |
| 26 | a | 710 | PHO | C1A-NA | 2.69 | 1.42 | 1.37 |
| 25 | C | 509 | CLA | C1D-C2D | 2.69 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | c | 502 | CLA | C1D-C2D | 2.69 | 1.48 | 1.42 |
| 25 | b | 616 | CLA | C1D-C2D | 2.69 | 1.48 | 1.42 |
| 25 | c | 505 | CLA | C1D-C2D | 2.68 | 1.48 | 1.42 |
| 25 | c | 503 | CLA | C1D-C2D | 2.68 | 1.48 | 1.42 |
| 25 | B | 612 | CLA | C1D-C2D | 2.68 | 1.48 | 1.42 |
| 25 | C | 503 | CLA | C1D-C2D | 2.68 | 1.48 | 1.42 |
| 25 | C | 507 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | C | 504 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | C | 510 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | b | 608 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | C | 506 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | B | 605 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | b | 615 | CLA | C1D-C2D | 2.67 | 1.48 | 1.42 |
| 25 | B | 611 | CLA | C1D-C2D | 2.66 | 1.48 | 1.42 |
| 25 | B | 610 | CLA | C1D-C2D | 2.66 | 1.48 | 1.42 |
| 25 | b | 619 | CLA | C1D-C2D | 2.65 | 1.48 | 1.42 |
| 25 | B | 616 | CLA | C1D-C2D | 2.64 | 1.48 | 1.42 |
| 25 | b | 622 | CLA | C1D-C2D | 2.64 | 1.48 | 1.42 |
| 25 | d | 402 | CLA | C1D-C2D | 2.63 | 1.48 | 1.42 |
| 25 | c | 511 | CLA | C1D-C2D | 2.63 | 1.48 | 1.42 |
| 25 | c | 508 | CLA | C1D-C2D | 2.63 | 1.48 | 1.42 |
| 25 | B | 614 | CLA | C1D-C2D | 2.62 | 1.48 | 1.42 |
| 25 | a | 707 | CLA | C1D-C2D | 2.62 | 1.48 | 1.42 |
| 25 | D | 403 | CLA | C1D-C2D | 2.62 | 1.48 | 1.42 |
| 25 | c | 510 | CLA | C1D-C2D | 2.62 | 1.48 | 1.42 |
| 25 | c | 507 | CLA | C1D-C2D | 2.61 | 1.48 | 1.42 |
| 25 | B | 607 | CLA | C1D-C2D | 2.61 | 1.48 | 1.42 |
| 25 | b | 618 | CLA | C1D-C2D | 2.59 | 1.48 | 1.42 |
| 25 | c | 513 | CLA | C1D-C2D | 2.58 | 1.48 | 1.42 |
| 25 | B | 617 | CLA | C1D-C2D | 2.57 | 1.48 | 1.42 |
| 28 | d | 405 | PL9 | C3-C4 | -2.56 | 1.45 | 1.49 |
| 25 | C | 513 | CLA | C1D-C2D | 2.56 | 1.48 | 1.42 |
| 25 | C | 508 | CLA | C1D-C2D | 2.56 | 1.48 | 1.42 |
| 25 | B | 604 | CLA | C1D-C2D | 2.54 | 1.48 | 1.42 |
| 25 | c | 512 | CLA | C1D-C2D | 2.54 | 1.48 | 1.42 |
| 25 | b | 621 | CLA | C1D-C2D | 2.54 | 1.48 | 1.42 |
| 28 | a | 713 | PL9 | C3-C4 | -2.53 | 1.45 | 1.49 |
| 23 | c | 520 | LMG | C1-C2 | 2.49 | 1.59 | 1.52 |
| 25 | c | 501 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 25 | C | 507 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 26 | D | 401 | PHO | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 25 | b | 617 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | C | 521 | LMG | C1-C2 | 2.46 | 1.59 | 1.52 |
| 25 | b | 607 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 25 | b | 615 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 25 | a | 708 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 25 | b | 616 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 25 | B | 605 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 25 | B | 612 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 25 | a | 711 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 25 | C | 510 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 26 | a | 709 | PHO | CHD-C1D | 2.43 | 1.43 | 1.38 |
| 25 | B | 606 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 25 | B | 602 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 25 | c | 511 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 25 | B | 603 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 25 | b | 614 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 25 | a | 719 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 25 | B | 611 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 25 | B | 607 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 26 | A | 608 | PHO | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 25 | C | 502 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 25 | c | 505 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 25 | C | 506 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | c | 504 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | c | 502 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | A | 609 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | C | 503 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | c | 506 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | A | 607 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | C | 508 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | B | 608 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | b | 618 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | c | 508 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 25 | B | 613 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 25 | D | 404 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 25 | D | 403 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 26 | a | 710 | PHO | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 25 | b | 611 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 25 | b | 612 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 25 | B | 615 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | b | 621 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | b | 613 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | B | 604 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | a | 707 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | c | 507 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 26 | a | 709 | PHO | C4C-C3C | 2.37 | 1.49 | 1.45 |
| 25 | D | 402 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 26 | a | 710 | PHO | CHD-C1D | 2.37 | 1.43 | 1.38 |
| 25 | B | 614 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | b | 620 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 25 | B | 610 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 25 | B | 616 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 25 | C | 513 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 25 | b | 609 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 25 | C | 505 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 25 | c | 509 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 25 | c | 510 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 25 | b | 608 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 25 | d | 402 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 26 | D | 401 | PHO | CHD-C1D | 2.35 | 1.43 | 1.38 |
| 25 | c | 503 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 26 | A | 608 | PHO | CHD-C1D | 2.35 | 1.43 | 1.38 |
| 25 | b | 610 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 25 | A | 606 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 25 | c | 513 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 25 | C | 504 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 25 | c | 512 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 25 | C | 511 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 25 | b | 619 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 25 | B | 609 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 25 | d | 403 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 33 | c | 517 | DGD | O1G-C1G | -2.33 | 1.39 | 1.45 |
| 25 | C | 509 | CLA | CMB-C2B | -2.32 | 1.46 | 1.51 |
| 26 | D | 401 | PHO | C1C-NC | -2.32 | 1.33 | 1.38 |
| 25 | B | 617 | CLA | CMB-C2B | -2.31 | 1.46 | 1.51 |
| 33 | C | 518 | DGD | O1G-C1G | -2.31 | 1.39 | 1.45 |
| 26 | A | 608 | PHO | C1C-NC | -2.31 | 1.33 | 1.38 |
| 25 | C | 512 | CLA | CMB-C2B | -2.30 | 1.46 | 1.51 |
| 26 | a | 709 | PHO | C1C-NC | -2.30 | 1.33 | 1.38 |
| 26 | a | 710 | PHO | C1C-NC | -2.28 | 1.33 | 1.38 |
| 25 | C | 514 | CLA | CMB-C2B | -2.28 | 1.46 | 1.51 |
| 25 | b | 622 | CLA | CMB-C2B | -2.28 | 1.46 | 1.51 |
| 32 | E | 101 | LHG | P-O6 | 2.27 | 1.68 | 1.59 |
| 33 | C | 518 | DGD | O2G-C2G | -2.25 | 1.41 | 1.46 |
| 33 | c | 517 | DGD | O2G-C2G | -2.25 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35 | V | 201 | HEC | CAD-C3D | 2.25 | 1.55 | 1.52 |
| 25 | c | 510 | CLA | CMD-C2D | -2.24 | 1.46 | 1.51 |
| 29 | A | 612 | SQD | O2-C2 | -2.23 | 1.37 | 1.43 |
| 25 | c | 505 | CLA | CMD-C2D | -2.23 | 1.46 | 1.51 |
| 29 | a | 714 | SQD | O2-C2 | -2.21 | 1.37 | 1.43 |
| 33 | C | 518 | DGD | O6D-C5D | -2.21 | 1.39 | 1.44 |
| 25 | C | 506 | CLA | CMD-C2D | -2.19 | 1.46 | 1.51 |
| 32 | b | 629 | LHG | O7-C5 | -2.18 | 1.41 | 1.46 |
| 29 | D | 410 | SQD | O2-C2 | -2.18 | 1.37 | 1.43 |
| 25 | B | 604 | CLA | CMD-C2D | -2.18 | 1.46 | 1.51 |
| 29 | b | 601 | SQD | O2-C2 | -2.17 | 1.37 | 1.43 |
| 32 | D | 407 | LHG | O7-C5 | -2.17 | 1.41 | 1.46 |
| 32 | L | 101 | LHG | O7-C5 | -2.17 | 1.41 | 1.46 |
| 25 | b | 618 | CLA | CMD-C2D | -2.17 | 1.46 | 1.51 |
| 25 | a | 707 | CLA | CMD-C2D | -2.16 | 1.46 | 1.51 |
| 23 | b | 626 | LMG | O6-C1 | 2.16 | 1.47 | 1.41 |
| 29 | f | 102 | SQD | O2-C2 | -2.16 | 1.37 | 1.43 |
| 35 | v | 201 | HEC | CAD-C3D | 2.16 | 1.55 | 1.52 |
| 29 | B | 626 | SQD | O2-C2 | -2.16 | 1.37 | 1.43 |
| 33 | H | 103 | DGD | O2G-C2G | -2.16 | 1.41 | 1.46 |
| 25 | A | 606 | CLA | CMD-C2D | -2.15 | 1.46 | 1.51 |
| 33 | C | 517 | DGD | O1G-C1G | -2.15 | 1.40 | 1.45 |
| 32 | e | 101 | LHG | P-O6 | 2.14 | 1.68 | 1.59 |
| 32 | d | 407 | LHG | O7-C5 | -2.14 | 1.41 | 1.46 |
| 25 | b | 609 | CLA | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 25 | c | 503 | CLA | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 25 | d | 402 | CLA | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 25 | D | 403 | CLA | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 25 | c | 511 | CLA | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 25 | b | 611 | CLA | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 26 | D | 401 | PHO | C4B-NB | 2.12 | 1.41 | 1.36 |
| 25 | c | 512 | CLA | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 25 | B | 609 | CLA | CMD-C2D | -2.11 | 1.46 | 1.51 |
| 25 | C | 504 | CLA | CMD-C2D | -2.11 | 1.46 | 1.51 |
| 26 | A | 608 | PHO | C4B-NB | 2.10 | 1.41 | 1.36 |
| 26 | a | 709 | PHO | C4B-NB | 2.10 | 1.41 | 1.36 |
| 32 | B | 625 | LHG | O7-C5 | -2.10 | 1.41 | 1.46 |
| 25 | C | 502 | CLA | CMD-C2D | -2.10 | 1.46 | 1.51 |
| 25 | C | 503 | CLA | CMD-C2D | -2.10 | 1.46 | 1.51 |
| 25 | a | 708 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |
| 25 | B | 614 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |
| 25 | c | 502 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33 | c | 516 | DGD | O1G-C1G | -2.09 | 1.40 | 1.45 |
| 25 | B | 602 | CLA | CMD-C2D | -2.09 | 1.46 | 1.51 |
| 25 | B | 615 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | b | 619 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | D | 404 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | C | 509 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | B | 610 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | c | 501 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | C | 507 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 29 | B | 623 | SQD | O2-C2 | -2.08 | 1.38 | 1.43 |
| 25 | B | 613 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | B | 606 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | C | 511 | CLA | CMD-C2D | -2.08 | 1.46 | 1.51 |
| 25 | B | 608 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | b | 608 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | b | 616 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 26 | a | 710 | PHO | C4B-NB | 2.07 | 1.41 | 1.36 |
| 25 | c | 504 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | b | 607 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | a | 719 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | b | 613 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | b | 615 | CLA | CMD-C2D | -2.07 | 1.46 | 1.51 |
| 25 | B | 605 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | C | 508 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | B | 607 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 33 | c | 516 | DGD | O2G-C2G | -2.06 | 1.41 | 1.46 |
| 33 | C | 518 | DGD | O5D-C6D | -2.06 | 1.40 | 1.43 |
| 25 | C | 513 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | D | 402 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | B | 617 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 29 | a | 714 | SQD | O3-C3 | -2.06 | 1.38 | 1.43 |
| 25 | A | 607 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | b | 617 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | b | 622 | CLA | CMD-C2D | -2.06 | 1.46 | 1.51 |
| 25 | B | 617 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 25 | b | 614 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 28 | d | 405 | PL9 | C53-C6 | -2.05 | 1.46 | 1.50 |
| 25 | c | 513 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 29 | f | 102 | SQD | O4-C4 | -2.05 | 1.38 | 1.43 |
| 25 | b | 621 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | d | 403 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | b | 620 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | c | 508 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | c | 506 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 33 | c | 517 | DGD | C1E-C2E | 2.05 | 1.58 | 1.52 |
| 25 | C | 505 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | C | 512 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 33 | c | 517 | DGD | O6E-C5E | -2.05 | 1.39 | 1.44 |
| 25 | C | 514 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | B | 611 | CLA | CMD-C2D | -2.05 | 1.46 | 1.51 |
| 25 | A | 609 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 25 | B | 612 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 25 | b | 610 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 29 | B | 626 | SQD | O3-C3 | -2.04 | 1.38 | 1.43 |
| 25 | c | 507 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 25 | a | 711 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 25 | B | 603 | CLA | CMD-C2D | -2.04 | 1.46 | 1.51 |
| 28 | A | 611 | PL9 | C53-C6 | -2.04 | 1.46 | 1.50 |
| 25 | c | 509 | CLA | CMD-C2D | -2.03 | 1.46 | 1.51 |
| 29 | D | 410 | SQD | O3-C3 | -2.03 | 1.38 | 1.43 |
| 29 | A | 612 | SQD | O3-C3 | -2.03 | 1.38 | 1.43 |
| 25 | b | 612 | CLA | CMD-C2D | -2.03 | 1.46 | 1.51 |
| 25 | C | 510 | CLA | CMD-C2D | -2.02 | 1.46 | 1.51 |
| 29 | D | 410 | SQD | O4-C4 | -2.02 | 1.38 | 1.43 |
| 28 | a | 713 | PL9 | C53-C6 | -2.02 | 1.46 | 1.50 |
| 33 | C | 517 | DGD | O2G-C2G | -2.02 | 1.41 | 1.46 |
| 33 | c | 518 | DGD | O1G-C1G | -2.02 | 1.40 | 1.45 |
| 29 | f | 102 | SQD | O3-C3 | -2.02 | 1.38 | 1.43 |
| 26 | A | 608 | PHO | C1B-C2B | 2.02 | 1.50 | 1.45 |
| 29 | A | 612 | SQD | O4-C4 | -2.02 | 1.38 | 1.43 |
| 28 | D | 406 | PL9 | C53-C6 | -2.02 | 1.46 | 1.50 |
| 29 | B | 626 | SQD | O4-C4 | -2.02 | 1.38 | 1.43 |
| 23 | b | 626 | LMG | O8-C9 | -2.01 | 1.40 | 1.45 |
| 23 | d | 408 | LMG | C7-C8 | 2.01 | 1.56 | 1.51 |
| 23 | C | 520 | LMG | C4-C5 | 2.01 | 1.57 | 1.53 |
| 33 | C | 519 | DGD | O1G-C1G | -2.01 | 1.40 | 1.45 |
| 25 | B | 616 | CLA | CMD-C2D | -2.01 | 1.46 | 1.51 |
| 33 | c | 518 | DGD | O2G-C2G | -2.01 | 1.41 | 1.46 |
| 32 | B | 625 | LHG | P-O6 | 2.01 | 1.67 | 1.59 |
| 29 | a | 714 | SQD | O4-C4 | -2.01 | 1.38 | 1.43 |
| 28 | A | 611 | PL9 | C6-C1 | -2.00 | 1.45 | 1.48 |
| 26 | a | 709 | PHO | C1B-C2B | 2.00 | 1.50 | 1.45 |

All (1149) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 25 | B | 605 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 25 | b | 610 | CLA | C4A-NA-C1A | 6.40 | 109.58 | 106.71 |
| 25 | C | 508 | CLA | C4A-NA-C1A | 6.36 | 109.57 | 106.71 |
| 25 | C | 513 | CLA | C4A-NA-C1A | 6.29 | 109.53 | 106.71 |
| 25 | b | 619 | CLA | C4A-NA-C1A | 6.21 | 109.50 | 106.71 |
| 25 | b | 621 | CLA | C4A-NA-C1A | 6.17 | 109.48 | 106.71 |
| 25 | c | 507 | CLA | C4A-NA-C1A | 6.13 | 109.46 | 106.71 |
| 25 | C | 504 | CLA | C4A-NA-C1A | 6.09 | 109.44 | 106.71 |
| 25 | c | 509 | CLA | C4A-NA-C1A | 6.07 | 109.44 | 106.71 |
| 25 | c | 511 | CLA | C4A-NA-C1A | 6.06 | 109.43 | 106.71 |
| 25 | c | 513 | CLA | C4A-NA-C1A | 6.04 | 109.42 | 106.71 |
| 25 | c | 503 | CLA | C4A-NA-C1A | 6.03 | 109.42 | 106.71 |
| 25 | c | 512 | CLA | C4A-NA-C1A | 5.97 | 109.39 | 106.71 |
| 25 | b | 615 | CLA | C4A-NA-C1A | 5.93 | 109.37 | 106.71 |
| 25 | C | 510 | CLA | C4A-NA-C1A | 5.91 | 109.36 | 106.71 |
| 25 | B | 616 | CLA | C4A-NA-C1A | 5.90 | 109.36 | 106.71 |
| 25 | B | 610 | CLA | C4A-NA-C1A | 5.89 | 109.36 | 106.71 |
| 25 | C | 512 | CLA | C4A-NA-C1A | 5.87 | 109.34 | 106.71 |
| 25 | b | 607 | CLA | C4A-NA-C1A | 5.86 | 109.34 | 106.71 |
| 25 | B | 617 | CLA | C4A-NA-C1A | 5.84 | 109.33 | 106.71 |
| 25 | B | 613 | CLA | C4A-NA-C1A | 5.80 | 109.31 | 106.71 |
| 25 | c | 502 | CLA | C4A-NA-C1A | 5.79 | 109.31 | 106.71 |
| 25 | b | 618 | CLA | C4A-NA-C1A | 5.78 | 109.31 | 106.71 |
| 25 | B | 612 | CLA | C4A-NA-C1A | 5.75 | 109.29 | 106.71 |
| 25 | C | 506 | CLA | C4A-NA-C1A | 5.73 | 109.28 | 106.71 |
| 25 | B | 602 | CLA | C4A-NA-C1A | 5.73 | 109.28 | 106.71 |
| 25 | b | 622 | CLA | C4A-NA-C1A | 5.68 | 109.26 | 106.71 |
| 25 | B | 614 | CLA | C4A-NA-C1A | 5.67 | 109.26 | 106.71 |
| 25 | C | 502 | CLA | C4A-NA-C1A | 5.64 | 109.24 | 106.71 |
| 25 | C | 503 | CLA | C4A-NA-C1A | 5.59 | 109.22 | 106.71 |
| 25 | d | 402 | CLA | C4A-NA-C1A | 5.56 | 109.21 | 106.71 |
| 25 | c | 510 | CLA | C4A-NA-C1A | 5.55 | 109.20 | 106.71 |
| 29 | B | 626 | SQD | O9-S-C6 | 5.54 | 113.53 | 106.94 |
| 25 | B | 607 | CLA | C4A-NA-C1A | 5.51 | 109.18 | 106.71 |
| 25 | C | 509 | CLA | C4A-NA-C1A | 5.46 | 109.16 | 106.71 |
| 25 | D | 404 | CLA | C4A-NA-C1A | 5.45 | 109.16 | 106.71 |
| 25 | C | 507 | CLA | C4A-NA-C1A | 5.43 | 109.15 | 106.71 |
| 25 | C | 514 | CLA | C4A-NA-C1A | 5.42 | 109.14 | 106.71 |
| 25 | c | 501 | CLA | C4A-NA-C1A | 5.41 | 109.14 | 106.71 |
| 25 | C | 511 | CLA | C4A-NA-C1A | 5.39 | 109.13 | 106.71 |
| 29 | b | 601 | SQD | O7-S-C6 | 5.38 | 113.34 | 106.94 |
| 25 | b | 617 | CLA | C4A-NA-C1A | 5.37 | 109.12 | 106.71 |
| 25 | B | 606 | CLA | C4A-NA-C1A | 5.36 | 109.11 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28 | a | 713 | PL9 | C7-C3-C4 | 5.33 | 121.21 | 116.88 |
| 25 | c | 508 | CLA | C4A-NA-C1A | 5.32 | 109.10 | 106.71 |
| 25 | a | 711 | CLA | C4A-NA-C1A | 5.27 | 109.08 | 106.71 |
| 25 | D | 403 | CLA | C4A-NA-C1A | 5.26 | 109.07 | 106.71 |
| 25 | A | 609 | CLA | C4A-NA-C1A | 5.23 | 109.06 | 106.71 |
| 28 | d | 405 | PL9 | C7-C3-C4 | 5.22 | 121.12 | 116.88 |
| 25 | b | 611 | CLA | C4A-NA-C1A | 5.22 | 109.05 | 106.71 |
| 25 | c | 504 | CLA | C4A-NA-C1A | 5.19 | 109.04 | 106.71 |
| 25 | d | 403 | CLA | C4A-NA-C1A | 5.17 | 109.03 | 106.71 |
| 25 | B | 611 | CLA | C4A-NA-C1A | 5.14 | 109.02 | 106.71 |
| 25 | B | 604 | CLA | C4A-NA-C1A | 5.14 | 109.02 | 106.71 |
| 25 | c | 506 | CLA | C4A-NA-C1A | 5.13 | 109.01 | 106.71 |
| 25 | B | 615 | CLA | C4A-NA-C1A | 5.13 | 109.01 | 106.71 |
| 28 | D | 406 | PL9 | C7-C3-C4 | 5.09 | 121.01 | 116.88 |
| 25 | c | 505 | CLA | C4A-NA-C1A | 5.08 | 108.99 | 106.71 |
| 25 | b | 614 | CLA | C4A-NA-C1A | 5.02 | 108.96 | 106.71 |
| 28 | A | 611 | PL9 | C7-C3-C4 | 5.00 | 120.94 | 116.88 |
| 25 | b | 616 | CLA | C4A-NA-C1A | 4.94 | 108.92 | 106.71 |
| 25 | A | 607 | CLA | C4A-NA-C1A | 4.92 | 108.92 | 106.71 |
| 25 | B | 603 | CLA | C4A-NA-C1A | 4.91 | 108.91 | 106.71 |
| 25 | a | 708 | CLA | C4A-NA-C1A | 4.89 | 108.91 | 106.71 |
| 25 | b | 612 | CLA | C4A-NA-C1A | 4.87 | 108.89 | 106.71 |
| 29 | A | 612 | SQD | O9-S-C6 | 4.86 | 112.71 | 106.94 |
| 29 | b | 601 | SQD | O6-C1-C2 | 4.82 | 115.82 | 108.30 |
| 25 | D | 402 | CLA | C4A-NA-C1A | 4.74 | 108.84 | 106.71 |
| 25 | a | 719 | CLA | C4A-NA-C1A | 4.73 | 108.83 | 106.71 |
| 25 | a | 707 | CLA | C4A-NA-C1A | 4.63 | 108.79 | 106.71 |
| 29 | B | 626 | SQD | O5-C5-C4 | 4.54 | 117.93 | 109.69 |
| 29 | b | 601 | SQD | O9-S-C6 | 4.52 | 112.31 | 106.94 |
| 29 | B | 623 | SQD | C4-C3-C2 | 4.48 | 118.64 | 110.82 |
| 33 | C | 519 | DGD | O3G-C3G-C2G | -4.39 | 100.32 | 110.90 |
| 25 | B | 608 | CLA | C4A-NA-C1A | 4.32 | 108.65 | 106.71 |
| 25 | b | 617 | CLA | CMB-C2B-C1B | -4.31 | 121.83 | 128.46 |
| 25 | d | 403 | CLA | CMB-C2B-C1B | -4.31 | 121.83 | 128.46 |
| 33 | C | 517 | DGD | O3G-C3G-C2G | -4.29 | 100.56 | 110.90 |
| 25 | C | 514 | CLA | CMB-C2B-C1B | -4.27 | 121.89 | 128.46 |
| 33 | c | 516 | DGD | O3G-C3G-C2G | -4.27 | 100.60 | 110.90 |
| 25 | B | 617 | CLA | CMB-C2B-C1B | -4.26 | 121.92 | 128.46 |
| 33 | C | 518 | DGD | O3G-C3G-C2G | -4.23 | 100.70 | 110.90 |
| 25 | b | 608 | CLA | C4A-NA-C1A | 4.23 | 108.61 | 106.71 |
| 29 | B | 626 | SQD | O7-S-C6 | 4.22 | 111.96 | 106.94 |
| 25 | B | 612 | CLA | CMB-C2B-C1B | -4.22 | 121.98 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | B | 613 | CLA | CMB-C2B-C1B | -4.21 | 122.00 | 128.46 |
| 32 | D | 408 | LHG | O4-P-O5 | 4.20 | 133.01 | 112.24 |
| 25 | c | 512 | CLA | CMB-C2B-C1B | -4.20 | 122.01 | 128.46 |
| 25 | C | 512 | CLA | CMB-C2B-C1B | -4.19 | 122.02 | 128.46 |
| 33 | c | 518 | DGD | O3G-C3G-C2G | -4.19 | 100.78 | 110.90 |
| 32 | B | 625 | LHG | O4-P-O5 | 4.19 | 132.94 | 112.24 |
| 32 | L | 101 | LHG | O4-P-O5 | 4.19 | 132.94 | 112.24 |
| 29 | a | 714 | SQD | O7-S-C6 | 4.18 | 111.91 | 106.94 |
| 32 | d | 407 | LHG | O4-P-O5 | 4.18 | 132.91 | 112.24 |
| 32 | d | 406 | LHG | O4-P-O5 | 4.18 | 132.91 | 112.24 |
| 32 | b | 629 | LHG | O4-P-O5 | 4.18 | 132.90 | 112.24 |
| 29 | a | 714 | SQD | O5-C5-C4 | 4.18 | 117.28 | 109.69 |
| 33 | c | 517 | DGD | O3G-C3G-C2G | -4.18 | 100.82 | 110.90 |
| 32 | a | 720 | LHG | O4-P-O5 | 4.18 | 132.89 | 112.24 |
| 32 | D | 407 | LHG | O4-P-O5 | 4.18 | 132.88 | 112.24 |
| 25 | C | 505 | CLA | C4A-NA-C1A | 4.17 | 108.58 | 106.71 |
| 25 | b | 622 | CLA | CMB-C2B-C1B | -4.17 | 122.06 | 128.46 |
| 32 | e | 101 | LHG | O4-P-O5 | 4.16 | 132.79 | 112.24 |
| 25 | b | 620 | CLA | C4A-NA-C1A | 4.15 | 108.57 | 106.71 |
| 32 | E | 101 | LHG | O4-P-O5 | 4.12 | 132.62 | 112.24 |
| 25 | b | 619 | CLA | CMB-C2B-C1B | -4.11 | 122.14 | 128.46 |
| 25 | c | 513 | CLA | CMB-C2B-C1B | -4.11 | 122.15 | 128.46 |
| 29 | I | 102 | SQD | O47-C7-C8 | 4.09 | 120.33 | 111.50 |
| 29 | f | 102 | SQD | O7-S-C6 | 4.08 | 111.79 | 106.94 |
| 29 | D | 410 | SQD | O7-S-C6 | 4.05 | 111.75 | 106.94 |
| 25 | c | 510 | CLA | CMB-C2B-C1B | -4.03 | 122.26 | 128.46 |
| 23 | c | 520 | LMG | O6-C1-O1 | -4.03 | 100.42 | 109.97 |
| 29 | A | 612 | SQD | O5-C5-C4 | 4.02 | 116.99 | 109.69 |
| 25 | b | 612 | CLA | CMB-C2B-C1B | -4.00 | 122.31 | 128.46 |
| 25 | c | 509 | CLA | CMB-C2B-C1B | -4.00 | 122.32 | 128.46 |
| 29 | D | 410 | SQD | O9-S-C6 | 3.99 | 111.68 | 106.94 |
| 29 | f | 102 | SQD | O9-S-C6 | 3.99 | 111.68 | 106.94 |
| 23 | b | 626 | LMG | O6-C1-C2 | 3.97 | 118.76 | 110.35 |
| 25 | a | 707 | CLA | CMB-C2B-C1B | -3.97 | 122.37 | 128.46 |
| 25 | C | 511 | CLA | CMB-C2B-C1B | -3.95 | 122.39 | 128.46 |
| 29 | B | 626 | SQD | O6-C1-C2 | 3.94 | 114.46 | 108.30 |
| 29 | D | 410 | SQD | O6-C1-C2 | 3.94 | 114.46 | 108.30 |
| 25 | A | 606 | CLA | C4A-NA-C1A | 3.93 | 108.47 | 106.71 |
| 25 | B | 614 | CLA | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |
| 29 | A | 612 | SQD | O9-S-O7 | -3.87 | 100.56 | 113.95 |
| 25 | c | 503 | CLA | CMB-C2B-C1B | -3.87 | 122.52 | 128.46 |
| 25 | C | 513 | CLA | CMB-C2B-C1B | -3.86 | 122.53 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | B | 609 | CLA | CMB-C2B-C1B | -3.86 | 122.53 | 128.46 |
| 25 | b | 613 | CLA | CMB-C2B-C1B | -3.86 | 122.53 | 128.46 |
| 25 | B | 604 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 25 | C | 509 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 29 | a | 714 | SQD | O9-S-C6 | 3.84 | 111.51 | 106.94 |
| 25 | D | 402 | CLA | CMB-C2B-C1B | -3.84 | 122.56 | 128.46 |
| 29 | B | 626 | SQD | O9-S-O7 | -3.84 | 100.66 | 113.95 |
| 23 | C | 521 | LMG | O6-C1-O1 | -3.83 | 100.91 | 109.97 |
| 25 | c | 506 | CLA | CMB-C2B-C1B | -3.81 | 122.60 | 128.46 |
| 33 | H | 103 | DGD | O3G-C3G-C2G | -3.81 | 101.71 | 110.90 |
| 25 | b | 609 | CLA | CMB-C2B-C1B | -3.81 | 122.61 | 128.46 |
| 25 | c | 511 | CLA | CMB-C2B-C1B | -3.81 | 122.61 | 128.46 |
| 29 | B | 623 | SQD | O9-S-O7 | -3.79 | 100.84 | 113.95 |
| 25 | B | 609 | CLA | C4A-NA-C1A | 3.79 | 108.41 | 106.71 |
| 25 | C | 504 | CLA | CMB-C2B-C1B | -3.75 | 122.71 | 128.46 |
| 25 | A | 606 | CLA | CMB-C2B-C1B | -3.73 | 122.72 | 128.46 |
| 25 | b | 609 | CLA | C4A-NA-C1A | 3.73 | 108.38 | 106.71 |
| 29 | B | 623 | SQD | O47-C7-C8 | 3.73 | 119.54 | 111.50 |
| 29 | B | 623 | SQD | O9-S-C6 | 3.72 | 111.36 | 106.94 |
| 29 | f | 102 | SQD | O9-S-O7 | -3.70 | 101.13 | 113.95 |
| 29 | A | 612 | SQD | O47-C7-C8 | 3.70 | 119.47 | 111.50 |
| 25 | c | 507 | CLA | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 27 | H | 102 | BCR | C2-C1-C6 | 3.69 | 116.16 | 110.48 |
| 29 | D | 410 | SQD | O9-S-O7 | -3.68 | 101.21 | 113.95 |
| 25 | b | 614 | CLA | CMB-C2B-C1B | -3.68 | 122.81 | 128.46 |
| 29 | A | 612 | SQD | O7-S-C6 | 3.68 | 111.31 | 106.94 |
| 25 | b | 610 | CLA | CMB-C2B-C1B | -3.66 | 122.83 | 128.46 |
| 25 | C | 514 | CLA | CMB-C2B-C3B | 3.66 | 131.53 | 124.68 |
| 25 | B | 607 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 25 | c | 504 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 29 | B | 623 | SQD | O5-C5-C4 | 3.63 | 116.29 | 109.69 |
| 29 | a | 714 | SQD | O9-S-O7 | -3.63 | 101.37 | 113.95 |
| 23 | b | 626 | LMG | O6-C5-C4 | 3.63 | 116.28 | 109.69 |
| 28 | a | 713 | PL9 | C7-C3-C2 | -3.63 | 118.53 | 123.30 |
| 25 | C | 506 | CLA | CMB-C2B-C1B | -3.62 | 122.90 | 128.46 |
| 25 | B | 617 | CLA | CMB-C2B-C3B | 3.60 | 131.42 | 124.68 |
| 25 | C | 510 | CLA | CMB-C2B-C1B | -3.60 | 122.93 | 128.46 |
| 25 | d | 403 | CLA | CMB-C2B-C3B | 3.60 | 131.41 | 124.68 |
| 29 | A | 614 | SQD | O47-C7-C8 | 3.59 | 119.24 | 111.50 |
| 25 | B | 608 | CLA | CMB-C2B-C1B | -3.59 | 122.95 | 128.46 |
| 25 | b | 620 | CLA | CMB-C2B-C1B | -3.59 | 122.95 | 128.46 |
| 25 | c | 512 | CLA | CMB-C2B-C3B | 3.58 | 131.38 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35 | v | 201 | HEC | CMB-C2B-C1B | -3.57 | 122.97 | 128.46 |
| 25 | b | 622 | CLA | CMB-C2B-C3B | 3.57 | 131.35 | 124.68 |
| 25 | c | 508 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 25 | c | 513 | CLA | CMB-C2B-C3B | 3.52 | 131.27 | 124.68 |
| 25 | C | 507 | CLA | CMB-C2B-C1B | -3.52 | 123.05 | 128.46 |
| 25 | b | 613 | CLA | C4A-NA-C1A | 3.52 | 108.29 | 106.71 |
| 25 | c | 501 | CLA | CMB-C2B-C1B | -3.51 | 123.07 | 128.46 |
| 29 | a | 714 | SQD | O47-C7-C8 | 3.51 | 119.06 | 111.50 |
| 25 | C | 505 | CLA | CMB-C2B-C1B | -3.50 | 123.08 | 128.46 |
| 28 | A | 611 | PL9 | C7-C3-C2 | -3.50 | 118.70 | 123.30 |
| 25 | B | 615 | CLA | CMB-C2B-C1B | -3.50 | 123.09 | 128.46 |
| 25 | C | 512 | CLA | CMB-C2B-C3B | 3.49 | 131.22 | 124.68 |
| 33 | C | 519 | DGD | O6D-C1D-O3G | -3.49 | 101.72 | 109.97 |
| 35 | V | 201 | HEC | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |
| 25 | b | 617 | CLA | CMB-C2B-C3B | 3.48 | 131.19 | 124.68 |
| 25 | b | 608 | CLA | CMB-C2B-C1B | -3.48 | 123.12 | 128.46 |
| 25 | C | 503 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 28 | D | 406 | PL9 | C7-C3-C2 | -3.46 | 118.75 | 123.30 |
| 29 | B | 623 | SQD | C3-C4-C5 | 3.46 | 116.41 | 110.24 |
| 25 | C | 508 | CLA | CMB-C2B-C1B | -3.46 | 123.15 | 128.46 |
| 33 | h | 102 | DGD | O3G-C3G-C2G | -3.45 | 102.56 | 110.90 |
| 25 | b | 611 | CLA | CMB-C2B-C1B | -3.45 | 123.16 | 128.46 |
| 25 | B | 613 | CLA | CMB-C2B-C3B | 3.45 | 131.14 | 124.68 |
| 28 | d | 405 | PL9 | C7-C3-C2 | -3.45 | 118.77 | 123.30 |
| 29 | B | 623 | SQD | O7-S-C6 | 3.43 | 111.02 | 106.94 |
| 33 | c | 518 | DGD | O6D-C1D-O3G | -3.43 | 101.85 | 109.97 |
| 29 | D | 410 | SQD | O47-C7-C8 | 3.43 | 118.89 | 111.50 |
| 25 | b | 607 | CLA | CMB-C2B-C1B | -3.43 | 123.20 | 128.46 |
| 25 | b | 619 | CLA | CMB-C2B-C3B | 3.41 | 131.05 | 124.68 |
| 25 | a | 708 | CLA | CMB-C2B-C1B | -3.40 | 123.25 | 128.46 |
| 25 | b | 618 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 33 | c | 517 | DGD | O6D-C1D-O3G | -3.39 | 101.94 | 109.97 |
| 25 | a | 711 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 25 | B | 612 | CLA | CMB-C2B-C3B | 3.39 | 131.02 | 124.68 |
| 29 | b | 601 | SQD | O47-C7-C8 | 3.39 | 118.81 | 111.50 |
| 25 | C | 502 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 33 | C | 518 | DGD | O5D-C6D-C5D | -3.38 | 102.80 | 109.05 |
| 25 | c | 510 | CLA | CMB-C2B-C3B | 3.37 | 130.99 | 124.68 |
| 25 | A | 609 | CLA | CMB-C2B-C1B | -3.37 | 123.29 | 128.46 |
| 29 | A | 612 | SQD | O6-C1-C2 | 3.37 | 113.56 | 108.30 |
| 25 | D | 404 | CLA | CMB-C2B-C1B | -3.36 | 123.29 | 128.46 |
| 29 | B | 626 | SQD | O47-C7-C8 | 3.36 | 118.75 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | C | 518 | DGD | O6D-C1D-O3G | -3.36 | 102.02 | 109.97 |
| 25 | b | 616 | CLA | CMB-C2B-C1B | -3.36 | 123.31 | 128.46 |
| 25 | b | 621 | CLA | CMB-C2B-C1B | -3.33 | 123.35 | 128.46 |
| 25 | c | 509 | CLA | CMB-C2B-C3B | 3.33 | 130.90 | 124.68 |
| 33 | C | 517 | DGD | O6D-C1D-O3G | -3.33 | 102.09 | 109.97 |
| 33 | c | 516 | DGD | O6D-C1D-O3G | -3.32 | 102.10 | 109.97 |
| 25 | B | 606 | CLA | CMB-C2B-C1B | -3.32 | 123.36 | 128.46 |
| 29 | a | 714 | SQD | C3-C4-C5 | 3.32 | 116.15 | 110.24 |
| 25 | C | 511 | CLA | CMB-C2B-C3B | 3.31 | 130.87 | 124.68 |
| 25 | B | 611 | CLA | CMB-C2B-C1B | -3.31 | 123.38 | 128.46 |
| 25 | a | 719 | CLA | CMB-C2B-C1B | -3.30 | 123.39 | 128.46 |
| 25 | B | 602 | CLA | CMB-C2B-C1B | -3.30 | 123.39 | 128.46 |
| 25 | B | 616 | CLA | CMB-C2B-C1B | -3.29 | 123.41 | 128.46 |
| 25 | a | 707 | CLA | CMB-C2B-C3B | 3.29 | 130.83 | 124.68 |
| 25 | b | 612 | CLA | CMB-C2B-C3B | 3.29 | 130.83 | 124.68 |
| 25 | B | 610 | CLA | CMB-C2B-C1B | -3.28 | 123.43 | 128.46 |
| 29 | b | 601 | SQD | O9-S-O7 | -3.28 | 102.61 | 113.95 |
| 25 | c | 502 | CLA | CMB-C2B-C1B | -3.27 | 123.43 | 128.46 |
| 25 | C | 513 | CLA | CMB-C2B-C3B | 3.27 | 130.79 | 124.68 |
| 25 | b | 615 | CLA | CMB-C2B-C1B | -3.26 | 123.45 | 128.46 |
| 25 | D | 403 | CLA | CMB-C2B-C1B | -3.26 | 123.46 | 128.46 |
| 25 | B | 603 | CLA | CMB-C2B-C1B | -3.26 | 123.46 | 128.46 |
| 25 | B | 609 | CLA | CMB-C2B-C3B | 3.25 | 130.77 | 124.68 |
| 25 | d | 402 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 25 | B | 605 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 25 | A | 607 | CLA | CMB-C2B-C1B | -3.24 | 123.48 | 128.46 |
| 25 | D | 402 | CLA | CMB-C2B-C3B | 3.24 | 130.74 | 124.68 |
| 29 | B | 623 | SQD | O8-S-C6 | 3.23 | 110.89 | 105.74 |
| 25 | C | 509 | CLA | CMB-C2B-C3B | 3.23 | 130.72 | 124.68 |
| 25 | B | 614 | CLA | CMB-C2B-C3B | 3.23 | 130.71 | 124.68 |
| 25 | c | 503 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 25 | B | 604 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 23 | B | 621 | LMG | O6-C1-O1 | -3.20 | 102.39 | 109.97 |
| 27 | C | 516 | BCR | C15-C16-C17 | -3.20 | 116.91 | 123.47 |
| 25 | c | 507 | CLA | CMB-C2B-C3B | 3.19 | 130.64 | 124.68 |
| 29 | f | 102 | SQD | O6-C1-C2 | 3.18 | 113.27 | 108.30 |
| 25 | b | 613 | CLA | CMB-C2B-C3B | 3.18 | 130.63 | 124.68 |
| 25 | c | 505 | CLA | CMB-C2B-C1B | -3.17 | 123.59 | 128.46 |
| 25 | b | 609 | CLA | CMB-C2B-C3B | 3.17 | 130.60 | 124.68 |
| 25 | c | 506 | CLA | CMB-C2B-C3B | 3.16 | 130.59 | 124.68 |
| 25 | c | 511 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 25 | C | 505 | CLA | CHB-C4A-NA | 3.14 | 128.85 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | H | 103 | DGD | O6D-C1D-O3G | -3.14 | 102.55 | 109.97 |
| 25 | C | 513 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 29 | B | 626 | SQD | C1-O5-C5 | 3.13 | 119.82 | 113.69 |
| 25 | B | 605 | CLA | CHB-C4A-NA | 3.12 | 128.82 | 124.51 |
| 25 | D | 402 | CLA | CHB-C4A-NA | 3.11 | 128.81 | 124.51 |
| 25 | b | 607 | CLA | O2D-CGD-O1D | -3.11 | 117.76 | 123.84 |
| 25 | B | 608 | CLA | CHB-C4A-NA | 3.10 | 128.81 | 124.51 |
| 29 | D | 410 | SQD | O5-C5-C4 | 3.10 | 115.33 | 109.69 |
| 25 | A | 606 | CLA | CMB-C2B-C3B | 3.10 | 130.48 | 124.68 |
| 25 | C | 506 | CLA | CMB-C2B-C3B | 3.09 | 130.46 | 124.68 |
| 25 | B | 602 | CLA | O2D-CGD-O1D | -3.08 | 117.81 | 123.84 |
| 25 | C | 504 | CLA | CMB-C2B-C3B | 3.07 | 130.42 | 124.68 |
| 29 | a | 714 | SQD | O6-C1-C2 | 3.07 | 113.09 | 108.30 |
| 25 | b | 612 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 25 | B | 607 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 29 | A | 612 | SQD | C3-C4-C5 | 3.04 | 115.67 | 110.24 |
| 23 | b | 626 | LMG | C1-O6-C5 | 3.04 | 119.65 | 113.69 |
| 25 | A | 606 | CLA | CHB-C4A-NA | 3.04 | 128.71 | 124.51 |
| 25 | b | 610 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 25 | C | 510 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |
| 29 | B | 623 | SQD | C1-O5-C5 | 3.00 | 119.58 | 113.69 |
| 29 | f | 102 | SQD | O47-C7-C8 | 3.00 | 119.18 | 110.80 |
| 25 | B | 604 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 25 | b | 610 | CLA | O2D-CGD-O1D | -3.00 | 117.98 | 123.84 |
| 25 | b | 621 | CLA | O2D-CGD-O1D | -3.00 | 117.98 | 123.84 |
| 25 | b | 613 | CLA | CHB-C4A-NA | 2.99 | 128.65 | 124.51 |
| 25 | c | 504 | CLA | CMB-C2B-C3B | 2.99 | 130.28 | 124.68 |
| 25 | b | 614 | CLA | CMB-C2B-C3B | 2.99 | 130.27 | 124.68 |
| 25 | b | 610 | CLA | CHB-C4A-NA | 2.99 | 128.64 | 124.51 |
| 25 | c | 507 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 25 | a | 708 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 28 | A | 611 | PL9 | C7-C8-C9 | -2.97 | 121.85 | 126.79 |
| 29 | b | 601 | SQD | C44-O6-C1 | 2.97 | 119.54 | 113.74 |
| 27 | h | 101 | BCR | C2-C1-C6 | 2.97 | 115.05 | 110.48 |
| 25 | C | 502 | CLA | O2D-CGD-O1D | -2.97 | 118.04 | 123.84 |
| 25 | b | 620 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 25 | C | 508 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 25 | C | 508 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 25 | b | 608 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 25 | c | 508 | CLA | CMB-C2B-C3B | 2.96 | 130.21 | 124.68 |
| 25 | B | 608 | CLA | CMB-C2B-C3B | 2.96 | 130.21 | 124.68 |
| 25 | D | 402 | CLA | O2D-CGD-O1D | -2.96 | 118.06 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | D | 404 | CLA | O2D-CGD-O1D | -2.96 | 118.06 | 123.84 |
| 25 | B | 605 | CLA | O2D-CGD-O1D | -2.95 | 118.07 | 123.84 |
| 25 | c | 504 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 25 | A | 607 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 25 | a | 719 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 33 | h | 102 | DGD | O6D-C1D-O3G | -2.94 | 103.00 | 109.97 |
| 25 | c | 504 | CLA | O2D-CGD-O1D | -2.94 | 118.08 | 123.84 |
| 27 | c | 515 | BCR | C15-C16-C17 | -2.94 | 117.45 | 123.47 |
| 25 | B | 607 | CLA | CMB-C2B-C3B | 2.94 | 130.18 | 124.68 |
| 25 | b | 613 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 25 | C | 506 | CLA | O2D-CGD-O1D | -2.94 | 118.10 | 123.84 |
| 25 | c | 508 | CLA | O2D-CGD-O1D | -2.94 | 118.10 | 123.84 |
| 25 | C | 505 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 25 | C | 508 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 25 | c | 501 | CLA | O2D-CGD-O1D | -2.91 | 118.14 | 123.84 |
| 25 | c | 502 | CLA | O2D-CGD-O1D | -2.91 | 118.14 | 123.84 |
| 25 | C | 509 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 25 | C | 513 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 27 | H | 102 | BCR | C24-C23-C22 | -2.90 | 121.85 | 126.23 |
| 25 | C | 507 | CLA | CMB-C2B-C3B | 2.90 | 130.11 | 124.68 |
| 25 | A | 609 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 25 | A | 607 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 25 | A | 609 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 25 | B | 616 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 25 | b | 617 | CLA | O2D-CGD-O1D | -2.90 | 118.18 | 123.84 |
| 25 | B | 616 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 25 | C | 503 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 25 | b | 620 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 25 | C | 503 | CLA | CMB-C2B-C3B | 2.89 | 130.08 | 124.68 |
| 27 | t | 103 | BCR | C15-C14-C13 | -2.89 | 123.19 | 127.31 |
| 28 | d | 405 | PL9 | C40-C39-C41 | 2.89 | 120.13 | 115.27 |
| 25 | B | 615 | CLA | CMB-C2B-C3B | 2.88 | 130.07 | 124.68 |
| 25 | B | 604 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 27 | b | 602 | BCR | C33-C5-C6 | -2.88 | 121.29 | 124.53 |
| 25 | c | 505 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 27 | t | 103 | BCR | C33-C5-C6 | -2.88 | 121.30 | 124.53 |
| 29 | B | 626 | SQD | C3-C4-C5 | 2.88 | 115.37 | 110.24 |
| 28 | A | 611 | PL9 | C40-C39-C41 | 2.87 | 120.11 | 115.27 |
| 25 | B | 603 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 25 | C | 505 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 25 | a | 711 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 26 | a | 710 | PHO | O2D-CGD-O1D | -2.86 | 118.24 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | B | 609 | CLA | O2D-CGD-O1D | -2.86 | 118.24 | 123.84 |
| 27 | B | 618 | BCR | C15-C16-C17 | -2.86 | 117.61 | 123.47 |
| 25 | d | 403 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 25 | b | 609 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 34 | e | 102 | HEM | CMD-C2D-C1D | -2.86 | 124.07 | 128.46 |
| 25 | b | 620 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 25 | B | 613 | CLA | CHB-C4A-NA | 2.86 | 128.46 | 124.51 |
| 25 | C | 510 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 25 | a | 711 | CLA | CHB-C4A-NA | 2.86 | 128.46 | 124.51 |
| 25 | b | 616 | CLA | CHB-C4A-NA | 2.86 | 128.46 | 124.51 |
| 25 | a | 719 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 25 | a | 707 | CLA | CHB-C4A-NA | 2.85 | 128.46 | 124.51 |
| 25 | c | 507 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 25 | c | 512 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 25 | c | 513 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 25 | B | 609 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 25 | C | 514 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 25 | b | 618 | CLA | CHB-C4A-NA | 2.84 | 128.45 | 124.51 |
| 25 | b | 618 | CLA | O2D-CGD-O1D | -2.84 | 118.28 | 123.84 |
| 25 | b | 621 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 25 | c | 501 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 25 | d | 402 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 26 | A | 608 | PHO | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 25 | a | 711 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 25 | c | 505 | CLA | C1B-CHB-C4A | -2.84 | 124.50 | 130.12 |
| 25 | C | 509 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 25 | a | 708 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 25 | c | 509 | CLA | CHB-C4A-NA | 2.84 | 128.43 | 124.51 |
| 25 | b | 607 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 23 | A | 603 | LMG | O6-C5-C4 | 2.83 | 114.84 | 109.69 |
| 33 | h | 102 | DGD | CDB-CCB-CBB | -2.83 | 100.04 | 114.42 |
| 25 | B | 613 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 25 | B | 615 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 25 | A | 609 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 32 | a | 720 | LHG | O8-C23-C24 | 2.83 | 120.78 | 111.91 |
| 25 | c | 511 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 25 | c | 512 | CLA | CMD-C2D-C3D | 2.82 | 129.96 | 124.68 |
| 32 | B | 625 | LHG | O8-C23-C24 | 2.82 | 120.76 | 111.91 |
| 25 | B | 603 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 25 | D | 404 | CLA | CMB-C2B-C3B | 2.82 | 129.94 | 124.68 |
| 25 | b | 621 | CLA | CMD-C2D-C3D | 2.82 | 129.94 | 124.68 |
| 33 | c | 517 | DGD | CDB-CCB-CBB | -2.81 | 100.14 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | b | 611 | CLA | CMB-C2B-C3B | 2.81 | 129.94 | 124.68 |
| 25 | a | 708 | CLA | CHB-C4A-NA | 2.81 | 128.40 | 124.51 |
| 25 | B | 606 | CLA | CMB-C2B-C3B | 2.81 | 129.93 | 124.68 |
| 25 | b | 618 | CLA | CMB-C2B-C3B | 2.81 | 129.93 | 124.68 |
| 29 | f | 102 | SQD | O5-C5-C4 | 2.81 | 114.79 | 109.69 |
| 25 | C | 511 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 23 | A | 603 | LMG | O6-C1-O1 | -2.80 | 103.33 | 109.97 |
| 25 | c | 512 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 23 | b | 626 | LMG | C4-C3-C2 | -2.80 | 105.94 | 110.82 |
| 27 | b | 623 | BCR | C15-C16-C17 | -2.79 | 117.75 | 123.47 |
| 25 | b | 614 | CLA | O2D-CGD-O1D | -2.79 | 118.38 | 123.84 |
| 25 | C | 504 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 25 | B | 611 | CLA | O2D-CGD-O1D | -2.79 | 118.38 | 123.84 |
| 27 | b | 602 | BCR | C15-C14-C13 | -2.79 | 123.33 | 127.31 |
| 25 | c | 503 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 25 | b | 609 | CLA | CHB-C4A-NA | 2.79 | 128.36 | 124.51 |
| 33 | C | 519 | DGD | CDB-CCB-CBB | -2.79 | 100.28 | 114.42 |
| 25 | b | 616 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 25 | B | 616 | CLA | CMB-C2B-C3B | 2.78 | 129.88 | 124.68 |
| 25 | B | 602 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 25 | B | 603 | CLA | CMB-C2B-C3B | 2.78 | 129.87 | 124.68 |
| 32 | D | 407 | LHG | O8-C23-C24 | 2.78 | 120.62 | 111.91 |
| 25 | c | 510 | CLA | O2D-CGD-O1D | -2.78 | 118.41 | 123.84 |
| 25 | d | 402 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 25 | b | 621 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 25 | b | 619 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 25 | D | 403 | CLA | CMB-C2B-C3B | 2.77 | 129.85 | 124.68 |
| 25 | a | 719 | CLA | CMB-C2B-C3B | 2.77 | 129.85 | 124.68 |
| 25 | D | 403 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 25 | c | 505 | CLA | CMB-C2B-C3B | 2.77 | 129.85 | 124.68 |
| 33 | C | 518 | DGD | CDB-CCB-CBB | -2.77 | 100.38 | 114.42 |
| 33 | c | 518 | DGD | O5D-C6D-C5D | -2.77 | 103.93 | 109.05 |
| 25 | b | 615 | CLA | CMB-C2B-C3B | 2.76 | 129.85 | 124.68 |
| 25 | c | 508 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 25 | B | 602 | CLA | CMB-C2B-C3B | 2.76 | 129.85 | 124.68 |
| 25 | b | 614 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 25 | B | 611 | CLA | CMB-C2B-C3B | 2.76 | 129.85 | 124.68 |
| 25 | b | 608 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 25 | b | 622 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 25 | B | 612 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 27 | b | 623 | BCR | C33-C5-C6 | -2.76 | 121.43 | 124.53 |
| 25 | C | 506 | CLA | C1B-CHB-C4A | -2.76 | 124.66 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | t | 103 | BCR | C15-C16-C17 | -2.76 | 117.83 | 123.47 |
| 33 | c | 516 | DGD | O5D-C6D-C5D | -2.76 | 103.95 | 109.05 |
| 25 | B | 614 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 25 | B | 611 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 25 | b | 619 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 33 | c | 516 | DGD | CDB-CCB-CBB | -2.75 | 100.48 | 114.42 |
| 25 | c | 501 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 32 | E | 101 | LHG | O8-C23-C24 | 2.74 | 120.51 | 111.91 |
| 25 | c | 508 | CLA | CMD-C2D-C3D | 2.74 | 129.81 | 124.68 |
| 25 | B | 606 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 25 | B | 608 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 25 | c | 503 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 25 | b | 616 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 25 | C | 502 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 27 | b | 602 | BCR | C15-C16-C17 | -2.74 | 117.87 | 123.47 |
| 25 | B | 610 | CLA | CMB-C2B-C3B | 2.73 | 129.79 | 124.68 |
| 25 | C | 510 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 25 | C | 504 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 25 | c | 506 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 26 | D | 401 | PHO | O2D-CGD-O1D | -2.73 | 118.51 | 123.84 |
| 27 | d | 404 | BCR | C27-C26-C25 | 2.73 | 126.69 | 122.73 |
| 25 | C | 512 | CLA | O2D-CGD-O1D | -2.73 | 118.51 | 123.84 |
| 32 | D | 408 | LHG | C11-C10-C9 | -2.72 | 100.59 | 114.42 |
| 25 | B | 610 | CLA | O2D-CGD-O1D | -2.72 | 118.51 | 123.84 |
| 25 | C | 507 | CLA | C1B-CHB-C4A | -2.72 | 124.73 | 130.12 |
| 25 | b | 609 | CLA | C1B-CHB-C4A | -2.72 | 124.73 | 130.12 |
| 25 | C | 514 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 25 | A | 607 | CLA | CMB-C2B-C3B | 2.72 | 129.76 | 124.68 |
| 25 | B | 612 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 25 | B | 617 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 32 | d | 406 | LHG | O8-C23-C24 | 2.71 | 120.42 | 111.91 |
| 29 | B | 623 | SQD | C44-O6-C1 | 2.71 | 119.04 | 113.74 |
| 33 | c | 518 | DGD | CDB-CCB-CBB | -2.71 | 100.66 | 114.42 |
| 28 | A | 611 | PL9 | C22-C23-C24 | -2.71 | 121.13 | 127.66 |
| 25 | d | 403 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 25 | A | 609 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 27 | B | 618 | BCR | C33-C5-C6 | -2.71 | 121.49 | 124.53 |
| 25 | c | 502 | CLA | CMB-C2B-C3B | 2.71 | 129.74 | 124.68 |
| 33 | H | 103 | DGD | CDB-CCB-CBB | -2.71 | 100.69 | 114.42 |
| 27 | b | 625 | BCR | C27-C26-C25 | 2.70 | 126.66 | 122.73 |
| 28 | a | 713 | PL9 | C40-C39-C41 | 2.70 | 119.82 | 115.27 |
| 25 | C | 513 | CLA | CMD-C2D-C3D | 2.70 | 129.73 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | b | 601 | SQD | O8-S-C6 | 2.70 | 110.05 | 105.74 |
| 25 | b | 607 | CLA | CMB-C2B-C3B | 2.70 | 129.73 | 124.68 |
| 25 | B | 607 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 25 | B | 615 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 25 | B | 614 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 25 | b | 617 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 25 | d | 402 | CLA | C1B-CHB-C4A | -2.69 | 124.78 | 130.12 |
| 27 | B | 620 | BCR | C27-C26-C25 | 2.69 | 126.64 | 122.73 |
| 25 | B | 617 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 25 | b | 615 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 27 | B | 618 | BCR | C11-C10-C9 | -2.69 | 123.47 | 127.31 |
| 25 | c | 506 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 25 | B | 605 | CLA | C1-C2-C3 | -2.69 | 121.39 | 126.04 |
| 23 | f | 101 | LMG | O6-C1-O1 | -2.69 | 103.61 | 109.97 |
| 25 | c | 502 | CLA | CHB-C4A-NA | 2.69 | 128.22 | 124.51 |
| 32 | d | 407 | LHG | O8-C23-C24 | 2.68 | 120.33 | 111.91 |
| 27 | B | 618 | BCR | C29-C30-C25 | 2.68 | 114.61 | 110.48 |
| 27 | k | 101 | BCR | C33-C5-C6 | -2.68 | 121.52 | 124.53 |
| 25 | b | 612 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 25 | C | 503 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 25 | b | 611 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 25 | c | 510 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 27 | b | 623 | BCR | C15-C14-C13 | -2.67 | 123.50 | 127.31 |
| 25 | c | 513 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 33 | C | 519 | DGD | C3G-C2G-C1G | -2.67 | 105.48 | 111.79 |
| 25 | B | 603 | CLA | C1B-CHB-C4A | -2.66 | 124.84 | 130.12 |
| 25 | B | 617 | CLA | CMD-C2D-C3D | 2.66 | 129.66 | 124.68 |
| 27 | C | 515 | BCR | C2-C1-C6 | 2.66 | 114.58 | 110.48 |
| 25 | b | 622 | CLA | C1B-CHB-C4A | -2.66 | 124.85 | 130.12 |
| 28 | D | 406 | PL9 | C7-C8-C9 | -2.66 | 122.36 | 126.79 |
| 25 | D | 403 | CLA | C1B-CHB-C4A | -2.66 | 124.86 | 130.12 |
| 25 | b | 615 | CLA | C1B-CHB-C4A | -2.66 | 124.86 | 130.12 |
| 28 | D | 406 | PL9 | C40-C39-C41 | 2.66 | 119.74 | 115.27 |
| 25 | C | 511 | CLA | CHB-C4A-NA | 2.66 | 128.18 | 124.51 |
| 27 | b | 623 | BCR | C27-C26-C25 | 2.65 | 126.58 | 122.73 |
| 25 | c | 511 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 27 | D | 405 | BCR | C33-C5-C6 | -2.65 | 121.56 | 124.53 |
| 25 | b | 617 | CLA | C1-C2-C3 | -2.65 | 121.47 | 126.04 |
| 25 | b | 608 | CLA | C1B-CHB-C4A | -2.65 | 124.88 | 130.12 |
| 25 | b | 611 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 26 | A | 608 | PHO | CBD-CHA-C4D | -2.64 | 105.56 | 108.54 |
| 29 | D | 410 | SQD | O8-S-C6 | 2.64 | 109.95 | 105.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | c | 515 | BCR | C15-C14-C13 | -2.64 | 123.54 | 127.31 |
| 25 | B | 605 | CLA | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 25 | c | 509 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 25 | D | 404 | CLA | C1B-CHB-C4A | -2.63 | 124.90 | 130.12 |
| 27 | C | 515 | BCR | C11-C10-C9 | -2.63 | 123.55 | 127.31 |
| 35 | V | 201 | HEC | CMB-C2B-C3B | 2.63 | 128.91 | 125.82 |
| 25 | C | 507 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 25 | C | 507 | CLA | CHB-C4A-NA | 2.63 | 128.14 | 124.51 |
| 29 | I | 102 | SQD | O48-C23-C24 | 2.62 | 120.14 | 111.91 |
| 23 | b | 627 | LMG | O6-C1-O1 | -2.62 | 103.77 | 109.97 |
| 25 | b | 608 | CLA | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 25 | B | 606 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 25 | B | 611 | CLA | C1B-CHB-C4A | -2.61 | 124.95 | 130.12 |
| 29 | A | 612 | SQD | O8-S-C6 | 2.61 | 109.89 | 105.74 |
| 26 | D | 401 | PHO | CBD-CHA-C4D | -2.60 | 105.61 | 108.54 |
| 27 | c | 514 | BCR | C27-C26-C25 | 2.60 | 126.51 | 122.73 |
| 33 | C | 517 | DGD | CDB-CCB-CBB | -2.60 | 101.22 | 114.42 |
| 25 | C | 509 | CLA | CMD-C2D-C3D | 2.60 | 129.54 | 124.68 |
| 25 | b | 618 | CLA | CMD-C2D-C3D | 2.60 | 129.54 | 124.68 |
| 32 | L | 101 | LHG | O8-C23-C24 | 2.60 | 120.06 | 111.91 |
| 25 | C | 512 | CLA | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 26 | a | 710 | PHO | O1D-CGD-CBD | 2.60 | 129.80 | 124.48 |
| 26 | a | 709 | PHO | O2D-CGD-O1D | -2.60 | 118.76 | 123.84 |
| 25 | c | 506 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 27 | B | 620 | BCR | C33-C5-C6 | -2.60 | 121.61 | 124.53 |
| 25 | B | 610 | CLA | CHB-C4A-NA | 2.60 | 128.10 | 124.51 |
| 25 | D | 404 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 23 | a | 701 | LMG | O6-C1-O1 | -2.59 | 103.84 | 109.97 |
| 27 | D | 405 | BCR | C27-C26-C25 | 2.59 | 126.49 | 122.73 |
| 25 | B | 609 | CLA | CMD-C2D-C3D | 2.59 | 129.52 | 124.68 |
| 27 | b | 624 | BCR | C27-C26-C25 | 2.59 | 126.49 | 122.73 |
| 27 | Y | 101 | BCR | C33-C5-C6 | -2.59 | 121.62 | 124.53 |
| 29 | f | 102 | SQD | O8-S-C6 | 2.59 | 109.86 | 105.74 |
| 25 | C | 502 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 25 | C | 503 | CLA | CMD-C2D-C3D | 2.59 | 129.52 | 124.68 |
| 29 | f | 102 | SQD | C44-O6-C1 | 2.58 | 118.79 | 113.74 |
| 29 | b | 601 | SQD | C4-C3-C2 | 2.58 | 115.33 | 110.82 |
| 29 | B | 623 | SQD | O48-C23-C24 | 2.58 | 120.01 | 111.91 |
| 25 | B | 609 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 28 | a | 713 | PL9 | C22-C23-C24 | -2.58 | 121.44 | 127.66 |
| 25 | B | 617 | CLA | C4D-C3D-CAD | -2.58 | 107.03 | 108.47 |
| 26 | a | 709 | PHO | CBD-CHA-C4D | -2.58 | 105.63 | 108.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | C | 506 | CLA | CHB-C4A-NA | 2.58 | 128.07 | 124.51 |
| 25 | b | 622 | CLA | CHB-C4A-NA | 2.58 | 128.07 | 124.51 |
| 28 | D | 406 | PL9 | C27-C28-C29 | -2.57 | 121.46 | 127.66 |
| 27 | b | 625 | BCR | C33-C5-C6 | -2.57 | 121.64 | 124.53 |
| 25 | b | 622 | CLA | CMD-C2D-C3D | 2.57 | 129.49 | 124.68 |
| 33 | C | 519 | DGD | O5D-C6D-C5D | -2.57 | 104.29 | 109.05 |
| 29 | a | 714 | SQD | O8-S-C6 | 2.57 | 109.83 | 105.74 |
| 25 | d | 402 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 25 | D | 403 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 23 | A | 603 | LMG | O6-C1-C2 | -2.56 | 104.92 | 110.35 |
| 27 | b | 624 | BCR | C15-C16-C17 | -2.56 | 118.22 | 123.47 |
| 32 | B | 625 | LHG | C11-C10-C9 | -2.56 | 101.42 | 114.42 |
| 28 | d | 405 | PL9 | C22-C23-C24 | -2.56 | 121.50 | 127.66 |
| 25 | D | 402 | CLA | C1B-CHB-C4A | -2.56 | 125.06 | 130.12 |
| 29 | A | 612 | SQD | O48-C23-C24 | 2.55 | 119.92 | 111.91 |
| 26 | a | 710 | PHO | CMB-C2B-C1B | -2.55 | 121.13 | 125.06 |
| 27 | D | 405 | BCR | C15-C16-C17 | -2.55 | 118.25 | 123.47 |
| 29 | a | 714 | SQD | O48-C23-C24 | 2.55 | 119.91 | 111.91 |
| 27 | t | 103 | BCR | C24-C23-C22 | -2.55 | 122.38 | 126.23 |
| 25 | c | 502 | CLA | CMD-C2D-C3D | 2.55 | 129.45 | 124.68 |
| 25 | a | 707 | CLA | C1B-CHB-C4A | -2.55 | 125.07 | 130.12 |
| 27 | C | 516 | BCR | C15-C14-C13 | -2.55 | 123.67 | 127.31 |
| 35 | v | 201 | HEC | CMB-C2B-C3B | 2.55 | 128.81 | 125.82 |
| 32 | d | 406 | LHG | C11-C10-C9 | -2.55 | 101.50 | 114.42 |
| 25 | c | 513 | CLA | CMD-C2D-C3D | 2.55 | 129.44 | 124.68 |
| 25 | A | 606 | CLA | C1B-CHB-C4A | -2.54 | 125.08 | 130.12 |
| 28 | a | 713 | PL9 | C7-C8-C9 | -2.54 | 122.56 | 126.79 |
| 27 | B | 619 | BCR | C27-C26-C25 | 2.54 | 126.42 | 122.73 |
| 29 | A | 614 | SQD | O48-C23-C24 | 2.54 | 119.87 | 111.91 |
| 27 | c | 514 | BCR | C33-C5-C6 | -2.54 | 121.68 | 124.53 |
| 29 | a | 714 | SQD | C4-C3-C2 | 2.54 | 115.25 | 110.82 |
| 25 | B | 617 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 25 | b | 619 | CLA | CMD-C2D-C3D | 2.54 | 129.42 | 124.68 |
| 25 | a | 711 | CLA | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 25 | B | 608 | CLA | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 26 | a | 710 | PHO | CBD-CHA-C4D | -2.53 | 105.69 | 108.54 |
| 23 | c | 519 | LMG | O6-C1-O1 | -2.53 | 103.99 | 109.97 |
| 26 | D | 401 | PHO | O1D-CGD-CBD | 2.53 | 129.66 | 124.48 |
| 27 | D | 405 | BCR | C24-C23-C22 | -2.53 | 122.42 | 126.23 |
| 27 | h | 101 | BCR | C27-C26-C25 | 2.53 | 126.40 | 122.73 |
| 25 | B | 604 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 25 | B | 616 | CLA | CMD-C2D-C3D | 2.53 | 129.40 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | b | 615 | CLA | O2D-CGD-O1D | -2.52 | 118.90 | 123.84 |
| 25 | d | 402 | CLA | CMD-C2D-C3D | 2.52 | 129.40 | 124.68 |
| 28 | d | 405 | PL9 | C27-C28-C29 | -2.52 | 121.58 | 127.66 |
| 25 | B | 610 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 25 | B | 606 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 32 | L | 101 | LHG | C11-C10-C9 | -2.52 | 101.63 | 114.42 |
| 23 | a | 701 | LMG | C38-C37-C36 | -2.52 | 101.63 | 114.42 |
| 33 | c | 517 | DGD | O5D-C6D-C5D | -2.52 | 104.38 | 109.05 |
| 23 | C | 501 | LMG | C38-C37-C36 | -2.52 | 101.64 | 114.42 |
| 25 | d | 403 | CLA | C4D-C3D-CAD | -2.52 | 107.07 | 108.47 |
| 29 | B | 626 | SQD | O48-C23-C24 | 2.52 | 119.81 | 111.91 |
| 33 | c | 518 | DGD | C3G-C2G-C1G | -2.52 | 105.84 | 111.79 |
| 27 | c | 514 | BCR | C15-C16-C17 | -2.52 | 118.32 | 123.47 |
| 27 | A | 610 | BCR | C24-C23-C22 | -2.51 | 122.44 | 126.23 |
| 27 | C | 516 | BCR | C33-C5-C6 | -2.51 | 121.71 | 124.53 |
| 23 | a | 701 | LMG | C40-C39-C38 | -2.51 | 101.67 | 114.42 |
| 27 | c | 515 | BCR | C33-C5-C6 | -2.51 | 121.71 | 124.53 |
| 26 | a | 709 | PHO | O1D-CGD-CBD | 2.51 | 129.61 | 124.48 |
| 27 | c | 515 | BCR | C27-C26-C25 | 2.51 | 126.37 | 122.73 |
| 33 | C | 517 | DGD | O5D-C6D-C5D | -2.51 | 104.41 | 109.05 |
| 23 | M | 101 | LMG | O6-C1-O1 | -2.51 | 104.04 | 109.97 |
| 25 | B | 610 | CLA | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 25 | A | 606 | CLA | O2D-CGD-O1D | -2.50 | 118.94 | 123.84 |
| 25 | B | 604 | CLA | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 25 | C | 508 | CLA | C1B-CHB-C4A | -2.50 | 125.16 | 130.12 |
| 25 | A | 609 | CLA | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 25 | b | 615 | CLA | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 28 | d | 405 | PL9 | C20-C19-C21 | 2.50 | 119.48 | 115.27 |
| 25 | B | 615 | CLA | C1B-CHB-C4A | -2.50 | 125.17 | 130.12 |
| 23 | a | 715 | LMG | O6-C1-O1 | -2.50 | 104.06 | 109.97 |
| 25 | c | 506 | CLA | CMD-C2D-C3D | 2.50 | 129.35 | 124.68 |
| 25 | C | 508 | CLA | CMD-C2D-C3D | 2.50 | 129.35 | 124.68 |
| 25 | d | 403 | CLA | CMD-C2D-C3D | 2.49 | 129.34 | 124.68 |
| 32 | b | 629 | LHG | O8-C23-C24 | 2.49 | 119.73 | 111.91 |
| 32 | b | 629 | LHG | C11-C10-C9 | -2.49 | 101.78 | 114.42 |
| 32 | D | 408 | LHG | O8-C23-C24 | 2.49 | 119.72 | 111.91 |
| 29 | B | 623 | SQD | C1-C2-C3 | 2.49 | 115.18 | 110.00 |
| 25 | a | 711 | CLA | CMD-C2D-C3D | 2.49 | 129.33 | 124.68 |
| 33 | C | 517 | DGD | C3G-C2G-C1G | -2.49 | 105.91 | 111.79 |
| 25 | D | 404 | CLA | CMD-C2D-C3D | 2.49 | 129.33 | 124.68 |
| 25 | C | 505 | CLA | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 27 | a | 712 | BCR | C27-C26-C25 | 2.48 | 126.34 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | M | 101 | LMG | C38-C37-C36 | -2.48 | 101.83 | 114.42 |
| 25 | c | 507 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 25 | a | 719 | CLA | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 25 | D | 403 | CLA | CMD-C2D-C3D | 2.48 | 129.31 | 124.68 |
| 27 | h | 101 | BCR | C15-C14-C13 | -2.48 | 123.78 | 127.31 |
| 29 | a | 714 | SQD | C44-O6-C1 | 2.47 | 118.57 | 113.74 |
| 28 | D | 406 | PL9 | C20-C19-C21 | 2.47 | 119.43 | 115.27 |
| 25 | b | 612 | CLA | C1B-CHB-C4A | -2.47 | 125.22 | 130.12 |
| 25 | a | 707 | CLA | O2D-CGD-O1D | -2.47 | 119.01 | 123.84 |
| 26 | D | 401 | PHO | CMB-C2B-C1B | -2.47 | 121.26 | 125.06 |
| 25 | B | 615 | CLA | CMD-C2D-C3D | 2.47 | 129.30 | 124.68 |
| 25 | b | 611 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 25 | B | 612 | CLA | CMD-C2D-C3D | 2.47 | 129.30 | 124.68 |
| 27 | b | 624 | BCR | C15-C14-C13 | -2.47 | 123.79 | 127.31 |
| 25 | C | 507 | CLA | CMD-C2D-C3D | 2.46 | 129.29 | 124.68 |
| 27 | k | 102 | BCR | C29-C30-C25 | 2.46 | 114.27 | 110.48 |
| 27 | K | 101 | BCR | C27-C26-C25 | 2.46 | 126.30 | 122.73 |
| 25 | B | 611 | CLA | CMD-C2D-C3D | 2.46 | 129.28 | 124.68 |
| 27 | c | 514 | BCR | C11-C10-C9 | -2.46 | 123.80 | 127.31 |
| 28 | A | 611 | PL9 | C27-C28-C29 | -2.46 | 121.75 | 127.66 |
| 25 | B | 607 | CLA | CMD-C2D-C3D | 2.46 | 129.27 | 124.68 |
| 25 | d | 403 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 27 | k | 102 | BCR | C33-C5-C6 | -2.45 | 121.77 | 124.53 |
| 23 | C | 501 | LMG | O6-C1-O1 | -2.45 | 104.16 | 109.97 |
| 27 | H | 102 | BCR | C27-C26-C25 | 2.45 | 126.29 | 122.73 |
| 32 | D | 408 | LHG | C20-C19-C18 | -2.45 | 101.98 | 114.42 |
| 25 | b | 620 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 25 | c | 507 | CLA | CMD-C2D-C3D | 2.45 | 129.26 | 124.68 |
| 25 | b | 614 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 25 | c | 508 | CLA | C4D-C3D-CAD | -2.45 | 107.11 | 108.47 |
| 25 | B | 614 | CLA | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 23 | B | 621 | LMG | O1-C7-C8 | -2.44 | 105.01 | 110.90 |
| 32 | D | 407 | LHG | C20-C19-C18 | -2.44 | 102.03 | 114.42 |
| 25 | b | 616 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 32 | d | 406 | LHG | C20-C19-C18 | -2.44 | 102.04 | 114.42 |
| 25 | B | 602 | CLA | C1B-CHB-C4A | -2.44 | 125.29 | 130.12 |
| 25 | c | 505 | CLA | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 25 | b | 616 | CLA | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 25 | c | 509 | CLA | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 32 | D | 407 | LHG | C11-C10-C9 | -2.44 | 102.06 | 114.42 |
| 23 | M | 101 | LMG | C40-C39-C38 | -2.43 | 102.08 | 114.42 |
| 32 | d | 407 | LHG | C20-C19-C18 | -2.43 | 102.08 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34 | e | 102 | HEM | CBA-CAA-C2A | -2.43 | 108.00 | 112.49 |
| 27 | K | 101 | BCR | C24-C23-C22 | -2.43 | 122.56 | 126.23 |
| 25 | b | 617 | CLA | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 25 | c | 512 | CLA | C1B-CHB-C4A | -2.43 | 125.31 | 130.12 |
| 25 | c | 511 | CLA | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 25 | b | 608 | CLA | CMD-C2D-C3D | 2.42 | 129.21 | 124.68 |
| 23 | f | 101 | LMG | C40-C39-C38 | -2.42 | 102.12 | 114.42 |
| 27 | d | 404 | BCR | C7-C8-C9 | -2.42 | 122.57 | 126.23 |
| 27 | C | 515 | BCR | C27-C26-C25 | 2.42 | 126.25 | 122.73 |
| 23 | D | 409 | LMG | O6-C1-O1 | -2.42 | 104.24 | 109.97 |
| 27 | B | 618 | BCR | C15-C14-C13 | -2.42 | 123.86 | 127.31 |
| 25 | C | 509 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 25 | B | 610 | CLA | C4D-C3D-CAD | -2.42 | 107.12 | 108.47 |
| 25 | B | 613 | CLA | CMD-C2D-C3D | 2.42 | 129.20 | 124.68 |
| 23 | C | 501 | LMG | C40-C39-C38 | -2.42 | 102.15 | 114.42 |
| 32 | B | 625 | LHG | C20-C19-C18 | -2.42 | 102.15 | 114.42 |
| 23 | A | 603 | LMG | C40-C39-C38 | -2.42 | 102.15 | 114.42 |
| 27 | a | 712 | BCR | C24-C23-C22 | -2.42 | 122.58 | 126.23 |
| 25 | B | 603 | CLA | CMD-C2D-C3D | 2.42 | 129.20 | 124.68 |
| 25 | c | 504 | CLA | CMD-C2D-C3D | 2.42 | 129.20 | 124.68 |
| 25 | C | 504 | CLA | CMD-C2D-C3D | 2.41 | 129.20 | 124.68 |
| 25 | C | 512 | CLA | CMD-C2D-C3D | 2.41 | 129.20 | 124.68 |
| 25 | b | 613 | CLA | CMD-C2D-C3D | 2.41 | 129.20 | 124.68 |
| 25 | C | 502 | CLA | CMD-C2D-C3D | 2.41 | 129.19 | 124.68 |
| 23 | B | 621 | LMG | C38-C37-C36 | -2.41 | 102.18 | 114.42 |
| 25 | b | 620 | CLA | CMD-C2D-C3D | 2.41 | 129.19 | 124.68 |
| 25 | B | 608 | CLA | CMD-C2D-C3D | 2.41 | 129.19 | 124.68 |
| 27 | h | 101 | BCR | C24-C23-C22 | -2.41 | 122.59 | 126.23 |
| 25 | c | 508 | CLA | C1B-CHB-C4A | -2.41 | 125.35 | 130.12 |
| 25 | b | 609 | CLA | CMD-C2D-C3D | 2.41 | 129.18 | 124.68 |
| 27 | c | 514 | BCR | C15-C14-C13 | -2.41 | 123.88 | 127.31 |
| 25 | C | 514 | CLA | CMD-C2D-C3D | 2.40 | 129.18 | 124.68 |
| 26 | a | 709 | PHO | CMB-C2B-C1B | -2.40 | 121.36 | 125.06 |
| 23 | C | 521 | LMG | C40-C39-C38 | -2.40 | 102.23 | 114.42 |
| 27 | a | 712 | BCR | C33-C5-C6 | -2.40 | 121.83 | 124.53 |
| 23 | B | 621 | LMG | C40-C39-C38 | -2.40 | 102.24 | 114.42 |
| 32 | e | 101 | LHG | C11-C10-C9 | -2.40 | 102.24 | 114.42 |
| 25 | b | 614 | CLA | CMD-C2D-C3D | 2.40 | 129.17 | 124.68 |
| 23 | C | 520 | LMG | O6-C1-O1 | -2.40 | 104.30 | 109.97 |
| 27 | c | 514 | BCR | C24-C23-C22 | -2.40 | 122.61 | 126.23 |
| 27 | h | 101 | BCR | C11-C10-C9 | -2.39 | 123.89 | 127.31 |
| 23 | b | 626 | LMG | O3-C3-C2 | -2.39 | 104.82 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32 | e | 101 | LHG | O8-C23-C24 | 2.39 | 119.42 | 111.91 |
| 28 | d | 405 | PL9 | C7-C8-C9 | -2.39 | 122.81 | 126.79 |
| 34 | E | 102 | HEM | CMD-C2D-C1D | -2.39 | 124.79 | 128.46 |
| 25 | c | 502 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 27 | Y | 101 | BCR | C27-C26-C25 | 2.39 | 126.20 | 122.73 |
| 27 | b | 624 | BCR | C33-C5-C6 | -2.39 | 121.84 | 124.53 |
| 25 | C | 511 | CLA | CMD-C2D-C3D | 2.39 | 129.15 | 124.68 |
| 23 | b | 627 | LMG | C38-C37-C36 | -2.39 | 102.30 | 114.42 |
| 23 | c | 520 | LMG | C40-C39-C38 | -2.39 | 102.30 | 114.42 |
| 27 | K | 101 | BCR | C15-C14-C13 | -2.39 | 123.90 | 127.31 |
| 25 | c | 505 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |
| 23 | c | 519 | LMG | C40-C39-C38 | -2.39 | 102.31 | 114.42 |
| 27 | K | 101 | BCR | C33-C5-C6 | -2.38 | 121.85 | 124.53 |
| 25 | a | 708 | CLA | C1B-CHB-C4A | -2.38 | 125.39 | 130.12 |
| 27 | a | 712 | BCR | C15-C16-C17 | -2.38 | 118.59 | 123.47 |
| 23 | b | 626 | LMG | O2-C2-C1 | -2.38 | 104.26 | 110.05 |
| 27 | A | 610 | BCR | C27-C26-C25 | 2.38 | 126.19 | 122.73 |
| 25 | c | 501 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 25 | A | 607 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 23 | a | 715 | LMG | C40-C39-C38 | -2.38 | 102.34 | 114.42 |
| 25 | C | 514 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 23 | D | 409 | LMG | C40-C39-C38 | -2.38 | 102.35 | 114.42 |
| 25 | b | 617 | CLA | C1B-CHB-C4A | -2.38 | 125.41 | 130.12 |
| 25 | b | 612 | CLA | CMD-C2D-C3D | 2.38 | 129.13 | 124.68 |
| 23 | b | 627 | LMG | C40-C39-C38 | -2.38 | 102.36 | 114.42 |
| 32 | L | 101 | LHG | C20-C19-C18 | -2.38 | 102.36 | 114.42 |
| 25 | C | 510 | CLA | CMD-C2D-C3D | 2.38 | 129.12 | 124.68 |
| 27 | B | 619 | BCR | C33-C5-C6 | -2.38 | 121.86 | 124.53 |
| 25 | B | 616 | CLA | C1B-CHB-C4A | -2.37 | 125.41 | 130.12 |
| 25 | B | 609 | CLA | C4D-C3D-CAD | -2.37 | 107.15 | 108.47 |
| 23 | d | 408 | LMG | O7-C10-O9 | -2.37 | 117.97 | 123.70 |
| 32 | d | 407 | LHG | C11-C10-C9 | -2.37 | 102.38 | 114.42 |
| 25 | a | 719 | CLA | CMD-C2D-C3D | 2.37 | 129.12 | 124.68 |
| 32 | e | 101 | LHG | C20-C19-C18 | -2.37 | 102.40 | 114.42 |
| 25 | a | 708 | CLA | CMD-C2D-C3D | 2.37 | 129.11 | 124.68 |
| 27 | d | 404 | BCR | C2-C3-C4 | 2.37 | 116.67 | 111.38 |
| 32 | b | 629 | LHG | C20-C19-C18 | -2.37 | 102.41 | 114.42 |
| 25 | b | 613 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 35 | V | 201 | HEC | CMD-C2D-C1D | -2.36 | 124.83 | 128.46 |
| 25 | B | 606 | CLA | CMD-C2D-C3D | 2.36 | 129.09 | 124.68 |
| 29 | D | 410 | SQD | C3-C4-C5 | 2.36 | 114.45 | 110.24 |
| 23 | c | 519 | LMG | C38-C37-C36 | -2.36 | 102.45 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | c | 501 | CLA | CMD-C2D-C3D | 2.36 | 129.09 | 124.68 |
| 25 | b | 607 | CLA | CMD-C2D-C3D | 2.36 | 129.09 | 124.68 |
| 27 | K | 101 | BCR | C15-C16-C17 | -2.36 | 118.65 | 123.47 |
| 25 | B | 607 | CLA | C1B-CHB-C4A | -2.35 | 125.45 | 130.12 |
| 25 | c | 503 | CLA | C1B-CHB-C4A | -2.35 | 125.45 | 130.12 |
| 25 | B | 605 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 33 | c | 516 | DGD | C3G-C2G-C1G | -2.35 | 106.23 | 111.79 |
| 27 | C | 515 | BCR | C33-C5-C6 | -2.35 | 121.89 | 124.53 |
| 25 | B | 605 | CLA | CMD-C2D-C3D | 2.35 | 129.07 | 124.68 |
| 25 | C | 506 | CLA | CMD-C2D-C3D | 2.35 | 129.07 | 124.68 |
| 25 | b | 610 | CLA | CMD-C2D-C3D | 2.35 | 129.07 | 124.68 |
| 27 | C | 516 | BCR | C27-C26-C25 | 2.35 | 126.14 | 122.73 |
| 27 | b | 625 | BCR | C24-C23-C22 | -2.34 | 122.69 | 126.23 |
| 32 | E | 101 | LHG | C20-C19-C18 | -2.34 | 102.53 | 114.42 |
| 27 | A | 610 | BCR | C33-C5-C6 | -2.34 | 121.90 | 124.53 |
| 25 | C | 503 | CLA | C1B-CHB-C4A | -2.34 | 125.48 | 130.12 |
| 27 | A | 610 | BCR | C15-C16-C17 | -2.34 | 118.68 | 123.47 |
| 28 | D | 406 | PL9 | C22-C23-C24 | -2.34 | 122.03 | 127.66 |
| 25 | B | 612 | CLA | C1-C2-C3 | -2.34 | 122.00 | 126.04 |
| 27 | Y | 101 | BCR | C15-C16-C17 | -2.33 | 118.69 | 123.47 |
| 27 | b | 623 | BCR | C11-C10-C9 | -2.33 | 123.98 | 127.31 |
| 23 | B | 621 | LMG | O7-C10-O9 | -2.33 | 118.06 | 123.70 |
| 25 | B | 613 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 23 | b | 626 | LMG | C40-C39-C38 | -2.33 | 102.58 | 114.42 |
| 27 | k | 101 | BCR | C27-C26-C25 | 2.33 | 126.12 | 122.73 |
| 25 | b | 621 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 27 | A | 610 | BCR | C15-C14-C13 | -2.33 | 123.98 | 127.31 |
| 25 | b | 610 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 23 | f | 101 | LMG | C38-C37-C36 | -2.33 | 102.60 | 114.42 |
| 23 | a | 715 | LMG | C38-C37-C36 | -2.32 | 102.62 | 114.42 |
| 26 | A | 608 | PHO | O1D-CGD-CBD | 2.32 | 129.24 | 124.48 |
| 25 | C | 509 | CLA | C4D-C3D-CAD | -2.32 | 107.17 | 108.47 |
| 29 | A | 612 | SQD | C1-O5-C5 | 2.32 | 118.25 | 113.69 |
| 25 | C | 505 | CLA | CMD-C2D-C3D | 2.32 | 129.01 | 124.68 |
| 23 | A | 603 | LMG | O3-C3-C2 | -2.32 | 104.99 | 110.35 |
| 25 | C | 510 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 27 | b | 625 | BCR | C15-C16-C17 | -2.31 | 118.74 | 123.47 |
| 25 | C | 513 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 27 | H | 102 | BCR | C15-C14-C13 | -2.31 | 124.01 | 127.31 |
| 23 | B | 621 | LMG | O3-C3-C2 | -2.31 | 105.02 | 110.35 |
| 33 | c | 518 | DGD | C3D-C4D-C5D | -2.30 | 106.13 | 110.24 |
| 25 | D | 402 | CLA | CMD-C2D-C3D | 2.30 | 128.99 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | b | 607 | CLA | O2D-CGD-CBD | 2.30 | 115.36 | 111.27 |
| 25 | C | 502 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 23 | c | 520 | LMG | C38-C37-C36 | -2.30 | 102.76 | 114.42 |
| 27 | k | 102 | BCR | C15-C16-C17 | -2.30 | 118.77 | 123.47 |
| 27 | C | 515 | BCR | C15-C14-C13 | -2.30 | 124.03 | 127.31 |
| 27 | b | 602 | BCR | C11-C10-C9 | -2.30 | 124.03 | 127.31 |
| 23 | C | 520 | LMG | C38-C37-C36 | -2.30 | 102.76 | 114.42 |
| 25 | c | 504 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 25 | C | 511 | CLA | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 25 | a | 707 | CLA | CMD-C2D-C3D | 2.30 | 128.97 | 124.68 |
| 23 | A | 603 | LMG | C38-C37-C36 | -2.30 | 102.77 | 114.42 |
| 23 | C | 521 | LMG | C38-C37-C36 | -2.30 | 102.77 | 114.42 |
| 23 | A | 603 | LMG | C1-C2-C3 | -2.29 | 105.22 | 110.00 |
| 25 | B | 614 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 23 | f | 101 | LMG | O1-C7-C8 | -2.29 | 105.37 | 110.90 |
| 25 | c | 513 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 23 | C | 520 | LMG | O3-C3-C2 | -2.29 | 105.06 | 110.35 |
| 23 | a | 701 | LMG | O1-C7-C8 | -2.29 | 105.38 | 110.90 |
| 29 | b | 601 | SQD | O5-C5-C4 | 2.29 | 113.85 | 109.69 |
| 27 | H | 102 | BCR | C3-C4-C5 | -2.29 | 109.99 | 114.08 |
| 27 | C | 515 | BCR | C15-C16-C17 | -2.29 | 118.79 | 123.47 |
| 25 | B | 602 | CLA | O2D-CGD-CBD | 2.28 | 115.33 | 111.27 |
| 27 | t | 103 | BCR | C27-C26-C25 | 2.28 | 126.05 | 122.73 |
| 25 | C | 504 | CLA | C1B-CHB-C4A | -2.28 | 125.59 | 130.12 |
| 25 | B | 602 | CLA | CMD-C2D-C3D | 2.28 | 128.95 | 124.68 |
| 33 | c | 517 | DGD | CBB-CAB-C9B | -2.28 | 102.84 | 114.42 |
| 27 | b | 602 | BCR | C27-C26-C25 | 2.28 | 126.04 | 122.73 |
| 27 | B | 620 | BCR | C24-C23-C22 | -2.28 | 122.79 | 126.23 |
| 25 | b | 607 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 25 | c | 509 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 27 | a | 712 | BCR | C15-C14-C13 | -2.28 | 124.06 | 127.31 |
| 23 | C | 520 | LMG | C40-C39-C38 | -2.28 | 102.86 | 114.42 |
| 27 | k | 102 | BCR | C27-C26-C25 | 2.28 | 126.03 | 122.73 |
| 23 | D | 409 | LMG | C38-C37-C36 | -2.27 | 102.88 | 114.42 |
| 32 | d | 406 | LHG | C18-C17-C16 | -2.27 | 102.89 | 114.42 |
| 32 | e | 101 | LHG | C5-O7-C7 | -2.27 | 112.20 | 117.79 |
| 28 | a | 713 | PL9 | C27-C28-C29 | -2.27 | 122.20 | 127.66 |
| 27 | B | 619 | BCR | C15-C14-C13 | -2.26 | 124.08 | 127.31 |
| 25 | b | 620 | CLA | C4D-C3D-CAD | -2.26 | 107.21 | 108.47 |
| 23 | f | 101 | LMG | O3-C3-C2 | -2.26 | 105.12 | 110.35 |
| 25 | A | 606 | CLA | CMD-C2D-C3D | 2.26 | 128.91 | 124.68 |
| 27 | B | 618 | BCR | C7-C8-C9 | -2.26 | 122.82 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | f | 102 | SQD | O48-C23-C24 | 2.26 | 119.00 | 111.91 |
| 25 | b | 613 | CLA | C4D-C3D-CAD | -2.26 | 107.21 | 108.47 |
| 27 | k | 102 | BCR | C24-C23-C22 | -2.26 | 122.82 | 126.23 |
| 25 | C | 511 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 27 | B | 619 | BCR | C15-C16-C17 | -2.26 | 118.85 | 123.47 |
| 25 | B | 612 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 34 | E | 102 | HEM | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |
| 26 | A | 608 | PHO | CMB-C2B-C1B | -2.25 | 121.60 | 125.06 |
| 25 | c | 503 | CLA | CMD-C2D-C3D | 2.25 | 128.89 | 124.68 |
| 27 | Y | 101 | BCR | C24-C23-C22 | -2.25 | 122.83 | 126.23 |
| 33 | h | 102 | DGD | C3G-C2G-C1G | -2.25 | 106.47 | 111.79 |
| 25 | c | 510 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 25 | c | 510 | CLA | CMD-C2D-C3D | 2.24 | 128.88 | 124.68 |
| 25 | b | 618 | CLA | C1B-CHB-C4A | -2.24 | 125.67 | 130.12 |
| 27 | d | 404 | BCR | C1-C6-C5 | -2.24 | 119.45 | 122.61 |
| 27 | d | 404 | BCR | C11-C10-C9 | -2.24 | 124.12 | 127.31 |
| 27 | D | 405 | BCR | C7-C8-C9 | -2.23 | 122.86 | 126.23 |
| 28 | a | 713 | PL9 | C20-C19-C21 | 2.23 | 119.03 | 115.27 |
| 25 | a | 708 | CLA | C4D-C3D-CAD | -2.23 | 107.23 | 108.47 |
| 26 | A | 608 | PHO | C1B-NB-C4B | 2.23 | 110.71 | 106.51 |
| 28 | D | 406 | PL9 | C36-C34-C33 | -2.23 | 116.61 | 121.12 |
| 28 | D | 406 | PL9 | C37-C38-C39 | -2.23 | 122.30 | 127.66 |
| 25 | c | 512 | CLA | C4D-C3D-CAD | -2.23 | 107.23 | 108.47 |
| 27 | H | 102 | BCR | C11-C10-C9 | -2.22 | 124.14 | 127.31 |
| 23 | b | 626 | LMG | C38-C37-C36 | -2.22 | 103.14 | 114.42 |
| 29 | b | 601 | SQD | O48-C23-O10 | -2.22 | 117.99 | 123.59 |
| 33 | C | 518 | DGD | C3D-C4D-C5D | -2.22 | 106.28 | 110.24 |
| 27 | d | 404 | BCR | C24-C23-C22 | -2.22 | 122.89 | 126.23 |
| 33 | C | 517 | DGD | O6E-C5E-C4E | 2.21 | 113.71 | 109.69 |
| 25 | b | 610 | CLA | C1-C2-C3 | -2.21 | 122.22 | 126.04 |
| 23 | c | 519 | LMG | O3-C3-C2 | -2.21 | 105.24 | 110.35 |
| 27 | h | 101 | BCR | C15-C16-C17 | -2.21 | 118.94 | 123.47 |
| 23 | a | 715 | LMG | O3-C3-C2 | -2.21 | 105.24 | 110.35 |
| 32 | D | 408 | LHG | C18-C17-C16 | -2.21 | 103.22 | 114.42 |
| 23 | C | 521 | LMG | O3-C3-C2 | -2.21 | 105.25 | 110.35 |
| 25 | d | 402 | CLA | C1D-CHD-C4C | 2.20 | 125.47 | 122.56 |
| 33 | H | 103 | DGD | C3G-C2G-C1G | -2.20 | 106.58 | 111.79 |
| 25 | b | 619 | CLA | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 23 | b | 626 | LMG | O6-C1-O1 | -2.20 | 104.77 | 109.97 |
| 32 | D | 408 | LHG | C27-C26-C25 | -2.20 | 103.28 | 114.42 |
| 25 | C | 504 | CLA | O2A-CGA-O1A | -2.19 | 118.05 | 123.59 |
| 33 | c | 517 | DGD | O3E-C3E-C2E | -2.19 | 105.28 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | B | 605 | CLA | O2A-CGA-O1A | -2.19 | 118.06 | 123.59 |
| 28 | A | 611 | PL9 | C20-C19-C21 | 2.19 | 118.96 | 115.27 |
| 27 | b | 624 | BCR | C11-C10-C9 | -2.19 | 124.18 | 127.31 |
| 25 | b | 618 | CLA | C1-C2-C3 | -2.19 | 122.25 | 126.04 |
| 32 | L | 101 | LHG | C18-C17-C16 | -2.19 | 103.30 | 114.42 |
| 25 | b | 615 | CLA | C4D-C3D-CAD | -2.19 | 107.25 | 108.47 |
| 25 | b | 617 | CLA | C4D-C3D-CAD | -2.19 | 107.25 | 108.47 |
| 33 | c | 516 | DGD | O6E-C5E-C4E | 2.19 | 113.67 | 109.69 |
| 32 | e | 101 | LHG | C27-C26-C25 | -2.19 | 103.32 | 114.42 |
| 32 | B | 625 | LHG | C27-C26-C25 | -2.19 | 103.33 | 114.42 |
| 25 | C | 509 | CLA | O2A-CGA-O1A | -2.19 | 118.08 | 123.59 |
| 32 | L | 101 | LHG | C27-C26-C25 | -2.19 | 103.33 | 114.42 |
| 25 | b | 614 | CLA | C4D-C3D-CAD | -2.18 | 107.25 | 108.47 |
| 25 | C | 512 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 23 | C | 501 | LMG | O3-C3-C2 | -2.18 | 105.30 | 110.35 |
| 25 | c | 511 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 32 | E | 101 | LHG | C11-C10-C9 | -2.18 | 103.35 | 114.42 |
| 25 | B | 614 | CLA | C1D-CHD-C4C | 2.18 | 125.44 | 122.56 |
| 25 | C | 507 | CLA | O2A-CGA-O1A | -2.18 | 118.09 | 123.59 |
| 32 | b | 629 | LHG | C18-C17-C16 | -2.18 | 103.35 | 114.42 |
| 28 | a | 713 | PL9 | O2-C1-C6 | 2.18 | 124.36 | 120.59 |
| 25 | b | 617 | CLA | O2A-CGA-O1A | -2.18 | 118.09 | 123.59 |
| 32 | d | 406 | LHG | C27-C26-C25 | -2.18 | 103.37 | 114.42 |
| 26 | D | 401 | PHO | C1B-NB-C4B | 2.18 | 110.61 | 106.51 |
| 28 | A | 611 | PL9 | O2-C1-C6 | 2.18 | 124.36 | 120.59 |
| 32 | B | 625 | LHG | C18-C17-C16 | -2.18 | 103.38 | 114.42 |
| 23 | d | 408 | LMG | O1-C7-C8 | -2.17 | 106.02 | 111.78 |
| 23 | M | 101 | LMG | O3-C3-C2 | -2.17 | 105.33 | 110.35 |
| 23 | a | 701 | LMG | C1-O6-C5 | -2.17 | 109.42 | 113.69 |
| 27 | H | 102 | BCR | C20-C21-C22 | -2.17 | 124.21 | 127.31 |
| 27 | B | 618 | BCR | C24-C23-C22 | -2.17 | 122.96 | 126.23 |
| 25 | b | 611 | CLA | CMD-C2D-C3D | 2.17 | 128.74 | 124.68 |
| 25 | C | 503 | CLA | C4D-C3D-CAD | -2.17 | 107.26 | 108.47 |
| 23 | C | 521 | LMG | O2-C2-C3 | -2.17 | 105.34 | 110.35 |
| 33 | C | 518 | DGD | CBB-CAB-C9B | -2.17 | 103.42 | 114.42 |
| 32 | a | 720 | LHG | C27-C26-C25 | -2.17 | 103.43 | 114.42 |
| 35 | v | 201 | HEC | CMD-C2D-C1D | -2.16 | 125.14 | 128.46 |
| 25 | D | 402 | CLA | C4D-C3D-CAD | -2.16 | 107.26 | 108.47 |
| 25 | D | 404 | CLA | C4D-C3D-CAD | -2.16 | 107.27 | 108.47 |
| 33 | c | 516 | DGD | CBB-CAB-C9B | -2.16 | 103.46 | 114.42 |
| 28 | D | 406 | PL9 | C31-C32-C33 | -2.16 | 104.79 | 111.88 |
| 32 | d | 407 | LHG | C18-C17-C16 | -2.16 | 103.48 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | b | 615 | CLA | C1-C2-C3 | -2.16 | 122.31 | 126.04 |
| 32 | e | 101 | LHG | C18-C17-C16 | -2.16 | 103.48 | 114.42 |
| 33 | C | 519 | DGD | CAB-C9B-C8B | -2.15 | 103.49 | 114.42 |
| 25 | c | 508 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 25 | C | 503 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 25 | B | 608 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 27 | C | 516 | BCR | C11-C10-C9 | -2.15 | 124.24 | 127.31 |
| 25 | B | 610 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 25 | D | 404 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 25 | b | 607 | CLA | C1D-CHD-C4C | 2.15 | 125.40 | 122.56 |
| 25 | B | 612 | CLA | O2A-CGA-O1A | -2.15 | 118.17 | 123.59 |
| 27 | d | 404 | BCR | C33-C5-C6 | -2.15 | 122.11 | 124.53 |
| 28 | D | 406 | PL9 | O2-C1-C6 | 2.15 | 124.31 | 120.59 |
| 25 | A | 607 | CLA | CMD-C2D-C3D | 2.15 | 128.70 | 124.68 |
| 27 | t | 103 | BCR | C35-C13-C14 | -2.15 | 119.92 | 122.92 |
| 25 | c | 501 | CLA | C4D-C3D-CAD | -2.15 | 107.27 | 108.47 |
| 28 | d | 405 | PL9 | O2-C1-C6 | 2.15 | 124.31 | 120.59 |
| 25 | B | 611 | CLA | C1-C2-C3 | -2.15 | 122.33 | 126.04 |
| 26 | a | 709 | PHO | C1B-NB-C4B | 2.15 | 110.55 | 106.51 |
| 25 | D | 403 | CLA | C1D-CHD-C4C | 2.15 | 125.39 | 122.56 |
| 25 | A | 606 | CLA | O2A-CGA-O1A | -2.15 | 118.18 | 123.59 |
| 25 | A | 609 | CLA | C4D-C3D-CAD | -2.14 | 107.28 | 108.47 |
| 25 | C | 505 | CLA | C4D-C3D-CAD | -2.14 | 107.28 | 108.47 |
| 25 | b | 614 | CLA | C1D-CHD-C4C | 2.14 | 125.39 | 122.56 |
| 25 | b | 619 | CLA | C1D-CHD-C4C | 2.14 | 125.39 | 122.56 |
| 25 | B | 617 | CLA | O2A-CGA-O1A | -2.14 | 118.19 | 123.59 |
| 25 | B | 602 | CLA | C1D-CHD-C4C | 2.14 | 125.38 | 122.56 |
| 26 | a | 710 | PHO | C1B-NB-C4B | 2.14 | 110.54 | 106.51 |
| 29 | D | 410 | SQD | O48-C23-C24 | 2.14 | 118.62 | 111.91 |
| 33 | c | 517 | DGD | C3G-C2G-C1G | -2.14 | 106.73 | 111.79 |
| 23 | c | 520 | LMG | C7-O1-C1 | 2.14 | 117.92 | 113.74 |
| 25 | B | 614 | CLA | O2A-CGA-O1A | -2.14 | 118.20 | 123.59 |
| 29 | A | 614 | SQD | C45-O47-C7 | 2.14 | 123.05 | 117.79 |
| 27 | c | 514 | BCR | C2-C1-C6 | 2.14 | 113.77 | 110.48 |
| 25 | C | 514 | CLA | O2A-CGA-O1A | -2.14 | 118.20 | 123.59 |
| 25 | c | 503 | CLA | O2A-CGA-O1A | -2.14 | 118.20 | 123.59 |
| 25 | c | 502 | CLA | O2A-CGA-O1A | -2.14 | 118.20 | 123.59 |
| 23 | B | 621 | LMG | C3-C4-C5 | -2.14 | 106.43 | 110.24 |
| 33 | C | 517 | DGD | CAB-C9B-C8B | -2.13 | 103.59 | 114.42 |
| 32 | d | 407 | LHG | C27-C26-C25 | -2.13 | 103.59 | 114.42 |
| 25 | A | 607 | CLA | C1D-CHD-C4C | 2.13 | 125.37 | 122.56 |
| 23 | C | 521 | LMG | C7-O1-C1 | 2.13 | 117.91 | 113.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | c | 502 | CLA | C4D-C3D-CAD | -2.13 | 107.28 | 108.47 |
| 23 | f | 101 | LMG | O1-C1-C2 | -2.13 | 104.98 | 108.30 |
| 33 | h | 102 | DGD | C1D-C2D-C3D | -2.13 | 105.56 | 110.00 |
| 25 | C | 511 | CLA | O2A-CGA-O1A | -2.13 | 118.22 | 123.59 |
| 23 | f | 101 | LMG | O2-C2-C1 | -2.13 | 104.87 | 110.05 |
| 27 | b | 625 | BCR | C15-C14-C13 | -2.13 | 124.27 | 127.31 |
| 28 | a | 713 | PL9 | O2-C1-C2 | -2.13 | 116.90 | 121.78 |
| 28 | d | 405 | PL9 | O1-C4-C3 | -2.13 | 118.38 | 120.72 |
| 27 | k | 102 | BCR | C15-C14-C13 | -2.13 | 124.27 | 127.31 |
| 23 | c | 520 | LMG | O2-C2-C3 | -2.13 | 105.43 | 110.35 |
| 25 | B | 615 | CLA | C4D-C3D-CAD | -2.13 | 107.28 | 108.47 |
| 33 | C | 518 | DGD | C3G-C2G-C1G | -2.12 | 106.76 | 111.79 |
| 25 | C | 506 | CLA | C1D-CHD-C4C | 2.12 | 125.36 | 122.56 |
| 32 | b | 629 | LHG | C27-C26-C25 | -2.12 | 103.65 | 114.42 |
| 28 | a | 713 | PL9 | C37-C38-C39 | -2.12 | 122.55 | 127.66 |
| 33 | H | 103 | DGD | CBB-CAB-C9B | -2.12 | 103.66 | 114.42 |
| 25 | C | 514 | CLA | C4D-C3D-CAD | -2.12 | 107.29 | 108.47 |
| 25 | B | 607 | CLA | C1D-CHD-C4C | 2.12 | 125.35 | 122.56 |
| 25 | C | 512 | CLA | O2A-CGA-O1A | -2.12 | 118.25 | 123.59 |
| 25 | b | 619 | CLA | O2A-CGA-O1A | -2.12 | 118.25 | 123.59 |
| 25 | B | 603 | CLA | C1D-CHD-C4C | 2.12 | 125.35 | 122.56 |
| 25 | C | 503 | CLA | C1D-CHD-C4C | 2.12 | 125.35 | 122.56 |
| 33 | c | 518 | DGD | CBB-CAB-C9B | -2.12 | 103.68 | 114.42 |
| 29 | B | 626 | SQD | C44-O6-C1 | 2.12 | 117.87 | 113.74 |
| 32 | D | 407 | LHG | C27-C26-C25 | -2.12 | 103.69 | 114.42 |
| 27 | C | 515 | BCR | C24-C23-C22 | -2.11 | 123.04 | 126.23 |
| 35 | V | 201 | HEC | C1D-C2D-C3D | 2.11 | 108.47 | 107.00 |
| 23 | c | 520 | LMG | O3-C3-C2 | -2.11 | 105.46 | 110.35 |
| 23 | a | 701 | LMG | O2-C2-C1 | -2.11 | 104.91 | 110.05 |
| 25 | B | 610 | CLA | C1D-CHD-C4C | 2.11 | 125.34 | 122.56 |
| 27 | C | 515 | BCR | C7-C8-C9 | -2.11 | 123.05 | 126.23 |
| 33 | c | 518 | DGD | CAB-C9B-C8B | -2.11 | 103.72 | 114.42 |
| 27 | d | 404 | BCR | C16-C15-C14 | -2.11 | 119.15 | 123.47 |
| 27 | D | 405 | BCR | C11-C10-C9 | -2.11 | 124.30 | 127.31 |
| 25 | c | 506 | CLA | O2A-CGA-O1A | -2.11 | 118.27 | 123.59 |
| 32 | E | 101 | LHG | C18-C17-C16 | -2.11 | 103.73 | 114.42 |
| 25 | C | 505 | CLA | O2A-CGA-O1A | -2.10 | 118.28 | 123.59 |
| 25 | b | 612 | CLA | C1D-CHD-C4C | 2.10 | 125.33 | 122.56 |
| 28 | A | 611 | PL9 | O2-C1-C2 | -2.10 | 116.96 | 121.78 |
| 25 | A | 609 | CLA | O2A-CGA-O1A | -2.10 | 118.29 | 123.59 |
| 23 | C | 520 | LMG | O2-C2-C1 | -2.10 | 104.95 | 110.05 |
| 25 | c | 512 | CLA | C1D-CHD-C4C | 2.10 | 125.33 | 122.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | c | 504 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 33 | h | 102 | DGD | CBB-CAB-C9B | -2.10 | 103.78 | 114.42 |
| 32 | D | 407 | LHG | C18-C17-C16 | -2.09 | 103.79 | 114.42 |
| 27 | D | 405 | BCR | C15-C14-C13 | -2.09 | 124.32 | 127.31 |
| 28 | A | 611 | PL9 | O1-C4-C3 | -2.09 | 118.42 | 120.72 |
| 28 | D | 406 | PL9 | O2-C1-C2 | -2.09 | 116.99 | 121.78 |
| 25 | B | 613 | CLA | C1D-CHD-C4C | 2.09 | 125.32 | 122.56 |
| 25 | b | 618 | CLA | C1D-CHD-C4C | 2.09 | 125.32 | 122.56 |
| 27 | c | 515 | BCR | C11-C10-C9 | -2.09 | 124.33 | 127.31 |
| 27 | Y | 101 | BCR | C15-C14-C13 | -2.09 | 124.33 | 127.31 |
| 25 | B | 613 | CLA | O2A-CGA-O1A | -2.09 | 118.32 | 123.59 |
| 25 | B | 603 | CLA | C4D-C3D-CAD | -2.09 | 107.31 | 108.47 |
| 27 | b | 625 | BCR | C11-C10-C9 | -2.09 | 124.33 | 127.31 |
| 23 | M | 101 | LMG | O2-C2-C1 | -2.09 | 104.97 | 110.05 |
| 33 | C | 519 | DGD | O6E-C1E-O5D | -2.09 | 105.03 | 109.97 |
| 34 | E | 102 | HEM | CBA-CAA-C2A | -2.09 | 108.64 | 112.49 |
| 28 | D | 406 | PL9 | O1-C4-C3 | -2.09 | 118.42 | 120.72 |
| 29 | A | 612 | SQD | O48-C23-O10 | -2.09 | 118.33 | 123.59 |
| 33 | H | 103 | DGD | C1D-C2D-C3D | -2.08 | 105.66 | 110.00 |
| 28 | a | 713 | PL9 | O1-C4-C3 | -2.08 | 118.43 | 120.72 |
| 27 | b | 623 | BCR | C24-C23-C22 | -2.08 | 123.09 | 126.23 |
| 23 | b | 627 | LMG | O2-C2-C1 | -2.08 | 104.99 | 110.05 |
| 25 | c | 513 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 25 | a | 711 | CLA | C4D-C3D-CAD | -2.08 | 107.31 | 108.47 |
| 27 | B | 618 | BCR | C27-C26-C25 | 2.08 | 125.75 | 122.73 |
| 25 | B | 608 | CLA | C1D-CHD-C4C | 2.08 | 125.30 | 122.56 |
| 25 | b | 615 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 25 | A | 607 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 29 | D | 410 | SQD | C4-C3-C2 | 2.08 | 114.45 | 110.82 |
| 33 | H | 103 | DGD | CAB-C9B-C8B | -2.08 | 103.87 | 114.42 |
| 33 | C | 518 | DGD | CAB-C9B-C8B | -2.08 | 103.88 | 114.42 |
| 25 | B | 605 | CLA | O2D-CGD-CBD | 2.08 | 114.96 | 111.27 |
| 25 | b | 615 | CLA | C1D-CHD-C4C | 2.08 | 125.30 | 122.56 |
| 28 | d | 405 | PL9 | O2-C1-C2 | -2.08 | 117.02 | 121.78 |
| 25 | b | 610 | CLA | C1D-CHD-C4C | 2.08 | 125.30 | 122.56 |
| 33 | c | 517 | DGD | CAB-C9B-C8B | -2.08 | 103.89 | 114.42 |
| 25 | A | 607 | CLA | C1-C2-C3 | -2.08 | 122.45 | 126.04 |
| 25 | C | 502 | CLA | C4D-C3D-CAD | -2.07 | 107.31 | 108.47 |
| 23 | a | 715 | LMG | O2-C2-C1 | -2.07 | 105.01 | 110.05 |
| 25 | a | 711 | CLA | C1D-CHD-C4C | 2.07 | 125.30 | 122.56 |
| 25 | a | 707 | CLA | O1D-CGD-CBD | 2.07 | 128.72 | 124.48 |
| 26 | D | 401 | PHO | O2A-CGA-O1A | -2.07 | 118.36 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | C | 517 | DGD | CBB-CAB-C9B | -2.07 | 103.91 | 114.42 |
| 23 | D | 409 | LMG | O3-C3-C2 | -2.07 | 105.56 | 110.35 |
| 32 | E | 101 | LHG | C27-C26-C25 | -2.07 | 103.93 | 114.42 |
| 26 | A | 608 | PHO | CBD-CHA-C1A | 2.07 | 131.20 | 126.40 |
| 25 | b | 613 | CLA | O2A-CGA-O1A | -2.07 | 118.38 | 123.59 |
| 25 | B | 603 | CLA | O2A-CGA-O1A | -2.07 | 118.38 | 123.59 |
| 25 | C | 512 | CLA | C1D-CHD-C4C | 2.07 | 125.28 | 122.56 |
| 25 | b | 607 | CLA | O2A-CGA-O1A | -2.07 | 118.38 | 123.59 |
| 25 | b | 621 | CLA | O2D-CGD-CBD | 2.07 | 114.94 | 111.27 |
| 25 | d | 402 | CLA | C4D-C3D-CAD | -2.06 | 107.32 | 108.47 |
| 25 | b | 614 | CLA | O2A-CGA-O1A | -2.06 | 118.38 | 123.59 |
| 27 | b | 602 | BCR | C7-C8-C9 | -2.06 | 123.12 | 126.23 |
| 33 | C | 518 | DGD | O3E-C3E-C2E | -2.06 | 105.58 | 110.35 |
| 23 | D | 409 | LMG | O2-C2-C1 | -2.06 | 105.04 | 110.05 |
| 25 | b | 610 | CLA | O2A-CGA-O1A | -2.06 | 118.39 | 123.59 |
| 25 | B | 611 | CLA | C1D-CHD-C4C | 2.06 | 125.28 | 122.56 |
| 25 | c | 506 | CLA | C4D-C3D-CAD | -2.06 | 107.32 | 108.47 |
| 27 | b | 623 | BCR | C7-C8-C9 | -2.06 | 123.12 | 126.23 |
| 23 | a | 715 | LMG | C1-C2-C3 | -2.06 | 105.71 | 110.00 |
| 25 | b | 621 | CLA | O2A-CGA-O1A | -2.06 | 118.40 | 123.59 |
| 25 | b | 619 | CLA | C4D-C3D-CAD | -2.06 | 107.32 | 108.47 |
| 27 | B | 619 | BCR | C24-C23-C22 | -2.06 | 123.13 | 126.23 |
| 25 | c | 502 | CLA | C1D-CHD-C4C | 2.06 | 125.27 | 122.56 |
| 25 | d | 403 | CLA | O2A-CGA-O1A | -2.05 | 118.41 | 123.59 |
| 25 | d | 403 | CLA | C1D-CHD-C4C | 2.05 | 125.27 | 122.56 |
| 25 | b | 612 | CLA | O2A-CGA-O1A | -2.05 | 118.41 | 123.59 |
| 25 | b | 610 | CLA | O2D-CGD-CBD | 2.05 | 114.91 | 111.27 |
| 27 | b | 625 | BCR | C2-C1-C6 | 2.05 | 113.64 | 110.48 |
| 27 | b | 625 | BCR | C38-C26-C25 | -2.05 | 122.23 | 124.53 |
| 25 | a | 711 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 25 | C | 511 | CLA | C1D-CHD-C4C | 2.05 | 125.26 | 122.56 |
| 33 | c | 516 | DGD | CAB-C9B-C8B | -2.05 | 104.03 | 114.42 |
| 23 | d | 408 | LMG | C38-C37-C36 | -2.05 | 104.03 | 114.42 |
| 33 | c | 517 | DGD | C3D-C4D-C5D | -2.05 | 106.59 | 110.24 |
| 28 | d | 405 | PL9 | C37-C38-C39 | -2.05 | 122.73 | 127.66 |
| 25 | D | 404 | CLA | C1D-CHD-C4C | 2.05 | 125.26 | 122.56 |
| 25 | B | 609 | CLA | O2A-CGA-O1A | -2.04 | 118.43 | 123.59 |
| 27 | a | 712 | BCR | C11-C10-C9 | -2.04 | 124.39 | 127.31 |
| 25 | c | 506 | CLA | C1D-CHD-C4C | 2.04 | 125.25 | 122.56 |
| 25 | C | 513 | CLA | C1D-CHD-C4C | 2.04 | 125.25 | 122.56 |
| 25 | c | 511 | CLA | O2A-CGA-O1A | -2.04 | 118.44 | 123.59 |
| 26 | A | 608 | PHO | C2B-C1B-NB | -2.04 | 106.71 | 109.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | d | 402 | CLA | O2A-CGA-O1A | -2.04 | 118.44 | 123.59 |
| 33 | h | 102 | DGD | CAB-C9B-C8B | -2.04 | 104.07 | 114.42 |
| 23 | d | 408 | LMG | C40-C39-C38 | -2.04 | 104.08 | 114.42 |
| 33 | C | 517 | DGD | C5B-C4B-C3B | -2.04 | 104.08 | 114.42 |
| 33 | c | 516 | DGD | C5B-C4B-C3B | -2.04 | 104.08 | 114.42 |
| 33 | c | 518 | DGD | O6E-C1E-O5D | -2.04 | 105.15 | 109.97 |
| 25 | b | 613 | CLA | C1D-CHD-C4C | 2.03 | 125.24 | 122.56 |
| 23 | C | 501 | LMG | C1-C2-C3 | -2.03 | 105.76 | 110.00 |
| 25 | D | 402 | CLA | O2A-CGA-O1A | -2.03 | 118.46 | 123.59 |
| 25 | a | 708 | CLA | C1D-CHD-C4C | 2.03 | 125.24 | 122.56 |
| 33 | c | 518 | DGD | O2D-C2D-C1D | -2.03 | 105.11 | 110.05 |
| 25 | c | 504 | CLA | C4D-C3D-CAD | -2.03 | 107.34 | 108.47 |
| 25 | c | 501 | CLA | C1D-CHD-C4C | 2.03 | 125.24 | 122.56 |
| 25 | C | 507 | CLA | C1D-CHD-C4C | 2.03 | 125.24 | 122.56 |
| 25 | C | 510 | CLA | C1D-CHD-C4C | 2.03 | 125.23 | 122.56 |
| 25 | b | 622 | CLA | O2A-CGA-O1A | -2.03 | 118.48 | 123.59 |
| 25 | B | 614 | CLA | C4D-C3D-CAD | -2.02 | 107.34 | 108.47 |
| 33 | C | 519 | DGD | C5B-C4B-C3B | -2.02 | 104.15 | 114.42 |
| 33 | C | 519 | DGD | CBB-CAB-C9B | -2.02 | 104.16 | 114.42 |
| 23 | a | 701 | LMG | O3-C3-C2 | -2.02 | 105.67 | 110.35 |
| 25 | c | 511 | CLA | C1D-CHD-C4C | 2.02 | 125.23 | 122.56 |
| 25 | B | 617 | CLA | OBD-CAD-CBD | -2.02 | 123.01 | 125.89 |
| 25 | a | 719 | CLA | O2A-CGA-O1A | -2.02 | 118.49 | 123.59 |
| 25 | b | 620 | CLA | O2A-CGA-O1A | -2.02 | 118.49 | 123.59 |
| 25 | b | 616 | CLA | C1D-CHD-C4C | 2.02 | 125.22 | 122.56 |
| 27 | B | 620 | BCR | C38-C26-C25 | -2.02 | 122.26 | 124.53 |
| 25 | C | 505 | CLA | C1D-CHD-C4C | 2.02 | 125.22 | 122.56 |
| 23 | c | 519 | LMG | O2-C2-C1 | -2.02 | 105.14 | 110.05 |
| 25 | B | 611 | CLA | O2A-CGA-O1A | -2.02 | 118.50 | 123.59 |
| 33 | c | 518 | DGD | C5B-C4B-C3B | -2.02 | 104.19 | 114.42 |
| 29 | A | 612 | SQD | C4-C3-C2 | 2.02 | 114.34 | 110.82 |
| 25 | c | 508 | CLA | C1-C2-C3 | -2.02 | 122.56 | 126.04 |
| 25 | B | 604 | CLA | O2A-CGA-O1A | -2.02 | 118.51 | 123.59 |
| 25 | B | 615 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 25 | c | 501 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 25 | c | 509 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 25 | a | 719 | CLA | C1D-CHD-C4C | 2.01 | 125.22 | 122.56 |
| 28 | a | 713 | PL9 | C32-C33-C34 | -2.01 | 122.81 | 127.66 |
| 25 | b | 616 | CLA | C4D-C3D-CAD | -2.01 | 107.35 | 108.47 |
| 25 | B | 615 | CLA | C1D-CHD-C4C | 2.01 | 125.21 | 122.56 |
| 27 | K | 101 | BCR | C11-C10-C9 | -2.01 | 124.44 | 127.31 |
| 25 | b | 609 | CLA | OBD-CAD-CBD | -2.01 | 123.02 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | A | 606 | CLA | O1D-CGD-CBD | 2.01 | 128.60 | 124.48 |
| 26 | a | 709 | PHO | C1-C2-C3 | -2.01 | 122.57 | 126.04 |
| 25 | A | 609 | CLA | C1D-CHD-C4C | 2.01 | 125.21 | 122.56 |
| 25 | C | 504 | CLA | C1D-CHD-C4C | 2.01 | 125.21 | 122.56 |
| 25 | D | 403 | CLA | C4D-C3D-CAD | -2.01 | 107.35 | 108.47 |
| 25 | b | 611 | CLA | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 29 | a | 714 | SQD | C1-O5-C5 | 2.01 | 117.63 | 113.69 |
| 26 | a | 709 | PHO | CBD-CHA-C1A | 2.01 | 131.06 | 126.40 |
| 26 | A | 608 | PHO | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 25 | c | 505 | CLA | C1D-CHD-C4C | 2.01 | 125.20 | 122.56 |
| 28 | A | 611 | PL9 | C36-C34-C33 | -2.00 | 117.06 | 121.12 |
| 25 | c | 509 | CLA | C1D-CHD-C4C | 2.00 | 125.20 | 122.56 |
| 25 | b | 619 | CLA | C1-C2-C3 | -2.00 | 122.58 | 126.04 |
| 26 | a | 709 | PHO | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |

