



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 12:50 AM EDT

PDB ID : 7RF8 / pdb_00007rf8
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.09 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 types of validation reports are described at

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

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

| | | |
|-----------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0rc1 |
| EDS | : | 3.0 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.006 (Gargrove) |

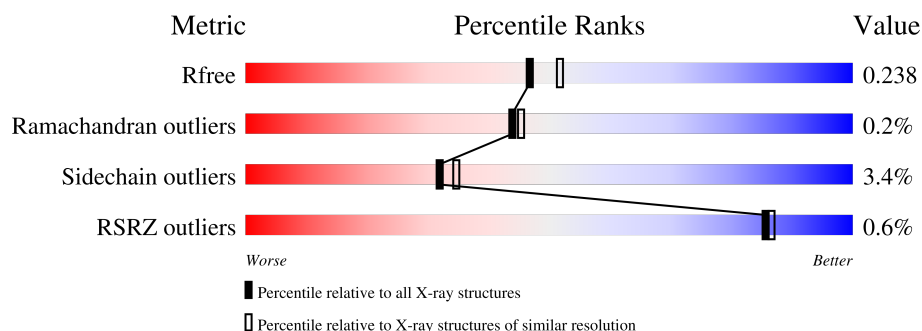
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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} | 164625 | 6234 (2.10-2.10) |
| Ramachandran outliers | 177936 | 6839 (2.10-2.10) |
| Sidechain outliers | 177891 | 6840 (2.10-2.10) |
| RSRZ outliers | 164620 | 6234 (2.10-2.10) |



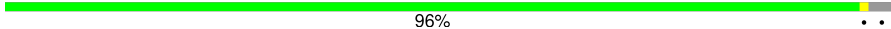

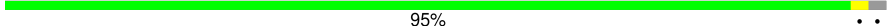
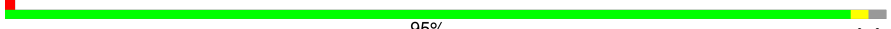










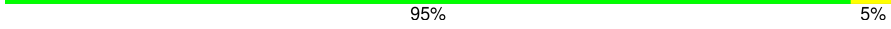








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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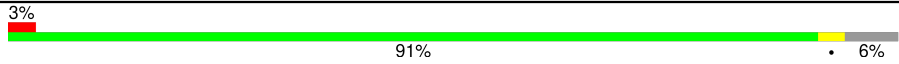




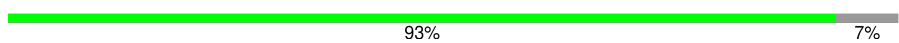




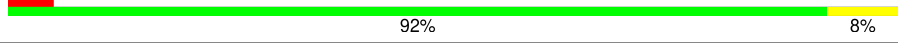
Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.42

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | C | 461 |  |
| 3 | c | 461 |  |
| 4 | D | 352 |  |
| 4 | d | 352 |  |
| 5 | E | 84 |  |
| 5 | e | 84 |  |
| 6 | F | 45 |  |
| 6 | f | 45 |  |
| 7 | H | 66 |  |
| 7 | h | 66 |  |
| 8 | I | 38 |  |
| 8 | i | 38 |  |
| 9 | J | 40 |  |
| 9 | j | 40 |  |
| 10 | K | 46 |  |
| 10 | k | 46 |  |
| 11 | L | 37 |  |
| 11 | l | 37 |  |
| 12 | M | 36 |  |
| 12 | m | 36 |  |
| 13 | O | 272 |  |
| 13 | o | 272 |  |
| 14 | R | 41 |  |
| 14 | r | 41 |  |
| 15 | T | 32 |  |