All (196) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | A | 606 | CLA | NA |
| 25 | A | 606 | CLA | NC |
| 25 | A | 606 | CLA | ND |
| 25 | A | 607 | CLA | NA |
| 25 | A | 607 | CLA | NC |
| 25 | A | 607 | CLA | ND |
| 25 | A | 609 | CLA | ND |
| 25 | A | 609 | CLA | NC |
| 25 | A | 609 | CLA | NA |
| 25 | B | 602 | CLA | ND |
| 25 | B | 602 | CLA | NC |
| 25 | B | 602 | CLA | NA |
| 25 | B | 603 | CLA | NC |
| 25 | B | 603 | CLA | NA |
| 25 | B | 604 | CLA | ND |
| 25 | B | 604 | CLA | NC |
| 25 | B | 604 | CLA | NA |
| 25 | B | 605 | CLA | ND |
| 25 | B | 605 | CLA | NC |
| 25 | B | 605 | CLA | NA |
| 25 | B | 606 | CLA | ND |
| 25 | B | 606 | CLA | NC |
| 25 | B | 606 | CLA | NA |
| 25 | B | 607 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | B | 607 | CLA | NC |
| 25 | B | 607 | CLA | NA |
| 25 | B | 608 | CLA | NA |
| 25 | B | 608 | CLA | NC |
| 25 | B | 608 | CLA | ND |
| 25 | B | 609 | CLA | NA |
| 25 | B | 609 | CLA | NC |
| 25 | B | 609 | CLA | ND |
| 25 | B | 610 | CLA | NC |
| 25 | B | 610 | CLA | NA |
| 25 | B | 611 | CLA | NA |
| 25 | B | 611 | CLA | ND |
| 25 | B | 611 | CLA | NC |
| 25 | B | 612 | CLA | ND |
| 25 | B | 612 | CLA | NC |
| 25 | B | 612 | CLA | NA |
| 25 | B | 613 | CLA | ND |
| 25 | B | 613 | CLA | NC |
| 25 | B | 613 | CLA | NA |
| 25 | B | 614 | CLA | ND |
| 25 | B | 614 | CLA | NC |
| 25 | B | 614 | CLA | NA |
| 25 | B | 615 | CLA | ND |
| 25 | B | 615 | CLA | NC |
| 25 | B | 615 | CLA | NA |
| 25 | B | 616 | CLA | ND |
| 25 | B | 616 | CLA | NC |
| 25 | B | 616 | CLA | NA |
| 25 | B | 617 | CLA | ND |
| 25 | B | 617 | CLA | NC |
| 25 | B | 617 | CLA | NA |
| 25 | C | 502 | CLA | ND |
| 25 | C | 502 | CLA | NC |
| 25 | C | 502 | CLA | NA |
| 25 | C | 503 | CLA | ND |
| 25 | C | 503 | CLA | NC |
| 25 | C | 503 | CLA | NA |
| 25 | C | 504 | CLA | ND |
| 25 | C | 504 | CLA | NC |
| 25 | C | 504 | CLA | NA |
| 25 | C | 505 | CLA | NA |
| 25 | C | 505 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | C | 505 | CLA | ND |
| 25 | C | 506 | CLA | NC |
| 25 | C | 506 | CLA | NA |
| 25 | C | 507 | CLA | NC |
| 25 | C | 507 | CLA | NA |
| 25 | C | 508 | CLA | ND |
| 25 | C | 508 | CLA | NC |
| 25 | C | 508 | CLA | NA |
| 25 | C | 509 | CLA | ND |
| 25 | C | 509 | CLA | NC |
| 25 | C | 509 | CLA | NA |
| 25 | C | 510 | CLA | ND |
| 25 | C | 510 | CLA | NC |
| 25 | C | 510 | CLA | NA |
| 25 | C | 511 | CLA | ND |
| 25 | C | 511 | CLA | NC |
| 25 | C | 511 | CLA | NA |
| 25 | C | 512 | CLA | ND |
| 25 | C | 512 | CLA | NC |
| 25 | C | 512 | CLA | NA |
| 25 | C | 513 | CLA | ND |
| 25 | C | 513 | CLA | NC |
| 25 | C | 513 | CLA | NA |
| 25 | C | 514 | CLA | ND |
| 25 | C | 514 | CLA | NC |
| 25 | C | 514 | CLA | NA |
| 25 | D | 402 | CLA | NA |
| 25 | D | 402 | CLA | NC |
| 25 | D | 403 | CLA | NC |
| 25 | D | 403 | CLA | NA |
| 25 | D | 404 | CLA | NC |
| 25 | D | 404 | CLA | NA |
| 25 | a | 707 | CLA | ND |
| 25 | a | 707 | CLA | NC |
| 25 | a | 707 | CLA | NA |
| 25 | a | 708 | CLA | NA |
| 25 | a | 708 | CLA | NC |
| 25 | a | 708 | CLA | ND |
| 25 | a | 711 | CLA | ND |
| 25 | a | 711 | CLA | NC |
| 25 | a | 711 | CLA | NA |
| 25 | a | 719 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | a | 719 | CLA | NC |
| 25 | a | 719 | CLA | ND |
| 25 | b | 607 | CLA | ND |
| 25 | b | 607 | CLA | NC |
| 25 | b | 607 | CLA | NA |
| 25 | b | 608 | CLA | ND |
| 25 | b | 608 | CLA | NC |
| 25 | b | 608 | CLA | NA |
| 25 | b | 609 | CLA | ND |
| 25 | b | 609 | CLA | NC |
| 25 | b | 609 | CLA | NA |
| 25 | b | 610 | CLA | ND |
| 25 | b | 610 | CLA | NC |
| 25 | b | 610 | CLA | NA |
| 25 | b | 611 | CLA | NC |
| 25 | b | 611 | CLA | NA |
| 25 | b | 612 | CLA | ND |
| 25 | b | 612 | CLA | NC |
| 25 | b | 612 | CLA | NA |
| 25 | b | 613 | CLA | NA |
| 25 | b | 613 | CLA | NC |
| 25 | b | 613 | CLA | ND |
| 25 | b | 614 | CLA | ND |
| 25 | b | 614 | CLA | NC |
| 25 | b | 614 | CLA | NA |
| 25 | b | 615 | CLA | NC |
| 25 | b | 615 | CLA | NA |
| 25 | b | 616 | CLA | NA |
| 25 | b | 616 | CLA | ND |
| 25 | b | 616 | CLA | NC |
| 25 | b | 617 | CLA | ND |
| 25 | b | 617 | CLA | NC |
| 25 | b | 617 | CLA | NA |
| 25 | b | 618 | CLA | ND |
| 25 | b | 618 | CLA | NC |
| 25 | b | 618 | CLA | NA |
| 25 | b | 619 | CLA | ND |
| 25 | b | 619 | CLA | NC |
| 25 | b | 619 | CLA | NA |
| 25 | b | 620 | CLA | ND |
| 25 | b | 620 | CLA | NC |
| 25 | b | 620 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | b | 621 | CLA | ND |
| 25 | b | 621 | CLA | NC |
| 25 | b | 621 | CLA | NA |
| 25 | b | 622 | CLA | ND |
| 25 | b | 622 | CLA | NC |
| 25 | b | 622 | CLA | NA |
| 25 | c | 501 | CLA | ND |
| 25 | c | 501 | CLA | NC |
| 25 | c | 501 | CLA | NA |
| 25 | c | 502 | CLA | ND |
| 25 | c | 502 | CLA | NC |
| 25 | c | 502 | CLA | NA |
| 25 | c | 503 | CLA | ND |
| 25 | c | 503 | CLA | NC |
| 25 | c | 503 | CLA | NA |
| 25 | c | 504 | CLA | ND |
| 25 | c | 504 | CLA | NC |
| 25 | c | 504 | CLA | NA |
| 25 | c | 505 | CLA | NC |
| 25 | c | 505 | CLA | NA |
| 25 | c | 506 | CLA | NC |
| 25 | c | 506 | CLA | NA |
| 25 | c | 507 | CLA | ND |
| 25 | c | 507 | CLA | NC |
| 25 | c | 507 | CLA | NA |
| 25 | c | 508 | CLA | NC |
| 25 | c | 508 | CLA | NA |
| 25 | c | 509 | CLA | ND |
| 25 | c | 509 | CLA | NC |
| 25 | c | 509 | CLA | NA |
| 25 | c | 510 | CLA | ND |
| 25 | c | 510 | CLA | NC |
| 25 | c | 510 | CLA | NA |
| 25 | c | 511 | CLA | ND |
| 25 | c | 511 | CLA | NC |
| 25 | c | 511 | CLA | NA |
| 25 | c | 512 | CLA | ND |
| 25 | c | 512 | CLA | NC |
| 25 | c | 512 | CLA | NA |
| 25 | c | 513 | CLA | ND |
| 25 | c | 513 | CLA | NC |
| 25 | c | 513 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25 | d | 402 | CLA | NC |
| 25 | d | 402 | CLA | NA |
| 25 | d | 403 | CLA | NC |
| 25 | d | 403 | CLA | NA |

All (1715) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 621 | LMG | C2-C1-O1-C7 |
| 23 | B | 621 | LMG | O6-C1-O1-C7 |
| 23 | C | 501 | LMG | C2-C1-O1-C7 |
| 23 | C | 501 | LMG | O6-C1-O1-C7 |
| 23 | C | 521 | LMG | O6-C1-O1-C7 |
| 23 | c | 520 | LMG | O6-C1-O1-C7 |
| 23 | d | 408 | LMG | C11-C10-O7-C8 |
| 25 | A | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 602 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 602 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 602 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 602 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 602 | CLA | C11-C10-C8-C9 |
| 25 | B | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 603 | CLA | C4-C3-C5-C6 |
| 25 | B | 604 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 604 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 608 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 608 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 615 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 615 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 615 | CLA | C2-C3-C5-C6 |
| 25 | B | 615 | CLA | C4-C3-C5-C6 |
| 25 | C | 503 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 503 | CLA | CHA-CBD-CGD-O2D |
| 25 | C | 503 | CLA | CAD-CBD-CGD-O1D |
| 25 | C | 503 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 503 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | C | 507 | CLA | C11-C12-C13-C14 |
| 25 | C | 510 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 510 | CLA | C11-C10-C8-C9 |
| 25 | D | 402 | CLA | CHA-CBD-CGD-O1D |
| 25 | D | 402 | CLA | CHA-CBD-CGD-O2D |
| 25 | D | 404 | CLA | C2-C3-C5-C6 |
| 25 | D | 404 | CLA | C4-C3-C5-C6 |
| 25 | a | 707 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 708 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 708 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 711 | CLA | C2-C3-C5-C6 |
| 25 | a | 711 | CLA | C4-C3-C5-C6 |
| 25 | a | 719 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 719 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 610 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 610 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 613 | CLA | C1A-C2A-CAA-CBA |
| 25 | b | 613 | CLA | C3A-C2A-CAA-CBA |
| 25 | b | 613 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 613 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 617 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 617 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 620 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 620 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 620 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 620 | CLA | CAD-CBD-CGD-O2D |
| 25 | c | 501 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 513 | CLA | C6-C7-C8-C9 |
| 25 | d | 402 | CLA | CBD-CGD-O2D-CED |
| 26 | a | 710 | PHO | CHA-CBD-CGD-O2D |
| 27 | B | 619 | BCR | C7-C8-C9-C34 |
| 27 | B | 620 | BCR | C1-C6-C7-C8 |
| 27 | B | 620 | BCR | C7-C8-C9-C34 |
| 27 | B | 620 | BCR | C23-C24-C25-C30 |
| 27 | D | 405 | BCR | C1-C6-C7-C8 |
| 27 | D | 405 | BCR | C7-C8-C9-C10 |
| 27 | D | 405 | BCR | C7-C8-C9-C34 |
| 27 | D | 405 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | H | 102 | BCR | C7-C8-C9-C34 |
| 27 | Y | 101 | BCR | C7-C8-C9-C34 |
| 27 | b | 602 | BCR | C5-C6-C7-C8 |
| 27 | b | 602 | BCR | C7-C8-C9-C34 |
| 27 | b | 602 | BCR | C21-C22-C23-C24 |
| 27 | b | 602 | BCR | C37-C22-C23-C24 |
| 27 | b | 624 | BCR | C7-C8-C9-C10 |
| 27 | b | 624 | BCR | C7-C8-C9-C34 |
| 27 | b | 625 | BCR | C1-C6-C7-C8 |
| 27 | b | 625 | BCR | C37-C22-C23-C24 |
| 27 | c | 514 | BCR | C7-C8-C9-C34 |
| 27 | c | 515 | BCR | C1-C6-C7-C8 |
| 27 | h | 101 | BCR | C7-C8-C9-C10 |
| 27 | h | 101 | BCR | C7-C8-C9-C34 |
| 27 | k | 101 | BCR | C20-C21-C22-C37 |
| 27 | t | 103 | BCR | C21-C22-C23-C24 |
| 28 | A | 611 | PL9 | C9-C11-C12-C13 |
| 28 | D | 406 | PL9 | C33-C34-C36-C37 |
| 28 | D | 406 | PL9 | C35-C34-C36-C37 |
| 29 | A | 612 | SQD | C5-C6-S-O8 |
| 29 | A | 612 | SQD | C5-C6-S-O9 |
| 29 | B | 623 | SQD | O5-C1-O6-C44 |
| 29 | B | 623 | SQD | O5-C5-C6-S |
| 29 | B | 626 | SQD | O5-C1-O6-C44 |
| 29 | B | 626 | SQD | O49-C7-O47-C45 |
| 29 | B | 626 | SQD | O10-C23-O48-C46 |
| 29 | D | 410 | SQD | C8-C7-O47-C45 |
| 29 | I | 102 | SQD | O6-C44-C45-O47 |
| 29 | I | 102 | SQD | C8-C7-O47-C45 |
| 29 | a | 714 | SQD | C5-C6-S-O7 |
| 29 | b | 601 | SQD | O5-C1-O6-C44 |
| 29 | b | 601 | SQD | C8-C7-O47-C45 |
| 29 | b | 601 | SQD | C4-C5-C6-S |
| 29 | f | 102 | SQD | C2-C1-O6-C44 |
| 29 | f | 102 | SQD | O5-C1-O6-C44 |
| 32 | B | 625 | LHG | C3-O3-P-O6 |
| 32 | B | 625 | LHG | C4-O6-P-O5 |
| 32 | D | 407 | LHG | O1-C1-C2-C3 |
| 32 | D | 407 | LHG | O2-C2-C3-O3 |
| 32 | D | 407 | LHG | C4-O6-P-O3 |
| 32 | D | 408 | LHG | O1-C1-C2-O2 |
| 32 | D | 408 | LHG | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | D | 408 | LHG | C4-O6-P-O4 |
| 32 | E | 101 | LHG | O1-C1-C2-C3 |
| 32 | E | 101 | LHG | C3-O3-P-O5 |
| 32 | a | 720 | LHG | C3-O3-P-O4 |
| 32 | a | 720 | LHG | C4-O6-P-O5 |
| 32 | d | 407 | LHG | C4-O6-P-O3 |
| 33 | C | 518 | DGD | C2E-C1E-O5D-C6D |
| 34 | e | 102 | HEM | C3D-CAD-CBD-CGD |
| 25 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 25 | C | 503 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 610 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 611 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | b | 613 | CLA | CBD-CGD-O2D-CED |
| 25 | b | 620 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 506 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 512 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 510 | CLA | O1D-CGD-O2D-CED |
| 25 | c | 501 | CLA | O1D-CGD-O2D-CED |
| 25 | d | 402 | CLA | O1D-CGD-O2D-CED |
| 29 | A | 614 | SQD | C24-C23-O48-C46 |
| 29 | B | 626 | SQD | C24-C23-O48-C46 |
| 25 | B | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 505 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 507 | CLA | CBD-CGD-O2D-CED |
| 25 | b | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 502 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 503 | CLA | CBD-CGD-O2D-CED |
| 29 | A | 614 | SQD | O10-C23-O48-C46 |
| 29 | B | 623 | SQD | O10-C23-O48-C46 |
| 32 | e | 101 | LHG | O10-C23-O8-C6 |
| 25 | a | 707 | CLA | O1D-CGD-O2D-CED |
| 25 | b | 609 | CLA | CBD-CGD-O2D-CED |
| 25 | b | 614 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 506 | CLA | O1D-CGD-O2D-CED |
| 25 | c | 512 | CLA | O1D-CGD-O2D-CED |
| 23 | a | 701 | LMG | O9-C10-O7-C8 |
| 29 | B | 623 | SQD | O49-C7-O47-C45 |
| 29 | I | 102 | SQD | O49-C7-O47-C45 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 602 | CLA | C3-C5-C6-C7 |
| 25 | C | 503 | CLA | C3-C5-C6-C7 |
| 33 | C | 518 | DGD | O6E-C5E-C6E-O5E |
| 29 | A | 614 | SQD | C8-C7-O47-C45 |
| 29 | B | 623 | SQD | C8-C7-O47-C45 |
| 29 | B | 626 | SQD | C8-C7-O47-C45 |
| 25 | B | 611 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 604 | CLA | C4-C3-C5-C6 |
| 25 | B | 603 | CLA | C2-C3-C5-C6 |
| 25 | B | 607 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 611 | CLA | C2A-CAA-CBA-CGA |
| 25 | b | 613 | CLA | O1D-CGD-O2D-CED |
| 29 | B | 623 | SQD | C24-C23-O48-C46 |
| 25 | B | 615 | CLA | O1D-CGD-O2D-CED |
| 28 | A | 611 | PL9 | C42-C43-C44-C45 |
| 25 | B | 613 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 512 | CLA | CBD-CGD-O2D-CED |
| 23 | d | 408 | LMG | O9-C10-O7-C8 |
| 29 | A | 614 | SQD | O49-C7-O47-C45 |
| 28 | A | 611 | PL9 | C42-C43-C44-C46 |
| 25 | D | 404 | CLA | O1A-CGA-O2A-C1 |
| 25 | b | 620 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 614 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 505 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 511 | CLA | CBD-CGD-O2D-CED |
| 26 | a | 710 | PHO | CBD-CGD-O2D-CED |
| 32 | d | 407 | LHG | O2-C2-C3-O3 |
| 25 | b | 610 | CLA | C3-C5-C6-C7 |
| 33 | C | 517 | DGD | O6E-C5E-C6E-O5E |
| 33 | h | 102 | DGD | C4E-C5E-C6E-O5E |
| 23 | a | 701 | LMG | C11-C10-O7-C8 |
| 25 | D | 404 | CLA | CBD-CGD-O2D-CED |
| 25 | b | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | c | 504 | CLA | CBD-CGD-O2D-CED |
| 23 | a | 701 | LMG | O6-C5-C6-O5 |
| 23 | b | 626 | LMG | O6-C5-C6-O5 |
| 23 | a | 715 | LMG | O6-C5-C6-O5 |
| 23 | b | 626 | LMG | C4-C5-C6-O5 |
| 25 | D | 404 | CLA | CBA-CGA-O2A-C1 |
| 32 | e | 101 | LHG | C24-C23-O8-C6 |
| 23 | A | 603 | LMG | O6-C5-C6-O5 |
| 33 | c | 517 | DGD | O6E-C5E-C6E-O5E |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | b | 609 | CLA | C4-C3-C5-C6 |
| 25 | b | 611 | CLA | C4-C3-C5-C6 |
| 33 | C | 518 | DGD | C4E-C5E-C6E-O5E |
| 25 | b | 609 | CLA | C2-C3-C5-C6 |
| 25 | b | 611 | CLA | C2-C3-C5-C6 |
| 25 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 610 | CLA | O1D-CGD-O2D-CED |
| 23 | b | 627 | LMG | O10-C28-O8-C9 |
| 29 | I | 102 | SQD | O10-C23-O48-C46 |
| 32 | E | 101 | LHG | O10-C23-O8-C6 |
| 33 | C | 518 | DGD | O6E-C1E-O5D-C6D |
| 28 | A | 611 | PL9 | C24-C26-C27-C28 |
| 28 | a | 713 | PL9 | C9-C11-C12-C13 |
| 23 | b | 627 | LMG | C29-C28-O8-C9 |
| 25 | c | 512 | CLA | CBA-CGA-O2A-C1 |
| 25 | b | 619 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 606 | CLA | O1D-CGD-O2D-CED |
| 32 | D | 407 | LHG | C28-C29-C30-C31 |
| 25 | c | 502 | CLA | O1D-CGD-O2D-CED |
| 32 | D | 407 | LHG | C1-C2-C3-O3 |
| 32 | d | 406 | LHG | C1-C2-C3-O3 |
| 33 | C | 517 | DGD | C4E-C5E-C6E-O5E |
| 33 | c | 517 | DGD | C4E-C5E-C6E-O5E |
| 25 | c | 512 | CLA | O1A-CGA-O2A-C1 |
| 25 | C | 505 | CLA | O1D-CGD-O2D-CED |
| 25 | c | 503 | CLA | O1D-CGD-O2D-CED |
| 23 | a | 701 | LMG | C29-C28-O8-C9 |
| 25 | C | 513 | CLA | CBA-CGA-O2A-C1 |
| 25 | b | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | c | 510 | CLA | CBA-CGA-O2A-C1 |
| 29 | I | 102 | SQD | C24-C23-O48-C46 |
| 32 | E | 101 | LHG | C24-C23-O8-C6 |
| 32 | B | 625 | LHG | C23-C24-C25-C26 |
| 23 | a | 715 | LMG | C4-C5-C6-O5 |
| 32 | E | 101 | LHG | O6-C4-C5-O7 |
| 25 | C | 510 | CLA | C8-C10-C11-C12 |
| 25 | c | 506 | CLA | C5-C6-C7-C8 |
| 25 | c | 502 | CLA | C3-C5-C6-C7 |
| 23 | a | 715 | LMG | C10-C11-C12-C13 |
| 23 | D | 409 | LMG | C16-C17-C18-C19 |
| 25 | b | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 604 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | A | 611 | PL9 | C38-C39-C41-C42 |
| 25 | B | 607 | CLA | C11-C12-C13-C14 |
| 25 | B | 615 | CLA | C11-C10-C8-C9 |
| 25 | B | 617 | CLA | C14-C13-C15-C16 |
| 25 | C | 504 | CLA | C11-C10-C8-C9 |
| 25 | C | 506 | CLA | C14-C13-C15-C16 |
| 25 | C | 510 | CLA | C11-C12-C13-C14 |
| 25 | D | 403 | CLA | C6-C7-C8-C9 |
| 25 | b | 611 | CLA | C14-C13-C15-C16 |
| 25 | b | 612 | CLA | C11-C10-C8-C9 |
| 25 | b | 616 | CLA | C14-C13-C15-C16 |
| 25 | c | 502 | CLA | C6-C7-C8-C9 |
| 25 | c | 509 | CLA | C11-C10-C8-C9 |
| 25 | b | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | C | 502 | CLA | CBD-CGD-O2D-CED |
| 25 | d | 403 | CLA | C13-C15-C16-C17 |
| 27 | D | 405 | BCR | C37-C22-C23-C24 |
| 27 | c | 515 | BCR | C7-C8-C9-C34 |
| 27 | d | 404 | BCR | C37-C22-C23-C24 |
| 27 | k | 101 | BCR | C11-C12-C13-C35 |
| 27 | t | 103 | BCR | C7-C8-C9-C34 |
| 27 | b | 602 | BCR | C7-C8-C9-C10 |
| 27 | d | 404 | BCR | C21-C22-C23-C24 |
| 27 | t | 103 | BCR | C7-C8-C9-C10 |
| 29 | b | 601 | SQD | O49-C7-O47-C45 |
| 29 | I | 102 | SQD | C23-C24-C25-C26 |
| 32 | a | 720 | LHG | C7-C8-C9-C10 |
| 32 | e | 101 | LHG | C23-C24-C25-C26 |
| 25 | C | 513 | CLA | O1A-CGA-O2A-C1 |
| 25 | C | 512 | CLA | C10-C11-C12-C13 |
| 26 | a | 709 | PHO | C13-C15-C16-C17 |
| 23 | c | 520 | LMG | O6-C5-C6-O5 |
| 23 | f | 101 | LMG | O6-C5-C6-O5 |
| 25 | B | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | d | 403 | CLA | C3-C5-C6-C7 |
| 25 | C | 508 | CLA | C15-C16-C17-C18 |
| 25 | b | 607 | CLA | C5-C6-C7-C8 |
| 25 | b | 608 | CLA | C13-C15-C16-C17 |
| 25 | c | 506 | CLA | C15-C16-C17-C18 |
| 23 | B | 621 | LMG | O6-C5-C6-O5 |
| 33 | H | 103 | DGD | O6E-C5E-C6E-O5E |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | B | 623 | SQD | C23-C24-C25-C26 |
| 26 | D | 401 | PHO | CBD-CGD-O2D-CED |
| 25 | B | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 604 | CLA | C8-C10-C11-C12 |
| 25 | B | 604 | CLA | C15-C16-C17-C18 |
| 25 | B | 607 | CLA | C8-C10-C11-C12 |
| 25 | C | 514 | CLA | C15-C16-C17-C18 |
| 25 | a | 711 | CLA | C8-C10-C11-C12 |
| 25 | b | 612 | CLA | C8-C10-C11-C12 |
| 25 | b | 612 | CLA | C13-C15-C16-C17 |
| 25 | b | 617 | CLA | C8-C10-C11-C12 |
| 25 | c | 503 | CLA | C15-C16-C17-C18 |
| 25 | c | 505 | CLA | C15-C16-C17-C18 |
| 25 | c | 512 | CLA | C10-C11-C12-C13 |
| 25 | d | 403 | CLA | C15-C16-C17-C18 |
| 23 | d | 408 | LMG | C10-C11-C12-C13 |
| 23 | d | 408 | LMG | C28-C29-C30-C31 |
| 29 | A | 614 | SQD | C7-C8-C9-C10 |
| 29 | A | 614 | SQD | C23-C24-C25-C26 |
| 29 | b | 601 | SQD | C7-C8-C9-C10 |
| 32 | E | 101 | LHG | C23-C24-C25-C26 |
| 33 | C | 518 | DGD | C1A-C2A-C3A-C4A |
| 23 | a | 701 | LMG | C4-C5-C6-O5 |
| 25 | C | 504 | CLA | C15-C16-C17-C18 |
| 25 | C | 512 | CLA | C15-C16-C17-C18 |
| 25 | a | 711 | CLA | C13-C15-C16-C17 |
| 25 | b | 610 | CLA | C10-C11-C12-C13 |
| 25 | b | 616 | CLA | C15-C16-C17-C18 |
| 25 | C | 503 | CLA | C13-C15-C16-C17 |
| 25 | D | 404 | CLA | C8-C10-C11-C12 |
| 25 | c | 508 | CLA | C15-C16-C17-C18 |
| 23 | C | 501 | LMG | C28-C29-C30-C31 |
| 23 | c | 519 | LMG | C10-C11-C12-C13 |
| 25 | B | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 604 | CLA | C5-C6-C7-C8 |
| 25 | B | 609 | CLA | C15-C16-C17-C18 |
| 25 | b | 607 | CLA | C13-C15-C16-C17 |
| 25 | b | 608 | CLA | C10-C11-C12-C13 |
| 25 | b | 611 | CLA | C13-C15-C16-C17 |
| 25 | b | 614 | CLA | C15-C16-C17-C18 |
| 25 | B | 611 | CLA | C12-C13-C15-C16 |
| 25 | C | 505 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | e | 101 | LHG | C7-C8-C9-C10 |
| 25 | b | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | C | 507 | CLA | O1D-CGD-O2D-CED |
| 25 | b | 614 | CLA | O1D-CGD-O2D-CED |
| 25 | D | 404 | CLA | C10-C11-C12-C13 |
| 25 | a | 719 | CLA | C15-C16-C17-C18 |
| 25 | b | 608 | CLA | C15-C16-C17-C18 |
| 25 | c | 511 | CLA | C15-C16-C17-C18 |
| 25 | c | 513 | CLA | C13-C15-C16-C17 |
| 33 | h | 102 | DGD | O6E-C5E-C6E-O5E |
| 23 | a | 715 | LMG | O10-C28-O8-C9 |
| 25 | c | 510 | CLA | O1A-CGA-O2A-C1 |
| 23 | C | 520 | LMG | O6-C1-O1-C7 |
| 23 | a | 715 | LMG | O6-C1-O1-C7 |
| 25 | b | 621 | CLA | C5-C6-C7-C8 |
| 28 | A | 611 | PL9 | C44-C46-C47-C48 |
| 28 | D | 406 | PL9 | C39-C41-C42-C43 |
| 28 | a | 713 | PL9 | C24-C26-C27-C28 |
| 27 | h | 101 | BCR | C18-C19-C20-C21 |
| 32 | d | 406 | LHG | O2-C2-C3-O3 |
| 29 | D | 410 | SQD | O49-C7-O47-C45 |
| 25 | B | 607 | CLA | C3-C5-C6-C7 |
| 25 | A | 606 | CLA | C15-C16-C17-C18 |
| 25 | C | 512 | CLA | C13-C15-C16-C17 |
| 25 | b | 607 | CLA | C8-C10-C11-C12 |
| 25 | b | 615 | CLA | C13-C15-C16-C17 |
| 25 | b | 617 | CLA | C13-C15-C16-C17 |
| 25 | c | 508 | CLA | C8-C10-C11-C12 |
| 25 | c | 511 | CLA | C8-C10-C11-C12 |
| 25 | B | 603 | CLA | C5-C6-C7-C8 |
| 25 | B | 616 | CLA | C5-C6-C7-C8 |
| 25 | B | 616 | CLA | C15-C16-C17-C18 |
| 25 | C | 507 | CLA | C10-C11-C12-C13 |
| 25 | C | 514 | CLA | C13-C15-C16-C17 |
| 25 | B | 609 | CLA | CBD-CGD-O2D-CED |
| 23 | D | 409 | LMG | C11-C10-O7-C8 |
| 25 | b | 609 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 602 | CLA | C10-C11-C12-C13 |
| 25 | B | 602 | CLA | C15-C16-C17-C18 |
| 25 | B | 607 | CLA | C10-C11-C12-C13 |
| 25 | b | 607 | CLA | C10-C11-C12-C13 |
| 25 | c | 509 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | c | 510 | CLA | C5-C6-C7-C8 |
| 25 | c | 511 | CLA | C13-C15-C16-C17 |
| 32 | a | 720 | LHG | C3-O3-P-O6 |
| 32 | a | 720 | LHG | C4-O6-P-O3 |
| 32 | d | 406 | LHG | C3-O3-P-O6 |
| 32 | d | 406 | LHG | C23-C24-C25-C26 |
| 25 | b | 615 | CLA | C3-C5-C6-C7 |
| 29 | f | 102 | SQD | C24-C23-O48-C46 |
| 25 | B | 605 | CLA | C13-C15-C16-C17 |
| 25 | B | 615 | CLA | C8-C10-C11-C12 |
| 25 | b | 621 | CLA | C10-C11-C12-C13 |
| 26 | a | 709 | PHO | C15-C16-C17-C18 |
| 23 | C | 520 | LMG | C28-C29-C30-C31 |
| 32 | d | 407 | LHG | C1-C2-C3-O3 |
| 25 | C | 508 | CLA | C4-C3-C5-C6 |
| 25 | b | 610 | CLA | C4-C3-C5-C6 |
| 25 | b | 620 | CLA | C4-C3-C5-C6 |
| 25 | b | 619 | CLA | C8-C10-C11-C12 |
| 25 | B | 605 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 711 | CLA | CBA-CGA-O2A-C1 |
| 29 | D | 410 | SQD | C24-C23-O48-C46 |
| 29 | b | 601 | SQD | C24-C23-O48-C46 |
| 29 | A | 612 | SQD | C29-C30-C31-C32 |
| 29 | B | 623 | SQD | C30-C31-C32-C33 |
| 32 | d | 406 | LHG | C32-C33-C34-C35 |
| 27 | d | 404 | BCR | C20-C21-C22-C37 |
| 23 | B | 621 | LMG | C18-C19-C20-C21 |
| 23 | C | 520 | LMG | C15-C16-C17-C18 |
| 23 | C | 520 | LMG | C16-C17-C18-C19 |
| 23 | a | 715 | LMG | C20-C21-C22-C23 |
| 23 | b | 627 | LMG | C17-C18-C19-C20 |
| 23 | b | 627 | LMG | C29-C30-C31-C32 |
| 29 | B | 623 | SQD | C28-C29-C30-C31 |
| 32 | e | 101 | LHG | C15-C16-C17-C18 |
| 33 | C | 518 | DGD | C8B-C9B-CAB-CBB |
| 33 | H | 103 | DGD | C7A-C8A-C9A-CAA |
| 33 | h | 102 | DGD | C5B-C6B-C7B-C8B |
| 25 | B | 613 | CLA | O1D-CGD-O2D-CED |
| 25 | C | 507 | CLA | C16-C17-C18-C19 |
| 25 | c | 512 | CLA | C16-C17-C18-C19 |
| 23 | a | 715 | LMG | C29-C28-O8-C9 |
| 23 | C | 501 | LMG | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 521 | LMG | C15-C16-C17-C18 |
| 23 | D | 409 | LMG | C17-C18-C19-C20 |
| 23 | b | 627 | LMG | C13-C14-C15-C16 |
| 23 | c | 519 | LMG | C31-C32-C33-C34 |
| 29 | B | 623 | SQD | C11-C10-C9-C8 |
| 29 | B | 626 | SQD | C13-C14-C15-C16 |
| 33 | C | 519 | DGD | C6B-C7B-C8B-C9B |
| 33 | c | 516 | DGD | C5B-C6B-C7B-C8B |
| 23 | a | 701 | LMG | C7-C8-O7-C10 |
| 29 | A | 614 | SQD | C44-C45-O47-C7 |
| 29 | B | 623 | SQD | C46-C45-O47-C7 |
| 25 | C | 512 | CLA | O1D-CGD-O2D-CED |
| 23 | A | 603 | LMG | C10-C11-C12-C13 |
| 23 | b | 627 | LMG | C28-C29-C30-C31 |
| 23 | M | 101 | LMG | C30-C31-C32-C33 |
| 29 | I | 102 | SQD | C13-C14-C15-C16 |
| 23 | B | 621 | LMG | C29-C30-C31-C32 |
| 23 | D | 409 | LMG | C20-C21-C22-C23 |
| 29 | B | 626 | SQD | C31-C32-C33-C34 |
| 29 | I | 102 | SQD | C10-C11-C12-C13 |
| 29 | b | 601 | SQD | C12-C13-C14-C15 |
| 32 | D | 407 | LHG | C32-C33-C34-C35 |
| 25 | C | 507 | CLA | C13-C15-C16-C17 |
| 23 | a | 715 | LMG | C13-C14-C15-C16 |
| 23 | b | 627 | LMG | C14-C15-C16-C17 |
| 29 | b | 601 | SQD | C11-C12-C13-C14 |
| 32 | B | 625 | LHG | C30-C31-C32-C33 |
| 23 | C | 520 | LMG | C2-C1-O1-C7 |
| 23 | a | 715 | LMG | C2-C1-O1-C7 |
| 27 | k | 101 | BCR | C20-C21-C22-C23 |
| 33 | c | 517 | DGD | C2E-C1E-O5D-C6D |
| 25 | c | 504 | CLA | CBA-CGA-O2A-C1 |
| 33 | C | 519 | DGD | C2A-C1A-O1G-C1G |
| 23 | A | 603 | LMG | C19-C20-C21-C22 |
| 23 | C | 501 | LMG | C31-C32-C33-C34 |
| 23 | b | 627 | LMG | C33-C34-C35-C36 |
| 23 | f | 101 | LMG | C21-C22-C23-C24 |
| 29 | I | 102 | SQD | C11-C12-C13-C14 |
| 29 | a | 714 | SQD | C15-C16-C17-C18 |
| 29 | f | 102 | SQD | C27-C28-C29-C30 |
| 32 | D | 408 | LHG | C17-C18-C19-C20 |
| 33 | C | 517 | DGD | C5B-C6B-C7B-C8B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | C | 518 | DGD | C2A-C3A-C4A-C5A |
| 33 | C | 518 | DGD | CCA-CDA-CEA-CFA |
| 33 | C | 519 | DGD | CBA-CCA-CDA-CEA |
| 33 | c | 516 | DGD | C4A-C5A-C6A-C7A |
| 25 | D | 404 | CLA | C15-C16-C17-C18 |
| 33 | C | 518 | DGD | O1A-C1A-O1G-C1G |
| 25 | C | 512 | CLA | C16-C17-C18-C20 |
| 25 | b | 617 | CLA | C16-C17-C18-C19 |
| 25 | d | 403 | CLA | C16-C17-C18-C19 |
| 23 | M | 101 | LMG | C35-C36-C37-C38 |
| 23 | c | 519 | LMG | C32-C33-C34-C35 |
| 23 | d | 408 | LMG | C30-C31-C32-C33 |
| 29 | D | 410 | SQD | C33-C34-C35-C36 |
| 32 | D | 408 | LHG | C30-C31-C32-C33 |
| 32 | e | 101 | LHG | C18-C19-C20-C21 |
| 33 | c | 516 | DGD | C4B-C5B-C6B-C7B |
| 25 | B | 605 | CLA | C14-C13-C15-C16 |
| 25 | B | 606 | CLA | C14-C13-C15-C16 |
| 25 | C | 511 | CLA | C6-C7-C8-C9 |
| 25 | b | 610 | CLA | C11-C12-C13-C14 |
| 25 | b | 617 | CLA | C11-C12-C13-C14 |
| 25 | c | 508 | CLA | C14-C13-C15-C16 |
| 26 | a | 709 | PHO | C14-C13-C15-C16 |
| 23 | M | 101 | LMG | C28-C29-C30-C31 |
| 23 | a | 715 | LMG | C28-C29-C30-C31 |
| 29 | I | 102 | SQD | C7-C8-C9-C10 |
| 23 | A | 603 | LMG | C18-C19-C20-C21 |
| 23 | C | 501 | LMG | C15-C16-C17-C18 |
| 23 | C | 501 | LMG | C29-C30-C31-C32 |
| 23 | D | 409 | LMG | C11-C12-C13-C14 |
| 23 | a | 701 | LMG | C32-C33-C34-C35 |
| 29 | A | 614 | SQD | C9-C10-C11-C12 |
| 29 | A | 614 | SQD | C24-C25-C26-C27 |
| 33 | C | 518 | DGD | CBA-CCA-CDA-CEA |
| 33 | h | 102 | DGD | C9A-CAA-CBA-CCA |
| 25 | b | 607 | CLA | C15-C16-C17-C18 |
| 25 | b | 618 | CLA | C15-C16-C17-C18 |
| 25 | c | 501 | CLA | C2A-CAA-CBA-CGA |
| 27 | t | 103 | BCR | C37-C22-C23-C24 |
| 23 | C | 521 | LMG | C30-C31-C32-C33 |
| 23 | b | 627 | LMG | C34-C35-C36-C37 |
| 23 | c | 520 | LMG | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | f | 101 | LMG | C16-C17-C18-C19 |
| 29 | D | 410 | SQD | C26-C27-C28-C29 |
| 32 | L | 101 | LHG | C32-C33-C34-C35 |
| 32 | a | 720 | LHG | O1-C1-C2-C3 |
| 32 | e | 101 | LHG | O1-C1-C2-C3 |
| 27 | H | 102 | BCR | C7-C8-C9-C10 |
| 23 | D | 409 | LMG | C31-C32-C33-C34 |
| 23 | b | 626 | LMG | C16-C17-C18-C19 |
| 23 | b | 627 | LMG | C35-C36-C37-C38 |
| 29 | B | 626 | SQD | C14-C15-C16-C17 |
| 29 | B | 626 | SQD | C34-C35-C36-C37 |
| 32 | D | 408 | LHG | C25-C26-C27-C28 |
| 32 | E | 101 | LHG | C13-C14-C15-C16 |
| 29 | D | 410 | SQD | C23-C24-C25-C26 |
| 25 | c | 511 | CLA | O1D-CGD-O2D-CED |
| 23 | A | 603 | LMG | C15-C16-C17-C18 |
| 23 | B | 621 | LMG | C33-C34-C35-C36 |
| 23 | C | 521 | LMG | C35-C36-C37-C38 |
| 23 | M | 101 | LMG | C31-C32-C33-C34 |
| 23 | a | 701 | LMG | C13-C14-C15-C16 |
| 23 | a | 715 | LMG | C16-C17-C18-C19 |
| 23 | b | 626 | LMG | C32-C33-C34-C35 |
| 23 | b | 627 | LMG | C37-C38-C39-C40 |
| 29 | I | 102 | SQD | C9-C10-C11-C12 |
| 32 | D | 407 | LHG | C30-C31-C32-C33 |
| 32 | D | 408 | LHG | C29-C30-C31-C32 |
| 32 | E | 101 | LHG | C32-C33-C34-C35 |
| 32 | a | 720 | LHG | C30-C31-C32-C33 |
| 32 | e | 101 | LHG | C14-C15-C16-C17 |
| 32 | e | 101 | LHG | C24-C25-C26-C27 |
| 33 | C | 519 | DGD | C7B-C8B-C9B-CAB |
| 33 | H | 103 | DGD | C5B-C6B-C7B-C8B |
| 33 | c | 517 | DGD | C9A-CAA-CBA-CCA |
| 33 | c | 518 | DGD | CBA-CCA-CDA-CEA |
| 25 | B | 604 | CLA | C16-C17-C18-C20 |
| 25 | C | 505 | CLA | C16-C17-C18-C20 |
| 25 | C | 507 | CLA | C16-C17-C18-C20 |
| 25 | b | 619 | CLA | C16-C17-C18-C20 |
| 25 | c | 512 | CLA | C16-C17-C18-C20 |
| 26 | A | 608 | PHO | C16-C17-C18-C20 |
| 23 | c | 519 | LMG | O6-C1-O1-C7 |
| 25 | B | 606 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | c | 506 | CLA | C10-C11-C12-C13 |
| 23 | C | 501 | LMG | C17-C18-C19-C20 |
| 23 | C | 521 | LMG | C20-C21-C22-C23 |
| 23 | D | 409 | LMG | C19-C20-C21-C22 |
| 23 | a | 701 | LMG | C30-C31-C32-C33 |
| 29 | B | 626 | SQD | C24-C25-C26-C27 |
| 29 | f | 102 | SQD | C32-C33-C34-C35 |
| 32 | B | 625 | LHG | C11-C10-C9-C8 |
| 32 | D | 408 | LHG | C32-C33-C34-C35 |
| 33 | C | 517 | DGD | C4B-C5B-C6B-C7B |
| 23 | D | 409 | LMG | C15-C16-C17-C18 |
| 23 | a | 701 | LMG | C21-C22-C23-C24 |
| 29 | A | 614 | SQD | C15-C16-C17-C18 |
| 29 | B | 626 | SQD | C29-C30-C31-C32 |
| 29 | I | 102 | SQD | C14-C15-C16-C17 |
| 29 | a | 714 | SQD | C13-C14-C15-C16 |
| 25 | c | 513 | CLA | C8-C10-C11-C12 |
| 23 | C | 521 | LMG | C21-C22-C23-C24 |
| 23 | d | 408 | LMG | C31-C32-C33-C34 |
| 29 | a | 714 | SQD | C28-C29-C30-C31 |
| 32 | D | 408 | LHG | C18-C19-C20-C21 |
| 32 | d | 406 | LHG | C25-C26-C27-C28 |
| 25 | D | 404 | CLA | C3-C5-C6-C7 |
| 26 | D | 401 | PHO | C3-C5-C6-C7 |
| 25 | C | 504 | CLA | CBA-CGA-O2A-C1 |
| 25 | b | 622 | CLA | CBA-CGA-O2A-C1 |
| 25 | c | 513 | CLA | CBA-CGA-O2A-C1 |
| 23 | c | 520 | LMG | C20-C21-C22-C23 |
| 29 | a | 714 | SQD | C9-C10-C11-C12 |
| 33 | C | 517 | DGD | C6A-C7A-C8A-C9A |
| 25 | B | 614 | CLA | O1D-CGD-O2D-CED |
| 26 | a | 710 | PHO | O1D-CGD-O2D-CED |
| 25 | D | 403 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 606 | CLA | C8-C10-C11-C12 |
| 23 | C | 520 | LMG | C29-C30-C31-C32 |
| 23 | C | 520 | LMG | C35-C36-C37-C38 |
| 23 | C | 521 | LMG | C38-C39-C40-C41 |
| 23 | f | 101 | LMG | C19-C20-C21-C22 |
| 29 | B | 626 | SQD | C18-C19-C20-C21 |
| 29 | I | 102 | SQD | C30-C31-C32-C33 |
| 32 | B | 625 | LHG | C32-C33-C34-C35 |
| 33 | C | 517 | DGD | C4A-C5A-C6A-C7A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | C | 505 | CLA | C16-C17-C18-C19 |
| 25 | b | 617 | CLA | C16-C17-C18-C20 |
| 25 | b | 619 | CLA | C16-C17-C18-C19 |
| 25 | c | 507 | CLA | C16-C17-C18-C20 |
| 23 | f | 101 | LMG | C12-C13-C14-C15 |
| 29 | I | 102 | SQD | C31-C32-C33-C34 |
| 32 | e | 101 | LHG | C12-C13-C14-C15 |
| 25 | b | 617 | CLA | CBD-CGD-O2D-CED |
| 29 | A | 614 | SQD | C13-C14-C15-C16 |
| 28 | d | 405 | PL9 | C15-C14-C16-C17 |
| 26 | A | 608 | PHO | C2-C3-C5-C6 |
| 28 | a | 713 | PL9 | C43-C44-C46-C47 |
| 23 | B | 621 | LMG | C30-C31-C32-C33 |
| 23 | C | 521 | LMG | C19-C20-C21-C22 |
| 25 | c | 505 | CLA | O1D-CGD-O2D-CED |
| 23 | A | 603 | LMG | C14-C15-C16-C17 |
| 23 | B | 621 | LMG | C12-C13-C14-C15 |
| 23 | C | 501 | LMG | C32-C33-C34-C35 |
| 23 | C | 520 | LMG | C17-C18-C19-C20 |
| 23 | a | 701 | LMG | C31-C32-C33-C34 |
| 23 | a | 715 | LMG | C32-C33-C34-C35 |
| 23 | d | 408 | LMG | C11-C12-C13-C14 |
| 29 | A | 612 | SQD | C12-C13-C14-C15 |
| 29 | A | 612 | SQD | C25-C26-C27-C28 |
| 29 | I | 102 | SQD | C26-C27-C28-C29 |
| 29 | b | 601 | SQD | C24-C25-C26-C27 |
| 33 | C | 518 | DGD | C4A-C5A-C6A-C7A |
| 33 | c | 517 | DGD | C5A-C6A-C7A-C8A |
| 33 | c | 518 | DGD | C2B-C3B-C4B-C5B |
| 25 | a | 711 | CLA | O1A-CGA-O2A-C1 |
| 25 | d | 403 | CLA | C16-C17-C18-C20 |
| 23 | c | 520 | LMG | C14-C15-C16-C17 |
| 25 | a | 707 | CLA | C13-C15-C16-C17 |
| 29 | I | 102 | SQD | C17-C18-C19-C20 |
| 32 | D | 408 | LHG | C9-C10-C11-C12 |
| 32 | L | 101 | LHG | C10-C11-C12-C13 |
| 25 | c | 504 | CLA | O1D-CGD-O2D-CED |
| 29 | I | 102 | SQD | C27-C28-C29-C30 |
| 32 | e | 101 | LHG | C9-C10-C11-C12 |
| 33 | h | 102 | DGD | CAA-CBA-CCA-CDA |
| 32 | D | 408 | LHG | C15-C16-C17-C18 |
| 25 | C | 506 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | D | 404 | CLA | C5-C6-C7-C8 |
| 25 | B | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | b | 622 | CLA | O1A-CGA-O2A-C1 |
| 25 | c | 504 | CLA | O1A-CGA-O2A-C1 |
| 23 | A | 603 | LMG | C32-C33-C34-C35 |
| 23 | C | 520 | LMG | C36-C37-C38-C39 |
| 23 | c | 519 | LMG | C17-C18-C19-C20 |
| 29 | A | 614 | SQD | C11-C10-C9-C8 |
| 32 | D | 408 | LHG | C11-C12-C13-C14 |
| 32 | d | 406 | LHG | C11-C12-C13-C14 |
| 33 | C | 519 | DGD | CBB-CCB-CDB-CEB |
| 25 | C | 507 | CLA | C3-C5-C6-C7 |
| 27 | B | 618 | BCR | C1-C6-C7-C8 |
| 27 | B | 618 | BCR | C5-C6-C7-C8 |
| 27 | B | 620 | BCR | C5-C6-C7-C8 |
| 27 | B | 620 | BCR | C23-C24-C25-C26 |
| 27 | D | 405 | BCR | C5-C6-C7-C8 |
| 27 | Y | 101 | BCR | C1-C6-C7-C8 |
| 27 | Y | 101 | BCR | C5-C6-C7-C8 |
| 27 | b | 602 | BCR | C1-C6-C7-C8 |
| 27 | b | 623 | BCR | C1-C6-C7-C8 |
| 27 | b | 623 | BCR | C5-C6-C7-C8 |
| 27 | b | 625 | BCR | C5-C6-C7-C8 |
| 27 | b | 625 | BCR | C23-C24-C25-C26 |
| 27 | b | 625 | BCR | C23-C24-C25-C30 |
| 27 | c | 514 | BCR | C1-C6-C7-C8 |
| 27 | c | 515 | BCR | C5-C6-C7-C8 |
| 27 | k | 101 | BCR | C1-C6-C7-C8 |
| 27 | k | 101 | BCR | C5-C6-C7-C8 |
| 27 | t | 103 | BCR | C1-C6-C7-C8 |
| 27 | t | 103 | BCR | C5-C6-C7-C8 |
| 23 | C | 520 | LMG | C29-C28-O8-C9 |
| 23 | C | 521 | LMG | C29-C28-O8-C9 |
| 25 | b | 620 | CLA | CBA-CGA-O2A-C1 |
| 25 | C | 510 | CLA | C10-C11-C12-C13 |
| 25 | c | 507 | CLA | C15-C16-C17-C18 |
| 23 | C | 520 | LMG | C32-C33-C34-C35 |
| 29 | B | 623 | SQD | C32-C33-C34-C35 |
| 32 | a | 720 | LHG | C31-C32-C33-C34 |
| 33 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 25 | c | 513 | CLA | O1A-CGA-O2A-C1 |
| 29 | b | 601 | SQD | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | c | 516 | DGD | O6E-C5E-C6E-O5E |
| 23 | A | 603 | LMG | C31-C32-C33-C34 |
| 25 | b | 615 | CLA | C4-C3-C5-C6 |
| 28 | D | 406 | PL9 | C15-C14-C16-C17 |
| 25 | b | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 605 | CLA | C11-C10-C8-C7 |
| 25 | B | 607 | CLA | C11-C12-C13-C15 |
| 25 | C | 504 | CLA | C11-C10-C8-C7 |
| 25 | C | 511 | CLA | C6-C7-C8-C10 |
| 25 | b | 609 | CLA | C6-C7-C8-C10 |
| 25 | b | 612 | CLA | C11-C10-C8-C7 |
| 25 | c | 508 | CLA | C12-C13-C15-C16 |
| 25 | c | 510 | CLA | C6-C7-C8-C10 |
| 25 | c | 511 | CLA | C6-C7-C8-C10 |
| 25 | d | 402 | CLA | C12-C13-C15-C16 |
| 25 | C | 504 | CLA | O1A-CGA-O2A-C1 |
| 23 | c | 520 | LMG | C32-C33-C34-C35 |
| 25 | B | 614 | CLA | C13-C15-C16-C17 |
| 25 | c | 508 | CLA | C16-C17-C18-C19 |
| 23 | b | 627 | LMG | O9-C10-O7-C8 |
| 29 | A | 614 | SQD | C16-C17-C18-C19 |
| 32 | a | 720 | LHG | C27-C28-C29-C30 |
| 32 | e | 101 | LHG | C26-C27-C28-C29 |
| 25 | b | 620 | CLA | C2A-CAA-CBA-CGA |
| 25 | C | 513 | CLA | C10-C11-C12-C13 |
| 25 | c | 510 | CLA | C8-C10-C11-C12 |
| 25 | D | 404 | CLA | O1D-CGD-O2D-CED |
| 29 | b | 601 | SQD | C30-C31-C32-C33 |
| 23 | a | 701 | LMG | C28-C29-C30-C31 |
| 32 | L | 101 | LHG | C23-C24-C25-C26 |
| 32 | E | 101 | LHG | C24-C25-C26-C27 |
| 33 | C | 518 | DGD | CCB-CDB-CEB-CFB |
| 33 | H | 103 | DGD | CBA-CCA-CDA-CEA |
| 33 | H | 103 | DGD | CCA-CDA-CEA-CFA |
| 32 | d | 406 | LHG | C10-C11-C12-C13 |
| 25 | C | 507 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 614 | CLA | C16-C17-C18-C20 |
| 25 | b | 611 | CLA | C16-C17-C18-C20 |
| 33 | C | 519 | DGD | O6D-C1D-O3G-C3G |
| 33 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 25 | b | 609 | CLA | C15-C16-C17-C18 |
| 25 | c | 510 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | a | 713 | PL9 | C39-C41-C42-C43 |
| 23 | c | 519 | LMG | C19-C20-C21-C22 |
| 29 | b | 601 | SQD | C32-C33-C34-C35 |
| 32 | E | 101 | LHG | C8-C7-O7-C5 |
| 23 | C | 501 | LMG | C13-C14-C15-C16 |
| 23 | C | 520 | LMG | C13-C14-C15-C16 |
| 32 | d | 407 | LHG | C16-C17-C18-C19 |
| 25 | b | 615 | CLA | C15-C16-C17-C18 |
| 25 | C | 509 | CLA | CBD-CGD-O2D-CED |
| 23 | c | 519 | LMG | C20-C21-C22-C23 |
| 23 | d | 408 | LMG | C18-C19-C20-C21 |
| 32 | d | 407 | LHG | C34-C35-C36-C37 |
| 33 | H | 103 | DGD | C4D-C5D-C6D-O5D |
| 23 | a | 701 | LMG | C17-C18-C19-C20 |
| 32 | D | 408 | LHG | C12-C13-C14-C15 |
| 23 | c | 519 | LMG | C2-C1-O1-C7 |
| 23 | c | 520 | LMG | C2-C1-O1-C7 |
| 29 | B | 623 | SQD | C2-C1-O6-C44 |
| 25 | c | 508 | CLA | CBA-CGA-O2A-C1 |
| 23 | C | 521 | LMG | C37-C38-C39-C40 |
| 23 | a | 715 | LMG | C21-C22-C23-C24 |
| 25 | C | 504 | CLA | C5-C6-C7-C8 |
| 25 | B | 606 | CLA | C4-C3-C5-C6 |
| 26 | A | 608 | PHO | C4-C3-C5-C6 |
| 28 | D | 406 | PL9 | C30-C29-C31-C32 |
| 28 | a | 713 | PL9 | C15-C14-C16-C17 |
| 23 | B | 621 | LMG | C10-C11-C12-C13 |
| 29 | B | 626 | SQD | C7-C8-C9-C10 |
| 25 | b | 610 | CLA | C2-C3-C5-C6 |
| 25 | b | 615 | CLA | C2-C3-C5-C6 |
| 28 | a | 713 | PL9 | C38-C39-C41-C42 |
| 25 | A | 607 | CLA | C6-C7-C8-C9 |
| 25 | B | 604 | CLA | C11-C12-C13-C14 |
| 25 | B | 605 | CLA | C11-C10-C8-C9 |
| 25 | B | 607 | CLA | C6-C7-C8-C9 |
| 25 | B | 616 | CLA | C11-C12-C13-C14 |
| 25 | B | 616 | CLA | C14-C13-C15-C16 |
| 25 | B | 617 | CLA | C11-C10-C8-C9 |
| 25 | C | 505 | CLA | C14-C13-C15-C16 |
| 25 | b | 609 | CLA | C6-C7-C8-C9 |
| 25 | c | 510 | CLA | C6-C7-C8-C9 |
| 25 | c | 511 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | M | 101 | LMG | C16-C17-C18-C19 |
| 25 | C | 512 | CLA | C3-C5-C6-C7 |
| 25 | c | 512 | CLA | C2A-CAA-CBA-CGA |
| 23 | a | 701 | LMG | O10-C28-O8-C9 |
| 25 | b | 620 | CLA | O1A-CGA-O2A-C1 |
| 25 | C | 504 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 719 | CLA | C1A-C2A-CAA-CBA |
| 25 | c | 503 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 614 | CLA | C16-C17-C18-C19 |
| 25 | C | 512 | CLA | C16-C17-C18-C19 |
| 25 | c | 508 | CLA | C16-C17-C18-C20 |
| 23 | D | 409 | LMG | O9-C10-O7-C8 |
| 23 | b | 628 | LMG | C11-C12-C13-C14 |
| 32 | E | 101 | LHG | C28-C29-C30-C31 |
| 33 | C | 519 | DGD | C5A-C6A-C7A-C8A |
| 25 | B | 608 | CLA | O1D-CGD-O2D-CED |
| 25 | b | 619 | CLA | O1D-CGD-O2D-CED |
| 32 | D | 407 | LHG | C3-O3-P-O6 |
| 32 | E | 101 | LHG | C4-O6-P-O3 |
| 23 | f | 101 | LMG | C31-C32-C33-C34 |
| 29 | B | 626 | SQD | C27-C28-C29-C30 |
| 29 | b | 601 | SQD | C33-C34-C35-C36 |
| 29 | f | 102 | SQD | C31-C32-C33-C34 |
| 32 | D | 407 | LHG | C34-C35-C36-C37 |
| 32 | a | 720 | LHG | C25-C26-C27-C28 |
| 33 | C | 518 | DGD | C6A-C7A-C8A-C9A |
| 33 | C | 519 | DGD | C4B-C5B-C6B-C7B |
| 23 | C | 520 | LMG | C31-C32-C33-C34 |
| 23 | b | 626 | LMG | C30-C31-C32-C33 |
| 32 | B | 625 | LHG | C27-C28-C29-C30 |
| 25 | b | 611 | CLA | C16-C17-C18-C19 |
| 23 | C | 521 | LMG | O6-C5-C6-O5 |
| 23 | C | 520 | LMG | C12-C13-C14-C15 |
| 33 | C | 519 | DGD | C8A-C9A-CAA-CBA |
| 25 | c | 507 | CLA | C3-C5-C6-C7 |
| 23 | c | 519 | LMG | C29-C30-C31-C32 |
| 23 | b | 626 | LMG | C37-C38-C39-C40 |
| 29 | I | 102 | SQD | C25-C26-C27-C28 |
| 29 | b | 601 | SQD | C27-C28-C29-C30 |
| 25 | a | 707 | CLA | C15-C16-C17-C18 |
| 26 | A | 608 | PHO | C15-C16-C17-C18 |
| 29 | A | 614 | SQD | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | f | 101 | LMG | C11-C12-C13-C14 |
| 32 | E | 101 | LHG | C31-C32-C33-C34 |
| 25 | B | 611 | CLA | C15-C16-C17-C18 |
| 29 | f | 102 | SQD | C44-C45-C46-O48 |
| 32 | E | 101 | LHG | C4-C5-C6-O8 |
| 32 | e | 101 | LHG | C4-C5-C6-O8 |
| 32 | e | 101 | LHG | C19-C20-C21-C22 |
| 23 | b | 627 | LMG | O6-C5-C6-O5 |
| 25 | d | 403 | CLA | C10-C11-C12-C13 |
| 23 | A | 603 | LMG | C20-C21-C22-C23 |
| 23 | C | 501 | LMG | C38-C39-C40-C41 |
| 23 | C | 521 | LMG | C8-C7-O1-C1 |
| 29 | b | 601 | SQD | C45-C44-O6-C1 |
| 23 | C | 501 | LMG | C22-C23-C24-C25 |
| 33 | C | 519 | DGD | C2B-C3B-C4B-C5B |
| 25 | C | 502 | CLA | O1D-CGD-O2D-CED |
| 26 | D | 401 | PHO | O1D-CGD-O2D-CED |
| 23 | c | 520 | LMG | C17-C18-C19-C20 |
| 23 | f | 101 | LMG | C33-C34-C35-C36 |
| 32 | B | 625 | LHG | C10-C11-C12-C13 |
| 23 | B | 621 | LMG | C28-C29-C30-C31 |
| 29 | A | 612 | SQD | C30-C31-C32-C33 |
| 23 | M | 101 | LMG | C19-C20-C21-C22 |
| 29 | A | 612 | SQD | C32-C33-C34-C35 |
| 25 | C | 506 | CLA | CBD-CGD-O2D-CED |
| 32 | E | 101 | LHG | O1-C1-C2-O2 |
| 32 | a | 720 | LHG | O1-C1-C2-O2 |
| 32 | e | 101 | LHG | O1-C1-C2-O2 |
| 32 | e | 101 | LHG | C28-C29-C30-C31 |
| 23 | D | 409 | LMG | O6-C5-C6-O5 |
| 23 | A | 603 | LMG | C38-C39-C40-C41 |
| 33 | c | 517 | DGD | C3B-C4B-C5B-C6B |
| 29 | D | 410 | SQD | O48-C23-C24-C25 |
| 23 | A | 603 | LMG | C4-C5-C6-O5 |
| 23 | b | 626 | LMG | C40-C41-C42-C43 |
| 25 | c | 503 | CLA | C5-C6-C7-C8 |
| 25 | c | 505 | CLA | C4-C3-C5-C6 |
| 28 | a | 713 | PL9 | C20-C19-C21-C22 |
| 28 | a | 713 | PL9 | C45-C44-C46-C47 |
| 25 | C | 508 | CLA | C2-C3-C5-C6 |
| 25 | b | 620 | CLA | C2-C3-C5-C6 |
| 25 | c | 505 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | D | 409 | LMG | C28-C29-C30-C31 |
| 25 | C | 508 | CLA | C16-C17-C18-C19 |
| 25 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 29 | B | 626 | SQD | C11-C12-C13-C14 |
| 29 | I | 102 | SQD | C18-C19-C20-C21 |
| 33 | C | 518 | DGD | C9B-CAB-CBB-CCB |
| 25 | c | 512 | CLA | C2-C1-O2A-CGA |
| 23 | b | 626 | LMG | C31-C32-C33-C34 |
| 32 | E | 101 | LHG | C12-C13-C14-C15 |
| 33 | h | 102 | DGD | CBB-CCB-CDB-CEB |
| 33 | C | 518 | DGD | C2A-C1A-O1G-C1G |
| 25 | C | 507 | CLA | O1A-CGA-O2A-C1 |
| 25 | c | 508 | CLA | O1A-CGA-O2A-C1 |
| 32 | D | 407 | LHG | C27-C28-C29-C30 |
| 23 | b | 626 | LMG | C19-C20-C21-C22 |
| 29 | I | 102 | SQD | C11-C10-C9-C8 |
| 25 | B | 612 | CLA | C13-C15-C16-C17 |
| 23 | C | 521 | LMG | C2-C1-O1-C7 |
| 23 | B | 621 | LMG | O1-C7-C8-O7 |
| 23 | a | 715 | LMG | O7-C8-C9-O8 |
| 29 | a | 714 | SQD | O6-C44-C45-O47 |
| 23 | b | 626 | LMG | C34-C35-C36-C37 |
| 25 | B | 617 | CLA | C15-C16-C17-C18 |
| 29 | f | 102 | SQD | C35-C36-C37-C38 |
| 23 | B | 621 | LMG | C40-C41-C42-C43 |
| 32 | L | 101 | LHG | C34-C35-C36-C37 |
| 25 | B | 610 | CLA | C15-C16-C17-C18 |
| 25 | b | 620 | CLA | C10-C11-C12-C13 |
| 25 | A | 607 | CLA | C6-C7-C8-C10 |
| 25 | A | 607 | CLA | C12-C13-C15-C16 |
| 25 | B | 602 | CLA | C11-C12-C13-C15 |
| 25 | B | 604 | CLA | C11-C12-C13-C15 |
| 25 | B | 607 | CLA | C6-C7-C8-C10 |
| 25 | B | 609 | CLA | C11-C12-C13-C15 |
| 25 | B | 616 | CLA | C11-C12-C13-C15 |
| 25 | B | 616 | CLA | C12-C13-C15-C16 |
| 25 | B | 617 | CLA | C11-C10-C8-C7 |
| 25 | C | 509 | CLA | C11-C10-C8-C7 |
| 25 | C | 510 | CLA | C11-C10-C8-C7 |
| 25 | C | 513 | CLA | C11-C10-C8-C7 |
| 25 | a | 711 | CLA | C11-C12-C13-C15 |
| 25 | b | 610 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | b | 611 | CLA | C12-C13-C15-C16 |
| 25 | b | 612 | CLA | C6-C7-C8-C10 |
| 25 | b | 621 | CLA | C11-C10-C8-C7 |
| 25 | c | 506 | CLA | C11-C12-C13-C15 |
| 25 | c | 507 | CLA | C12-C13-C15-C16 |
| 25 | d | 403 | CLA | C6-C7-C8-C10 |
| 28 | D | 406 | PL9 | C28-C29-C31-C32 |
| 23 | C | 520 | LMG | O10-C28-O8-C9 |
| 33 | c | 517 | DGD | CCB-CDB-CEB-CFB |
| 25 | B | 604 | CLA | C6-C7-C8-C9 |
| 25 | B | 612 | CLA | C14-C13-C15-C16 |
| 25 | C | 509 | CLA | C11-C10-C8-C9 |
| 25 | C | 513 | CLA | C11-C10-C8-C9 |
| 25 | a | 708 | CLA | C6-C7-C8-C9 |
| 25 | a | 711 | CLA | C11-C12-C13-C14 |
| 25 | b | 617 | CLA | C6-C7-C8-C9 |
| 25 | b | 621 | CLA | C11-C10-C8-C9 |
| 25 | b | 621 | CLA | C14-C13-C15-C16 |
| 25 | c | 506 | CLA | C11-C12-C13-C14 |
| 25 | c | 507 | CLA | C14-C13-C15-C16 |
| 25 | c | 510 | CLA | C11-C12-C13-C14 |
| 25 | c | 512 | CLA | C14-C13-C15-C16 |
| 25 | c | 513 | CLA | C11-C12-C13-C14 |
| 25 | d | 403 | CLA | C6-C7-C8-C9 |
| 23 | b | 626 | LMG | C17-C18-C19-C20 |
| 29 | B | 626 | SQD | C32-C33-C34-C35 |
| 23 | A | 603 | LMG | C29-C28-O8-C9 |
| 23 | c | 519 | LMG | C29-C28-O8-C9 |
| 25 | C | 503 | CLA | C5-C6-C7-C8 |
| 25 | C | 505 | CLA | C8-C10-C11-C12 |
| 29 | A | 612 | SQD | C9-C10-C11-C12 |
| 29 | B | 623 | SQD | C7-C8-C9-C10 |
| 23 | a | 715 | LMG | C29-C30-C31-C32 |
| 32 | D | 408 | LHG | C19-C20-C21-C22 |
| 25 | c | 503 | CLA | CBA-CGA-O2A-C1 |
| 32 | D | 407 | LHG | C14-C15-C16-C17 |
| 33 | h | 102 | DGD | C7A-C8A-C9A-CAA |
| 33 | h | 102 | DGD | C2B-C3B-C4B-C5B |
| 23 | C | 501 | LMG | C21-C22-C23-C24 |
| 29 | B | 623 | SQD | C12-C13-C14-C15 |
| 29 | a | 714 | SQD | C14-C15-C16-C17 |
| 32 | e | 101 | LHG | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | t | 103 | BCR | C22-C23-C24-C25 |
| 33 | c | 518 | DGD | C9B-CAB-CBB-CCB |
| 32 | E | 101 | LHG | O6-C4-C5-C6 |
| 32 | d | 407 | LHG | O6-C4-C5-C6 |
| 23 | c | 519 | LMG | C30-C31-C32-C33 |
| 23 | d | 408 | LMG | C12-C13-C14-C15 |
| 23 | A | 603 | LMG | C16-C17-C18-C19 |
| 25 | B | 604 | CLA | CBA-CGA-O2A-C1 |
| 25 | C | 504 | CLA | C4-C3-C5-C6 |
| 23 | f | 101 | LMG | C10-C11-C12-C13 |
| 23 | C | 501 | LMG | C36-C37-C38-C39 |
| 32 | L | 101 | LHG | C31-C32-C33-C34 |
| 25 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 23 | C | 521 | LMG | C12-C13-C14-C15 |
| 23 | C | 520 | LMG | C30-C31-C32-C33 |
| 23 | f | 101 | LMG | C13-C14-C15-C16 |
| 23 | f | 101 | LMG | C4-C5-C6-O5 |
| 33 | h | 102 | DGD | CBA-CCA-CDA-CEA |
| 29 | A | 612 | SQD | C10-C11-C12-C13 |
| 25 | B | 616 | CLA | C13-C15-C16-C17 |
| 25 | b | 608 | CLA | C8-C10-C11-C12 |
| 25 | c | 506 | CLA | C8-C10-C11-C12 |
| 33 | c | 516 | DGD | C5A-C6A-C7A-C8A |
| 25 | c | 507 | CLA | C16-C17-C18-C19 |
| 25 | C | 502 | CLA | CBA-CGA-O2A-C1 |
| 29 | B | 623 | SQD | C33-C34-C35-C36 |
| 32 | L | 101 | LHG | C16-C17-C18-C19 |
| 25 | B | 616 | CLA | C8-C10-C11-C12 |
| 25 | C | 510 | CLA | C13-C15-C16-C17 |
| 25 | B | 609 | CLA | O1D-CGD-O2D-CED |
| 23 | B | 621 | LMG | O1-C7-C8-C9 |
| 23 | C | 520 | LMG | O1-C7-C8-C9 |
| 23 | a | 715 | LMG | C7-C8-C9-O8 |
| 29 | A | 614 | SQD | C44-C45-C46-O48 |
| 29 | D | 410 | SQD | C44-C45-C46-O48 |
| 29 | a | 714 | SQD | O6-C44-C45-C46 |
| 33 | c | 516 | DGD | C1G-C2G-C3G-O3G |
| 23 | c | 520 | LMG | C30-C31-C32-C33 |
| 32 | B | 625 | LHG | C11-C12-C13-C14 |
| 32 | L | 101 | LHG | C9-C10-C11-C12 |
| 25 | c | 508 | CLA | C10-C11-C12-C13 |
| 23 | c | 519 | LMG | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 611 | CLA | C13-C15-C16-C17 |
| 25 | b | 611 | CLA | CBA-CGA-O2A-C1 |
| 23 | c | 519 | LMG | C14-C15-C16-C17 |
| 23 | a | 701 | LMG | C36-C37-C38-C39 |
| 32 | D | 408 | LHG | C4-O6-P-O3 |
| 23 | C | 521 | LMG | C10-C11-C12-C13 |
| 23 | C | 521 | LMG | C36-C37-C38-C39 |
| 32 | D | 407 | LHG | O1-C1-C2-O2 |
| 25 | b | 621 | CLA | C15-C16-C17-C18 |
| 23 | C | 501 | LMG | C16-C17-C18-C19 |
| 23 | c | 519 | LMG | C15-C16-C17-C18 |
| 33 | H | 103 | DGD | C5A-C6A-C7A-C8A |
| 32 | D | 407 | LHG | O6-C4-C5-O7 |
| 32 | a | 720 | LHG | O6-C4-C5-O7 |
| 33 | c | 516 | DGD | O6D-C5D-C6D-O5D |
| 25 | C | 508 | CLA | C16-C17-C18-C20 |
| 32 | a | 720 | LHG | C9-C10-C11-C12 |
| 32 | L | 101 | LHG | O2-C2-C3-O3 |
| 23 | a | 701 | LMG | C18-C19-C20-C21 |
| 32 | d | 406 | LHG | C18-C19-C20-C21 |
| 23 | a | 715 | LMG | C37-C38-C39-C40 |
| 23 | A | 603 | LMG | C34-C35-C36-C37 |
| 29 | a | 714 | SQD | C16-C17-C18-C19 |
| 23 | C | 501 | LMG | O1-C7-C8-O7 |
| 23 | a | 715 | LMG | O1-C7-C8-O7 |
| 29 | B | 623 | SQD | O47-C45-C46-O48 |
| 29 | b | 601 | SQD | O6-C44-C45-O47 |
| 32 | E | 101 | LHG | O7-C5-C6-O8 |
| 33 | c | 516 | DGD | O2G-C2G-C3G-O3G |
| 25 | B | 608 | CLA | CBA-CGA-O2A-C1 |
| 23 | M | 101 | LMG | C38-C39-C40-C41 |
| 33 | C | 519 | DGD | C3B-C4B-C5B-C6B |
| 33 | c | 517 | DGD | C4B-C5B-C6B-C7B |
| 23 | a | 715 | LMG | C11-C10-O7-C8 |
| 26 | A | 608 | PHO | C16-C17-C18-C19 |
| 26 | a | 710 | PHO | C16-C17-C18-C20 |
| 23 | b | 626 | LMG | C35-C36-C37-C38 |
| 29 | A | 614 | SQD | C33-C34-C35-C36 |
| 28 | d | 405 | PL9 | C39-C41-C42-C43 |
| 29 | I | 102 | SQD | O6-C44-C45-C46 |
| 23 | C | 520 | LMG | C38-C39-C40-C41 |
| 29 | B | 623 | SQD | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 609 | CLA | C2-C1-O2A-CGA |
| 25 | B | 614 | CLA | C2-C1-O2A-CGA |
| 28 | a | 713 | PL9 | C18-C19-C21-C22 |
| 25 | B | 612 | CLA | C11-C12-C13-C14 |
| 25 | C | 512 | CLA | C11-C10-C8-C9 |
| 25 | C | 513 | CLA | C14-C13-C15-C16 |
| 25 | c | 505 | CLA | C11-C10-C8-C9 |
| 25 | c | 513 | CLA | C14-C13-C15-C16 |
| 25 | d | 402 | CLA | C6-C7-C8-C9 |
| 29 | I | 102 | SQD | C35-C36-C37-C38 |
| 32 | E | 101 | LHG | C2-C3-O3-P |
| 23 | C | 501 | LMG | C33-C34-C35-C36 |
| 25 | B | 609 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 615 | CLA | C16-C17-C18-C20 |
| 25 | a | 711 | CLA | C16-C17-C18-C20 |
| 25 | a | 719 | CLA | C16-C17-C18-C20 |
| 27 | A | 610 | BCR | C1-C6-C7-C8 |
| 27 | A | 610 | BCR | C5-C6-C7-C8 |
| 27 | B | 619 | BCR | C1-C6-C7-C8 |
| 27 | B | 619 | BCR | C5-C6-C7-C8 |
| 27 | B | 619 | BCR | C23-C24-C25-C26 |
| 27 | B | 619 | BCR | C23-C24-C25-C30 |
| 27 | C | 515 | BCR | C1-C6-C7-C8 |
| 27 | C | 516 | BCR | C1-C6-C7-C8 |
| 27 | D | 405 | BCR | C23-C24-C25-C26 |
| 27 | D | 405 | BCR | C23-C24-C25-C30 |
| 27 | H | 102 | BCR | C23-C24-C25-C26 |
| 27 | H | 102 | BCR | C23-C24-C25-C30 |
| 27 | K | 101 | BCR | C1-C6-C7-C8 |
| 27 | K | 101 | BCR | C23-C24-C25-C26 |
| 27 | a | 712 | BCR | C1-C6-C7-C8 |
| 27 | a | 712 | BCR | C5-C6-C7-C8 |
| 27 | b | 624 | BCR | C1-C6-C7-C8 |
| 27 | b | 624 | BCR | C5-C6-C7-C8 |
| 27 | b | 624 | BCR | C23-C24-C25-C26 |
| 27 | c | 514 | BCR | C5-C6-C7-C8 |
| 27 | c | 515 | BCR | C23-C24-C25-C26 |
| 27 | c | 515 | BCR | C23-C24-C25-C30 |
| 27 | d | 404 | BCR | C1-C6-C7-C8 |
| 27 | d | 404 | BCR | C5-C6-C7-C8 |
| 27 | h | 101 | BCR | C23-C24-C25-C26 |
| 27 | k | 102 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | k | 102 | BCR | C5-C6-C7-C8 |
| 27 | k | 102 | BCR | C23-C24-C25-C30 |
| 25 | C | 509 | CLA | C5-C6-C7-C8 |
| 25 | c | 513 | CLA | C15-C16-C17-C18 |
| 23 | D | 409 | LMG | C30-C31-C32-C33 |
| 25 | b | 617 | CLA | O1D-CGD-O2D-CED |
| 23 | f | 101 | LMG | C14-C15-C16-C17 |
| 32 | D | 408 | LHG | C24-C23-O8-C6 |
| 27 | Y | 101 | BCR | C7-C8-C9-C10 |
| 27 | b | 623 | BCR | C21-C22-C23-C24 |
| 27 | c | 514 | BCR | C21-C22-C23-C24 |
| 33 | c | 516 | DGD | C4D-C5D-C6D-O5D |
| 25 | B | 602 | CLA | C8-C10-C11-C12 |
| 23 | C | 501 | LMG | C12-C13-C14-C15 |
| 23 | d | 408 | LMG | C20-C21-C22-C23 |
| 25 | B | 604 | CLA | C16-C17-C18-C19 |
| 25 | B | 609 | CLA | C16-C17-C18-C20 |
| 23 | C | 521 | LMG | C39-C40-C41-C42 |
| 32 | D | 407 | LHG | C11-C10-C9-C8 |
| 33 | c | 516 | DGD | C2A-C3A-C4A-C5A |
| 25 | B | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 607 | CLA | C13-C15-C16-C17 |
| 25 | C | 504 | CLA | C8-C10-C11-C12 |
| 32 | D | 407 | LHG | O6-C4-C5-C6 |
| 25 | B | 604 | CLA | C6-C7-C8-C10 |
| 25 | B | 612 | CLA | C12-C13-C15-C16 |
| 25 | B | 615 | CLA | C11-C10-C8-C7 |
| 25 | B | 617 | CLA | C11-C12-C13-C15 |
| 25 | C | 503 | CLA | C6-C7-C8-C10 |
| 25 | C | 503 | CLA | C11-C10-C8-C7 |
| 25 | C | 507 | CLA | C11-C12-C13-C15 |
| 25 | C | 511 | CLA | C11-C10-C8-C7 |
| 25 | C | 512 | CLA | C6-C7-C8-C10 |
| 25 | C | 512 | CLA | C11-C10-C8-C7 |
| 25 | C | 513 | CLA | C12-C13-C15-C16 |
| 25 | a | 708 | CLA | C6-C7-C8-C10 |
| 25 | a | 708 | CLA | C12-C13-C15-C16 |
| 25 | b | 617 | CLA | C6-C7-C8-C10 |
| 25 | b | 617 | CLA | C11-C12-C13-C15 |
| 25 | b | 617 | CLA | C12-C13-C15-C16 |
| 25 | b | 621 | CLA | C12-C13-C15-C16 |
| 25 | c | 502 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | c | 513 | CLA | C6-C7-C8-C10 |
| 25 | c | 513 | CLA | C11-C12-C13-C15 |
| 25 | c | 513 | CLA | C12-C13-C15-C16 |
| 33 | C | 518 | DGD | C4B-C5B-C6B-C7B |
| 33 | c | 518 | DGD | C7A-C8A-C9A-CAA |
| 25 | C | 514 | CLA | C8-C10-C11-C12 |
| 23 | a | 715 | LMG | C33-C34-C35-C36 |
| 23 | B | 621 | LMG | C14-C15-C16-C17 |
| 25 | C | 510 | CLA | C5-C6-C7-C8 |
| 25 | C | 511 | CLA | C8-C10-C11-C12 |
| 23 | C | 501 | LMG | C11-C10-O7-C8 |
| 33 | C | 517 | DGD | C4D-C5D-C6D-O5D |
| 27 | C | 516 | BCR | C16-C17-C18-C36 |
| 27 | a | 712 | BCR | C16-C17-C18-C36 |
| 29 | a | 714 | SQD | C26-C27-C28-C29 |
| 25 | C | 506 | CLA | CBA-CGA-O2A-C1 |
| 32 | L | 101 | LHG | C33-C34-C35-C36 |
| 23 | B | 621 | LMG | C34-C35-C36-C37 |
| 23 | D | 409 | LMG | C18-C19-C20-C21 |
| 23 | b | 628 | LMG | C13-C14-C15-C16 |
| 25 | c | 512 | CLA | C5-C6-C7-C8 |
| 23 | a | 715 | LMG | C38-C39-C40-C41 |
| 29 | A | 612 | SQD | C14-C15-C16-C17 |
| 25 | B | 609 | CLA | CAD-CBD-CGD-O2D |
| 25 | C | 514 | CLA | CAD-CBD-CGD-O2D |
| 25 | b | 616 | CLA | CAD-CBD-CGD-O2D |
| 25 | c | 509 | CLA | CAD-CBD-CGD-O2D |
| 26 | A | 608 | PHO | CAD-CBD-CGD-O2D |
| 29 | B | 626 | SQD | C46-C45-O47-C7 |
| 25 | C | 507 | CLA | C5-C6-C7-C8 |
| 23 | B | 621 | LMG | C39-C40-C41-C42 |
| 23 | M | 101 | LMG | C40-C41-C42-C43 |
| 29 | A | 612 | SQD | C13-C14-C15-C16 |
| 23 | c | 520 | LMG | C29-C28-O8-C9 |
| 33 | C | 517 | DGD | O6D-C5D-C6D-O5D |
| 25 | B | 616 | CLA | C10-C11-C12-C13 |
| 23 | D | 409 | LMG | C22-C23-C24-C25 |
| 23 | a | 701 | LMG | O1-C7-C8-C9 |
| 23 | b | 627 | LMG | C7-C8-C9-O8 |
| 29 | B | 623 | SQD | C44-C45-C46-O48 |
| 32 | L | 101 | LHG | C4-C5-C6-O8 |
| 32 | a | 720 | LHG | C4-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 604 | CLA | O1A-CGA-O2A-C1 |
| 25 | c | 508 | CLA | C13-C15-C16-C17 |
| 23 | a | 715 | LMG | C15-C16-C17-C18 |
| 33 | C | 519 | DGD | CAA-CBA-CCA-CDA |
| 25 | B | 615 | CLA | C16-C17-C18-C19 |
| 25 | C | 509 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 610 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 610 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 613 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 504 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 509 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 509 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 618 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 618 | CLA | CHA-CBD-CGD-O2D |
| 25 | c | 502 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 506 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 508 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 508 | CLA | CHA-CBD-CGD-O2D |
| 26 | a | 710 | PHO | CHA-CBD-CGD-O1D |
| 23 | a | 715 | LMG | C36-C37-C38-C39 |
| 25 | C | 502 | CLA | O1A-CGA-O2A-C1 |
| 25 | c | 503 | CLA | O1A-CGA-O2A-C1 |
| 23 | c | 520 | LMG | O7-C8-C9-O8 |
| 32 | a | 720 | LHG | O7-C5-C6-O8 |
| 25 | b | 611 | CLA | O1A-CGA-O2A-C1 |
| 23 | D | 409 | LMG | C32-C33-C34-C35 |
| 32 | B | 625 | LHG | C24-C25-C26-C27 |
| 33 | c | 517 | DGD | CDA-CEA-CFA-CGA |
| 23 | A | 603 | LMG | O10-C28-O8-C9 |
| 28 | d | 405 | PL9 | C4-C3-C7-C8 |
| 25 | C | 503 | CLA | C11-C10-C8-C9 |
| 25 | C | 512 | CLA | C6-C7-C8-C9 |
| 25 | C | 514 | CLA | C11-C10-C8-C9 |
| 25 | b | 617 | CLA | C14-C13-C15-C16 |
| 25 | B | 608 | CLA | O1A-CGA-O2A-C1 |
| 32 | e | 101 | LHG | C25-C26-C27-C28 |
| 33 | c | 518 | DGD | C4A-C5A-C6A-C7A |
| 29 | a | 714 | SQD | C5-C6-S-O8 |
| 23 | C | 520 | LMG | C11-C12-C13-C14 |
| 23 | c | 520 | LMG | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | C | 506 | CLA | O1A-CGA-O2A-C1 |
| 23 | D | 409 | LMG | C34-C35-C36-C37 |
| 23 | f | 101 | LMG | C18-C19-C20-C21 |
| 25 | D | 403 | CLA | C1A-C2A-CAA-CBA |
| 25 | c | 501 | CLA | C1A-C2A-CAA-CBA |
| 26 | a | 709 | PHO | C1A-C2A-CAA-CBA |
| 25 | B | 609 | CLA | C16-C17-C18-C19 |
| 25 | C | 503 | CLA | C16-C17-C18-C20 |
| 25 | b | 618 | CLA | CBD-CGD-O2D-CED |
| 29 | b | 601 | SQD | C11-C10-C9-C8 |
| 32 | E | 101 | LHG | C3-O3-P-O6 |
| 25 | B | 611 | CLA | C5-C6-C7-C8 |
| 25 | c | 513 | CLA | C3-C5-C6-C7 |
| 25 | B | 606 | CLA | C2-C3-C5-C6 |
| 33 | h | 102 | DGD | O1A-C1A-O1G-C1G |
| 32 | B | 625 | LHG | C3-O3-P-O5 |
| 32 | D | 407 | LHG | C3-O3-P-O4 |
| 32 | D | 407 | LHG | C4-O6-P-O5 |
| 32 | E | 101 | LHG | C4-O6-P-O4 |
| 32 | a | 720 | LHG | C3-O3-P-O5 |
| 32 | d | 406 | LHG | C3-O3-P-O5 |
| 32 | d | 407 | LHG | C4-O6-P-O5 |
| 25 | C | 510 | CLA | C16-C17-C18-C20 |
| 25 | a | 711 | CLA | C16-C17-C18-C19 |
| 25 | a | 719 | CLA | C16-C17-C18-C19 |
| 25 | b | 609 | CLA | C16-C17-C18-C19 |
| 25 | c | 513 | CLA | C16-C17-C18-C20 |
| 29 | A | 612 | SQD | O5-C1-O6-C44 |
| 25 | B | 606 | CLA | C10-C11-C12-C13 |
| 23 | M | 101 | LMG | C20-C21-C22-C23 |
| 29 | b | 601 | SQD | C26-C27-C28-C29 |
| 25 | b | 609 | CLA | C2A-CAA-CBA-CGA |
| 32 | D | 408 | LHG | C10-C11-C12-C13 |
| 25 | B | 604 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 606 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 610 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 613 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 615 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 607 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 610 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 613 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 618 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | A | 612 | SQD | C5-C6-S-O7 |
| 25 | B | 613 | CLA | C10-C11-C12-C13 |
| 23 | a | 701 | LMG | C20-C21-C22-C23 |
| 32 | L | 101 | LHG | C1-C2-C3-O3 |
| 32 | L | 101 | LHG | C17-C18-C19-C20 |
| 25 | B | 610 | CLA | C16-C17-C18-C20 |
| 25 | B | 615 | CLA | C6-C7-C8-C10 |
| 25 | B | 616 | CLA | C11-C10-C8-C7 |
| 25 | C | 510 | CLA | C11-C12-C13-C15 |
| 25 | C | 514 | CLA | C11-C10-C8-C7 |
| 25 | b | 607 | CLA | C11-C12-C13-C15 |
| 25 | b | 609 | CLA | C11-C10-C8-C7 |
| 25 | b | 610 | CLA | C11-C10-C8-C7 |
| 25 | b | 619 | CLA | C6-C7-C8-C10 |
| 25 | c | 502 | CLA | C6-C7-C8-C10 |
| 25 | c | 509 | CLA | C11-C10-C8-C7 |
| 26 | A | 608 | PHO | C6-C7-C8-C10 |
| 32 | d | 407 | LHG | O6-C4-C5-O7 |
| 33 | c | 517 | DGD | C6A-C7A-C8A-C9A |
| 33 | c | 518 | DGD | C6A-C7A-C8A-C9A |
| 23 | M | 101 | LMG | C34-C35-C36-C37 |
| 23 | M | 101 | LMG | C32-C33-C34-C35 |
| 23 | a | 701 | LMG | C37-C38-C39-C40 |
| 25 | D | 404 | CLA | C16-C17-C18-C20 |
| 23 | C | 501 | LMG | O1-C7-C8-C9 |
| 23 | a | 715 | LMG | O1-C7-C8-C9 |
| 29 | D | 410 | SQD | C2-C1-O6-C44 |
| 29 | b | 601 | SQD | O6-C44-C45-C46 |
| 32 | d | 406 | LHG | C17-C18-C19-C20 |
| 23 | C | 520 | LMG | O1-C7-C8-O7 |
| 23 | a | 701 | LMG | O1-C7-C8-O7 |
| 29 | A | 614 | SQD | O47-C45-C46-O48 |
| 29 | B | 623 | SQD | O6-C44-C45-O47 |
| 29 | D | 410 | SQD | O47-C45-C46-O48 |
| 32 | L | 101 | LHG | O7-C5-C6-O8 |
| 32 | e | 101 | LHG | O7-C5-C6-O8 |
| 33 | C | 517 | DGD | O2G-C2G-C3G-O3G |
| 29 | B | 623 | SQD | C25-C26-C27-C28 |
| 23 | a | 701 | LMG | C39-C40-C41-C42 |
| 32 | D | 408 | LHG | C13-C14-C15-C16 |
| 32 | d | 406 | LHG | C27-C28-C29-C30 |
| 29 | D | 410 | SQD | O10-C23-O48-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | a | 701 | LMG | C8-C7-O1-C1 |
| 26 | a | 710 | PHO | C16-C17-C18-C19 |
| 23 | d | 408 | LMG | C37-C38-C39-C40 |
| 25 | C | 506 | CLA | O1D-CGD-O2D-CED |
| 23 | f | 101 | LMG | C30-C31-C32-C33 |
| 25 | a | 711 | CLA | C10-C11-C12-C13 |
| 25 | c | 510 | CLA | C4-C3-C5-C6 |
| 25 | C | 512 | CLA | CBA-CGA-O2A-C1 |
| 23 | c | 519 | LMG | C37-C38-C39-C40 |
| 33 | c | 517 | DGD | C3A-C4A-C5A-C6A |
| 28 | D | 406 | PL9 | C13-C14-C16-C17 |
| 33 | H | 103 | DGD | O2G-C1B-C2B-C3B |
| 25 | B | 605 | CLA | C10-C11-C12-C13 |
| 25 | B | 609 | CLA | C11-C12-C13-C14 |
| 25 | C | 511 | CLA | C11-C10-C8-C9 |
| 25 | a | 708 | CLA | C14-C13-C15-C16 |
| 25 | b | 612 | CLA | C14-C13-C15-C16 |
| 25 | b | 617 | CLA | C11-C10-C8-C9 |
| 25 | b | 618 | CLA | C6-C7-C8-C9 |
| 25 | c | 501 | CLA | C11-C12-C13-C14 |
| 25 | c | 502 | CLA | C11-C10-C8-C9 |
| 26 | A | 608 | PHO | C6-C7-C8-C9 |
| 23 | C | 521 | LMG | O10-C28-O8-C9 |
| 23 | C | 520 | LMG | C37-C38-C39-C40 |
| 23 | c | 520 | LMG | C15-C16-C17-C18 |
| 29 | b | 601 | SQD | C18-C19-C20-C21 |
| 33 | C | 518 | DGD | C1B-C2B-C3B-C4B |
| 33 | h | 102 | DGD | C4D-C5D-C6D-O5D |
| 29 | f | 102 | SQD | C8-C7-O47-C45 |
| 23 | B | 621 | LMG | C32-C33-C34-C35 |
| 23 | C | 520 | LMG | C22-C23-C24-C25 |
| 23 | c | 519 | LMG | C38-C39-C40-C41 |
| 33 | C | 518 | DGD | CDA-CEA-CFA-CGA |
| 25 | C | 504 | CLA | C2-C3-C5-C6 |
| 23 | a | 701 | LMG | C15-C16-C17-C18 |
| 33 | C | 519 | DGD | O6E-C5E-C6E-O5E |
| 25 | C | 512 | CLA | O1A-CGA-O2A-C1 |
| 32 | E | 101 | LHG | C30-C31-C32-C33 |
| 25 | C | 506 | CLA | C2A-CAA-CBA-CGA |
| 25 | D | 402 | CLA | C15-C16-C17-C18 |
| 25 | D | 403 | CLA | C2-C1-O2A-CGA |
| 25 | a | 707 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | b | 619 | CLA | C2-C1-O2A-CGA |
| 33 | c | 516 | DGD | C7B-C8B-C9B-CAB |
| 25 | D | 403 | CLA | C3-C5-C6-C7 |
| 23 | c | 520 | LMG | C31-C32-C33-C34 |
| 32 | D | 408 | LHG | C34-C35-C36-C37 |
| 32 | d | 406 | LHG | C15-C16-C17-C18 |
| 23 | C | 501 | LMG | C29-C28-O8-C9 |
| 32 | e | 101 | LHG | O6-C4-C5-O7 |
| 23 | c | 520 | LMG | C40-C41-C42-C43 |
| 25 | b | 618 | CLA | O1D-CGD-O2D-CED |
| 27 | A | 610 | BCR | C23-C24-C25-C26 |
| 27 | A | 610 | BCR | C23-C24-C25-C30 |
| 27 | C | 515 | BCR | C5-C6-C7-C8 |
| 27 | C | 516 | BCR | C5-C6-C7-C8 |
| 27 | C | 516 | BCR | C23-C24-C25-C30 |
| 27 | K | 101 | BCR | C5-C6-C7-C8 |
| 27 | K | 101 | BCR | C23-C24-C25-C30 |
| 27 | a | 712 | BCR | C23-C24-C25-C30 |
| 27 | b | 624 | BCR | C23-C24-C25-C30 |
| 27 | h | 101 | BCR | C23-C24-C25-C30 |
| 27 | k | 102 | BCR | C23-C24-C25-C26 |
| 32 | E | 101 | LHG | O9-C7-O7-C5 |
| 25 | C | 508 | CLA | C13-C15-C16-C17 |
| 29 | b | 601 | SQD | C2-C1-O6-C44 |
| 33 | C | 519 | DGD | C2D-C1D-O3G-C3G |
| 32 | L | 101 | LHG | C4-O6-P-O3 |
| 32 | d | 407 | LHG | C3-O3-P-O6 |
| 33 | C | 517 | DGD | C7A-C8A-C9A-CAA |
| 33 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 23 | c | 519 | LMG | O1-C7-C8-C9 |
| 33 | C | 517 | DGD | C1G-C2G-C3G-O3G |
| 23 | C | 520 | LMG | C20-C21-C22-C23 |
| 23 | D | 409 | LMG | C39-C40-C41-C42 |
| 32 | D | 407 | LHG | C12-C13-C14-C15 |
| 32 | d | 406 | LHG | C12-C13-C14-C15 |
| 25 | C | 502 | CLA | C12-C13-C15-C16 |
| 25 | C | 510 | CLA | C6-C7-C8-C10 |
| 25 | b | 617 | CLA | C11-C10-C8-C7 |
| 25 | b | 618 | CLA | C6-C7-C8-C10 |
| 25 | c | 512 | CLA | C12-C13-C15-C16 |
| 25 | A | 607 | CLA | C14-C13-C15-C16 |
| 25 | B | 602 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 606 | CLA | C6-C7-C8-C9 |
| 25 | B | 616 | CLA | C11-C10-C8-C9 |
| 25 | B | 617 | CLA | C11-C12-C13-C14 |
| 25 | b | 609 | CLA | C11-C10-C8-C9 |
| 25 | b | 619 | CLA | C6-C7-C8-C9 |
| 25 | c | 501 | CLA | C11-C10-C8-C9 |
| 25 | c | 508 | CLA | C11-C12-C13-C14 |
| 25 | d | 402 | CLA | C14-C13-C15-C16 |
| 27 | d | 404 | BCR | C19-C20-C21-C22 |
| 25 | B | 608 | CLA | C16-C17-C18-C20 |
| 23 | a | 701 | LMG | C34-C35-C36-C37 |
| 33 | h | 102 | DGD | CCB-CDB-CEB-CFB |
| 25 | B | 613 | CLA | C13-C15-C16-C17 |
| 25 | C | 510 | CLA | C16-C17-C18-C19 |
| 25 | c | 513 | CLA | C16-C17-C18-C19 |
| 23 | d | 408 | LMG | C36-C37-C38-C39 |
| 32 | d | 406 | LHG | O1-C1-C2-C3 |
| 32 | d | 407 | LHG | C25-C26-C27-C28 |
| 29 | f | 102 | SQD | O10-C23-O48-C46 |
| 27 | b | 625 | BCR | C21-C22-C23-C24 |
| 33 | C | 517 | DGD | C7B-C8B-C9B-CAB |
| 25 | B | 606 | CLA | C5-C6-C7-C8 |
| 25 | C | 511 | CLA | C4-C3-C5-C6 |
| 28 | d | 405 | PL9 | C13-C14-C16-C17 |
| 28 | d | 405 | PL9 | C28-C29-C31-C32 |
| 25 | B | 610 | CLA | C16-C17-C18-C19 |
| 23 | b | 628 | LMG | C10-C11-C12-C13 |
| 32 | B | 625 | LHG | C25-C26-C27-C28 |
| 33 | h | 102 | DGD | C5A-C6A-C7A-C8A |
| 23 | b | 626 | LMG | O8-C28-C29-C30 |
| 25 | B | 606 | CLA | C13-C15-C16-C17 |
| 25 | B | 617 | CLA | C5-C6-C7-C8 |
| 33 | C | 517 | DGD | O1A-C1A-O1G-C1G |
| 25 | C | 502 | CLA | C2A-CAA-CBA-CGA |
| 25 | D | 404 | CLA | C16-C17-C18-C19 |
| 23 | b | 627 | LMG | O6-C1-O1-C7 |
| 29 | a | 714 | SQD | O5-C1-O6-C44 |
| 33 | c | 517 | DGD | CBA-CCA-CDA-CEA |
| 27 | B | 618 | BCR | C10-C11-C12-C13 |
| 27 | b | 624 | BCR | C10-C11-C12-C13 |
| 27 | k | 101 | BCR | C10-C11-C12-C13 |
| 27 | t | 103 | BCR | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | A | 607 | CLA | C3-C5-C6-C7 |
| 29 | A | 614 | SQD | C34-C35-C36-C37 |
| 28 | D | 406 | PL9 | C45-C44-C46-C47 |
| 25 | C | 505 | CLA | C15-C16-C17-C18 |
| 25 | C | 511 | CLA | C2-C3-C5-C6 |
| 28 | a | 713 | PL9 | C13-C14-C16-C17 |
| 25 | B | 613 | CLA | C15-C16-C17-C18 |
| 33 | c | 517 | DGD | C8B-C9B-CAB-CBB |
| 25 | C | 504 | CLA | C2-C1-O2A-CGA |
| 33 | C | 518 | DGD | CBB-CCB-CDB-CEB |
| 33 | C | 518 | DGD | C7B-C8B-C9B-CAB |
| 23 | b | 627 | LMG | O7-C8-C9-O8 |
| 23 | c | 519 | LMG | O1-C7-C8-O7 |
| 25 | B | 615 | CLA | C2A-CAA-CBA-CGA |
| 25 | a | 707 | CLA | C2A-CAA-CBA-CGA |
| 33 | c | 517 | DGD | C1B-C2B-C3B-C4B |
| 25 | b | 611 | CLA | C15-C16-C17-C18 |
| 26 | D | 401 | PHO | C16-C17-C18-C20 |
| 23 | d | 408 | LMG | C29-C30-C31-C32 |
| 23 | f | 101 | LMG | C39-C40-C41-C42 |
| 25 | C | 513 | CLA | C4-C3-C5-C6 |
| 29 | A | 614 | SQD | C11-C12-C13-C14 |
| 25 | c | 510 | CLA | C2-C3-C5-C6 |
| 28 | a | 713 | PL9 | C4-C3-C7-C8 |
| 23 | d | 408 | LMG | C14-C15-C16-C17 |
| 32 | d | 407 | LHG | C32-C33-C34-C35 |
| 25 | B | 611 | CLA | C11-C12-C13-C14 |
| 25 | B | 611 | CLA | C14-C13-C15-C16 |
| 25 | b | 609 | CLA | C14-C13-C15-C16 |
| 25 | b | 613 | CLA | C11-C12-C13-C14 |
| 25 | b | 615 | CLA | C11-C10-C8-C9 |
| 25 | c | 507 | CLA | C6-C7-C8-C9 |
| 25 | c | 509 | CLA | C11-C12-C13-C14 |
| 25 | c | 512 | CLA | C11-C12-C13-C14 |
| 23 | c | 519 | LMG | C7-C8-C9-O8 |
| 33 | H | 103 | DGD | O1A-C1A-O1G-C1G |
| 23 | c | 519 | LMG | C4-C5-C6-O5 |
| 25 | a | 708 | CLA | C16-C17-C18-C19 |
| 25 | b | 615 | CLA | CBA-CGA-O2A-C1 |
| 33 | c | 516 | DGD | O6D-C1D-O3G-C3G |
| 33 | c | 518 | DGD | O6D-C1D-O3G-C3G |
| 33 | C | 519 | DGD | CCB-CDB-CEB-CFB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | C | 516 | BCR | C7-C8-C9-C34 |
| 33 | c | 516 | DGD | CAA-CBA-CCA-CDA |
| 27 | B | 620 | BCR | C7-C8-C9-C10 |
| 23 | d | 408 | LMG | C16-C17-C18-C19 |
| 32 | a | 720 | LHG | C35-C36-C37-C38 |
| 33 | C | 518 | DGD | C6B-C7B-C8B-C9B |
| 25 | D | 404 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 608 | CLA | C12-C13-C15-C16 |
| 25 | D | 403 | CLA | C6-C7-C8-C10 |
| 25 | D | 403 | CLA | C11-C12-C13-C15 |
| 25 | c | 506 | CLA | C12-C13-C15-C16 |
| 23 | B | 621 | LMG | C19-C20-C21-C22 |
| 23 | b | 627 | LMG | C40-C41-C42-C43 |
| 32 | E | 101 | LHG | C10-C11-C12-C13 |
| 33 | c | 518 | DGD | O6E-C5E-C6E-O5E |
| 29 | B | 626 | SQD | C10-C11-C12-C13 |
| 25 | C | 502 | CLA | C15-C16-C17-C18 |
| 25 | B | 602 | CLA | C16-C17-C18-C20 |
| 23 | f | 101 | LMG | C20-C21-C22-C23 |
| 32 | d | 406 | LHG | C33-C34-C35-C36 |
| 32 | d | 407 | LHG | C26-C27-C28-C29 |
| 25 | B | 615 | CLA | C13-C15-C16-C17 |
| 23 | a | 715 | LMG | C22-C23-C24-C25 |
| 25 | B | 610 | CLA | C8-C10-C11-C12 |
| 23 | b | 626 | LMG | C20-C21-C22-C23 |
| 23 | d | 408 | LMG | C15-C16-C17-C18 |
| 25 | C | 513 | CLA | C5-C6-C7-C8 |
| 25 | b | 609 | CLA | C10-C11-C12-C13 |
| 32 | D | 408 | LHG | C27-C28-C29-C30 |
| 23 | A | 603 | LMG | C37-C38-C39-C40 |
| 25 | C | 510 | CLA | C3-C5-C6-C7 |
| 29 | f | 102 | SQD | O47-C45-C46-O48 |
| 23 | b | 627 | LMG | C16-C17-C18-C19 |
| 25 | B | 617 | CLA | C13-C15-C16-C17 |
| 23 | b | 626 | LMG | C18-C19-C20-C21 |
| 32 | E | 101 | LHG | C26-C27-C28-C29 |
| 25 | b | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | D | 404 | CLA | C6-C7-C8-C9 |
| 25 | c | 502 | CLA | O1A-CGA-O2A-C1 |
| 33 | c | 518 | DGD | C5B-C6B-C7B-C8B |
| 23 | A | 603 | LMG | C13-C14-C15-C16 |
| 32 | D | 408 | LHG | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | B | 618 | BCR | C23-C24-C25-C30 |
| 27 | C | 515 | BCR | C23-C24-C25-C26 |
| 27 | C | 515 | BCR | C23-C24-C25-C30 |
| 27 | C | 516 | BCR | C23-C24-C25-C26 |
| 27 | H | 102 | BCR | C1-C6-C7-C8 |
| 27 | Y | 101 | BCR | C23-C24-C25-C30 |
| 27 | a | 712 | BCR | C23-C24-C25-C26 |
| 27 | h | 101 | BCR | C1-C6-C7-C8 |
| 27 | k | 101 | BCR | C23-C24-C25-C30 |
| 29 | D | 410 | SQD | C31-C32-C33-C34 |
| 32 | L | 101 | LHG | C28-C29-C30-C31 |
| 33 | h | 102 | DGD | C6A-C7A-C8A-C9A |
| 25 | B | 612 | CLA | C8-C10-C11-C12 |
| 25 | B | 617 | CLA | C8-C10-C11-C12 |
| 25 | c | 506 | CLA | C13-C15-C16-C17 |
| 23 | D | 409 | LMG | C8-C7-O1-C1 |
| 29 | B | 626 | SQD | C26-C27-C28-C29 |
| 29 | D | 410 | SQD | C27-C28-C29-C30 |
| 33 | C | 517 | DGD | C8A-C9A-CAA-CBA |
| 25 | c | 502 | CLA | CBA-CGA-O2A-C1 |
| 23 | d | 408 | LMG | O7-C10-C11-C12 |
| 25 | B | 603 | CLA | C16-C17-C18-C20 |
| 25 | b | 608 | CLA | O1D-CGD-O2D-CED |
| 29 | A | 612 | SQD | C34-C35-C36-C37 |
| 29 | B | 626 | SQD | C12-C13-C14-C15 |
| 25 | B | 607 | CLA | CBA-CGA-O2A-C1 |
| 33 | c | 517 | DGD | CDB-CEB-CFB-CGB |
| 25 | B | 607 | CLA | O1A-CGA-O2A-C1 |
| 23 | d | 408 | LMG | O9-C10-C11-C12 |
| 29 | D | 410 | SQD | O5-C1-O6-C44 |
| 25 | C | 503 | CLA | C4-C3-C5-C6 |
| 25 | C | 505 | CLA | C4-C3-C5-C6 |
| 25 | b | 608 | CLA | C4-C3-C5-C6 |
| 25 | d | 402 | CLA | C4-C3-C5-C6 |
| 25 | B | 610 | CLA | C11-C12-C13-C15 |
| 25 | b | 612 | CLA | C12-C13-C15-C16 |
| 25 | b | 615 | CLA | C6-C7-C8-C10 |
| 25 | c | 501 | CLA | C11-C10-C8-C7 |
| 25 | c | 508 | CLA | C11-C12-C13-C15 |
| 25 | c | 510 | CLA | C12-C13-C15-C16 |
| 33 | c | 517 | DGD | C4A-C5A-C6A-C7A |
| 25 | a | 719 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | b | 619 | CLA | CAA-CBA-CGA-O2A |
| 33 | h | 102 | DGD | O2G-C1B-C2B-C3B |
| 29 | B | 626 | SQD | C19-C20-C21-C22 |
| 29 | B | 626 | SQD | O47-C45-C46-O48 |
| 33 | C | 519 | DGD | O1A-C1A-O1G-C1G |
| 29 | I | 102 | SQD | C33-C34-C35-C36 |
| 33 | c | 516 | DGD | C6A-C7A-C8A-C9A |
| 23 | c | 520 | LMG | C16-C17-C18-C19 |
| 23 | B | 621 | LMG | C29-C28-O8-C9 |
| 27 | b | 625 | BCR | C20-C21-C22-C37 |
| 27 | c | 514 | BCR | C20-C21-C22-C37 |
| 25 | b | 618 | CLA | CAA-CBA-CGA-O2A |
| 28 | A | 611 | PL9 | C40-C39-C41-C42 |
| 28 | d | 405 | PL9 | C35-C34-C36-C37 |
| 25 | c | 502 | CLA | C8-C10-C11-C12 |
| 25 | B | 615 | CLA | C6-C7-C8-C9 |
| 25 | C | 510 | CLA | C6-C7-C8-C9 |
| 25 | D | 403 | CLA | C11-C12-C13-C14 |
| 25 | b | 607 | CLA | C6-C7-C8-C9 |
| 25 | b | 610 | CLA | C11-C10-C8-C9 |
| 29 | b | 601 | SQD | C31-C32-C33-C34 |
| 33 | c | 517 | DGD | CBB-CCB-CDB-CEB |
| 25 | c | 506 | CLA | C3A-C2A-CAA-CBA |
| 26 | a | 709 | PHO | C3A-C2A-CAA-CBA |
| 29 | b | 601 | SQD | O48-C23-C24-C25 |
| 25 | B | 611 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 614 | CLA | CAD-CBD-CGD-O2D |
| 25 | C | 504 | CLA | CAD-CBD-CGD-O2D |
| 25 | C | 507 | CLA | CAD-CBD-CGD-O2D |
| 25 | C | 513 | CLA | CAD-CBD-CGD-O2D |
| 25 | b | 611 | CLA | CAD-CBD-CGD-O2D |
| 25 | b | 615 | CLA | CAD-CBD-CGD-O2D |
| 25 | c | 503 | CLA | CAD-CBD-CGD-O2D |
| 25 | c | 504 | CLA | CAD-CBD-CGD-O2D |
| 25 | c | 506 | CLA | CAD-CBD-CGD-O2D |
| 25 | d | 403 | CLA | CAD-CBD-CGD-O2D |
| 23 | d | 408 | LMG | C29-C28-O8-C9 |
| 25 | B | 602 | CLA | C16-C17-C18-C19 |
| 23 | A | 603 | LMG | C11-C12-C13-C14 |
| 25 | c | 503 | CLA | C8-C10-C11-C12 |
| 25 | d | 402 | CLA | C2-C1-O2A-CGA |
| 23 | A | 603 | LMG | O7-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 29 | A | 614 | SQD | C10-C11-C12-C13 |
| 28 | D | 406 | PL9 | C43-C44-C46-C47 |
| 23 | C | 501 | LMG | O8-C28-C29-C30 |
| 25 | B | 614 | CLA | CAA-CBA-CGA-O2A |
| 29 | I | 102 | SQD | C12-C13-C14-C15 |
| 23 | M | 101 | LMG | C33-C34-C35-C36 |
| 32 | B | 625 | LHG | C9-C10-C11-C12 |
| 29 | D | 410 | SQD | C29-C30-C31-C32 |
| 29 | a | 714 | SQD | C30-C31-C32-C33 |
| 23 | A | 603 | LMG | O8-C28-C29-C30 |
| 29 | D | 410 | SQD | C7-C8-C9-C10 |
| 29 | B | 623 | SQD | C11-C12-C13-C14 |
| 25 | A | 606 | CLA | O2A-C1-C2-C3 |
| 25 | C | 514 | CLA | O2A-C1-C2-C3 |
| 25 | c | 512 | CLA | O2A-C1-C2-C3 |
| 23 | A | 603 | LMG | C22-C23-C24-C25 |
| 25 | B | 613 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 617 | CLA | CHA-CBD-CGD-O2D |
| 25 | C | 505 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 508 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 508 | CLA | CHA-CBD-CGD-O2D |
| 25 | C | 510 | CLA | CHA-CBD-CGD-O1D |
| 25 | C | 510 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | b | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | b | 609 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 502 | CLA | CHA-CBD-CGD-O2D |
| 25 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 511 | CLA | CHA-CBD-CGD-O1D |
| 25 | c | 511 | CLA | CHA-CBD-CGD-O2D |
| 25 | c | 512 | CLA | CHA-CBD-CGD-O1D |
| 26 | D | 401 | PHO | CHA-CBD-CGD-O1D |
| 26 | D | 401 | PHO | CHA-CBD-CGD-O2D |
| 26 | a | 709 | PHO | CHA-CBD-CGD-O2D |
| 25 | D | 402 | CLA | C4C-C3C-CAC-CBC |
| 23 | C | 520 | LMG | C10-C11-C12-C13 |
| 33 | C | 517 | DGD | O1G-C1A-C2A-C3A |
| 23 | D | 409 | LMG | C37-C38-C39-C40 |
| 23 | c | 519 | LMG | O7-C8-C9-O8 |
| 32 | d | 407 | LHG | C10-C11-C12-C13 |
| 25 | B | 617 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | a | 701 | LMG | C40-C41-C42-C43 |
| 29 | A | 612 | SQD | C33-C34-C35-C36 |
| 32 | B | 625 | LHG | C29-C30-C31-C32 |
| 25 | B | 610 | CLA | C13-C15-C16-C17 |
| 25 | C | 511 | CLA | CAA-CBA-CGA-O2A |
| 29 | a | 714 | SQD | O47-C7-C8-C9 |
| 25 | D | 403 | CLA | CAA-CBA-CGA-O2A |
| 32 | L | 101 | LHG | O7-C7-C8-C9 |
| 25 | d | 402 | CLA | C11-C10-C8-C7 |
| 28 | A | 611 | PL9 | C4-C3-C7-C8 |
| 25 | D | 402 | CLA | C2C-C3C-CAC-CBC |
| 25 | b | 607 | CLA | C11-C12-C13-C14 |
| 25 | b | 609 | CLA | C11-C12-C13-C14 |
| 32 | B | 625 | LHG | C28-C29-C30-C31 |
| 26 | a | 710 | PHO | C8-C10-C11-C12 |
| 25 | a | 708 | CLA | C16-C17-C18-C20 |
| 23 | c | 519 | LMG | O10-C28-O8-C9 |
| 25 | C | 508 | CLA | C2A-CAA-CBA-CGA |
| 29 | B | 623 | SQD | O49-C7-C8-C9 |
| 33 | c | 516 | DGD | CBA-CCA-CDA-CEA |
| 25 | C | 503 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 614 | CLA | CAA-CBA-CGA-O1A |
| 27 | d | 404 | BCR | C7-C8-C9-C10 |
| 25 | C | 503 | CLA | CBA-CGA-O2A-C1 |
| 25 | b | 618 | CLA | CBA-CGA-O2A-C1 |
| 23 | b | 626 | LMG | C38-C39-C40-C41 |
| 33 | C | 517 | DGD | C2B-C3B-C4B-C5B |
| 25 | B | 609 | CLA | C1A-C2A-CAA-CBA |
| 25 | C | 503 | CLA | C1A-C2A-CAA-CBA |
| 25 | c | 506 | CLA | C1A-C2A-CAA-CBA |
| 26 | A | 608 | PHO | C1A-C2A-CAA-CBA |
| 29 | A | 614 | SQD | C25-C26-C27-C28 |
| 29 | a | 714 | SQD | O49-C7-C8-C9 |
| 32 | D | 408 | LHG | O10-C23-C24-C25 |
| 33 | C | 518 | DGD | O1B-C1B-C2B-C3B |
| 25 | b | 613 | CLA | C10-C11-C12-C13 |
| 28 | d | 405 | PL9 | C11-C12-C13-C14 |
| 25 | b | 621 | CLA | C13-C15-C16-C17 |
| 23 | A | 603 | LMG | O10-C28-C29-C30 |
| 25 | b | 618 | CLA | CAA-CBA-CGA-O1A |
| 25 | b | 619 | CLA | CAA-CBA-CGA-O1A |
| 32 | e | 101 | LHG | O10-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | c | 518 | DGD | C8A-C9A-CAA-CBA |
| 25 | b | 616 | CLA | C2A-CAA-CBA-CGA |
| 29 | b | 601 | SQD | C29-C30-C31-C32 |
| 23 | A | 603 | LMG | O9-C10-C11-C12 |
| 23 | M | 101 | LMG | O10-C28-C29-C30 |
| 29 | I | 102 | SQD | C28-C29-C30-C31 |
| 32 | D | 408 | LHG | C2-C3-O3-P |
| 25 | C | 511 | CLA | CAA-CBA-CGA-O1A |
| 29 | A | 612 | SQD | O49-C7-C8-C9 |
| 32 | D | 408 | LHG | C4-O6-P-O5 |
| 32 | E | 101 | LHG | C4-O6-P-O5 |
| 32 | L | 101 | LHG | C4-O6-P-O5 |
| 32 | d | 407 | LHG | C3-O3-P-O5 |
| 32 | a | 720 | LHG | O6-C4-C5-C6 |
| 29 | B | 626 | SQD | C35-C36-C37-C38 |
| 27 | H | 102 | BCR | C5-C6-C7-C8 |
| 27 | Y | 101 | BCR | C23-C24-C25-C26 |
| 27 | k | 101 | BCR | C23-C24-C25-C26 |
| 32 | L | 101 | LHG | O9-C7-C8-C9 |
| 32 | B | 625 | LHG | O8-C23-C24-C25 |
| 27 | c | 514 | BCR | C18-C19-C20-C21 |
| 25 | c | 510 | CLA | CAA-CBA-CGA-O1A |
| 25 | b | 609 | CLA | C5-C6-C7-C8 |
| 25 | b | 621 | CLA | C8-C10-C11-C12 |
| 32 | B | 625 | LHG | C17-C18-C19-C20 |
| 33 | c | 518 | DGD | O1G-C1A-C2A-C3A |
| 25 | C | 507 | CLA | C15-C16-C17-C18 |
| 32 | e | 101 | LHG | C11-C12-C13-C14 |
| 33 | c | 517 | DGD | C1A-C2A-C3A-C4A |
| 28 | a | 713 | PL9 | C21-C22-C23-C24 |
| 23 | a | 701 | LMG | C22-C23-C24-C25 |
| 25 | B | 605 | CLA | C2C-C3C-CAC-CBC |
| 25 | C | 505 | CLA | CAD-CBD-CGD-O1D |
| 25 | D | 404 | CLA | CAD-CBD-CGD-O1D |
| 25 | b | 609 | CLA | CAD-CBD-CGD-O1D |
| 25 | c | 502 | CLA | CAD-CBD-CGD-O1D |
| 25 | c | 510 | CLA | CAD-CBD-CGD-O1D |
| 25 | c | 511 | CLA | CAD-CBD-CGD-O1D |
| 29 | a | 714 | SQD | O5-C5-C6-S |
| 29 | b | 601 | SQD | O5-C5-C6-S |
| 25 | b | 618 | CLA | O1A-CGA-O2A-C1 |
| 32 | B | 625 | LHG | O10-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | B | 608 | CLA | C14-C13-C15-C16 |
| 25 | B | 613 | CLA | C11-C10-C8-C9 |
| 25 | a | 719 | CLA | C11-C10-C8-C9 |
| 25 | b | 615 | CLA | C6-C7-C8-C9 |
| 23 | C | 520 | LMG | C14-C15-C16-C17 |
| 25 | c | 505 | CLA | CAA-CBA-CGA-O2A |
| 29 | A | 612 | SQD | O47-C7-C8-C9 |
| 33 | H | 103 | DGD | C6A-C7A-C8A-C9A |
| 25 | b | 608 | CLA | CBD-CGD-O2D-CED |
| 23 | A | 603 | LMG | C33-C34-C35-C36 |
| 32 | B | 625 | LHG | C33-C34-C35-C36 |
| 25 | C | 502 | CLA | CAA-CBA-CGA-O2A |
| 32 | D | 408 | LHG | O8-C23-C24-C25 |
| 33 | C | 518 | DGD | C5A-C6A-C7A-C8A |
| 28 | d | 405 | PL9 | C30-C29-C31-C32 |
| 25 | B | 602 | CLA | C11-C10-C8-C7 |
| 25 | B | 606 | CLA | C11-C12-C13-C15 |
| 25 | B | 613 | CLA | C11-C10-C8-C7 |
| 25 | C | 513 | CLA | C2-C3-C5-C6 |
| 25 | D | 404 | CLA | C6-C7-C8-C10 |
| 25 | a | 719 | CLA | C11-C10-C8-C7 |
| 25 | b | 616 | CLA | C12-C13-C15-C16 |
| 25 | c | 513 | CLA | C11-C10-C8-C7 |
| 28 | a | 713 | PL9 | C33-C34-C36-C37 |
| 29 | A | 612 | SQD | C7-C8-C9-C10 |
| 25 | D | 403 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | c | 501 | CLA | C15-C16-C17-C18 |
| 27 | c | 515 | BCR | C7-C8-C9-C10 |
| 27 | H | 102 | BCR | C9-C10-C11-C12 |
| 33 | C | 518 | DGD | O2G-C1B-C2B-C3B |
| 25 | d | 402 | CLA | C2C-C3C-CAC-CBC |
| 25 | B | 607 | CLA | C15-C16-C17-C18 |
| 25 | D | 402 | CLA | C13-C15-C16-C17 |
| 23 | c | 519 | LMG | O9-C10-C11-C12 |
| 32 | E | 101 | LHG | C17-C18-C19-C20 |
| 32 | E | 101 | LHG | C29-C30-C31-C32 |
| 25 | B | 603 | CLA | C13-C15-C16-C17 |
| 25 | B | 609 | CLA | C13-C15-C16-C17 |
| 25 | b | 607 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 602 | CLA | C2A-CAA-CBA-CGA |
| 25 | c | 510 | CLA | C2A-CAA-CBA-CGA |