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

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | A | 402 | X | - | - | - |
| 22 | CLA | A | 405 | X | - | - | - |
| 22 | CLA | A | 410 | X | - | - | - |
| 22 | CLA | B | 601 | X | - | - | - |
| 22 | CLA | B | 603 | X | - | - | - |
| 22 | CLA | B | 604 | X | - | - | - |
| 22 | CLA | B | 605 | X | - | - | - |
| 22 | CLA | B | 606 | X | - | - | - |
| 22 | CLA | B | 607 | X | - | - | - |
| 22 | CLA | B | 608 | X | - | - | - |
| 22 | CLA | B | 610 | X | - | - | - |
| 22 | CLA | B | 611 | X | - | - | - |
| 22 | CLA | B | 612 | X | - | - | - |
| 22 | CLA | B | 613 | X | - | - | - |
| 22 | CLA | B | 614 | X | - | - | - |
| 22 | CLA | B | 615 | X | - | - | - |
| 22 | CLA | B | 616 | X | - | - | - |
| 22 | CLA | C | 501 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | C | 502 | X | - | - | - |
| 22 | CLA | C | 503 | X | - | - | - |
| 22 | CLA | C | 504 | X | - | - | - |
| 22 | CLA | C | 505 | X | - | - | - |
| 22 | CLA | C | 506 | X | - | - | - |
| 22 | CLA | C | 507 | X | - | - | - |
| 22 | CLA | C | 509 | X | - | - | - |
| 22 | CLA | C | 510 | X | - | - | - |
| 22 | CLA | C | 511 | X | - | - | - |
| 22 | CLA | C | 512 | X | - | - | - |
| 22 | CLA | C | 513 | X | - | - | - |
| 22 | CLA | D | 403 | X | - | - | - |
| 22 | CLA | a | 402 | X | - | - | - |
| 22 | CLA | a | 404 | X | - | - | - |
| 22 | CLA | b | 601 | X | - | - | - |
| 22 | CLA | b | 603 | X | - | - | - |
| 22 | CLA | b | 604 | X | - | - | - |
| 22 | CLA | b | 605 | X | - | - | - |
| 22 | CLA | b | 606 | X | - | - | - |
| 22 | CLA | b | 607 | X | - | - | - |
| 22 | CLA | b | 608 | X | - | - | - |
| 22 | CLA | b | 609 | X | - | - | - |
| 22 | CLA | b | 610 | X | - | - | - |
| 22 | CLA | b | 611 | X | - | - | - |
| 22 | CLA | b | 612 | X | - | - | - |
| 22 | CLA | b | 613 | X | - | - | - |
| 22 | CLA | b | 614 | X | - | - | - |
| 22 | CLA | b | 615 | X | - | - | - |
| 22 | CLA | b | 616 | X | - | - | - |
| 22 | CLA | c | 501 | X | - | - | - |
| 22 | CLA | c | 502 | X | - | - | - |
| 22 | CLA | c | 503 | X | - | - | - |
| 22 | CLA | c | 504 | X | - | - | - |
| 22 | CLA | c | 505 | X | - | - | - |
| 22 | CLA | c | 506 | X | - | - | - |
| 22 | CLA | c | 507 | X | - | - | - |
| 22 | CLA | c | 509 | X | - | - | - |
| 22 | CLA | c | 510 | X | - | - | - |
| 22 | CLA | c | 511 | X | - | - | - |
| 22 | CLA | c | 512 | X | - | - | - |
| 22 | CLA | c | 513 | X | - | - | - |
| 22 | CLA | d | 404 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | d | 405 | X | - | - | - |

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105937 atoms, of which 52685 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| M | 1 | FME | - | initiating methionine | UNP Q8DHA7 |
| m | 1 | FME | - | initiating methionine | 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 | H | N | O | 0 | 1 | 0 |
| | | | 3700 | 1168 | 1830 | 313 | 385 | | | |
| 13 | o | 244 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 3720 | 1170 | 1846 | 317 | 383 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 15 | T | 30 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 519 | 181 | 261 | 36 | 39 | 2 | | | |
| 15 | t | 30 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 512 | 180 | 256 | 36 | 38 | 2 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| T | 1 | FME | - | initiating methionine | UNP Q8DIQ0 |
| t | 1 | FME | - | initiating methionine | UNP Q8DIQ0 |

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

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

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

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

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

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

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

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

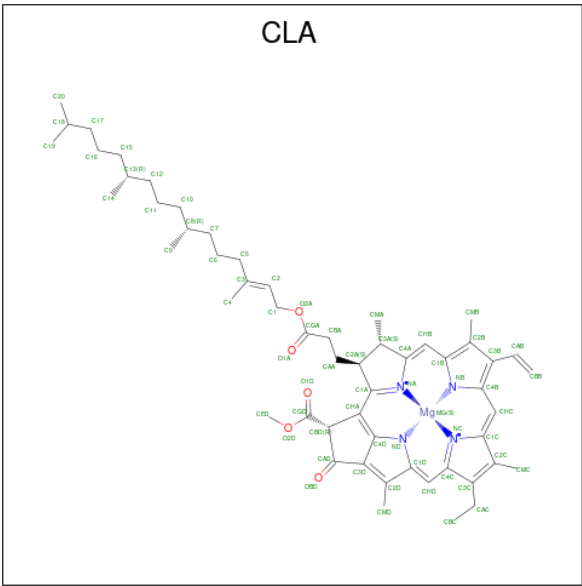
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 102 | 44 | 48 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 117 | 49 | 58 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|---------|--------|--------|---------|---------|
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | D | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | D | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | a | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 137 | C 55 | H 72 | Mg 1 | N 4 | O 5 | 0 | 0 |