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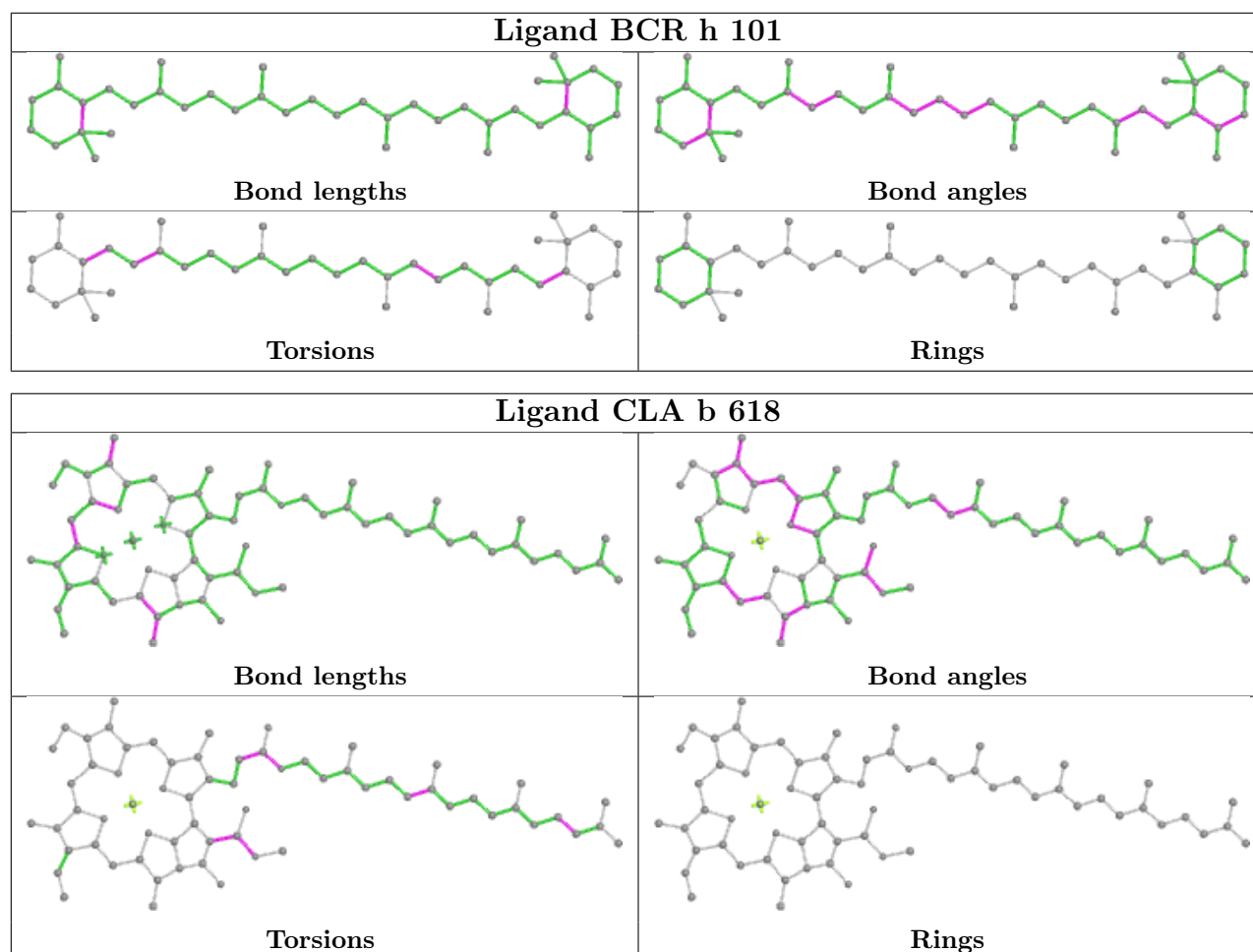
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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | C | 513 | CLA | CAA-CBA-CGA-O2A |

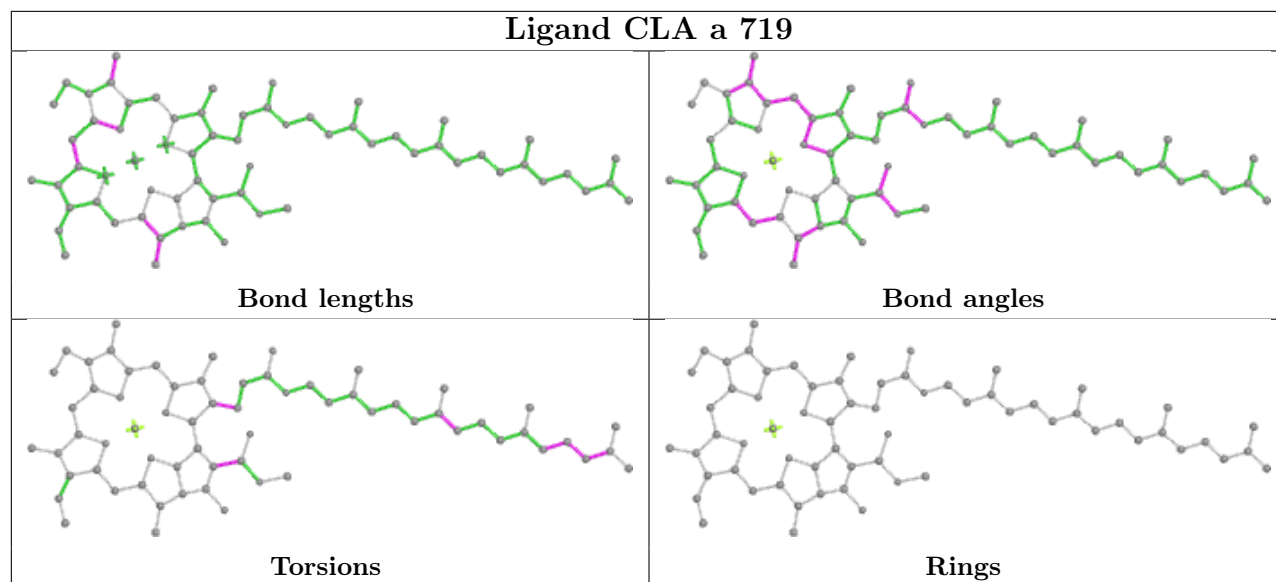
There are no ring outliers.

No monomer is involved in short contacts.

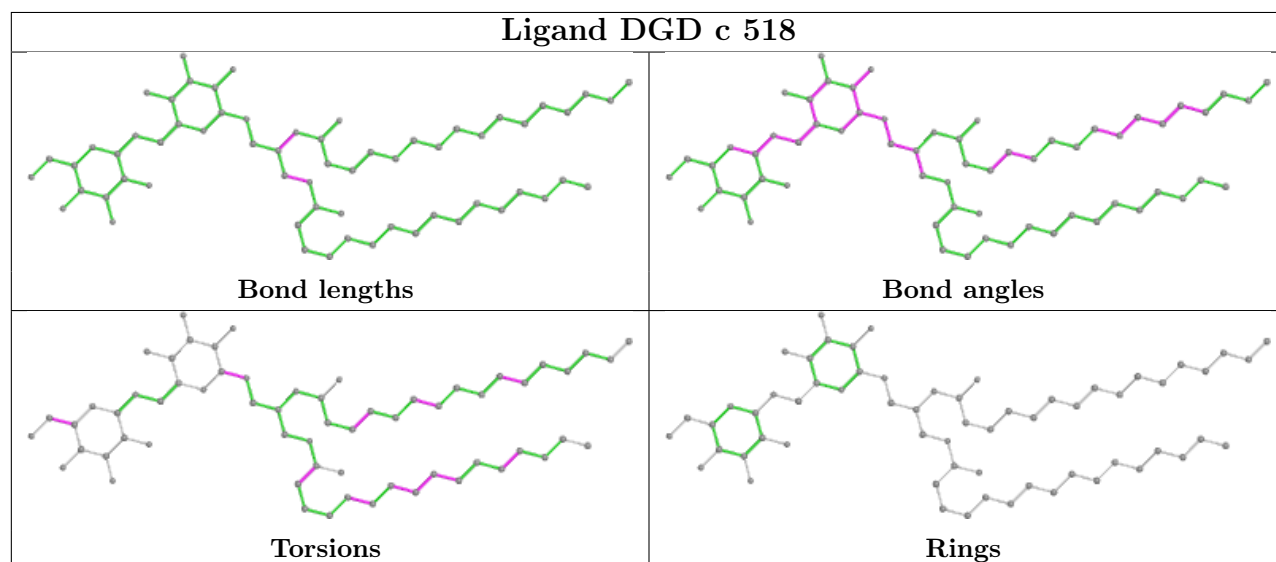
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



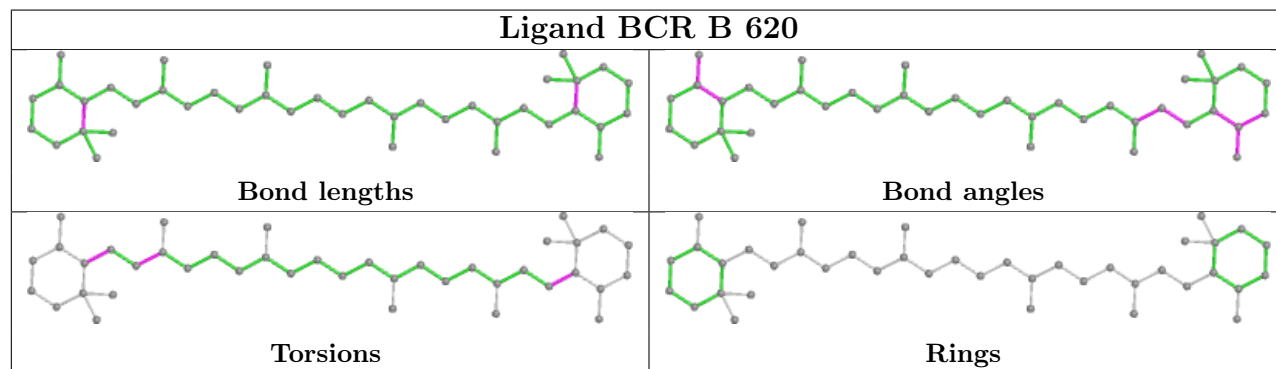
Ligand CLA a 719

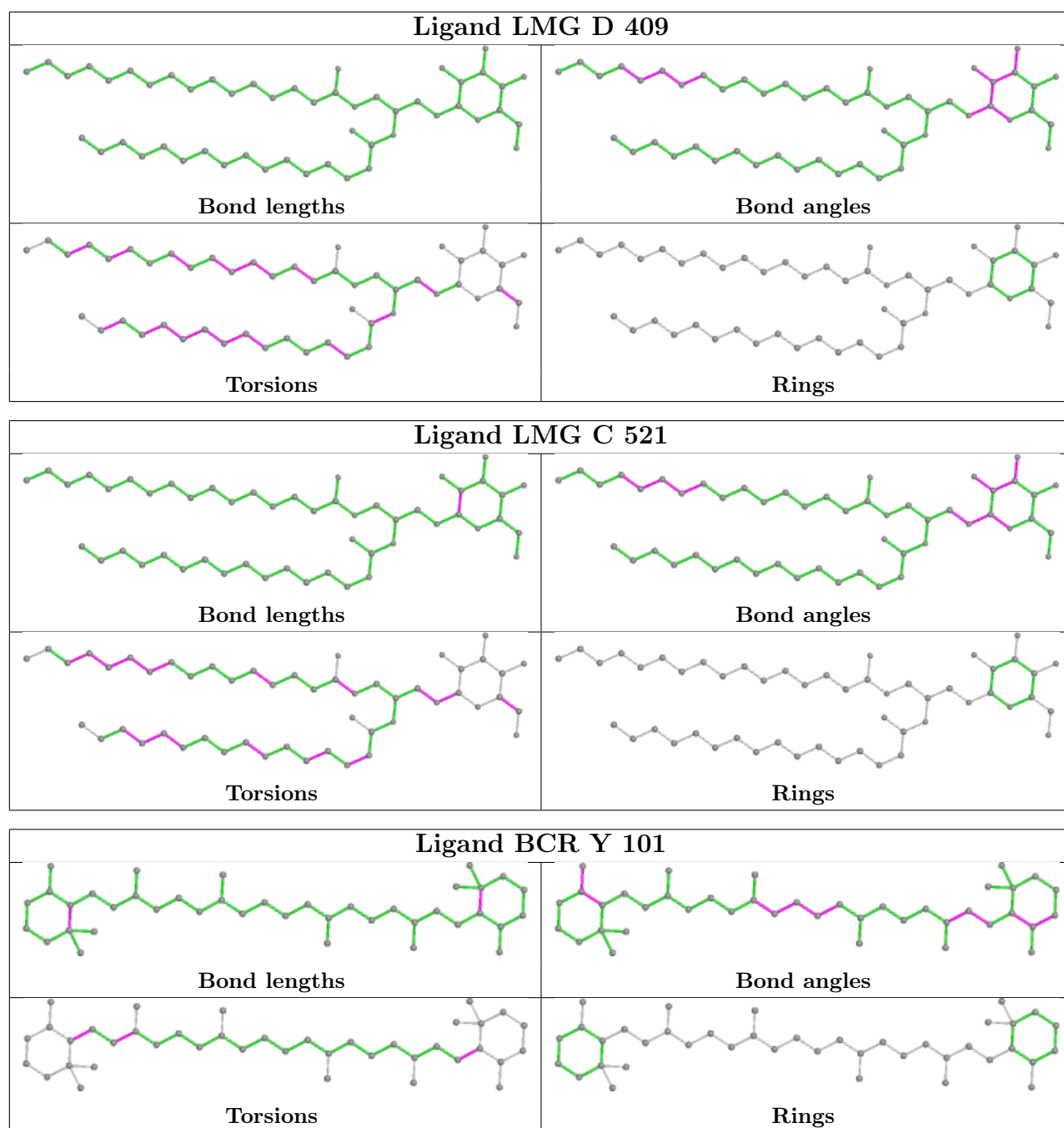


Ligand DGD c 518

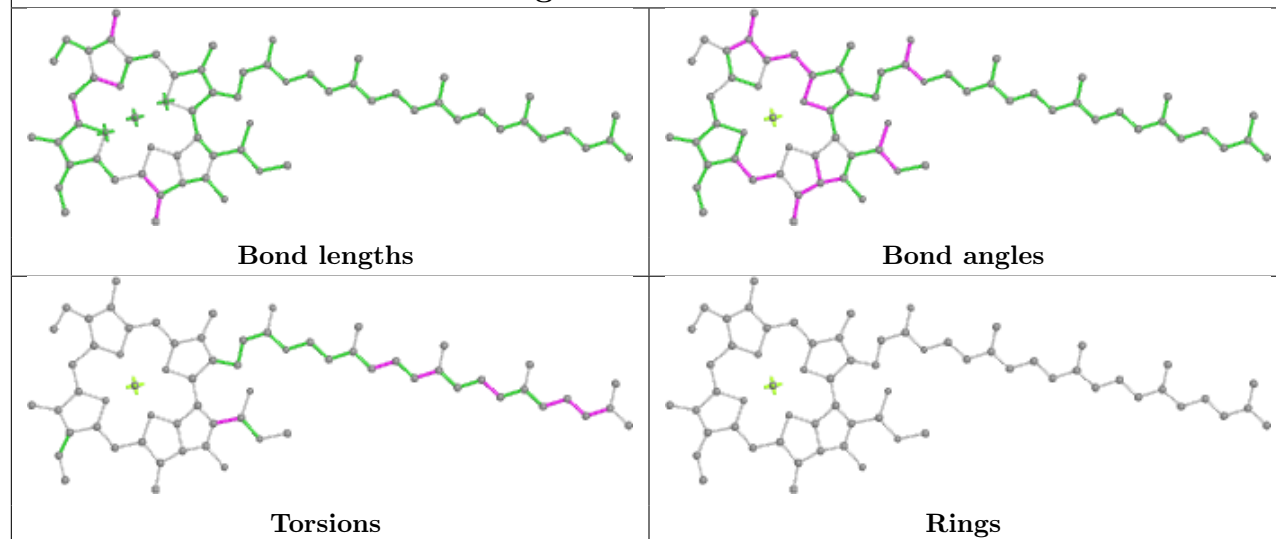


Ligand BCR B 620

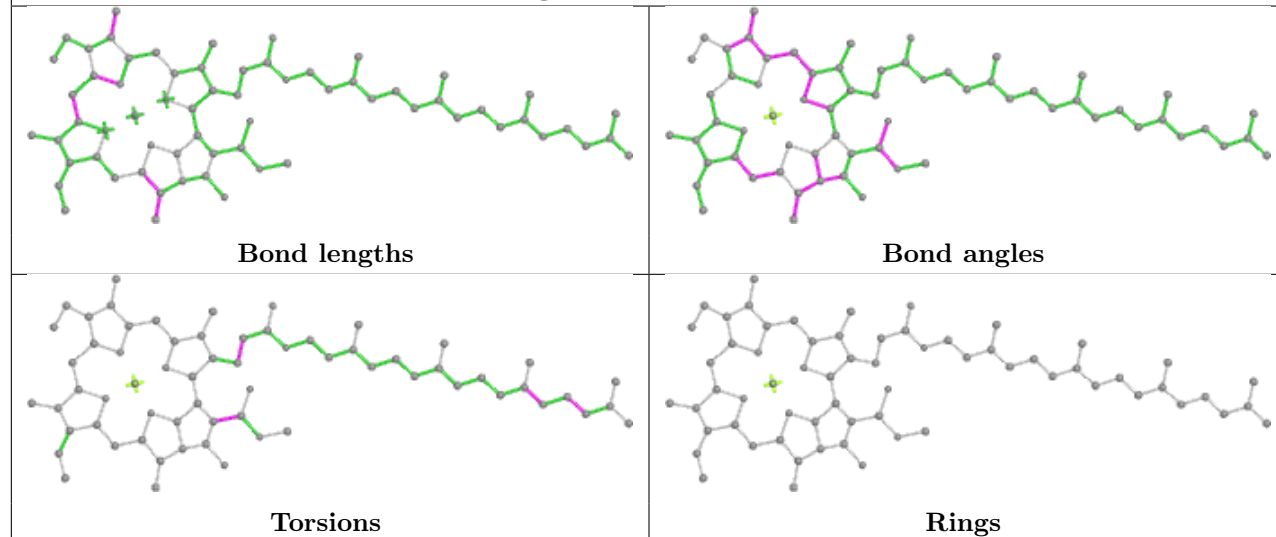




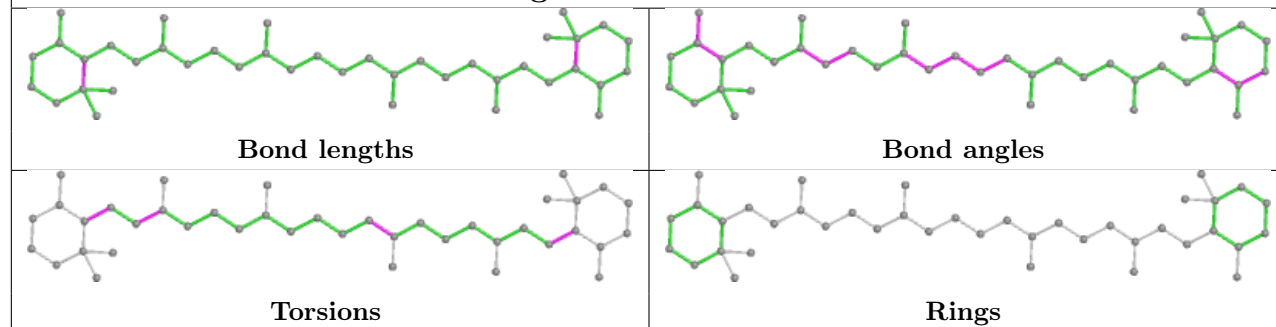
Ligand CLA d 403

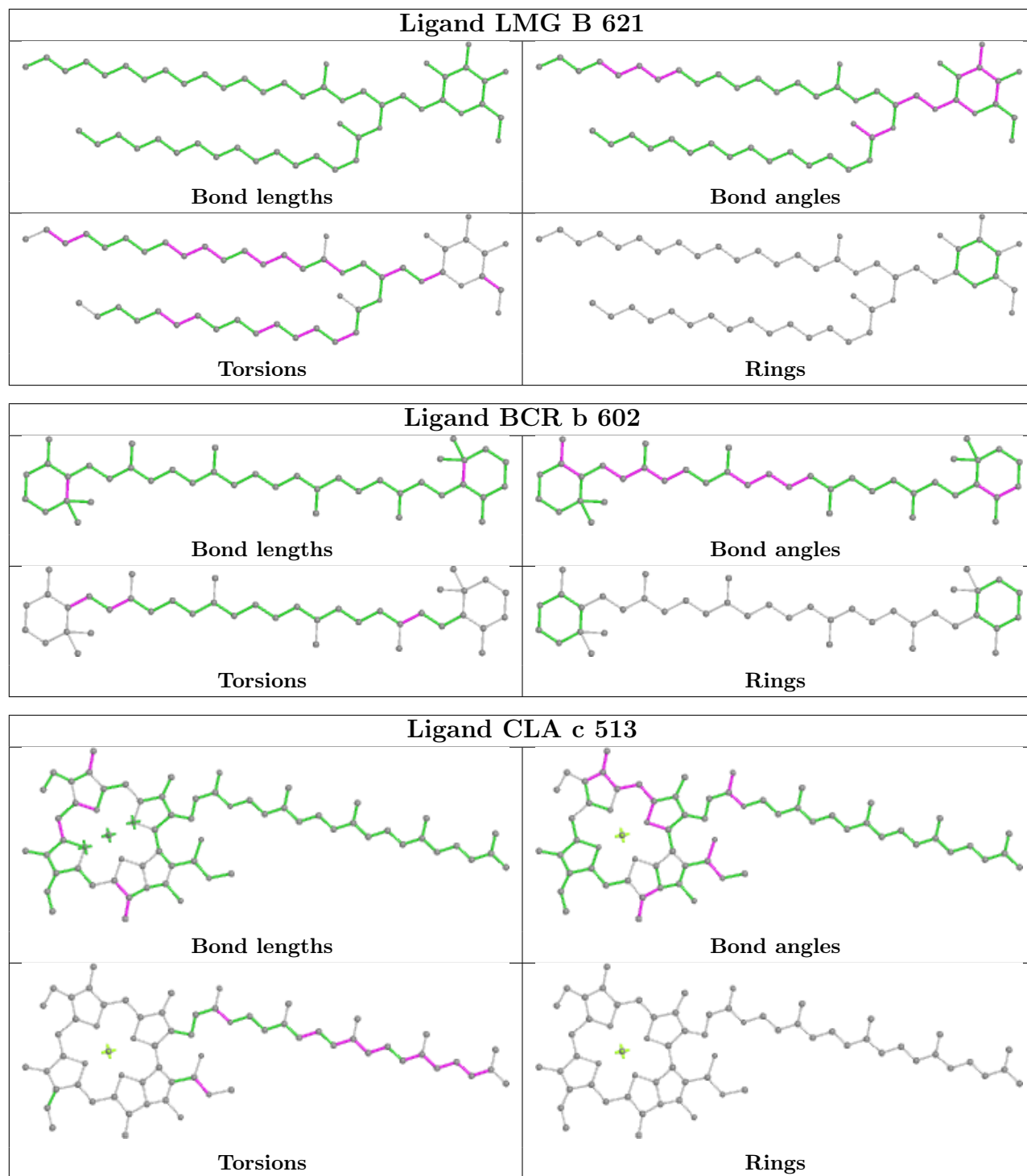


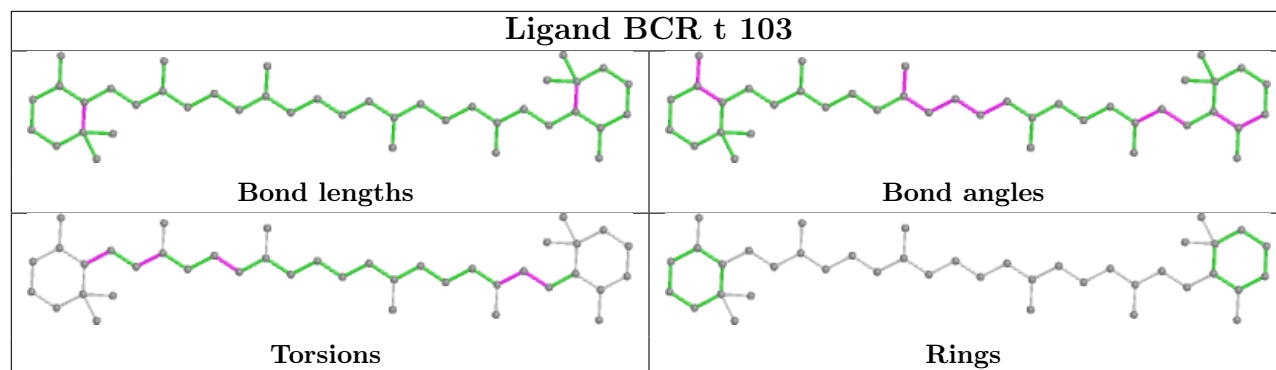
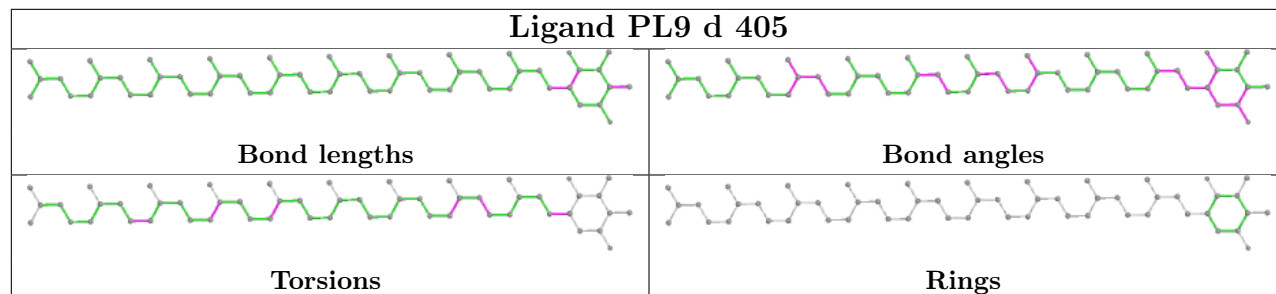
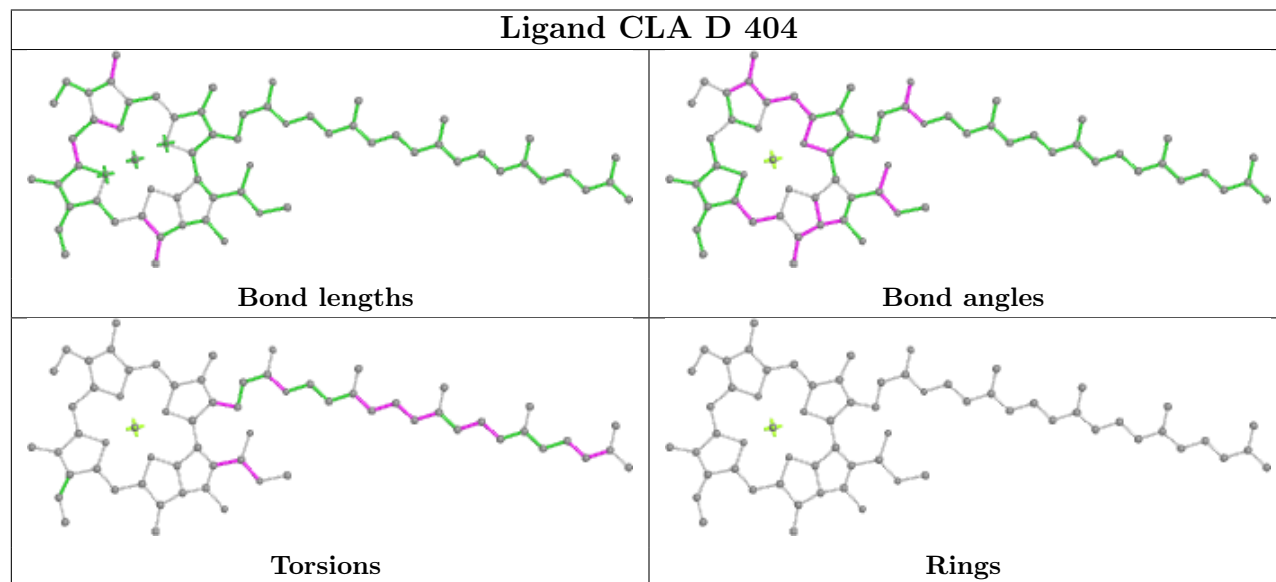
Ligand CLA b 616



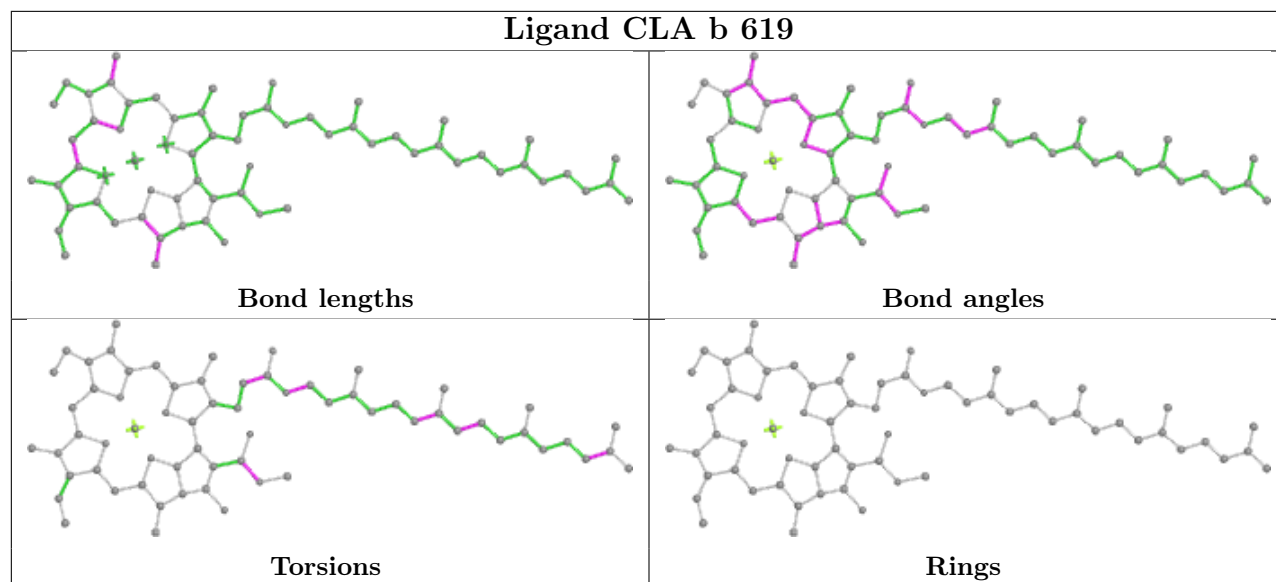
Ligand BCR C 516



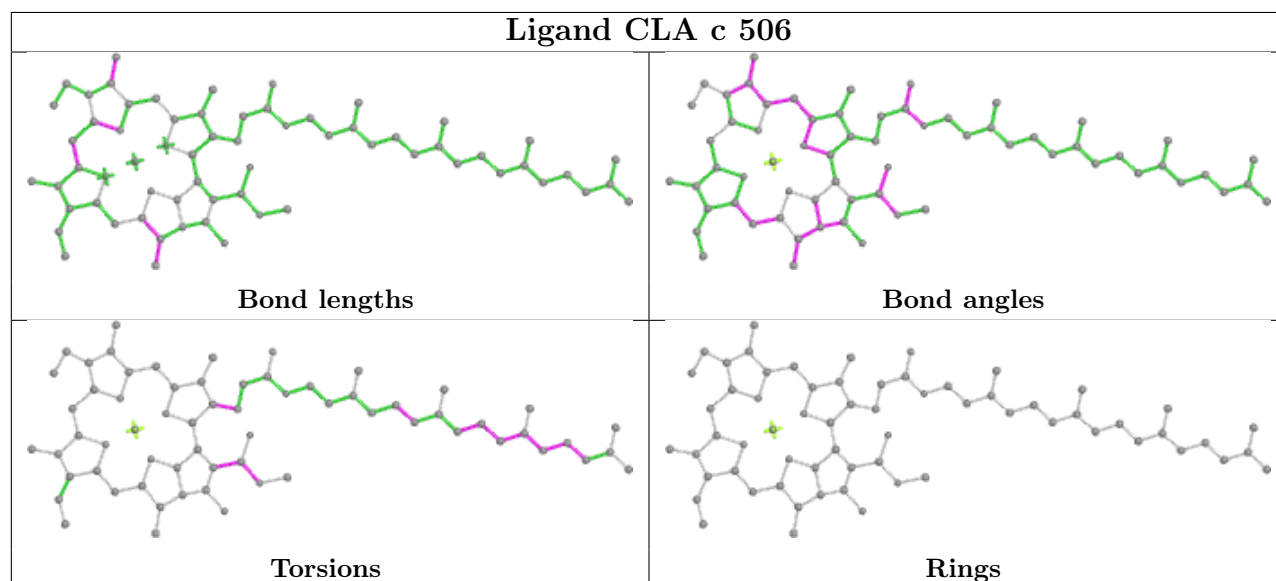


Ligand BCR t 103**Ligand PL9 d 405****Ligand CLA D 404**

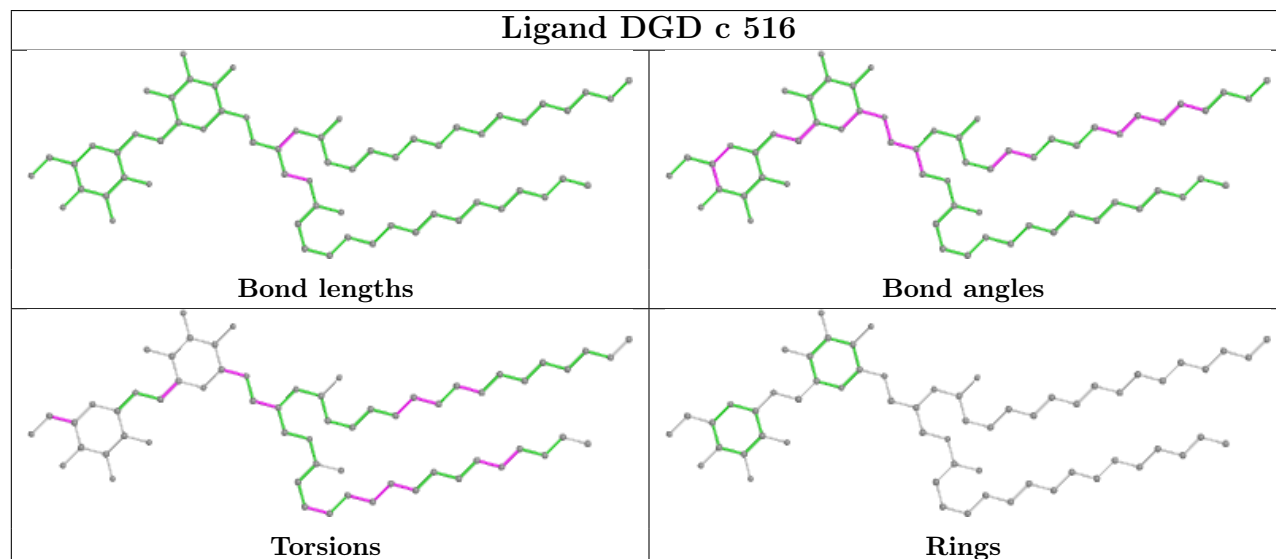
Ligand CLA b 619



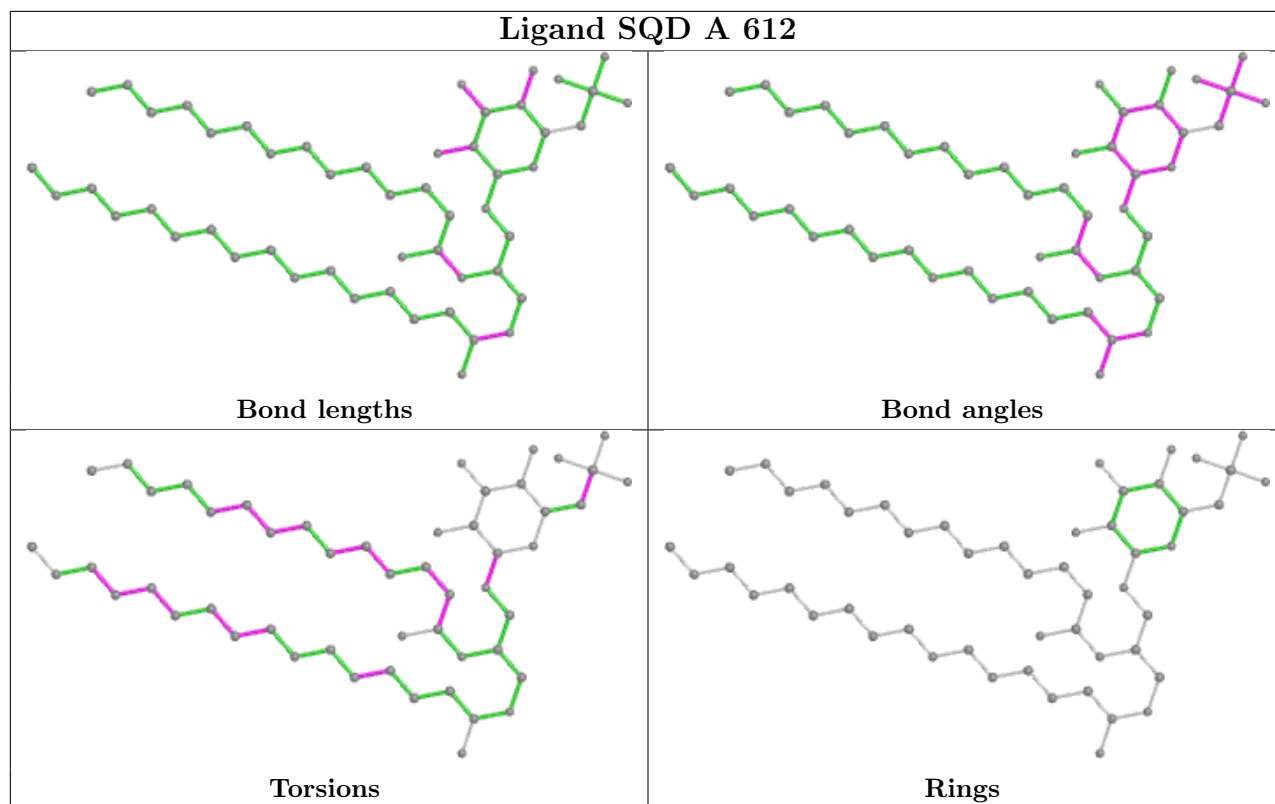
Ligand CLA c 506



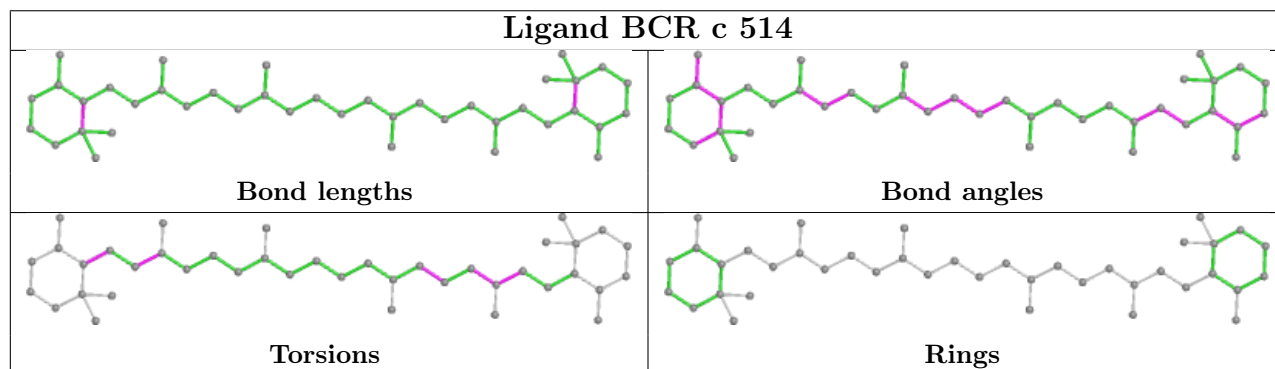
Ligand DGD c 516

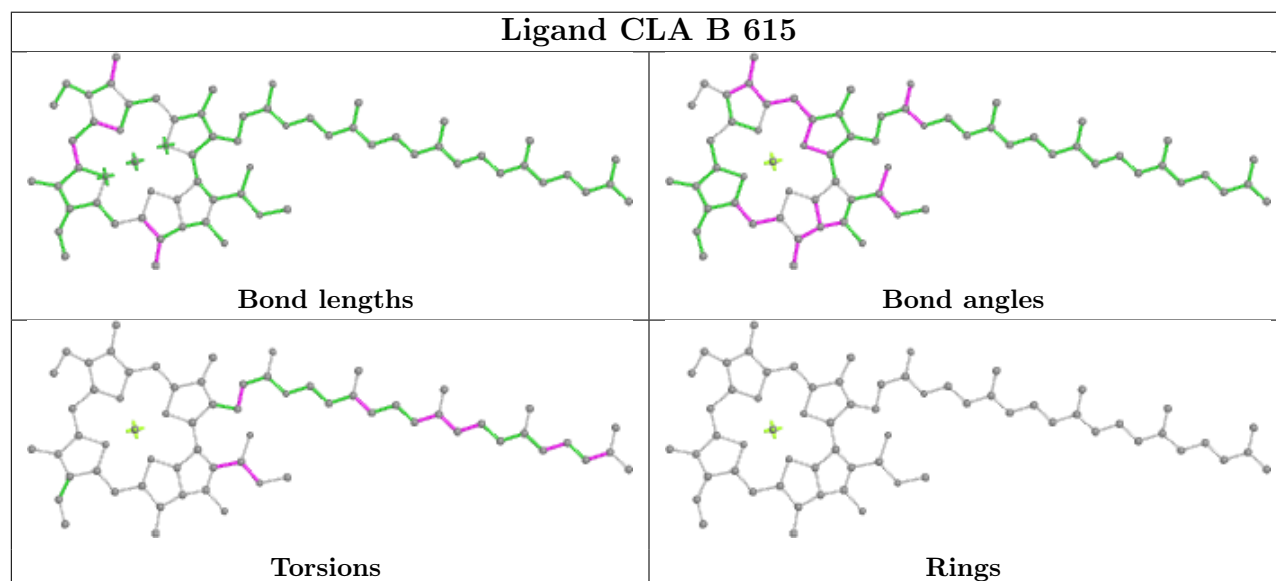
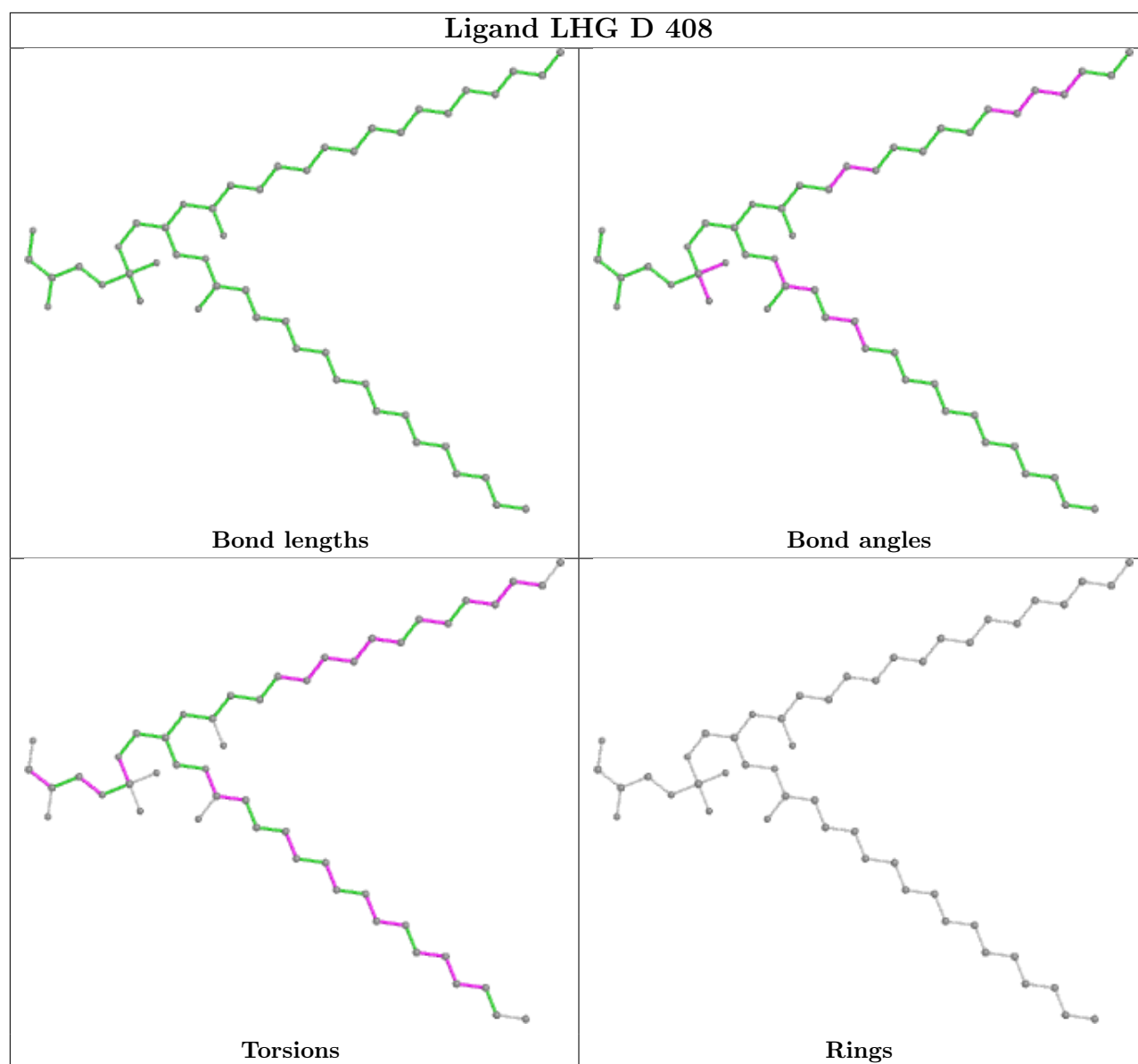


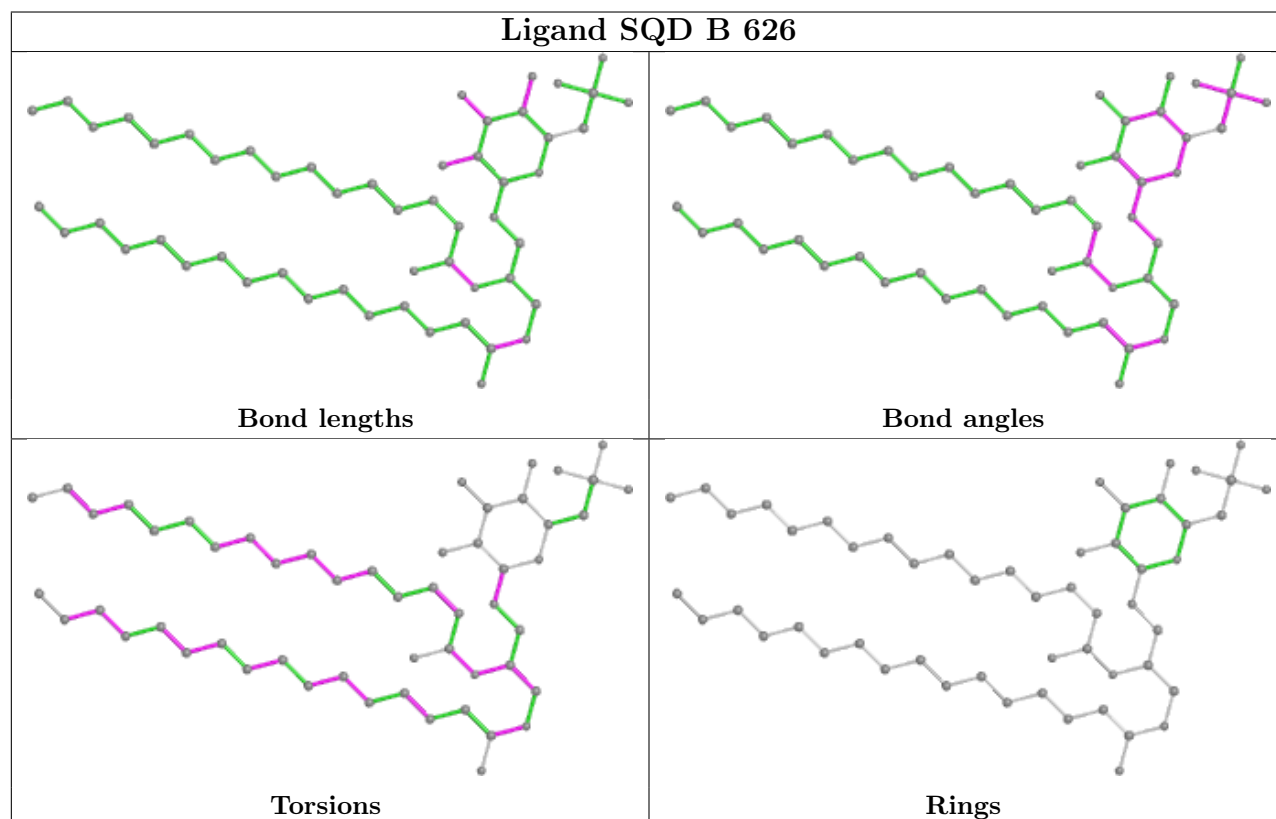
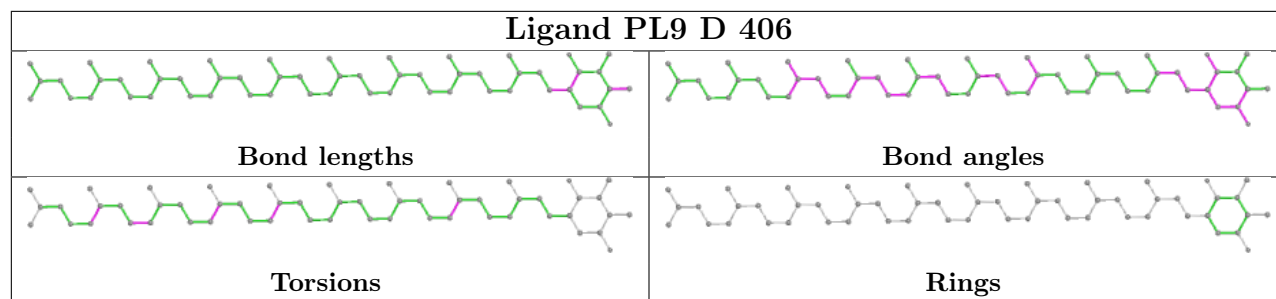
Ligand SQD A 612

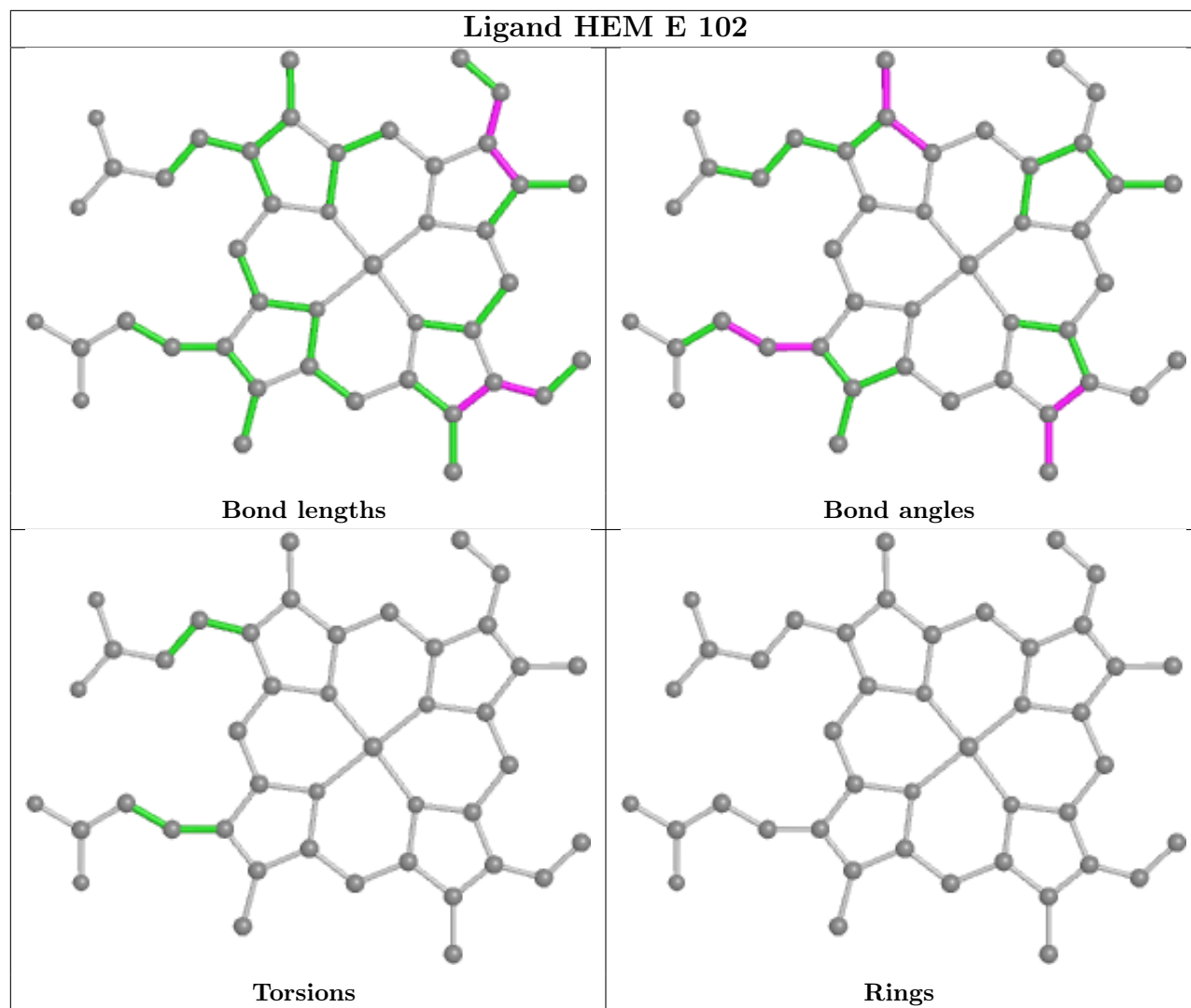


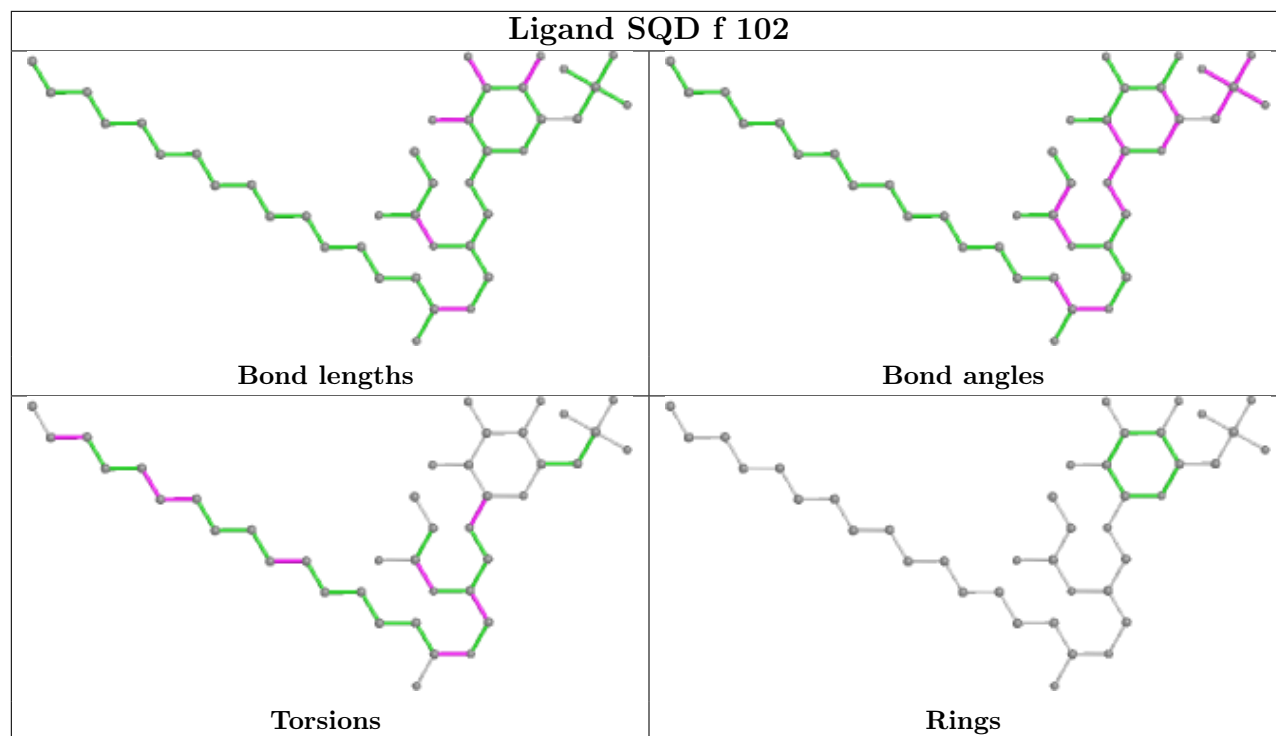
Ligand BCR c 514



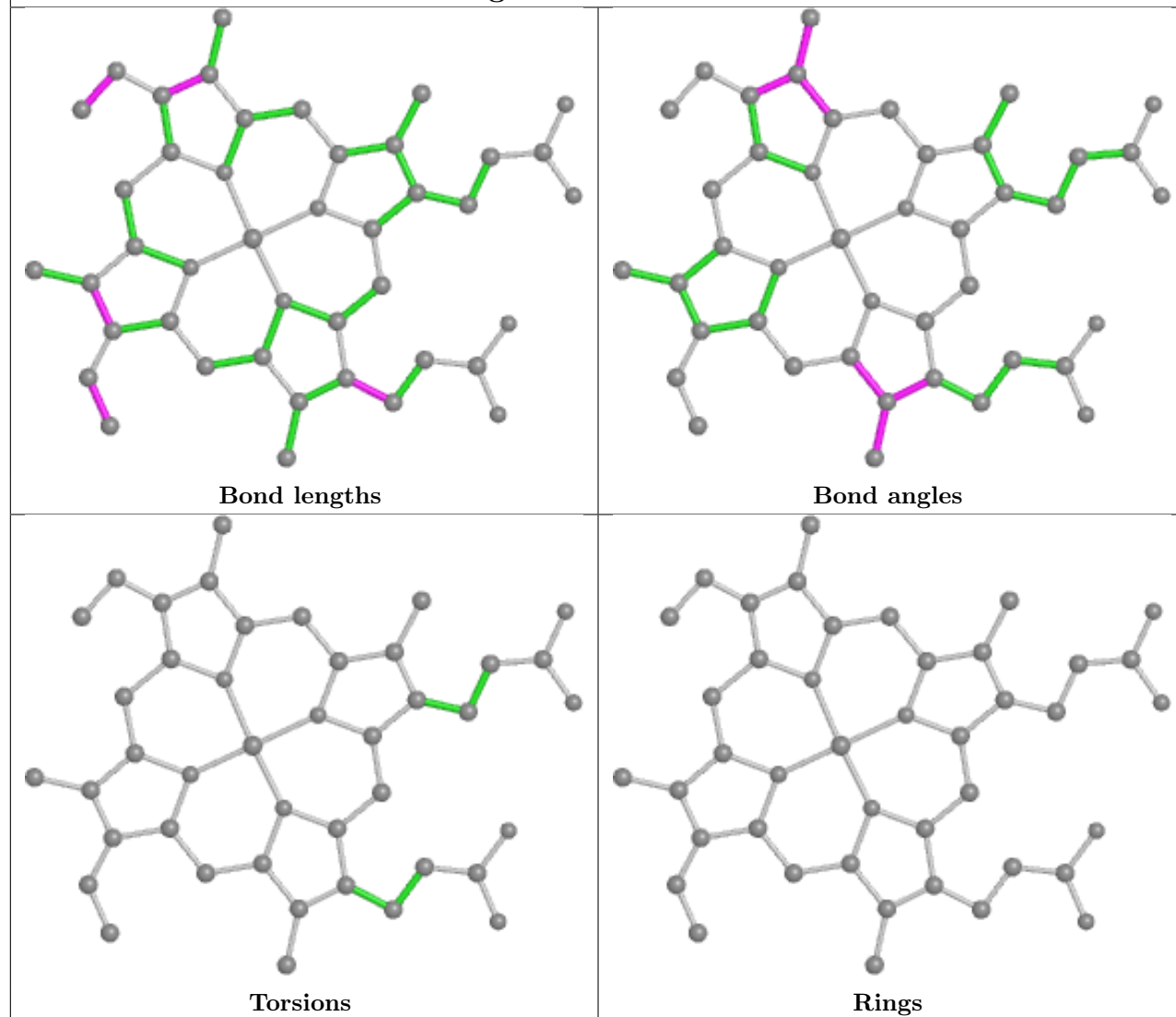




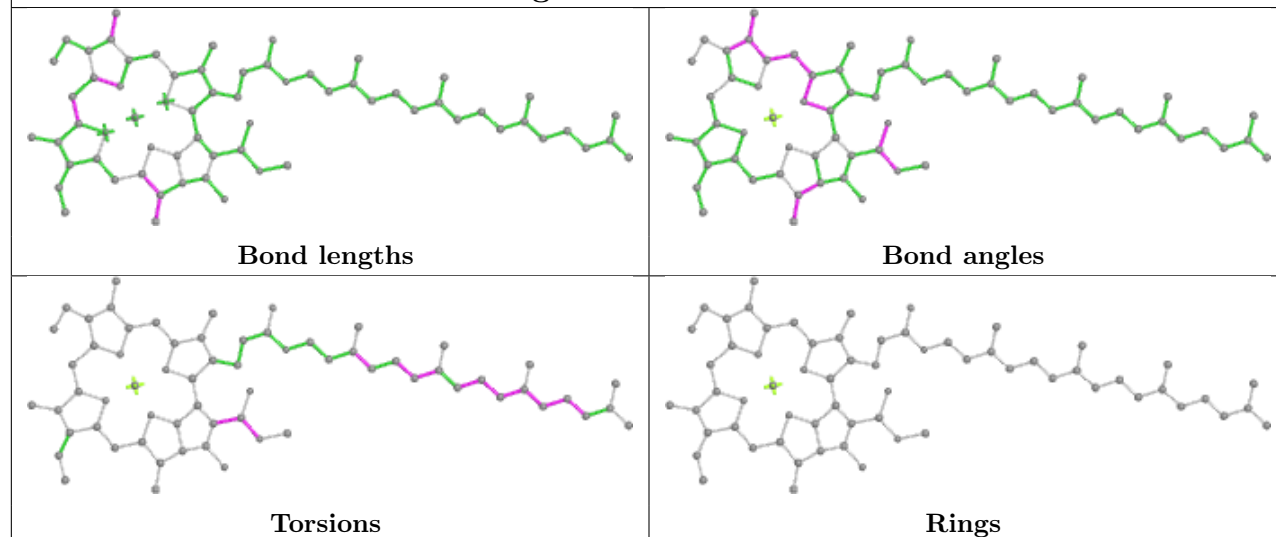




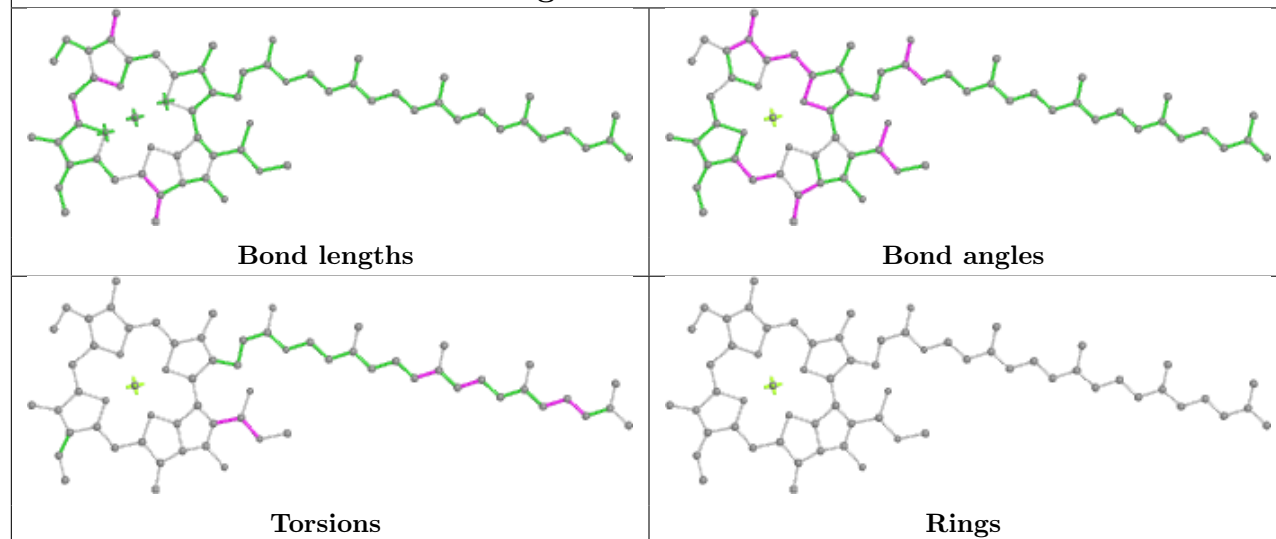
Ligand HEC V 201



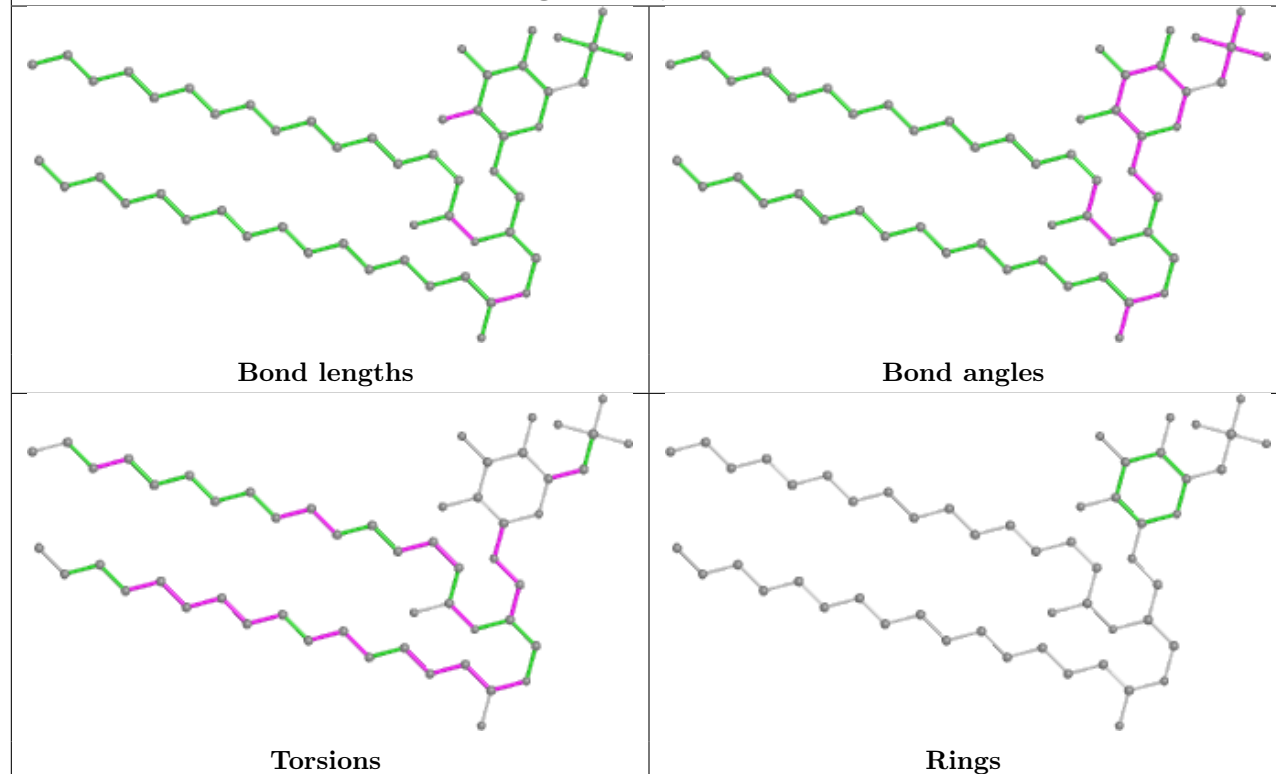
Ligand CLA B 606



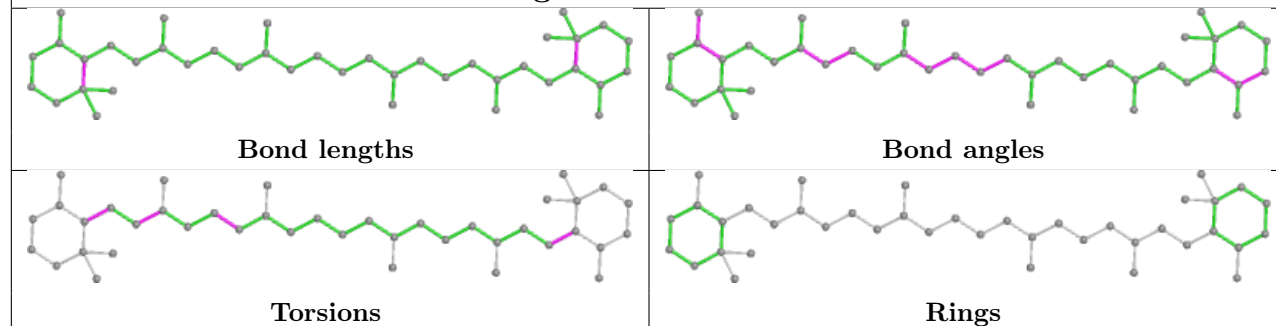
Ligand CLA c 511



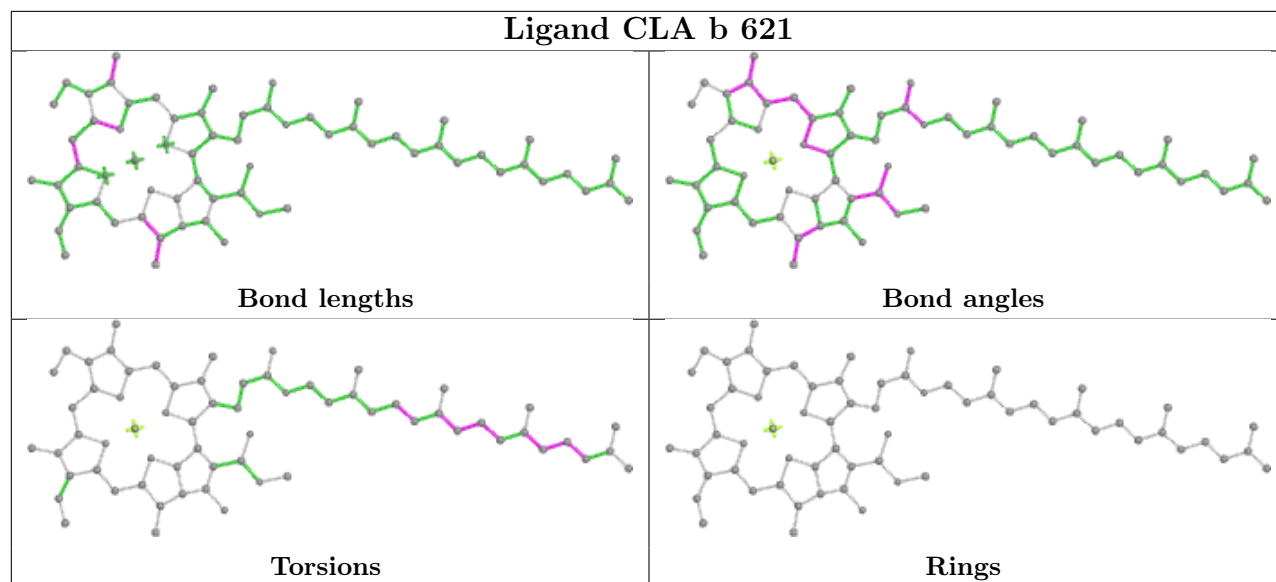
Ligand SQD b 601



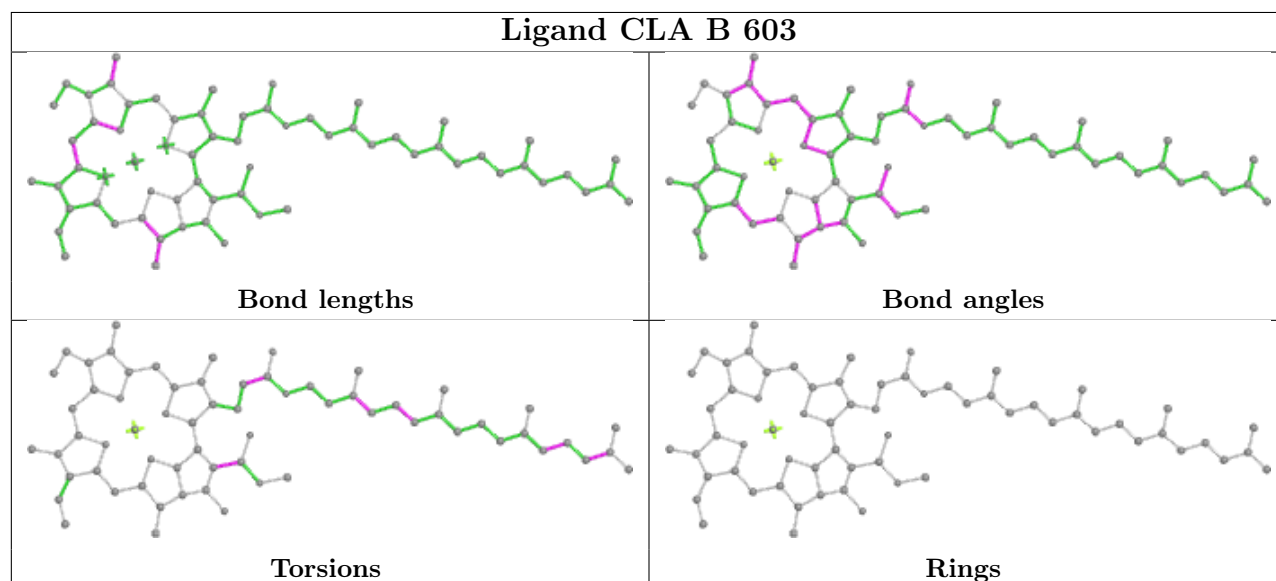
Ligand BCR b 624



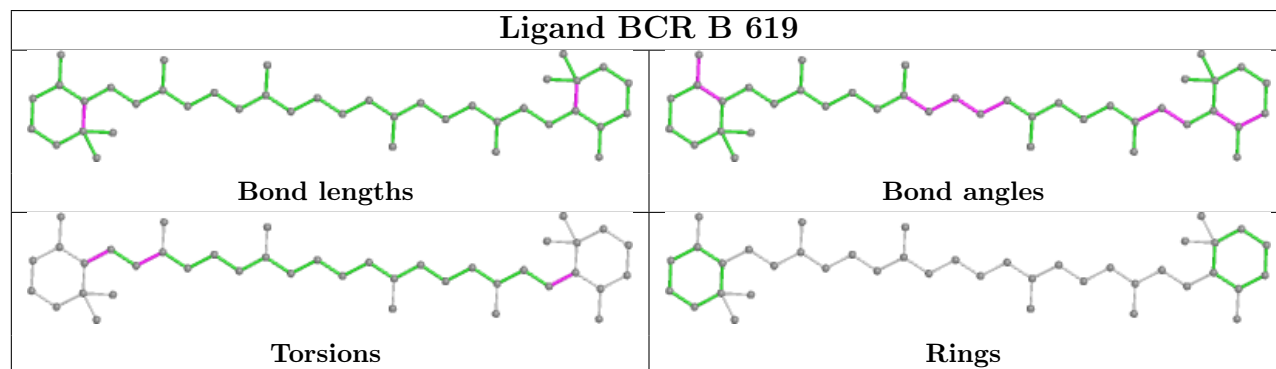
Ligand CLA b 621

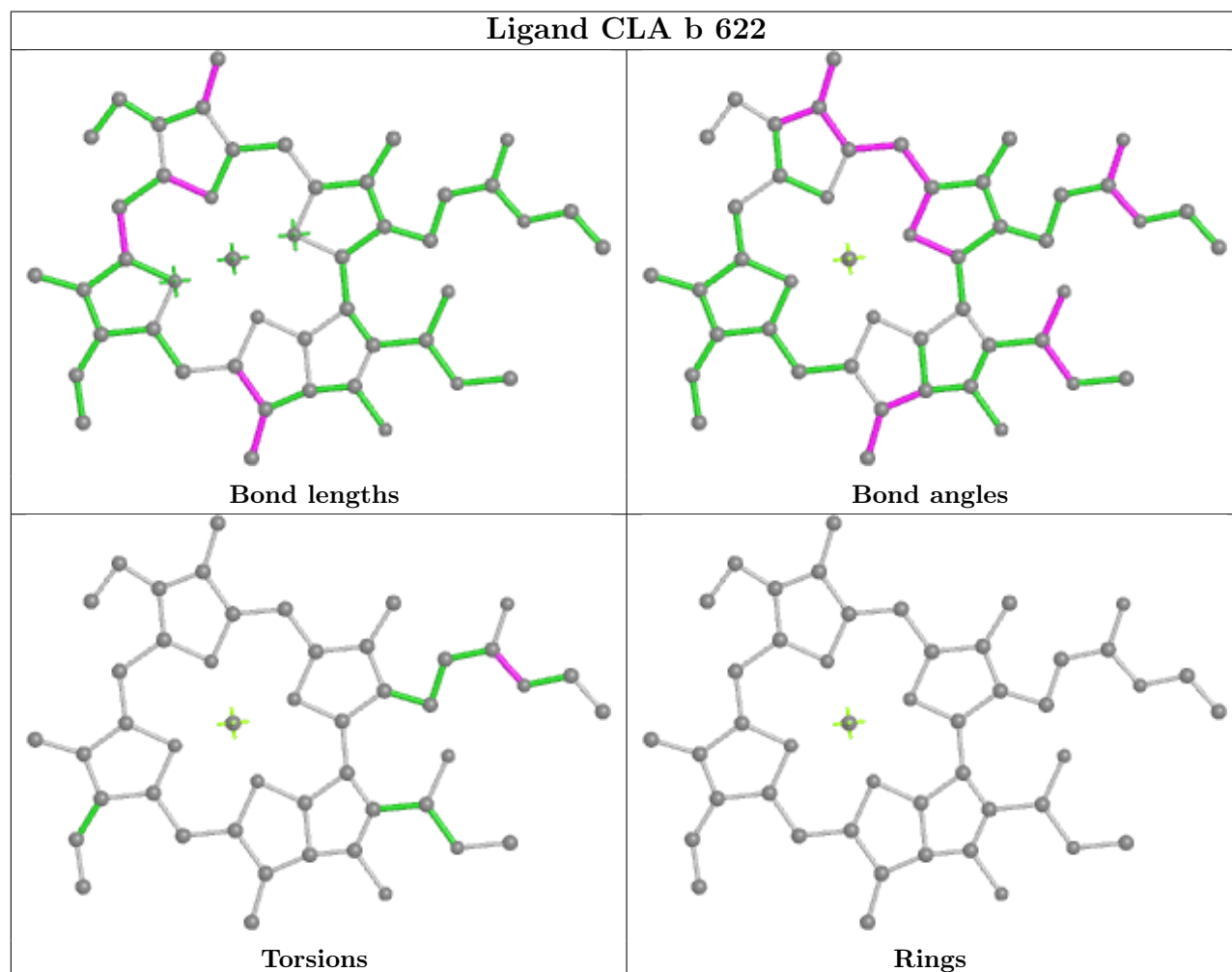
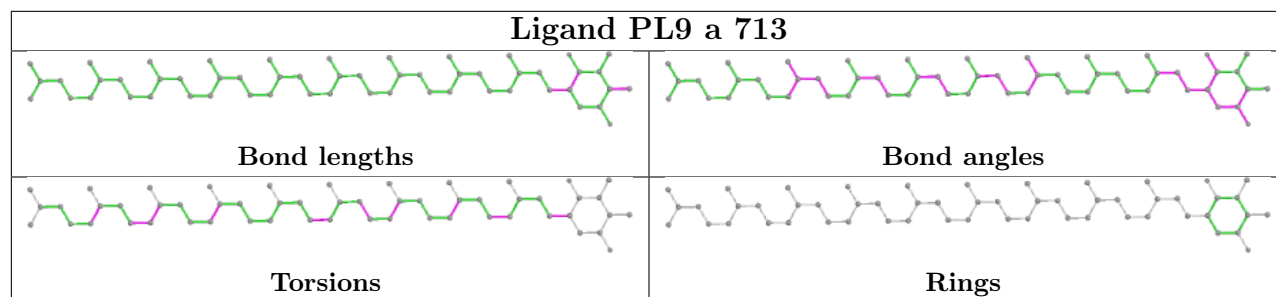