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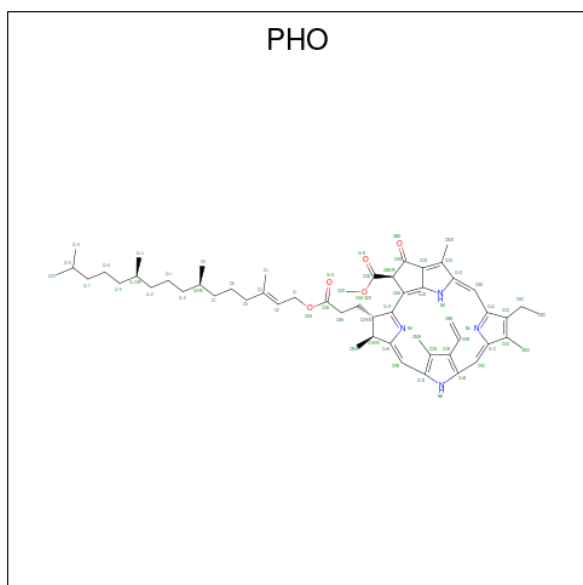
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 132 | 54 | 68 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

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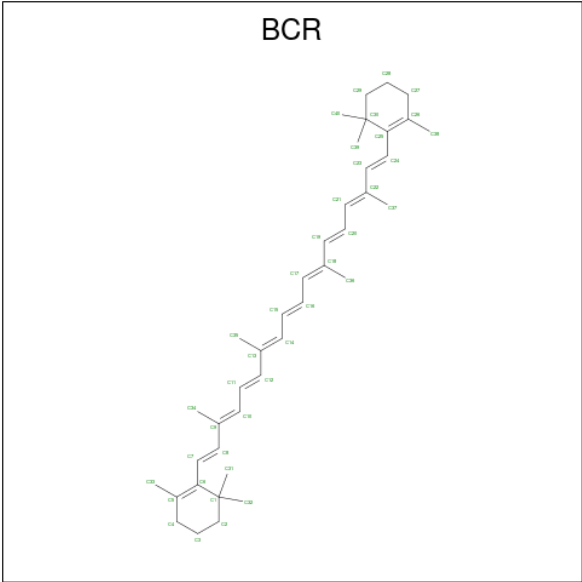
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 22 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | d | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|--|---------|---------|
| 23 | A | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 23 | D | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 23 | d | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |
| 23 | d | 1 | Total | C | H | N | O | | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | | |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24 | A | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | D | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | H | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | K | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | T | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | Y | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | a | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

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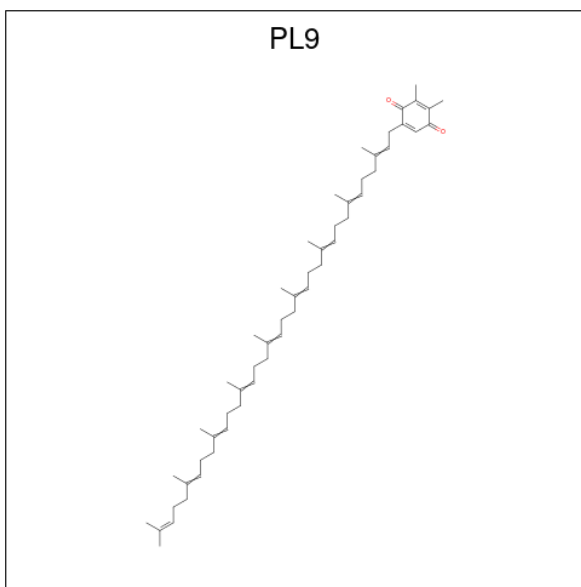
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | d | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | h | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | k | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 24 | t | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

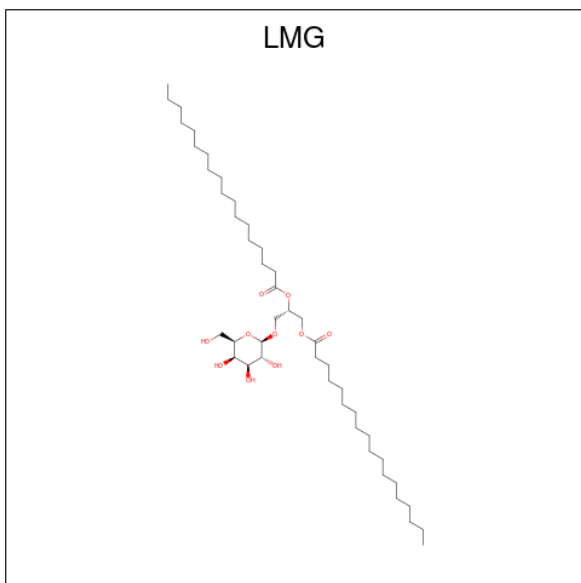
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 25 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



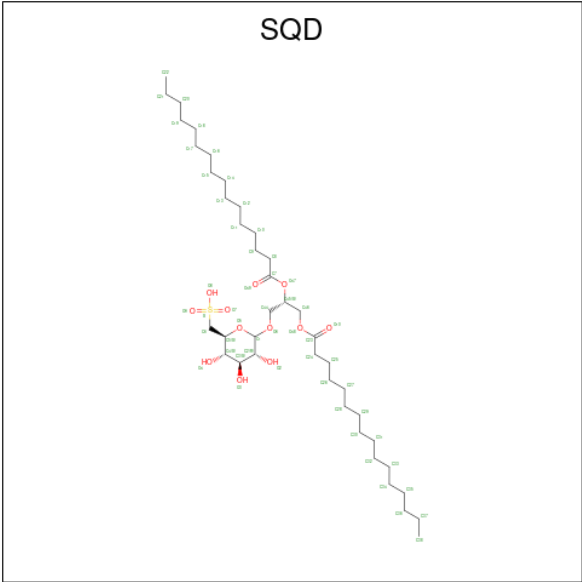
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | a | 1 | Total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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



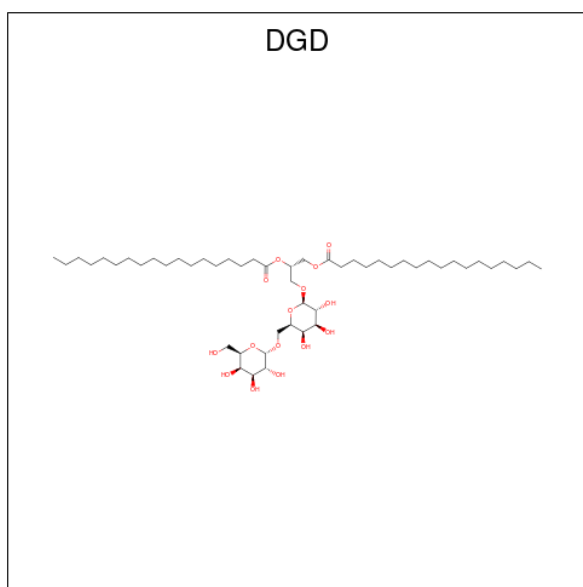
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 27 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 114 | 38 | 66 | 10 | | |
| 27 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 68 | 24 | 40 | 4 | | |
| 27 | C | 1 | Total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

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



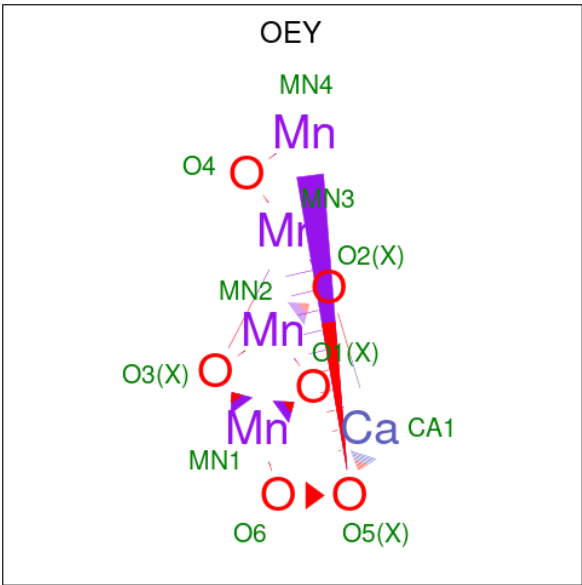
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 28 | A | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 123 | 39 | 71 | 12 | 1 | | |
| 28 | A | 1 | Total | C | H | O | | 0 | 0 |
| | | | 104 | 35 | 65 | 4 | | | |
|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

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



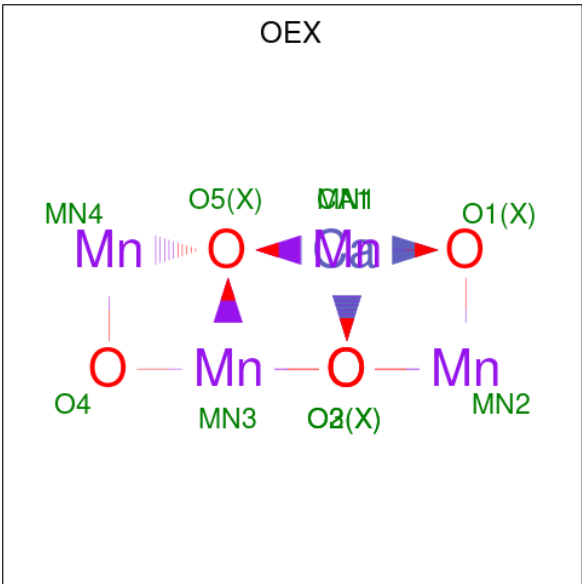
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 29 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 162 | 51 | 96 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | H | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 119 | 39 | 75 | 5 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | h | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30 | A | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 11 | 1 | 4 | 6 | | |
| 30 | a | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 11 | 1 | 4 | 6 | | |