Ligand CLA B 603

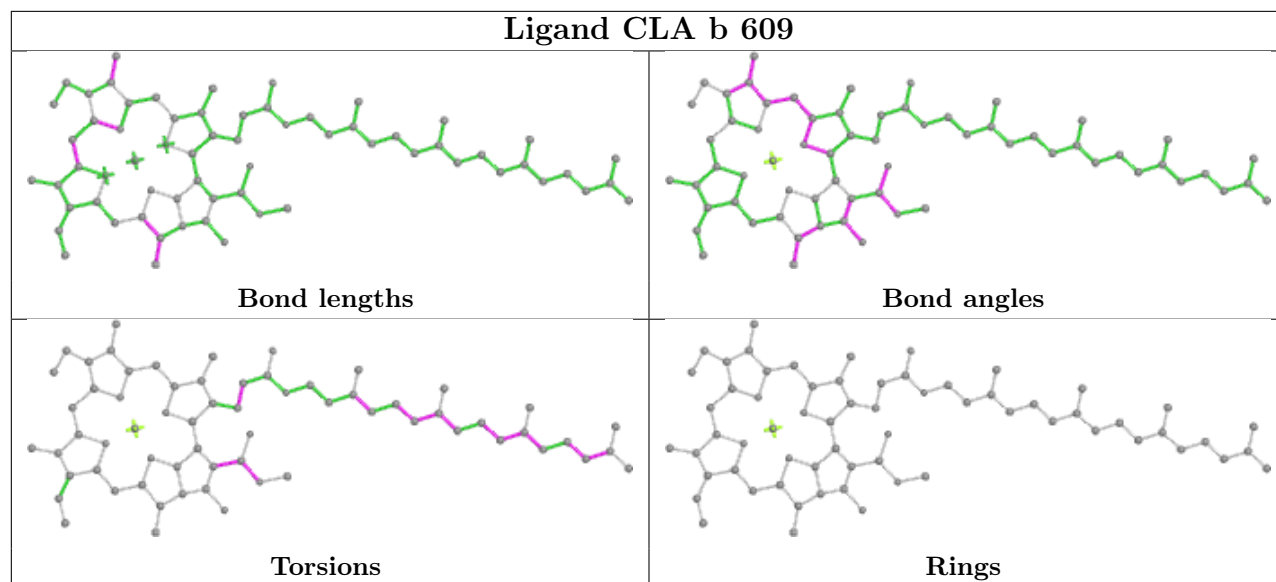


Ligand BCR B 619

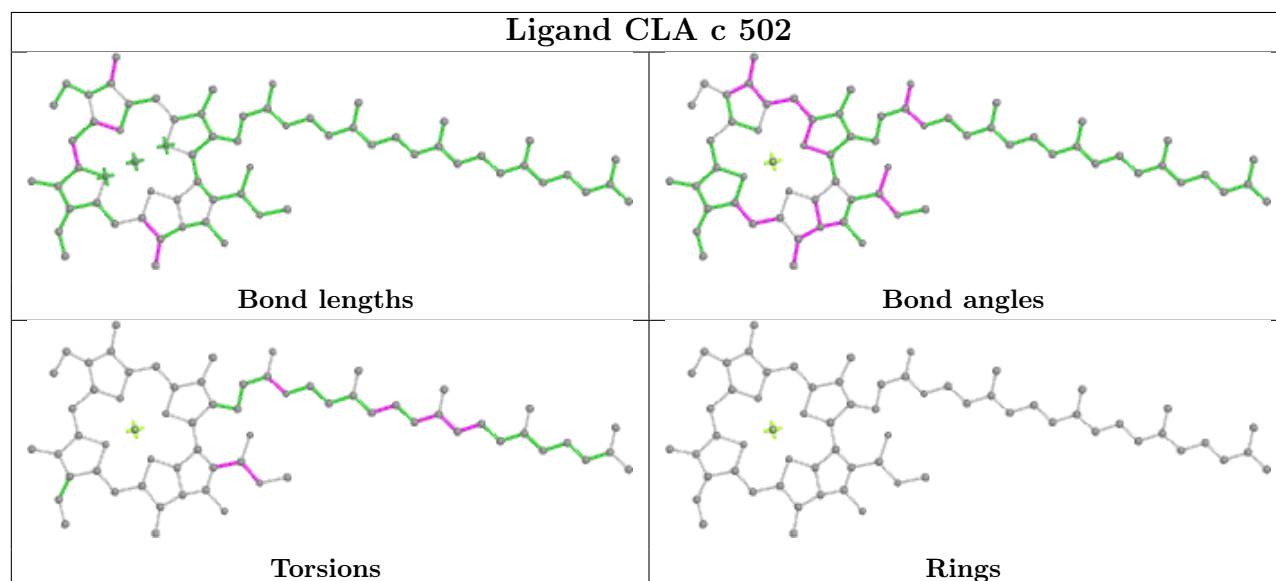




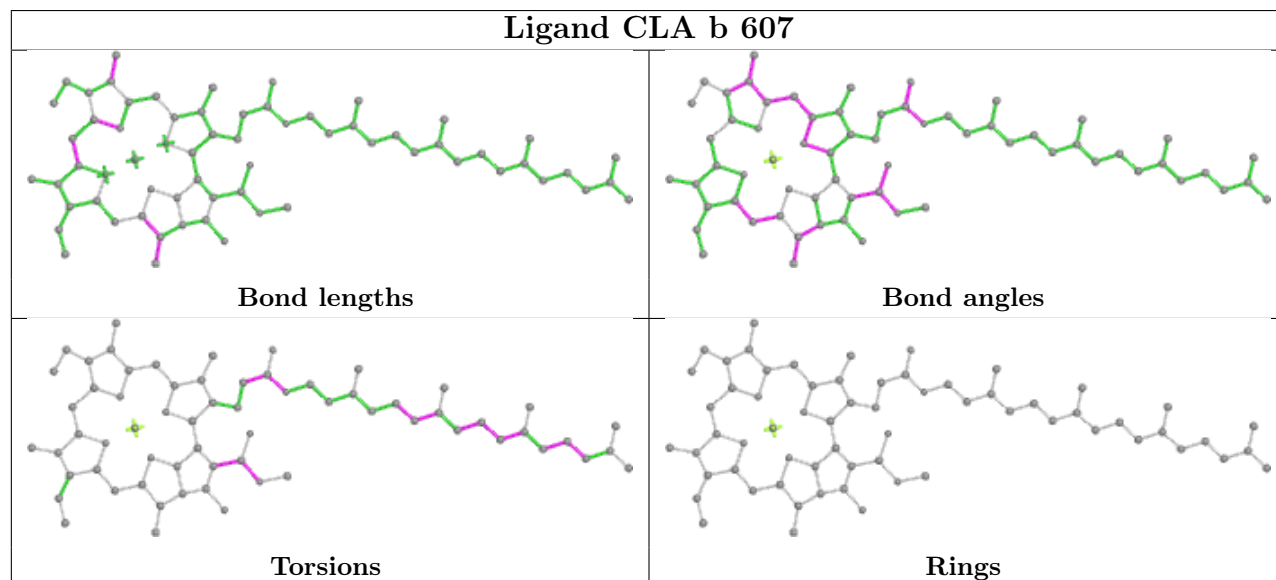
Ligand CLA b 609



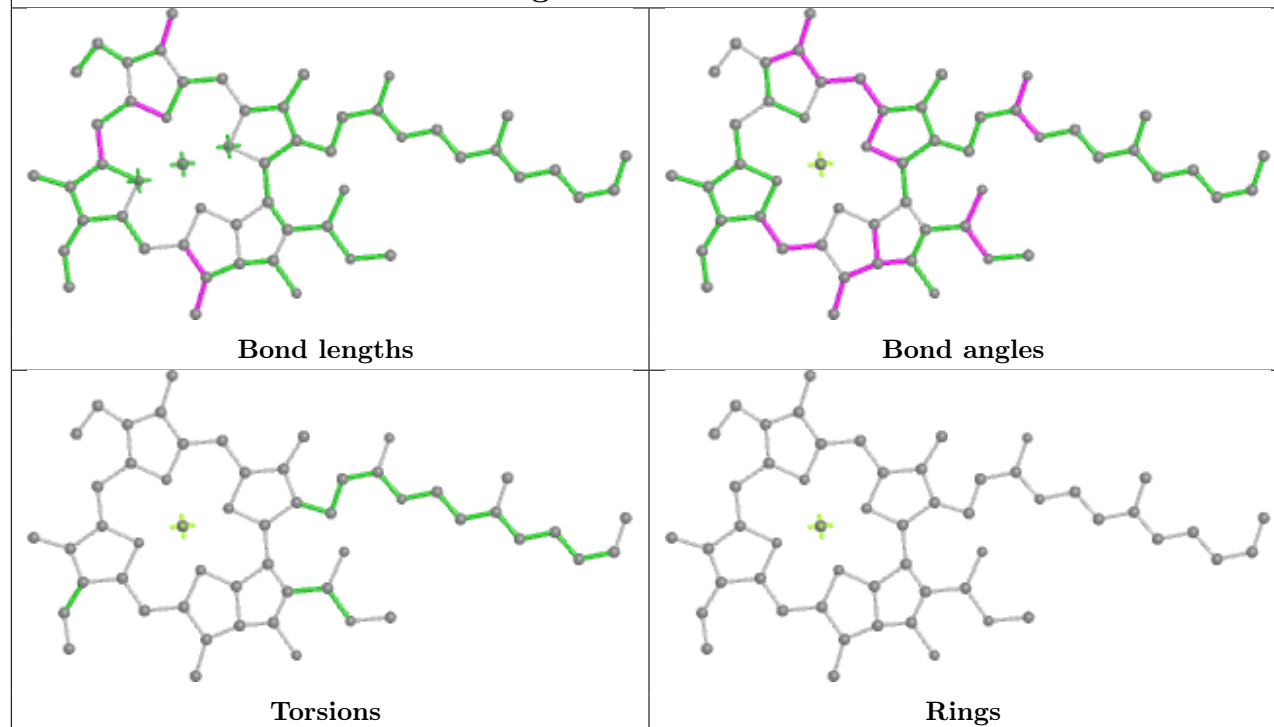
Ligand CLA c 502



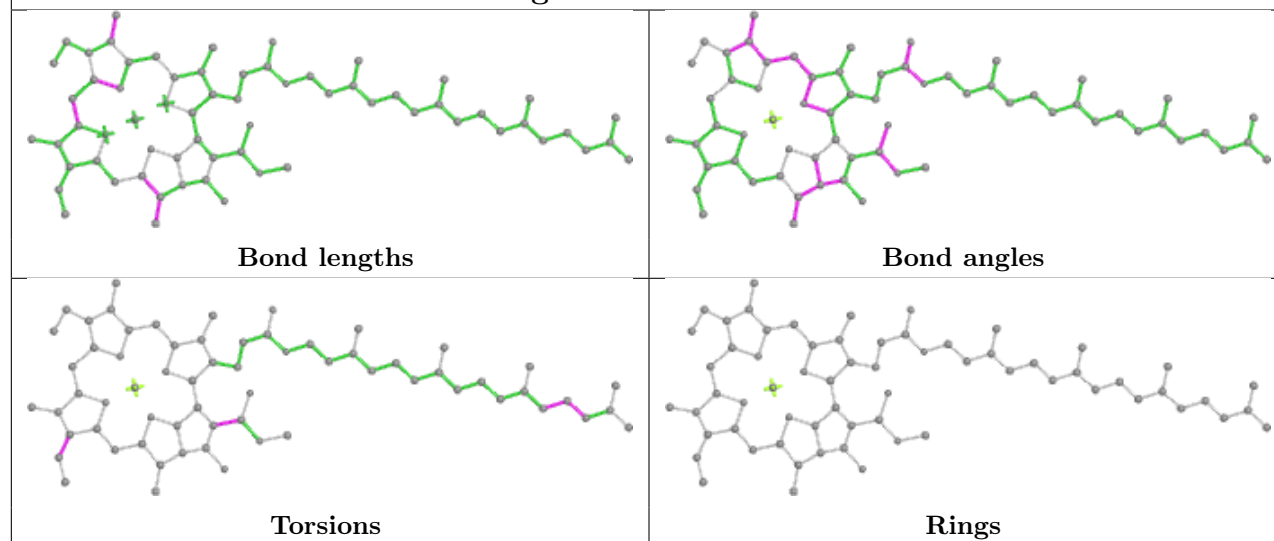
Ligand CLA b 607



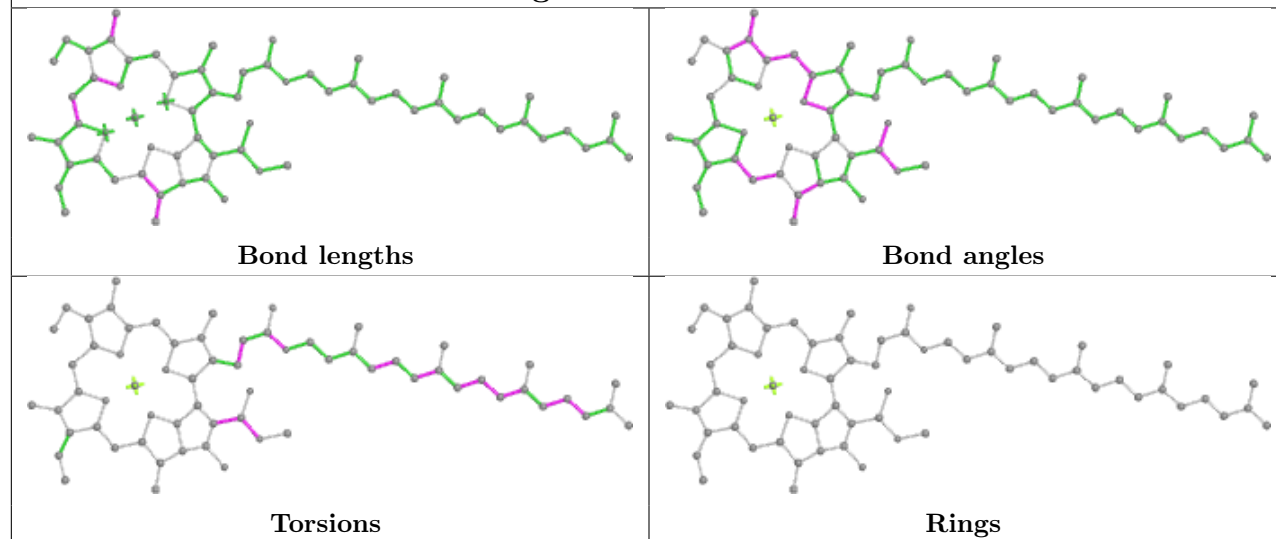
Ligand CLA A 609



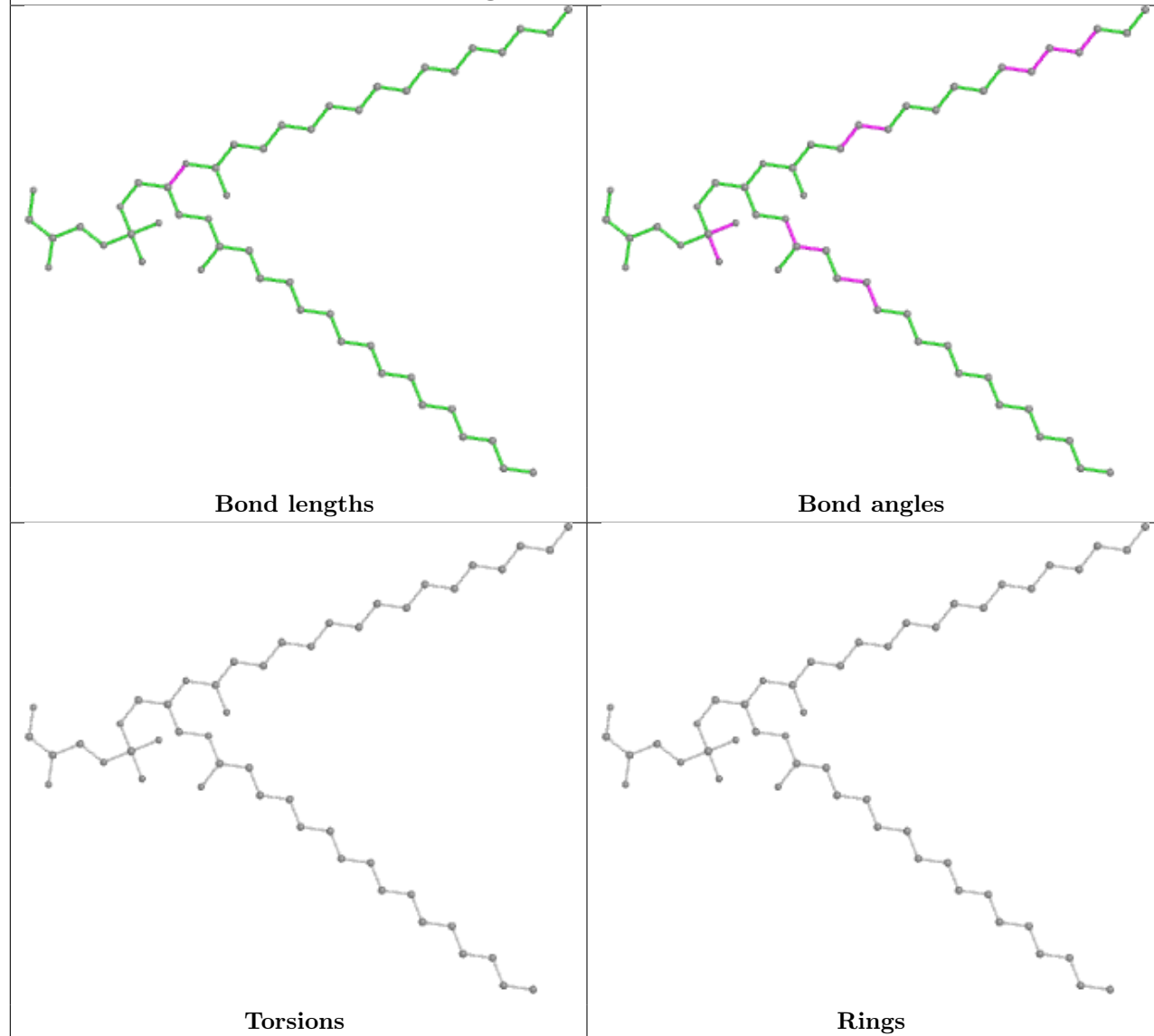
Ligand CLA D 402



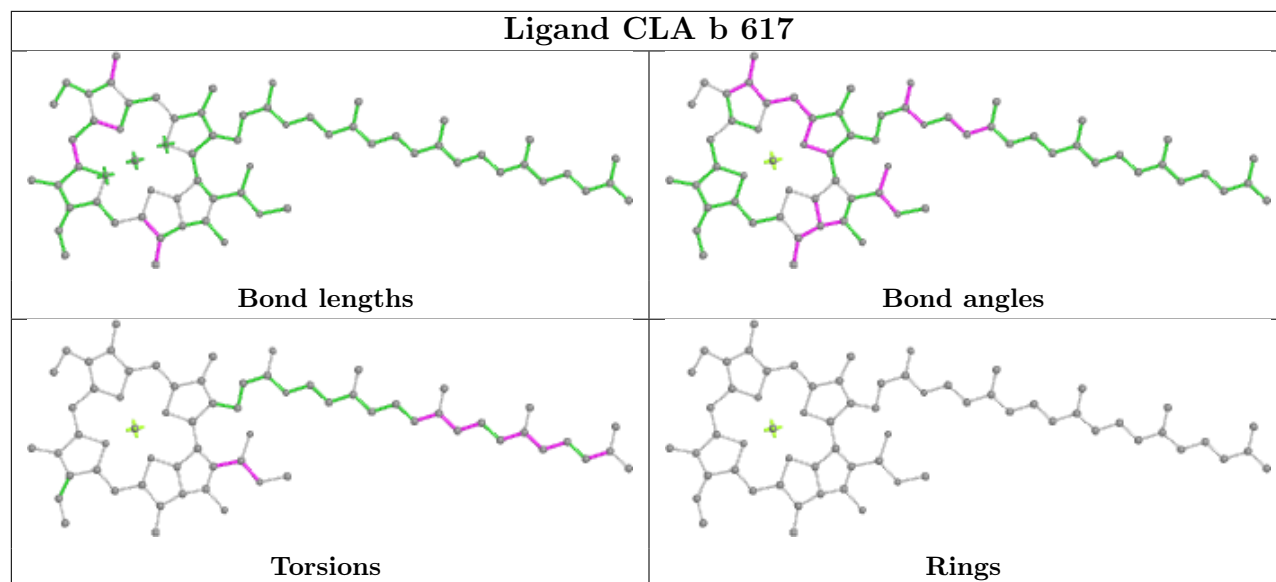
Ligand CLA B 607



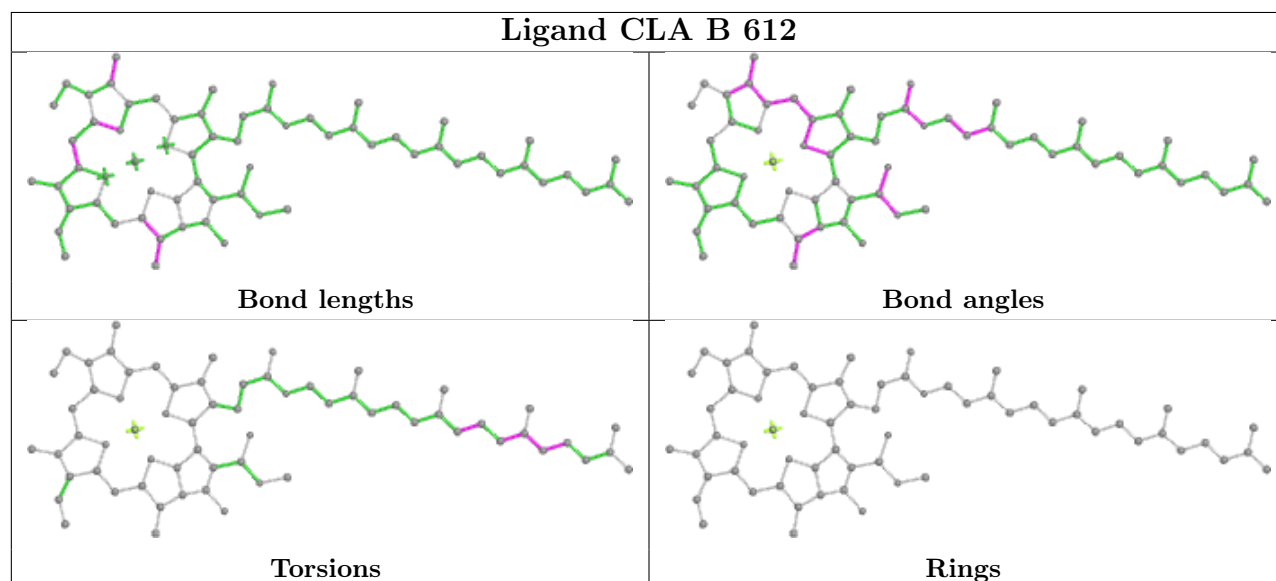
Ligand LHG b 629



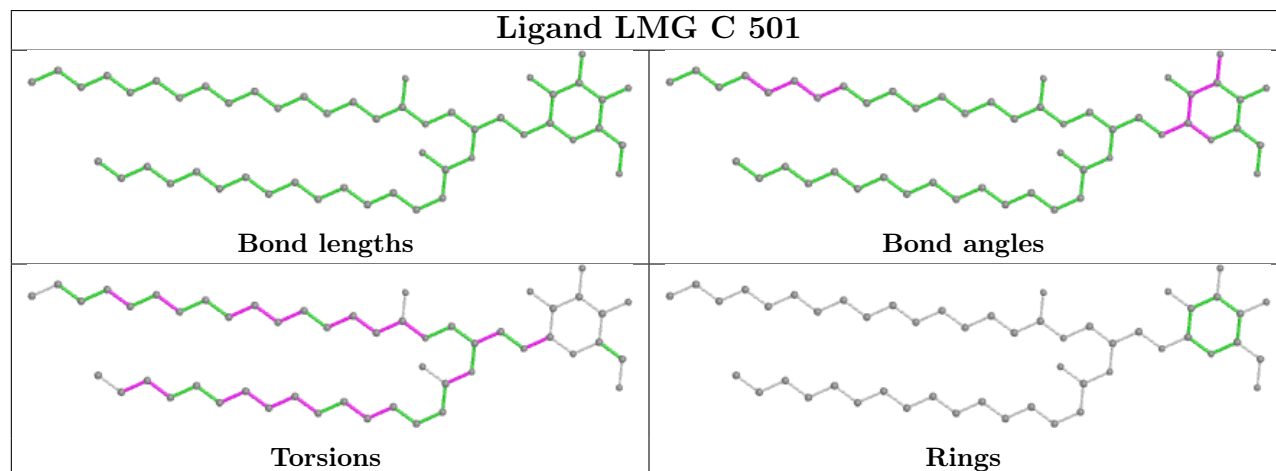
Ligand CLA b 617



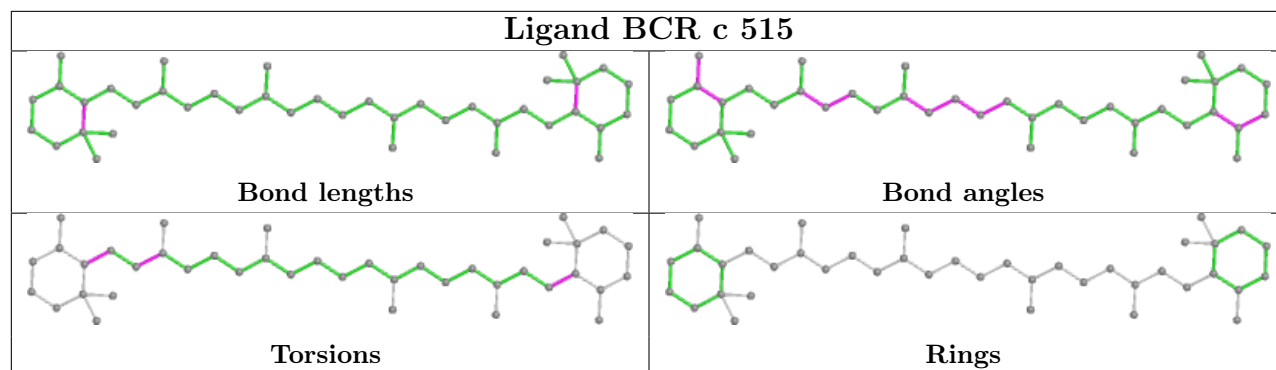
Ligand CLA B 612



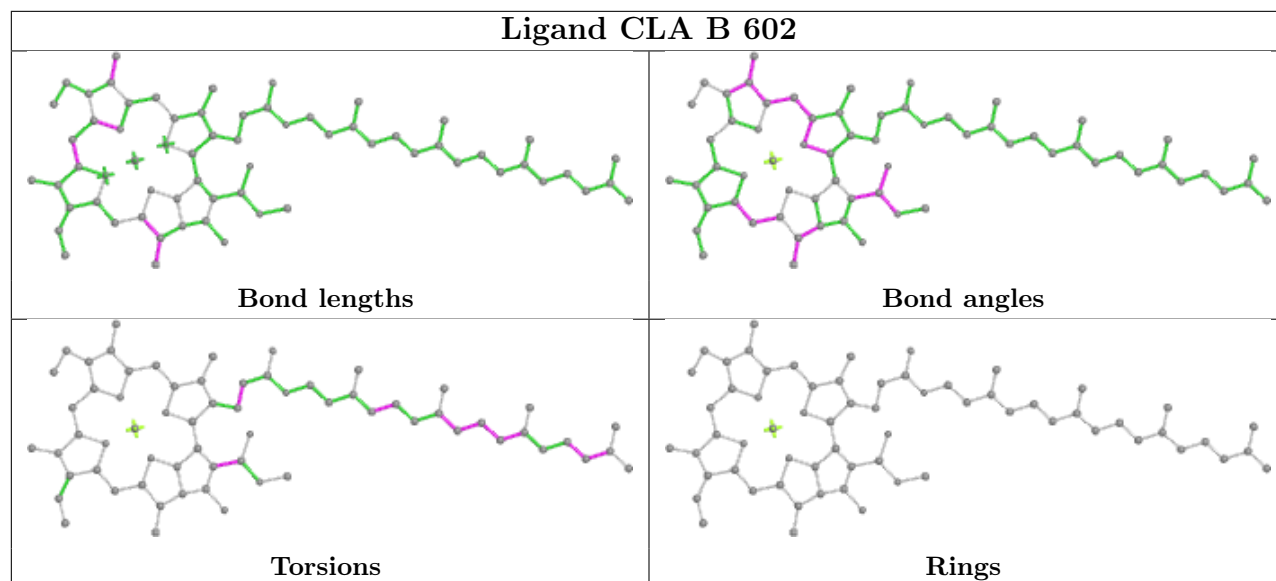
Ligand LMG C 501



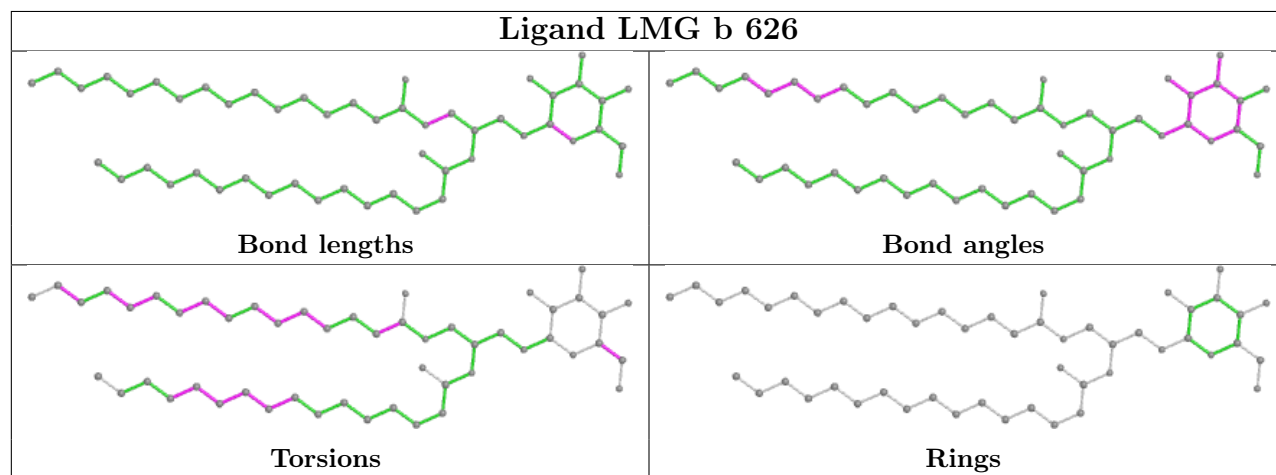
Ligand BCR c 515

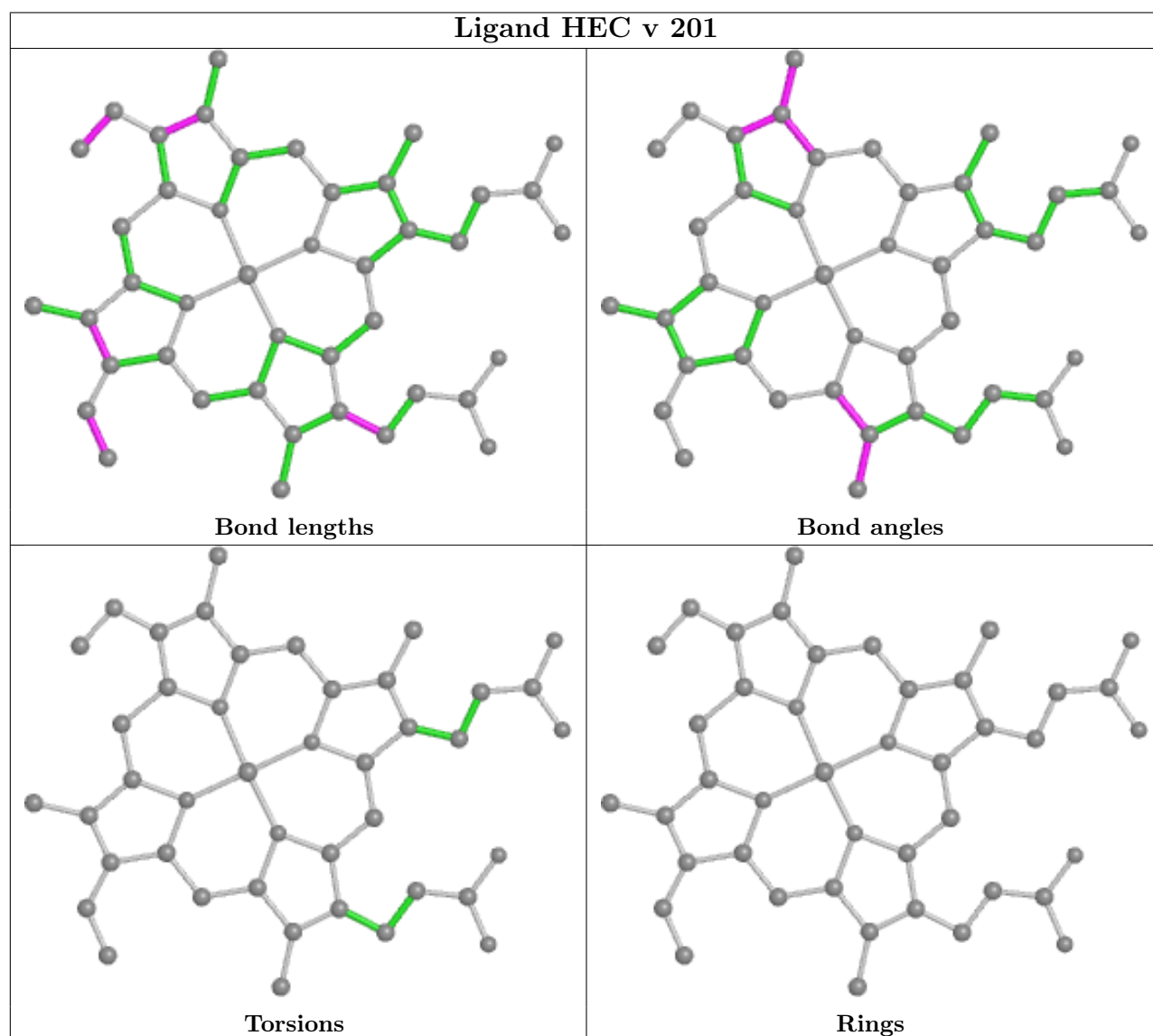
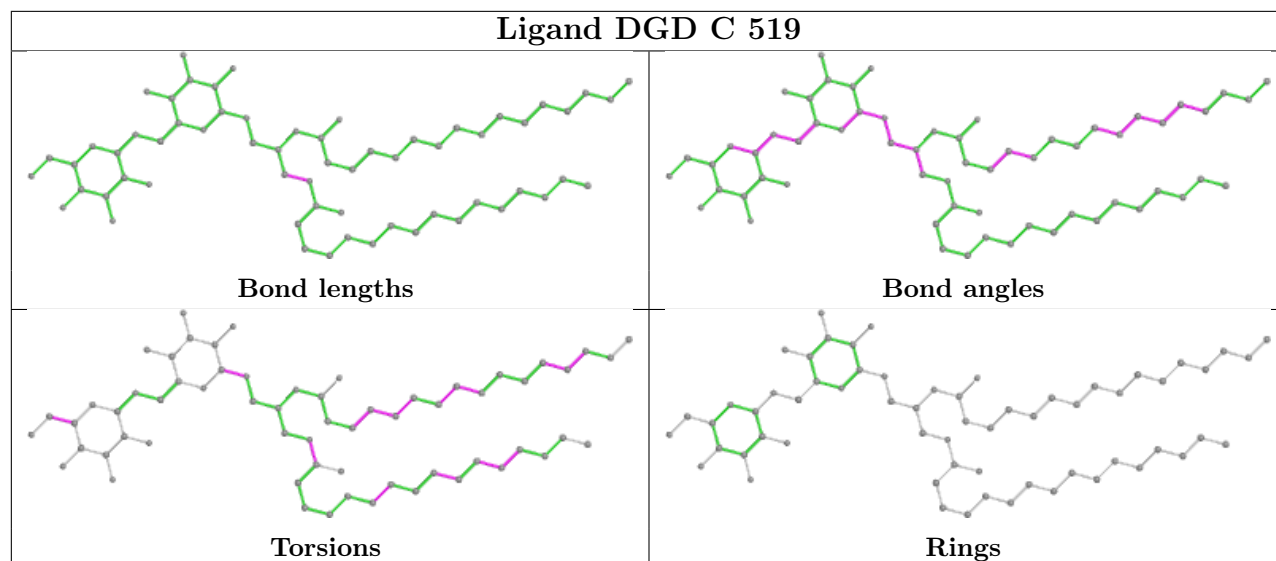


Ligand CLA B 602

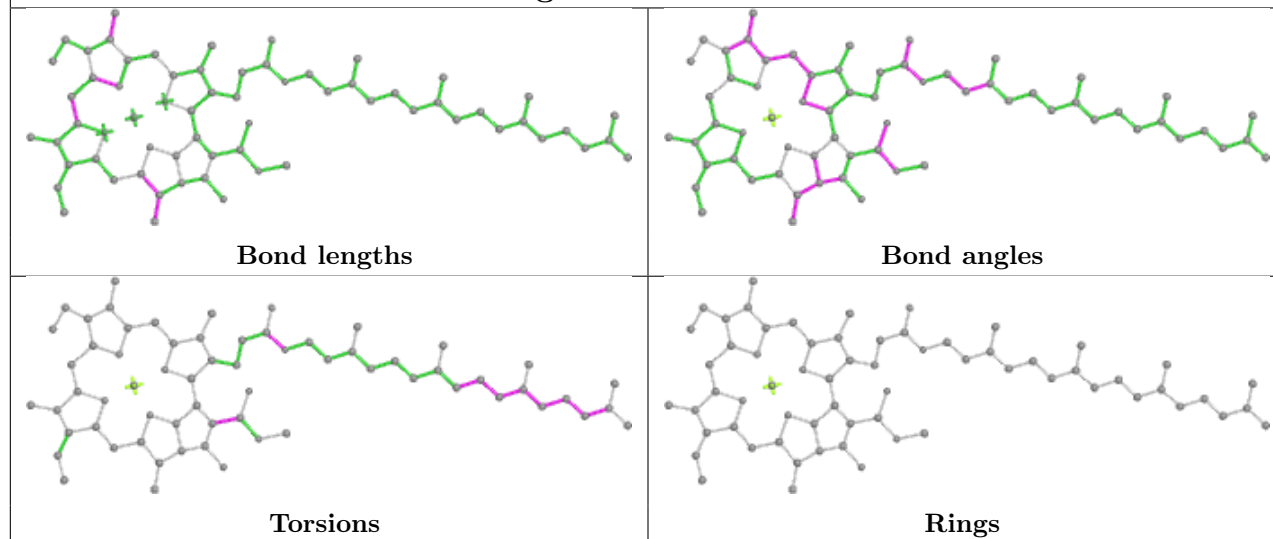


Ligand LMG b 626

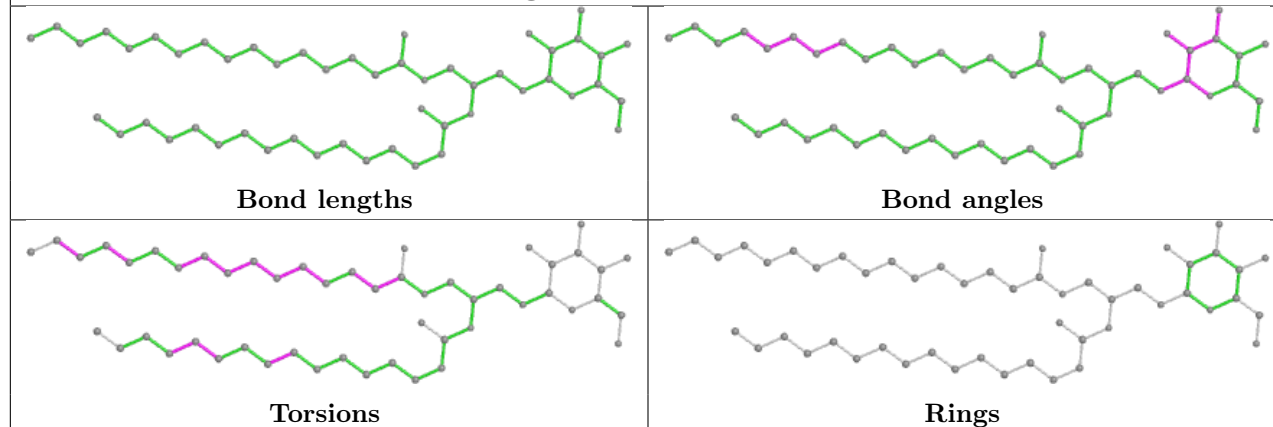




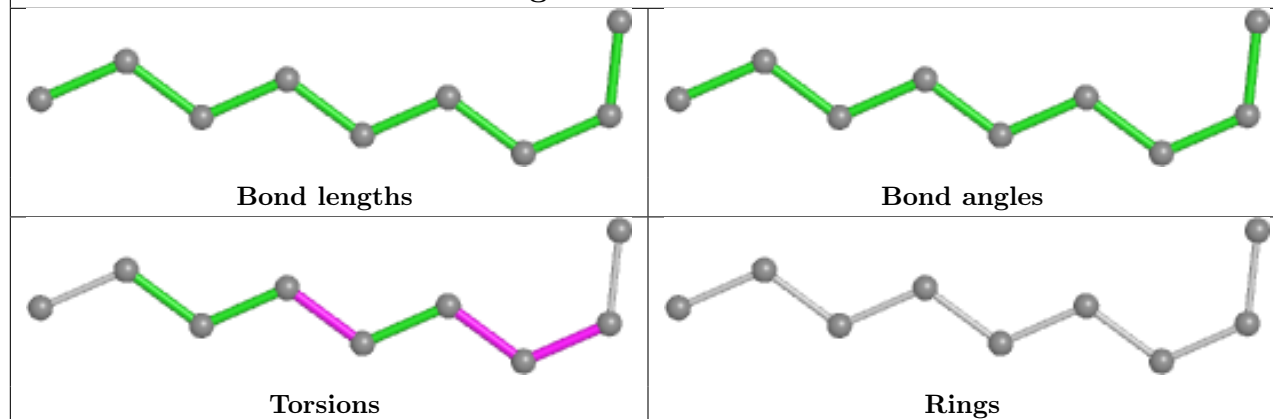
Ligand CLA c 508



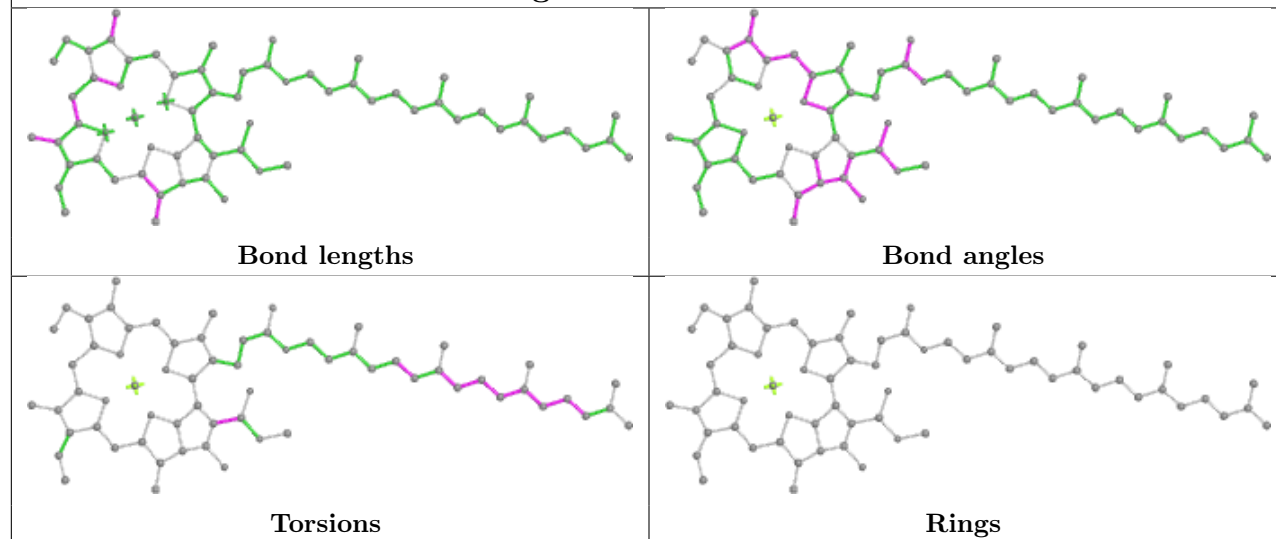
Ligand LMG M 101



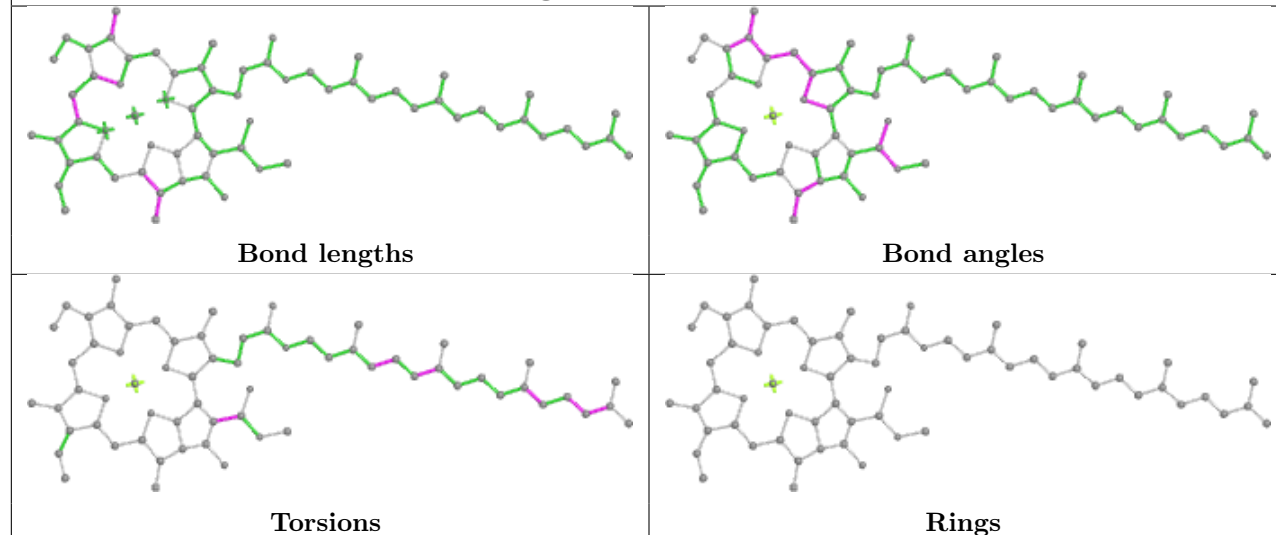
Ligand LMG b 628



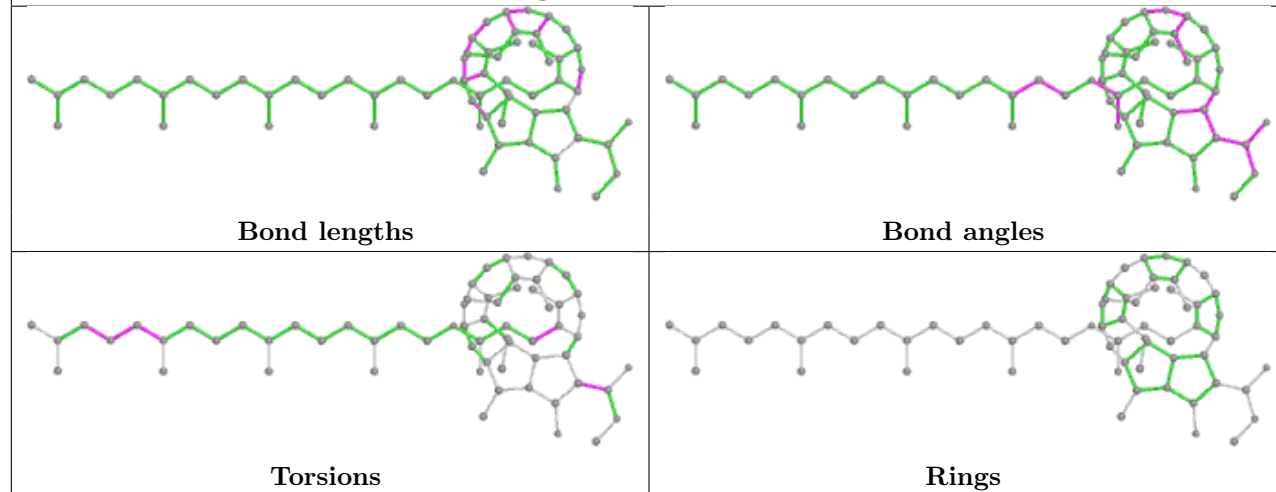
Ligand CLA B 617



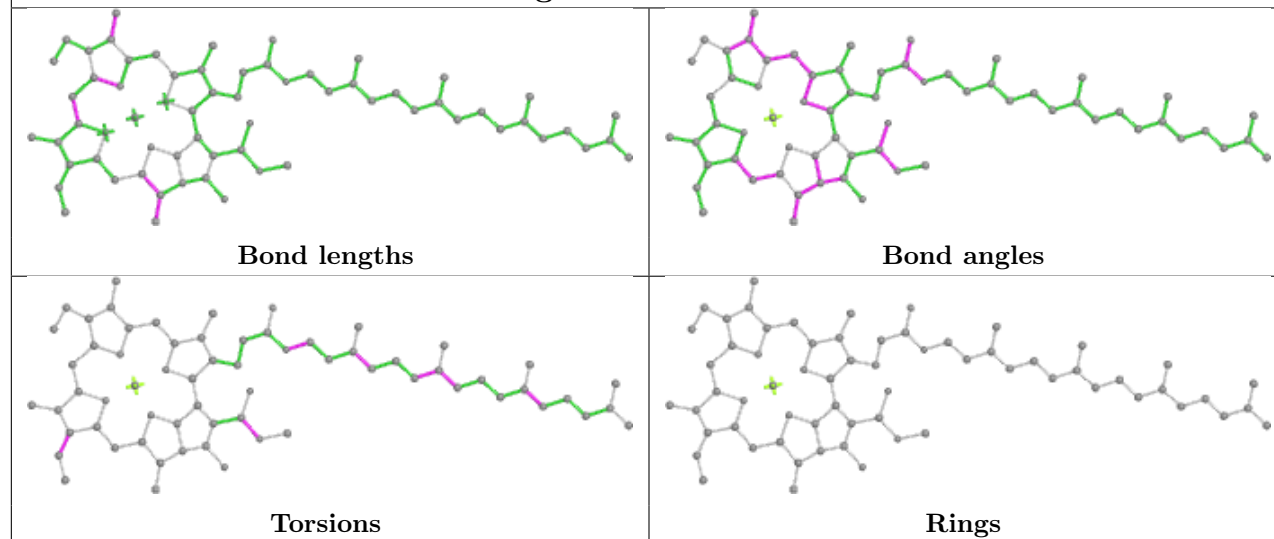
Ligand CLA c 507



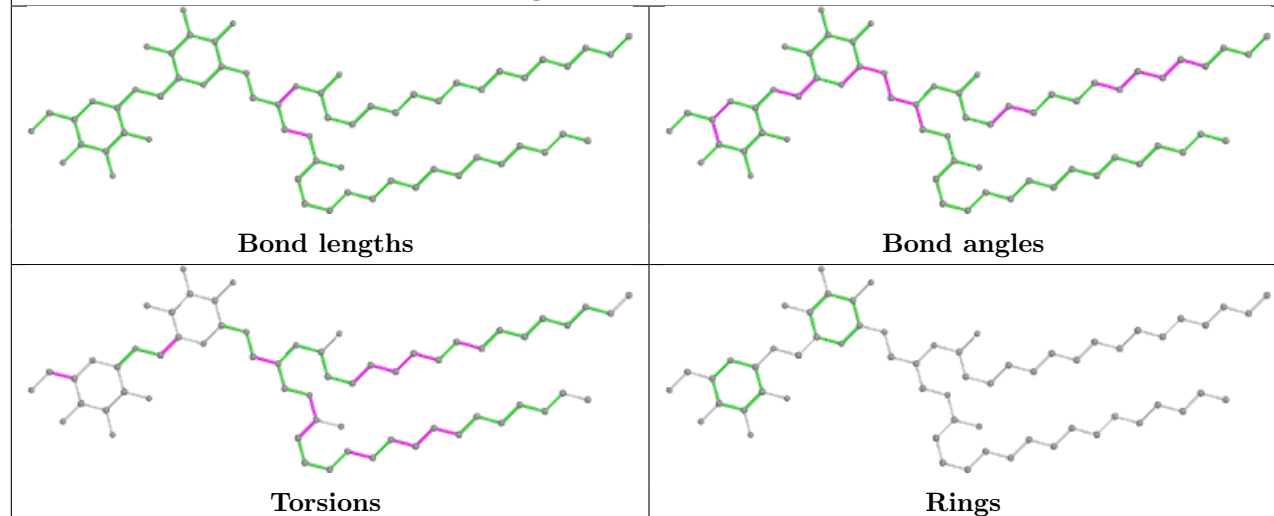
Ligand PHO a 709



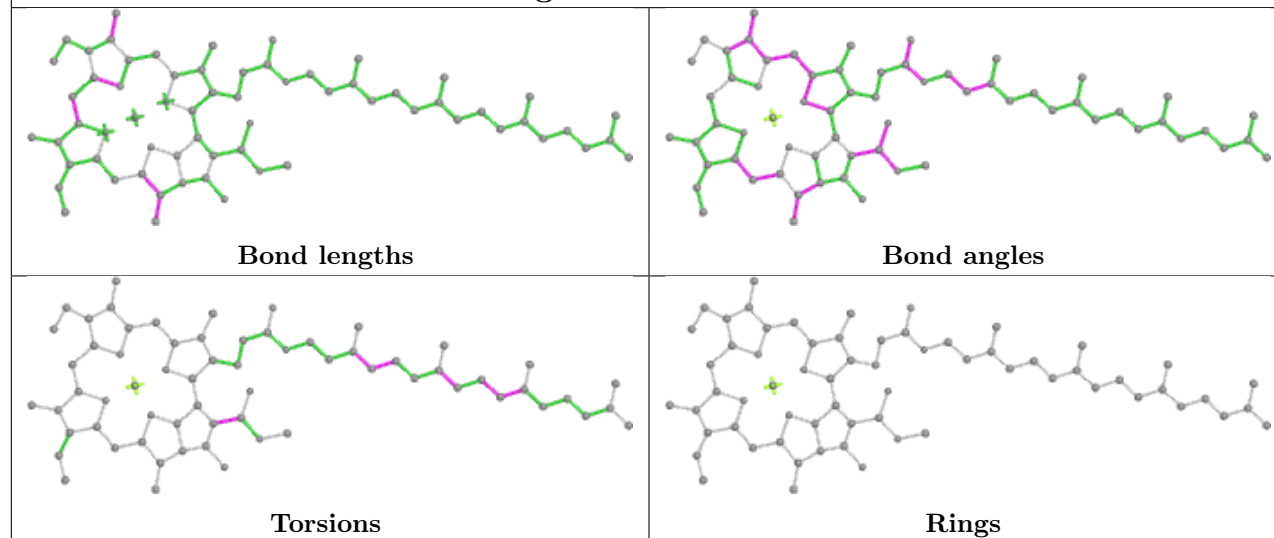
Ligand CLA d 402



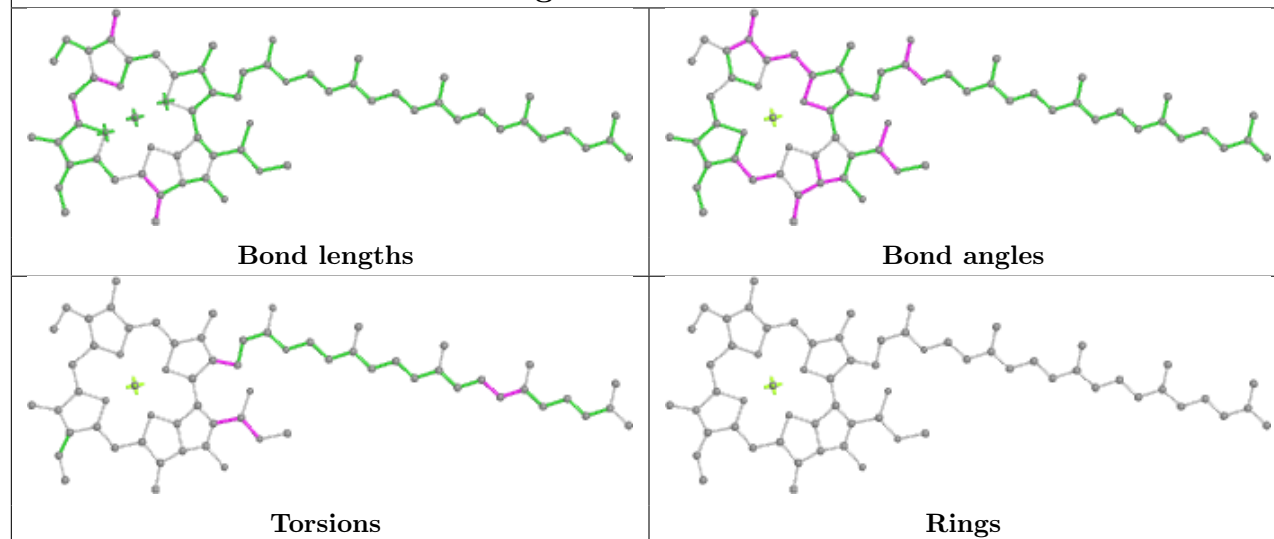
Ligand DGD C 517



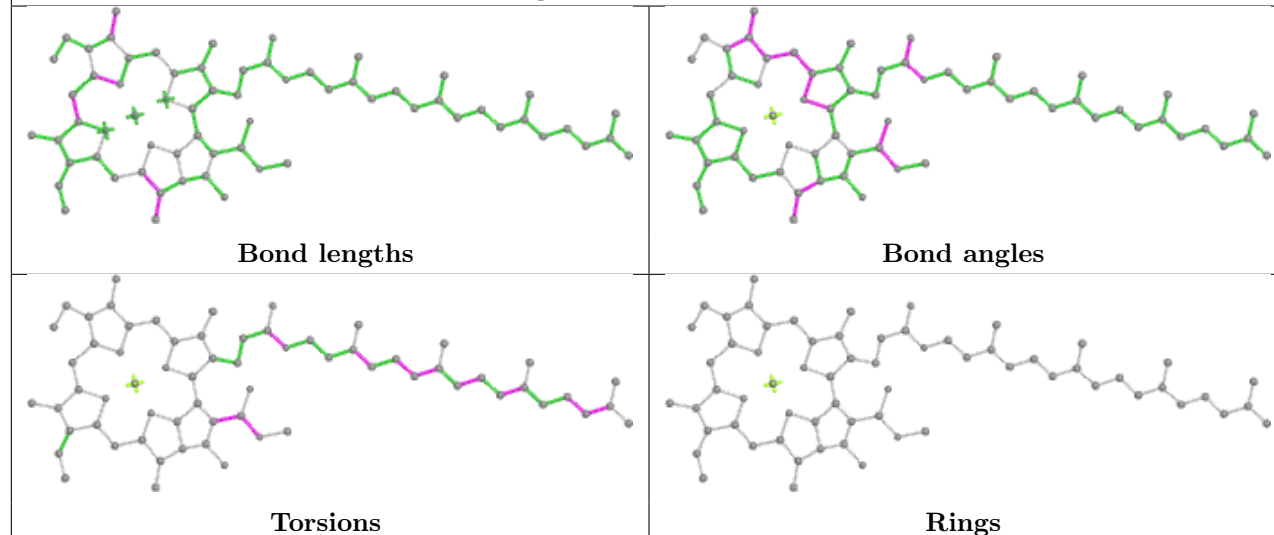
Ligand CLA b 610



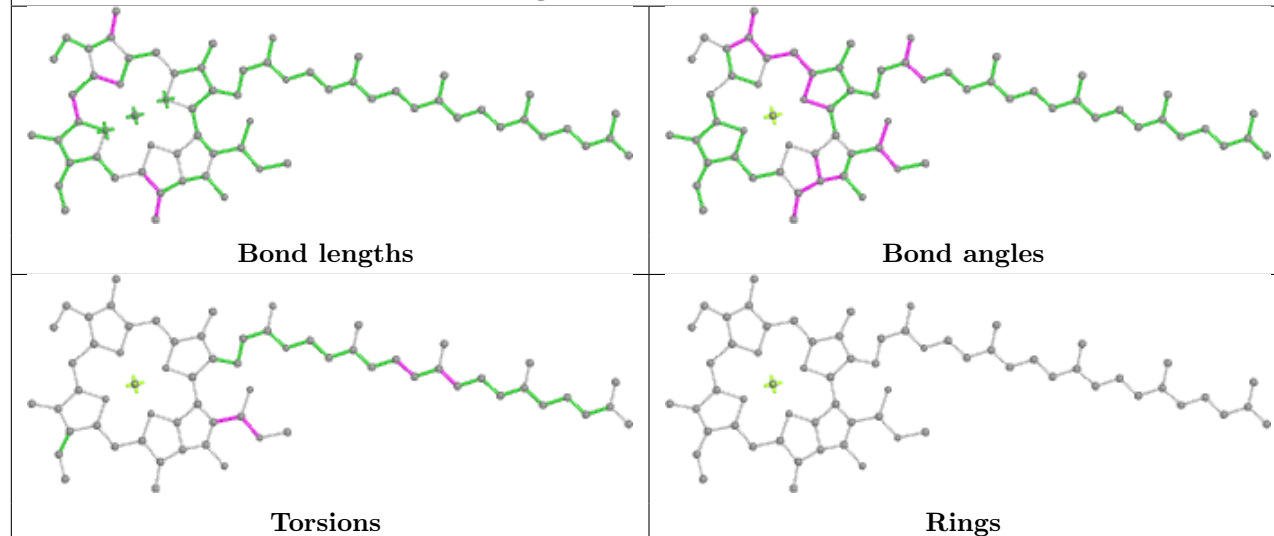
Ligand CLA b 613



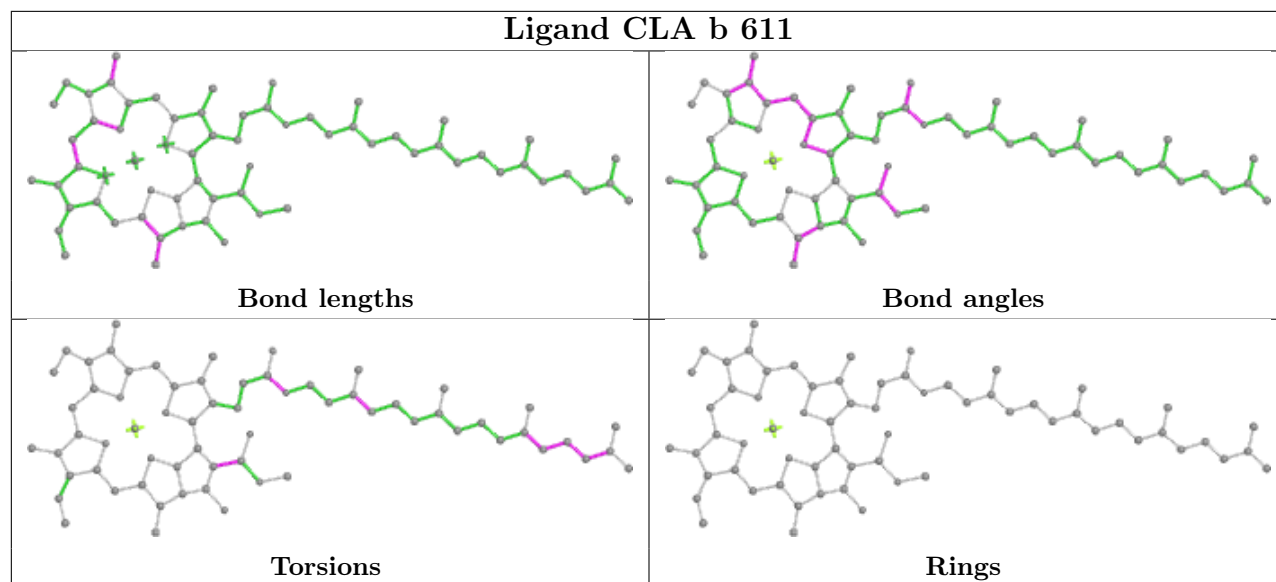
Ligand CLA B 604



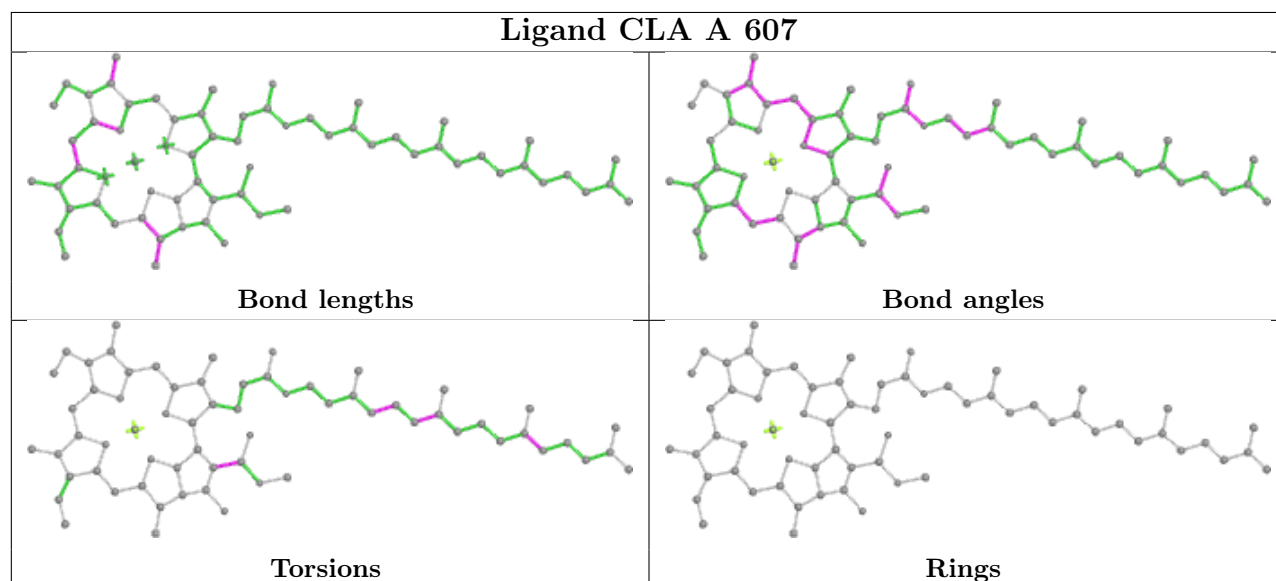
Ligand CLA C 509



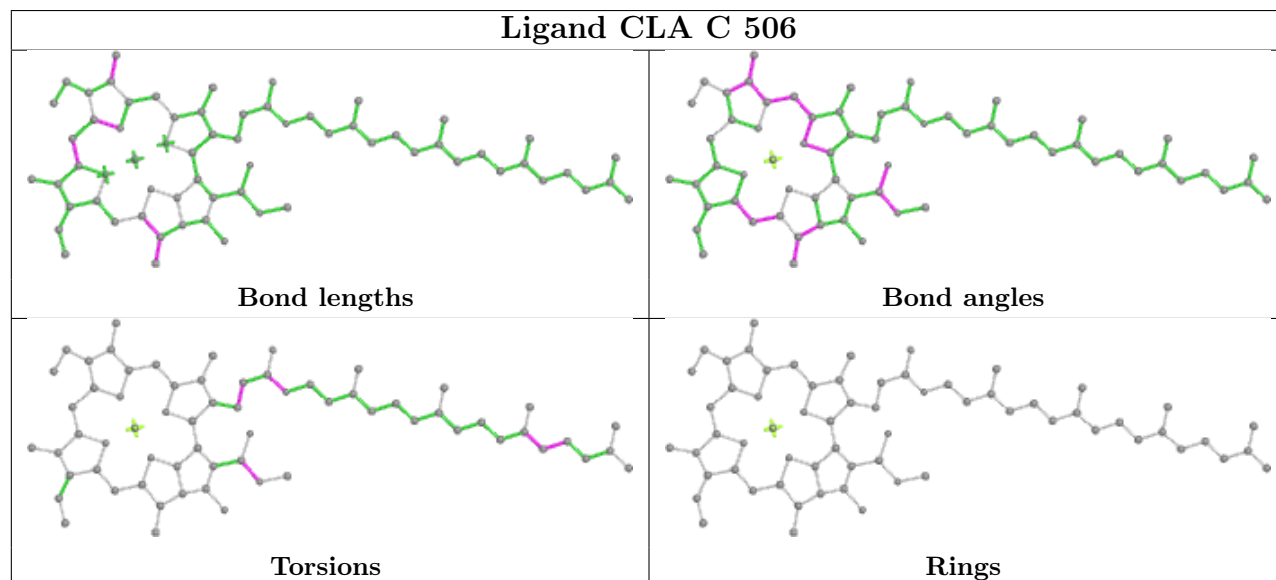
Ligand CLA b 611

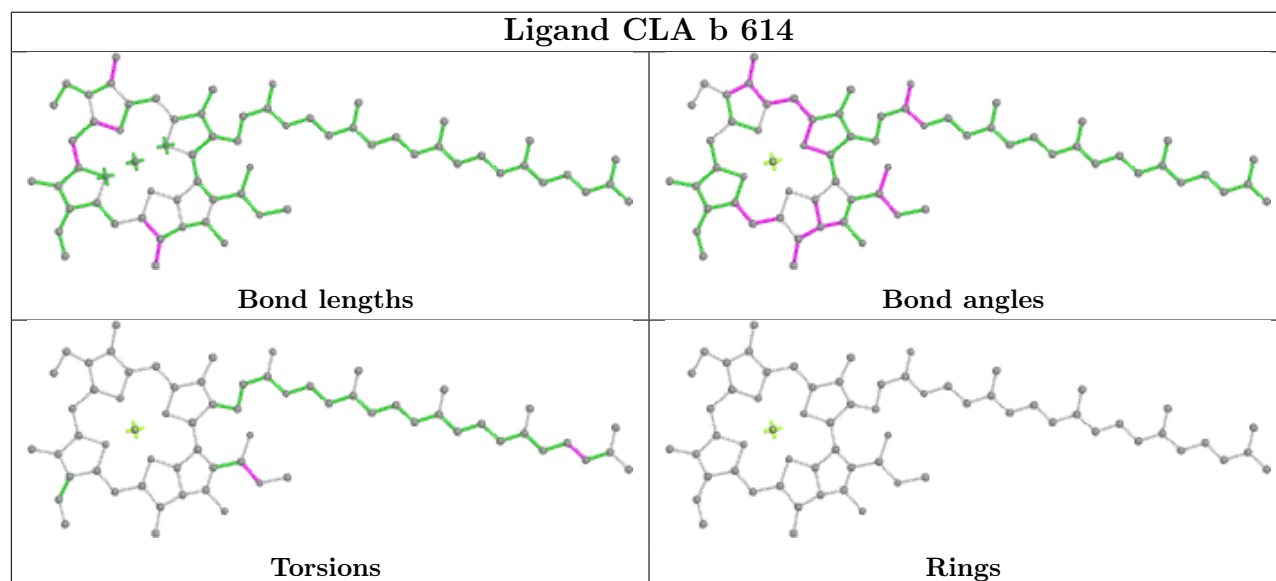
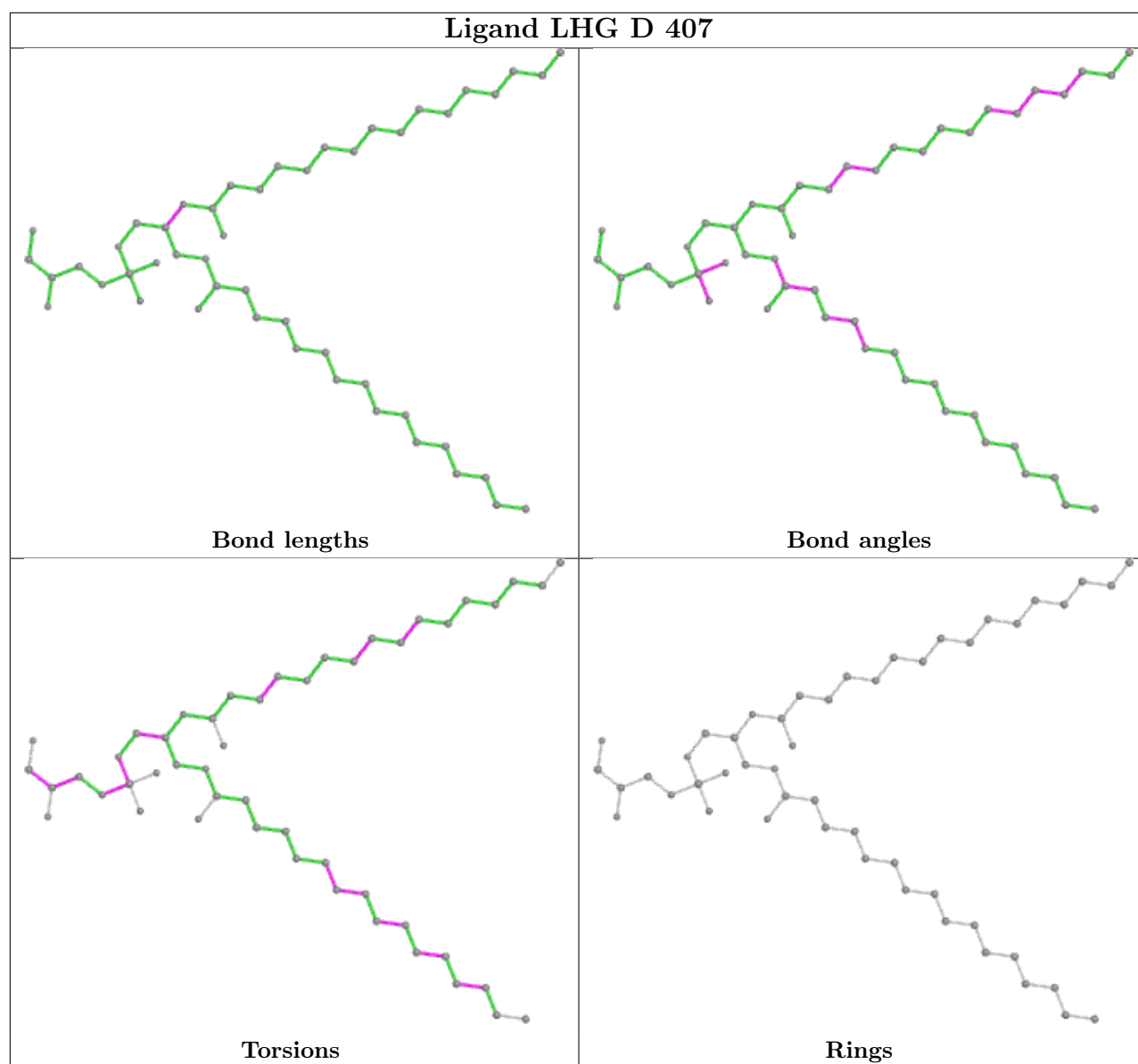


Ligand CLA A 607

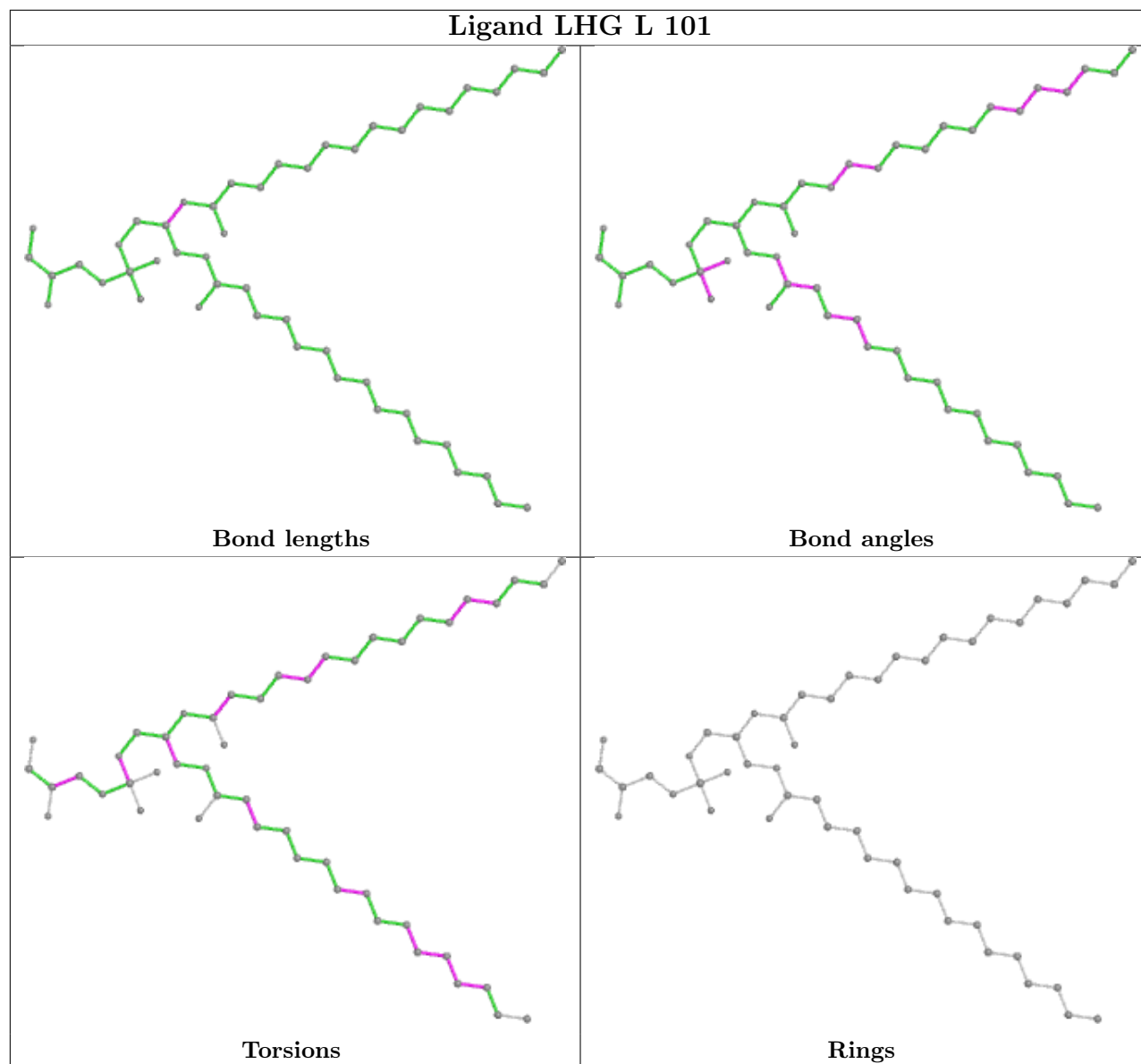


Ligand CLA C 506

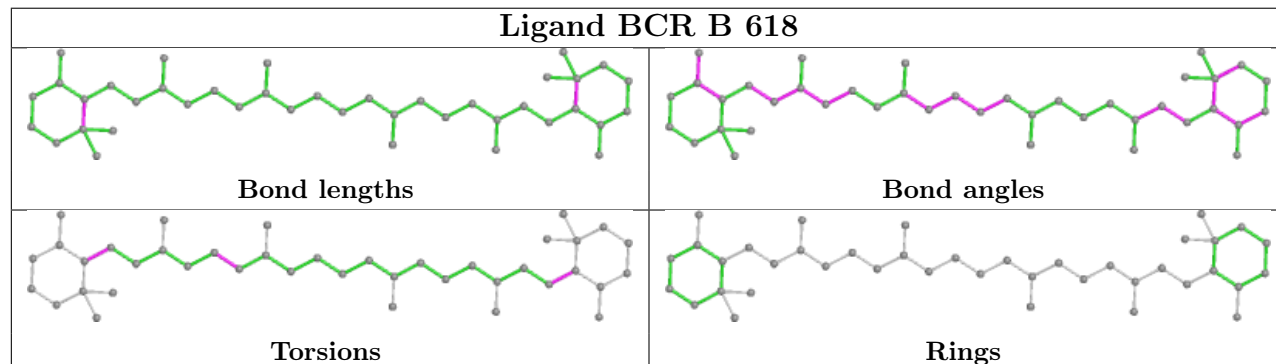


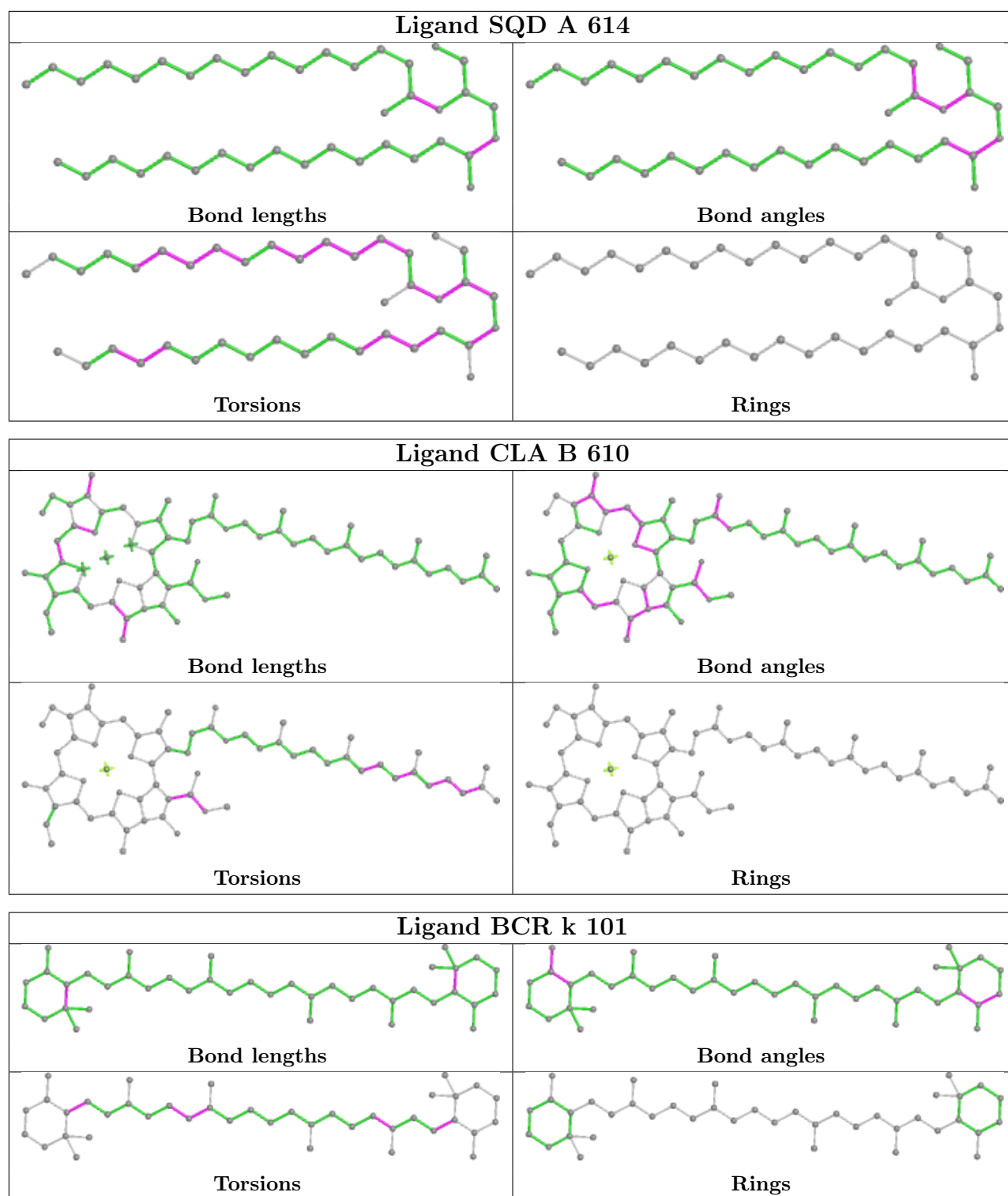


Ligand LHG L 101

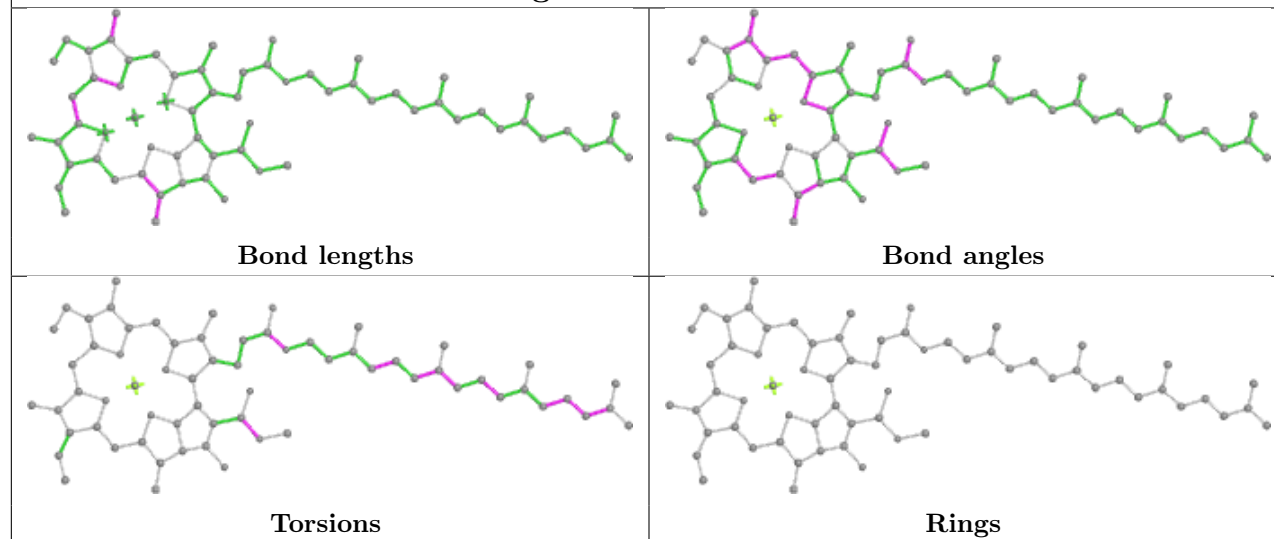


Ligand BCR B 618

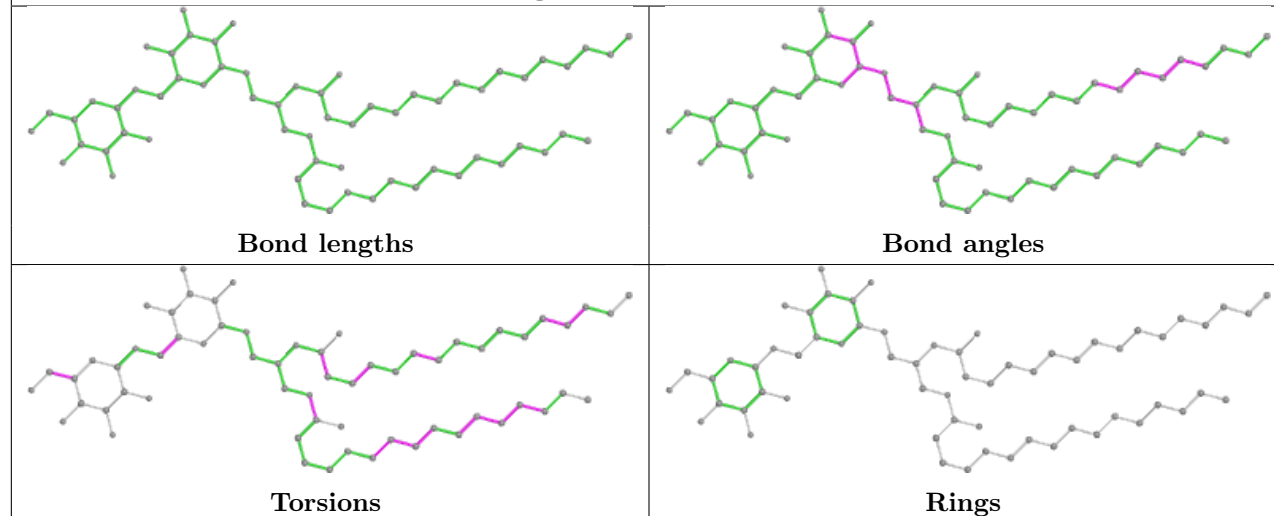




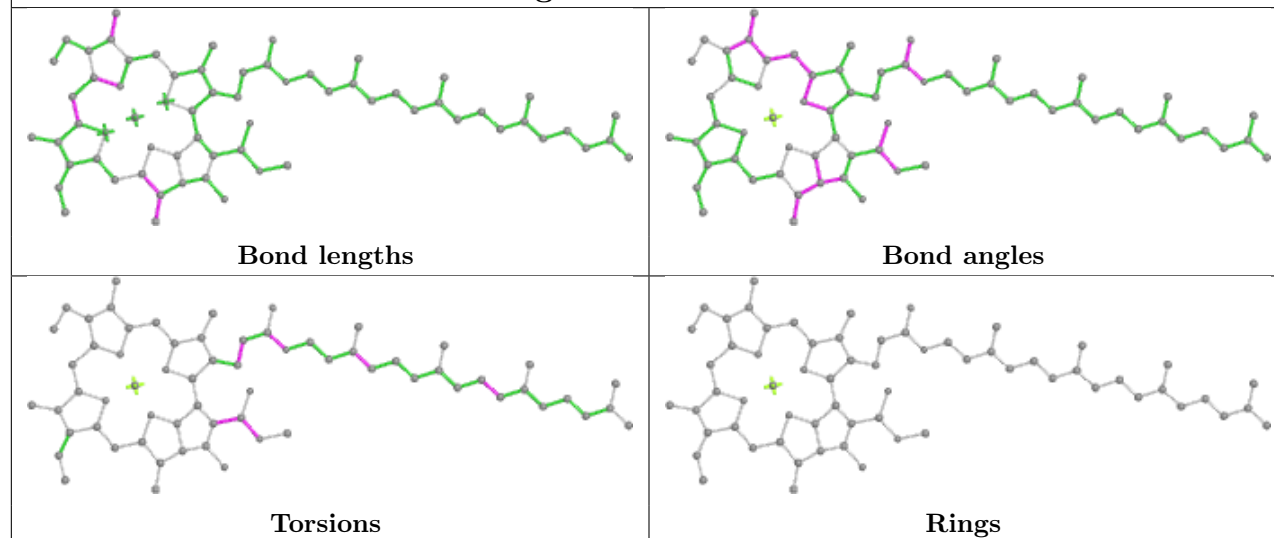
Ligand CLA C 512

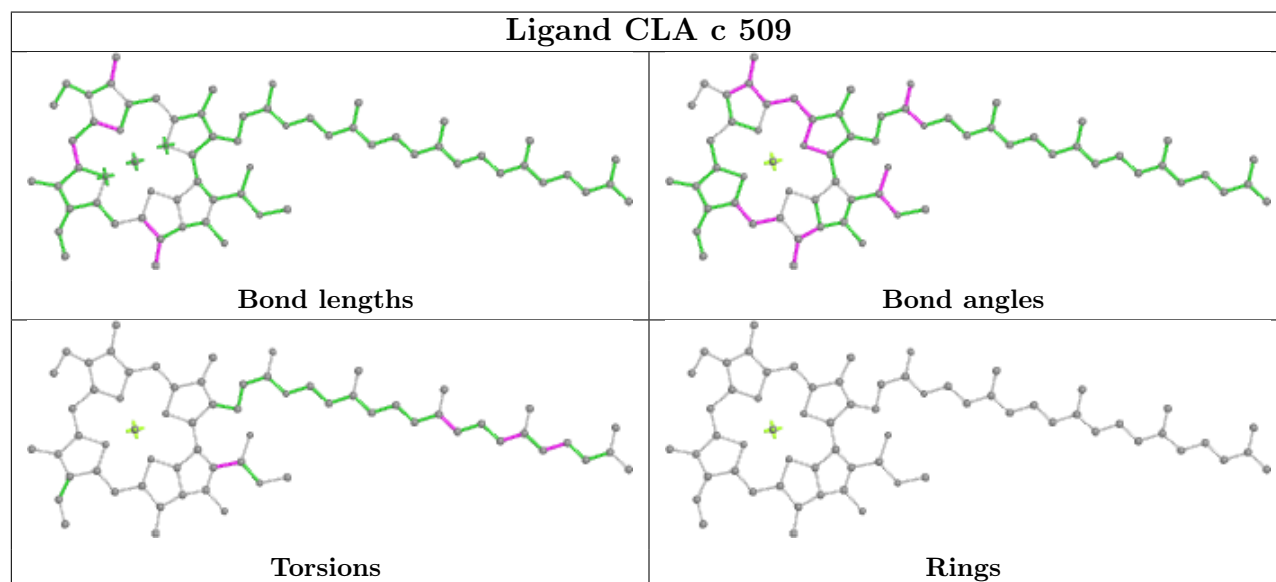
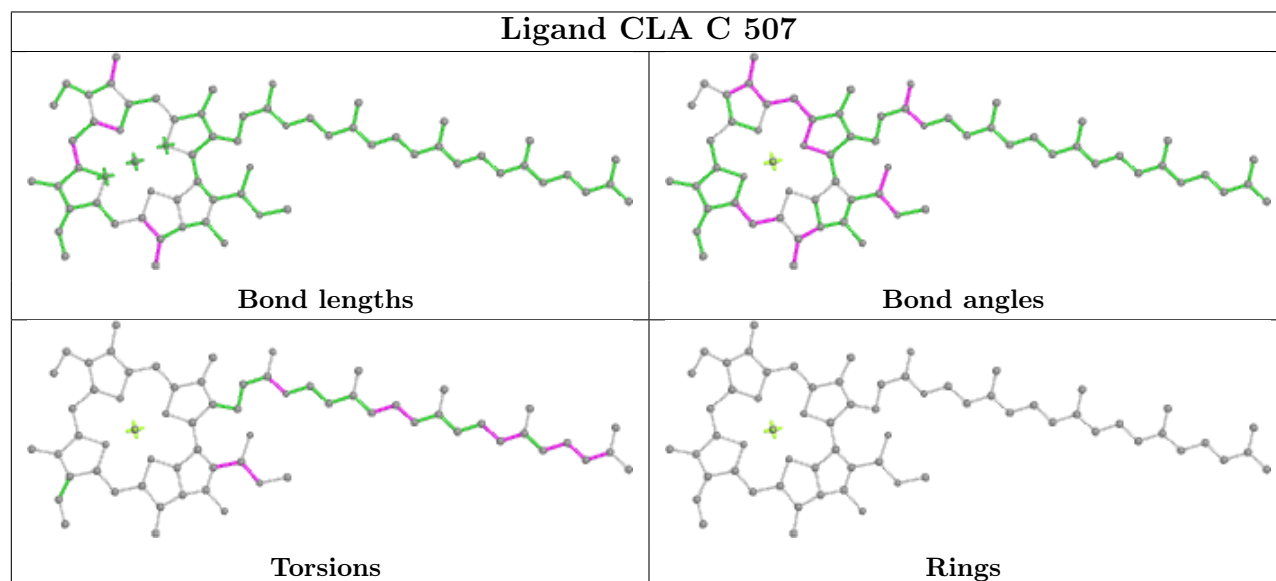
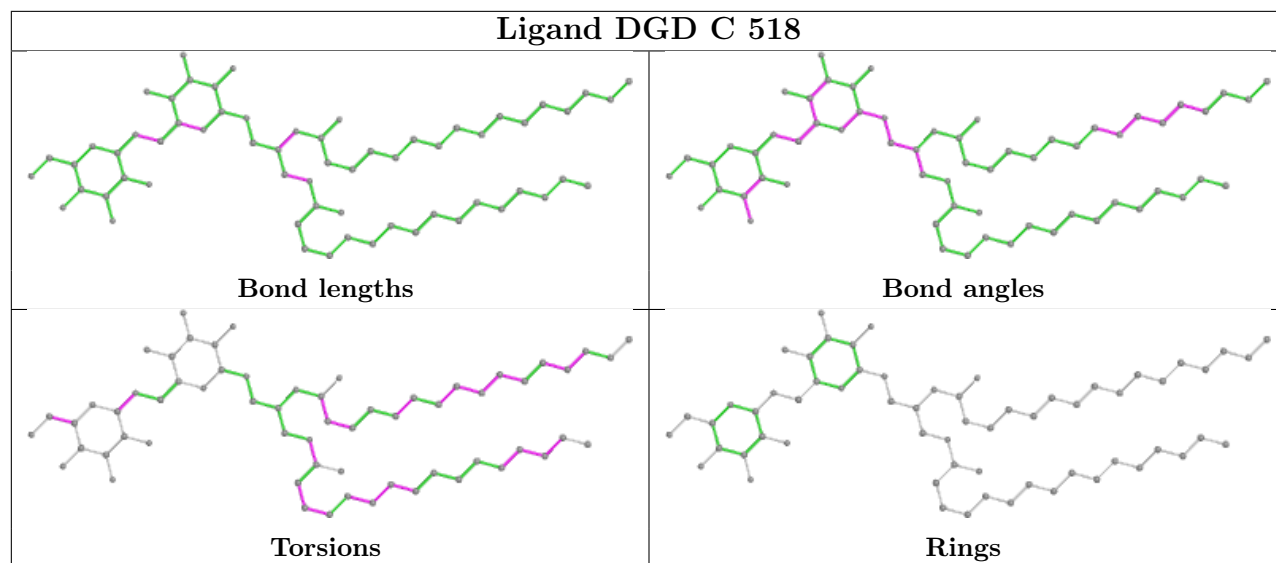


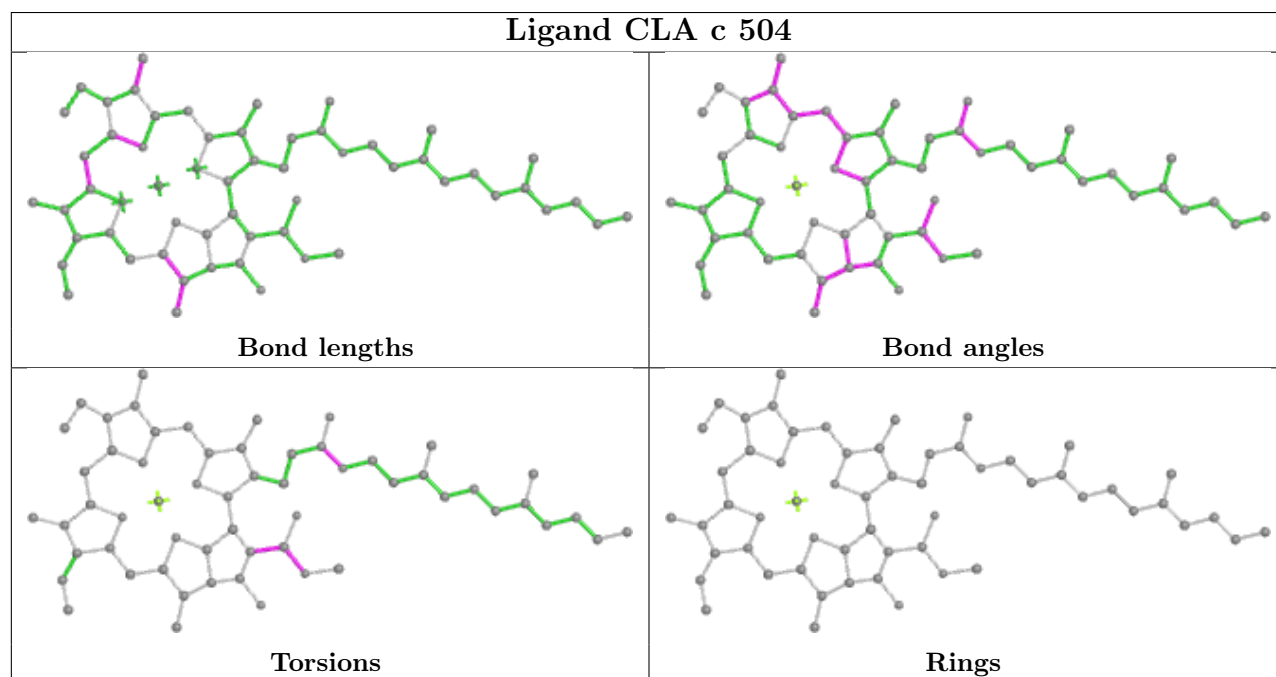
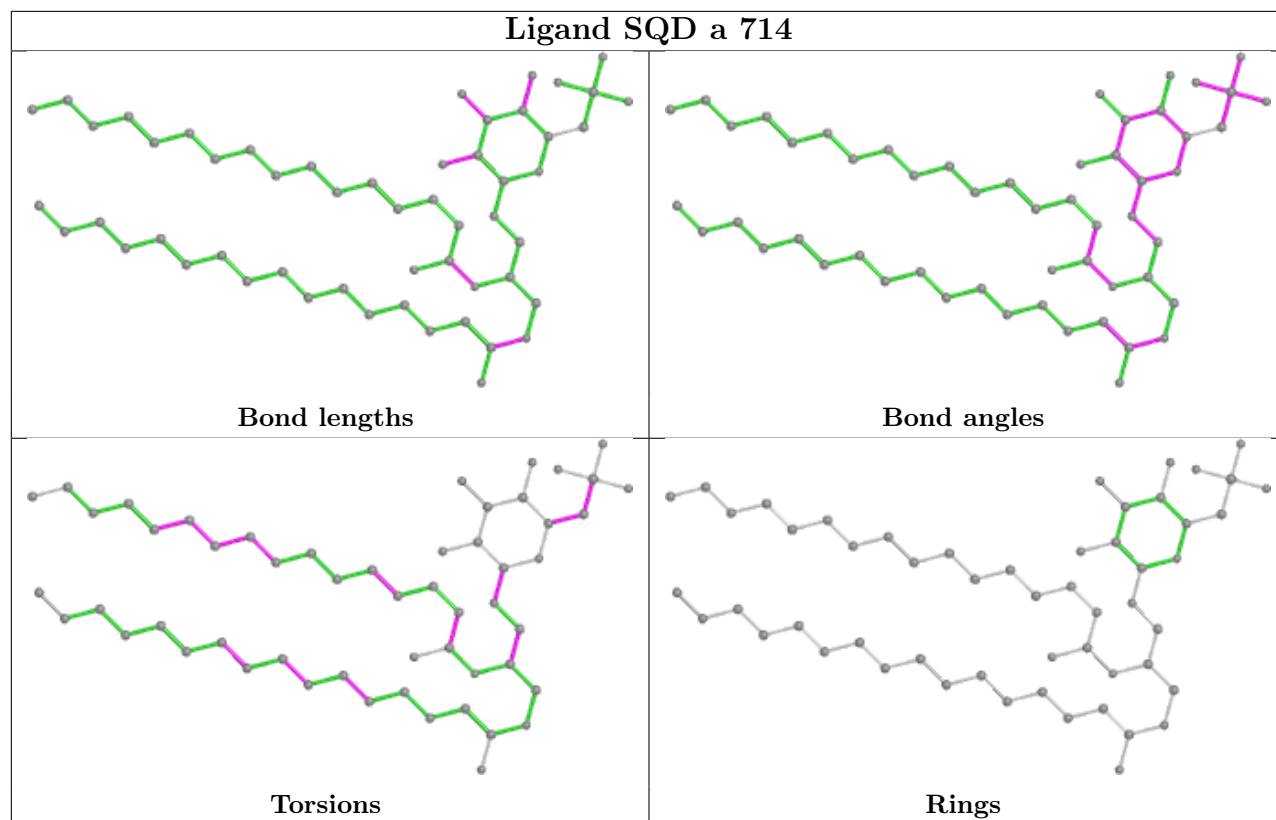
Ligand DGD h 102