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



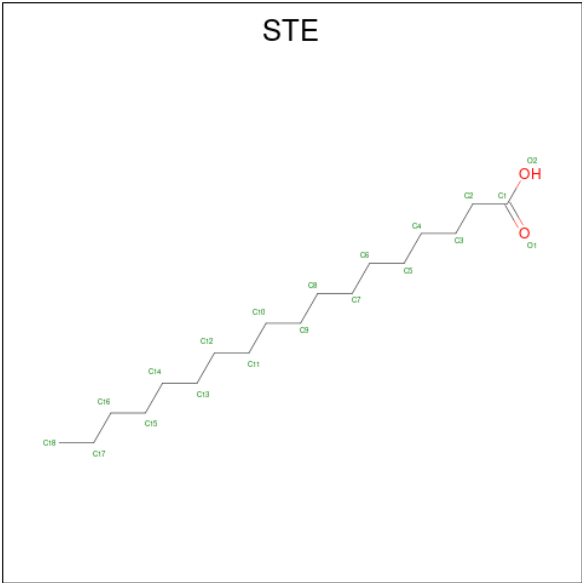
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | A | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 10 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | a | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 10 | 1 | 4 | 5 | | |

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



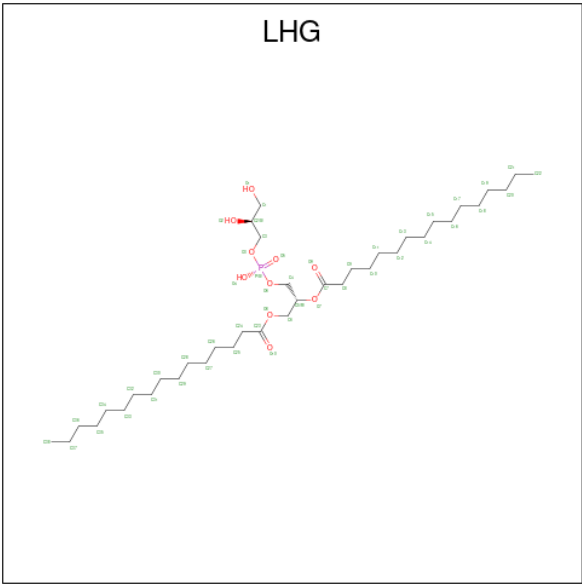
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 32 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 43 | 15 | 26 | 2 | | |
| 32 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 46 | 16 | 28 | 2 | | |
| 32 | B | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 32 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | C | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 32 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 32 | E | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |

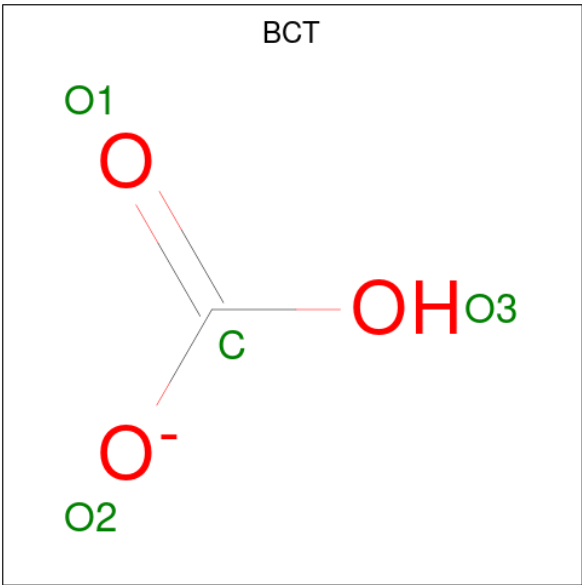
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 32 | H | 1 | Total C H 53 18 35 | 0 | 0 |
| 32 | I | 1 | Total C H 41 15 26 | 0 | 0 |
| 32 | J | 1 | Total C H O 28 10 16 2 | 0 | 0 |
| 32 | M | 1 | Total C H O 37 13 22 2 | 0 | 0 |
| 32 | M | 1 | Total C H 26 10 16 | 0 | 0 |
| 32 | T | 1 | Total C H 47 16 31 | 0 | 0 |
| 32 | T | 1 | Total C H 44 15 29 | 0 | 0 |
| 32 | a | 1 | Total C H 26 10 16 | 0 | 0 |
| 32 | a | 1 | Total C H O 28 10 16 2 | 0 | 0 |
| 32 | b | 1 | Total C H O 55 18 35 2 | 0 | 0 |
| 32 | b | 1 | Total C H O 40 14 24 2 | 0 | 0 |
| 32 | b | 1 | Total C H O 55 18 35 2 | 0 | 0 |
| 32 | b | 1 | Total C H 26 10 16 | 0 | 0 |
| 32 | c | 1 | Total C H O 55 18 35 2 | 0 | 0 |
| 32 | c | 1 | Total C H O 28 10 16 2 | 0 | 0 |
| 32 | d | 1 | Total C H O 43 15 26 2 | 0 | 0 |
| 32 | j | 1 | Total C H O 28 10 16 2 | 0 | 0 |
| 32 | l | 1 | Total C H 53 18 35 | 0 | 0 |
| 32 | m | 1 | Total C H O 28 10 16 2 | 0 | 0 |
| 32 | t | 1 | Total C H O 34 12 20 2 | 0 | 0 |
| 32 | x | 1 | Total C H O 55 18 35 2 | 0 | 0 |

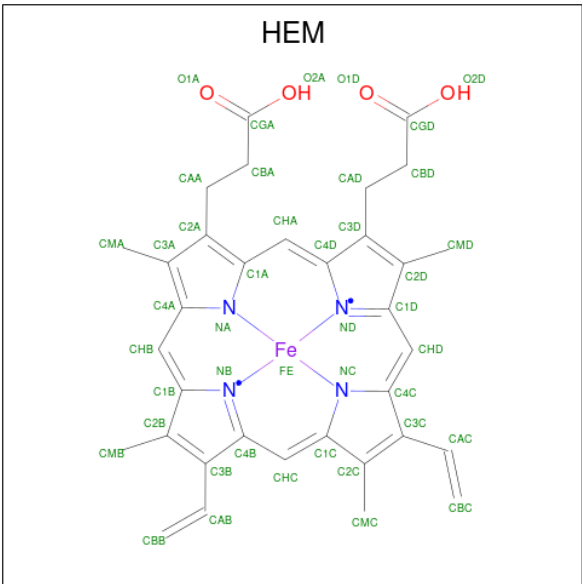
- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).





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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



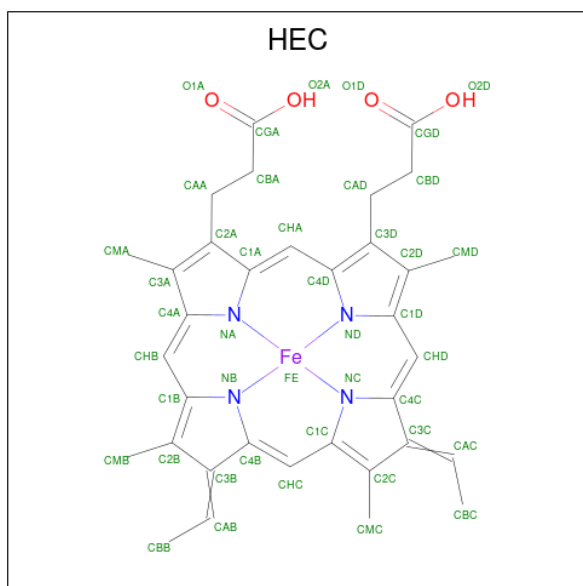
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 35 | E | 1 | Total | C | Fe | H | N | O | 0 | 0 |
| | | | 73 | 34 | 1 | 30 | 4 | 4 | | |

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

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



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

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 37 | A | 136 | Total | O | 1 | 12 |
| | | | 136 | 136 | | |
| 37 | B | 213 | Total | O | 0 | 0 |
| | | | 213 | 213 | | |
| 37 | C | 159 | Total | O | 0 | 0 |
| | | | 159 | 159 | | |
| 37 | D | 130 | Total | O | 0 | 0 |
| | | | 130 | 130 | | |
| 37 | E | 40 | Total | O | 0 | 0 |
| | | | 40 | 40 | | |
| 37 | F | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 37 | H | 42 | Total 42 | O 42 | 0 | 0 |
| 37 | I | 12 | Total 12 | O 12 | 0 | 0 |
| 37 | J | 13 | Total 13 | O 13 | 0 | 0 |
| 37 | K | 4 | Total 4 | O 4 | 0 | 0 |
| 37 | L | 9 | Total 9 | O 9 | 0 | 0 |
| 37 | M | 9 | Total 9 | O 9 | 0 | 0 |
| 37 | O | 99 | Total 99 | O 99 | 0 | 0 |
| 37 | R | 4 | Total 4 | O 4 | 0 | 0 |
| 37 | T | 9 | Total 9 | O 9 | 0 | 0 |
| 37 | U | 33 | Total 33 | O 33 | 0 | 0 |
| 37 | V | 64 | Total 64 | O 64 | 0 | 0 |
| 37 | X | 14 | Total 14 | O 14 | 0 | 0 |
| 37 | Y | 4 | Total 4 | O 4 | 0 | 0 |
| 37 | Z | 3 | Total 3 | O 3 | 0 | 0 |
| 37 | a | 118 | Total 118 | O 118 | 0 | 8 |
| 37 | b | 191 | Total 191 | O 191 | 0 | 0 |
| 37 | c | 157 | Total 157 | O 157 | 0 | 0 |
| 37 | d | 105 | Total 105 | O 105 | 0 | 0 |
| 37 | e | 17 | Total 17 | O 17 | 0 | 0 |
| 37 | f | 6 | Total 6 | O 6 | 0 | 0 |
| 37 | h | 30 | Total 30 | O 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 37 | i | 21 | Total 21 | O 21 | 0 | 0 |
| 37 | j | 6 | Total 6 | O 6 | 0 | 0 |
| 37 | k | 4 | Total 4 | O 4 | 0 | 0 |
| 37 | l | 12 | Total 12 | O 12 | 0 | 0 |
| 37 | m | 5 | Total 5 | O 5 | 0 | 0 |
| 37 | o | 93 | Total 93 | O 93 | 0 | 0 |
| 37 | r | 5 | Total 5 | O 5 | 0 | 0 |
| 37 | t | 8 | Total 8 | O 8 | 0 | 0 |
| 37 | u | 65 | Total 65 | O 65 | 0 | 0 |
| 37 | v | 59 | Total 59 | O 59 | 0 | 0 |
| 37 | x | 9 | Total 9 | O 9 | 0 | 0 |
| 37 | y | 4 | Total 4 | O 4 | 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