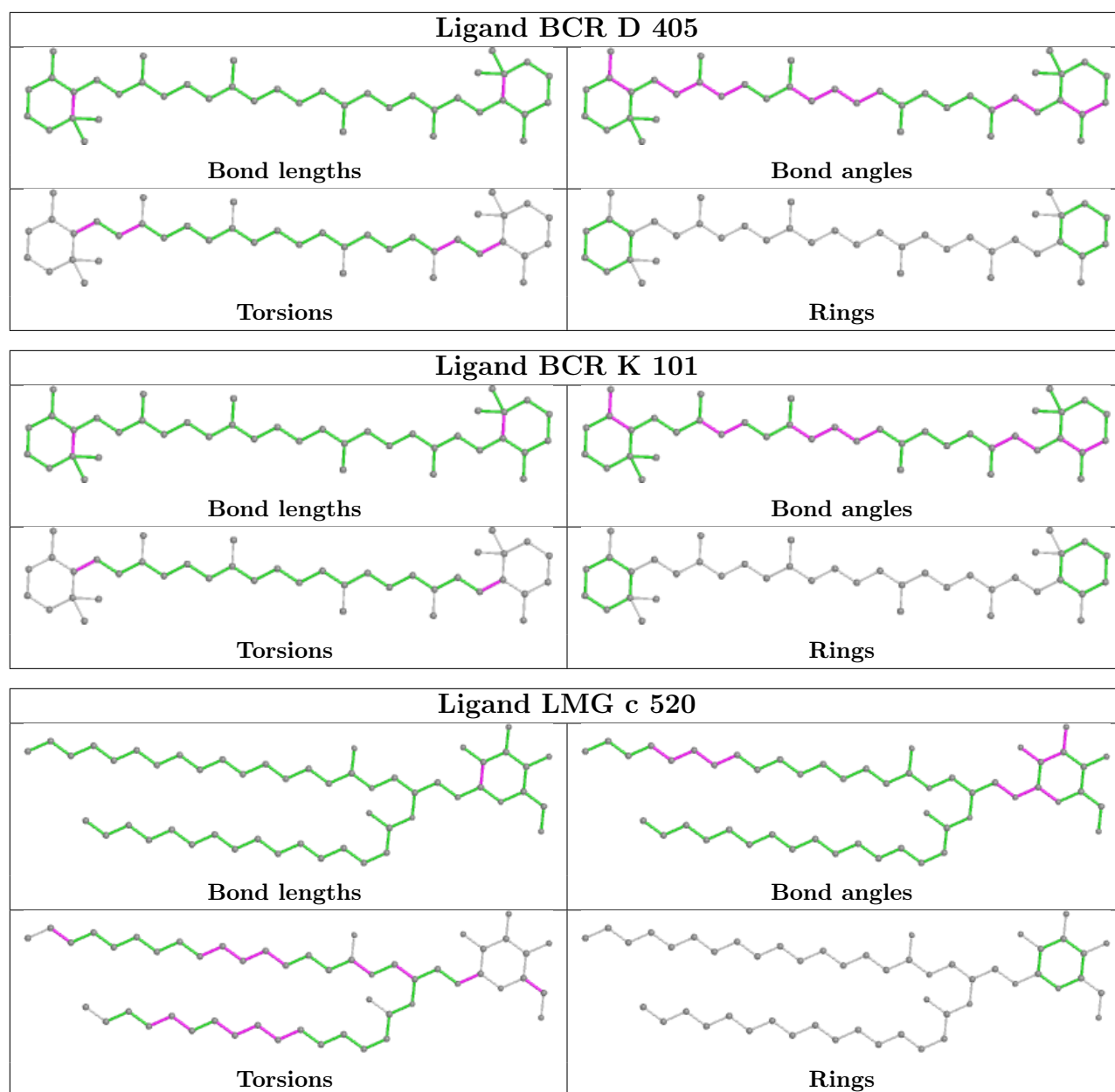


Ligand CLA b 620

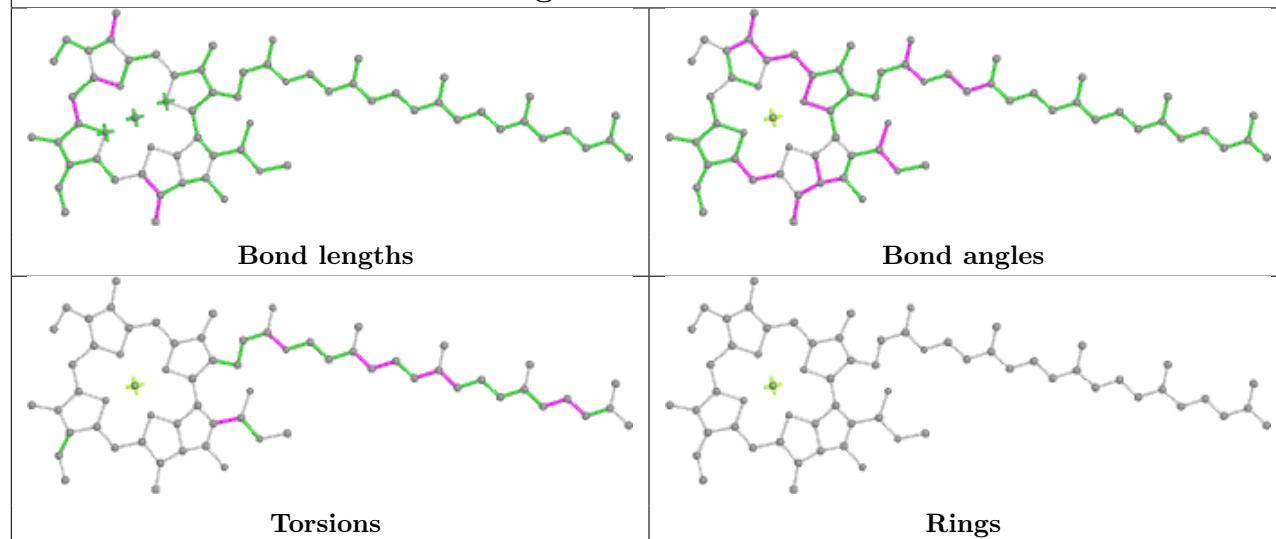




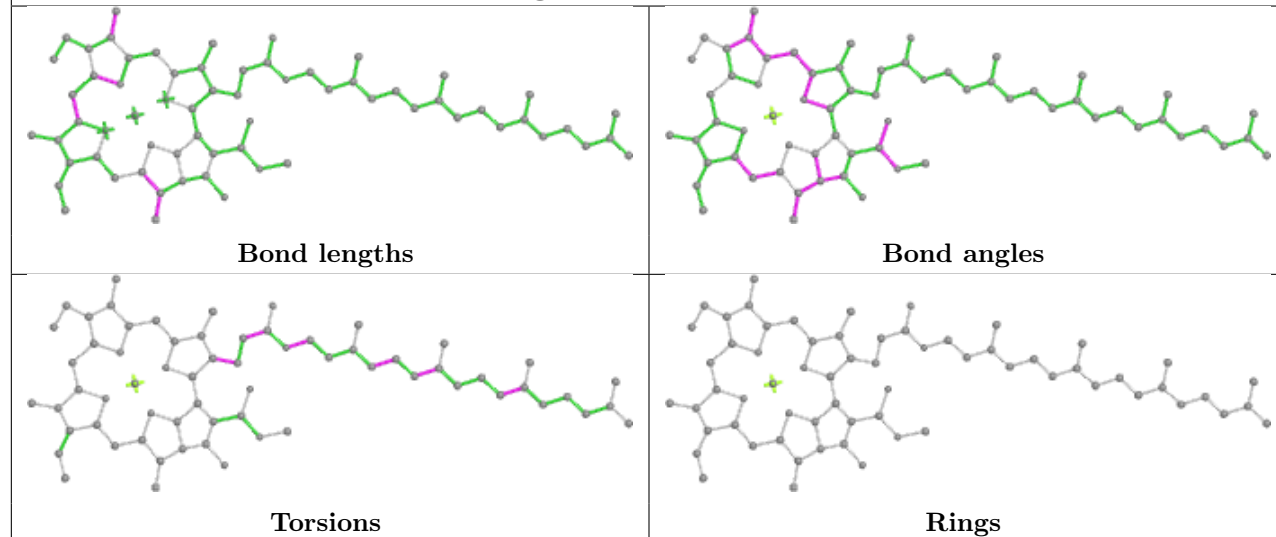




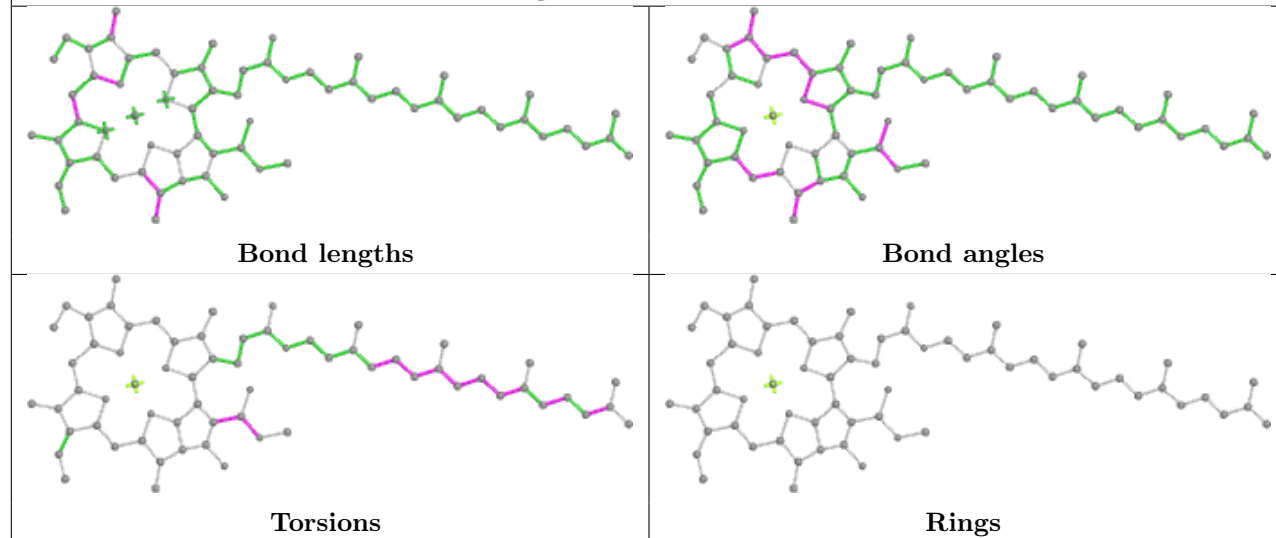
Ligand CLA b 615



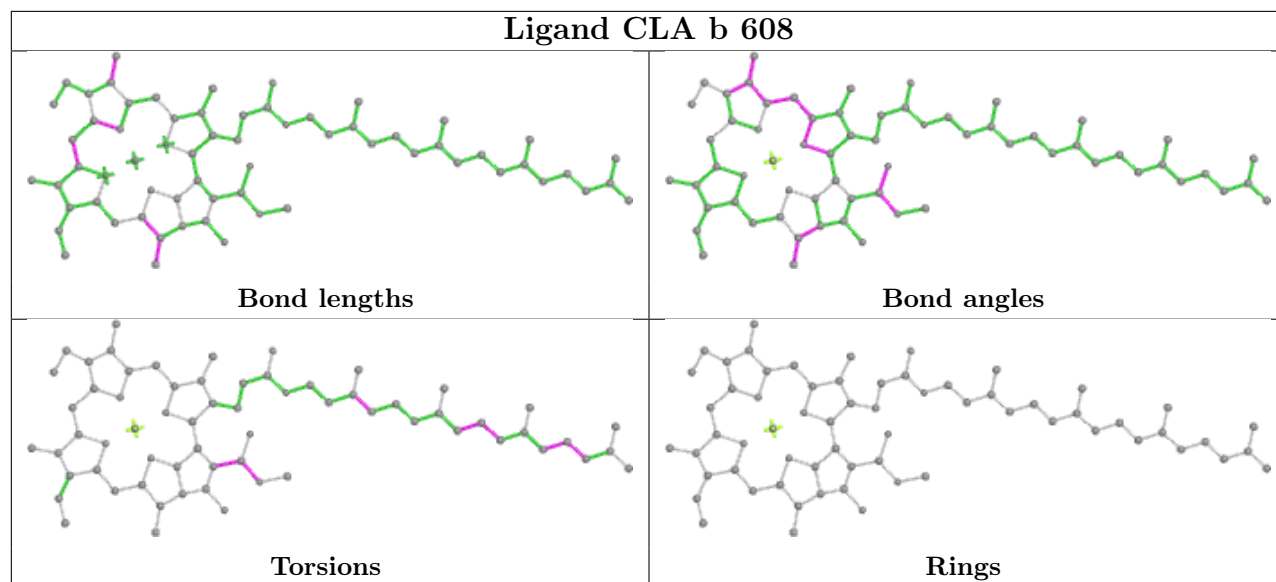
Ligand CLA D 403



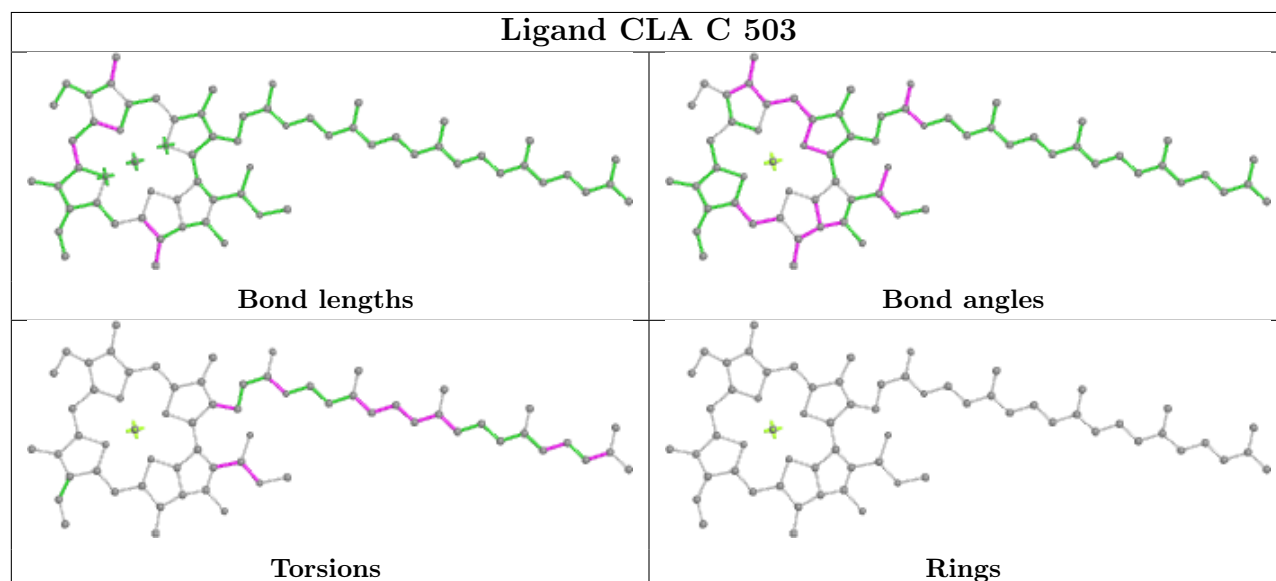
Ligand CLA C 510



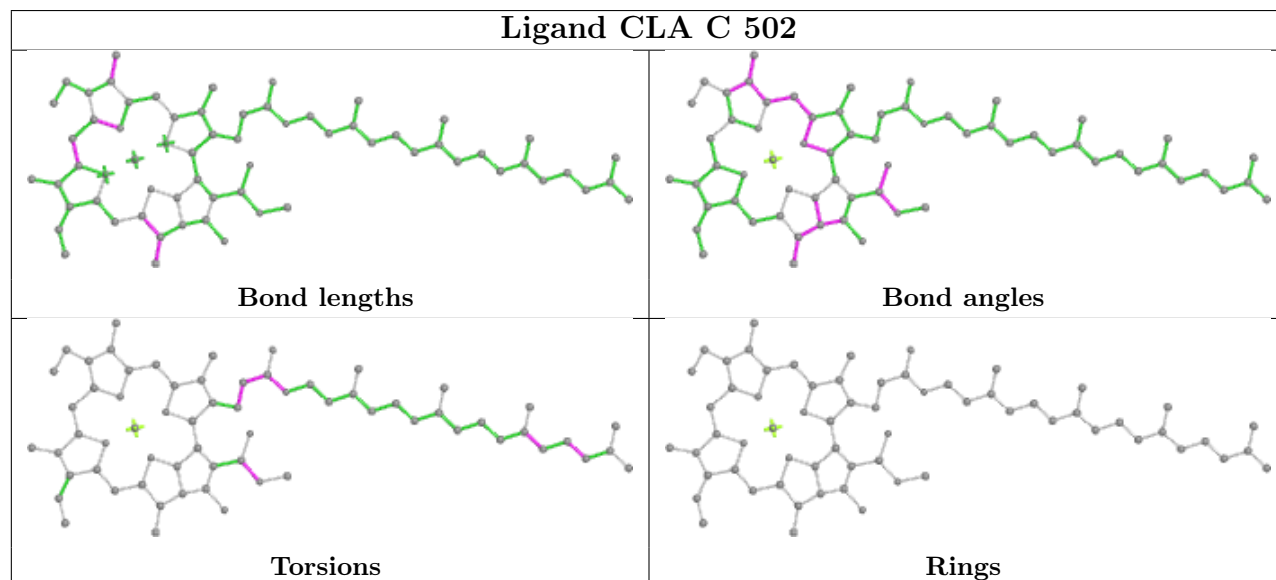
Ligand CLA b 608

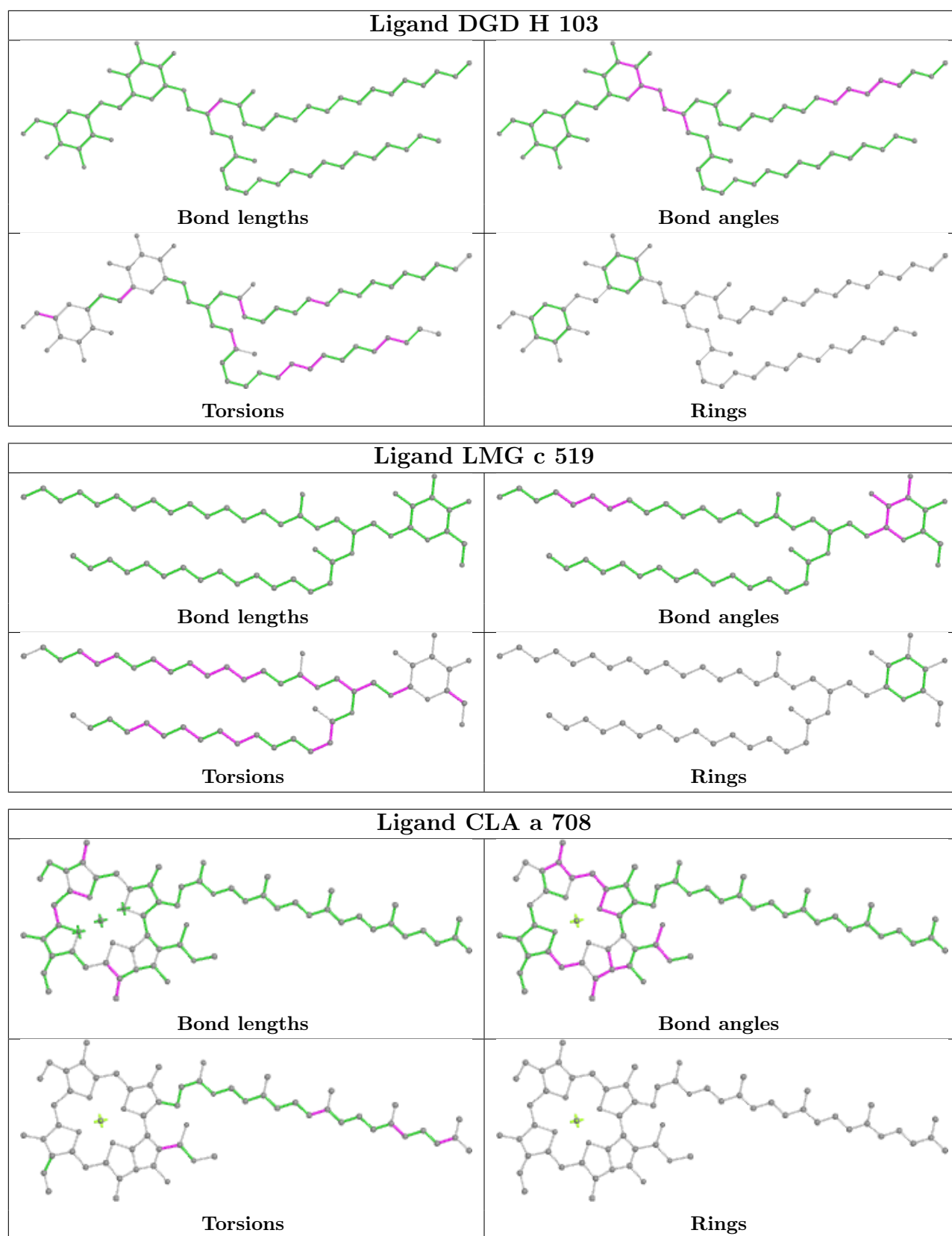


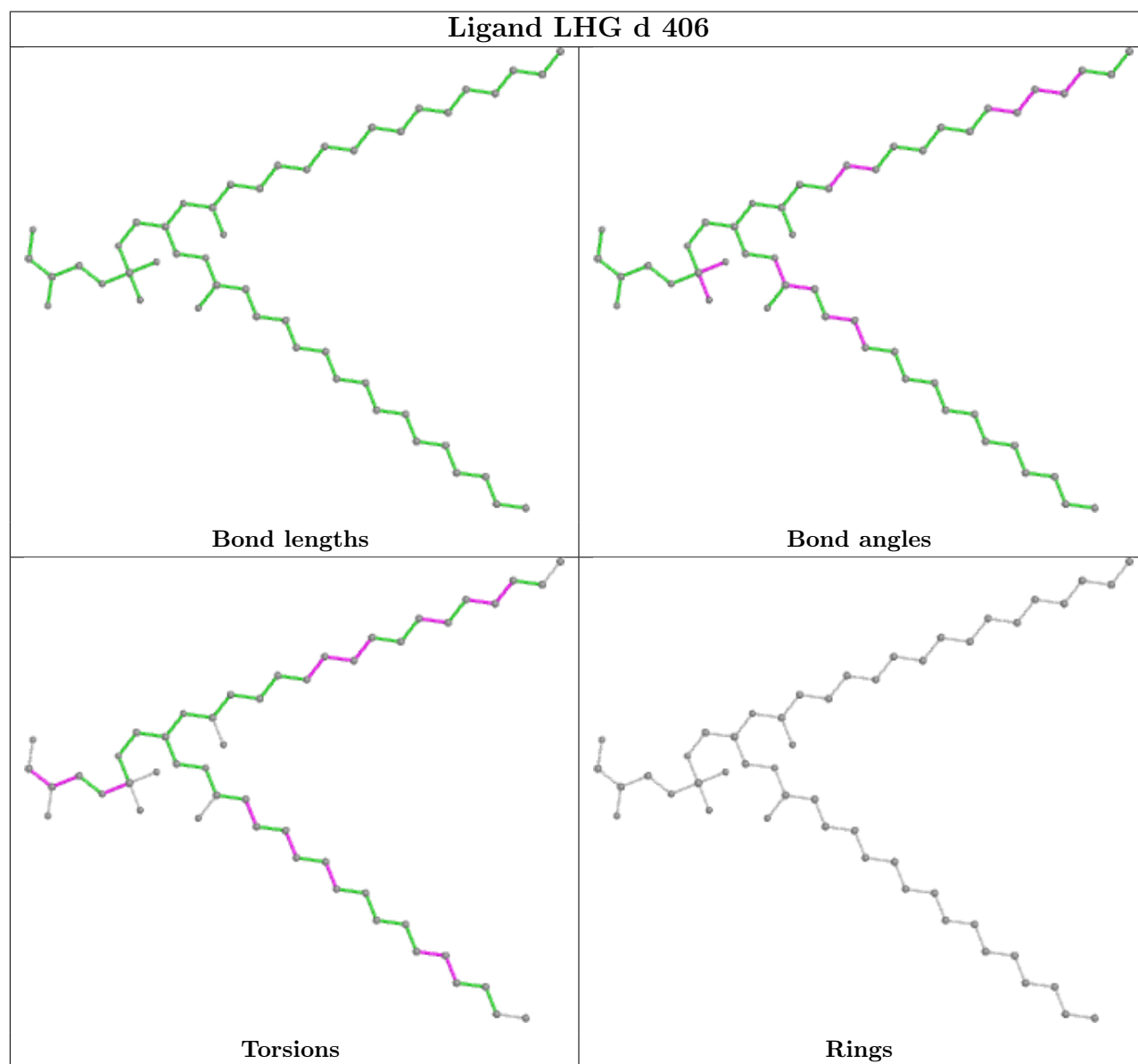
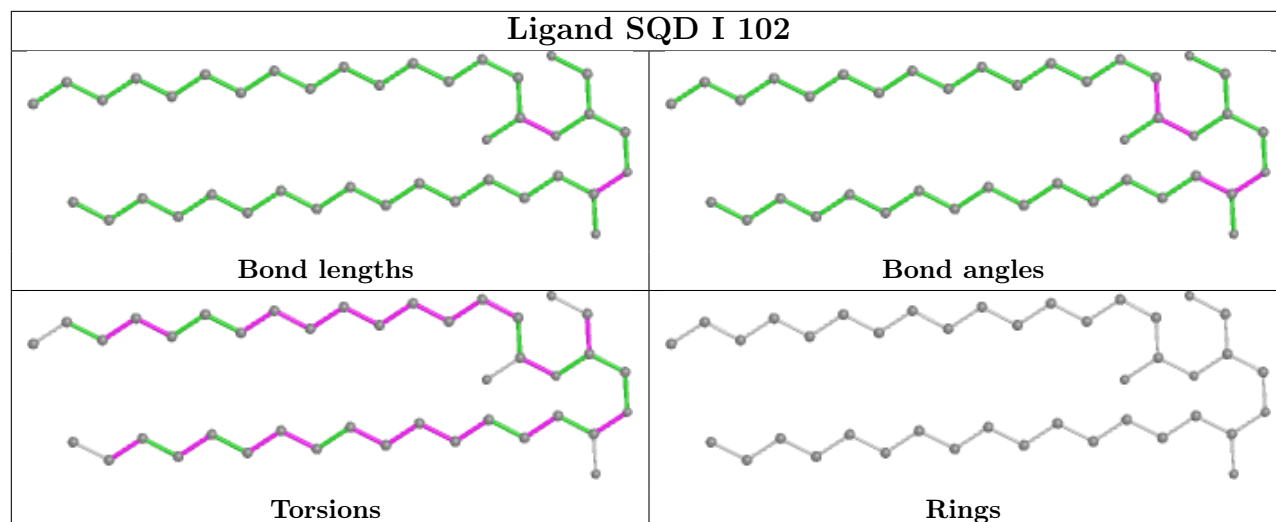
Ligand CLA C 503

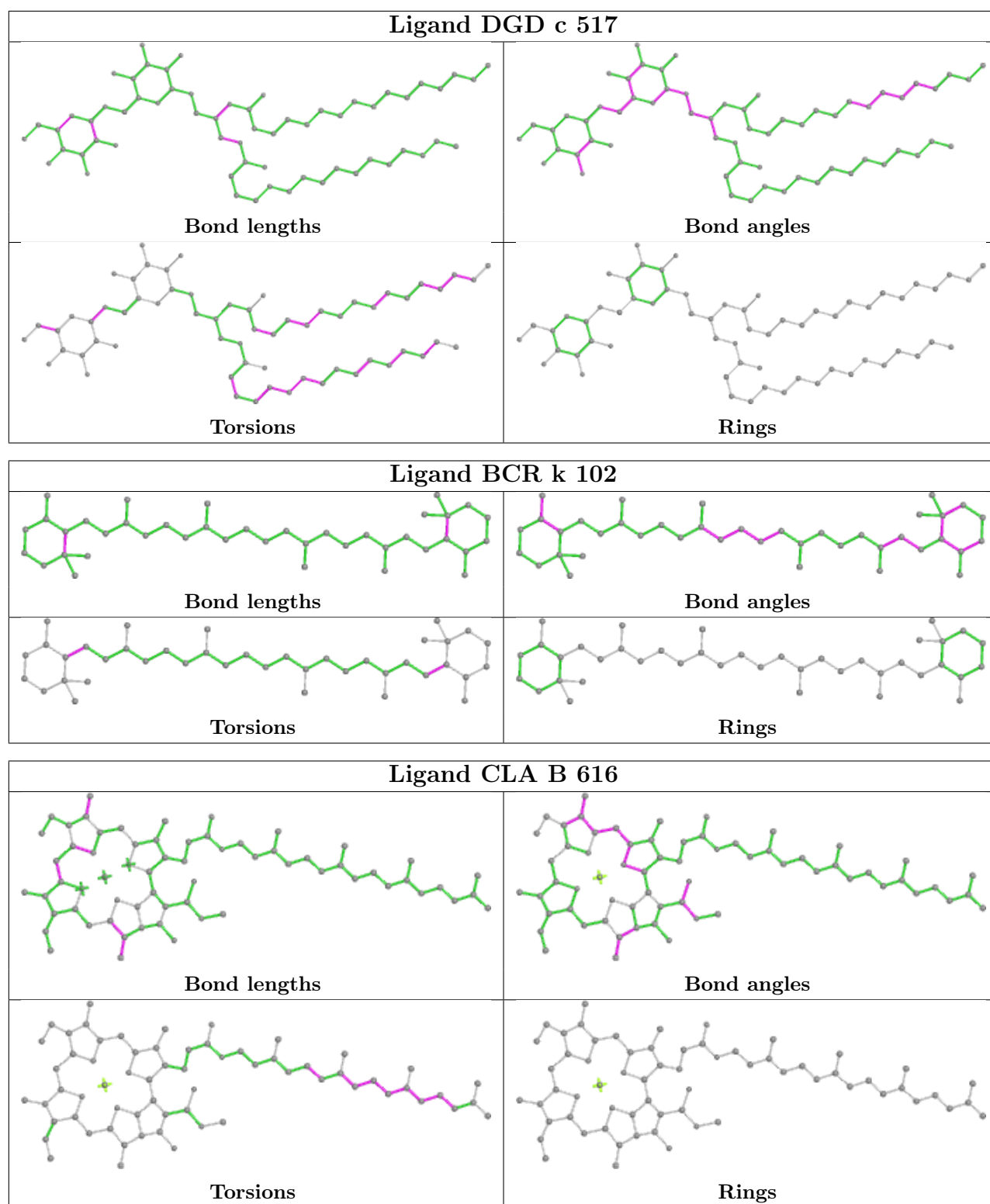


Ligand CLA C 502

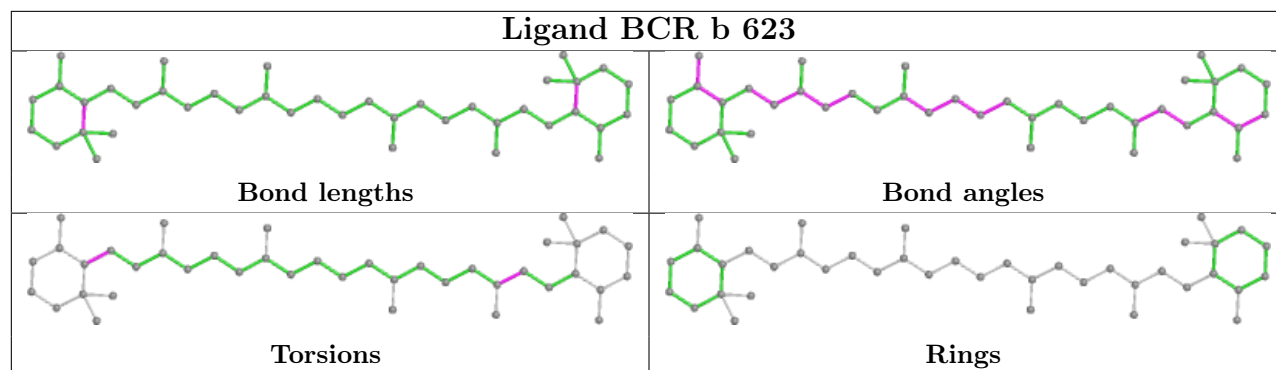




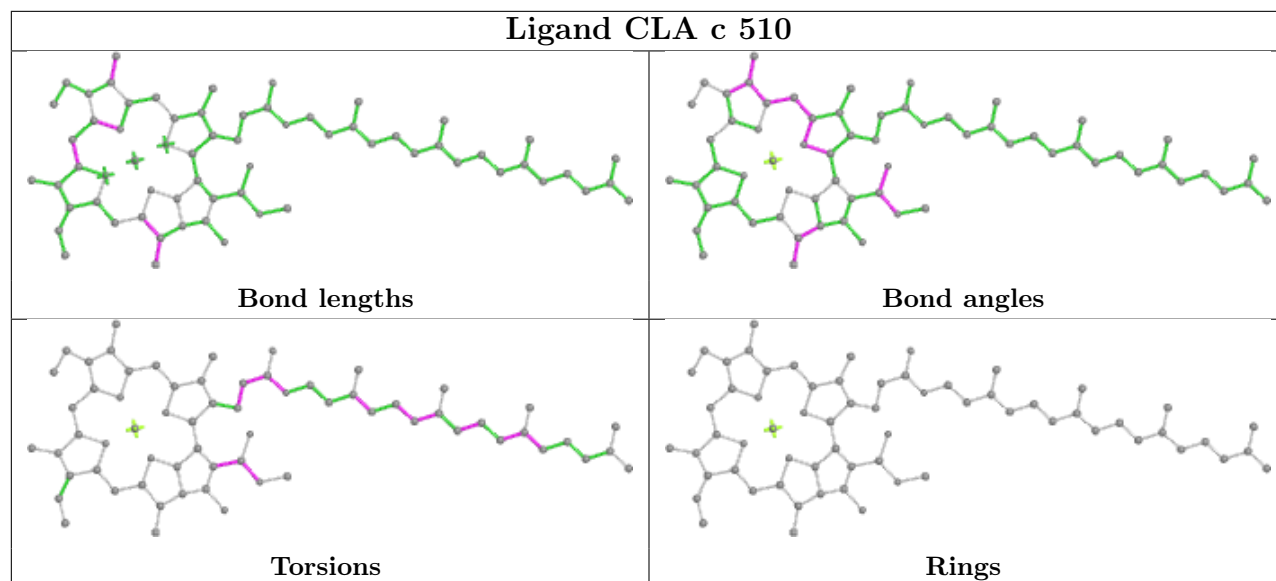




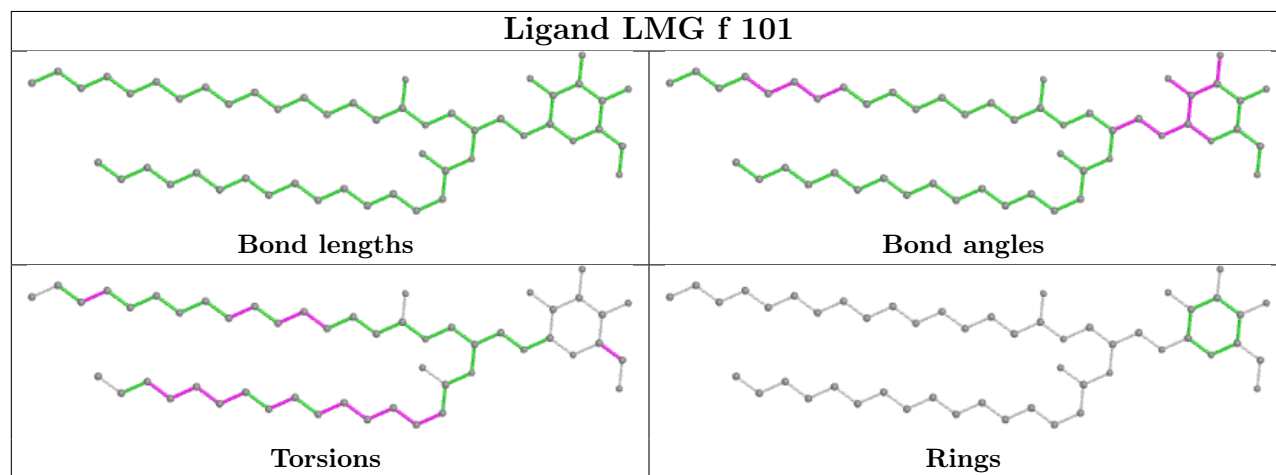
Ligand BCR b 623

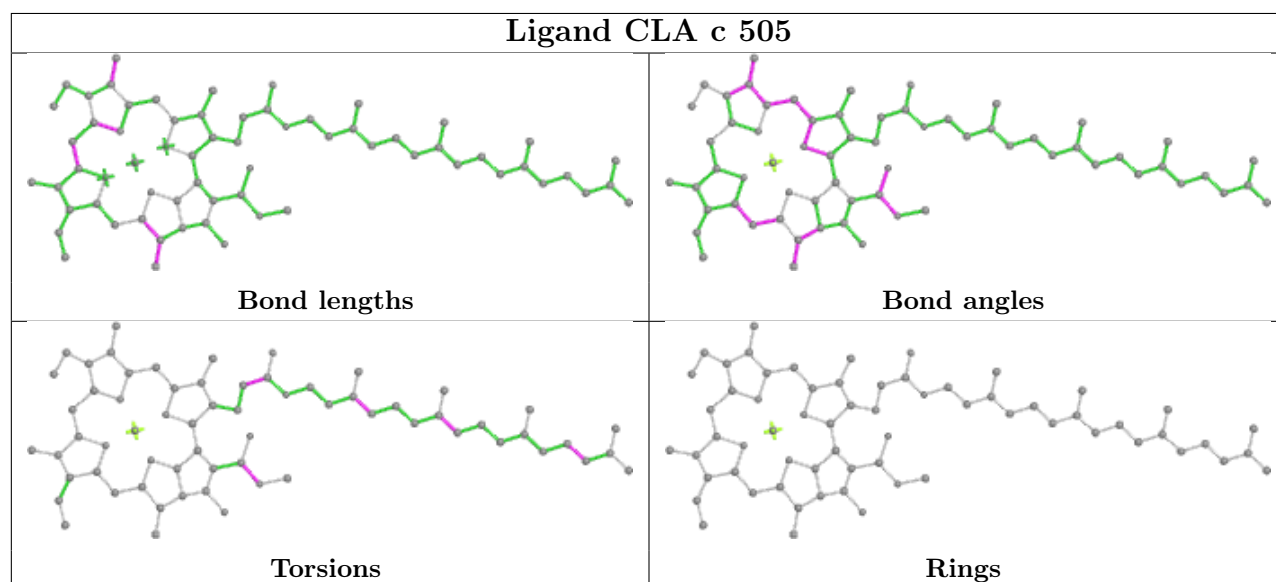
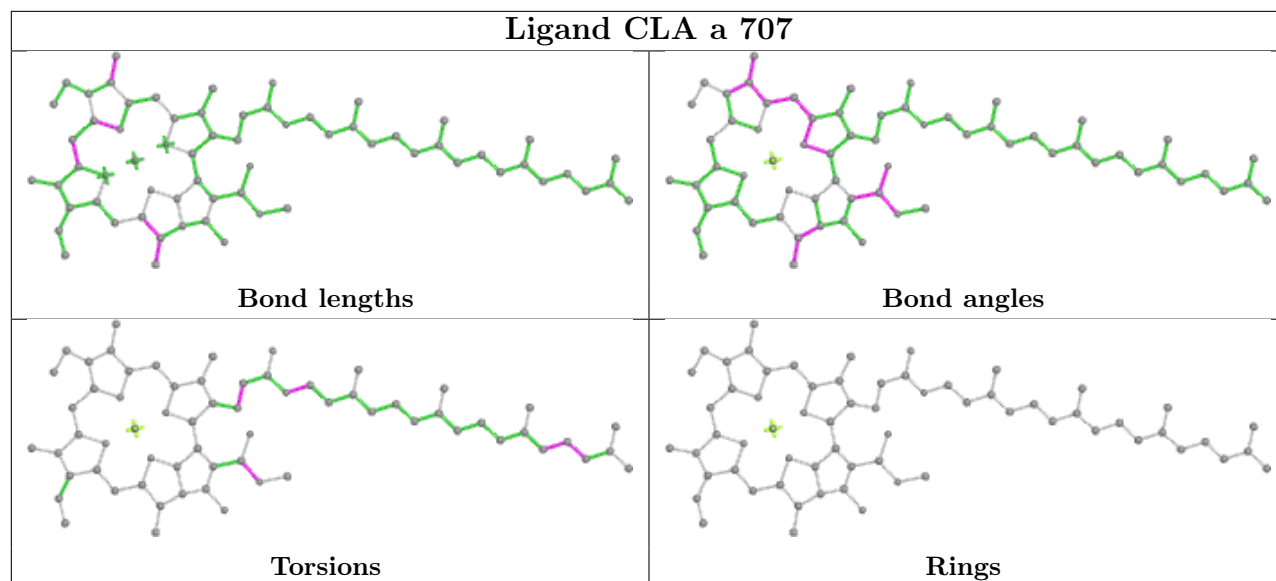
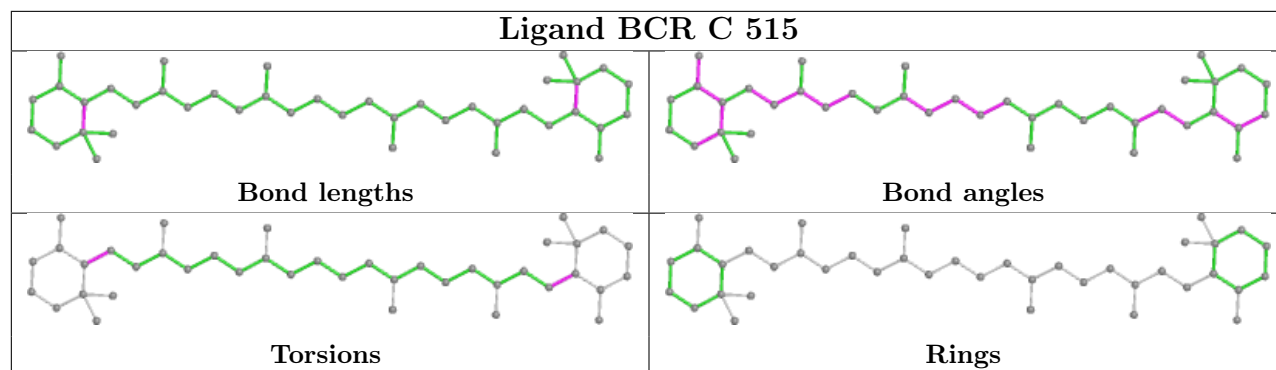


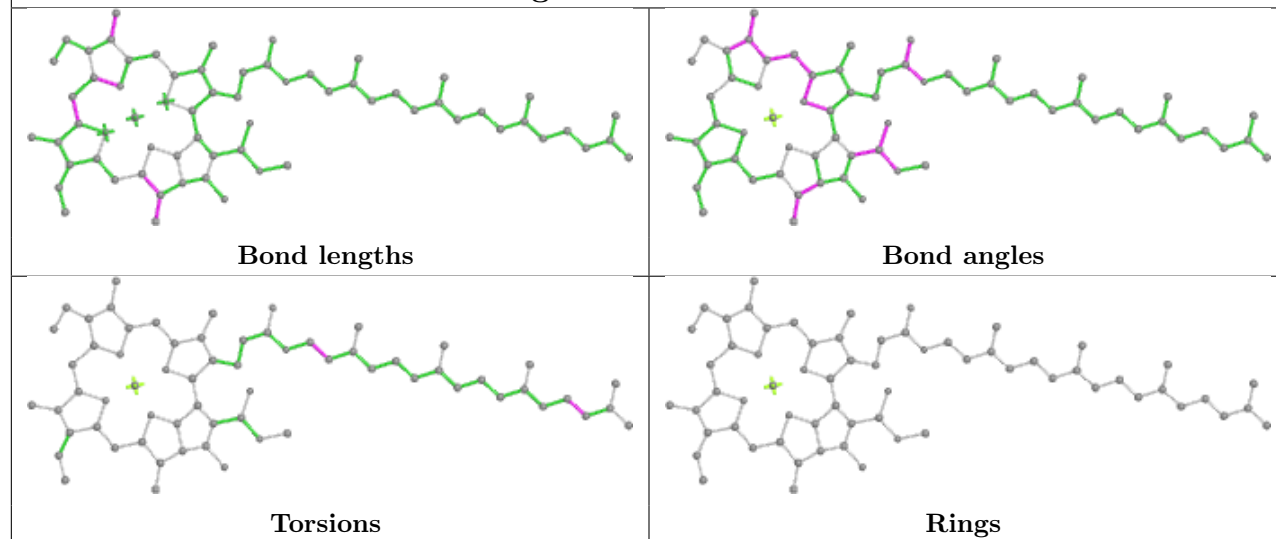
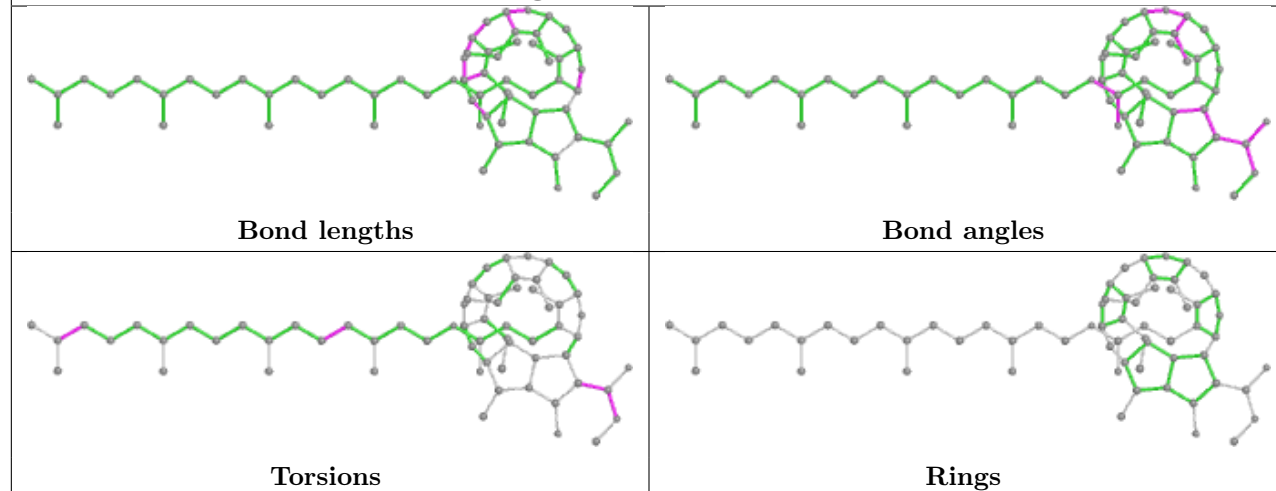
Ligand CLA c 510

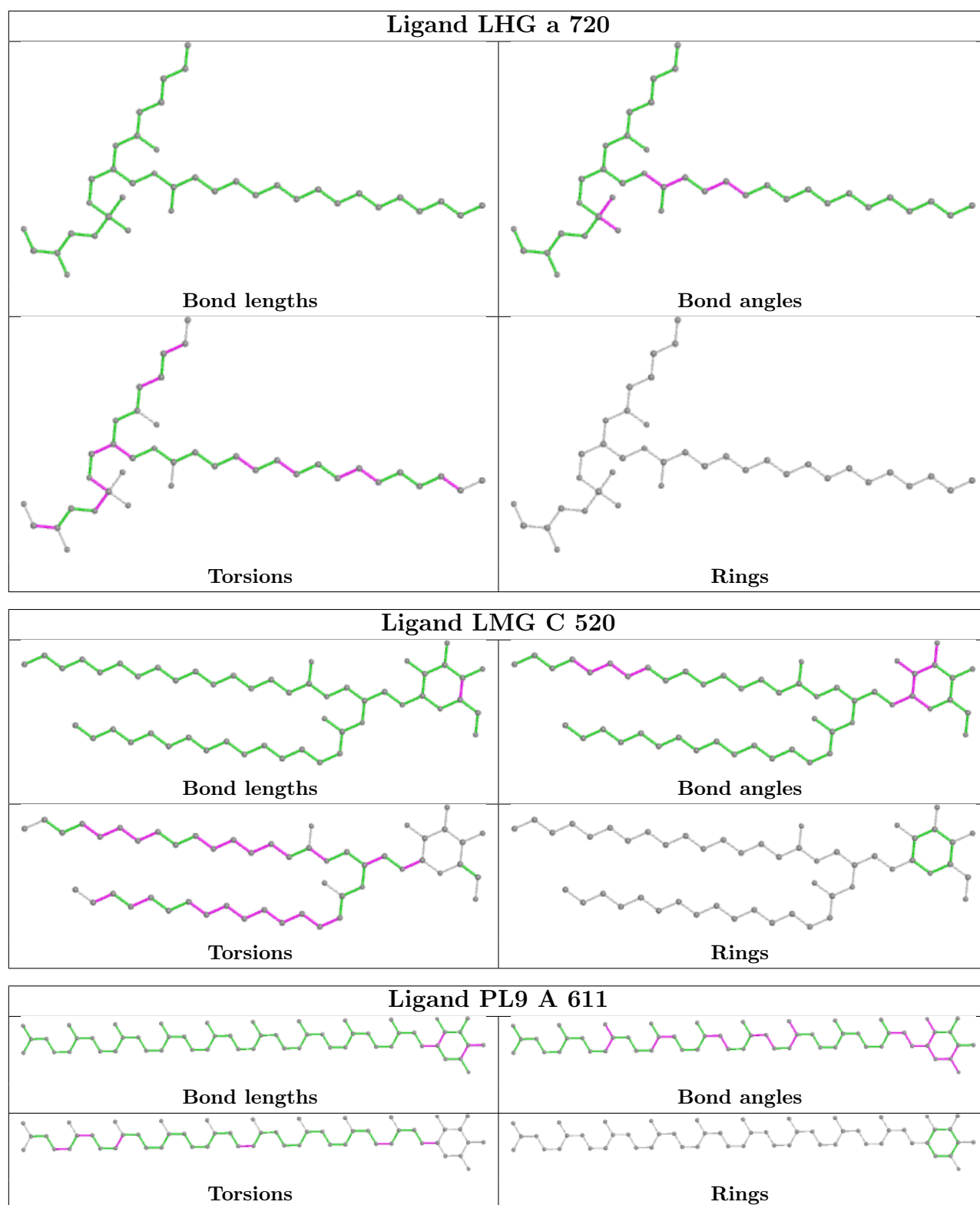


Ligand LMG f 101

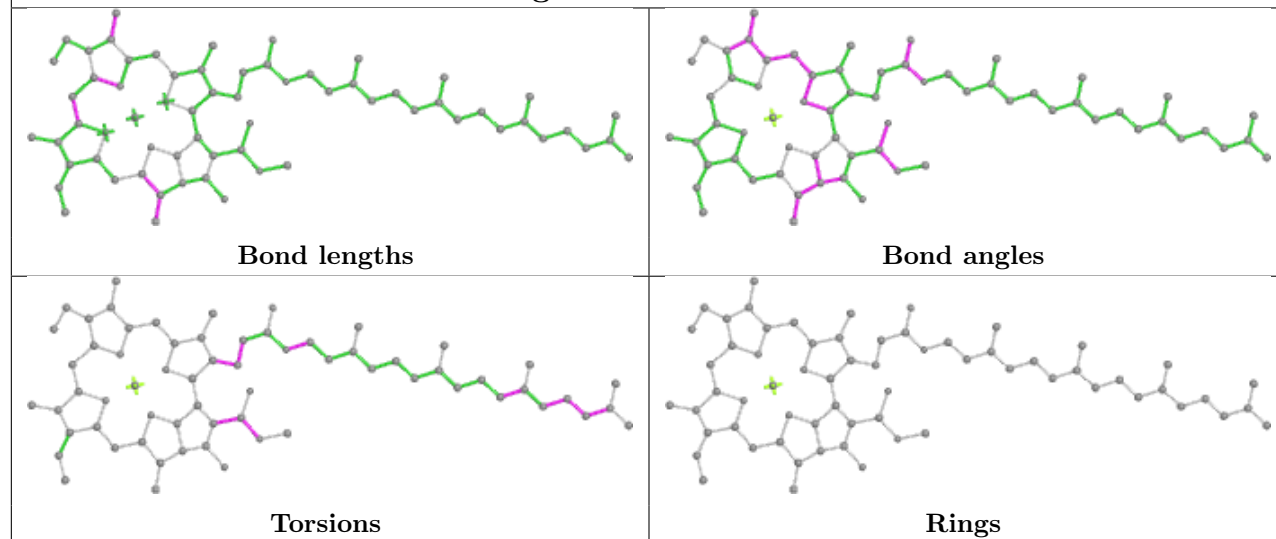




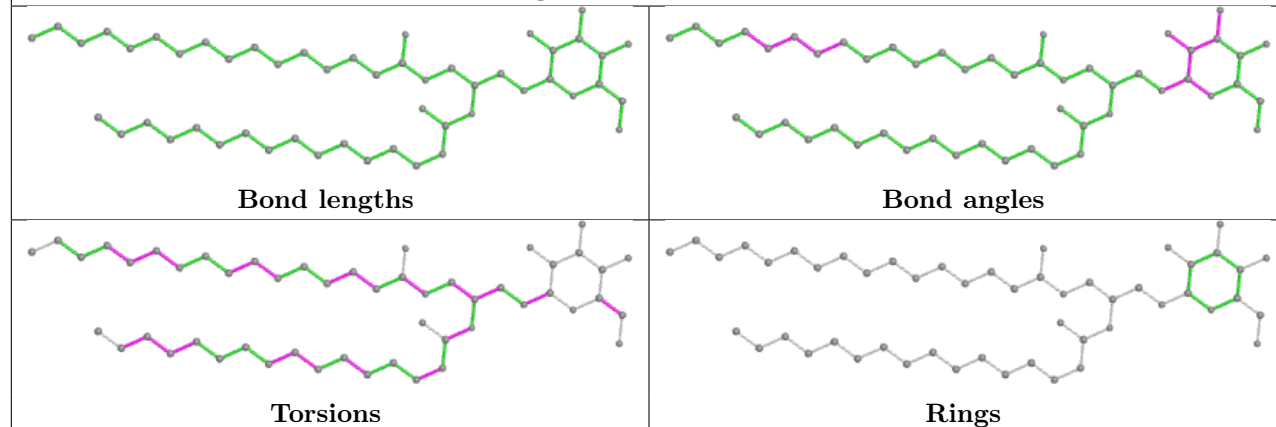
Ligand CLA A 606**Ligand PHO D 401**



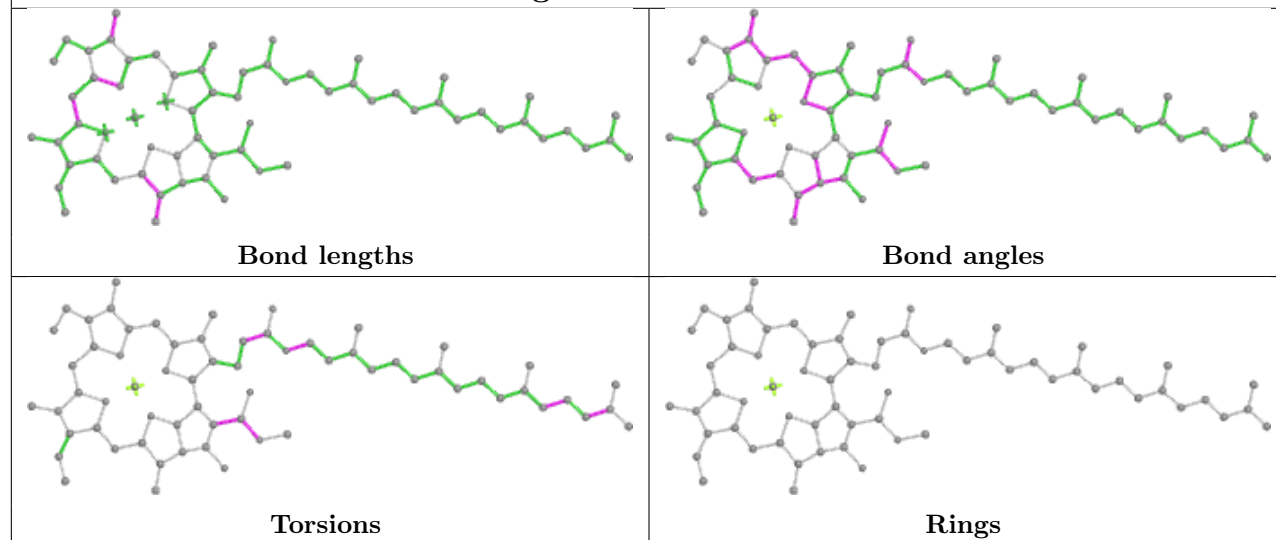
Ligand CLA B 609

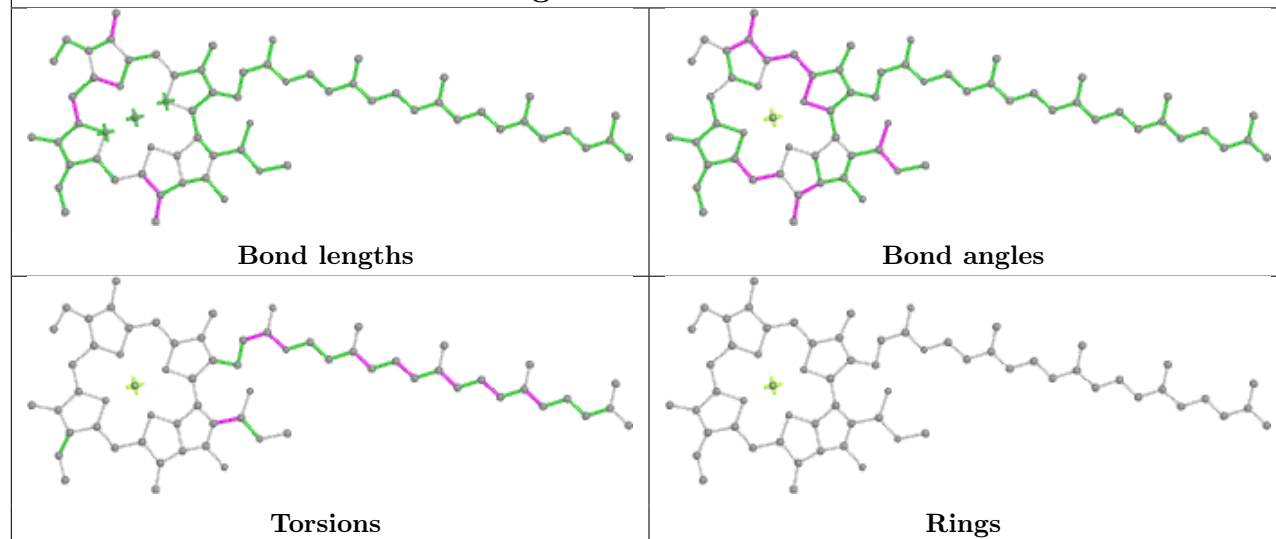
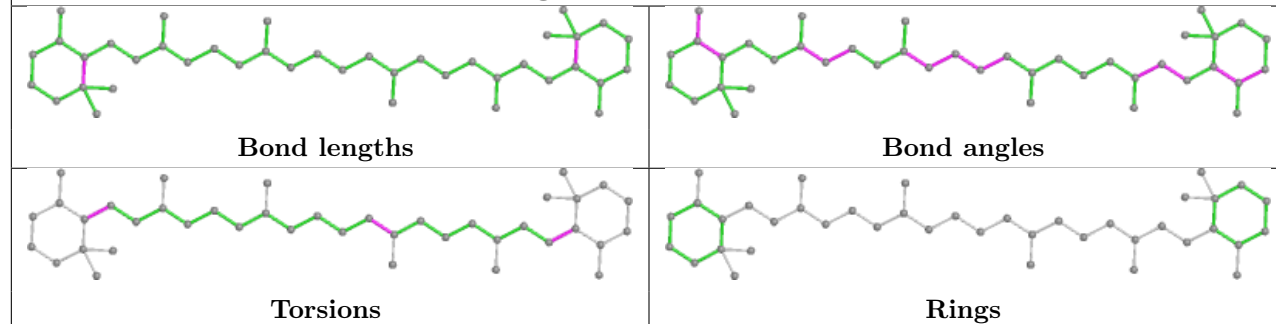
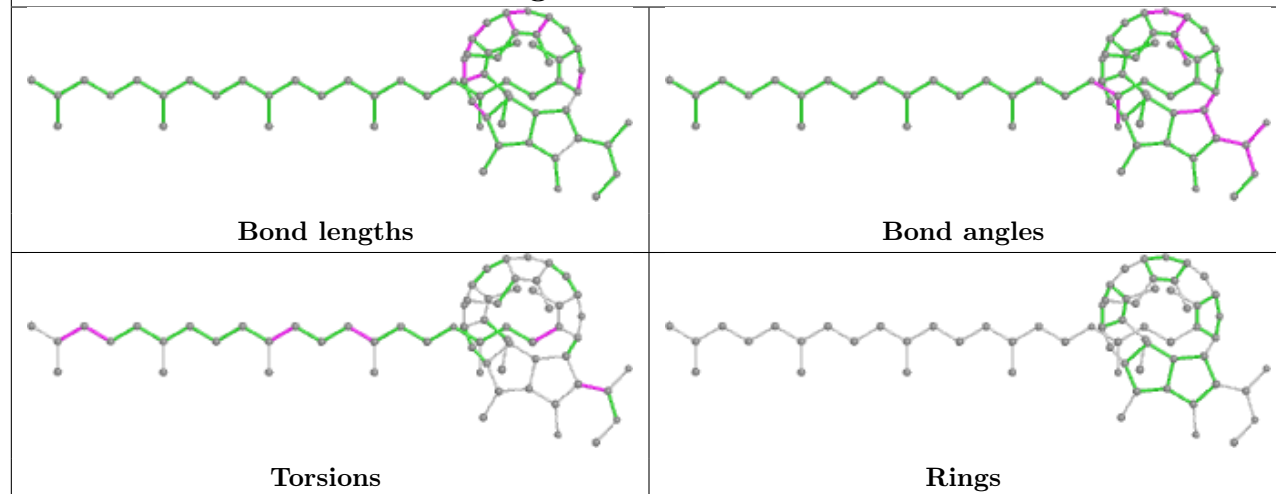


Ligand LMG a 715

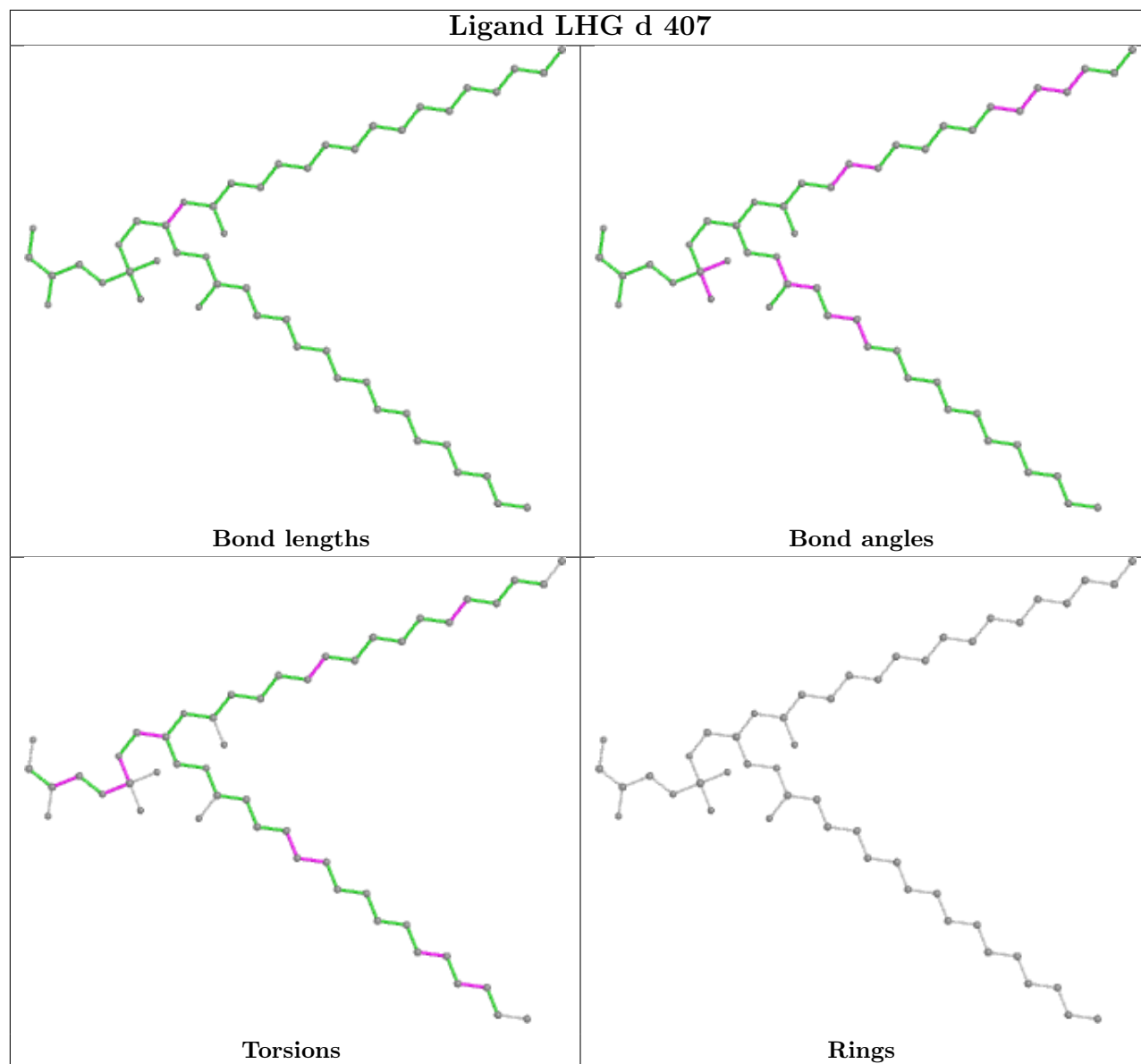


Ligand CLA B 614

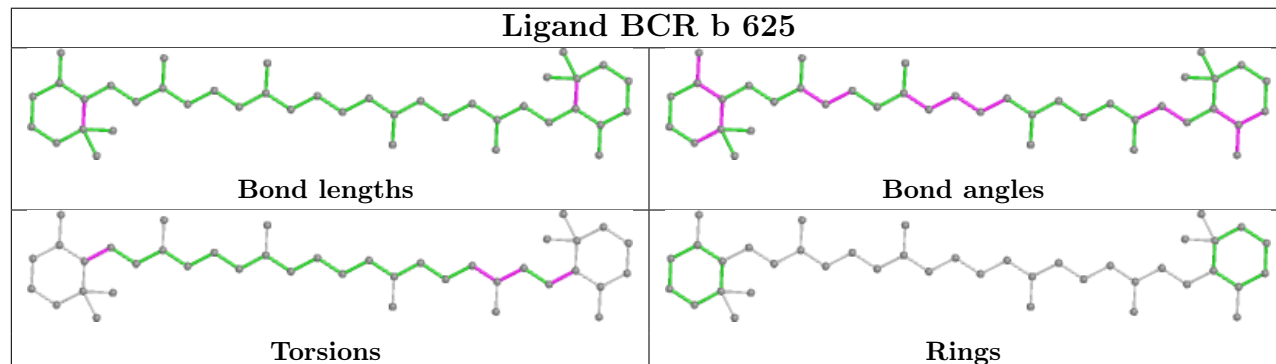


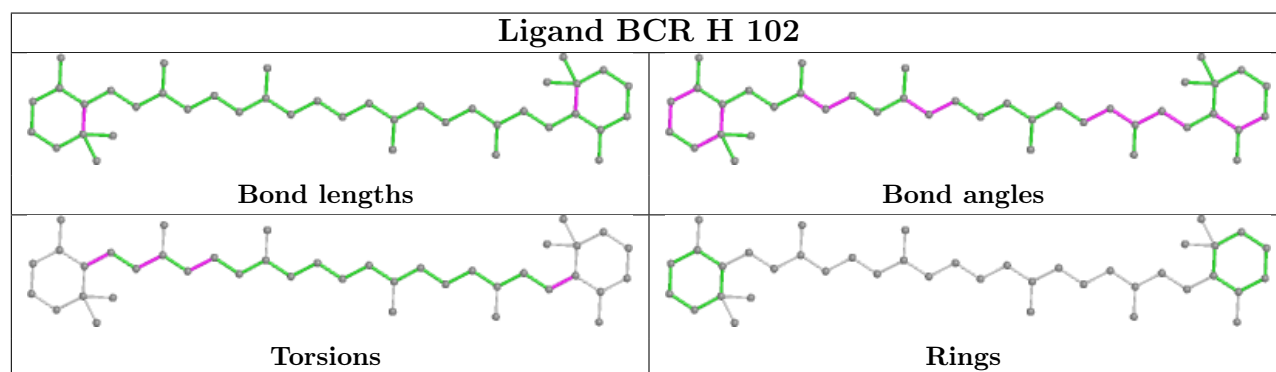
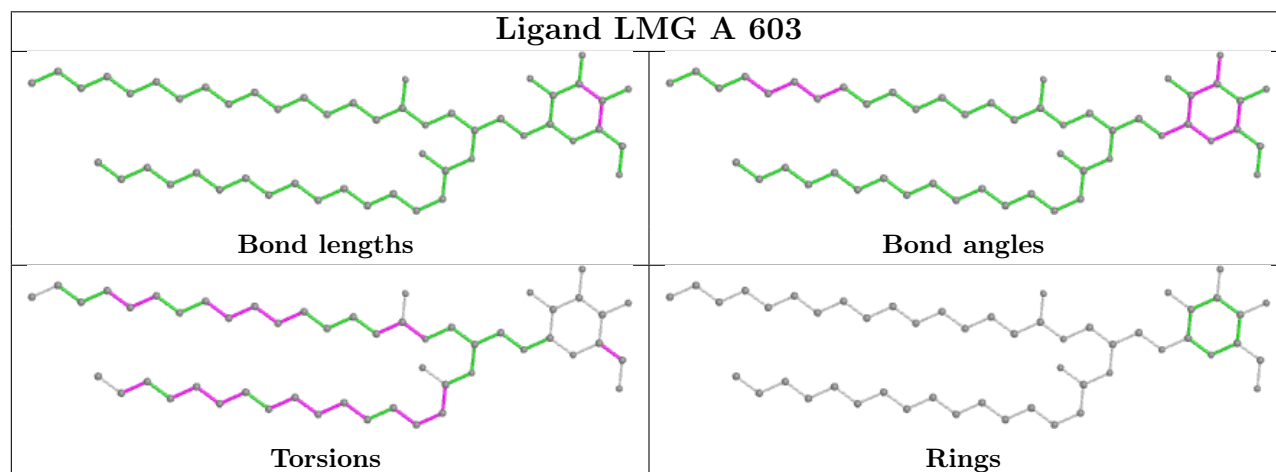
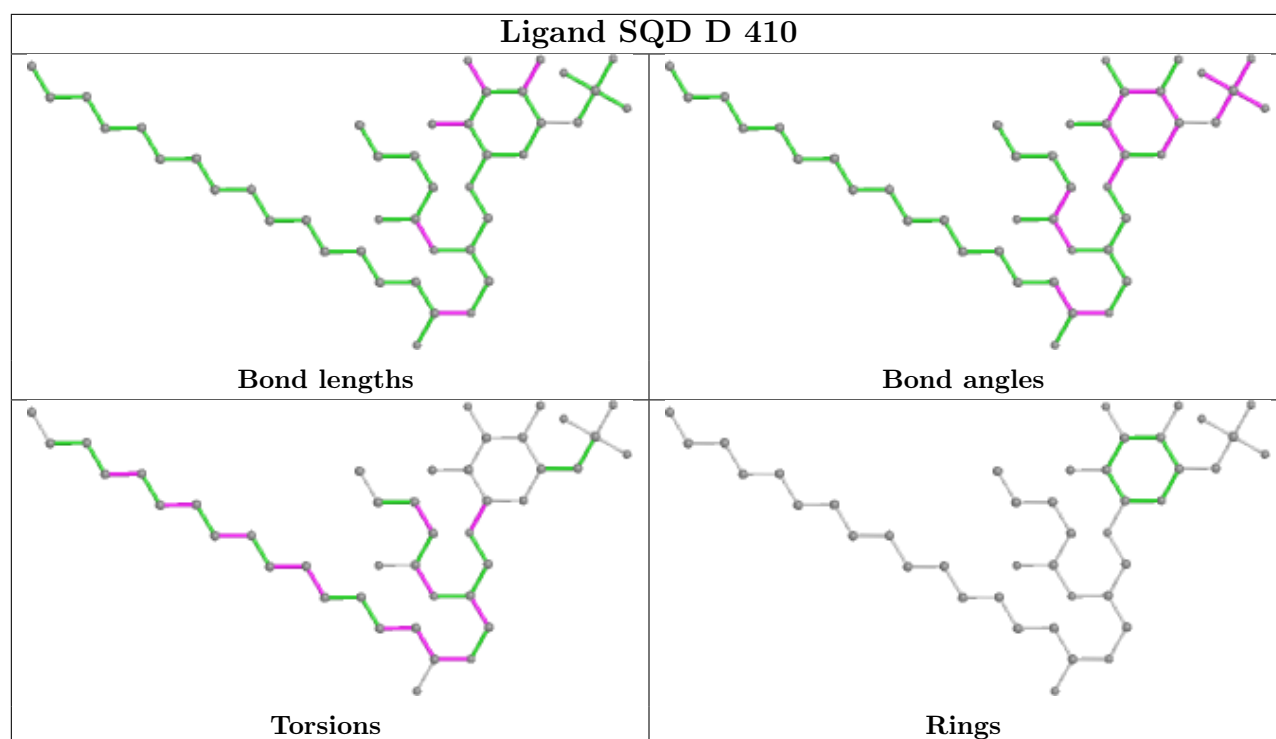
Ligand CLA C 513**Ligand BCR a 712****Ligand PHO A 608**

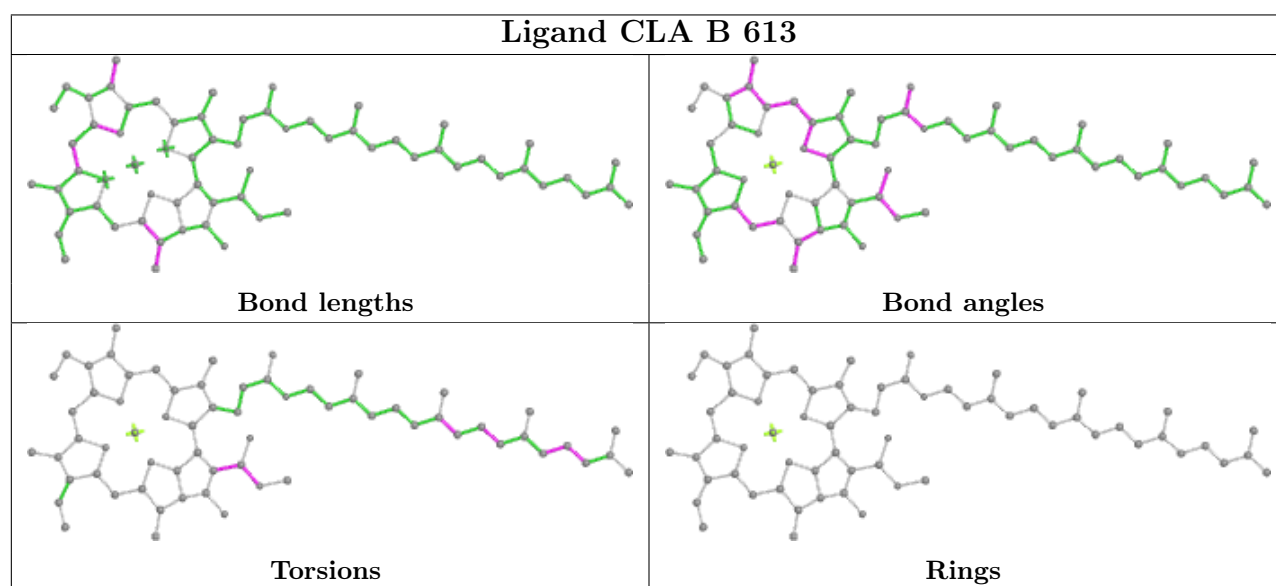
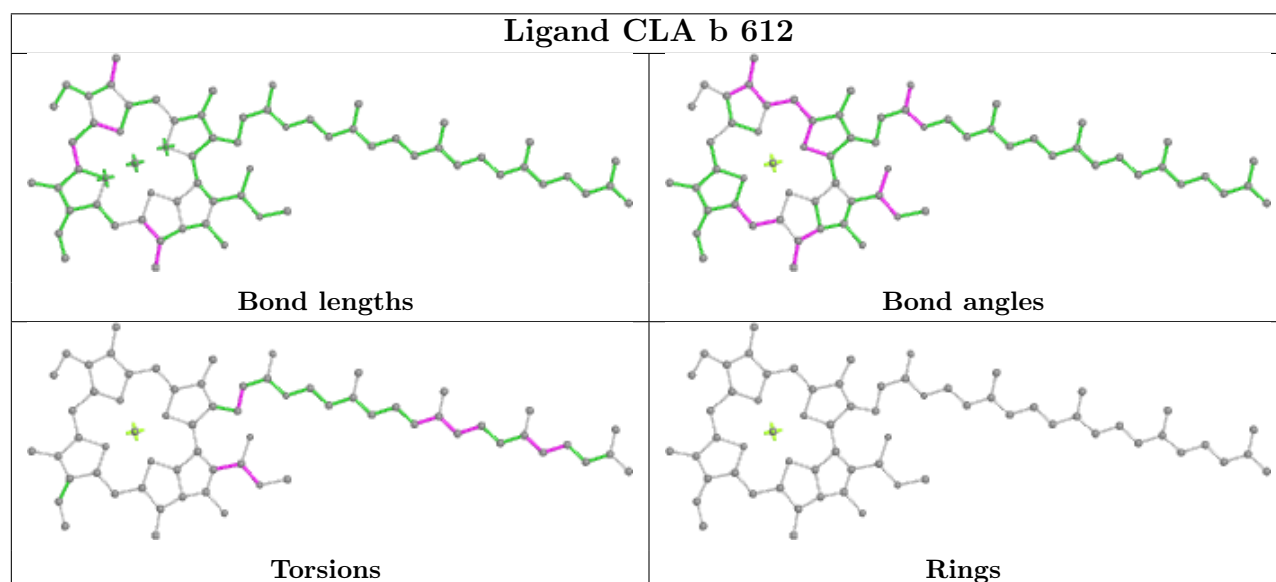
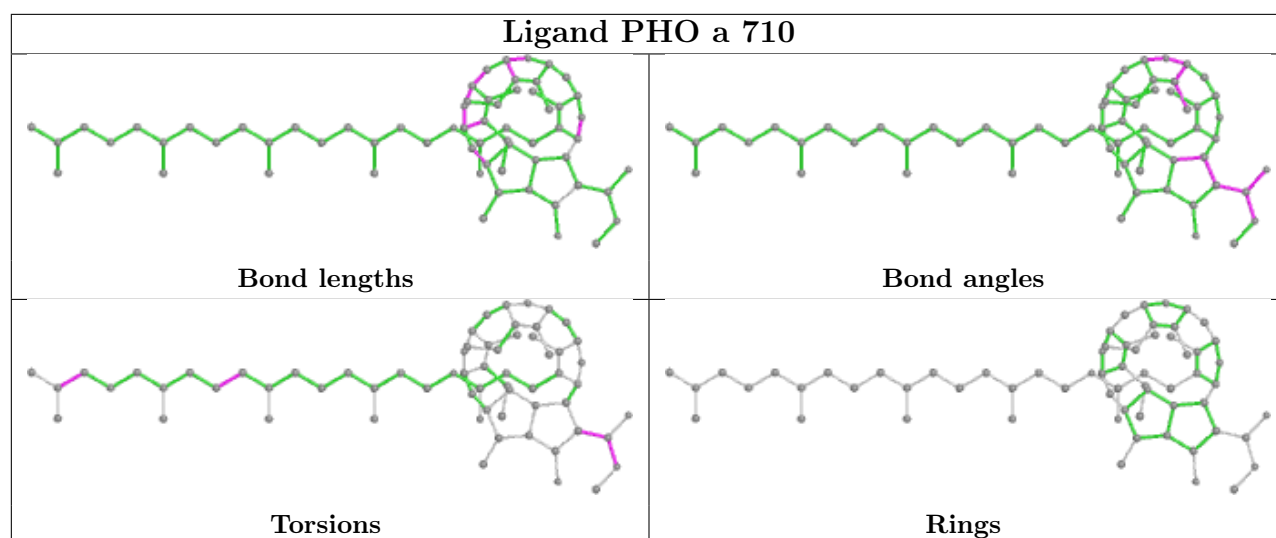
Ligand LHG d 407



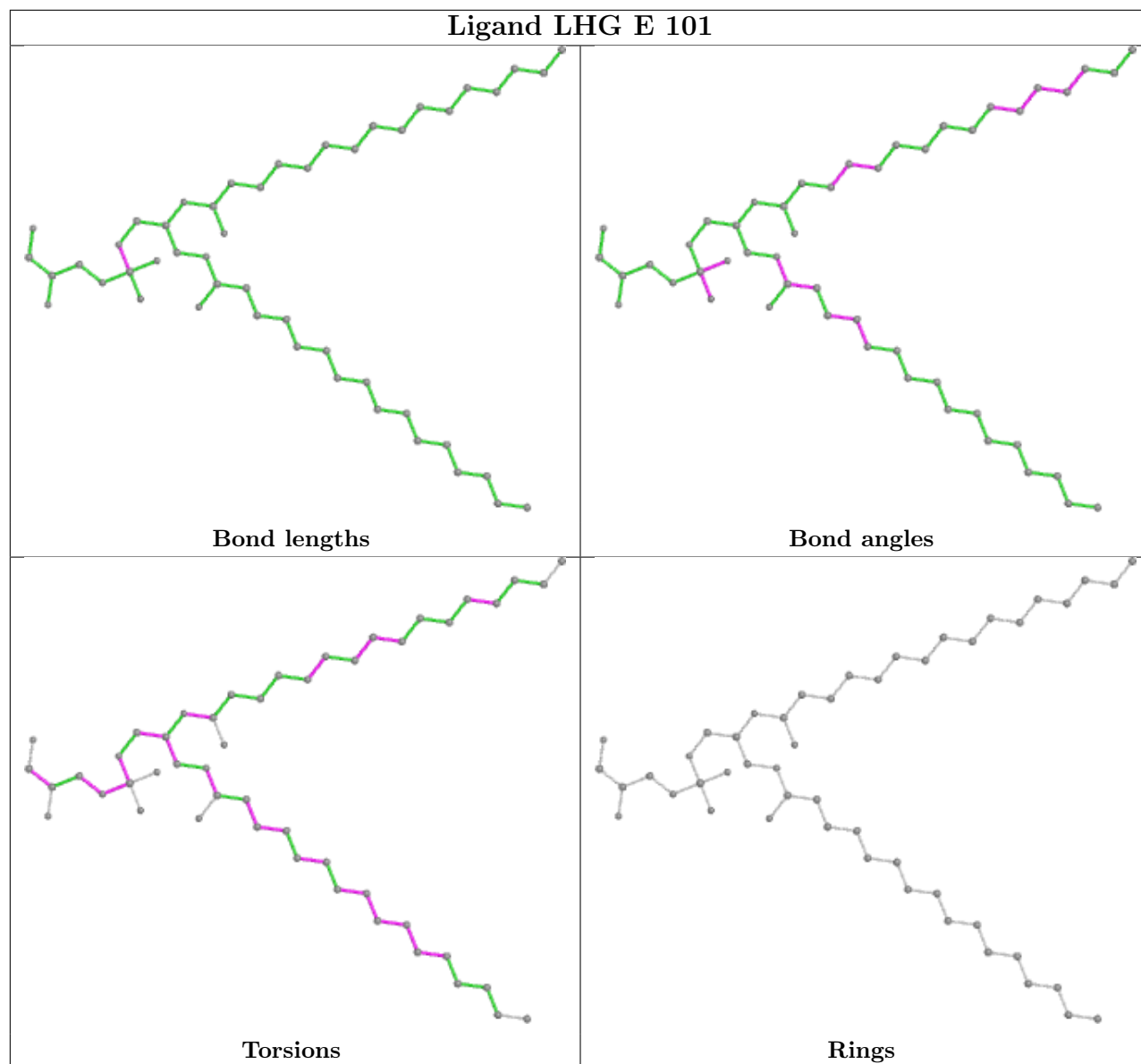
Ligand BCR b 625



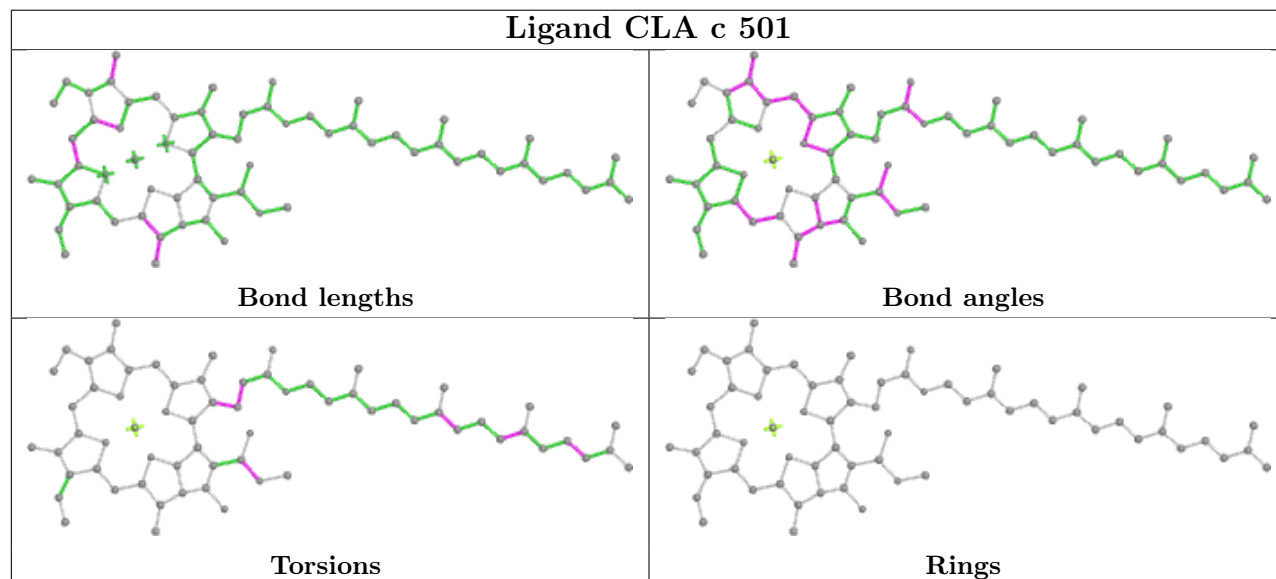


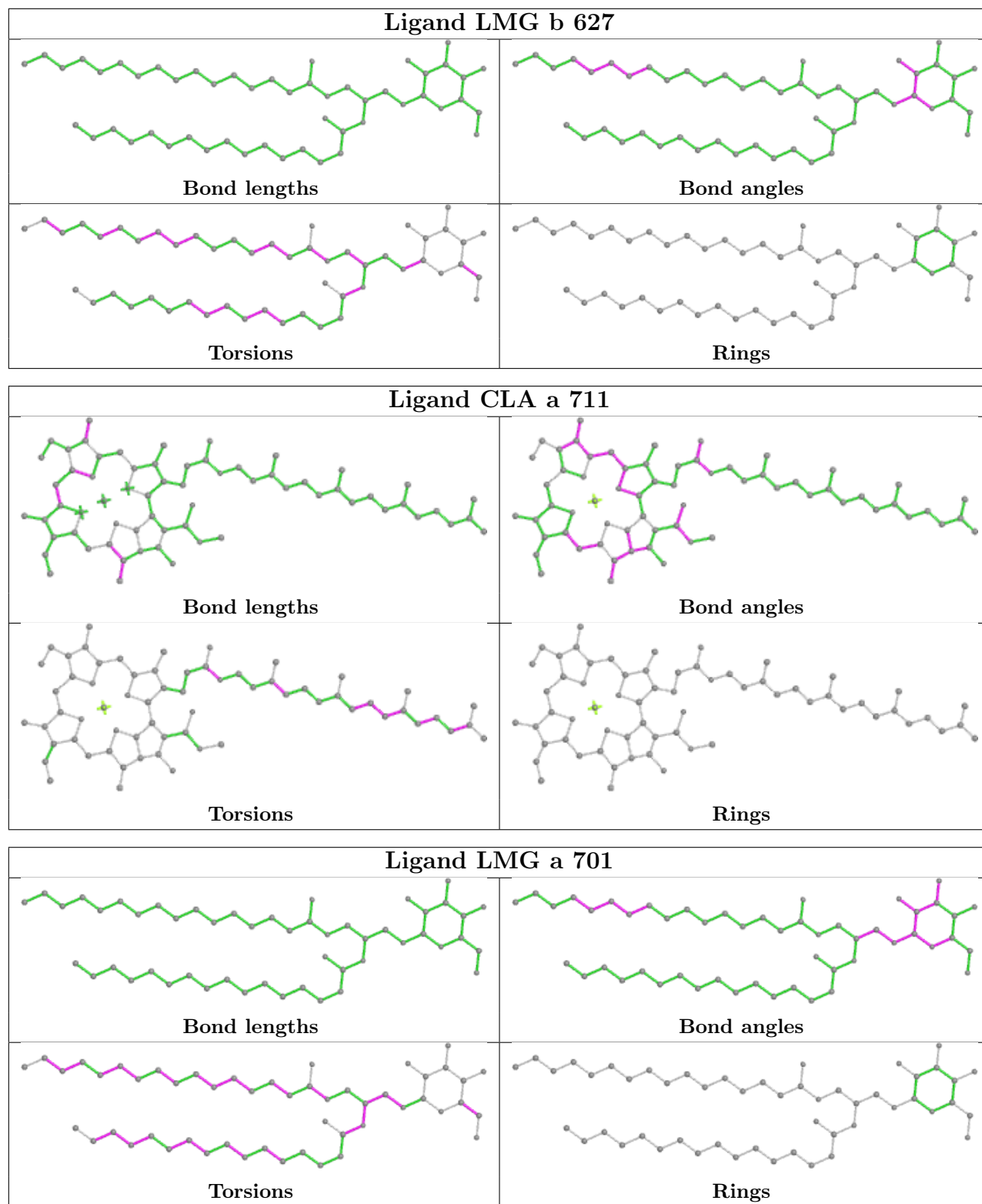


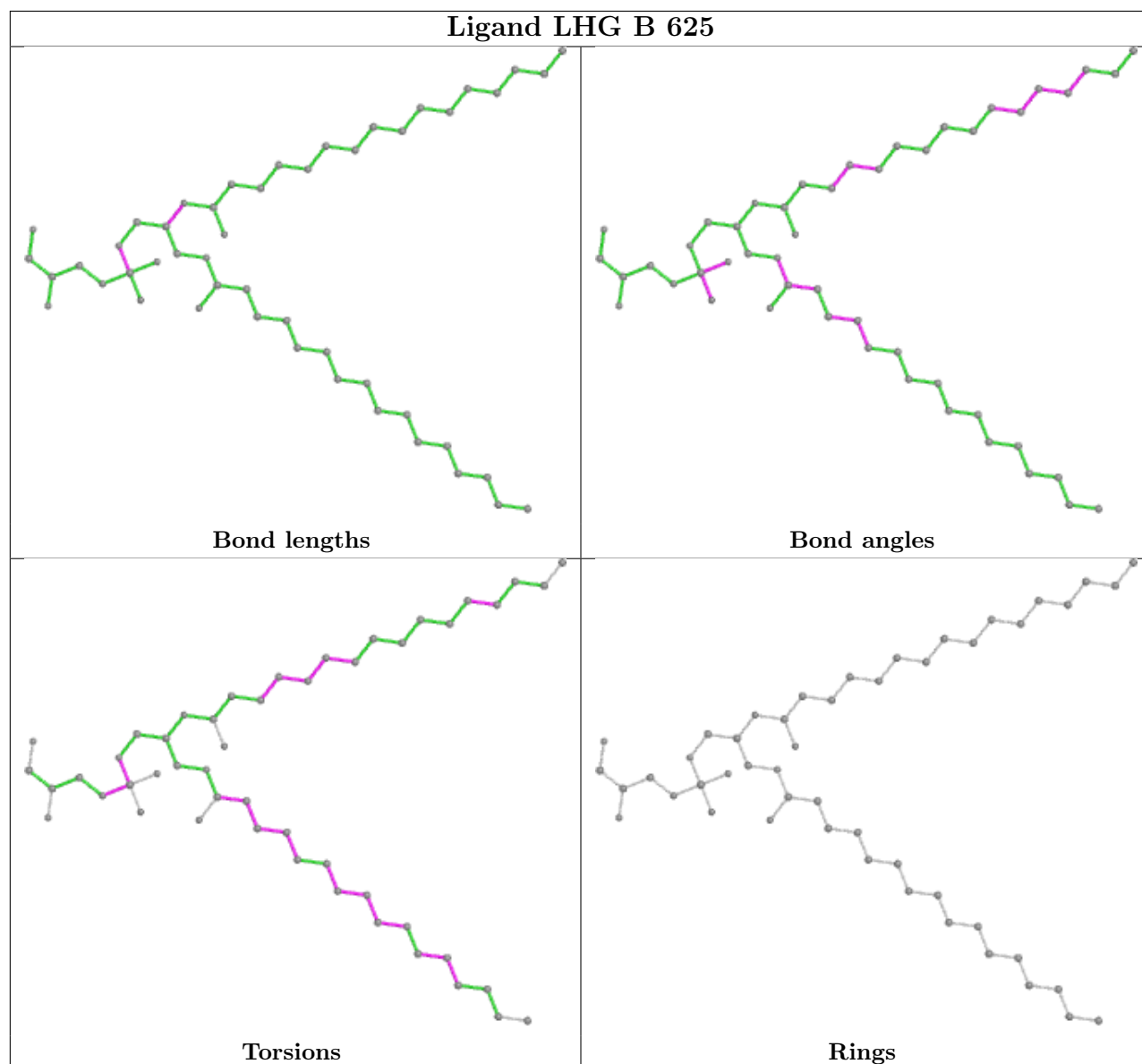
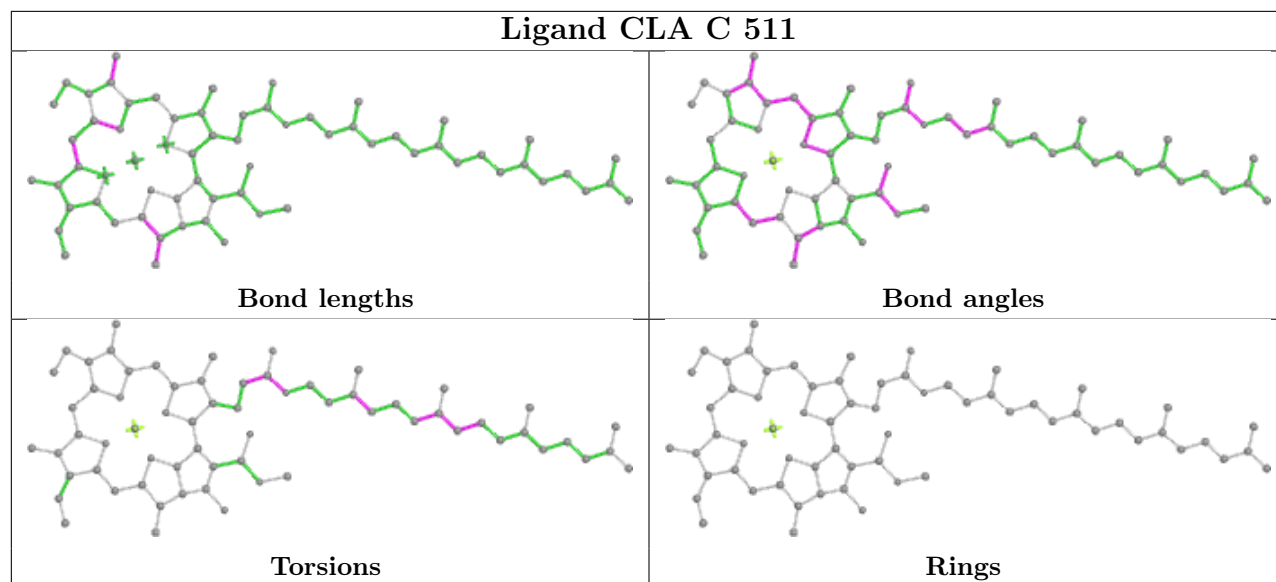
Ligand LHG E 101