Chain A:  95%



- Molecule 1: Photosystem II protein D1 1

Chain a:  93%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  97%



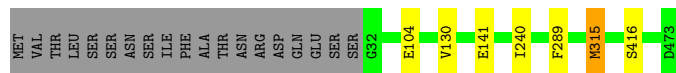
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  97%

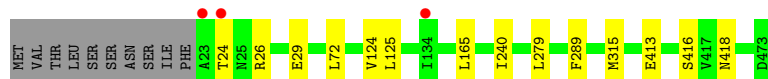
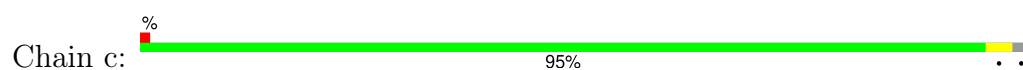


- Molecule 3: Photosystem II CP43 reaction center protein

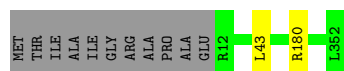
Chain C:  94%



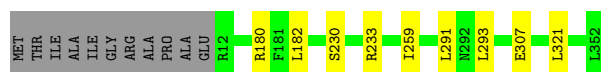
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



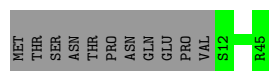
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



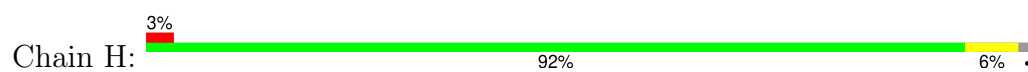
- Molecule 6: Cytochrome b559 subunit beta



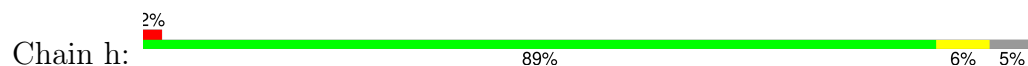
- Molecule 6: Cytochrome b559 subunit beta



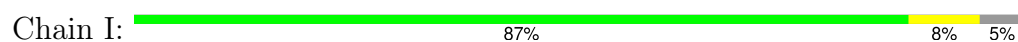
- Molecule 7: Photosystem II reaction center protein H



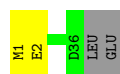
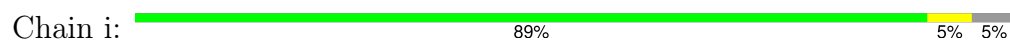
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



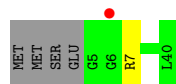
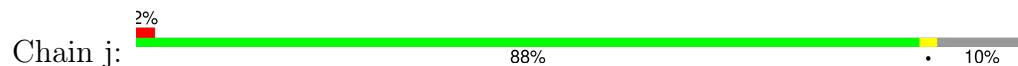
- Molecule 8: Photosystem II reaction center protein I



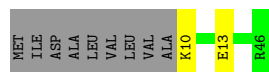
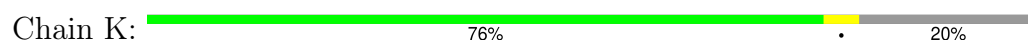
- Molecule 9: Photosystem II reaction center protein J




- Molecule 9: Photosystem II reaction center protein J

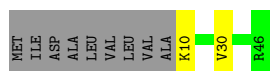


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  76% 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%

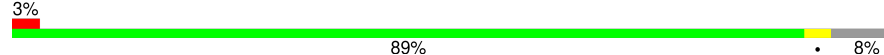


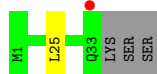
- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 8% 3%




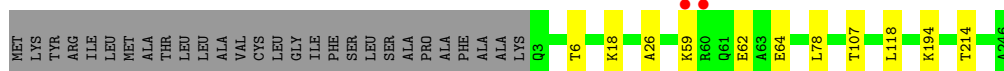
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%



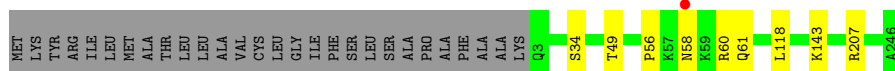
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 10% 4%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  86% 10% 4%



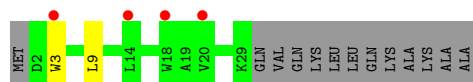
- Molecule 14: Photosystem II protein Y

Chain R:  61% 7% 32%




- Molecule 14: Photosystem II protein Y

Chain r:  10% 63% 5% 32%



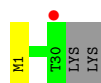
- Molecule 15: Photosystem II reaction center protein T