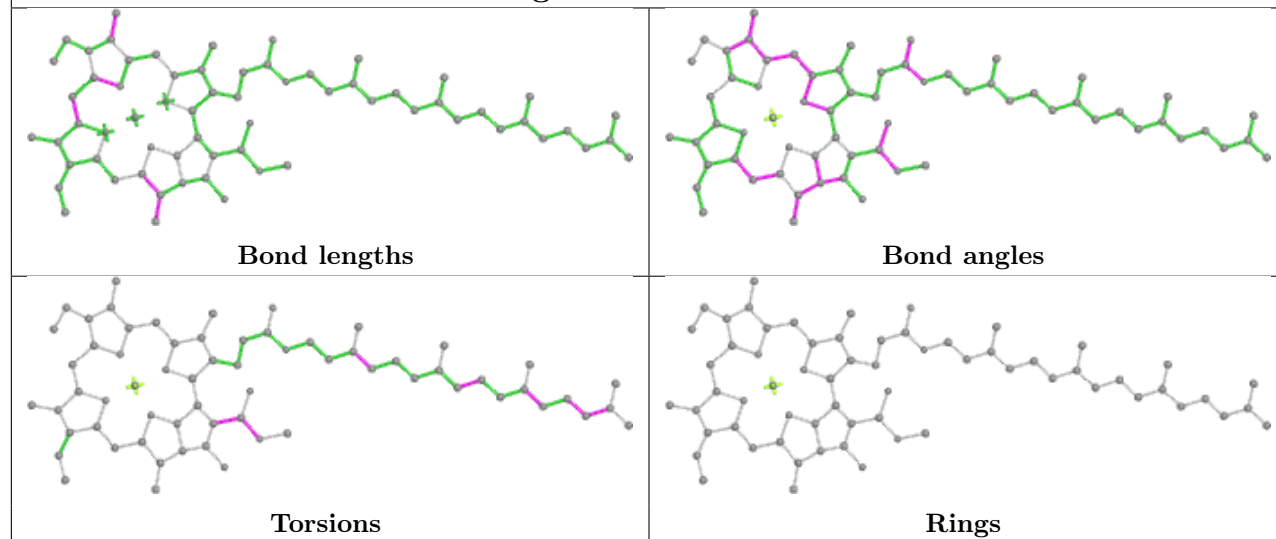
Ligand CLA c 501



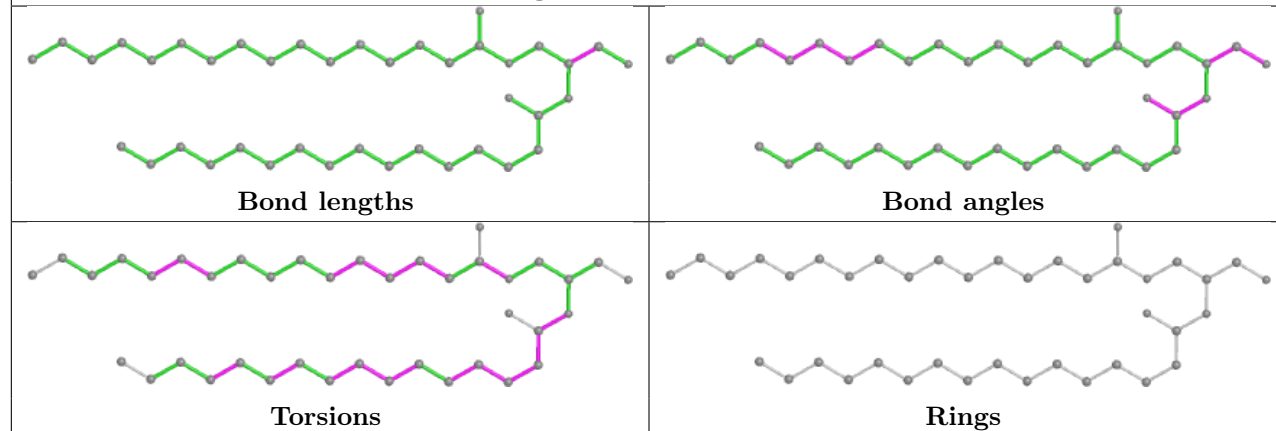




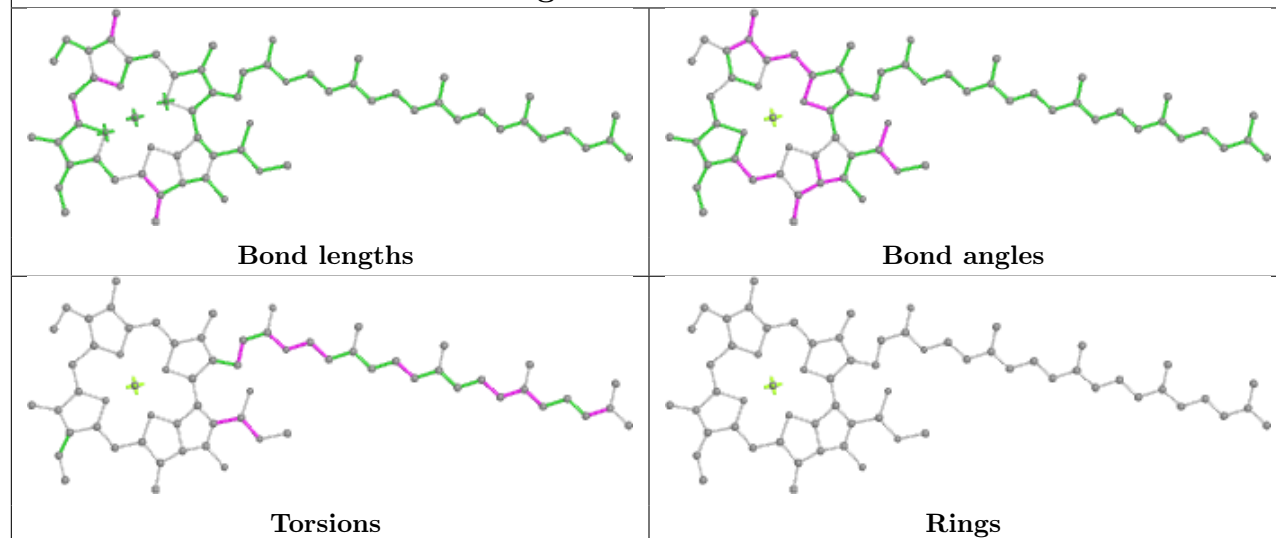
Ligand CLA C 505



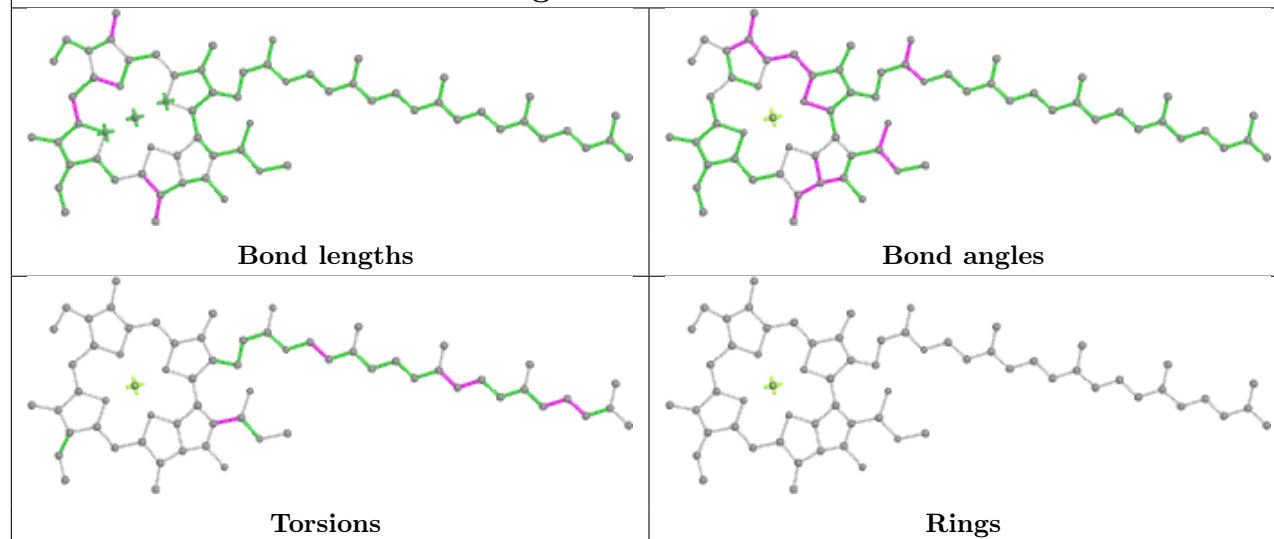
Ligand LMG d 408



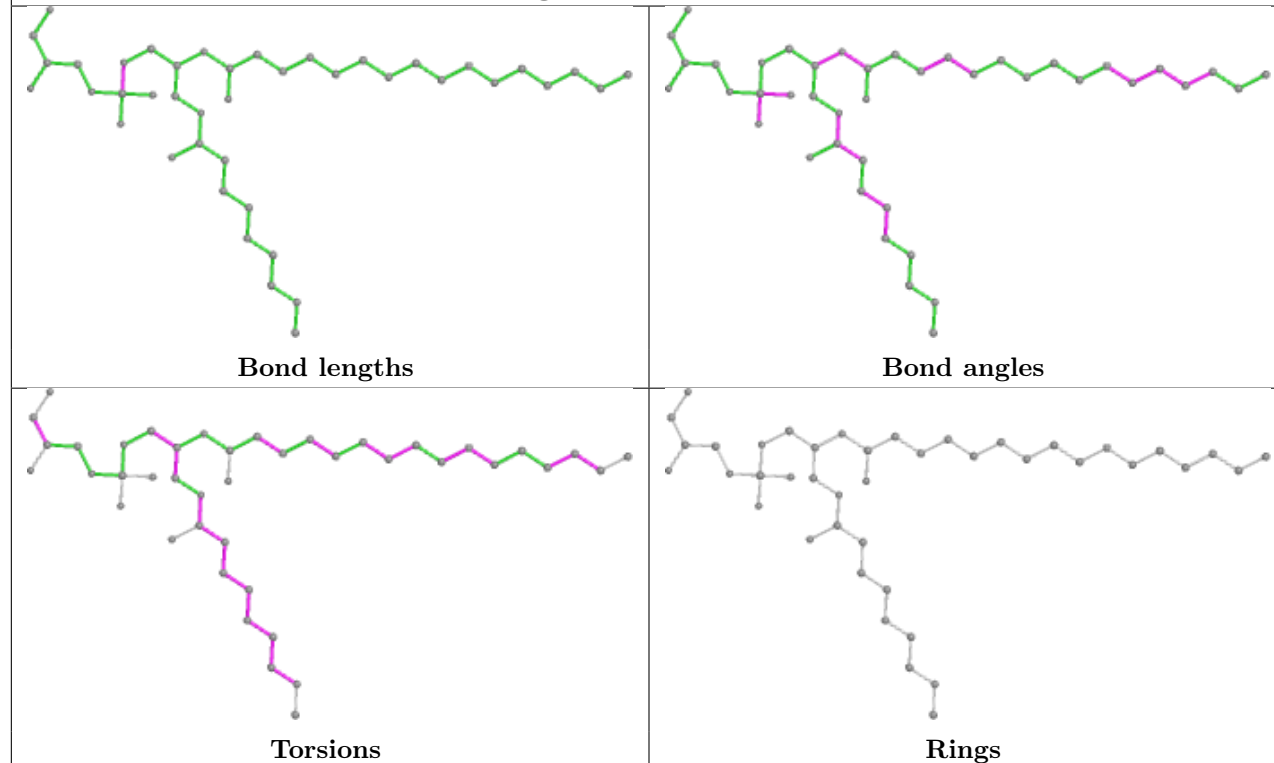
Ligand CLA c 512



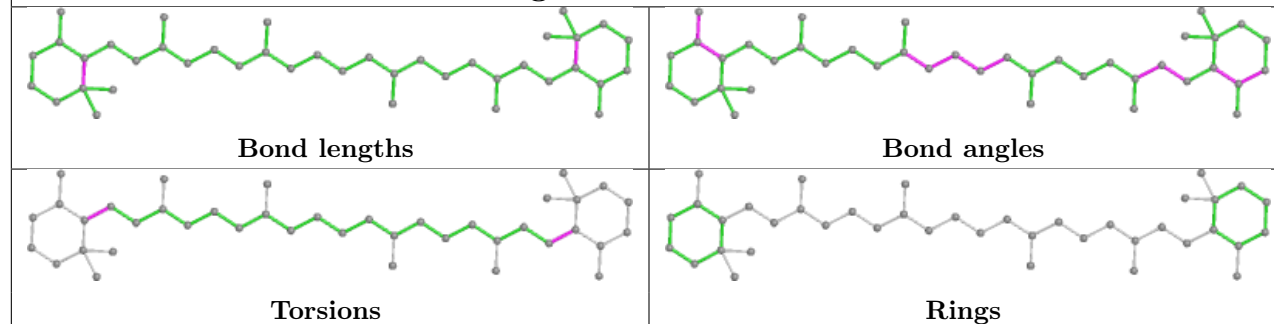
Ligand CLA C 514



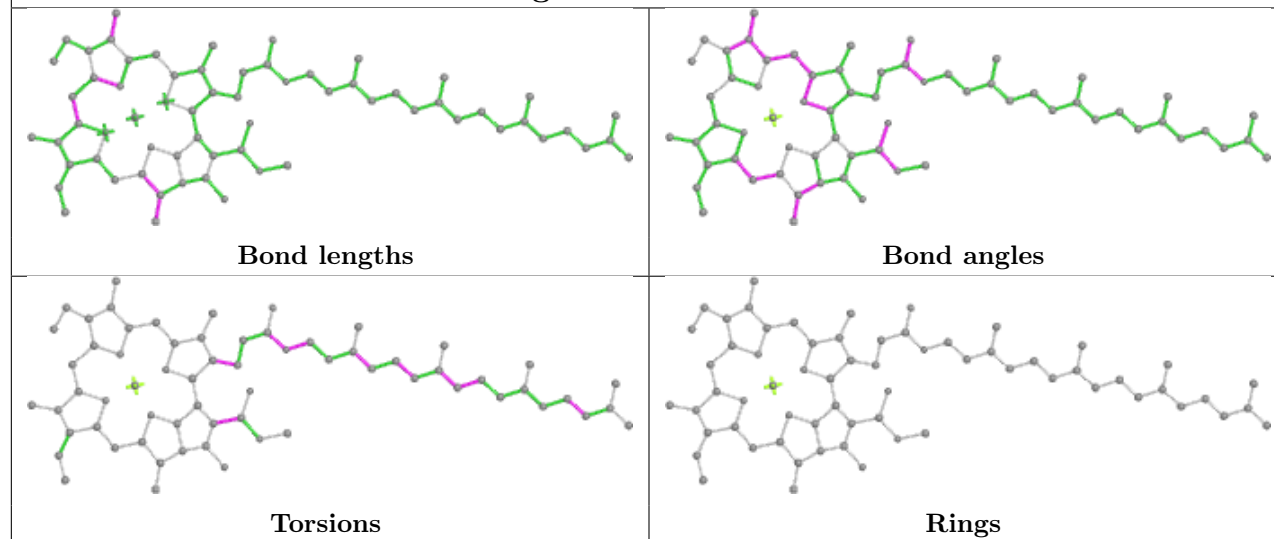
Ligand LHG e 101



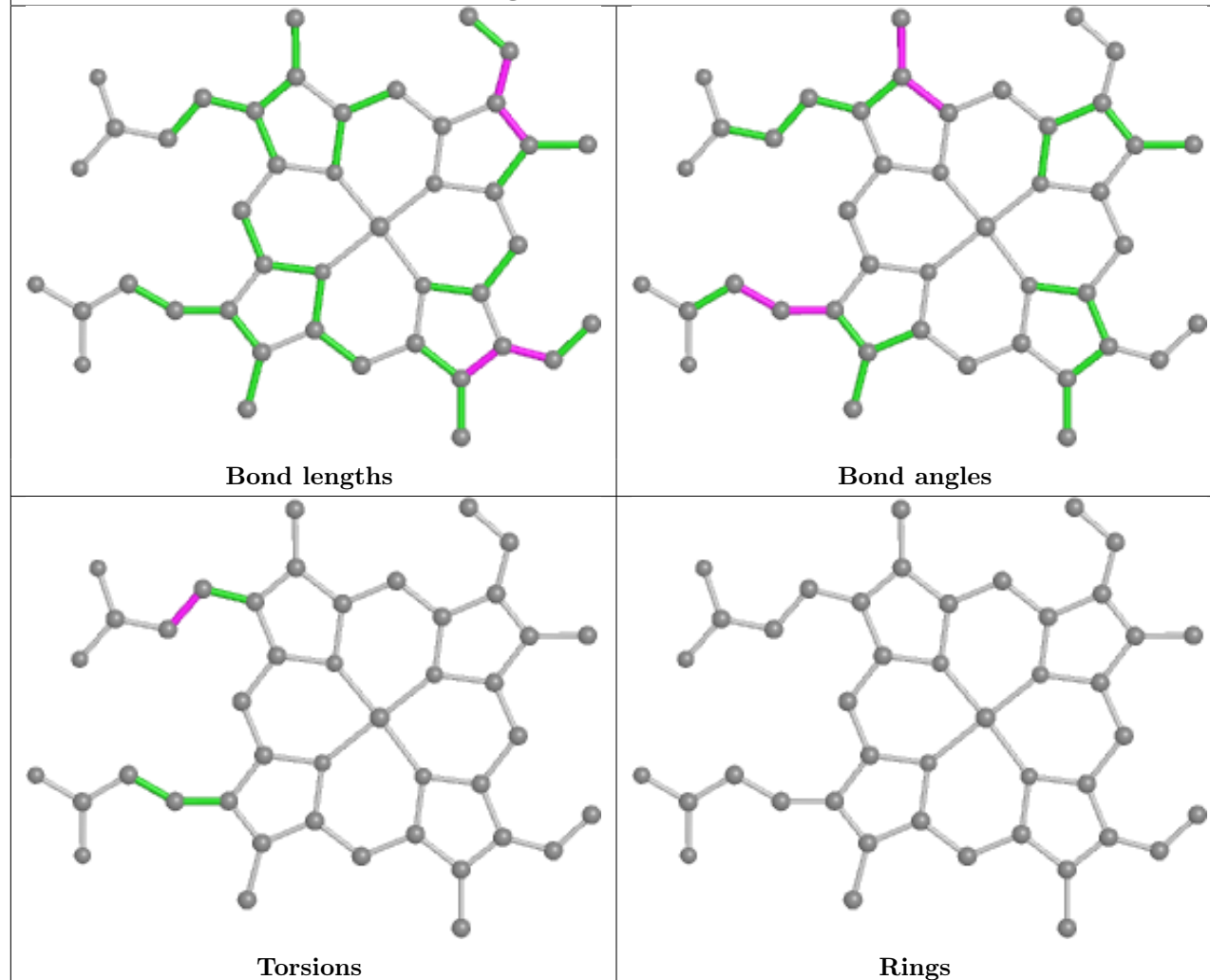
Ligand BCR A 610



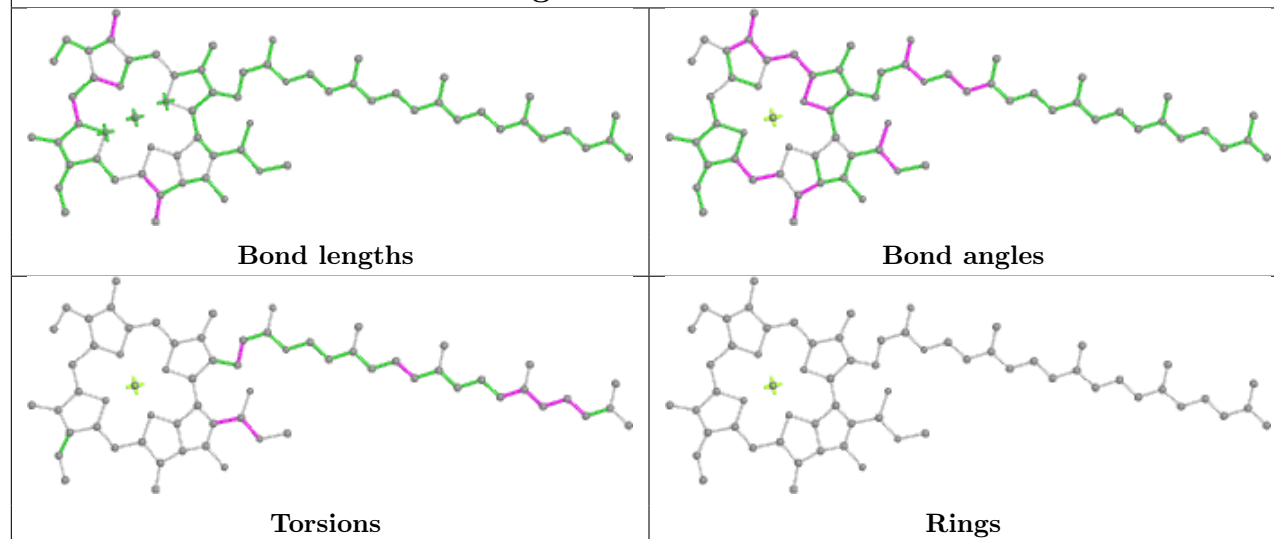
Ligand CLA C 504



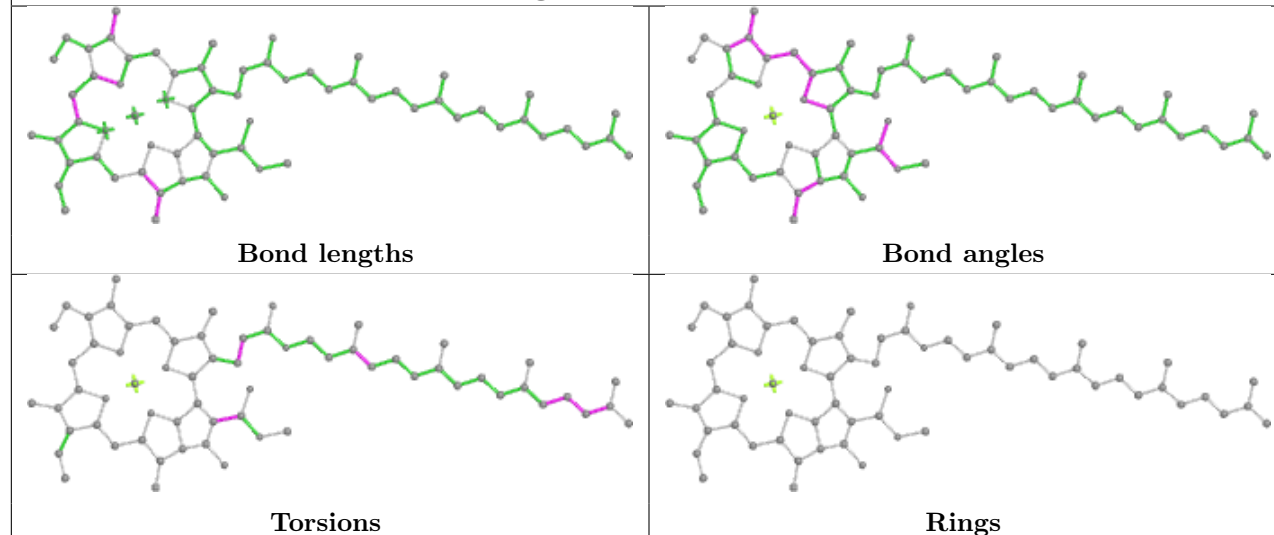
Ligand HEM e 102



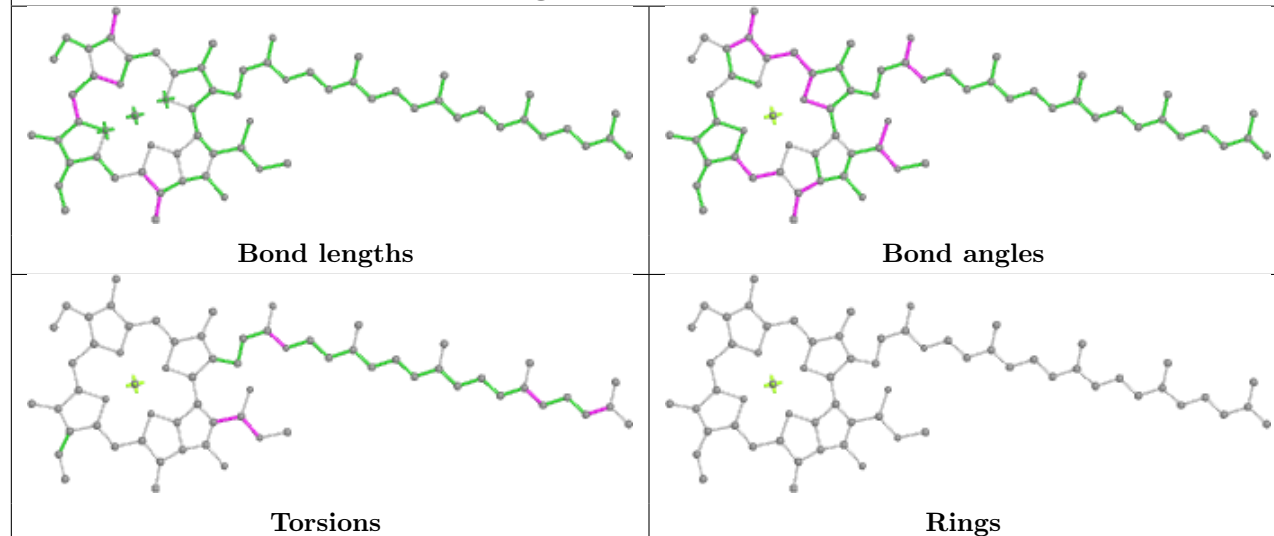
Ligand CLA B 611



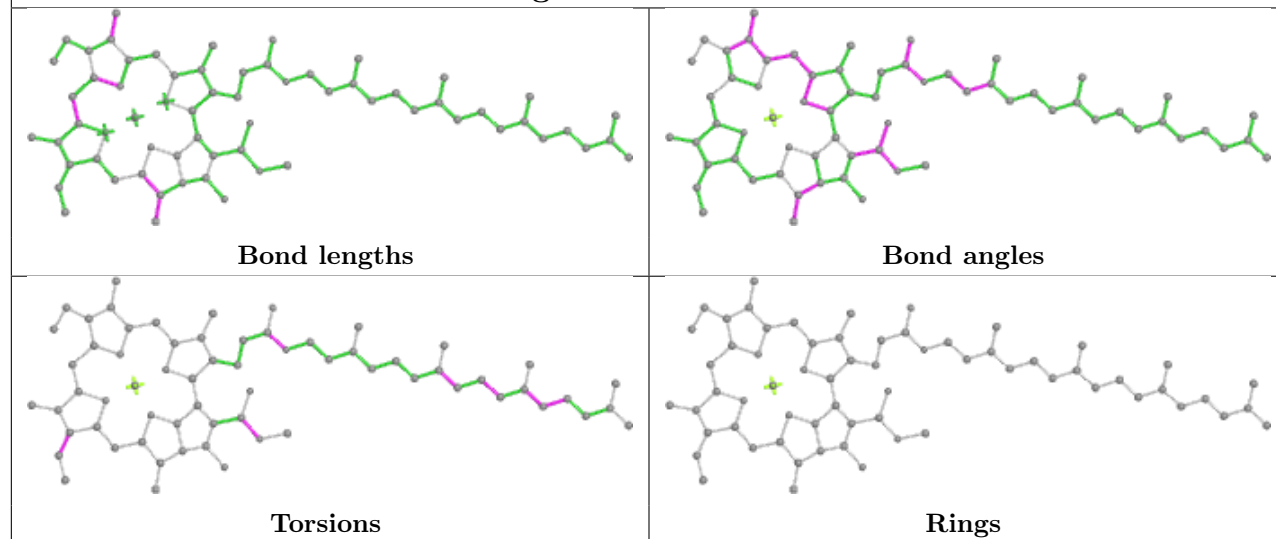
Ligand CLA C 508



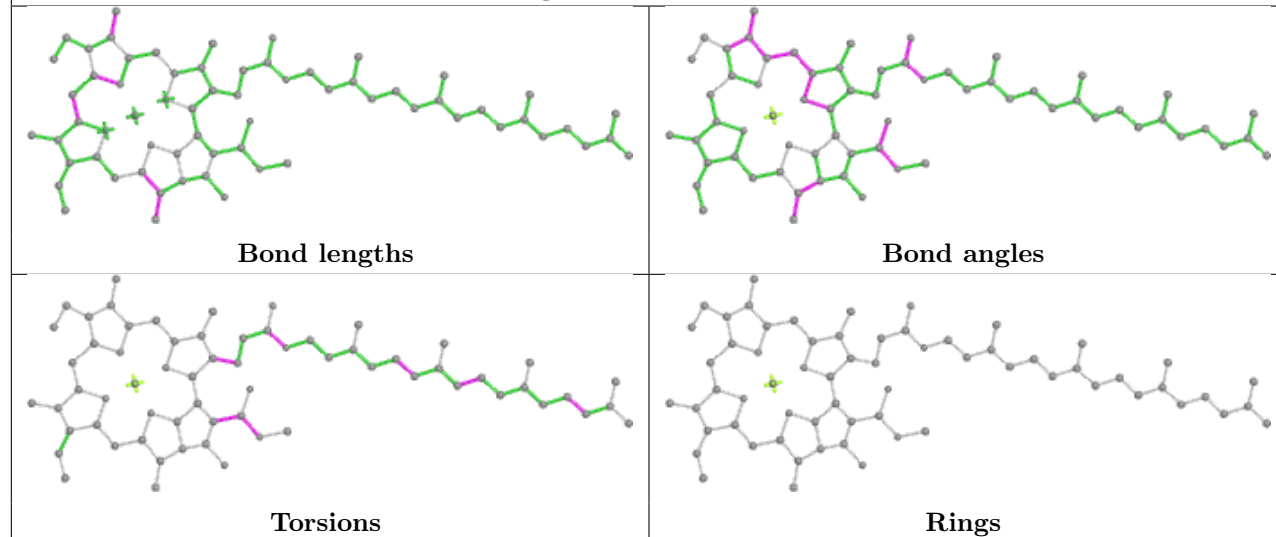
Ligand CLA B 608

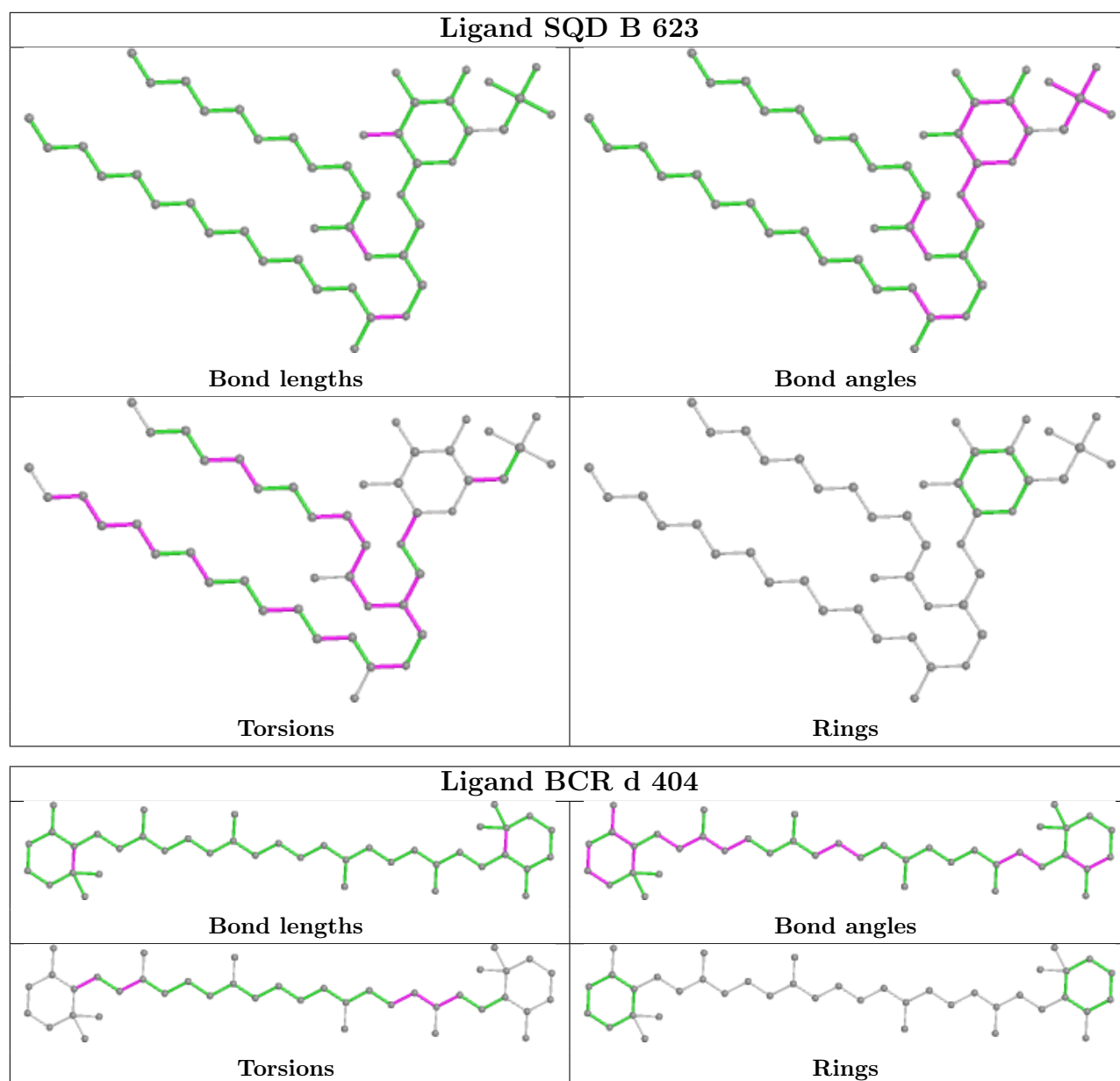


Ligand CLA B 605



Ligand CLA c 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 334/344 (97%) | -0.32 | 2 (0%) 89 86 | 38, 46, 69, 82 | 0 |
| 1 | a | 334/344 (97%) | -0.21 | 4 (1%) 79 73 | 35, 48, 71, 82 | 0 |
| 2 | B | 504/510 (98%) | -0.11 | 9 (1%) 68 61 | 38, 50, 74, 98 | 0 |
| 2 | b | 504/510 (98%) | -0.11 | 24 (4%) 30 21 | 38, 50, 76, 94 | 0 |
| 3 | C | 451/461 (97%) | -0.14 | 3 (0%) 87 84 | 41, 54, 71, 90 | 0 |
| 3 | c | 451/461 (97%) | -0.10 | 3 (0%) 87 84 | 39, 55, 74, 90 | 0 |
| 4 | D | 341/352 (96%) | -0.35 | 1 (0%) 94 93 | 37, 48, 63, 82 | 0 |
| 4 | d | 341/352 (96%) | -0.21 | 2 (0%) 89 86 | 40, 50, 67, 85 | 0 |
| 5 | E | 81/84 (96%) | 0.29 | 8 (9%) 7 4 | 47, 67, 79, 85 | 0 |
| 5 | e | 82/84 (97%) | 0.71 | 12 (14%) 2 1 | 52, 70, 85, 87 | 0 |
| 6 | F | 34/45 (75%) | -0.17 | 0 100 100 | 54, 64, 78, 84 | 0 |
| 6 | f | 34/45 (75%) | -0.35 | 0 100 100 | 56, 63, 77, 80 | 0 |
| 7 | H | 63/63 (100%) | 0.13 | 2 (3%) 47 37 | 43, 55, 68, 73 | 0 |
| 7 | h | 63/63 (100%) | 0.02 | 0 100 100 | 48, 56, 64, 68 | 0 |
| 8 | I | 35/38 (92%) | 0.14 | 2 (5%) 23 15 | 43, 53, 83, 94 | 0 |
| 8 | i | 35/38 (92%) | 0.13 | 3 (8%) 10 5 | 44, 51, 82, 89 | 0 |
| 9 | J | 36/40 (90%) | -0.01 | 2 (5%) 24 16 | 56, 64, 86, 99 | 0 |
| 9 | j | 36/40 (90%) | 0.12 | 2 (5%) 24 16 | 55, 66, 85, 89 | 0 |
| 10 | K | 37/46 (80%) | 0.34 | 4 (10%) 5 3 | 62, 68, 83, 89 | 0 |
| 10 | k | 37/46 (80%) | 0.19 | 0 100 100 | 60, 70, 84, 89 | 0 |
| 11 | L | 37/37 (100%) | -0.32 | 0 100 100 | 34, 45, 82, 93 | 0 |
| 11 | l | 37/37 (100%) | -0.43 | 1 (2%) 54 44 | 36, 47, 81, 90 | 0 |
| 12 | M | 32/36 (88%) | -0.40 | 1 (3%) 49 39 | 38, 47, 71, 83 | 0 |
| 12 | m | 32/36 (88%) | -0.31 | 1 (3%) 49 39 | 36, 47, 71, 77 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | O | 244/272 (89%) | -0.03 | 10 (4%) 37 27 | 42, 57, 87, 106 | 0 |
| 13 | o | 244/272 (89%) | -0.06 | 9 (3%) 41 31 | 43, 56, 89, 116 | 0 |
| 14 | T | 29/32 (90%) | -0.08 | 1 (3%) 45 35 | 37, 46, 69, 87 | 0 |
| 14 | t | 29/32 (90%) | -0.52 | 0 100 100 | 38, 48, 70, 79 | 0 |
| 15 | U | 97/134 (72%) | 0.04 | 3 (3%) 49 39 | 45, 58, 75, 86 | 0 |
| 15 | u | 97/134 (72%) | -0.20 | 0 100 100 | 47, 55, 69, 84 | 0 |
| 16 | V | 137/163 (84%) | -0.13 | 0 100 100 | 45, 55, 67, 85 | 0 |
| 16 | v | 137/163 (84%) | 0.17 | 4 (2%) 51 41 | 49, 63, 79, 100 | 0 |
| 17 | Y | 27/46 (58%) | 0.34 | 1 (3%) 41 31 | 68, 75, 87, 95 | 0 |
| 17 | y | 30/46 (65%) | 0.39 | 1 (3%) 46 36 | 69, 79, 89, 90 | 0 |
| 18 | X | 38/41 (92%) | 0.25 | 2 (5%) 26 17 | 52, 60, 82, 93 | 0 |
| 18 | x | 38/41 (92%) | 0.25 | 4 (10%) 6 3 | 54, 63, 80, 92 | 0 |
| 19 | Z | 62/62 (100%) | 0.87 | 18 (29%) 0 0 | 62, 76, 100, 113 | 0 |
| 19 | z | 62/62 (100%) | 0.64 | 9 (14%) 2 1 | 67, 82, 101, 112 | 0 |
| 20 | R | 34/41 (82%) | 1.69 | 14 (41%) 0 0 | 70, 82, 94, 95 | 0 |
| 20 | r | 34/41 (82%) | 1.58 | 12 (35%) 0 0 | 70, 84, 94, 101 | 0 |
| All | All | 5310/5694 (93%) | -0.06 | 174 (3%) 46 36 | 34, 53, 81, 116 | 0 |

All (174) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | R | 28 | VAL | 5.5 |
| 13 | o | 56 | PRO | 5.4 |
| 14 | T | 30 | THR | 5.3 |
| 16 | v | 18 | THR | 5.3 |
| 3 | C | 142 | GLU | 5.1 |
| 19 | Z | 7 | LEU | 4.7 |
| 13 | O | 35 | SER | 4.7 |
| 9 | J | 5 | GLY | 4.6 |
| 2 | b | 487 | SER | 4.5 |
| 19 | Z | 2 | THR | 4.5 |
| 13 | o | 58 | ASN | 4.4 |
| 2 | B | 488 | PRO | 4.3 |
| 13 | o | 61 | GLN | 4.2 |
| 13 | O | 63 | ALA | 4.2 |
| 19 | Z | 8 | ALA | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | b | 495 | PHE | 4.1 |
| 19 | Z | 62 | VAL | 4.1 |
| 20 | R | 23 | ILE | 4.0 |
| 19 | z | 34 | ASP | 3.9 |
| 2 | b | 496 | TYR | 3.9 |
| 20 | R | 25 | PRO | 3.8 |
| 20 | r | 25 | PRO | 3.8 |
| 12 | M | 33 | GLN | 3.7 |
| 19 | z | 32 | ASP | 3.7 |
| 15 | U | 8 | GLU | 3.7 |
| 20 | r | 3 | TRP | 3.7 |
| 9 | j | 6 | GLY | 3.6 |
| 2 | b | 504 | THR | 3.6 |
| 8 | i | 36 | ASP | 3.6 |
| 8 | I | 34 | ARG | 3.6 |
| 8 | I | 36 | ASP | 3.6 |
| 13 | o | 4 | THR | 3.5 |
| 2 | b | 293 | ALA | 3.5 |
| 3 | c | 454 | GLY | 3.4 |
| 1 | a | 13 | LEU | 3.4 |
| 2 | b | 294 | SER | 3.4 |
| 20 | R | 18 | TRP | 3.4 |
| 13 | O | 61 | GLN | 3.4 |
| 20 | r | 32 | GLN | 3.3 |
| 2 | B | 128 | THR | 3.3 |
| 10 | K | 14 | ALA | 3.3 |
| 7 | H | 2 | ALA | 3.3 |
| 13 | o | 3 | GLN | 3.3 |
| 19 | z | 1 | MET | 3.2 |
| 19 | z | 31 | GLN | 3.2 |
| 2 | b | 482 | ILE | 3.2 |
| 2 | b | 503 | THR | 3.2 |
| 18 | X | 2 | THR | 3.2 |
| 2 | b | 485 | GLU | 3.2 |
| 13 | O | 4 | THR | 3.2 |
| 2 | b | 500 | GLY | 3.2 |
| 19 | Z | 9 | LEU | 3.1 |
| 16 | v | 19 | ILE | 3.1 |
| 15 | U | 73 | GLN | 3.1 |
| 1 | a | 12 | ASN | 3.1 |
| 19 | Z | 1 | MET | 3.1 |
| 13 | o | 5 | LEU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | r | 26 | TYR | 3.1 |
| 16 | v | 16 | GLY | 3.1 |
| 20 | R | 24 | LEU | 3.0 |
| 20 | R | 26 | TYR | 3.0 |
| 5 | E | 15 | THR | 3.0 |
| 18 | x | 2 | THR | 3.0 |
| 19 | z | 62 | VAL | 3.0 |
| 13 | O | 245 | PRO | 3.0 |
| 20 | r | 18 | TRP | 3.0 |
| 20 | r | 2 | ASP | 3.0 |
| 2 | b | 497 | GLN | 3.0 |
| 19 | z | 29 | SER | 2.9 |
| 19 | z | 56 | VAL | 2.9 |
| 20 | R | 27 | ALA | 2.9 |
| 19 | Z | 3 | ILE | 2.9 |
| 19 | Z | 61 | VAL | 2.9 |
| 3 | c | 453 | ALA | 2.9 |
| 20 | R | 5 | VAL | 2.8 |
| 20 | R | 21 | ARG | 2.8 |
| 9 | J | 7 | ARG | 2.8 |
| 13 | o | 62 | GLU | 2.8 |
| 5 | e | 79 | PHE | 2.8 |
| 2 | B | 487 | SER | 2.8 |
| 19 | Z | 32 | ASP | 2.8 |
| 20 | r | 22 | ASN | 2.8 |
| 17 | y | 20 | ALA | 2.8 |
| 19 | Z | 6 | GLN | 2.8 |
| 20 | R | 29 | LYS | 2.8 |
| 2 | b | 486 | LEU | 2.8 |
| 2 | b | 502 | VAL | 2.8 |
| 5 | E | 60 | GLN | 2.8 |
| 5 | e | 16 | SER | 2.8 |
| 5 | e | 82 | GLN | 2.8 |
| 5 | e | 4 | THR | 2.7 |
| 2 | B | 126 | PRO | 2.7 |
| 1 | a | 243 | GLU | 2.7 |
| 13 | o | 60 | ARG | 2.7 |
| 2 | B | 292 | LEU | 2.6 |
| 12 | m | 33 | GLN | 2.6 |
| 9 | j | 5 | GLY | 2.6 |
| 13 | O | 62 | GLU | 2.6 |
| 19 | Z | 30 | PRO | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | d | 240 | ALA | 2.6 |
| 20 | r | 34 | LEU | 2.6 |
| 2 | B | 127 | ARG | 2.6 |
| 2 | b | 127 | ARG | 2.6 |
| 5 | E | 13 | ILE | 2.5 |
| 5 | e | 83 | LEU | 2.5 |
| 2 | b | 295 | GLY | 2.5 |
| 5 | e | 5 | THR | 2.5 |
| 20 | r | 20 | VAL | 2.5 |
| 20 | R | 31 | VAL | 2.5 |
| 20 | R | 3 | TRP | 2.5 |
| 1 | a | 225 | ARG | 2.5 |
| 19 | Z | 4 | LEU | 2.4 |
| 11 | l | 1 | MET | 2.4 |
| 2 | b | 85 | GLY | 2.4 |
| 5 | e | 60 | GLN | 2.4 |
| 19 | z | 35 | ARG | 2.4 |
| 2 | b | 489 | GLU | 2.4 |
| 2 | B | 484 | PRO | 2.4 |
| 10 | K | 17 | ILE | 2.4 |
| 19 | Z | 60 | PHE | 2.4 |
| 20 | R | 30 | GLN | 2.4 |
| 2 | b | 505 | ARG | 2.4 |
| 20 | r | 35 | LEU | 2.4 |
| 13 | O | 180 | GLU | 2.3 |
| 20 | r | 19 | ALA | 2.3 |
| 17 | Y | 43 | ARG | 2.3 |
| 5 | E | 20 | TRP | 2.3 |
| 20 | r | 14 | LEU | 2.3 |
| 4 | D | 238 | THR | 2.3 |
| 1 | A | 12 | ASN | 2.3 |
| 3 | c | 23 | ALA | 2.3 |
| 13 | o | 6 | THR | 2.2 |
| 19 | z | 2 | THR | 2.2 |
| 13 | O | 246 | ALA | 2.2 |
| 16 | v | 106 | ASN | 2.2 |
| 2 | b | 501 | ASP | 2.2 |
| 19 | Z | 59 | PHE | 2.2 |
| 5 | E | 17 | VAL | 2.2 |
| 18 | x | 37 | VAL | 2.2 |
| 2 | B | 489 | GLU | 2.2 |
| 5 | E | 16 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 2 | b | 84 | THR | 2.2 |
| 2 | b | 129 | GLY | 2.2 |
| 19 | Z | 33 | TRP | 2.2 |
| 19 | Z | 57 | LEU | 2.1 |
| 10 | K | 20 | PRO | 2.1 |
| 18 | x | 36 | LYS | 2.1 |
| 20 | R | 33 | LYS | 2.1 |
| 3 | C | 192 | GLY | 2.1 |
| 5 | e | 78 | THR | 2.1 |
| 10 | K | 13 | GLU | 2.1 |
| 8 | i | 31 | ASN | 2.1 |
| 5 | e | 77 | GLU | 2.1 |
| 15 | U | 53 | ALA | 2.1 |
| 2 | b | 478 | VAL | 2.1 |
| 2 | b | 239[A] | SER | 2.1 |
| 18 | x | 38 | GLN | 2.1 |
| 5 | e | 81 | GLU | 2.1 |
| 2 | b | 477 | ASP | 2.1 |
| 4 | d | 17 | ILE | 2.1 |
| 5 | E | 61 | ARG | 2.1 |
| 19 | Z | 52 | LEU | 2.0 |
| 5 | e | 11 | SER | 2.0 |
| 18 | X | 34 | ILE | 2.0 |
| 2 | B | 485 | GLU | 2.0 |
| 7 | H | 23 | PRO | 2.0 |
| 1 | A | 228 | THR | 2.0 |
| 3 | C | 191 | PRO | 2.0 |
| 8 | i | 34 | ARG | 2.0 |
| 13 | O | 3 | GLN | 2.0 |
| 5 | e | 6 | GLY | 2.0 |
| 13 | O | 37 | THR | 2.0 |
| 5 | E | 14 | ILE | 2.0 |
| 19 | Z | 10 | ALA | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8 | FME | I | 1 | 10/11 | 0.90 | 0.28 | 50,60,70,76 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.90 | 0.34 | 49,61,69,69 | 0 |
| 14 | FME | T | 1 | 10/11 | 0.92 | 0.15 | 51,58,70,77 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.92 | 0.29 | 54,63,77,87 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.94 | 0.12 | 52,59,74,79 | 0 |
| 14 | FME | t | 1 | 10/11 | 0.94 | 0.12 | 42,56,71,77 | 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(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 29 | SQD | I | 102 | 40/54 | 0.65 | 0.48 | 44,69,94,102 | 0 |
| 29 | SQD | B | 623 | 47/54 | 0.74 | 0.27 | 44,61,109,124 | 0 |
| 32 | LHG | e | 101 | 42/49 | 0.76 | 0.31 | 57,76,98,101 | 0 |
| 23 | LMG | C | 501 | 51/55 | 0.77 | 0.31 | 46,67,81,88 | 0 |
| 23 | LMG | C | 520 | 51/55 | 0.78 | 0.28 | 43,74,86,89 | 0 |
| 23 | LMG | d | 408 | 40/55 | 0.79 | 0.25 | 47,61,84,89 | 0 |
| 23 | LMG | B | 621 | 51/55 | 0.80 | 0.24 | 52,70,78,88 | 0 |
| 30 | UNL | b | 606 | 13/- | 0.80 | 0.24 | 45,51,57,59 | 0 |
| 32 | LHG | E | 101 | 49/49 | 0.80 | 0.28 | 48,77,92,95 | 0 |
| 23 | LMG | b | 626 | 51/55 | 0.80 | 0.30 | 38,56,72,77 | 0 |
| 30 | UNL | d | 401 | 22/- | 0.81 | 0.23 | 39,54,63,66 | 0 |
| 30 | UNL | z | 101 | 11/- | 0.81 | 0.29 | 48,65,72,72 | 0 |
| 23 | LMG | C | 521 | 51/55 | 0.81 | 0.34 | 49,71,81,91 | 0 |
| 23 | LMG | A | 603 | 51/55 | 0.81 | 0.26 | 40,62,77,83 | 0 |
| 30 | UNL | b | 603 | 11/- | 0.82 | 0.24 | 44,54,62,62 | 0 |
| 23 | LMG | a | 715 | 51/55 | 0.82 | 0.24 | 47,65,85,91 | 0 |
| 28 | PL9 | A | 611 | 55/55 | 0.82 | 0.29 | 46,68,78,83 | 0 |
| 23 | LMG | c | 519 | 51/55 | 0.82 | 0.30 | 42,75,90,91 | 0 |
| 23 | LMG | c | 520 | 51/55 | 0.82 | 0.40 | 61,75,95,100 | 0 |
| 30 | UNL | a | 716 | 4/- | 0.82 | 0.31 | 31,46,50,51 | 0 |
| 29 | SQD | b | 601 | 54/54 | 0.83 | 0.24 | 45,66,94,105 | 0 |
| 27 | BCR | H | 102 | 40/40 | 0.84 | 0.25 | 41,54,62,62 | 0 |
| 27 | BCR | k | 101 | 40/40 | 0.84 | 0.24 | 53,69,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23 | LMG | b | 627 | 51/55 | 0.84 | 0.31 | 51,70,80,82 | 0 |
| 30 | UNL | I | 101 | 9/- | 0.84 | 0.20 | 44,52,61,61 | 0 |
| 29 | SQD | A | 614 | 40/54 | 0.84 | 0.22 | 47,59,68,72 | 0 |
| 30 | UNL | a | 717 | 7/- | 0.84 | 0.26 | 48,53,61,67 | 0 |
| 30 | UNL | B | 601 | 12/- | 0.85 | 0.18 | 31,49,56,56 | 0 |
| 30 | UNL | B | 622 | 6/- | 0.85 | 0.26 | 40,51,56,56 | 0 |
| 30 | UNL | i | 101 | 22/- | 0.85 | 0.22 | 36,50,58,62 | 0 |
| 30 | UNL | j | 101 | 9/- | 0.85 | 0.24 | 52,61,65,65 | 0 |
| 30 | UNL | a | 718 | 13/- | 0.85 | 0.21 | 45,54,61,62 | 0 |
| 23 | LMG | a | 701 | 51/55 | 0.85 | 0.23 | 42,64,87,90 | 0 |
| 30 | UNL | b | 604 | 11/- | 0.85 | 0.26 | 38,48,57,59 | 0 |
| 28 | PL9 | a | 713 | 55/55 | 0.86 | 0.25 | 57,68,77,84 | 0 |
| 25 | CLA | C | 514 | 65/65 | 0.86 | 0.24 | 44,73,81,89 | 0 |
| 25 | CLA | b | 607 | 65/65 | 0.86 | 0.26 | 48,63,81,91 | 0 |
| 27 | BCR | k | 102 | 40/40 | 0.86 | 0.26 | 53,65,81,84 | 0 |
| 25 | CLA | c | 513 | 65/65 | 0.86 | 0.24 | 57,68,82,96 | 0 |
| 27 | BCR | D | 405 | 40/40 | 0.87 | 0.24 | 48,61,77,81 | 0 |
| 25 | CLA | B | 602 | 65/65 | 0.87 | 0.22 | 44,62,75,80 | 0 |
| 29 | SQD | f | 102 | 41/54 | 0.87 | 0.30 | 54,73,85,89 | 0 |
| 25 | CLA | c | 512 | 65/65 | 0.87 | 0.26 | 60,67,89,91 | 0 |
| 30 | UNL | m | 101 | 5/- | 0.87 | 0.24 | 36,39,42,45 | 0 |
| 23 | LMG | b | 628 | 9/55 | 0.87 | 0.22 | 36,50,54,54 | 0 |
| 30 | UNL | H | 101 | 8/- | 0.87 | 0.18 | 43,53,58,64 | 0 |
| 30 | UNL | b | 605 | 13/- | 0.87 | 0.21 | 42,54,62,62 | 0 |
| 27 | BCR | C | 515 | 40/40 | 0.88 | 0.23 | 53,63,72,76 | 0 |
| 27 | BCR | t | 103 | 40/40 | 0.88 | 0.23 | 36,47,60,63 | 0 |
| 23 | LMG | M | 101 | 51/55 | 0.88 | 0.20 | 34,58,74,77 | 0 |
| 25 | CLA | C | 513 | 65/65 | 0.88 | 0.23 | 52,66,80,86 | 0 |
| 27 | BCR | b | 602 | 40/40 | 0.88 | 0.22 | 45,53,70,76 | 0 |
| 27 | BCR | h | 101 | 40/40 | 0.88 | 0.22 | 40,54,68,71 | 0 |
| 30 | UNL | M | 102 | 6/- | 0.88 | 0.31 | 45,51,51,53 | 0 |
| 30 | UNL | M | 103 | 16/- | 0.88 | 0.21 | 41,51,57,58 | 0 |
| 29 | SQD | B | 626 | 54/54 | 0.88 | 0.25 | 46,67,90,99 | 0 |
| 29 | SQD | D | 410 | 43/54 | 0.88 | 0.29 | 56,75,87,96 | 0 |
| 25 | CLA | d | 403 | 65/65 | 0.88 | 0.20 | 45,54,65,66 | 0 |
| 30 | UNL | A | 613 | 7/- | 0.89 | 0.18 | 34,49,53,55 | 0 |
| 25 | CLA | D | 404 | 65/65 | 0.89 | 0.22 | 34,44,80,84 | 0 |
| 25 | CLA | C | 508 | 65/65 | 0.89 | 0.20 | 41,50,57,66 | 0 |
| 25 | CLA | C | 511 | 65/65 | 0.89 | 0.24 | 44,57,64,70 | 0 |
| 25 | CLA | B | 617 | 65/65 | 0.89 | 0.20 | 39,52,80,84 | 0 |
| 27 | BCR | c | 514 | 40/40 | 0.89 | 0.25 | 61,67,74,75 | 0 |
| 25 | CLA | C | 505 | 65/65 | 0.89 | 0.22 | 48,63,71,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 33 | DGD | c | 517 | 62/66 | 0.89 | 0.22 | 54,61,81,92 | 0 |
| 25 | CLA | c | 511 | 65/65 | 0.90 | 0.18 | 50,62,71,74 | 0 |
| 27 | BCR | K | 101 | 40/40 | 0.90 | 0.20 | 51,60,70,75 | 0 |
| 25 | CLA | B | 610 | 65/65 | 0.90 | 0.19 | 36,51,58,63 | 0 |
| 23 | LMG | f | 101 | 51/55 | 0.90 | 0.20 | 48,58,84,93 | 0 |
| 27 | BCR | d | 404 | 40/40 | 0.90 | 0.23 | 45,59,70,77 | 0 |
| 25 | CLA | B | 607 | 65/65 | 0.90 | 0.20 | 41,50,64,75 | 0 |
| 25 | CLA | c | 503 | 65/65 | 0.90 | 0.21 | 48,61,68,73 | 0 |
| 25 | CLA | c | 504 | 58/65 | 0.90 | 0.19 | 52,59,66,67 | 0 |
| 33 | DGD | h | 102 | 62/66 | 0.90 | 0.23 | 41,55,63,66 | 0 |
| 25 | CLA | b | 612 | 65/65 | 0.91 | 0.17 | 32,46,56,69 | 0 |
| 23 | LMG | D | 409 | 51/55 | 0.91 | 0.20 | 39,61,82,88 | 0 |
| 27 | BCR | Y | 101 | 40/40 | 0.91 | 0.20 | 46,66,71,72 | 0 |
| 25 | CLA | C | 512 | 65/65 | 0.91 | 0.19 | 52,60,69,71 | 0 |
| 27 | BCR | b | 624 | 40/40 | 0.91 | 0.20 | 38,49,58,59 | 0 |
| 25 | CLA | c | 506 | 65/65 | 0.91 | 0.21 | 47,57,79,92 | 0 |
| 27 | BCR | c | 515 | 40/40 | 0.91 | 0.18 | 38,53,64,72 | 0 |
| 25 | CLA | C | 506 | 65/65 | 0.91 | 0.19 | 41,51,57,60 | 0 |
| 25 | CLA | C | 507 | 65/65 | 0.91 | 0.19 | 44,55,75,88 | 0 |
| 25 | CLA | A | 606 | 65/65 | 0.91 | 0.19 | 29,43,48,53 | 0 |
| 30 | UNL | m | 102 | 12/- | 0.91 | 0.19 | 41,47,50,52 | 0 |
| 25 | CLA | a | 707 | 65/65 | 0.91 | 0.18 | 33,47,51,53 | 0 |
| 25 | CLA | C | 509 | 65/65 | 0.91 | 0.21 | 46,55,91,100 | 0 |
| 27 | BCR | C | 516 | 40/40 | 0.91 | 0.20 | 42,51,58,58 | 0 |
| 33 | DGD | C | 518 | 62/66 | 0.91 | 0.19 | 51,62,81,88 | 0 |
| 33 | DGD | H | 103 | 62/66 | 0.91 | 0.21 | 39,49,59,62 | 0 |
| 28 | PL9 | D | 406 | 55/55 | 0.91 | 0.21 | 31,43,52,55 | 0 |
| 25 | CLA | b | 610 | 65/65 | 0.91 | 0.22 | 37,47,59,62 | 0 |
| 25 | CLA | b | 616 | 65/65 | 0.92 | 0.20 | 34,42,50,56 | 0 |
| 25 | CLA | b | 621 | 65/65 | 0.92 | 0.17 | 38,49,55,60 | 0 |
| 29 | SQD | A | 612 | 52/54 | 0.92 | 0.21 | 45,67,80,92 | 0 |
| 25 | CLA | D | 402 | 65/65 | 0.92 | 0.18 | 31,41,47,51 | 0 |
| 25 | CLA | C | 510 | 65/65 | 0.92 | 0.20 | 45,57,64,68 | 0 |
| 25 | CLA | c | 505 | 65/65 | 0.92 | 0.19 | 41,52,60,69 | 0 |
| 27 | BCR | b | 623 | 40/40 | 0.92 | 0.19 | 42,53,60,61 | 0 |
| 25 | CLA | B | 616 | 65/65 | 0.92 | 0.16 | 42,51,60,64 | 0 |
| 29 | SQD | a | 714 | 54/54 | 0.92 | 0.22 | 48,68,83,90 | 0 |
| 27 | BCR | b | 625 | 40/40 | 0.92 | 0.16 | 36,49,55,58 | 0 |
| 25 | CLA | c | 510 | 65/65 | 0.92 | 0.21 | 43,54,63,68 | 0 |
| 25 | CLA | a | 711 | 65/65 | 0.92 | 0.19 | 34,46,79,87 | 0 |
| 30 | UNL | t | 101 | 10/- | 0.92 | 0.17 | 26,44,49,50 | 0 |
| 25 | CLA | B | 605 | 65/65 | 0.92 | 0.22 | 35,47,62,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 32 | LHG | D | 408 | 49/49 | 0.92 | 0.21 | 42,59,72,84 | 0 |
| 25 | CLA | C | 503 | 65/65 | 0.92 | 0.23 | 43,56,62,68 | 0 |
| 32 | LHG | a | 720 | 39/49 | 0.92 | 0.20 | 41,54,65,66 | 0 |
| 30 | UNL | B | 624 | 11/- | 0.92 | 0.20 | 34,49,52,53 | 0 |
| 33 | DGD | C | 517 | 62/66 | 0.92 | 0.20 | 36,46,65,71 | 0 |
| 25 | CLA | B | 615 | 65/65 | 0.92 | 0.17 | 38,48,67,73 | 0 |
| 27 | BCR | B | 620 | 40/40 | 0.92 | 0.18 | 39,48,56,71 | 0 |
| 33 | DGD | c | 516 | 62/66 | 0.92 | 0.20 | 34,50,68,76 | 0 |
| 25 | CLA | b | 613 | 65/65 | 0.92 | 0.19 | 37,44,55,58 | 0 |
| 33 | DGD | c | 518 | 62/66 | 0.92 | 0.19 | 44,57,76,81 | 0 |
| 25 | CLA | b | 615 | 65/65 | 0.92 | 0.17 | 42,50,55,60 | 0 |
| 25 | CLA | B | 608 | 65/65 | 0.93 | 0.17 | 30,42,52,56 | 0 |
| 25 | CLA | B | 609 | 65/65 | 0.93 | 0.25 | 32,45,51,59 | 0 |
| 25 | CLA | b | 608 | 65/65 | 0.93 | 0.19 | 39,49,60,64 | 0 |
| 24 | CL | a | 704 | 1/1 | 0.93 | 0.12 | 59,59,59,59 | 0 |
| 25 | CLA | d | 402 | 65/65 | 0.93 | 0.16 | 35,45,51,55 | 0 |
| 25 | CLA | B | 612 | 65/65 | 0.93 | 0.19 | 32,42,49,54 | 0 |
| 26 | PHO | a | 710 | 64/64 | 0.93 | 0.22 | 38,46,55,62 | 0 |
| 28 | PL9 | d | 405 | 55/55 | 0.93 | 0.20 | 32,41,53,56 | 0 |
| 27 | BCR | B | 618 | 40/40 | 0.93 | 0.18 | 37,52,60,63 | 0 |
| 27 | BCR | B | 619 | 40/40 | 0.93 | 0.20 | 35,47,51,52 | 0 |
| 25 | CLA | B | 614 | 65/65 | 0.93 | 0.20 | 34,43,57,69 | 0 |
| 25 | CLA | B | 603 | 65/65 | 0.93 | 0.21 | 42,52,59,62 | 0 |
| 25 | CLA | B | 604 | 65/65 | 0.93 | 0.20 | 33,44,54,57 | 0 |
| 30 | UNL | t | 102 | 5/- | 0.93 | 0.20 | 32,38,43,47 | 0 |
| 25 | CLA | b | 620 | 65/65 | 0.93 | 0.17 | 35,52,61,64 | 0 |
| 32 | LHG | B | 625 | 49/49 | 0.93 | 0.20 | 41,51,58,61 | 0 |
| 24 | CL | A | 605 | 1/1 | 0.93 | 0.14 | 51,51,51,51 | 0 |
| 25 | CLA | b | 622 | 47/65 | 0.93 | 0.16 | 40,48,58,64 | 0 |
| 25 | CLA | c | 502 | 65/65 | 0.93 | 0.21 | 45,55,67,81 | 0 |
| 27 | BCR | a | 712 | 40/40 | 0.93 | 0.17 | 26,44,53,54 | 0 |
| 25 | CLA | C | 502 | 65/65 | 0.93 | 0.21 | 38,50,57,64 | 0 |
| 25 | CLA | B | 606 | 65/65 | 0.93 | 0.18 | 37,45,52,53 | 0 |
| 33 | DGD | C | 519 | 62/66 | 0.93 | 0.17 | 43,56,67,76 | 0 |
| 25 | CLA | C | 504 | 65/65 | 0.93 | 0.20 | 43,57,62,68 | 0 |
| 25 | CLA | A | 607 | 65/65 | 0.93 | 0.19 | 31,46,91,99 | 0 |
| 25 | CLA | c | 507 | 65/65 | 0.93 | 0.17 | 41,50,61,67 | 0 |
| 25 | CLA | c | 508 | 65/65 | 0.93 | 0.19 | 46,57,72,82 | 0 |
| 25 | CLA | c | 509 | 65/65 | 0.93 | 0.19 | 49,57,70,73 | 0 |
| 34 | HEM | E | 102 | 43/43 | 0.93 | 0.22 | 52,66,76,80 | 0 |
| 34 | HEM | e | 102 | 43/43 | 0.93 | 0.20 | 60,71,81,91 | 0 |
| 27 | BCR | A | 610 | 40/40 | 0.94 | 0.15 | 31,44,52,56 | 0 |

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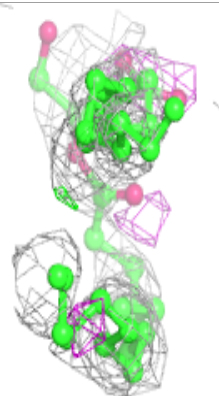
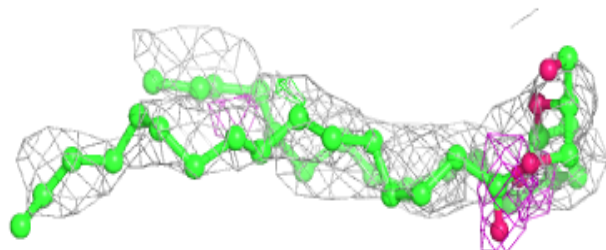
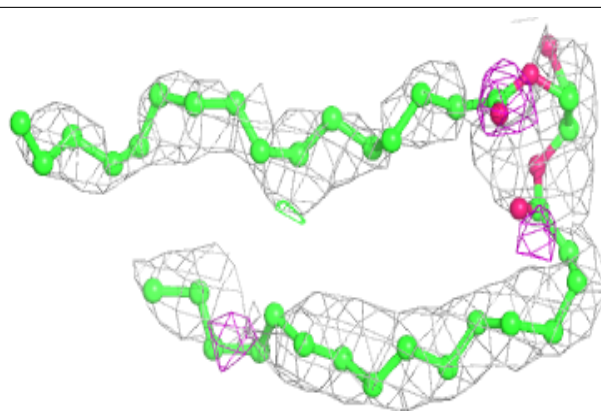
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 32 | LHG | L | 101 | 49/49 | 0.94 | 0.17 | 39,50,57,64 | 0 |
| 25 | CLA | b | 619 | 65/65 | 0.94 | 0.20 | 31,42,59,67 | 0 |
| 32 | LHG | b | 629 | 49/49 | 0.94 | 0.16 | 36,50,57,64 | 0 |
| 32 | LHG | d | 406 | 49/49 | 0.94 | 0.19 | 32,53,61,65 | 0 |
| 32 | LHG | d | 407 | 49/49 | 0.94 | 0.18 | 36,46,54,61 | 0 |
| 25 | CLA | b | 609 | 65/65 | 0.94 | 0.19 | 34,45,55,61 | 0 |
| 25 | CLA | A | 609 | 54/65 | 0.94 | 0.16 | 34,43,60,71 | 0 |
| 25 | CLA | B | 613 | 65/65 | 0.94 | 0.19 | 36,43,55,59 | 0 |
| 25 | CLA | c | 501 | 65/65 | 0.94 | 0.19 | 37,49,55,59 | 0 |
| 25 | CLA | a | 719 | 65/65 | 0.94 | 0.16 | 32,43,49,54 | 0 |
| 25 | CLA | b | 614 | 65/65 | 0.94 | 0.22 | 39,48,58,60 | 0 |
| 25 | CLA | D | 403 | 65/65 | 0.94 | 0.16 | 33,42,54,61 | 0 |
| 25 | CLA | B | 611 | 65/65 | 0.94 | 0.20 | 40,47,55,60 | 0 |
| 26 | PHO | D | 401 | 64/64 | 0.94 | 0.20 | 37,46,55,59 | 0 |
| 32 | LHG | D | 407 | 49/49 | 0.94 | 0.23 | 34,49,59,60 | 0 |
| 25 | CLA | b | 617 | 65/65 | 0.94 | 0.19 | 36,45,50,57 | 0 |
| 25 | CLA | a | 708 | 65/65 | 0.95 | 0.16 | 37,47,89,101 | 0 |
| 25 | CLA | b | 611 | 65/65 | 0.95 | 0.16 | 30,46,52,56 | 0 |
| 26 | PHO | A | 608 | 64/64 | 0.95 | 0.18 | 32,40,46,50 | 0 |
| 25 | CLA | b | 618 | 65/65 | 0.95 | 0.20 | 32,43,50,52 | 0 |
| 26 | PHO | a | 709 | 64/64 | 0.95 | 0.19 | 26,41,47,50 | 0 |
| 22 | FE2 | a | 703 | 1/1 | 0.95 | 0.03 | 60,60,60,60 | 0 |
| 35 | HEC | V | 201 | 43/43 | 0.95 | 0.16 | 41,51,57,63 | 0 |
| 35 | HEC | v | 201 | 43/43 | 0.95 | 0.15 | 46,58,64,72 | 0 |
| 24 | CL | a | 705 | 1/1 | 0.97 | 0.12 | 50,50,50,50 | 0 |
| 31 | BCT | A | 615 | 4/4 | 0.97 | 0.10 | 46,49,51,54 | 0 |
| 22 | FE2 | A | 602 | 1/1 | 0.97 | 0.03 | 60,60,60,60 | 0 |
| 21 | OEX | a | 702 | 10/10 | 0.97 | 0.11 | 44,52,59,60 | 0 |
| 21 | OEX | A | 601 | 10/10 | 0.98 | 0.11 | 42,54,59,60 | 0 |
| 31 | BCT | a | 706 | 4/4 | 0.98 | 0.09 | 50,56,56,59 | 0 |
| 24 | CL | A | 604 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |

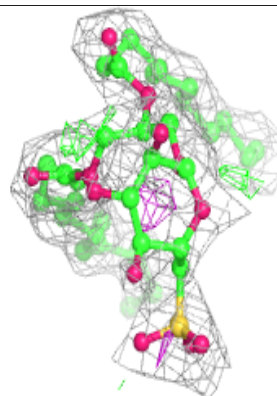
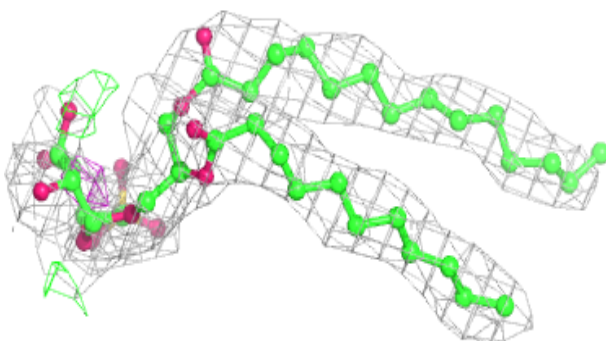
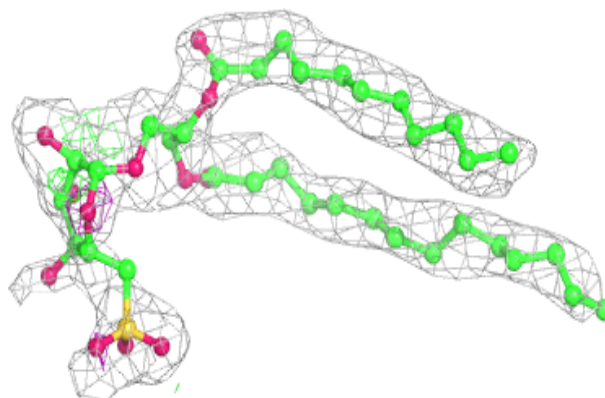
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD I 102:

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

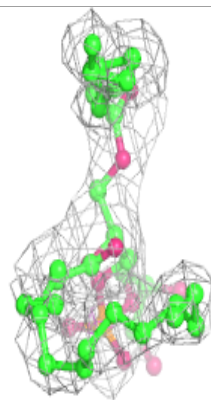
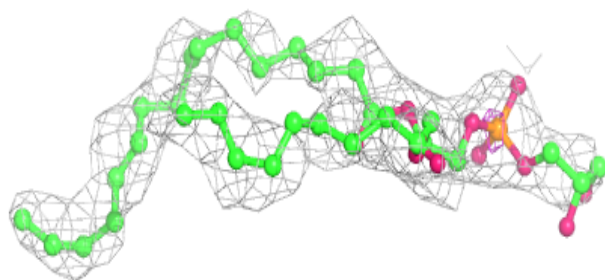
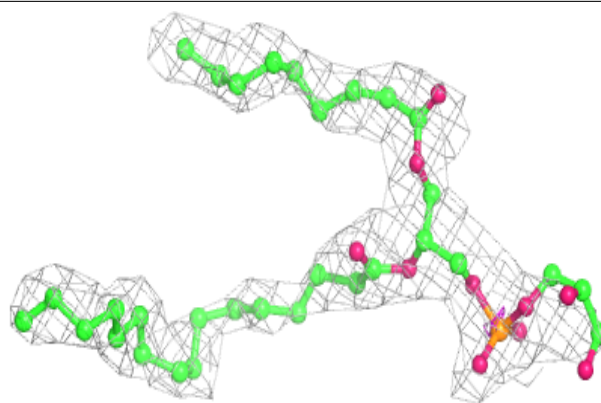
**Electron density around SQD B 623:**

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

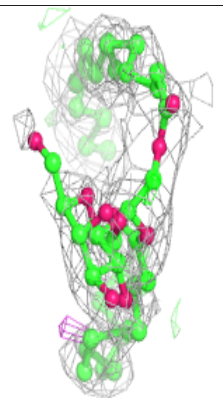
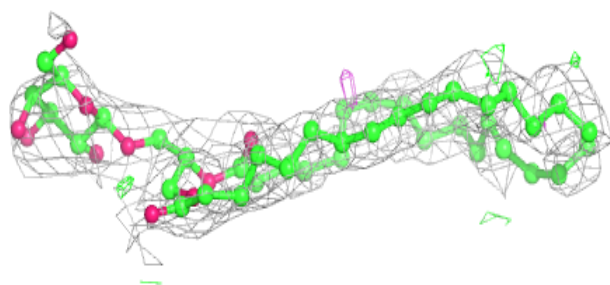
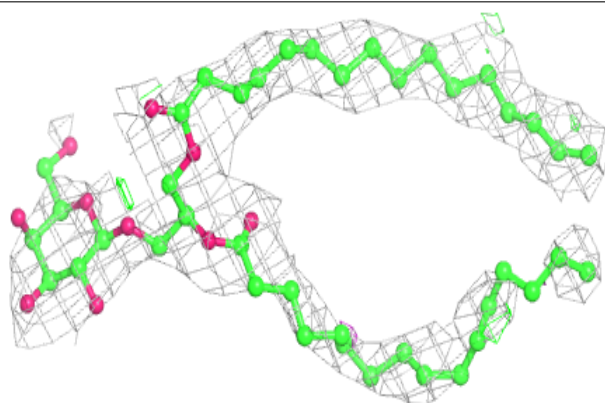


Electron density around LHG e 101:

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

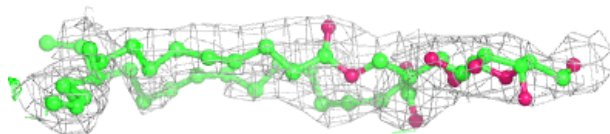
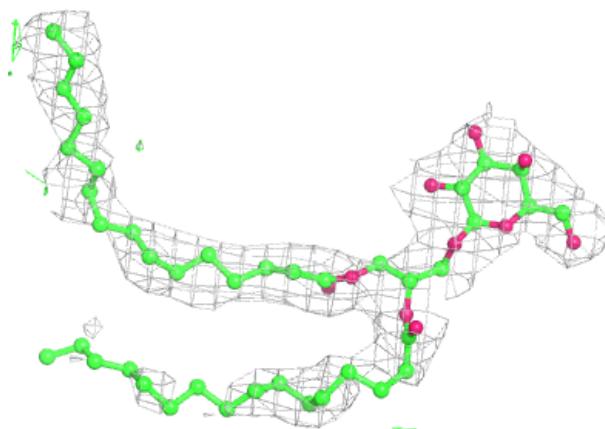
**Electron density around LMG C 501:**

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

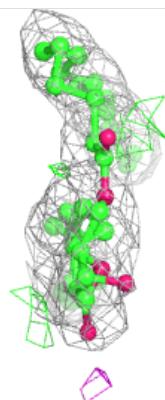
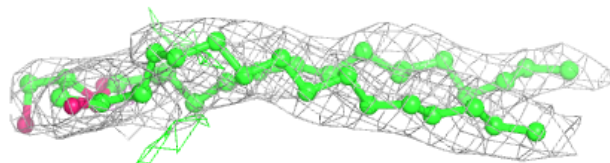
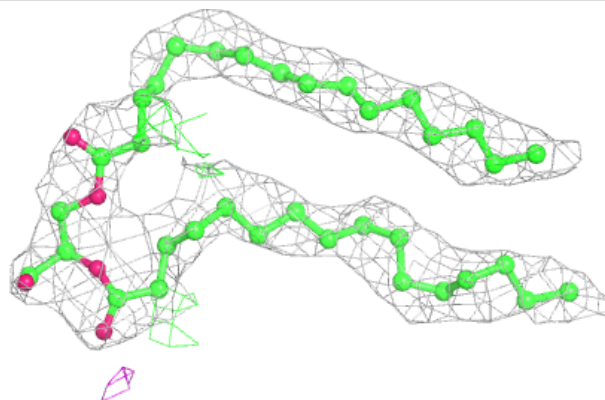


Electron density around LMG C 520:

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

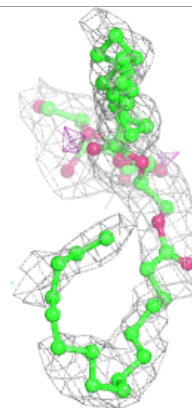
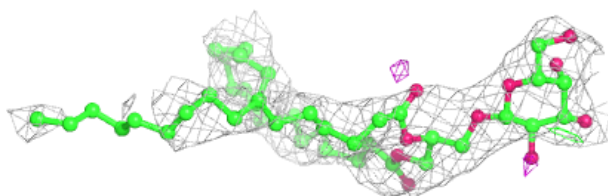
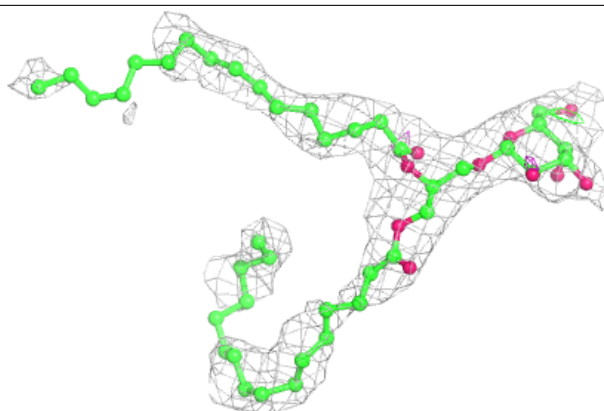
**Electron density around LMG d 408:**

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

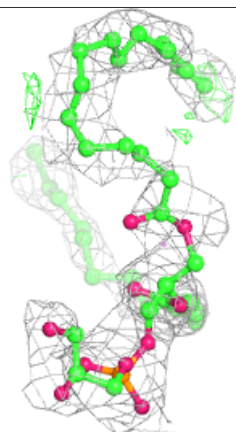
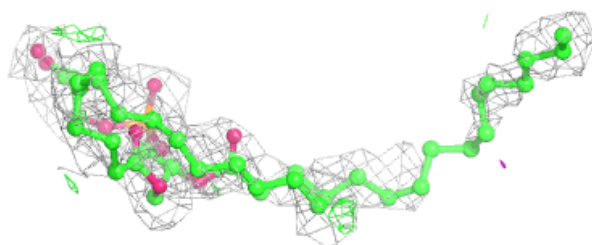
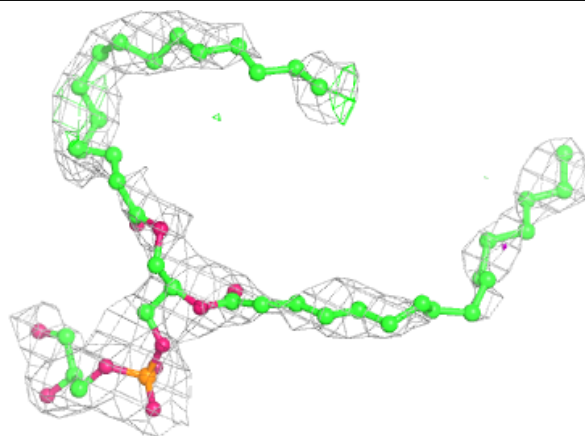


Electron density around LMG B 621:

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

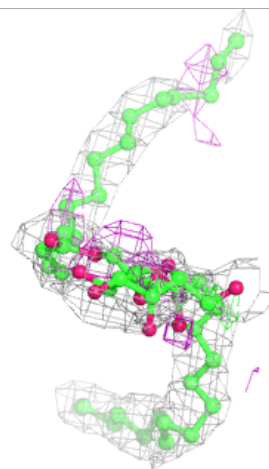
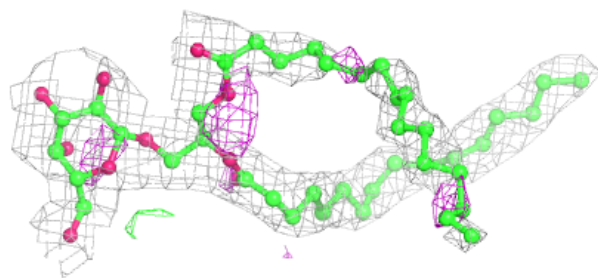
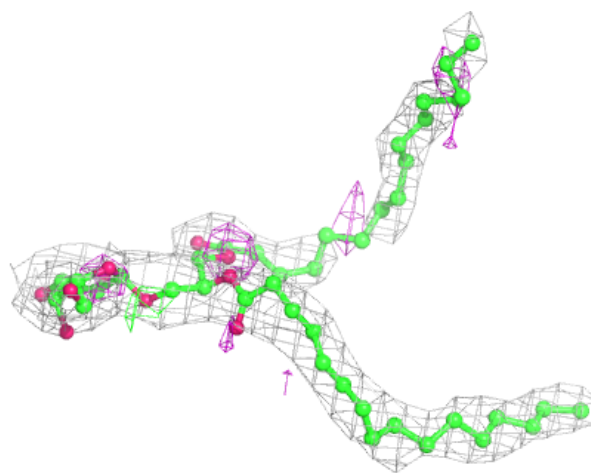
**Electron density around LHG E 101:**

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



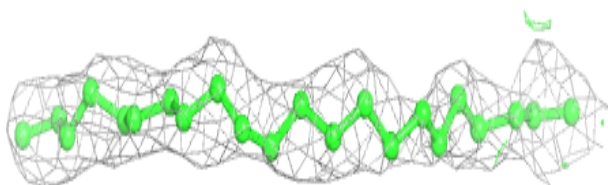
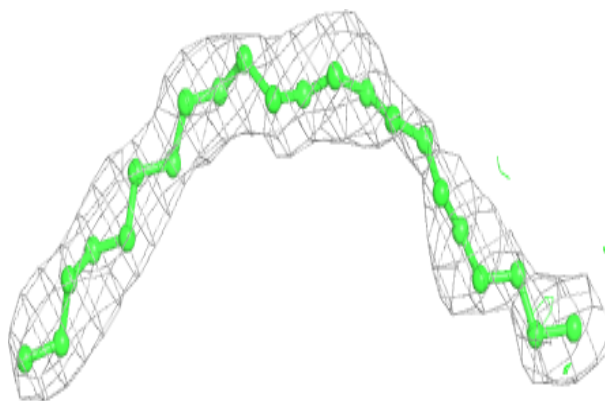
Electron density around LMG b 626:

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

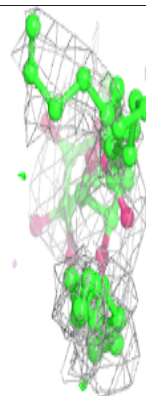
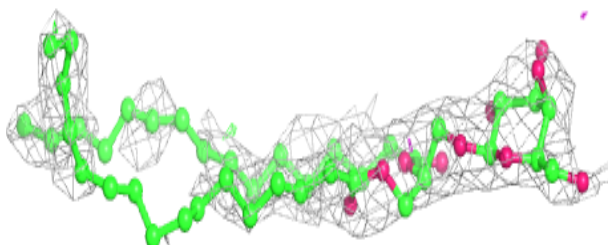
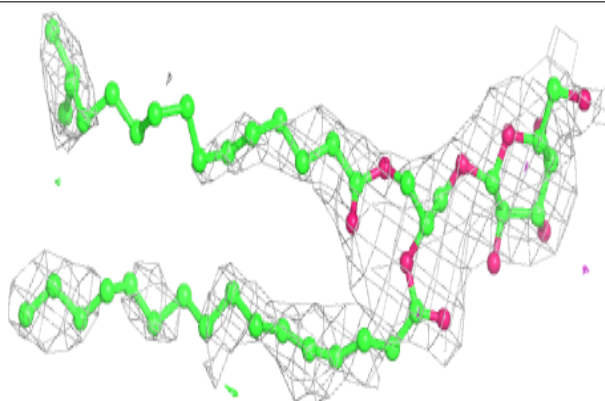


Electron density around UNL d 401:

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

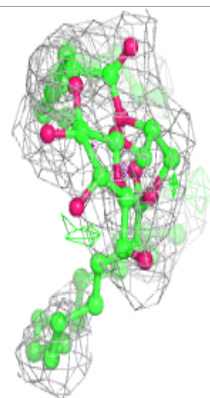
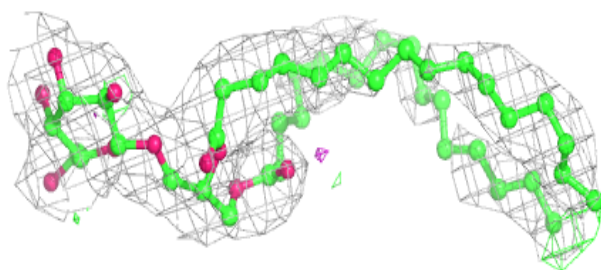
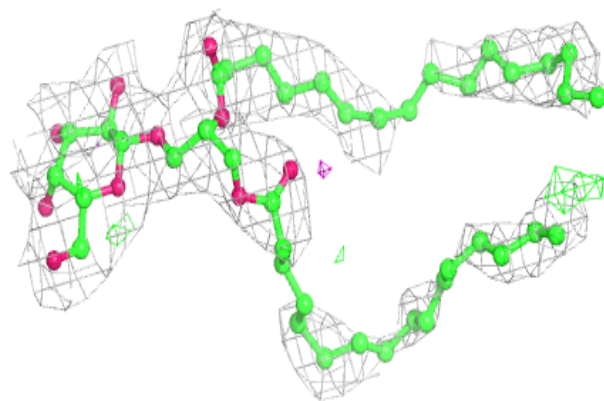
**Electron density around LMG C 521:**

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

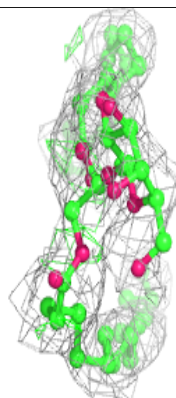
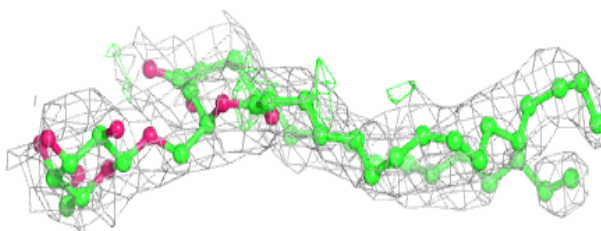
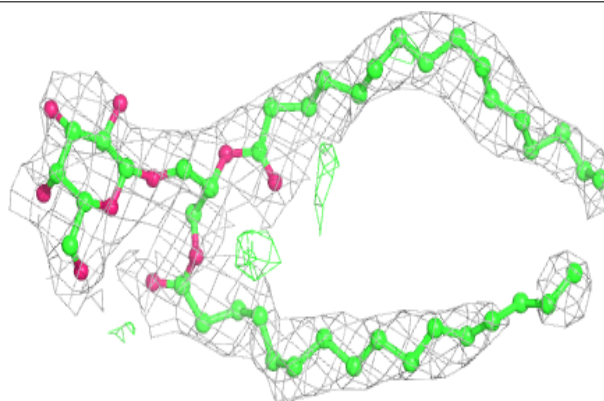


Electron density around LMG A 603:

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

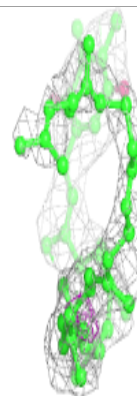
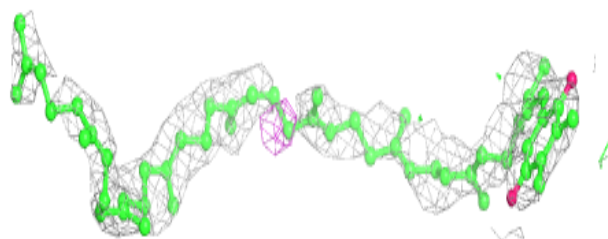
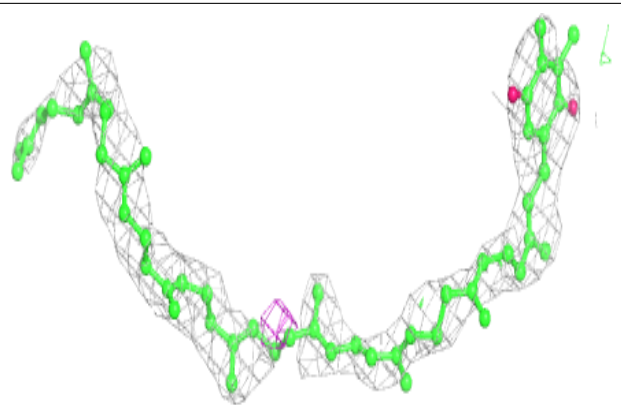
**Electron density around LMG a 715:**

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



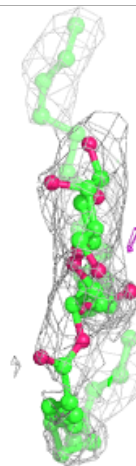
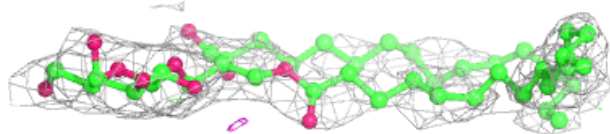
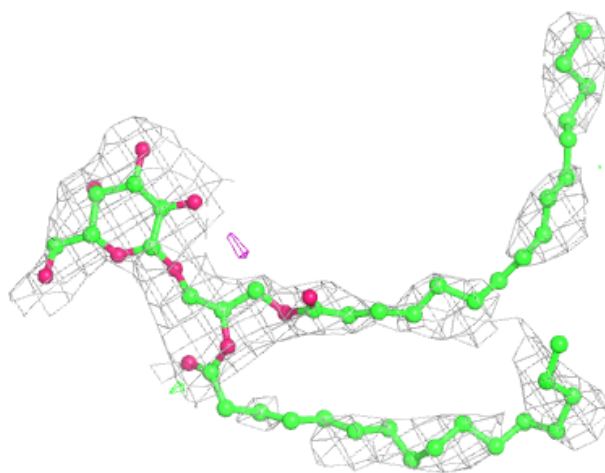
Electron density around PL9 A 611:

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



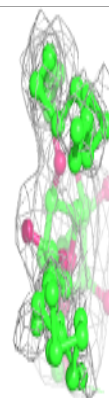
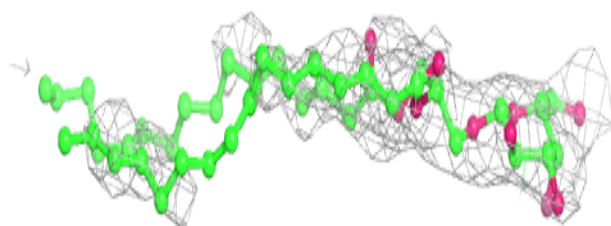
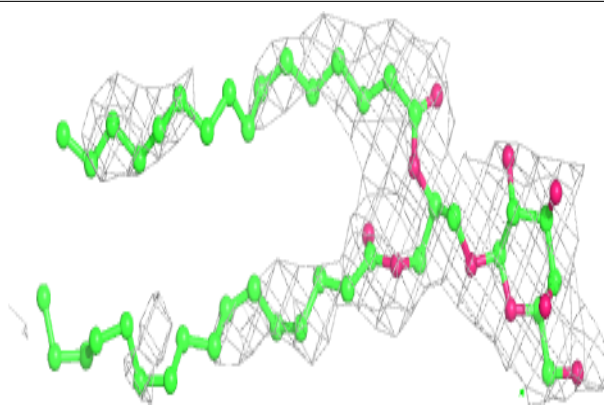
Electron density around LMG c 519:

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

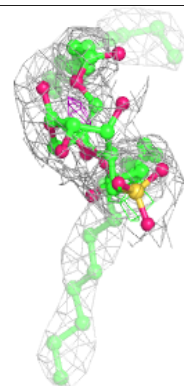
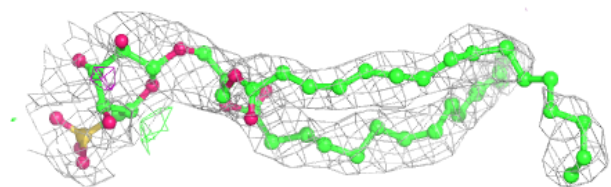
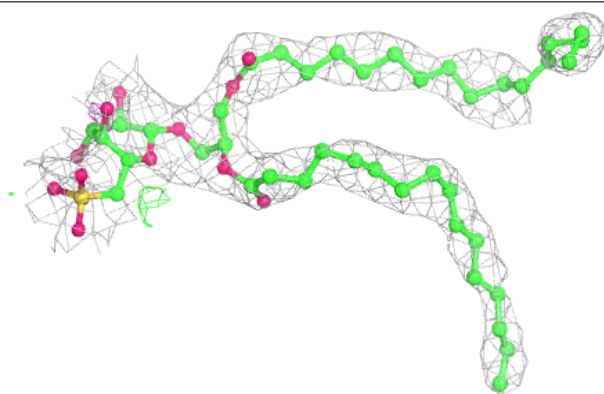


Electron density around LMG c 520:

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

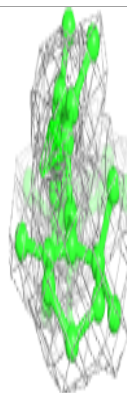
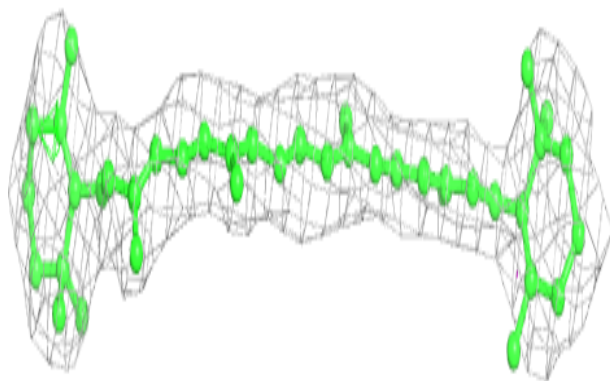
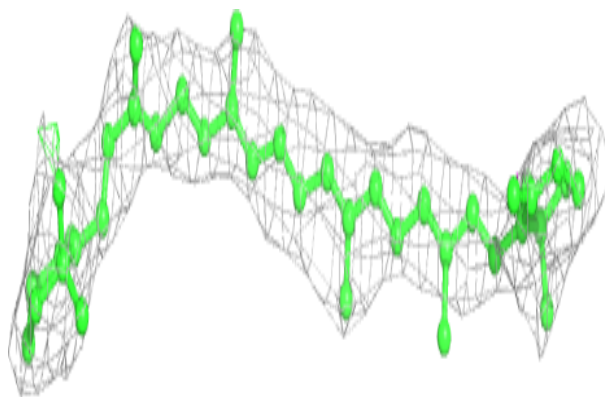
**Electron density around SQD b 601:**

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

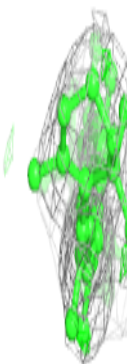
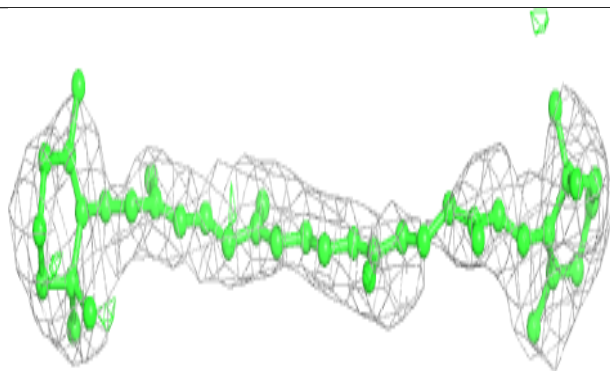
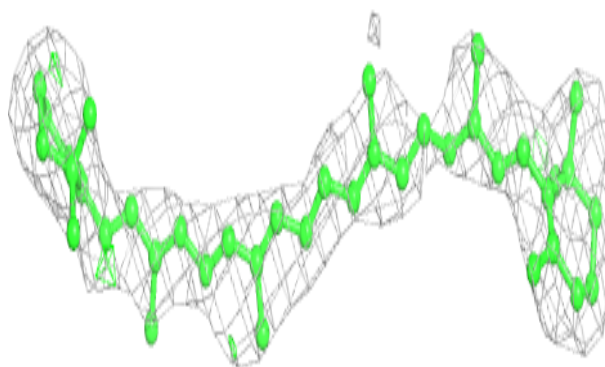


Electron density around BCR H 102:

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

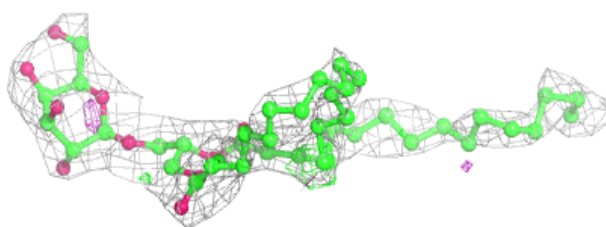
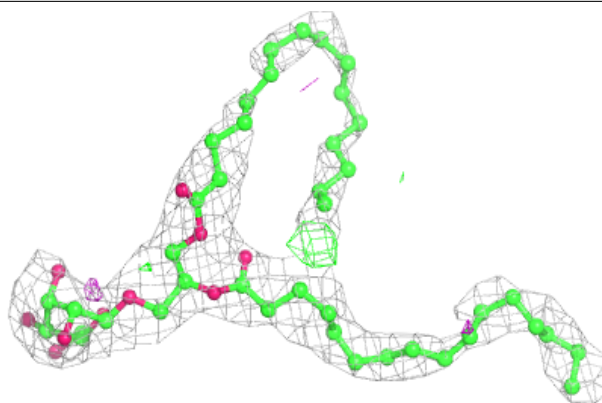
**Electron density around BCR k 101:**

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

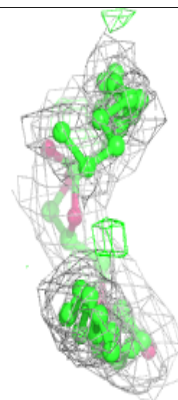
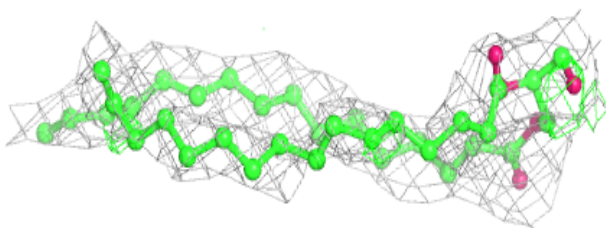
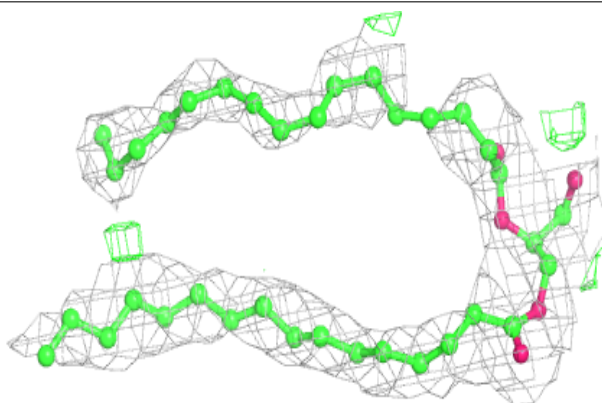


Electron density around LMG b 627:

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

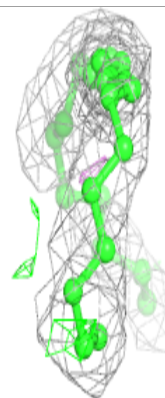
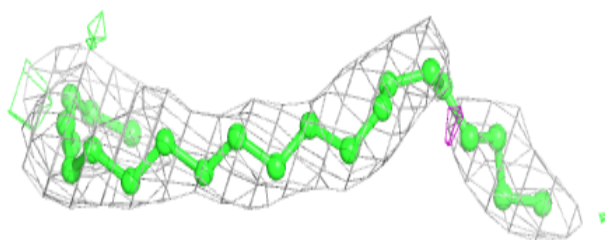
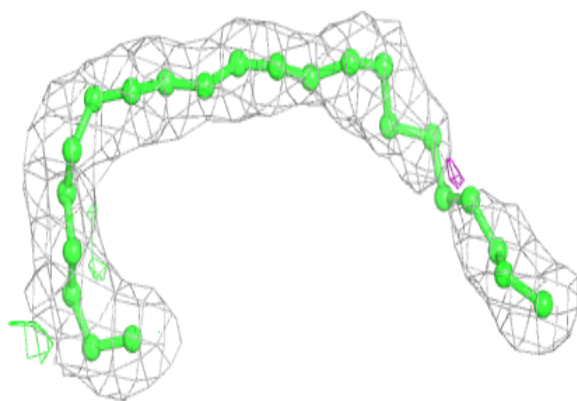
**Electron density around SQD A 614:**

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

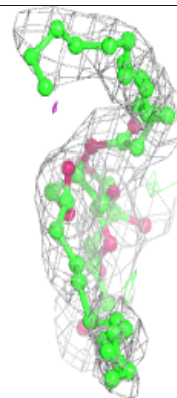
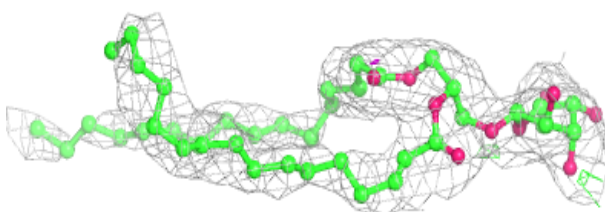
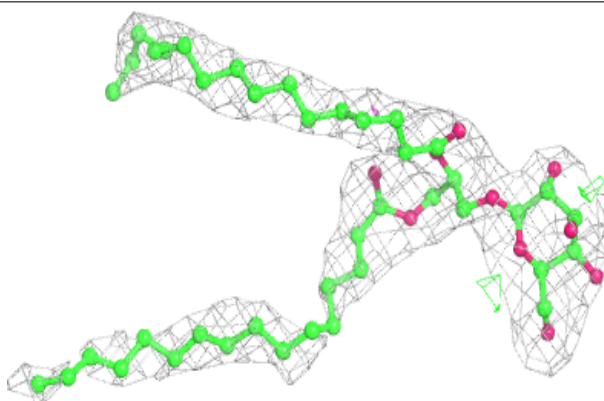


Electron density around UNL i 101:

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

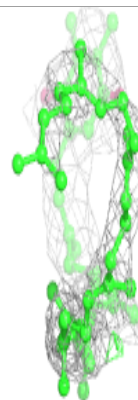
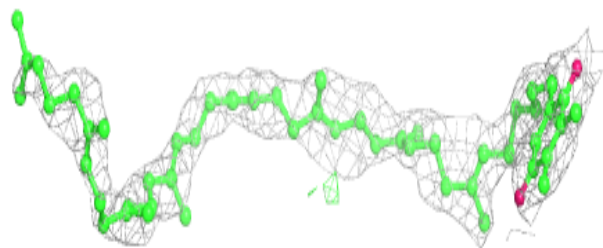
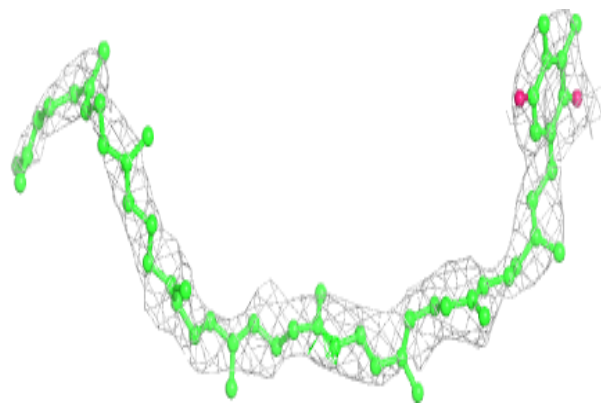
**Electron density around LMG a 701:**

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

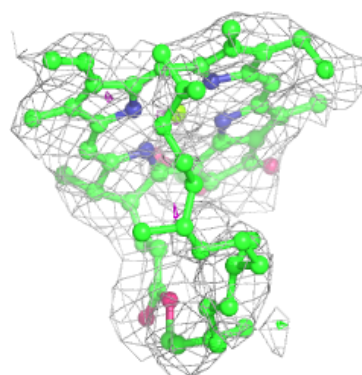
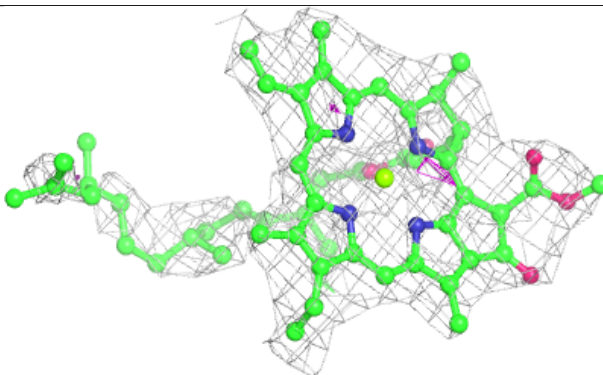
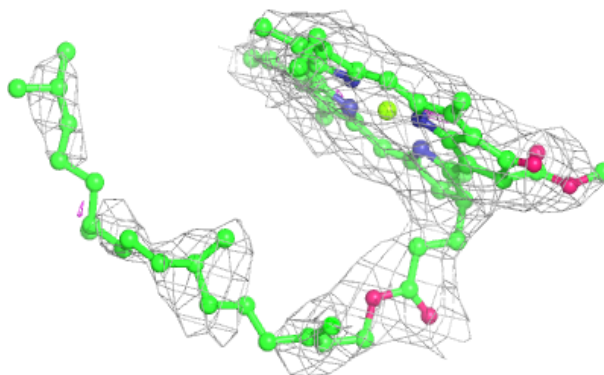


Electron density around PL9 a 713:

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

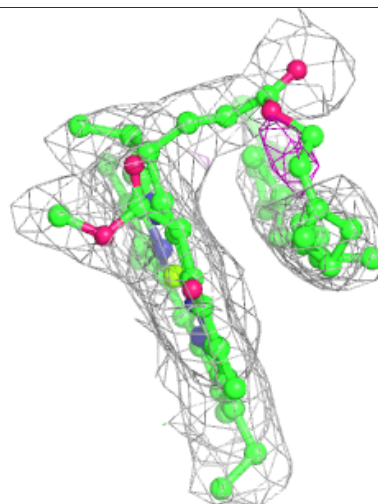
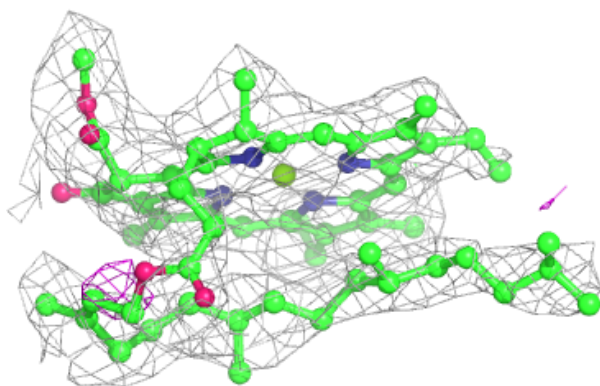
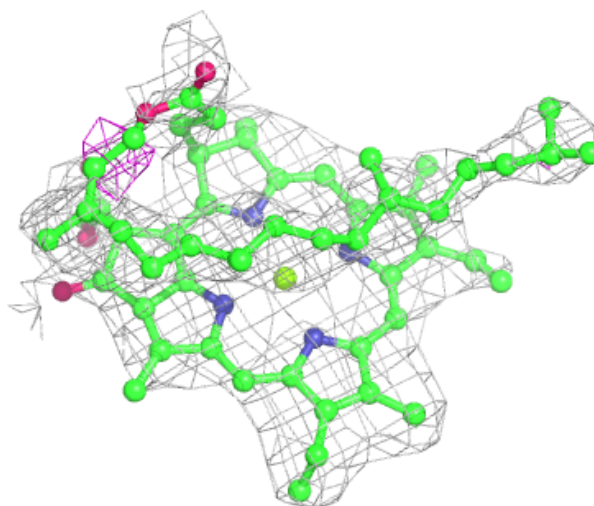
**Electron density around CLA C 514:**

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



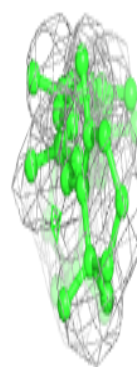
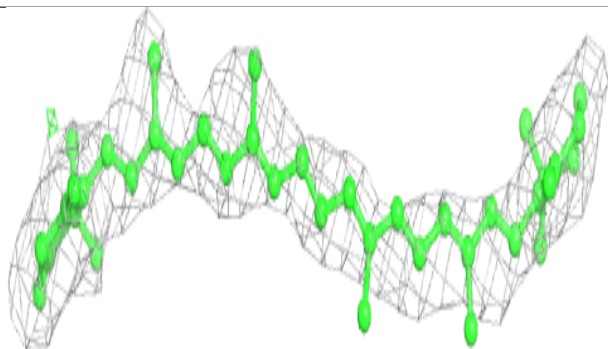
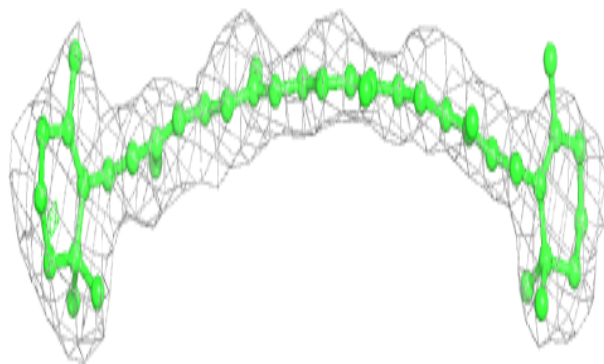
Electron density around CLA b 607:

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

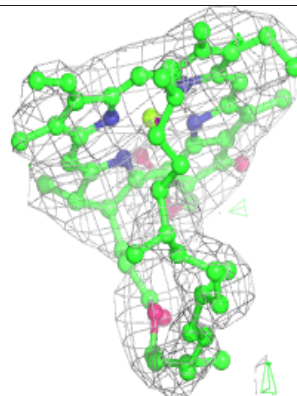
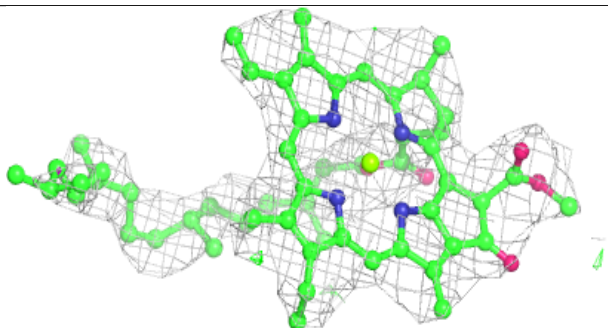
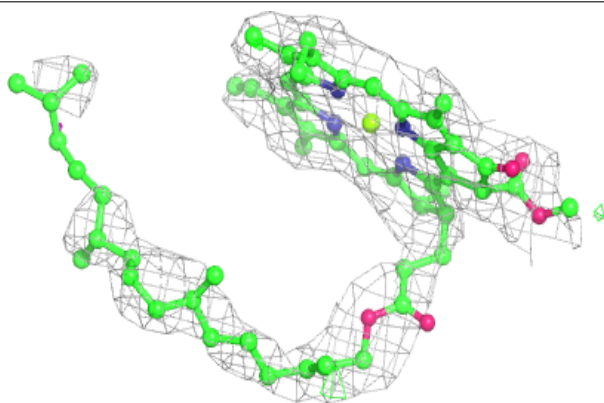


Electron density around BCR k 102:

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

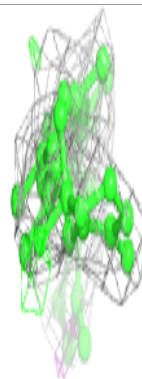
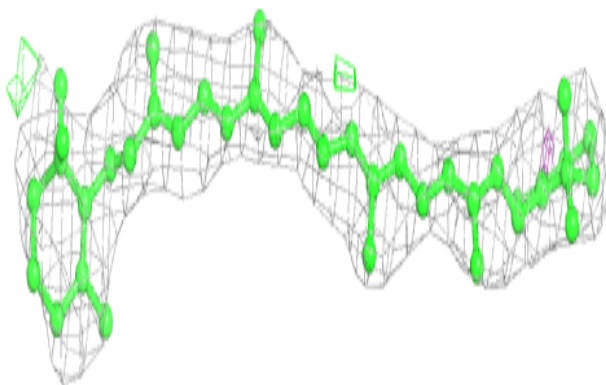
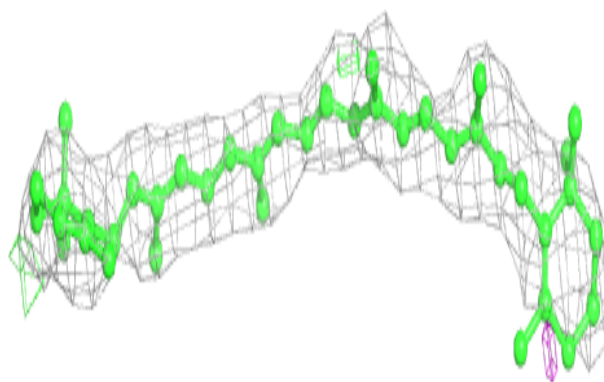
**Electron density around CLA c 513:**

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

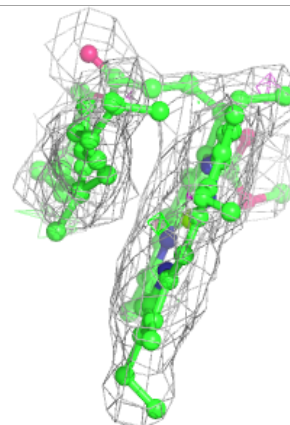
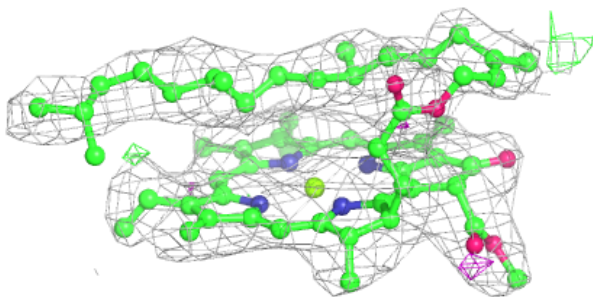
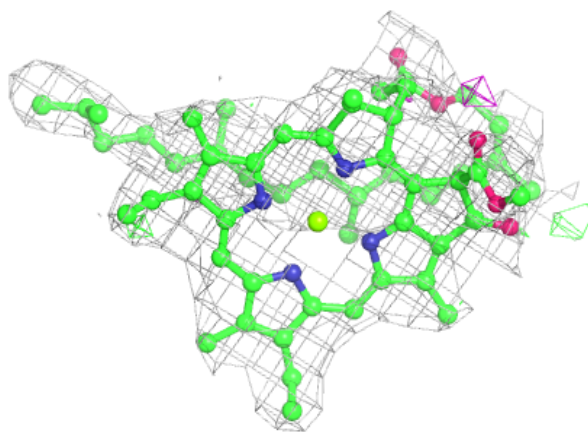


Electron density around BCR D 405:

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

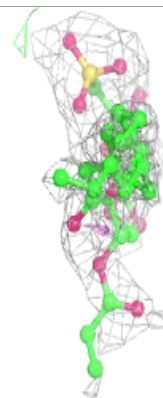
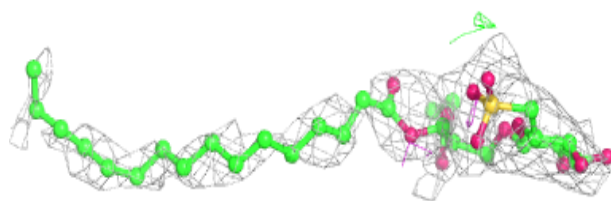
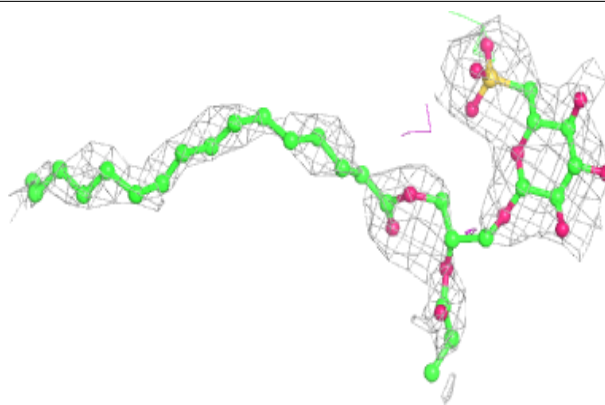
**Electron density around CLA B 602:**

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



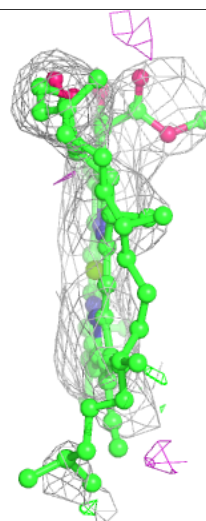
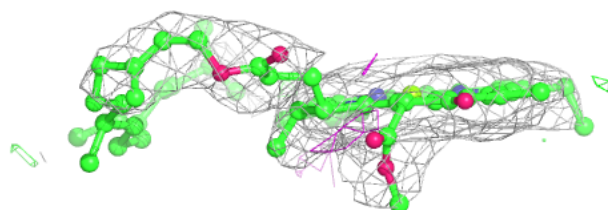
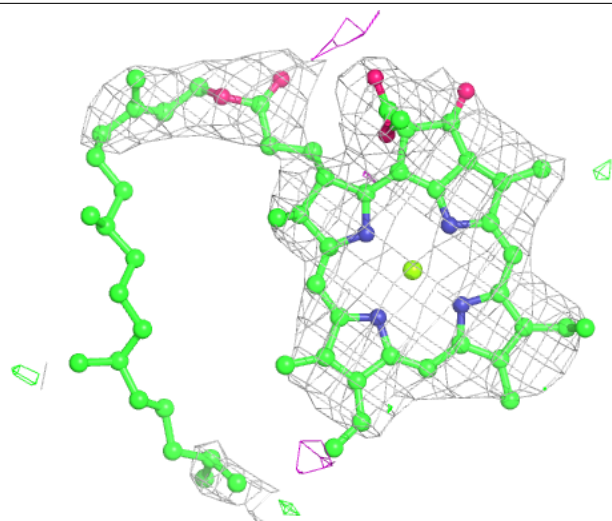
Electron density around SQD f 102:

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



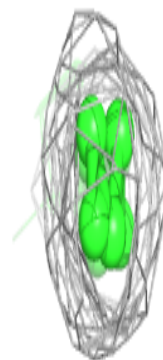
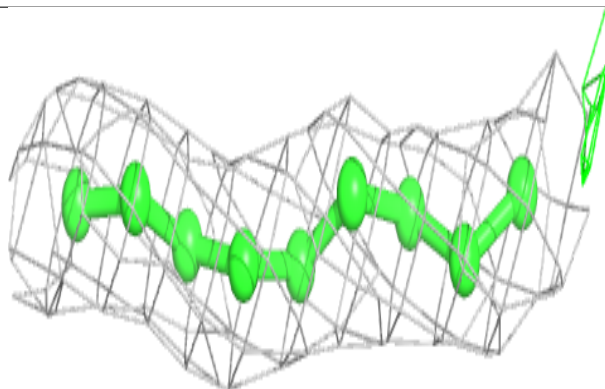
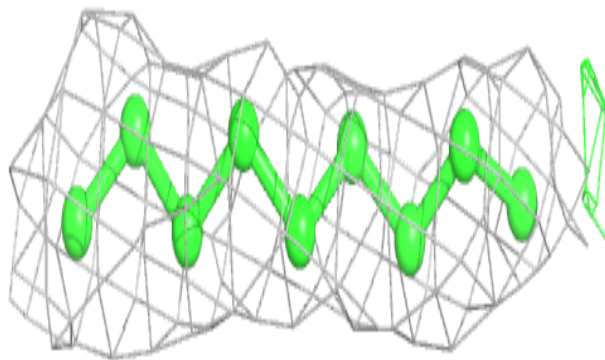
Electron density around CLA c 512:

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

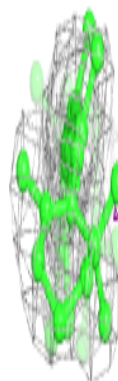
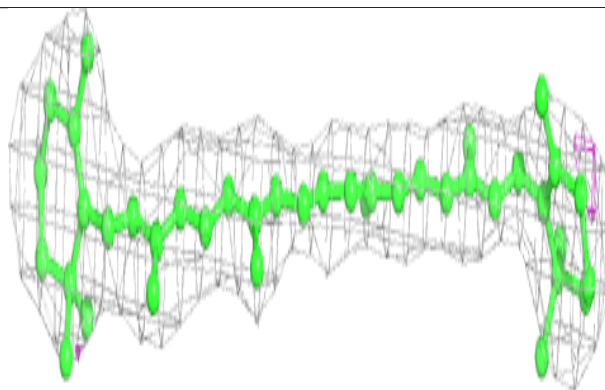
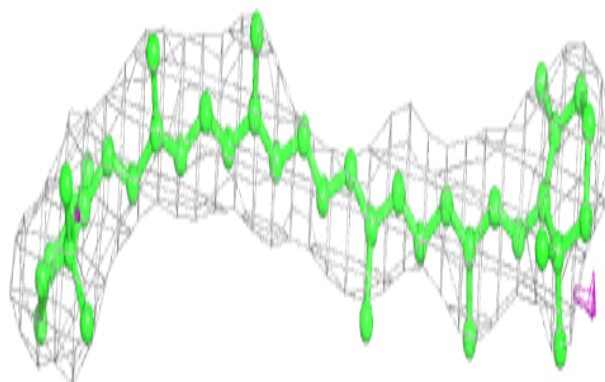


Electron density around LMG b 628:

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

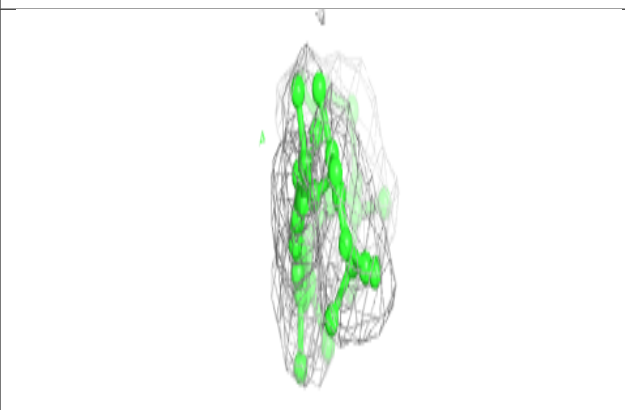
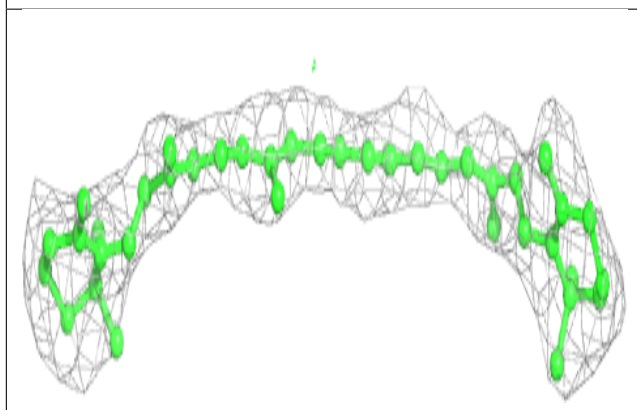
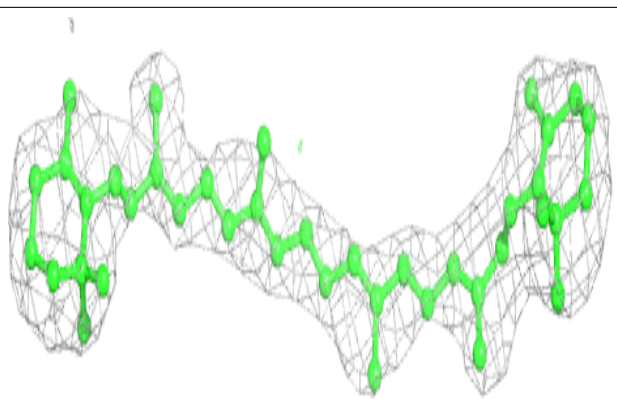
**Electron density around BCR C 515:**

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

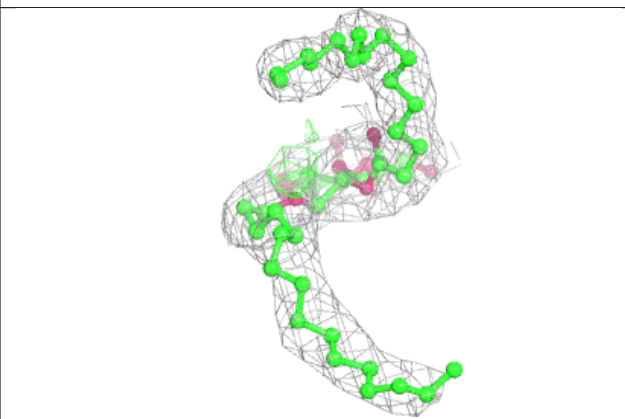
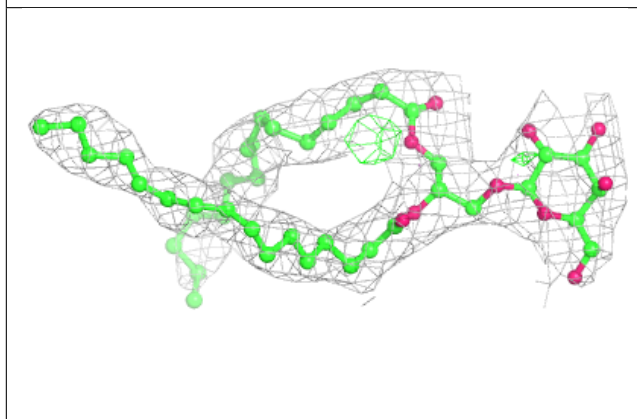
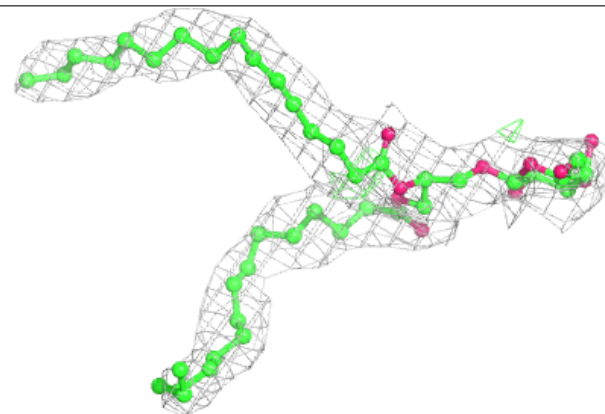


Electron density around BCR t 103:

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

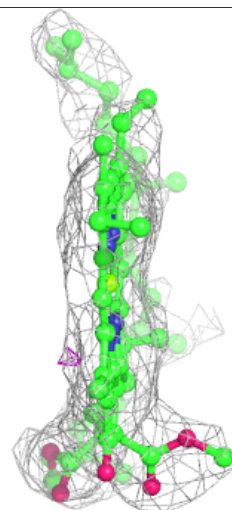
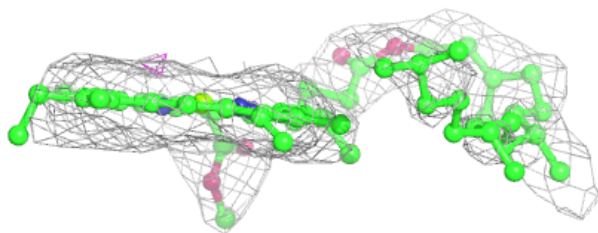
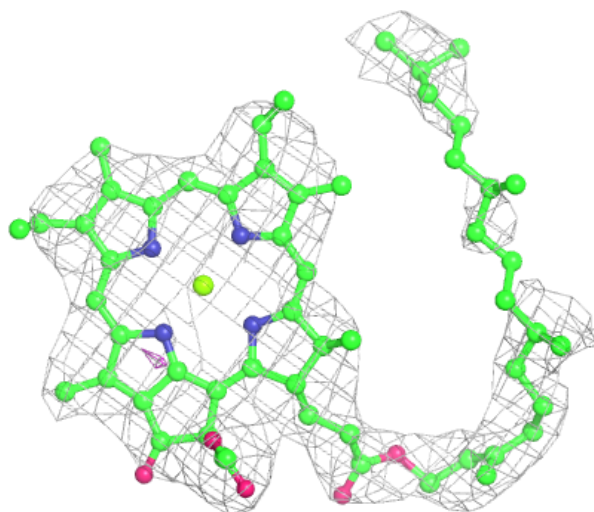
**Electron density around LMG M 101:**

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



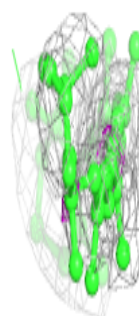
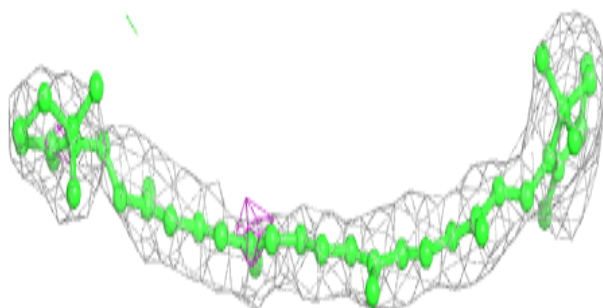
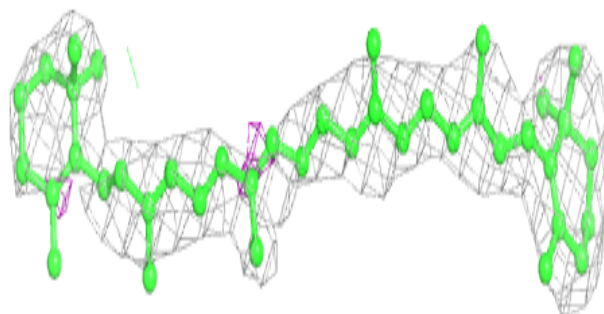
Electron density around CLA C 513:

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

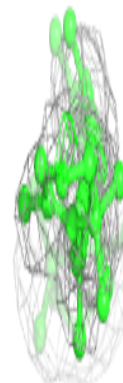
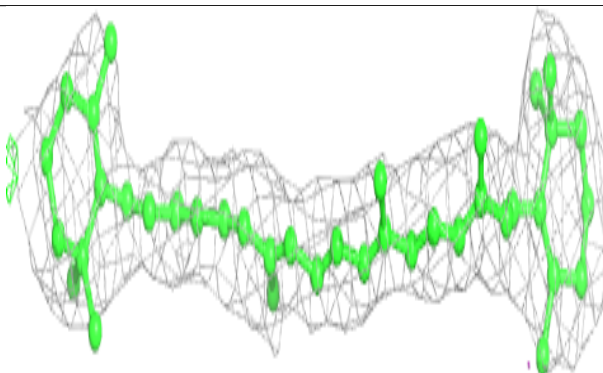
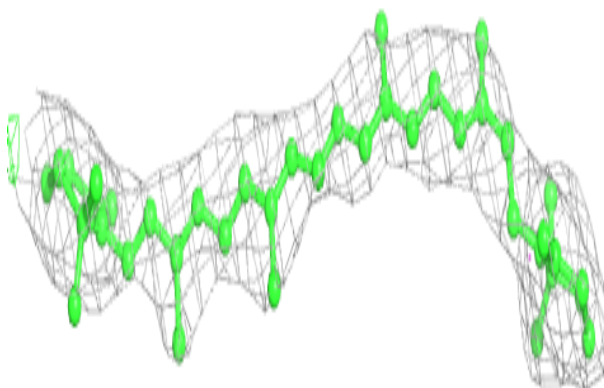


Electron density around BCR b 602:

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

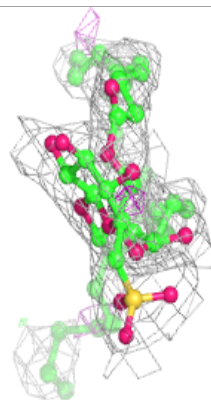
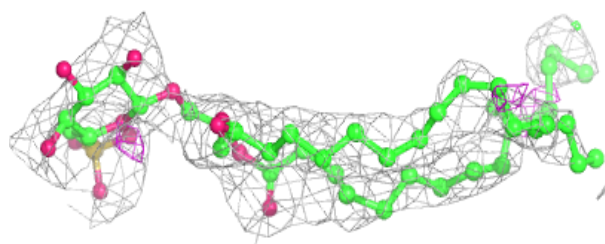
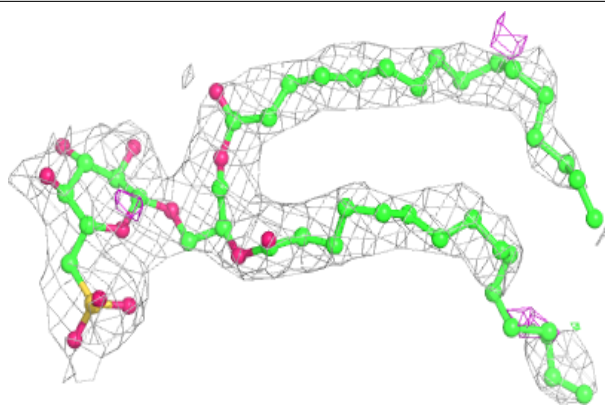
**Electron density around BCR h 101:**

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

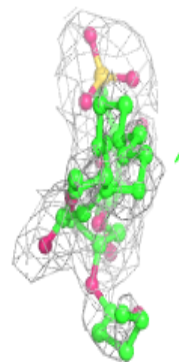
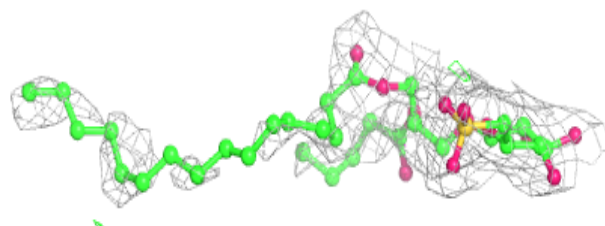
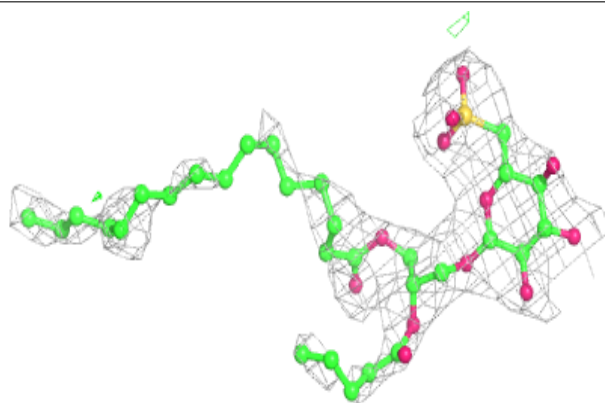


Electron density around SQD B 626:

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

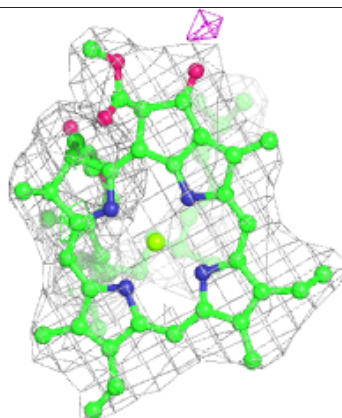
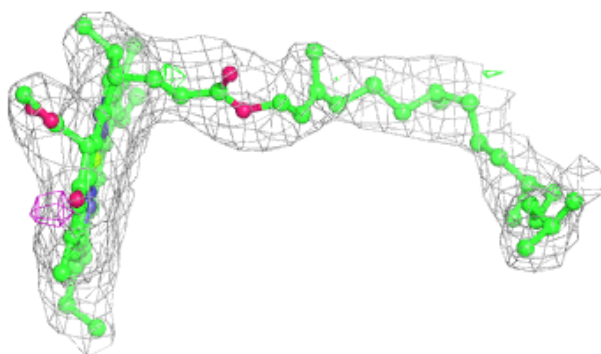
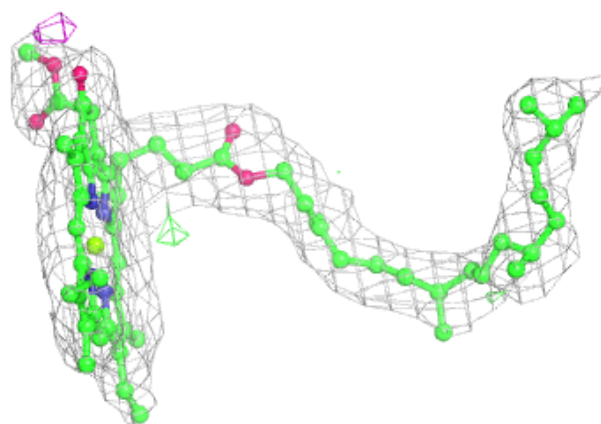
**Electron density around SQD D 410:**

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

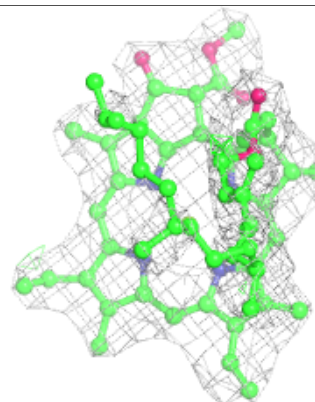
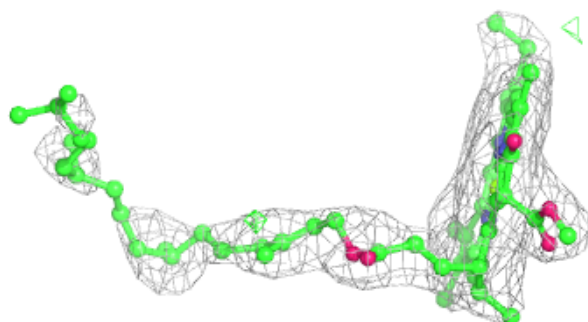
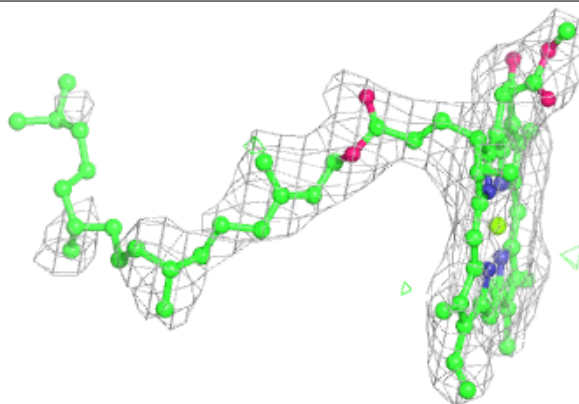


Electron density around CLA d 403:

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

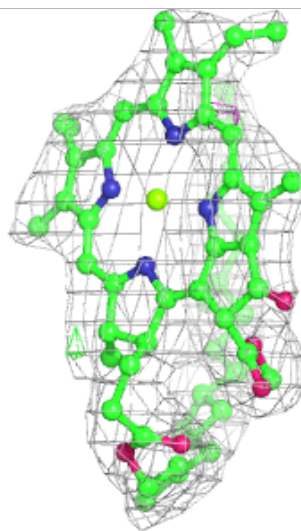
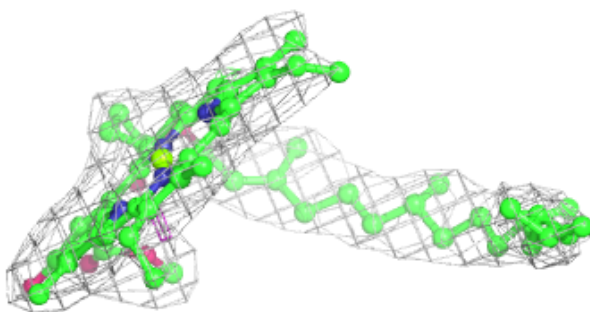
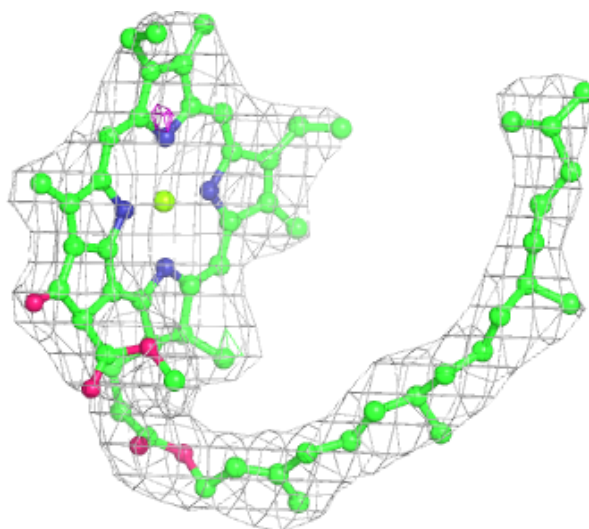
**Electron density around CLA D 404:**

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



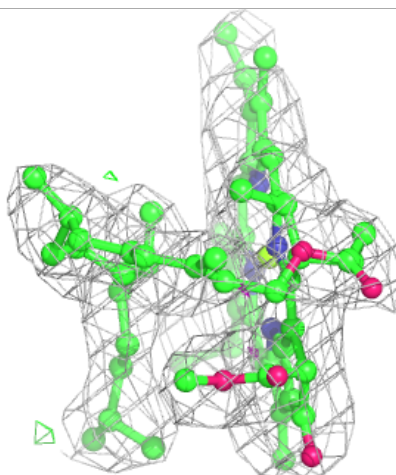
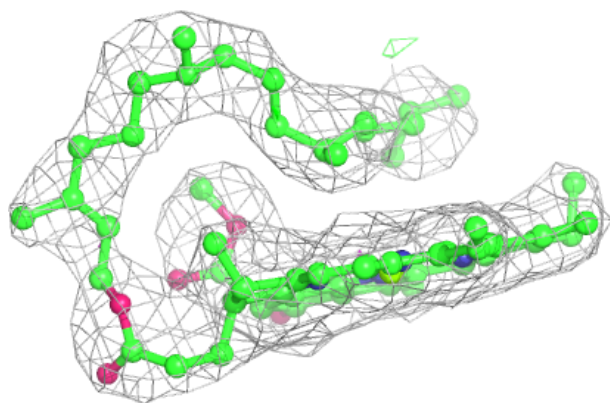
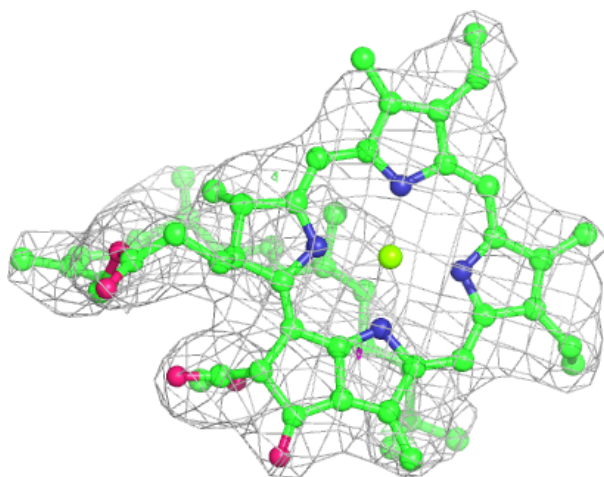
Electron density around CLA C 508:

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



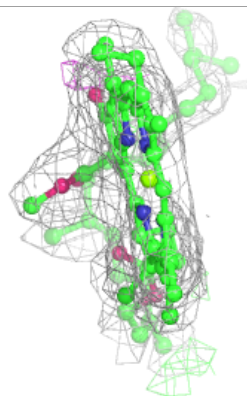
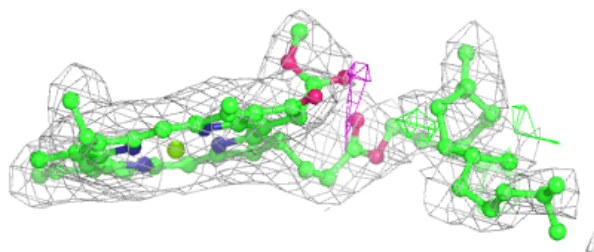
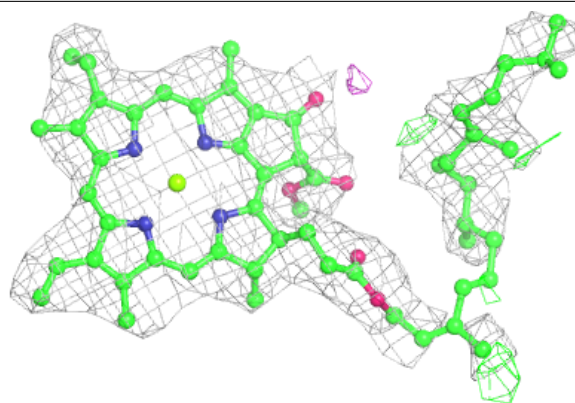
Electron density around CLA C 511:

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

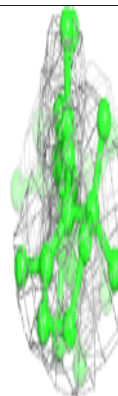
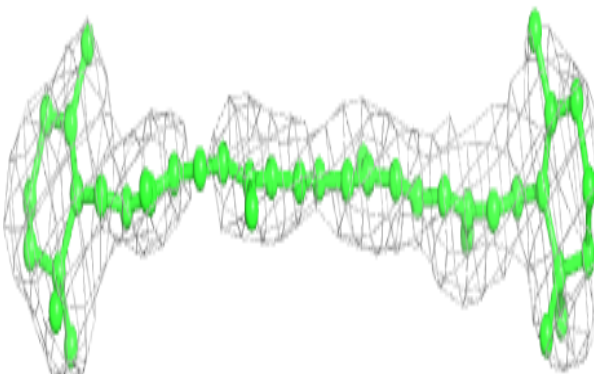
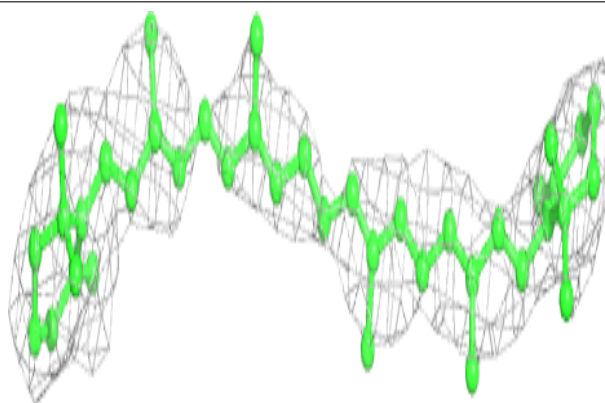


Electron density around CLA B 617:

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

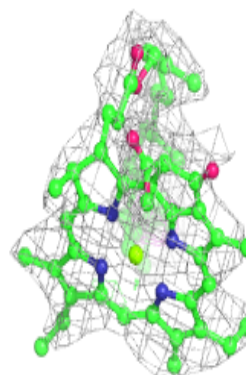
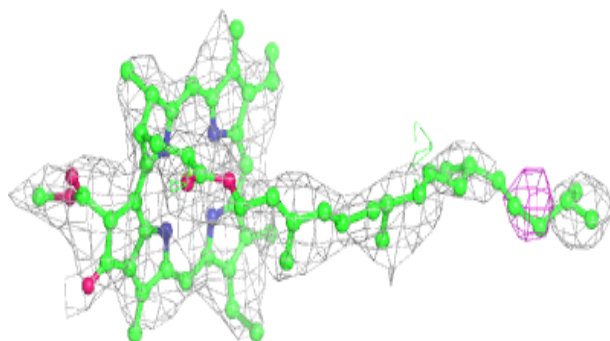
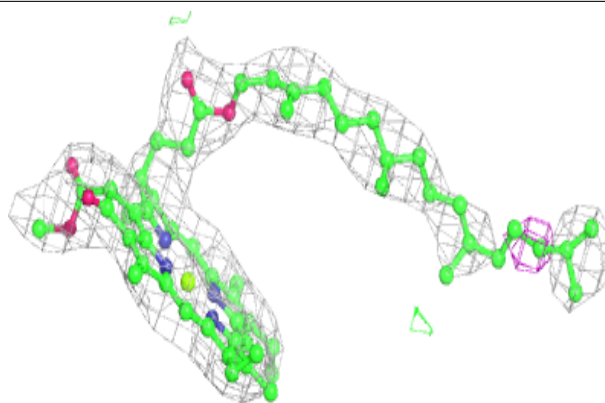
**Electron density around BCR c 514:**

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

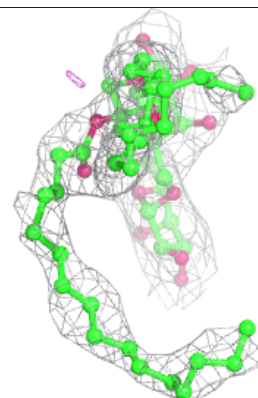
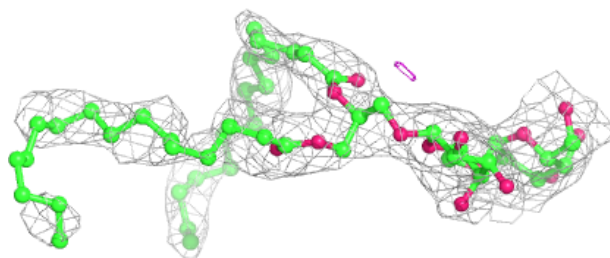
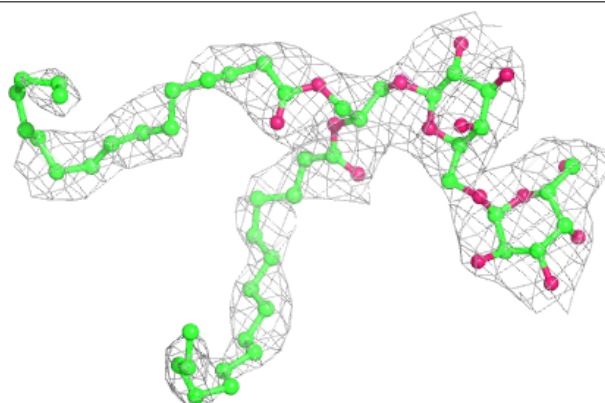


Electron density around CLA C 505:

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

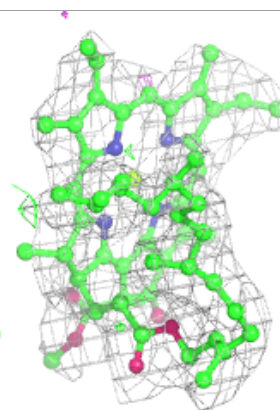
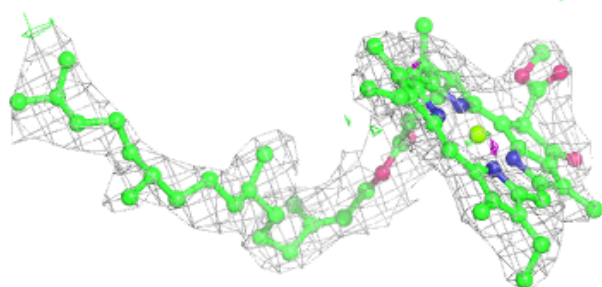
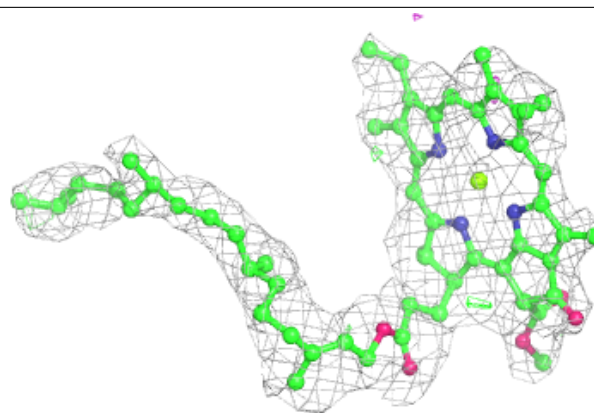
**Electron density around DGD c 517:**

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

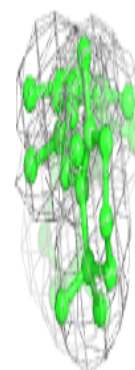
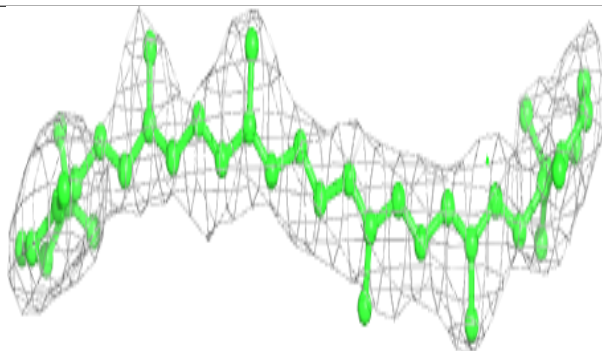
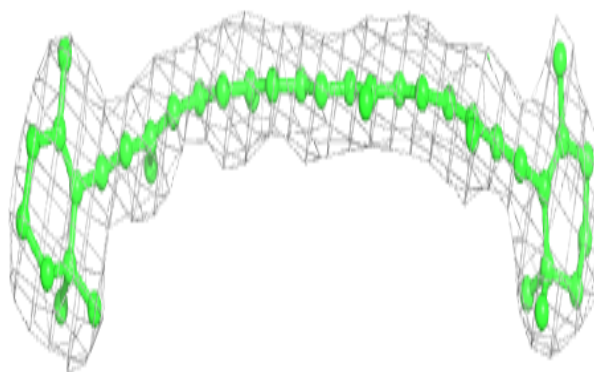


Electron density around CLA c 511:

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

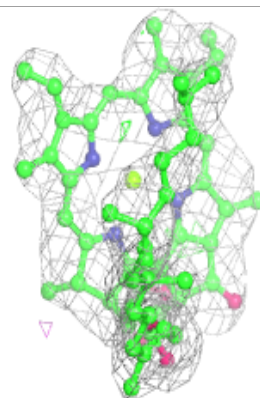
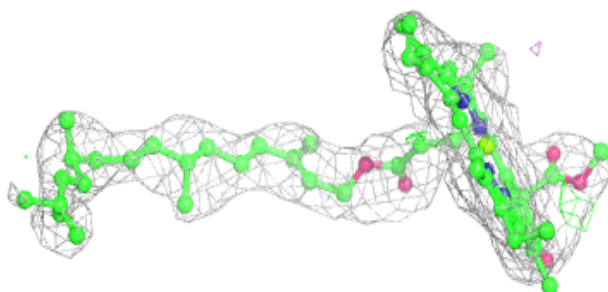
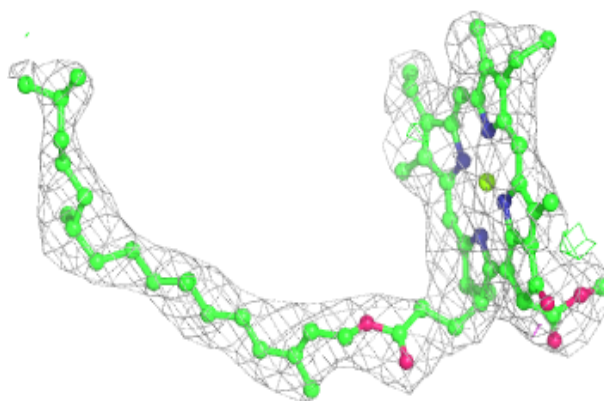
**Electron density around BCR K 101:**

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

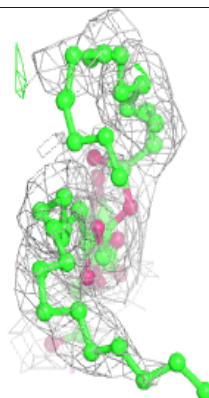
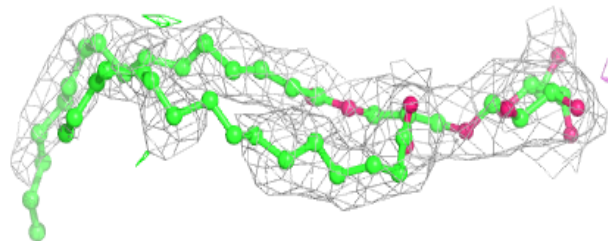
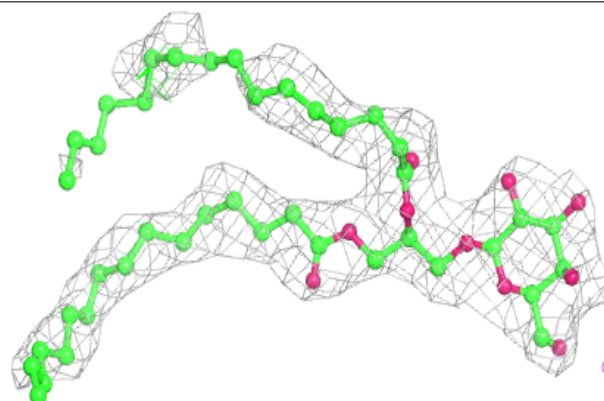


Electron density around CLA B 610:

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

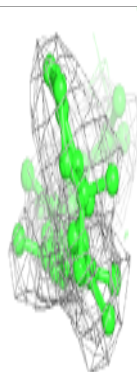
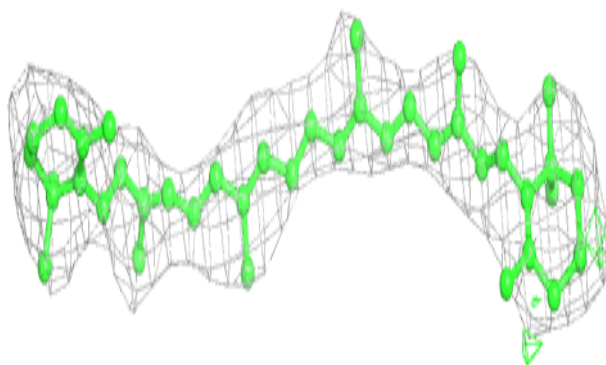
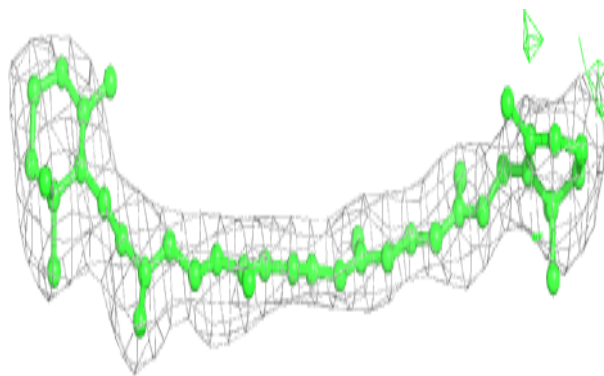
**Electron density around LMG f 101:**

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



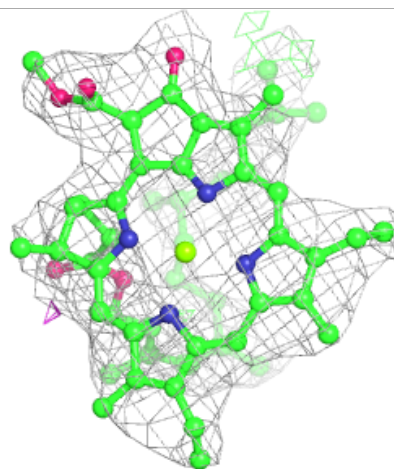
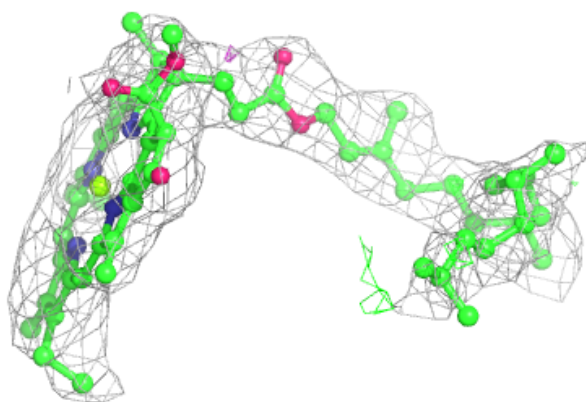
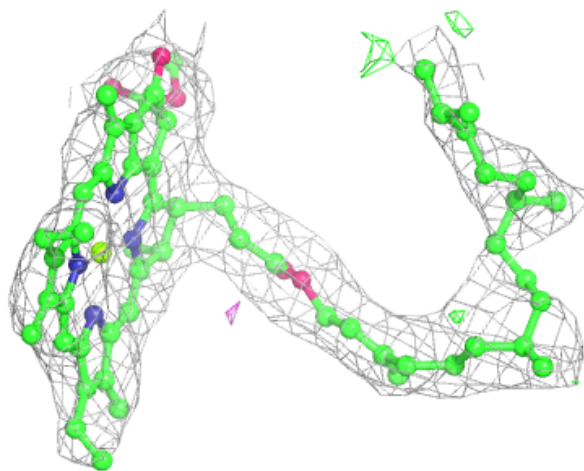
Electron density around BCR d 404:

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



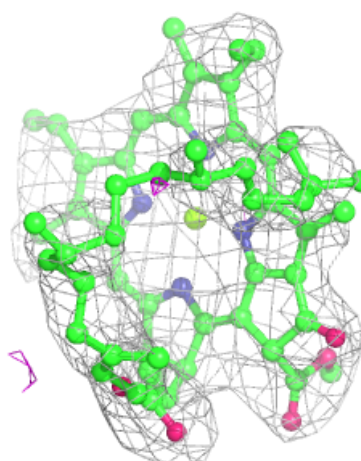
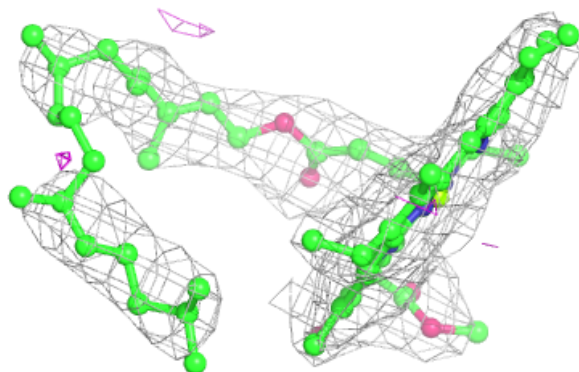
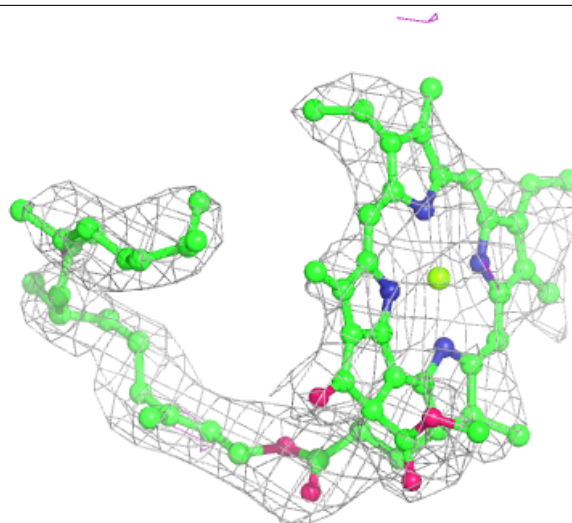
Electron density around CLA B 607:

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



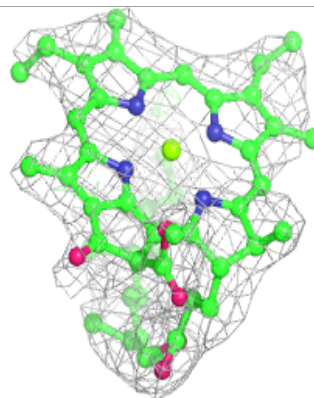
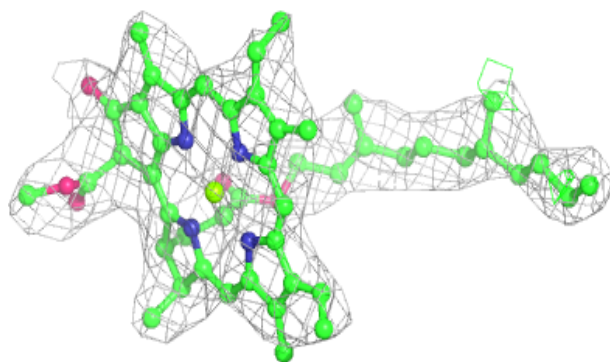
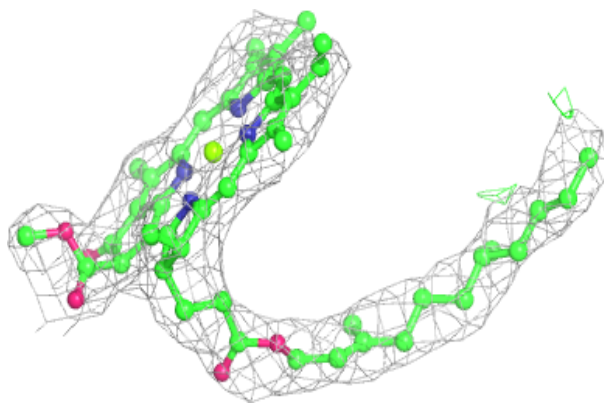
Electron density around CLA c 503:

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

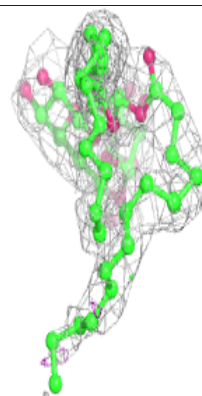
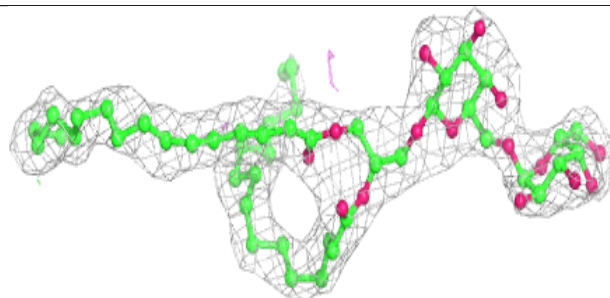
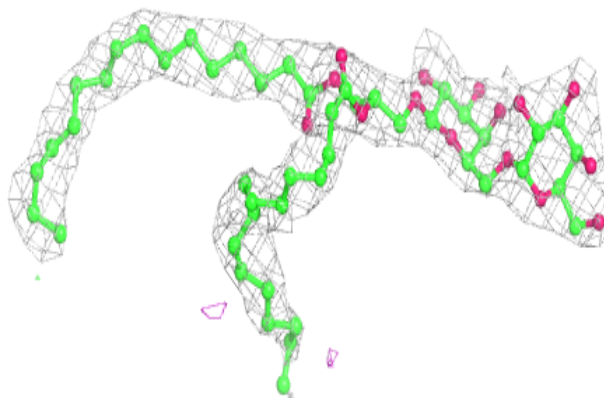


Electron density around CLA c 504:

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

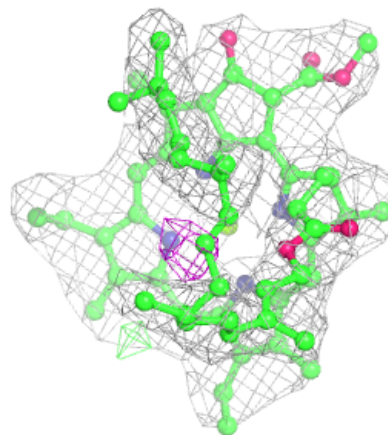
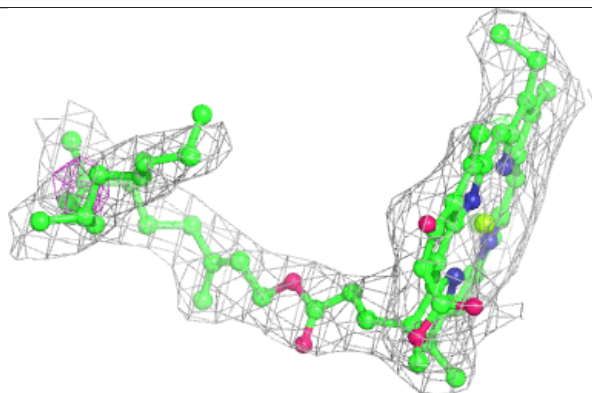
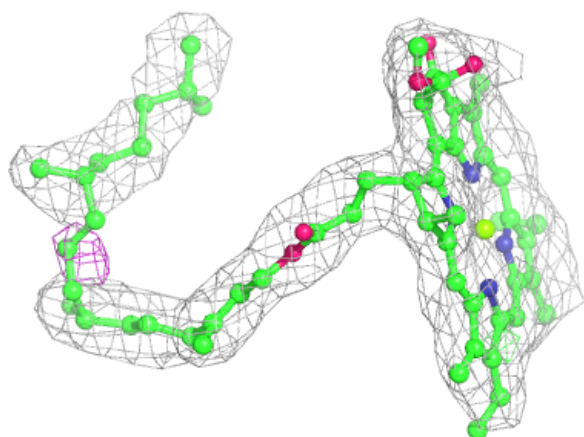
**Electron density around DGD h 102:**

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

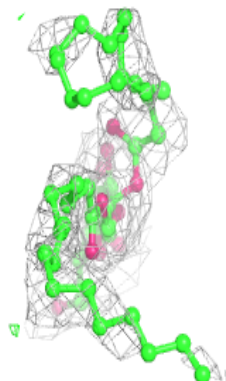
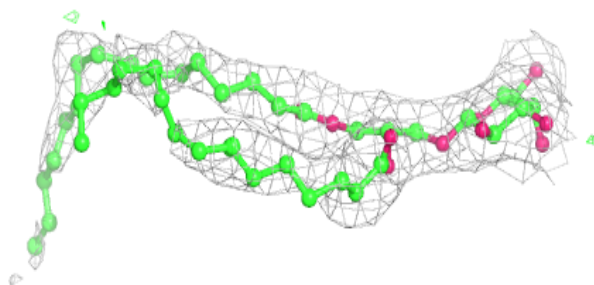
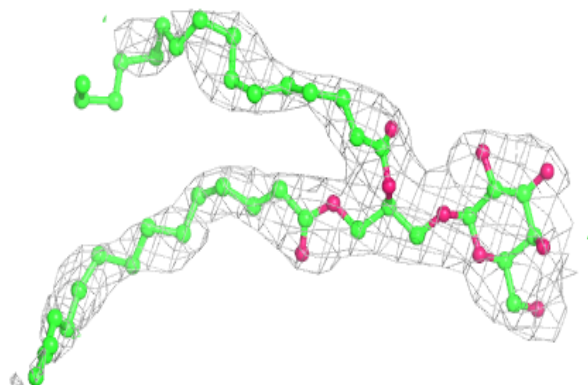


Electron density around CLA b 612:

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

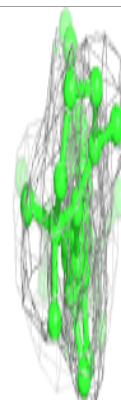
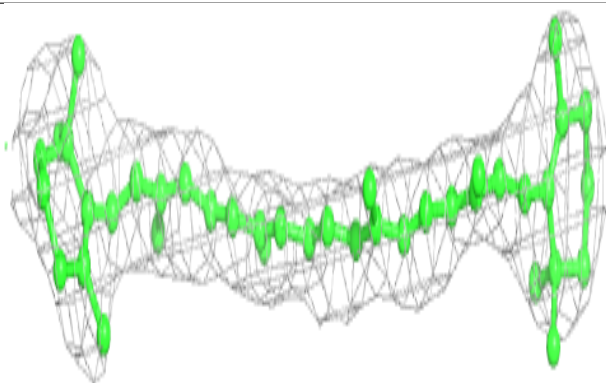
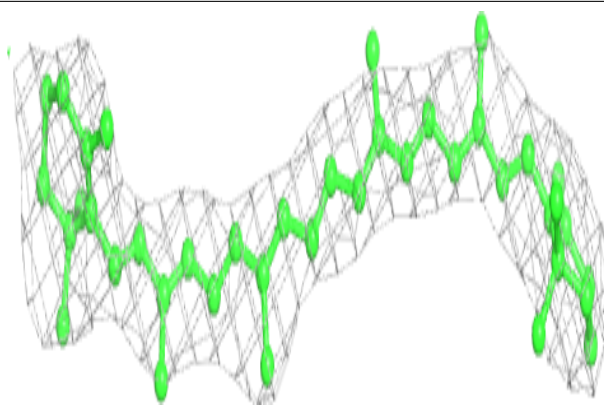
**Electron density around LMG D 409:**

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

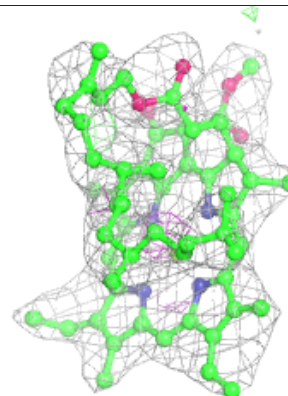
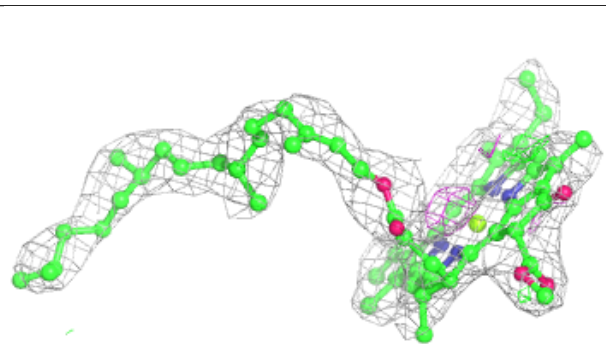
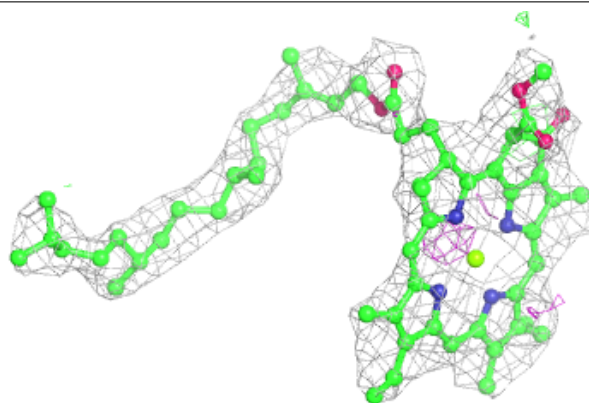


Electron density around BCR Y 101:

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

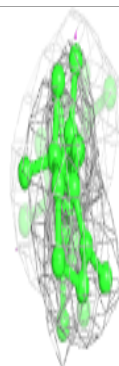
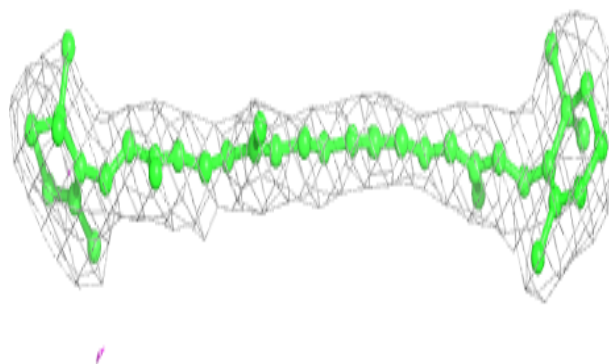
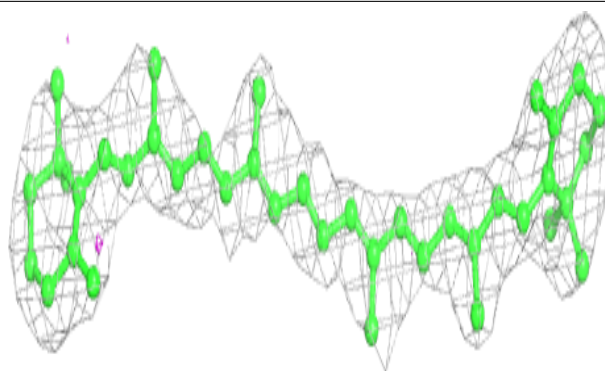
**Electron density around CLA C 512:**

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

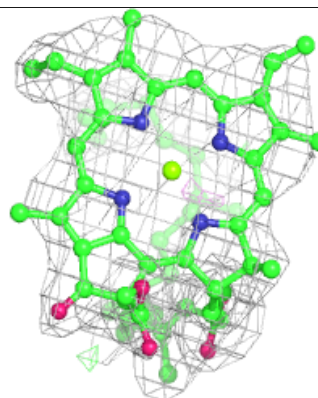
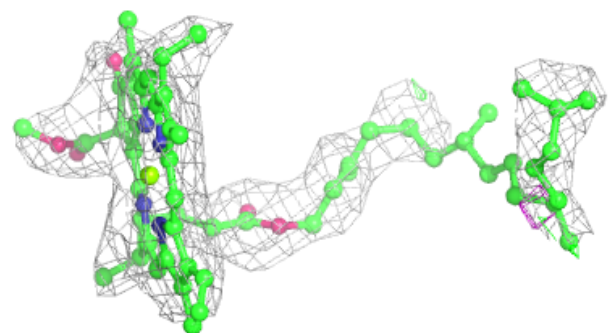
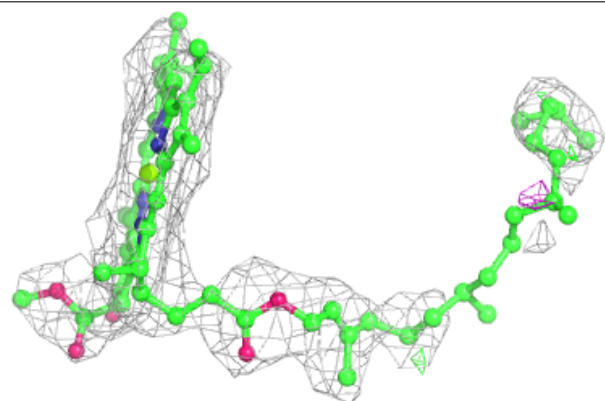


Electron density around BCR b 624:

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

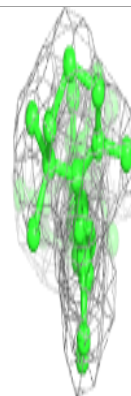
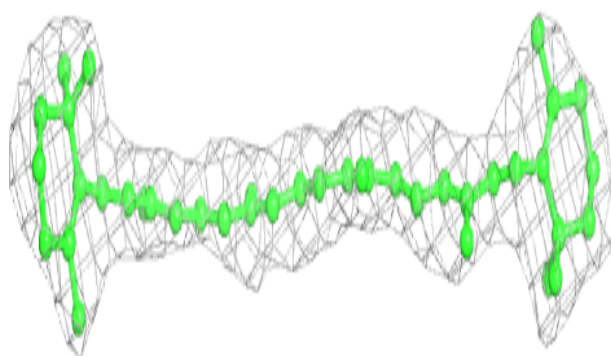
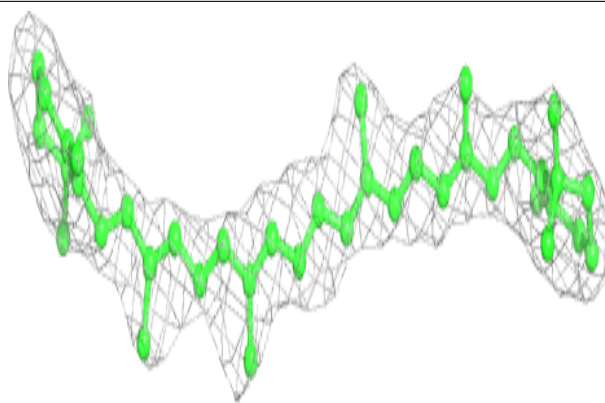
**Electron density around CLA c 506:**

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

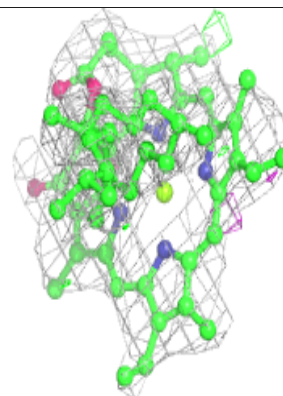
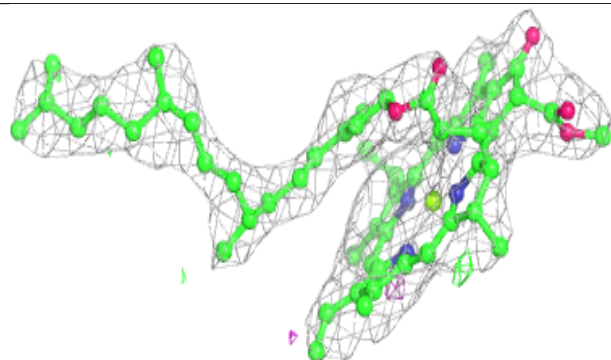
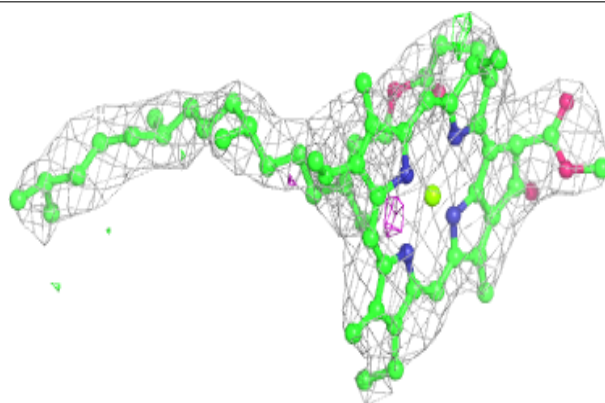


Electron density around BCR c 515:

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

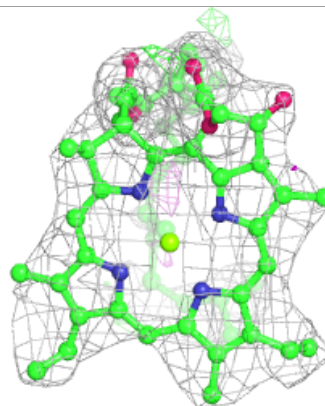
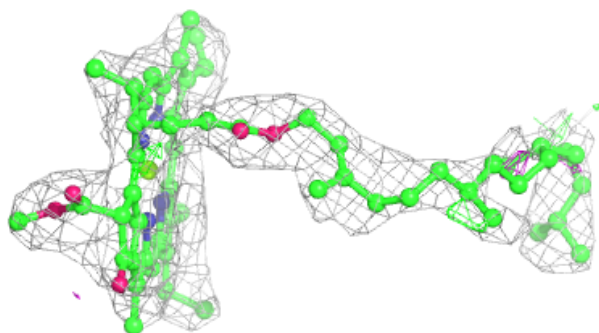
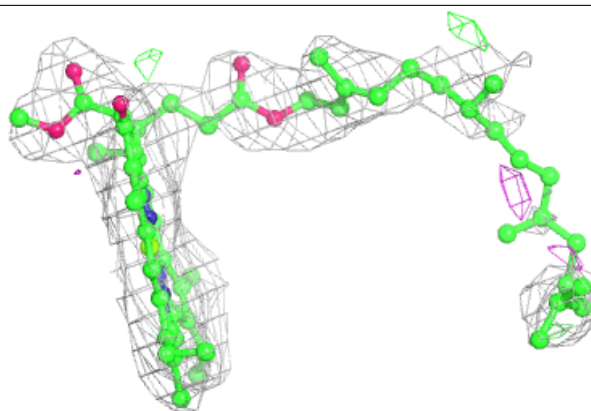
**Electron density around CLA C 506:**

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

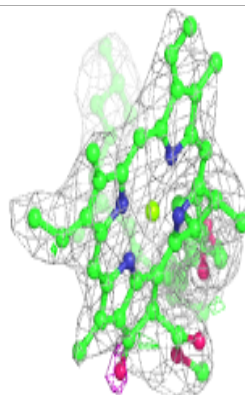
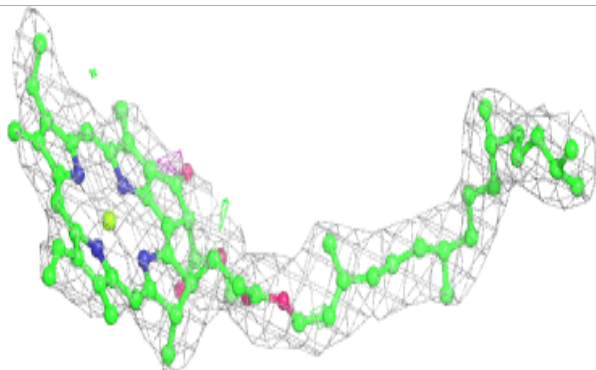
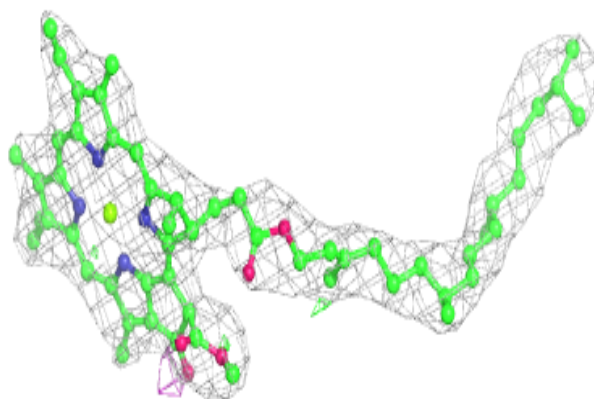


Electron density around CLA C 507:

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

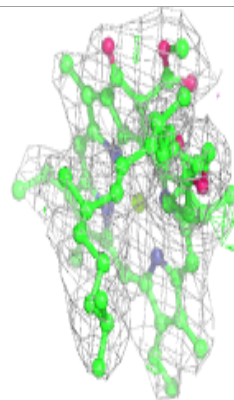
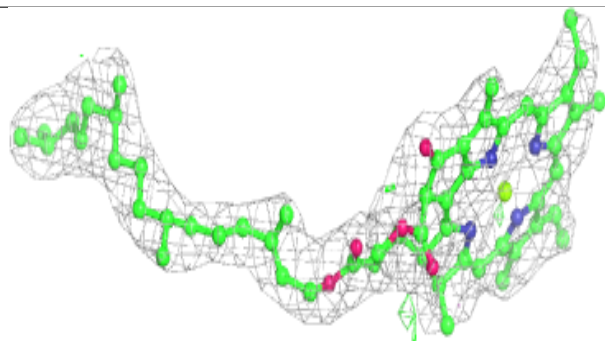
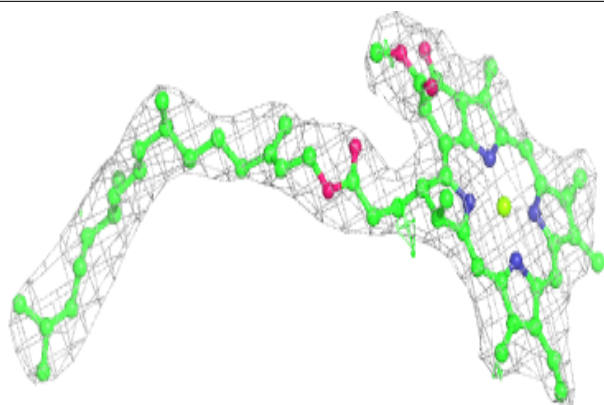
**Electron density around CLA A 606:**

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

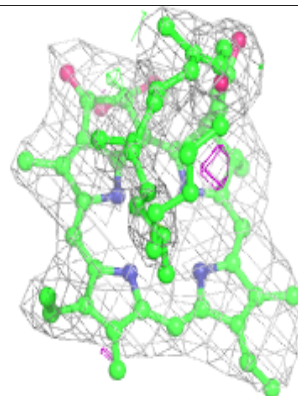
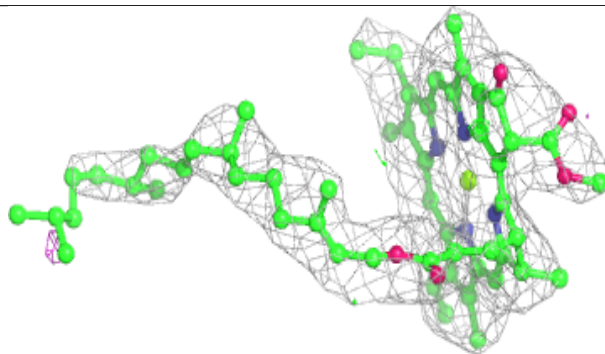
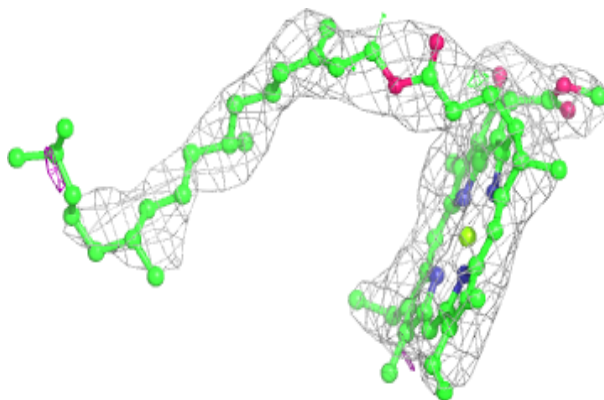


Electron density around CLA a 707:

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

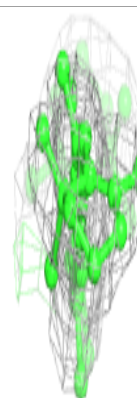
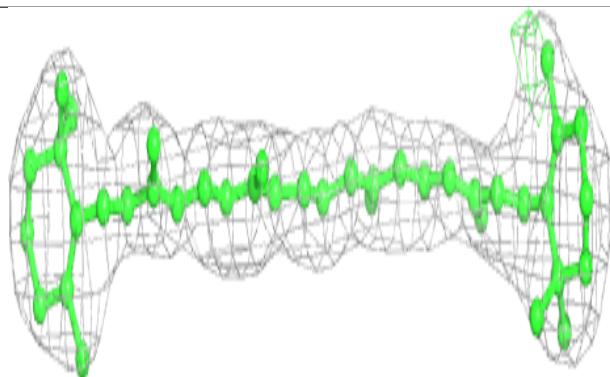
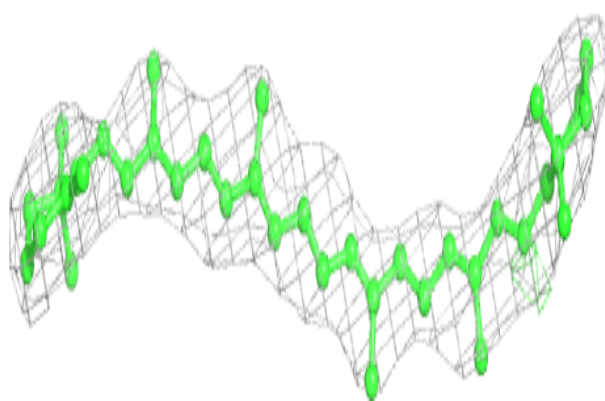
**Electron density around CLA C 509:**

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

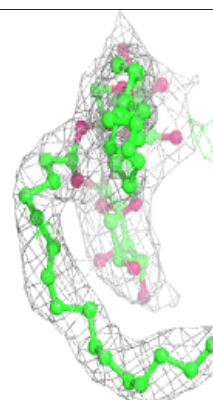
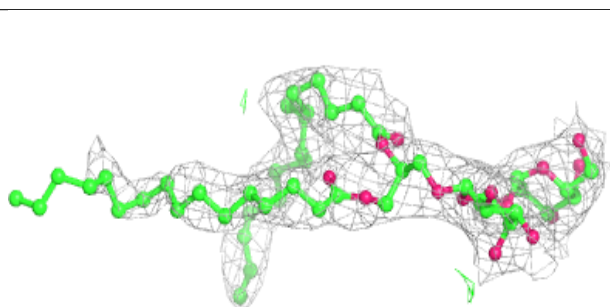
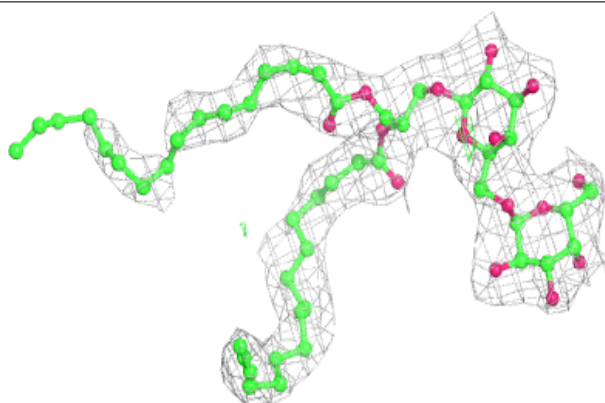


Electron density around BCR C 516:

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

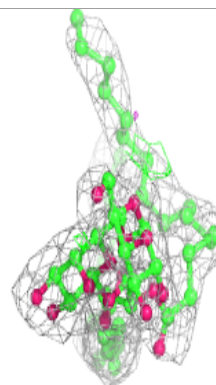
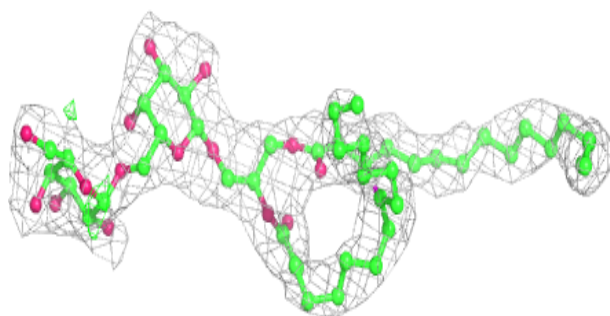
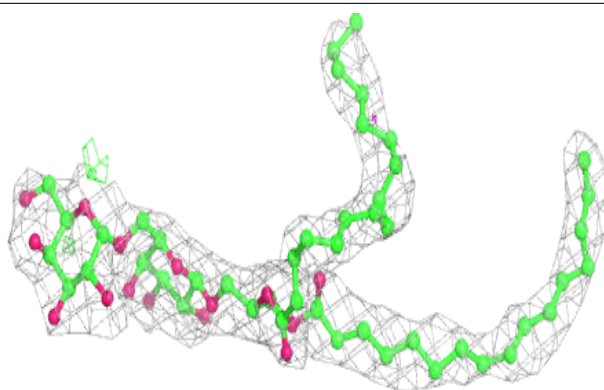
**Electron density around DGD C 518:**

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

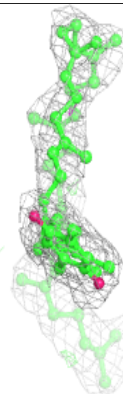
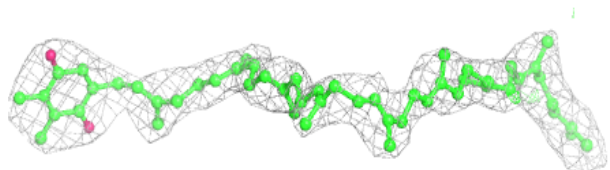
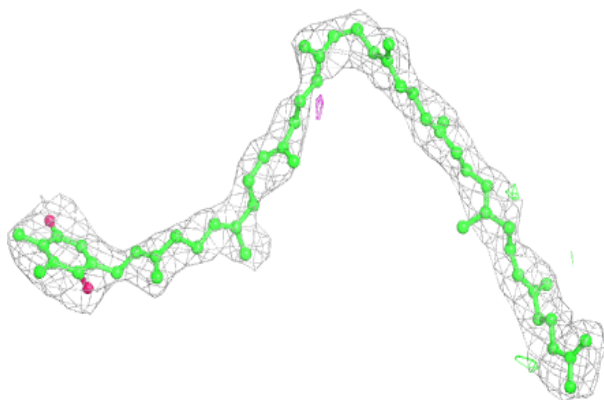


Electron density around DGD H 103:

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

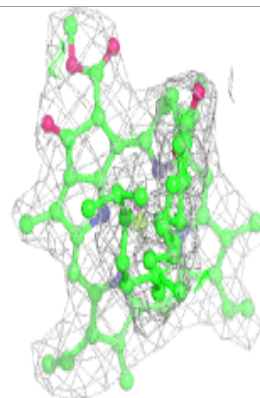
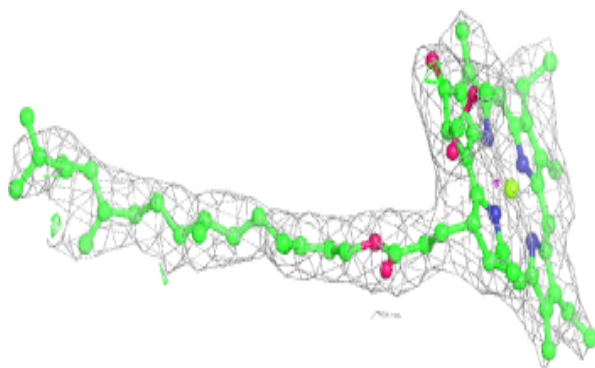
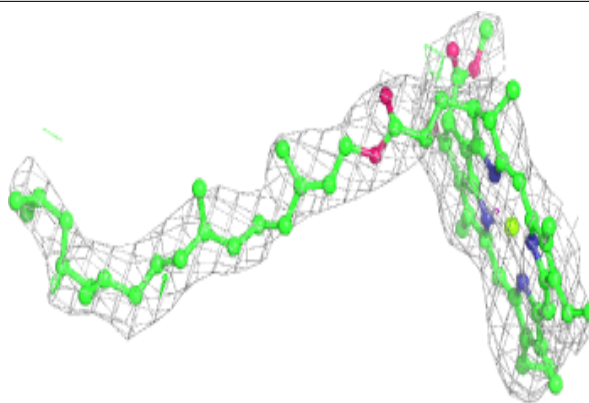
**Electron density around PL9 D 406:**

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

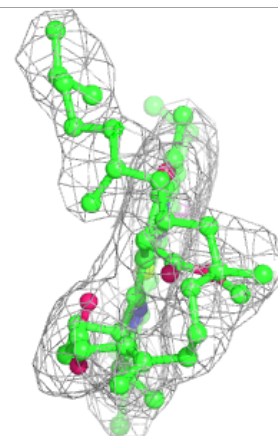
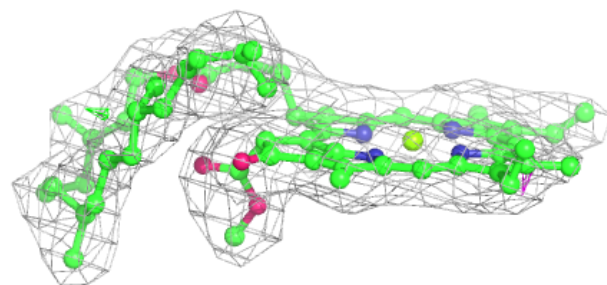
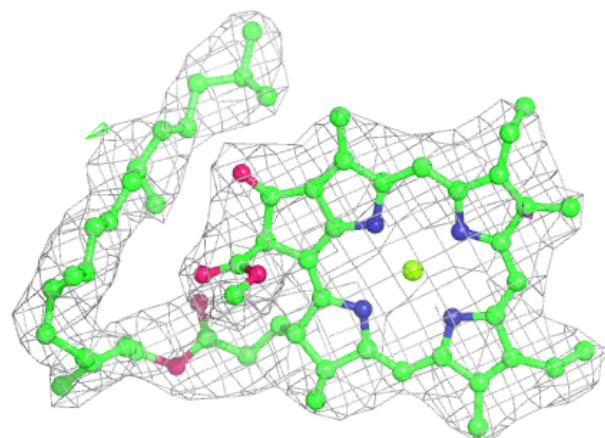


Electron density around CLA b 610:

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

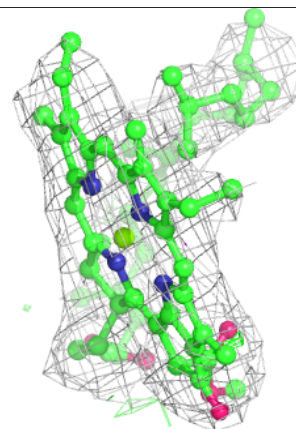
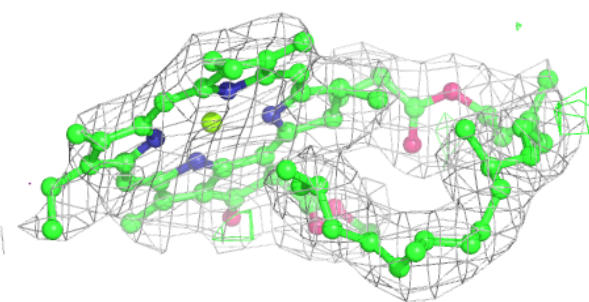
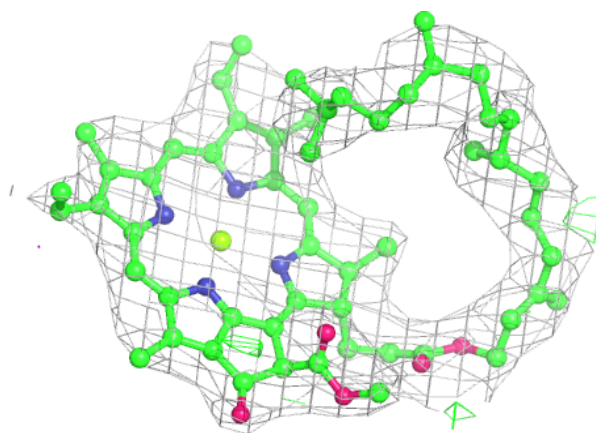
**Electron density around CLA b 616:**

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



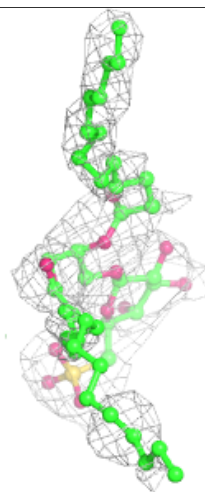
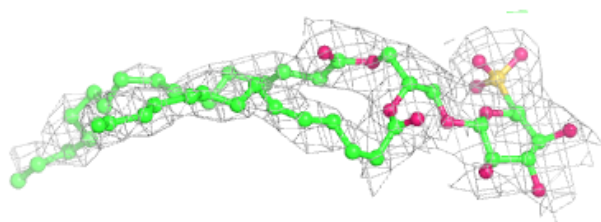
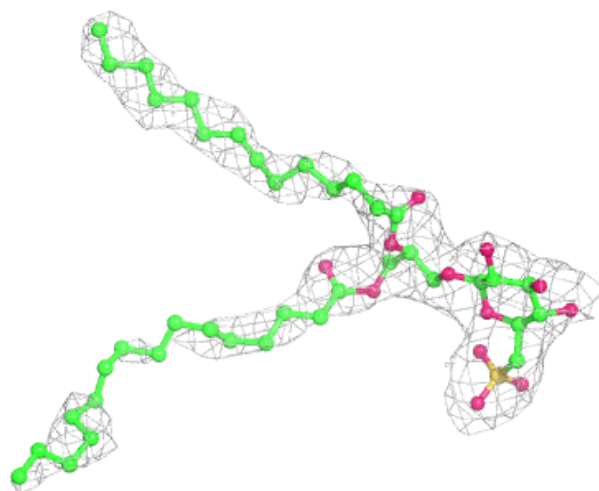
Electron density around CLA b 621:

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



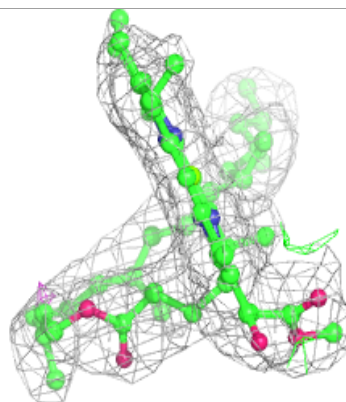
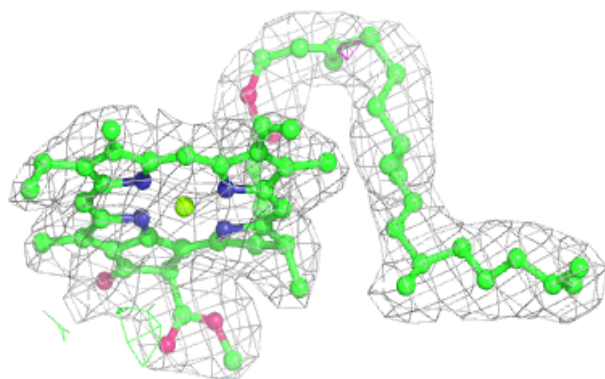
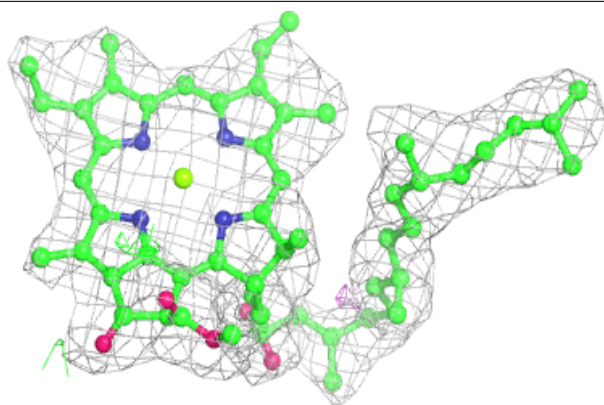
Electron density around SQD A 612:

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



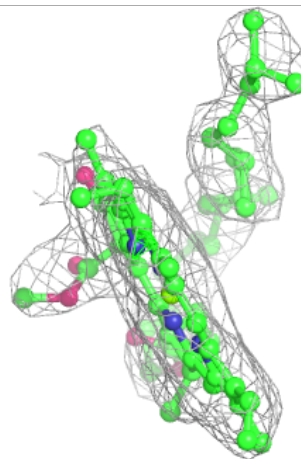
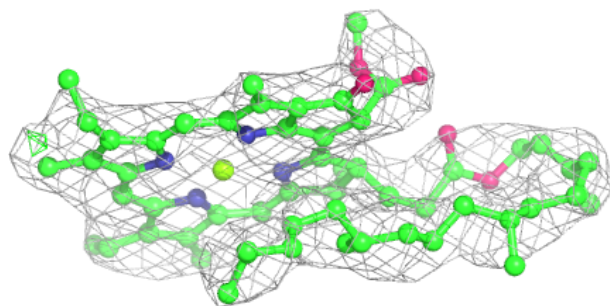
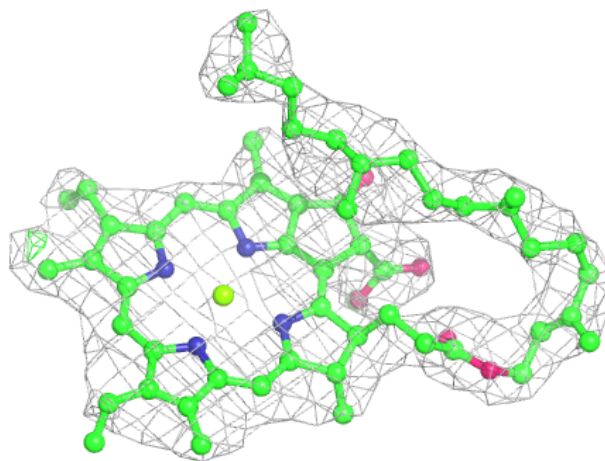
Electron density around CLA D 402:

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



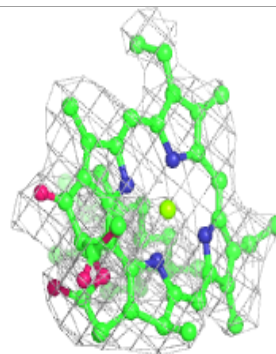
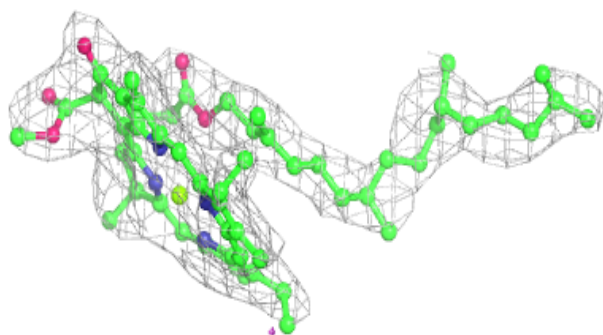
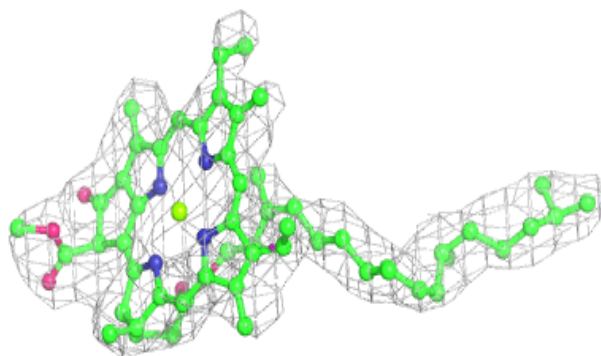
Electron density around CLA C 510:

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

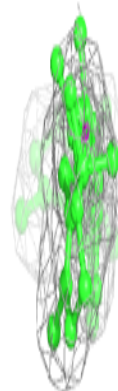
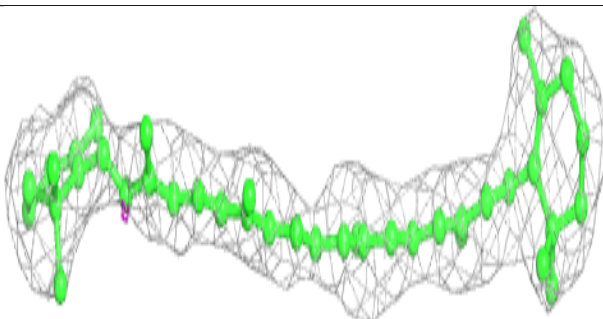
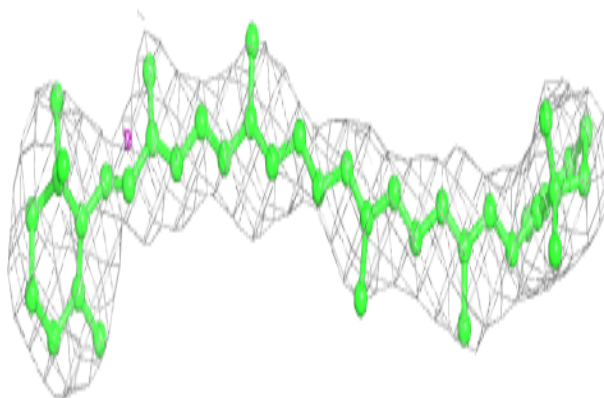


Electron density around CLA c 505:

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

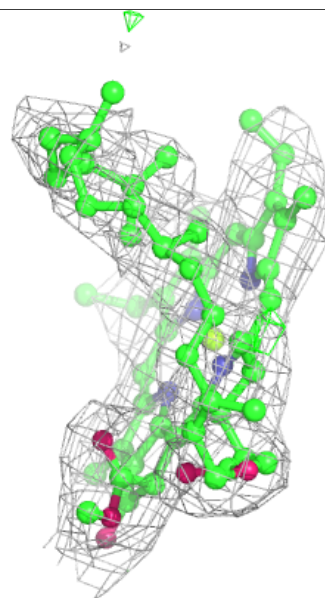
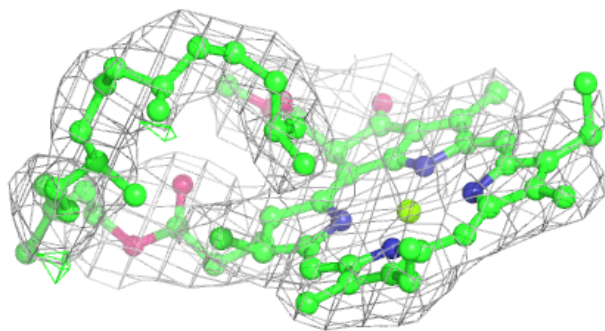
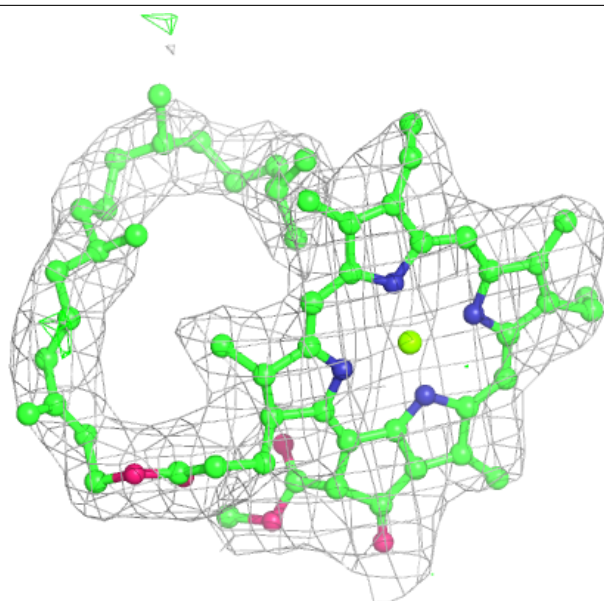
**Electron density around BCR b 623:**

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



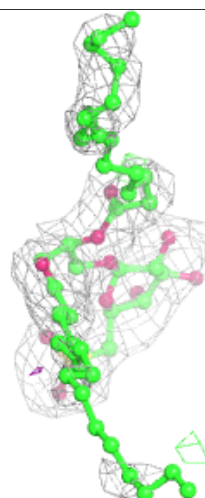
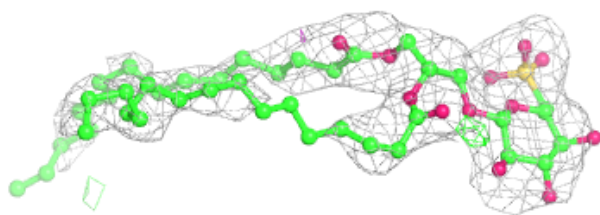
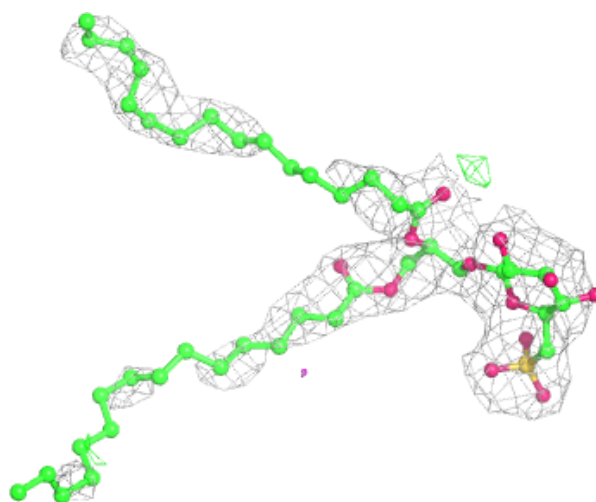
Electron density around CLA B 616:

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



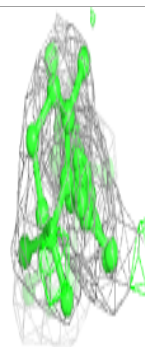
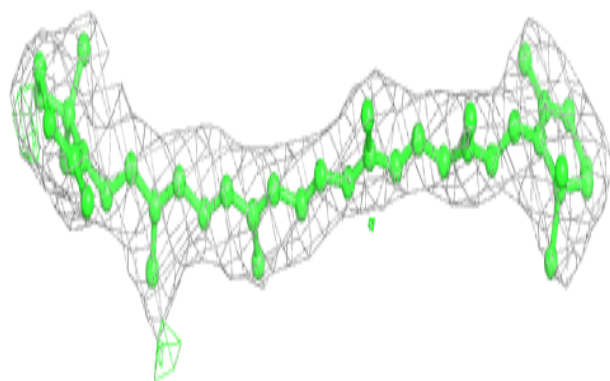
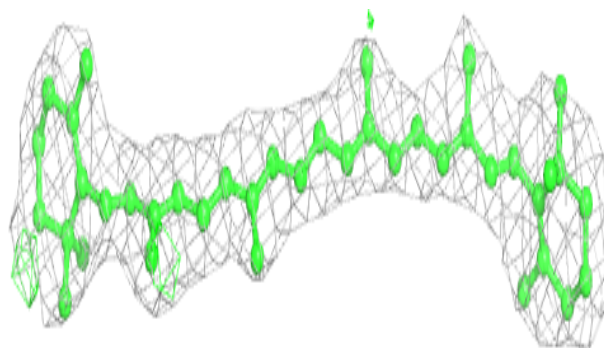
Electron density around SQD a 714:

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

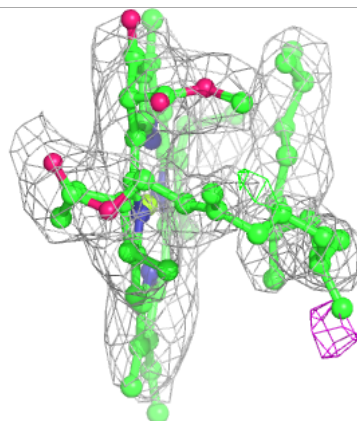
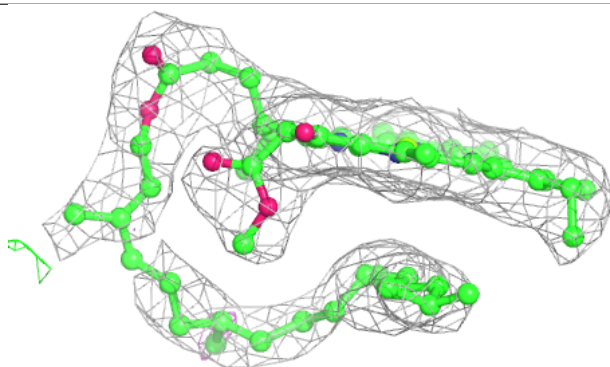
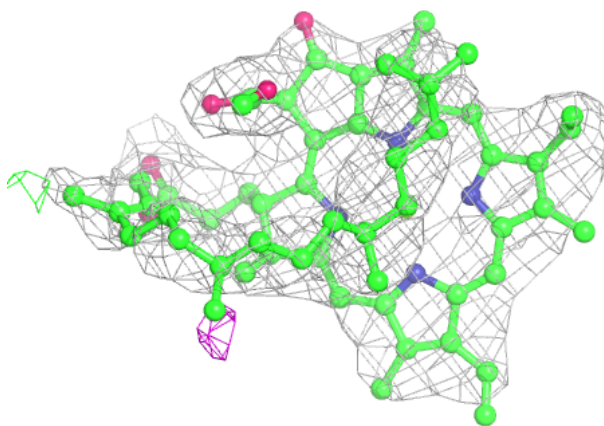


Electron density around BCR b 625:

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

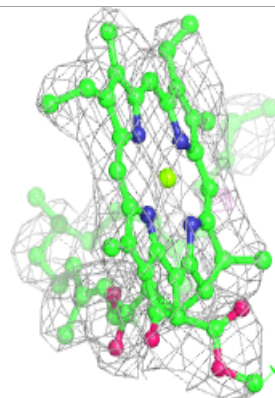
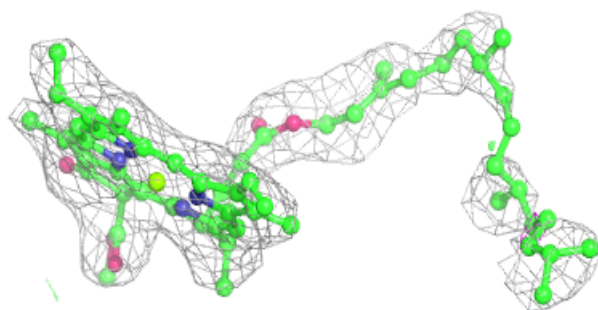
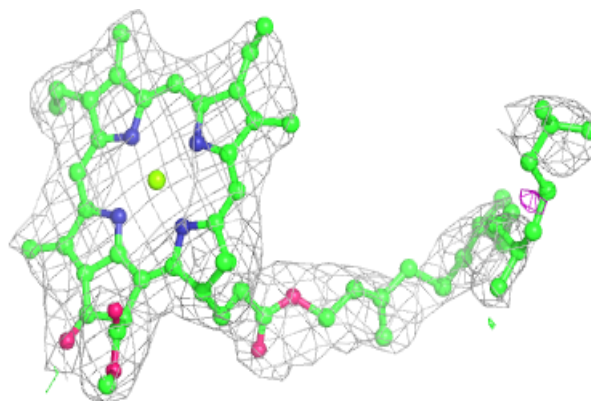
**Electron density around CLA c 510:**

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

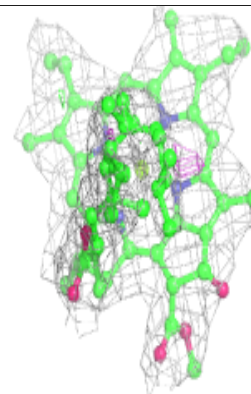
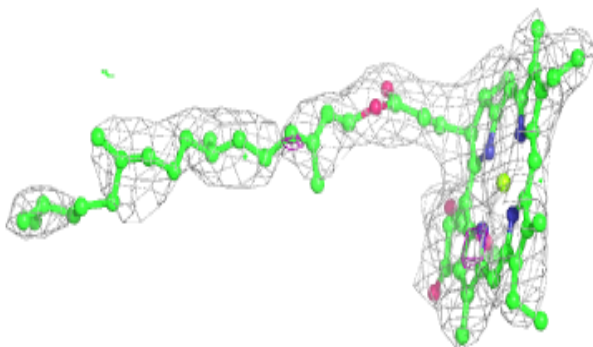
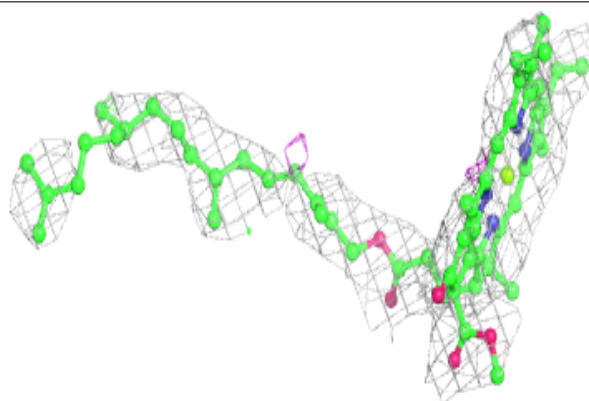


Electron density around CLA a 711:

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

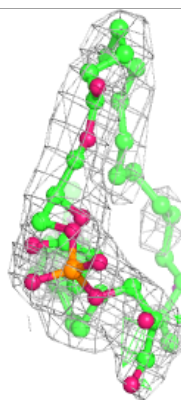
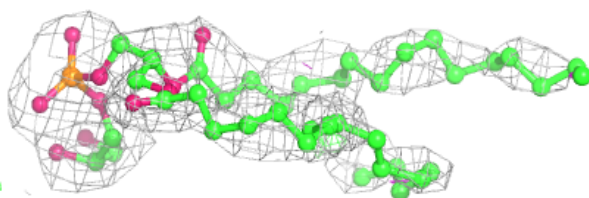
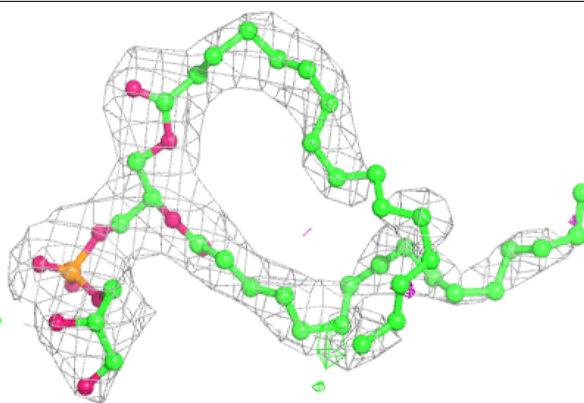
**Electron density around CLA B 605:**

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

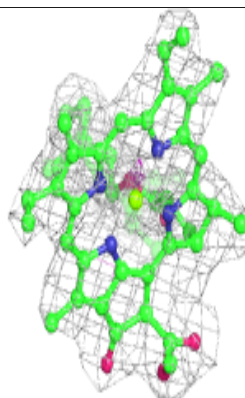
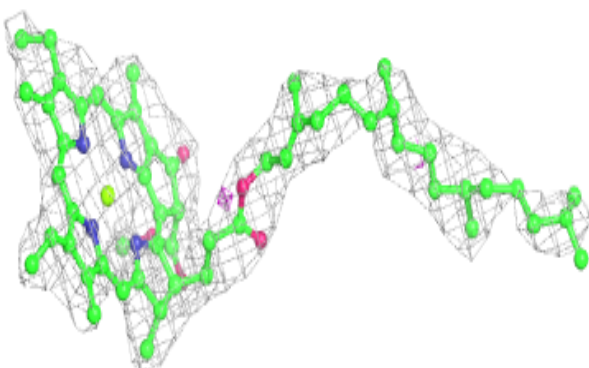
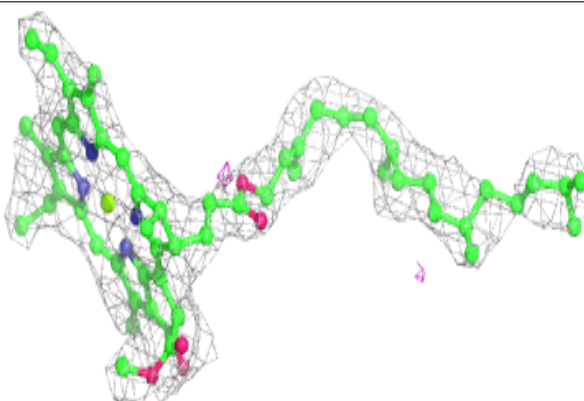


Electron density around LHG D 408:

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

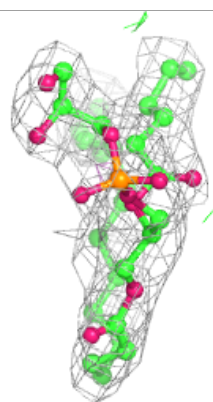
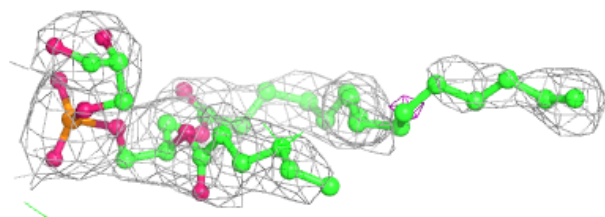
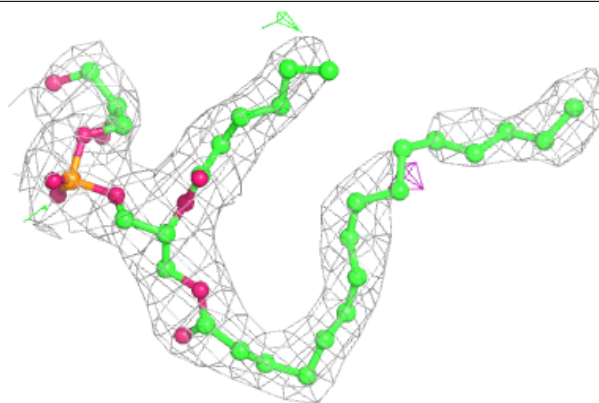
**Electron density around CLA C 503:**

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

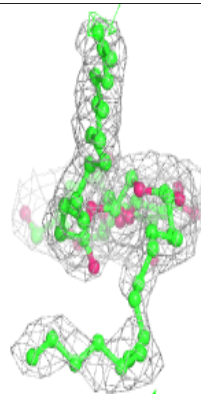
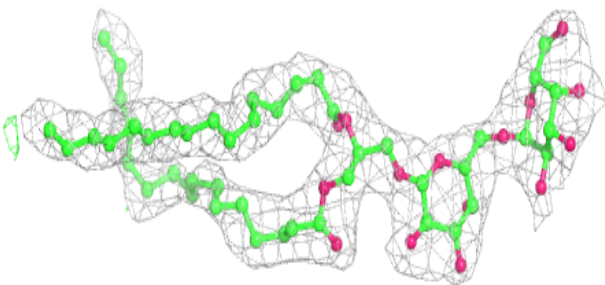
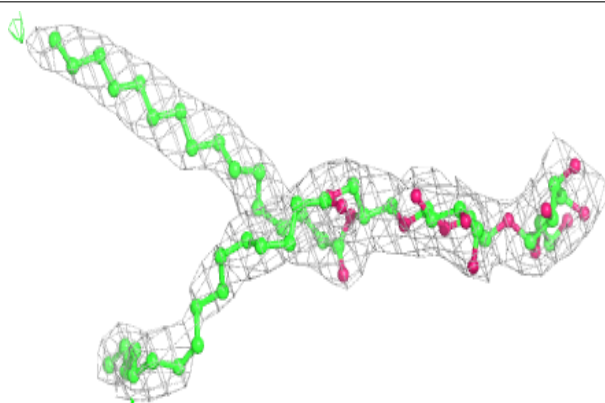


Electron density around LHG a 720:

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

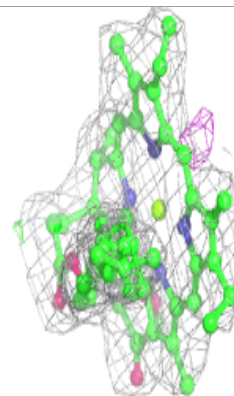
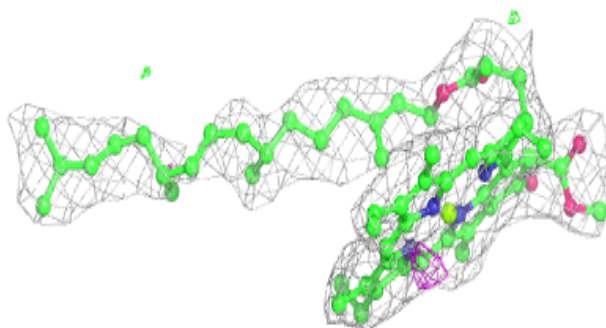
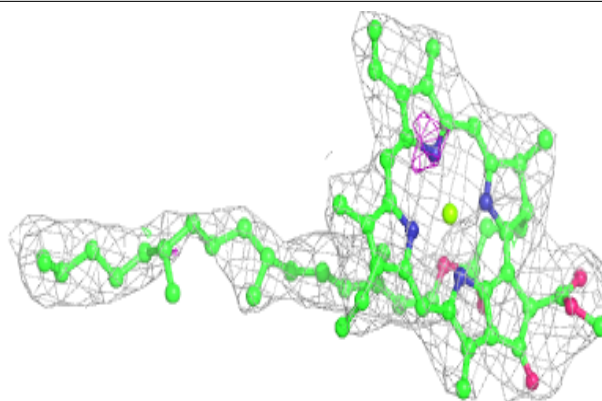
**Electron density around DGD C 517:**

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

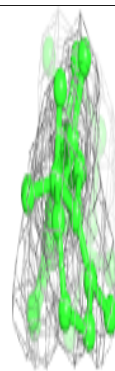
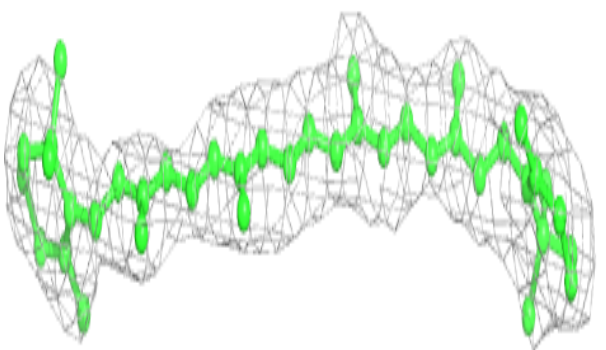
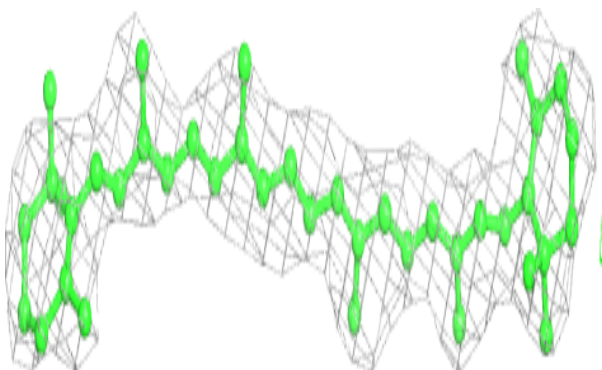


Electron density around CLA B 615:

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

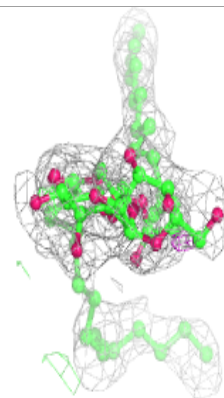
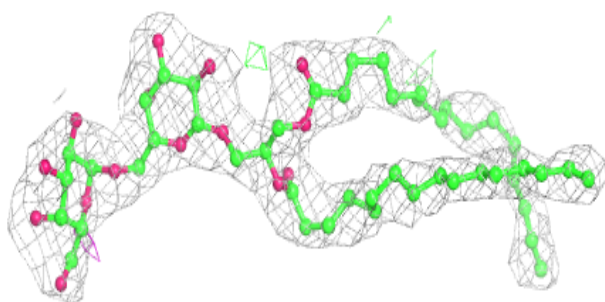
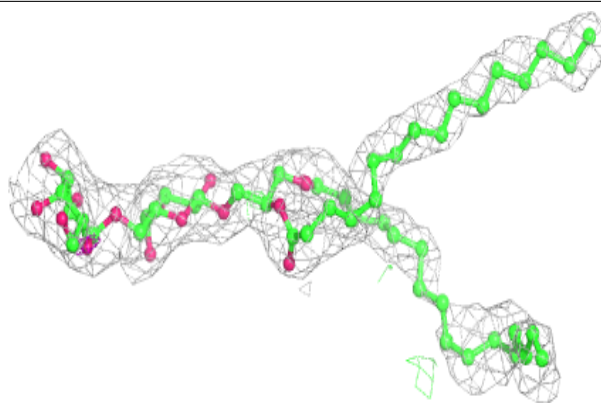
**Electron density around BCR B 620:**

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

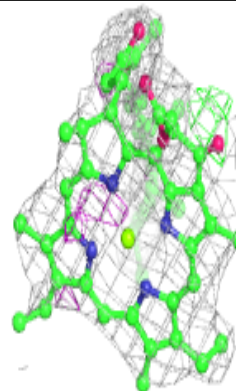
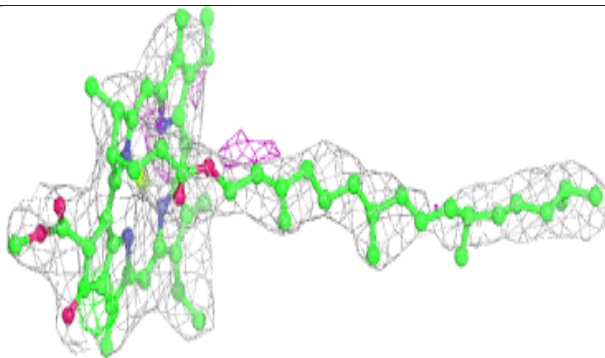
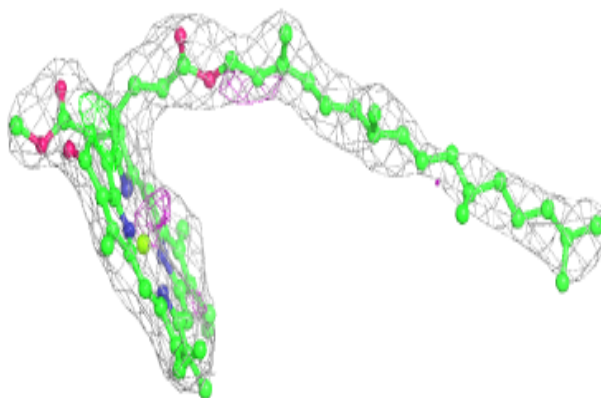


Electron density around DGD c 516:

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

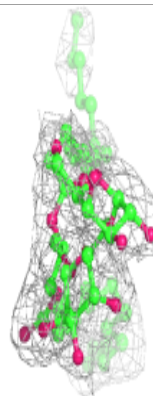
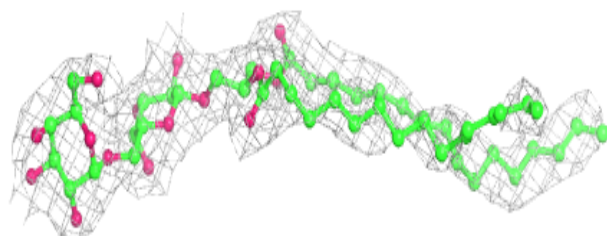
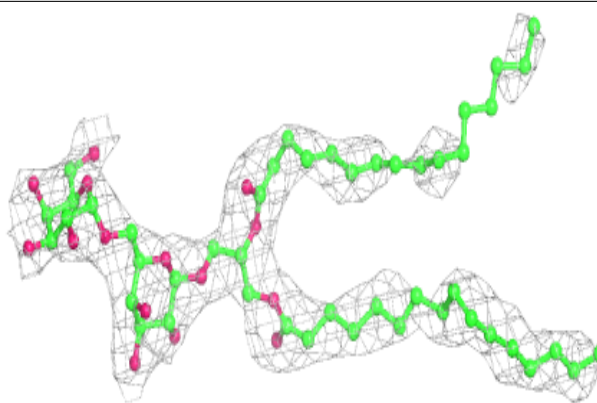
**Electron density around CLA b 613:**

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

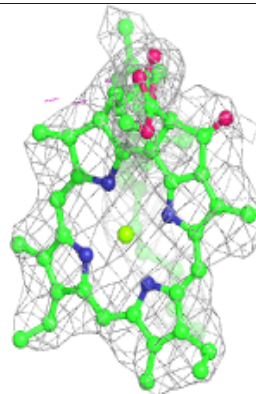
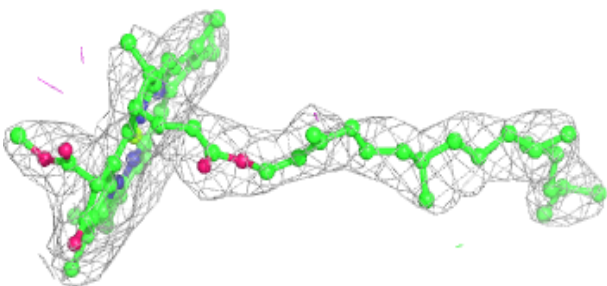
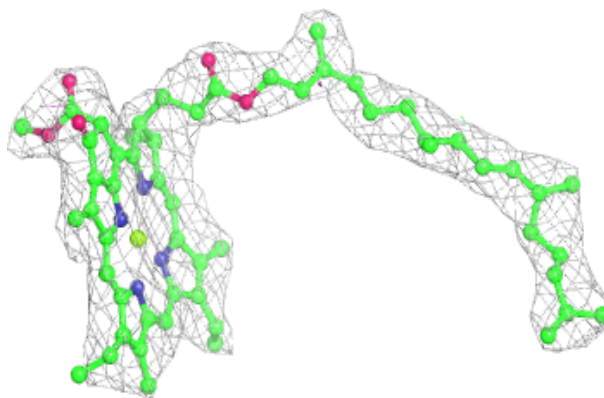


Electron density around DGD c 518:

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

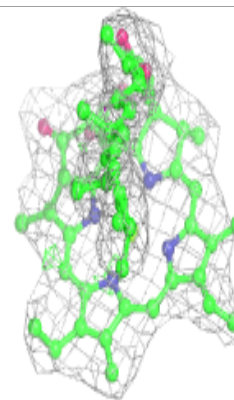
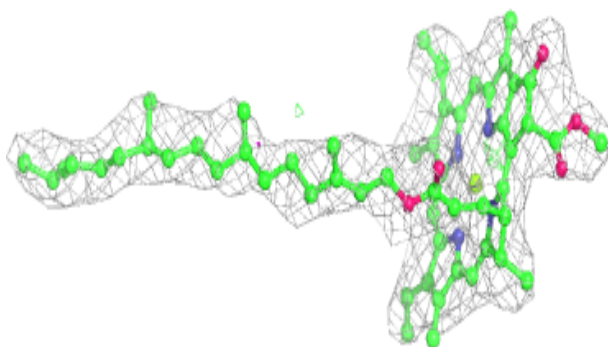
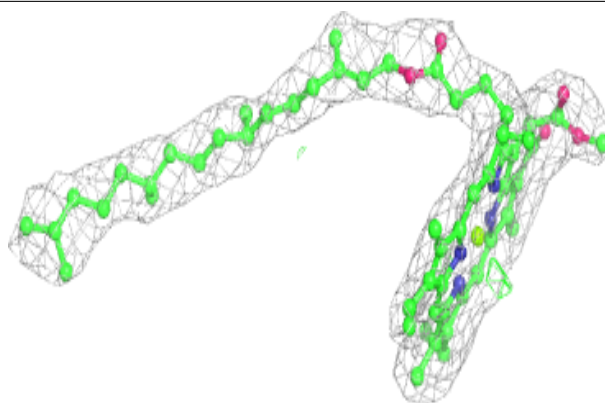
**Electron density around CLA b 615:**

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

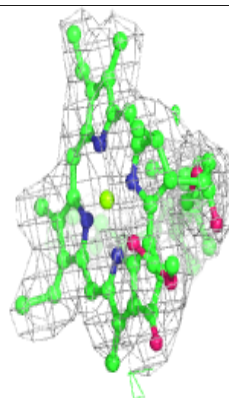
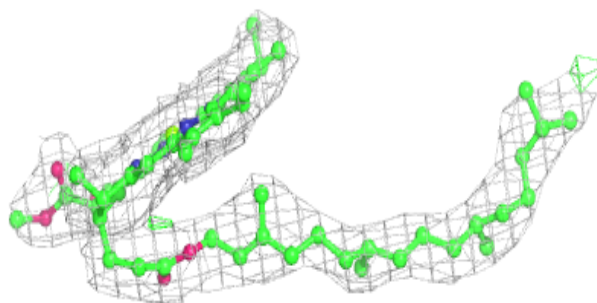
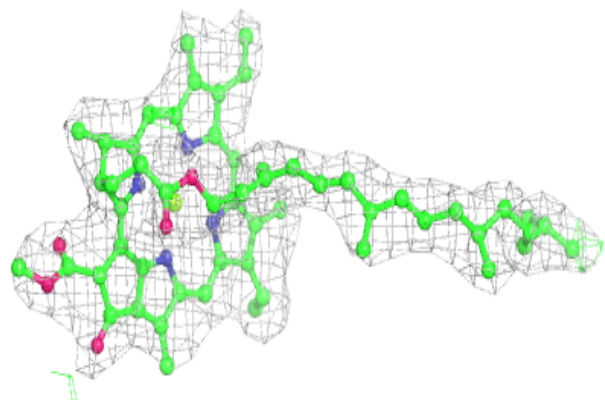


Electron density around CLA B 608:

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

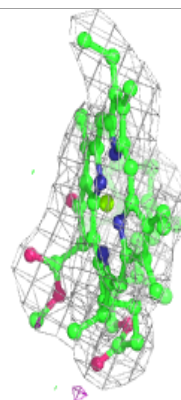
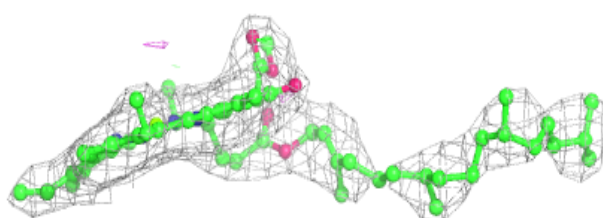
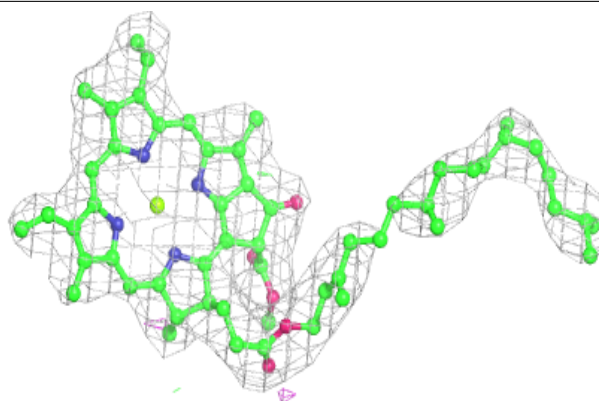
**Electron density around CLA B 609:**

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

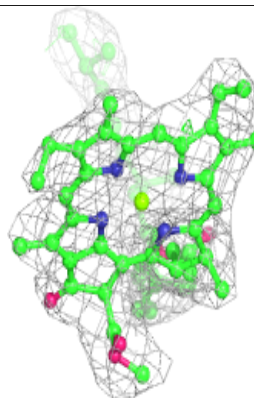
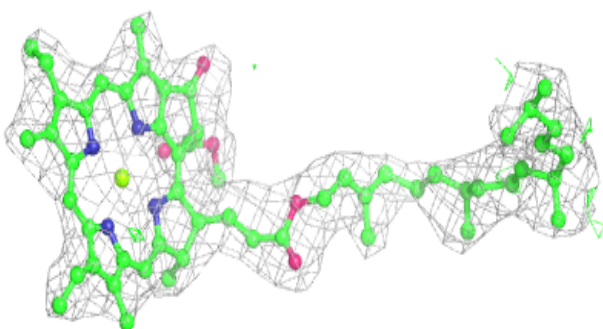
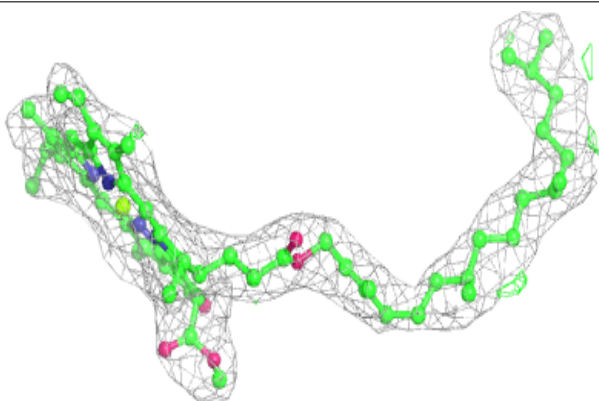


Electron density around CLA b 608:

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

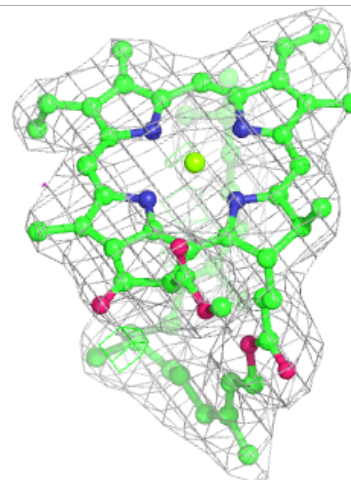
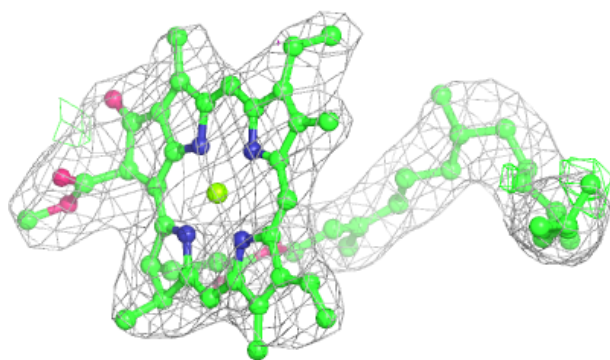
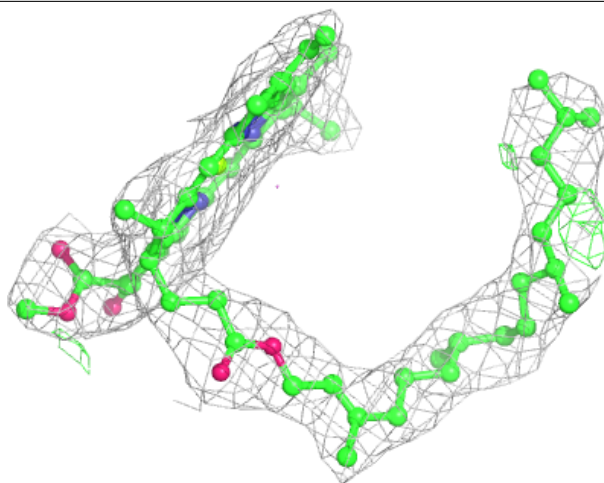
**Electron density around CLA d 402:**

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



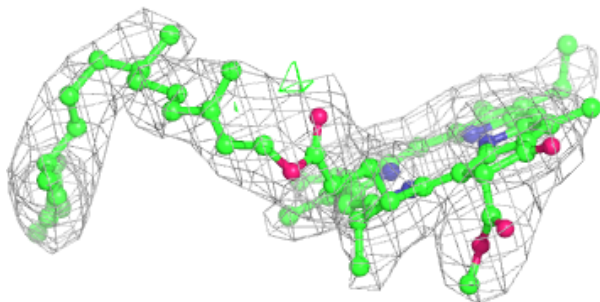
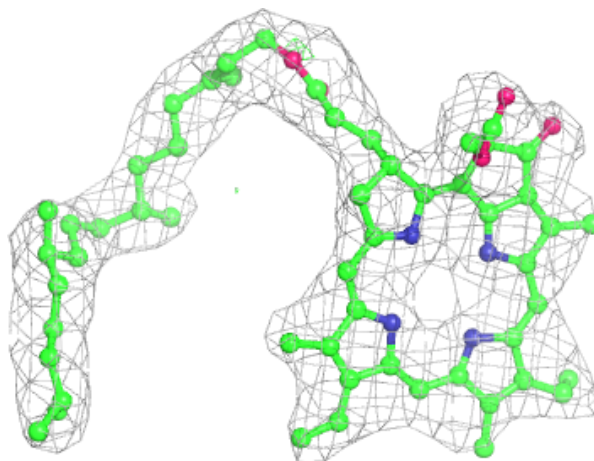
Electron density around CLA B 612:

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



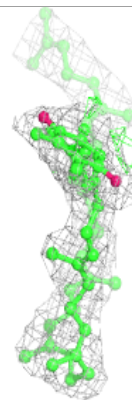
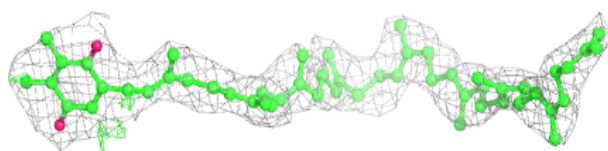
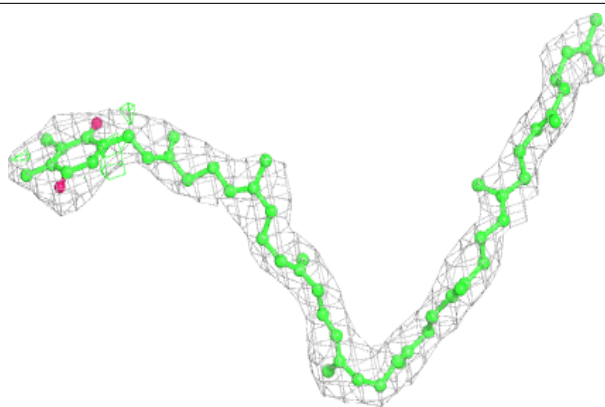
Electron density around PHO a 710:

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

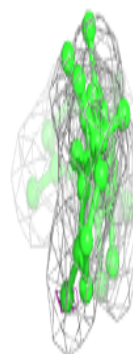
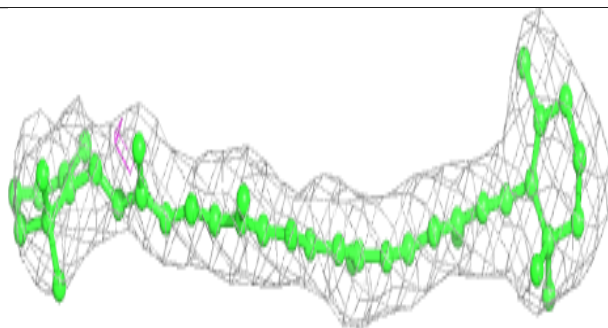
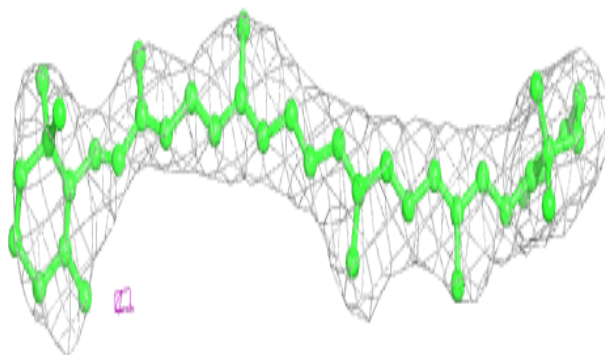


Electron density around PL9 d 405:

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

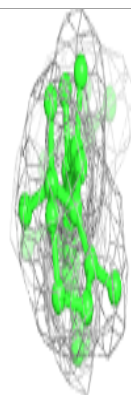
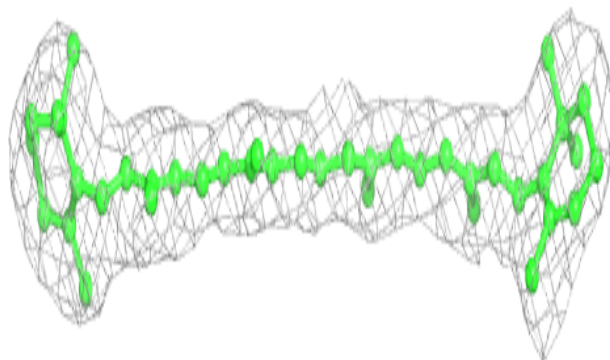
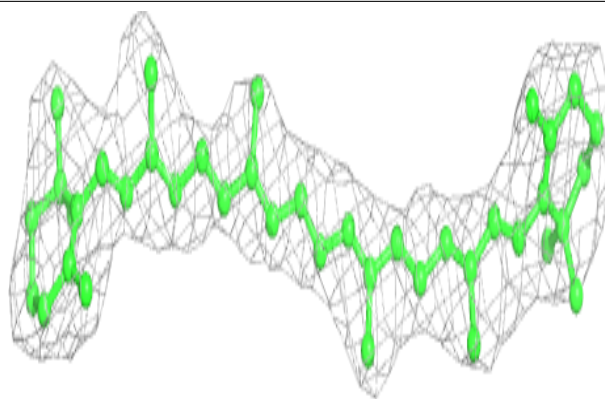
**Electron density around BCR B 618:**

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



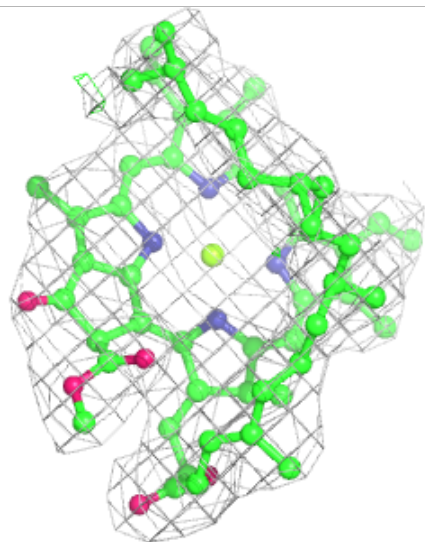
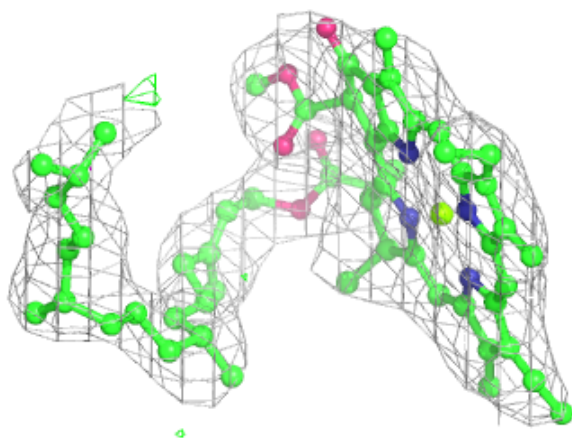
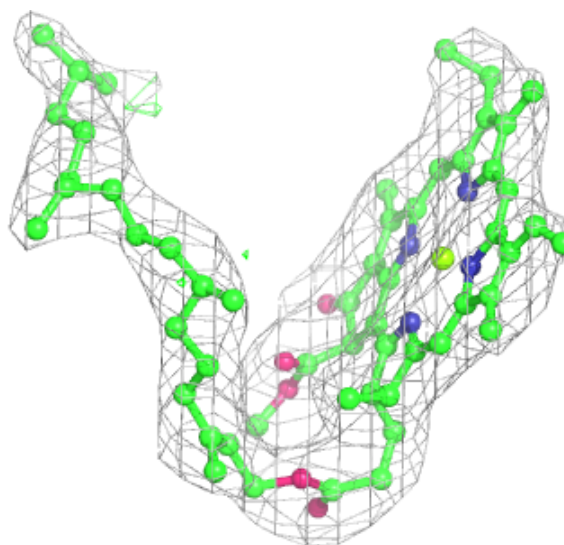
Electron density around BCR B 619:

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



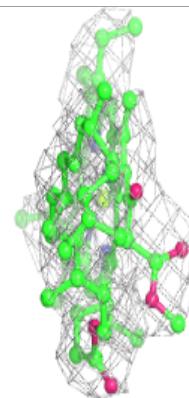
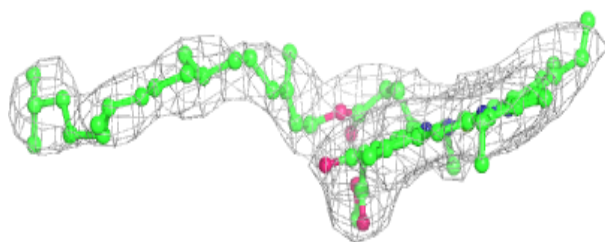
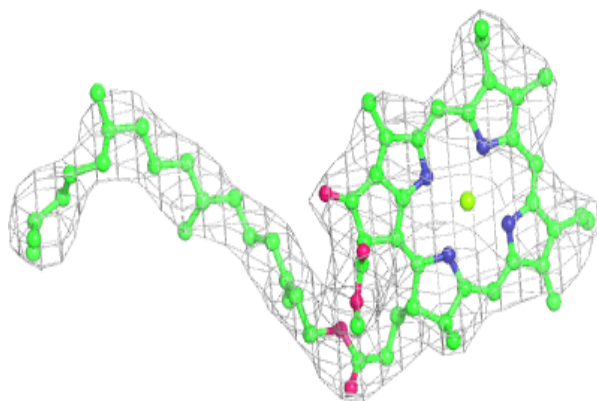
Electron density around CLA B 614:

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

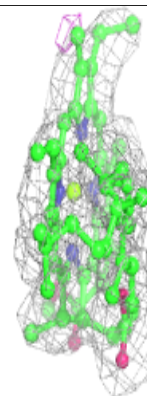
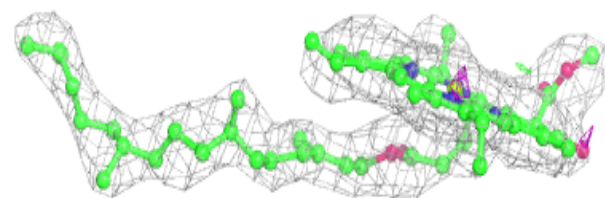
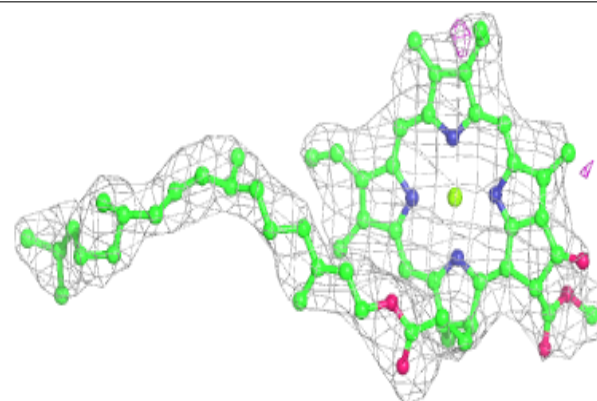


Electron density around CLA B 603:

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

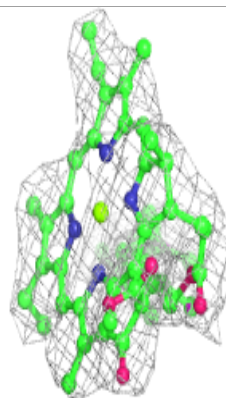
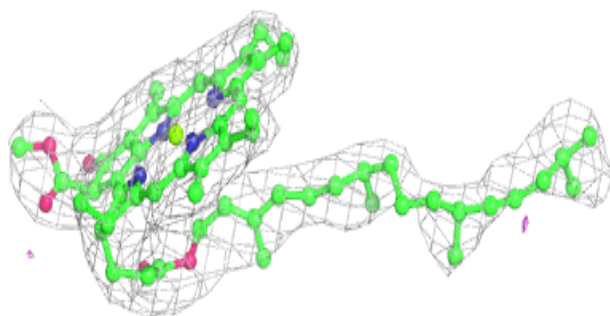
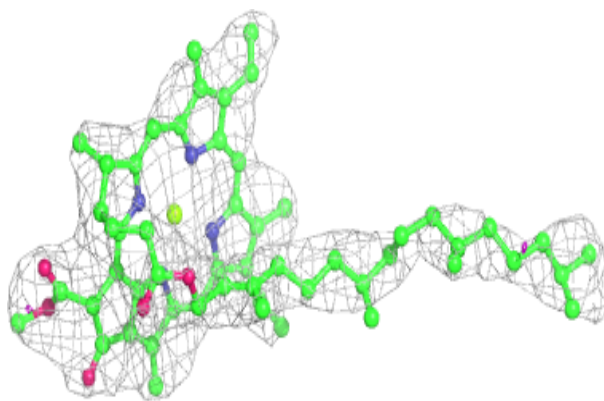
**Electron density around CLA B 604:**

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

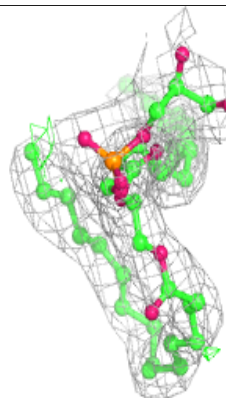
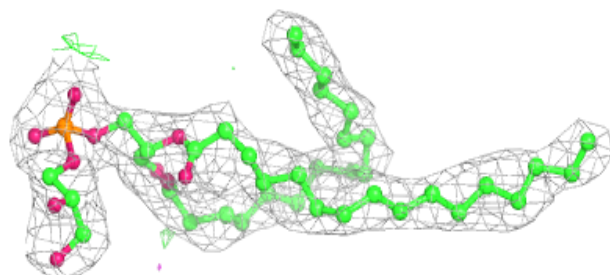
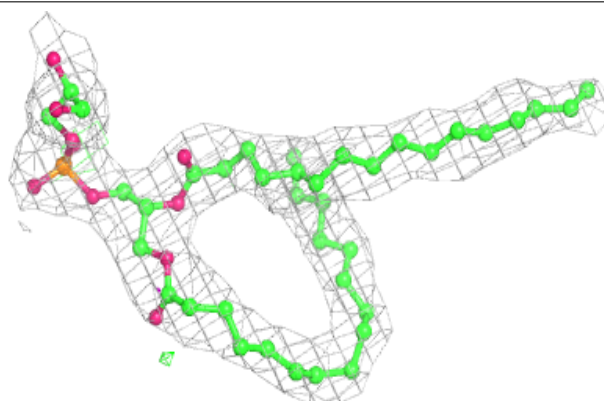


Electron density around CLA b 620:

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

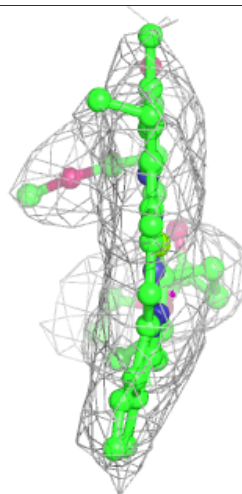
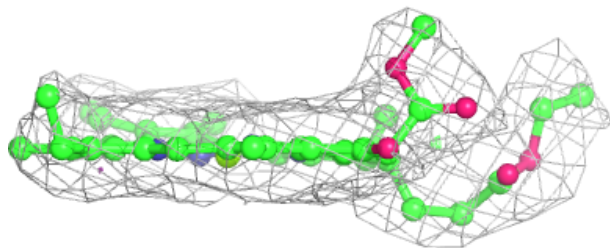
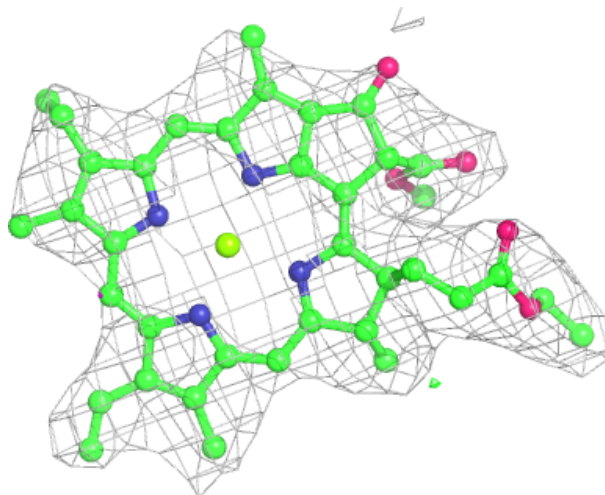
**Electron density around LHG B 625:**

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



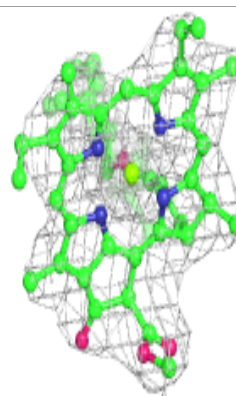
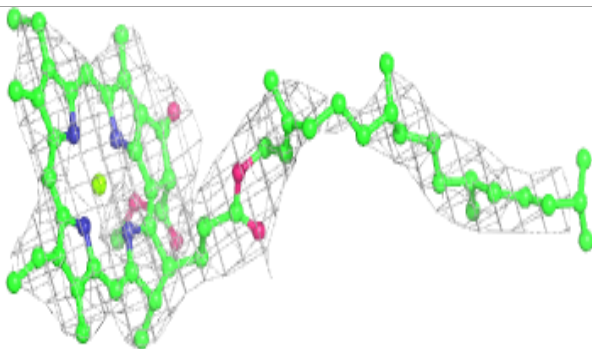
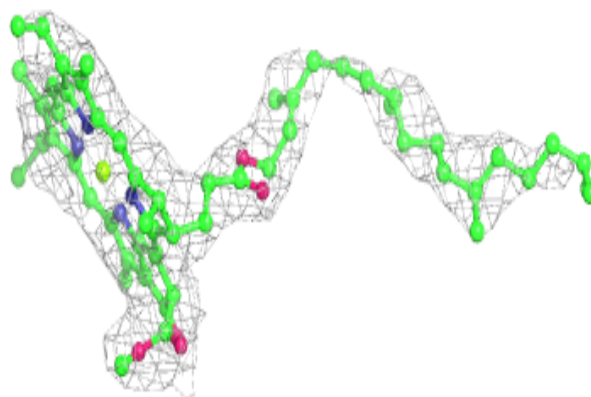
Electron density around CLA b 622:

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

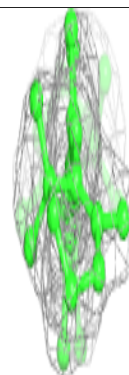
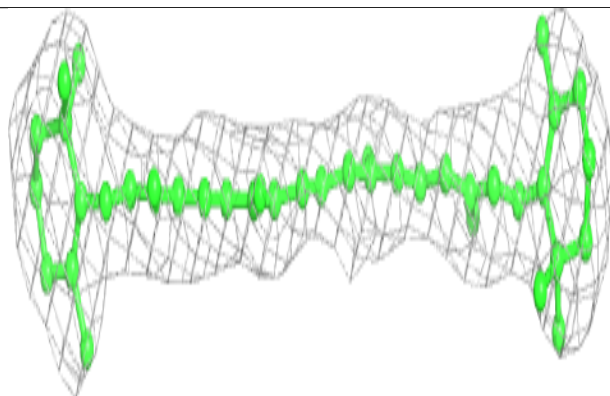
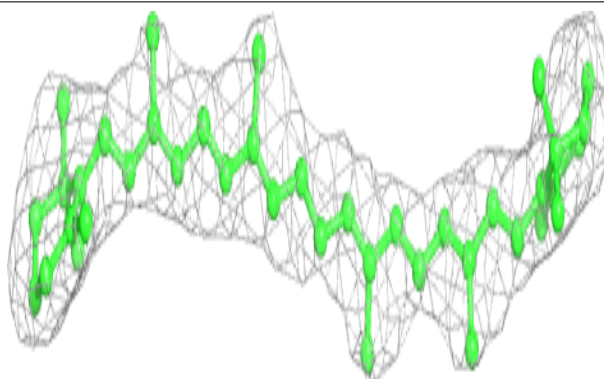


Electron density around CLA c 502:

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

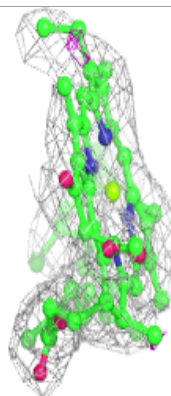
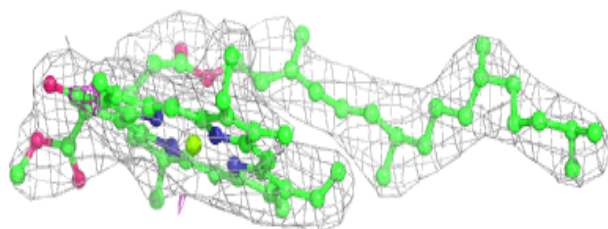
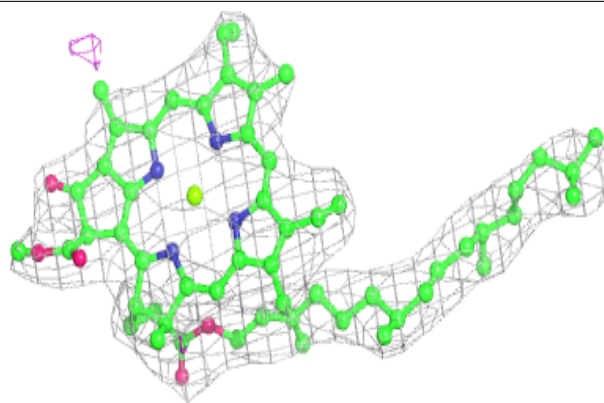
**Electron density around BCR a 712:**

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

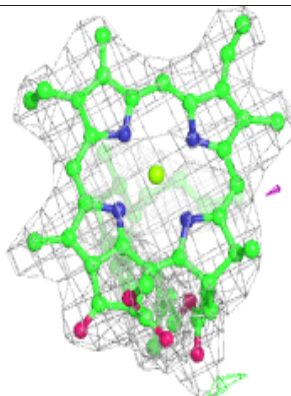
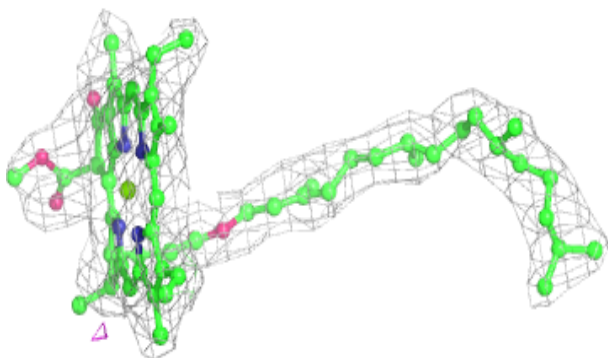
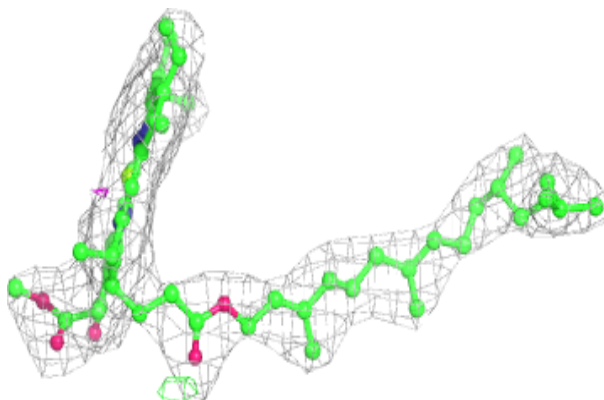


Electron density around CLA C 502:

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

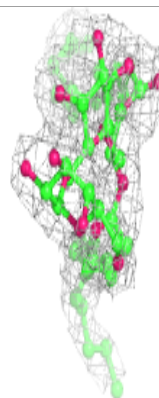
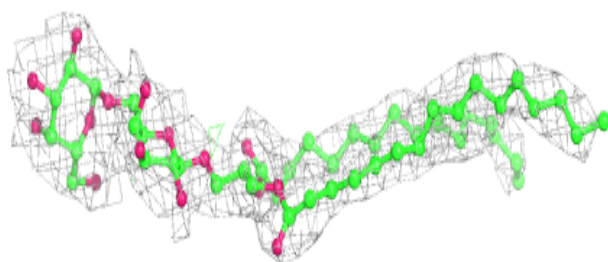
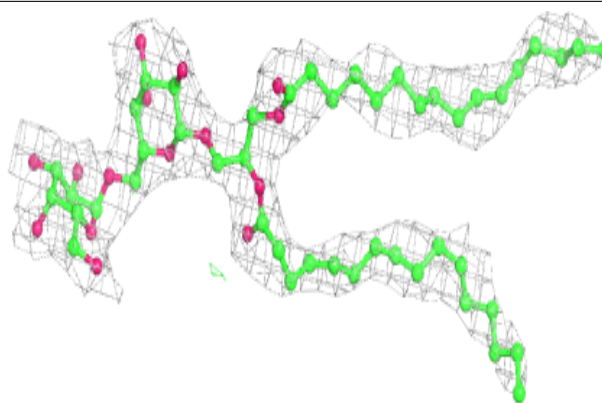
**Electron density around CLA B 606:**

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



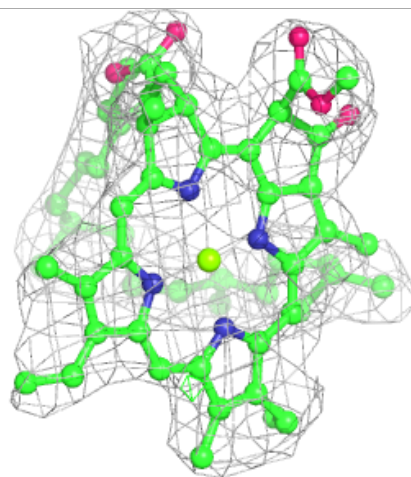
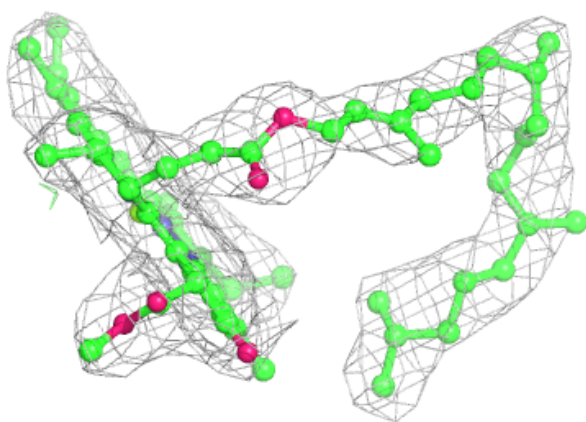
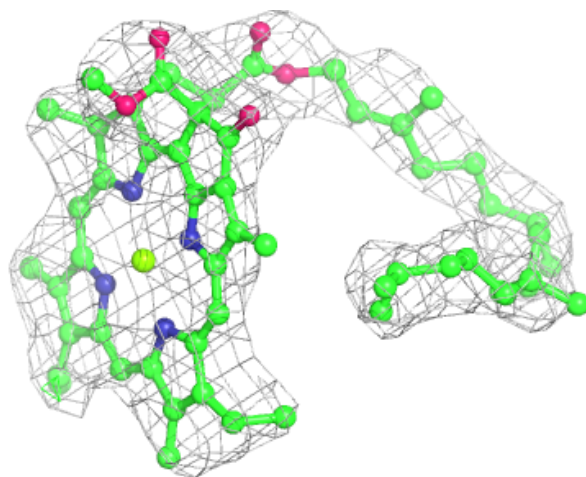
Electron density around DGD C 519:

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



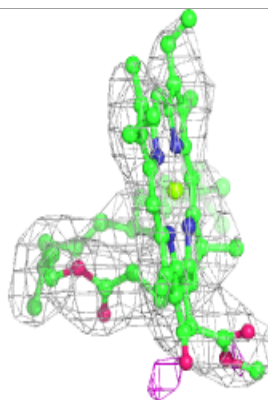
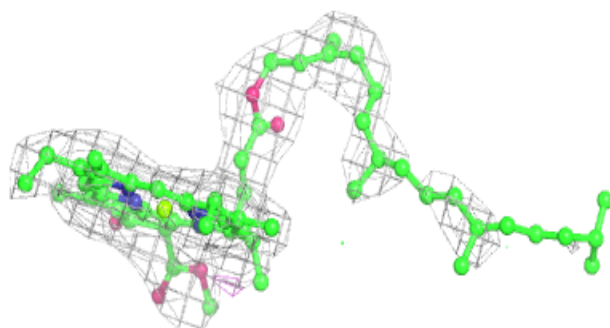
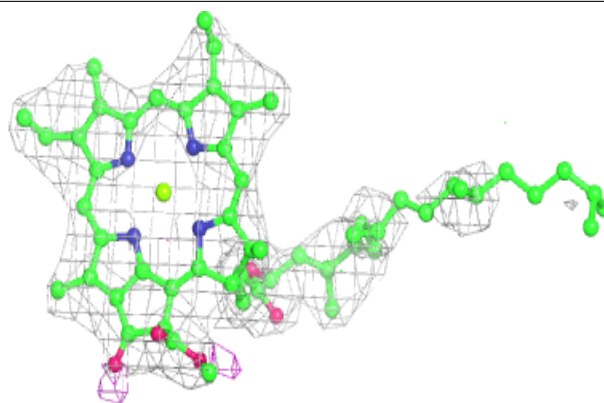
Electron density around CLA C 504:

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



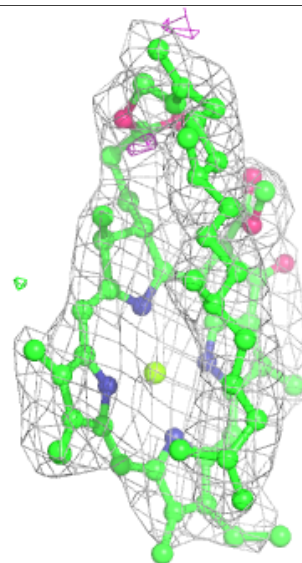
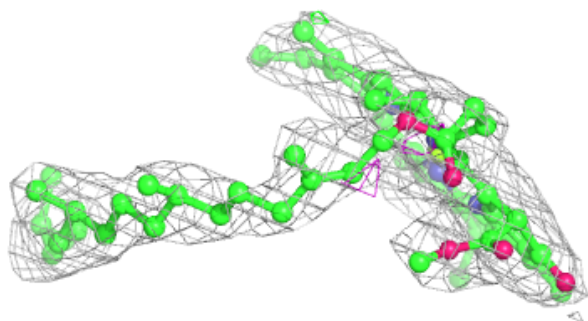
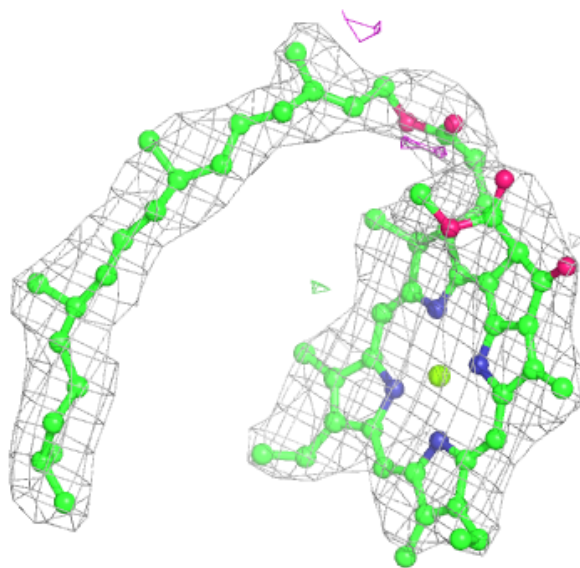
Electron density around CLA A 607:

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



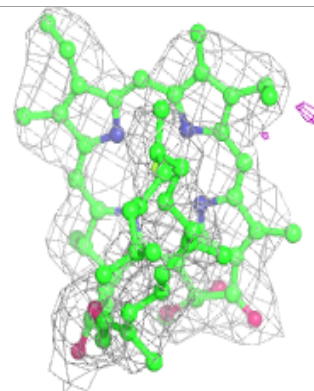
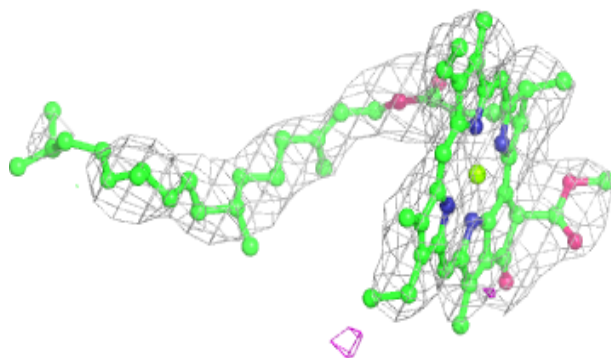
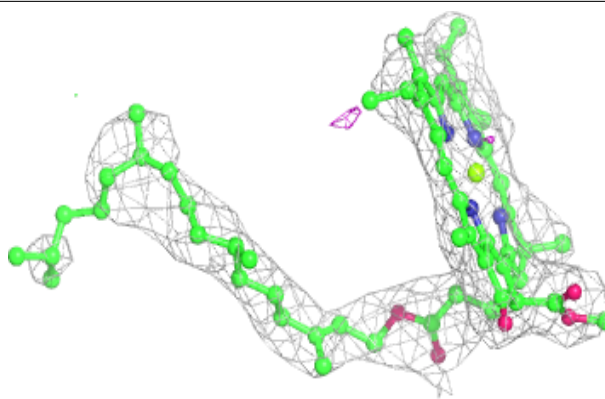
Electron density around CLA c 507:

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



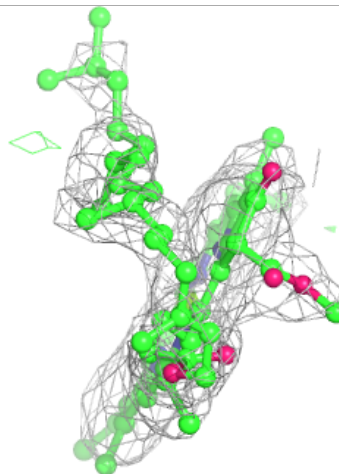
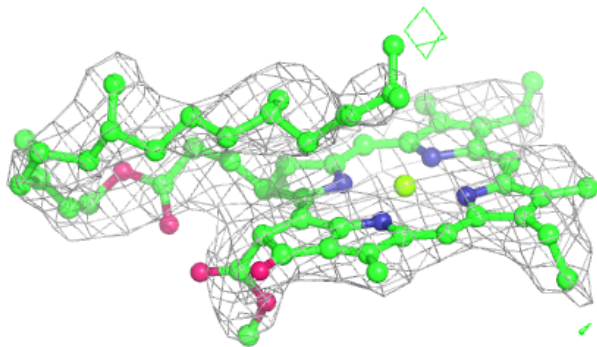
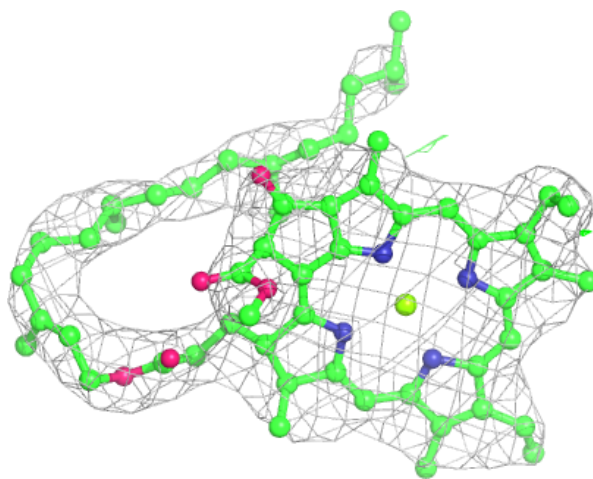
Electron density around CLA c 508:

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



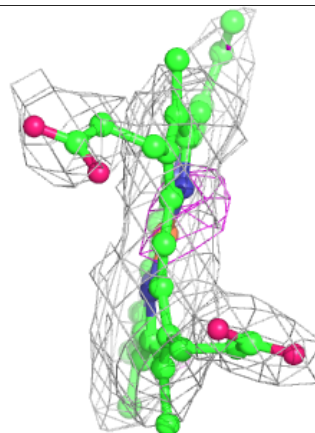
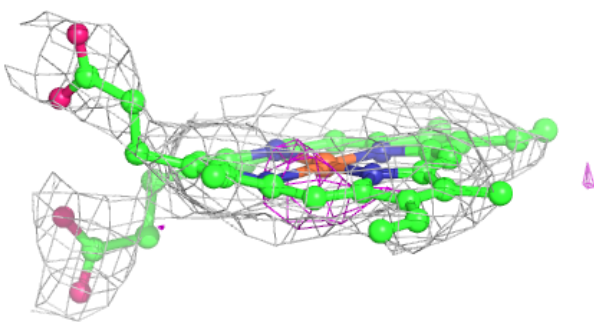
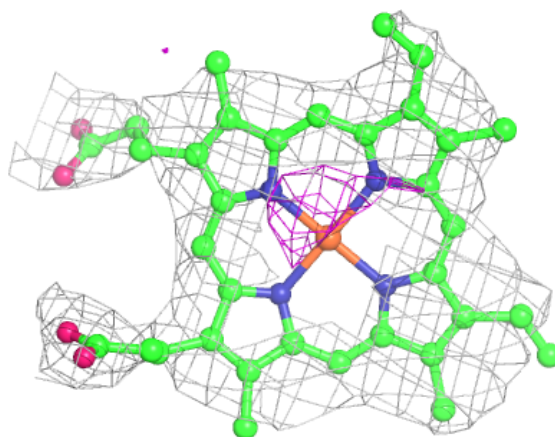
Electron density around CLA c 509:

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



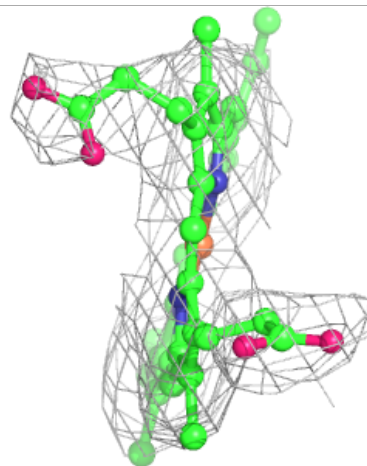
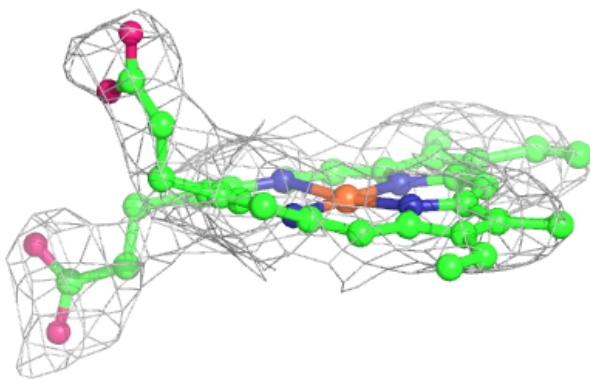
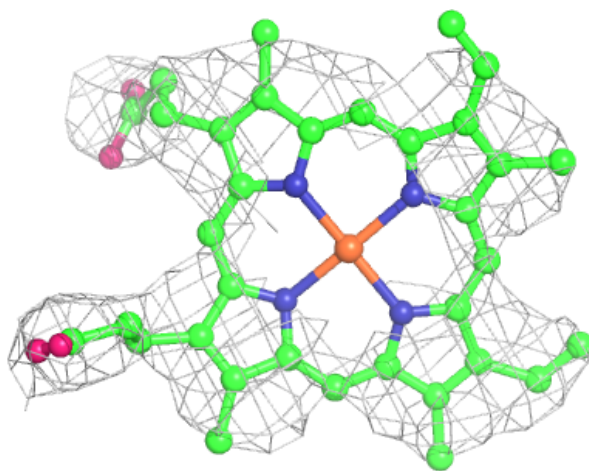
Electron density around HEM E 102:

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



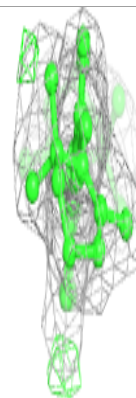
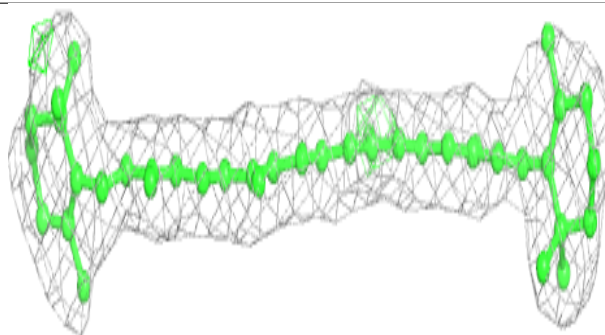
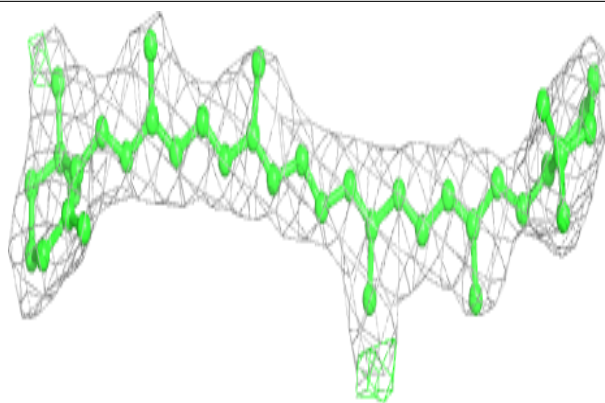
Electron density around HEM e 102:

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



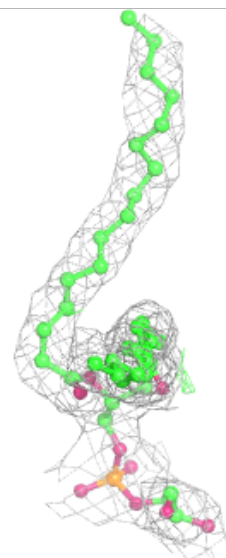
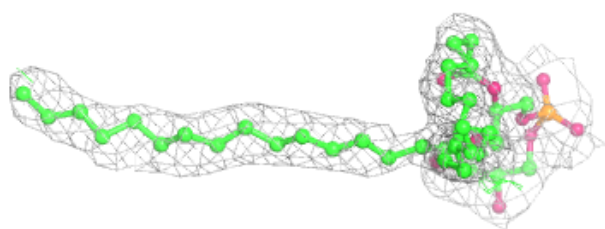
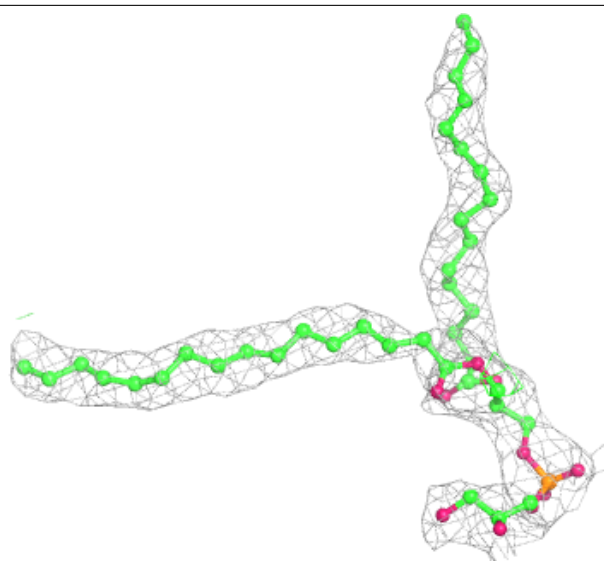
Electron density around BCR A 610:

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



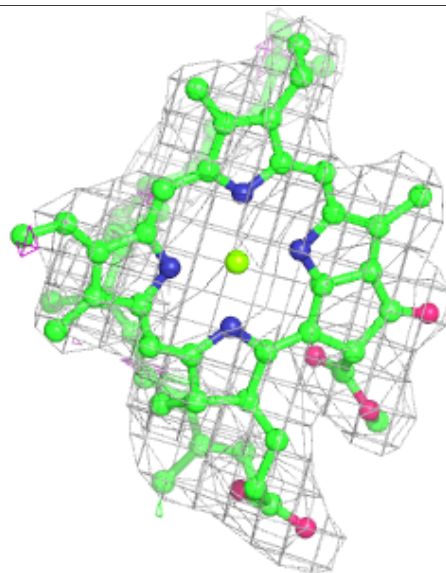
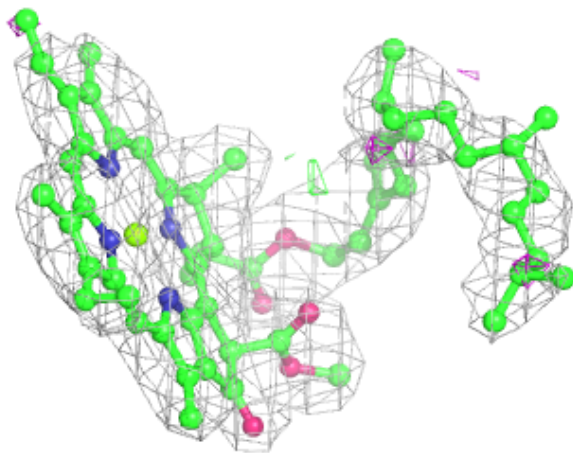
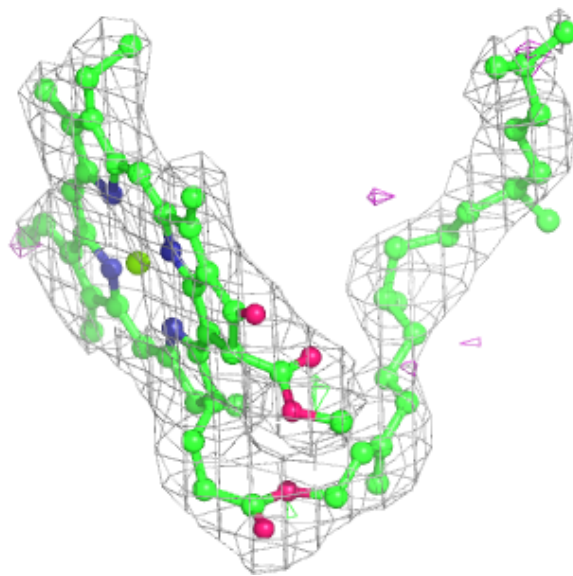
Electron density around LHG L 101:

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



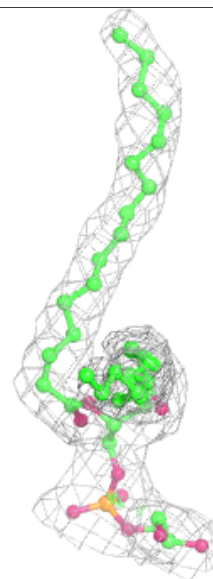
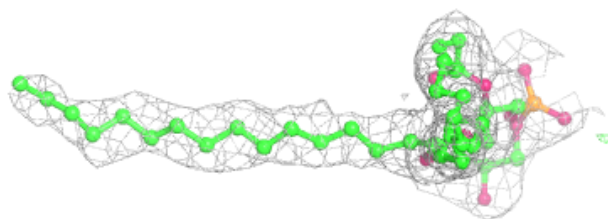
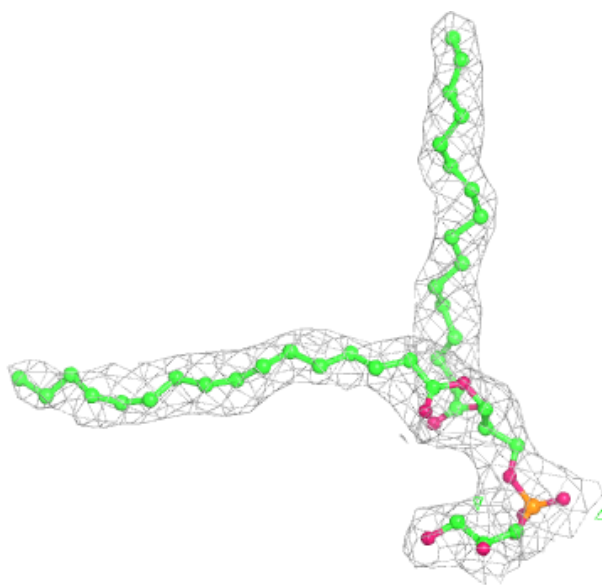
Electron density around CLA b 619:

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



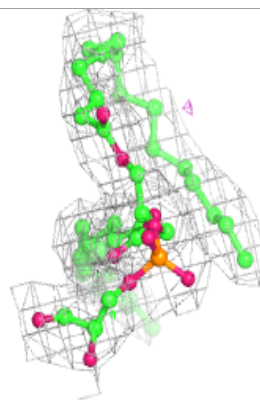
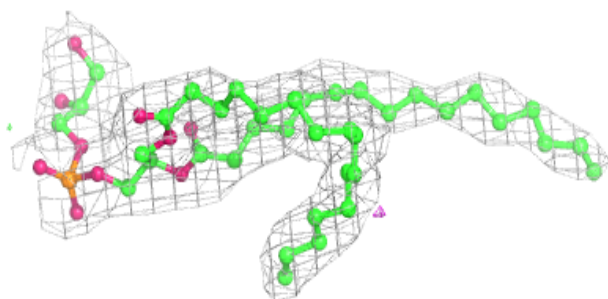
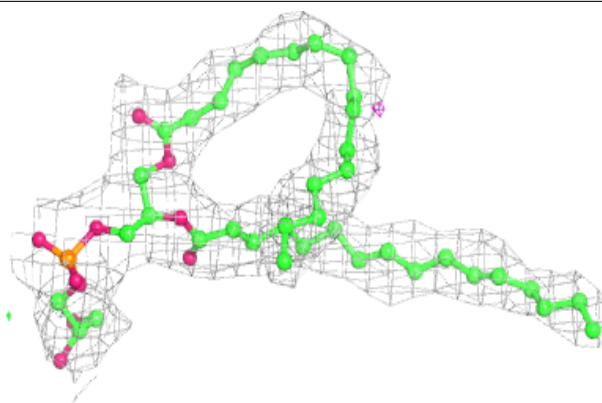
Electron density around LHG b 629:

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

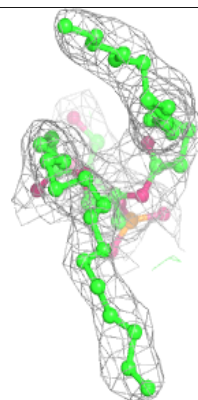
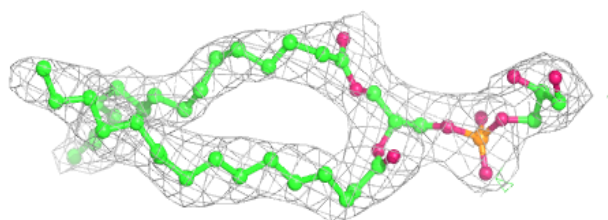
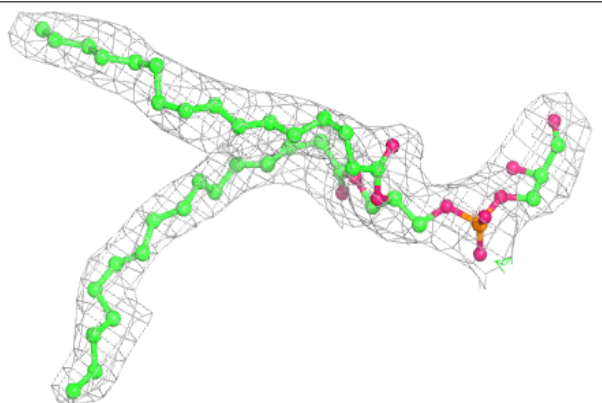


Electron density around LHG d 406:

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

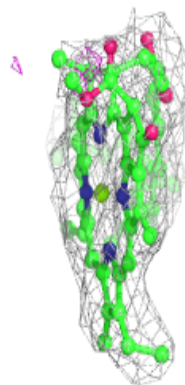
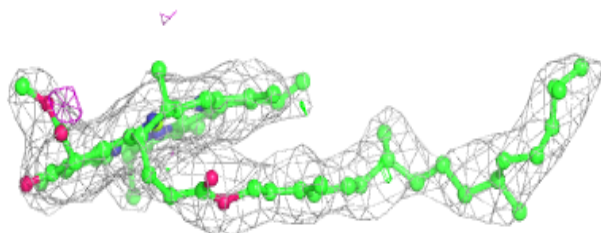
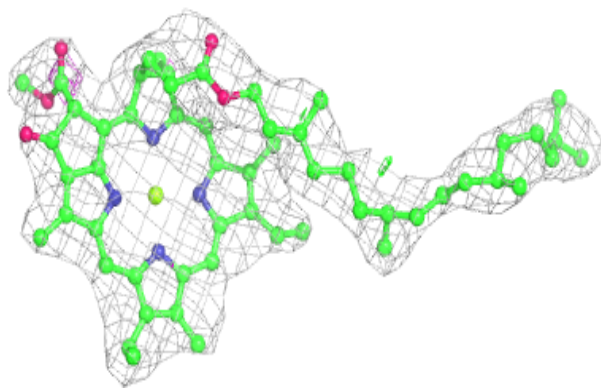
**Electron density around LHG d 407:**

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



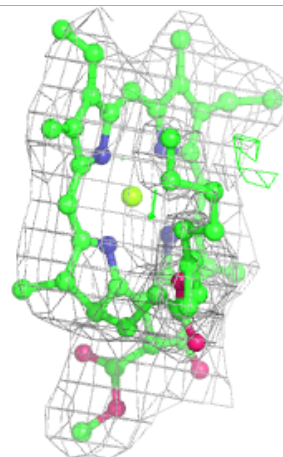
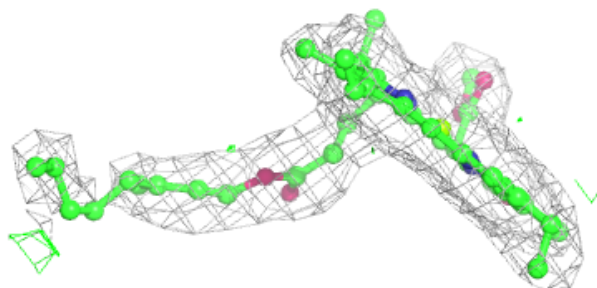
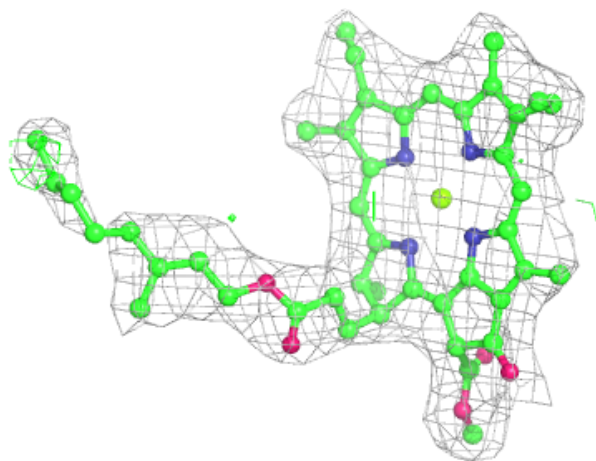
Electron density around CLA b 609:

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



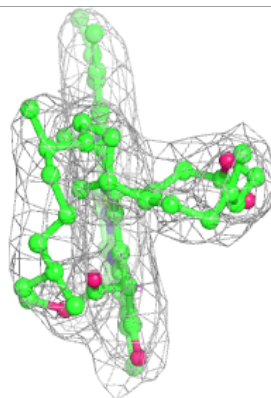
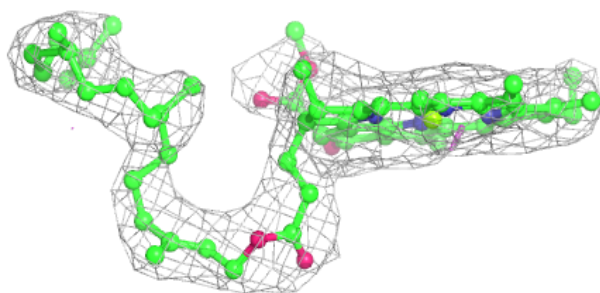
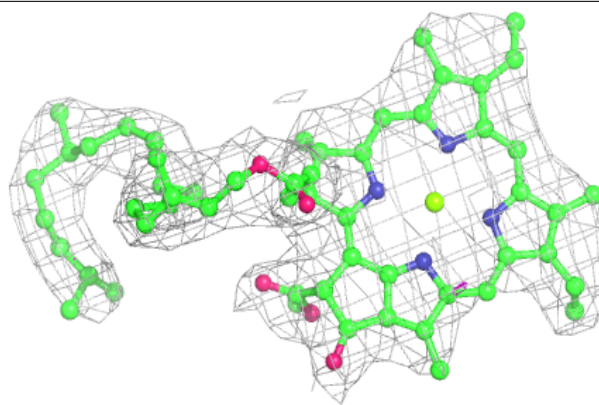
Electron density around CLA A 609:

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

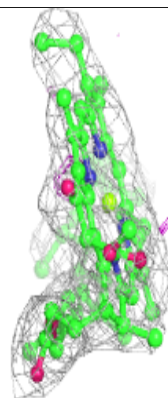
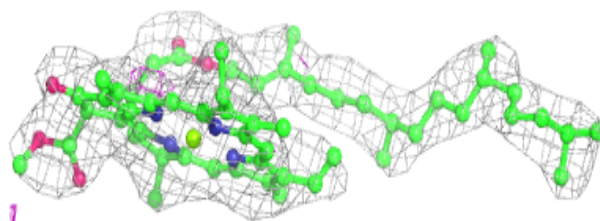
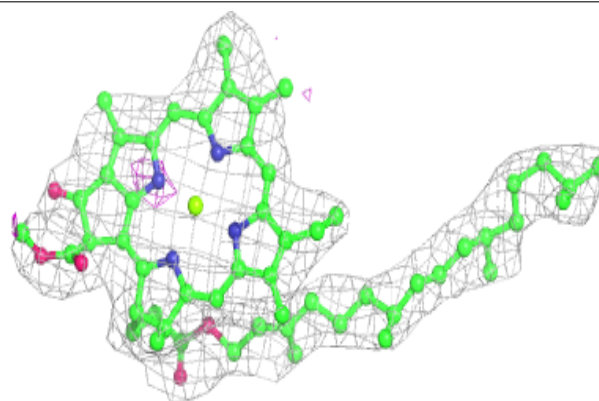


Electron density around CLA B 613:

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

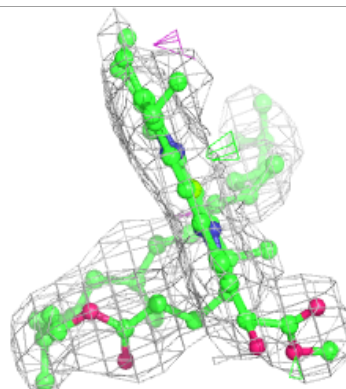
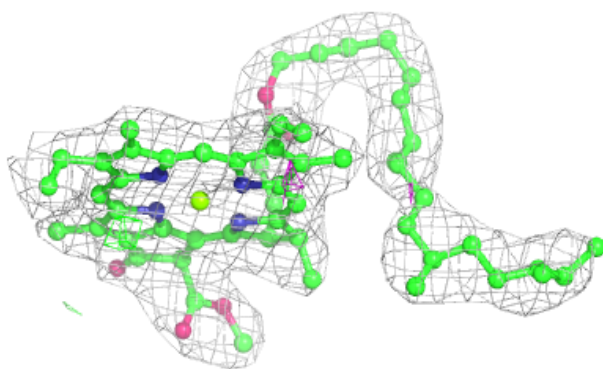
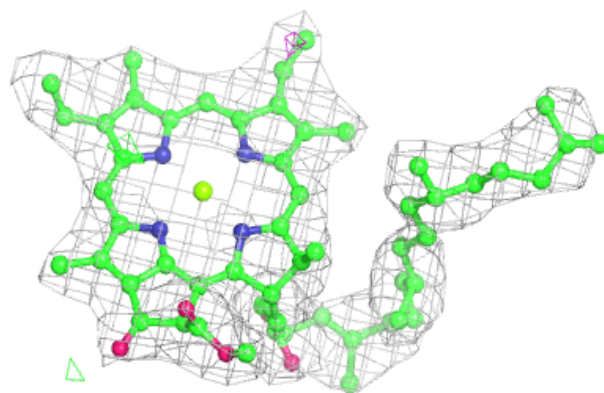
**Electron density around CLA c 501:**

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

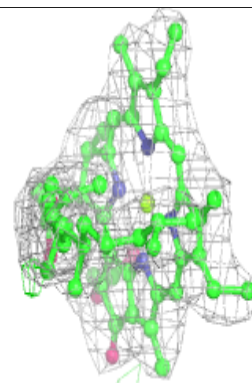
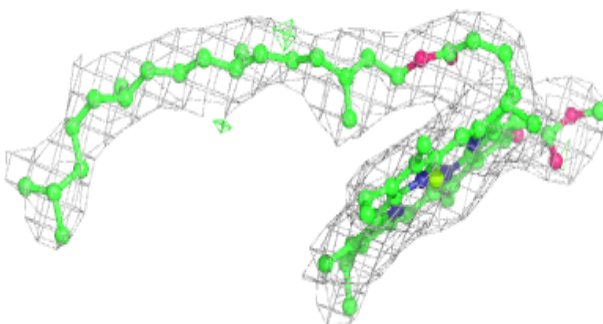
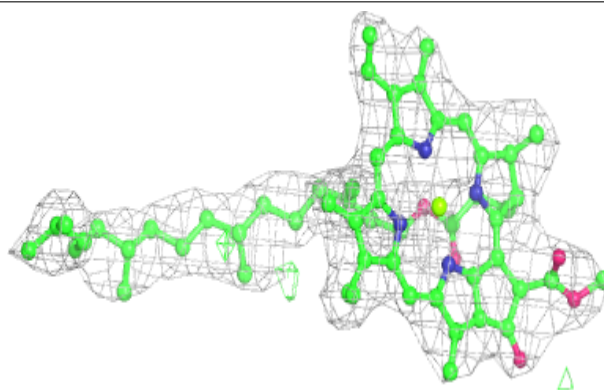


Electron density around CLA a 719:

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

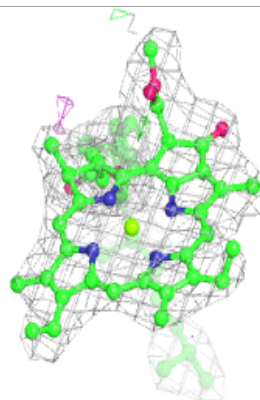
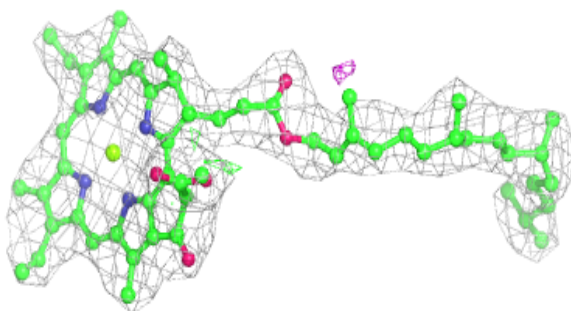
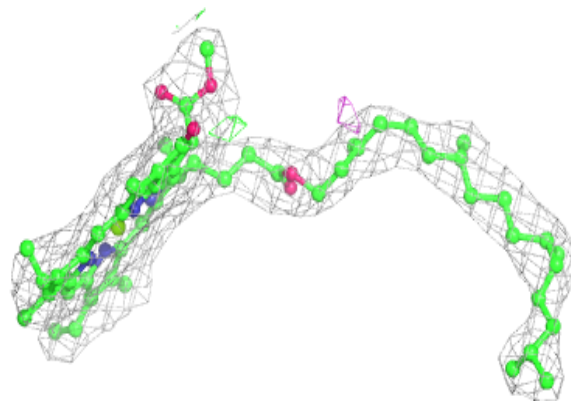
**Electron density around CLA b 614:**

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

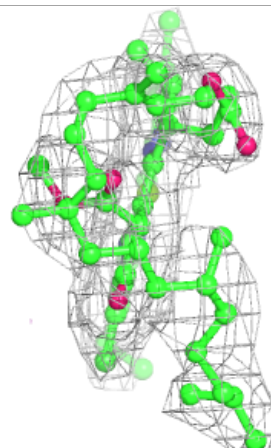
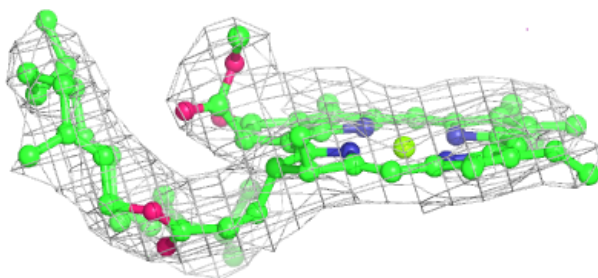
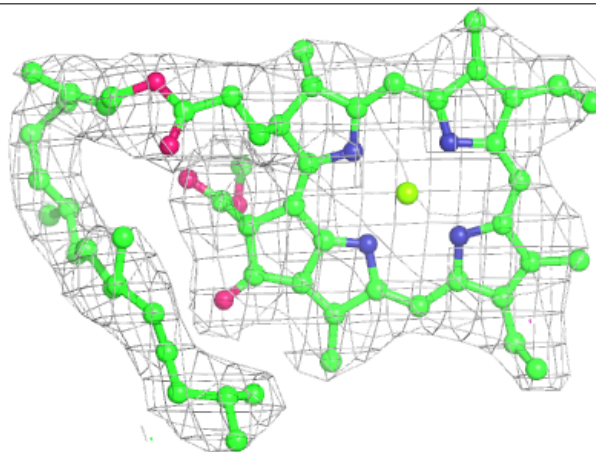


Electron density around CLA D 403:

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

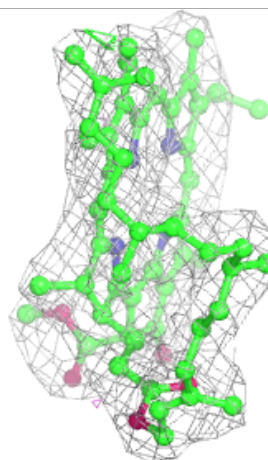
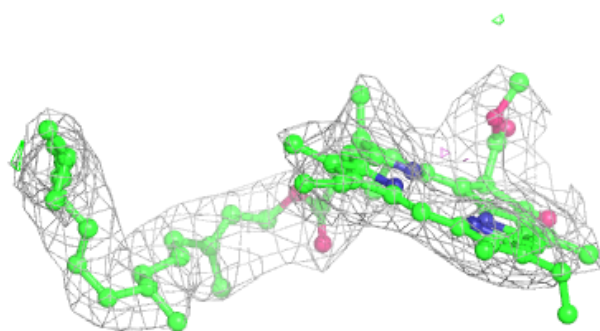
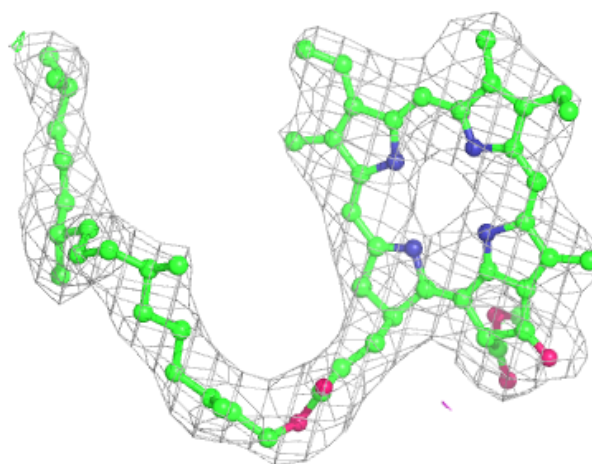
**Electron density around CLA B 611:**

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



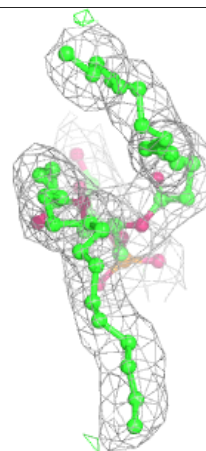
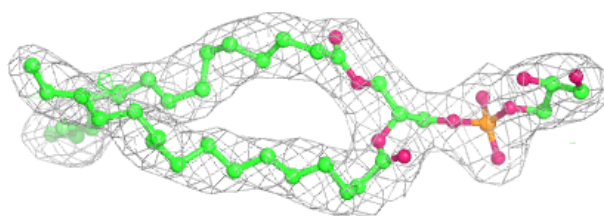
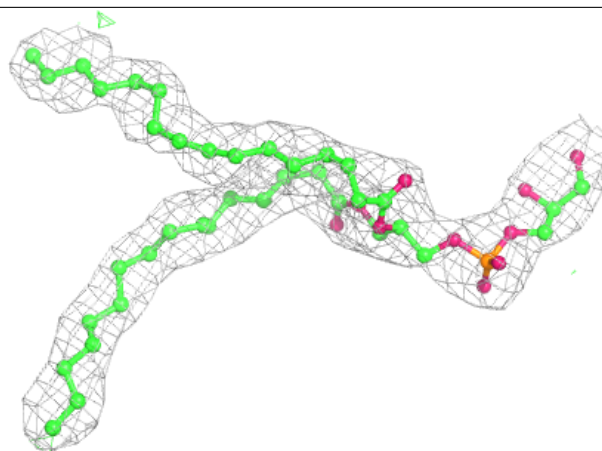
Electron density around PHO D 401:

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



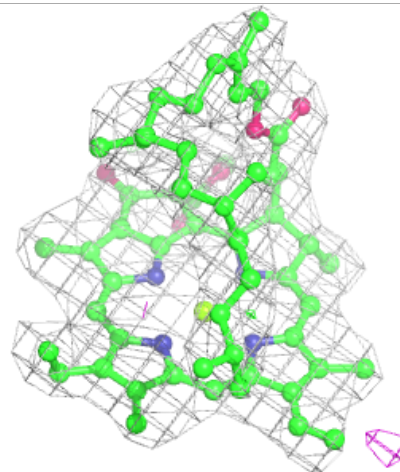
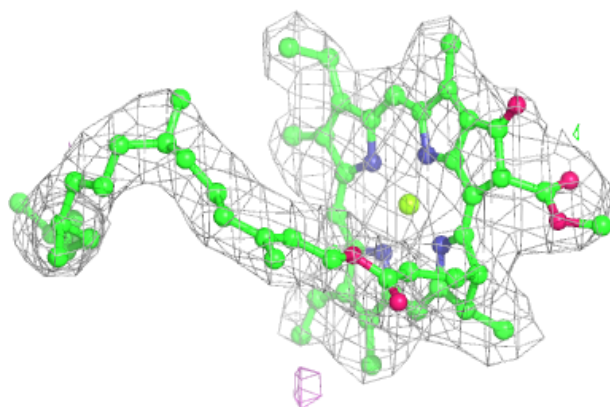
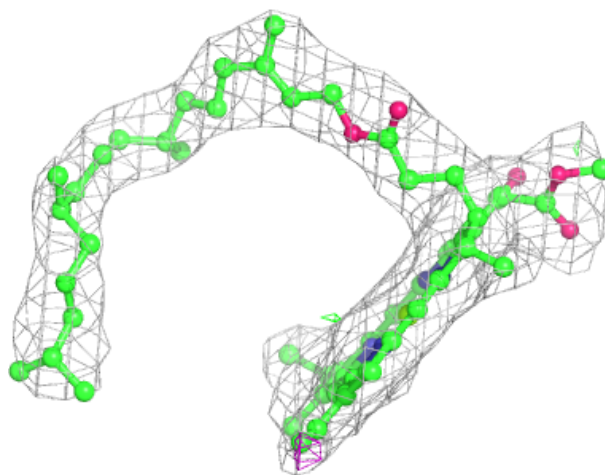
Electron density around LHG D 407:

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



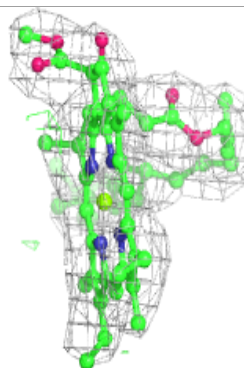
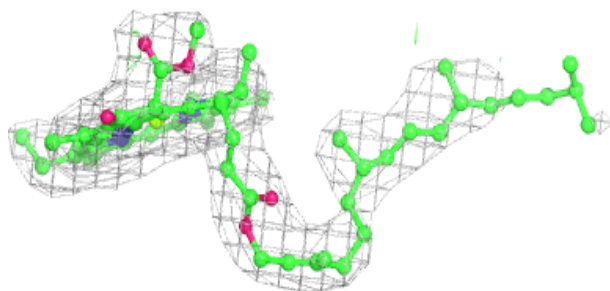
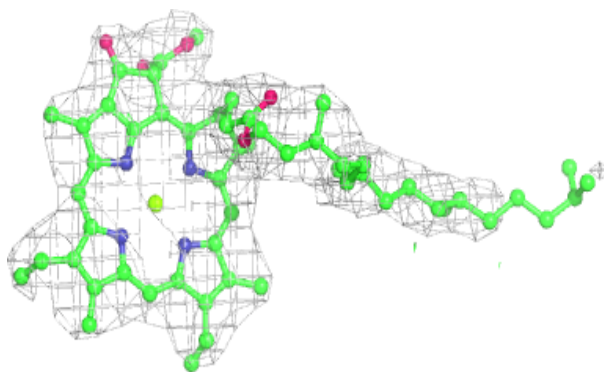
Electron density around CLA b 617:

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

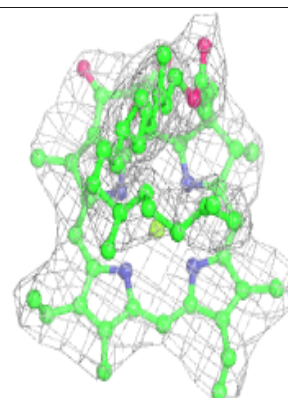
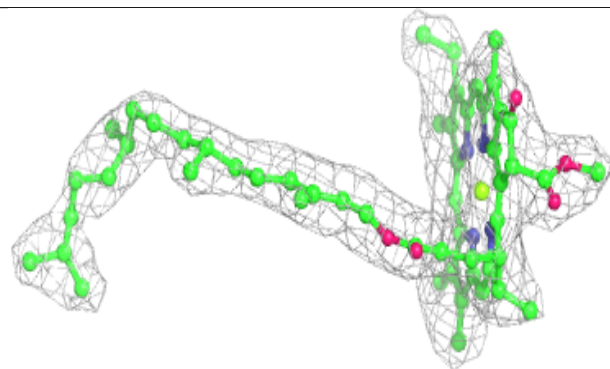
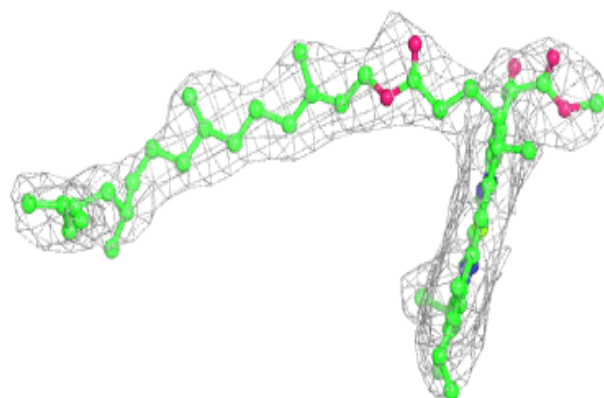


Electron density around CLA a 708:

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

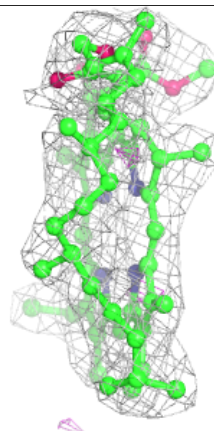
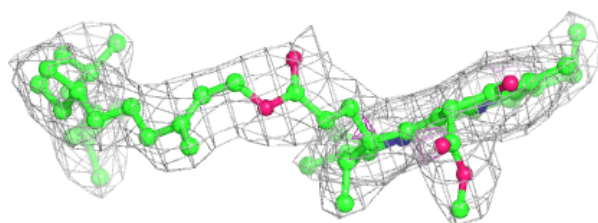
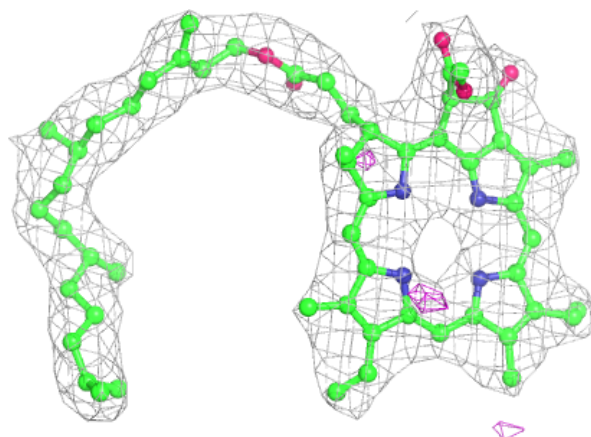
**Electron density around CLA b 611:**

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

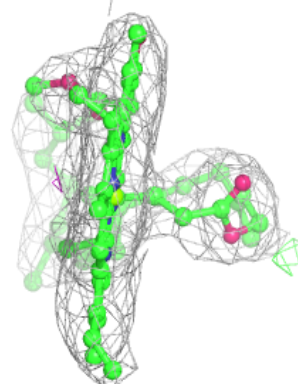
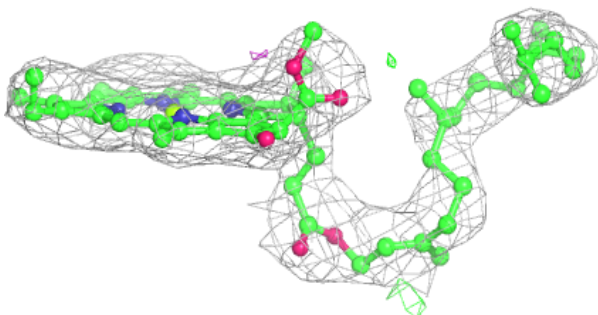
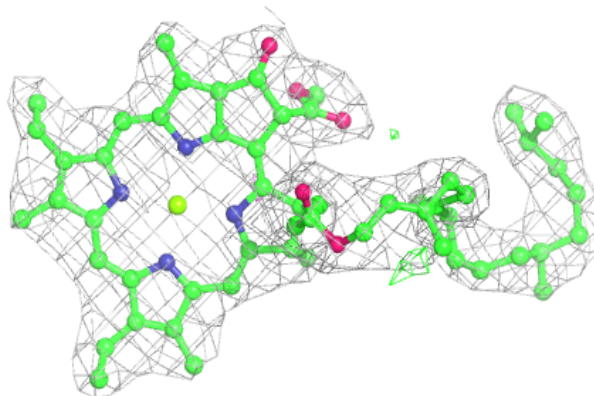


Electron density around PHO A 608:

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

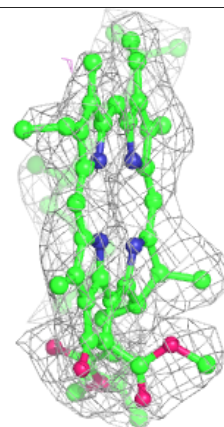
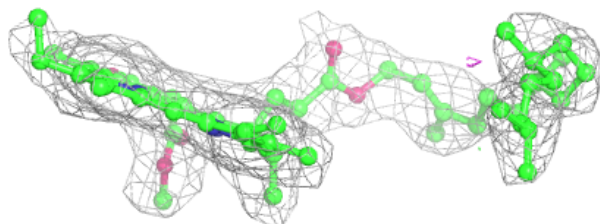
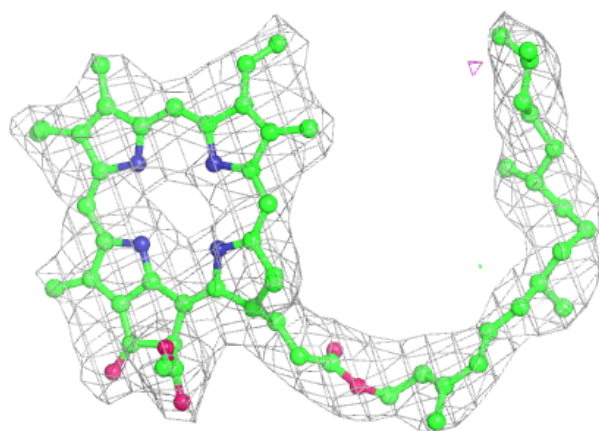
**Electron density around CLA b 618:**

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



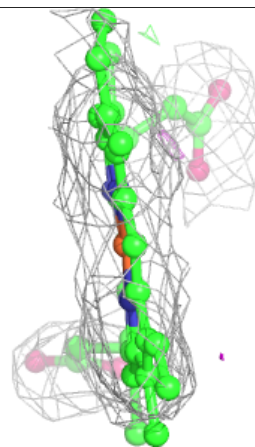
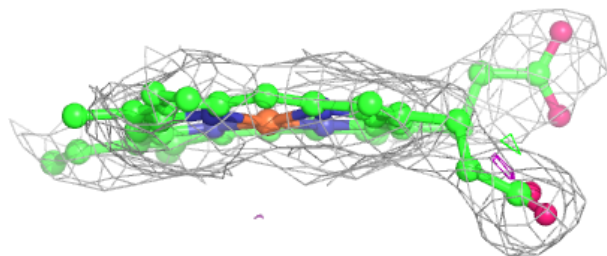
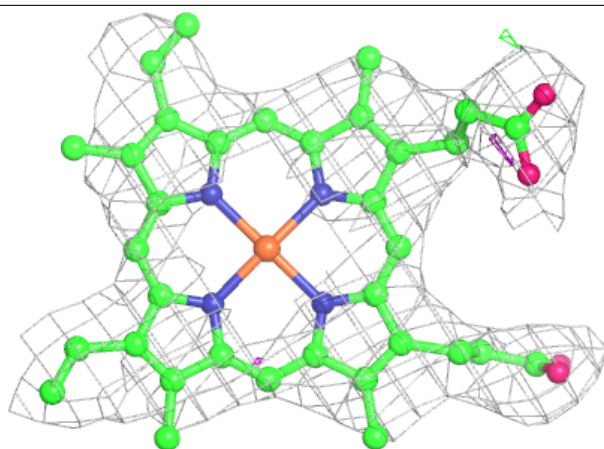
Electron density around PHO a 709:

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



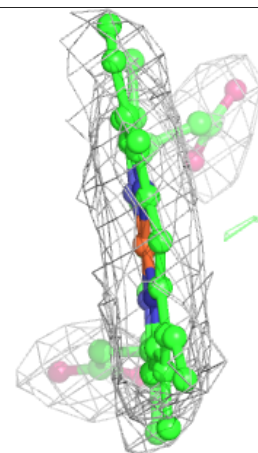
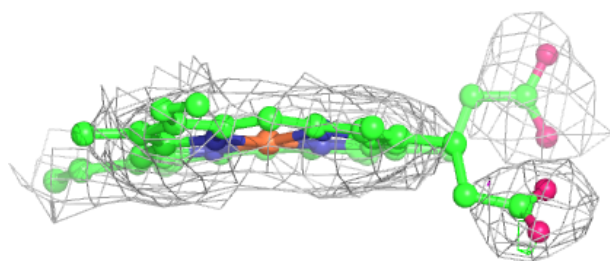
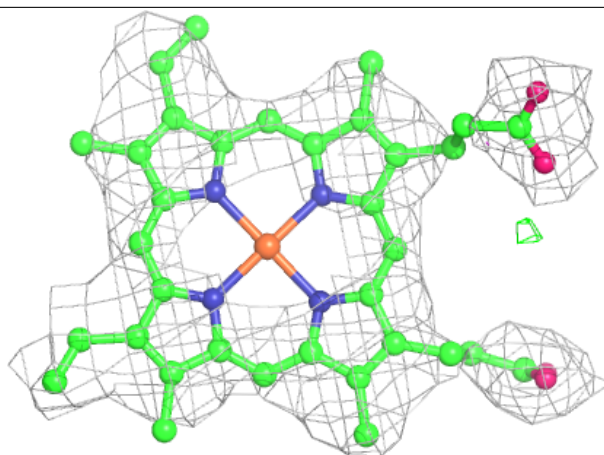
Electron density around HEC V 201:

$2mF_o-DF_c$ (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.