Chain T:  88% 6% 6%



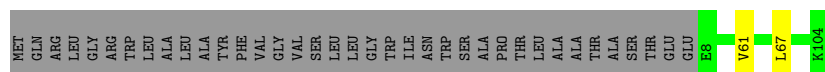
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 91% 6%



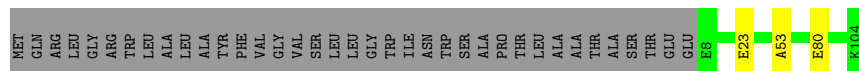
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  71% 28%




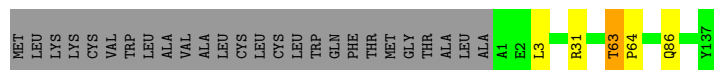
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  70% 28%




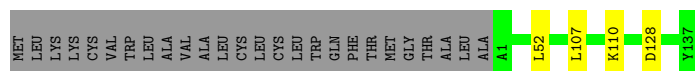
- Molecule 17: Cytochrome c-550

Chain V:  81% 16%



- Molecule 17: Cytochrome c-550

Chain v:  82% 16%




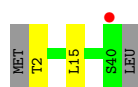
- Molecule 18: Photosystem II reaction center X protein

Chain X:  93% 7%



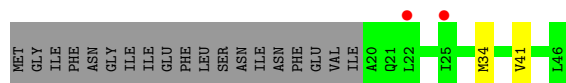
- Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5% 2%



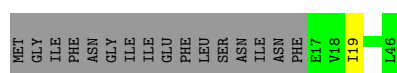
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  54% 41% 4%




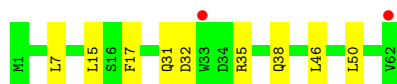
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  63% 35%

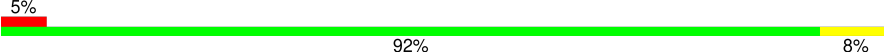


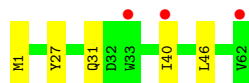
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  85% 15% 3%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  92% 8% 5%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 33.65 – 2.09 33.65 – 2.09 | Depositor EDS |
| % Data completeness (in resolution range) | 99.3 (33.65-2.09) 85.3 (33.65-2.09) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.51 (at 2.08Å) | Xtriage |
| Refinement program | PHENIX 1.19.2_4158 | Depositor |
| R, R_{free} | 0.181 , 0.239 0.181 , 0.238 | Depositor DCC |
| R_{free} test set | 4165 reflections (0.89%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 28.1 | Xtriage |
| Anisotropy | 0.219 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 58.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 105937 | wwPDB-VP |
| Average B, all atoms (Å ²) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.61 | 0/3227 | 0.66 | 1/4397 (0.0%) |
| 1 | a | 0.59 | 0/3224 | 0.65 | 0/4393 |
| 2 | B | 0.63 | 0/4161 | 0.68 | 1/5669 (0.0%) |
| 2 | b | 0.60 | 0/4118 | 0.66 | 2/5611 (0.0%) |
| 3 | C | 0.60 | 0/3647 | 0.65 | 1/4965 (0.0%) |
| 3 | c | 0.56 | 0/3719 | 0.65 | 0/5061 |
| 4 | D | 0.65 | 0/2825 | 0.66 | 0/3847 |
| 4 | d | 0.60 | 0/2834 | 0.68 | 0/3859 |
| 5 | E | 0.58 | 0/688 | 0.62 | 0/940 |
| 5 | e | 0.53 | 0/683 | 0.63 | 0/932 |
| 6 | F | 0.56 | 0/284 | 0.58 | 0/387 |
| 6 | f | 0.53 | 0/284 | 0.66 | 0/387 |
| 7 | H | 0.69 | 1/523 (0.2%) | 0.70 | 0/713 |
| 7 | h | 0.66 | 0/511 | 0.74 | 0/697 |
| 8 | I | 0.62 | 0/293 | 0.67 | 0/396 |
| 8 | i | 0.78 | 0/293 | 0.71 | 0/396 |
| 9 | J | 0.60 | 0/263 | 0.67 | 0/356 |
| 9 | j | 0.57 | 0/263 | 0.68 | 0/356 |
| 10 | K | 0.57 | 0/303 | 0.64 | 0/416 |
| 10 | k | 0.54 | 0/303 | 0.65 | 0/416 |
| 11 | L | 0.72 | 0/311 | 0.73 | 0/422 |
| 11 | l | 0.71 | 0/303 | 0.76 | 0/412 |
| 12 | M | 0.68 | 0/249 | 0.69 | 0/341 |
| 12 | m | 0.80 | 0/244 | 0.70 | 0/334 |
| 13 | O | 0.67 | 0/1904 | 0.77 | 0/2585 |
| 13 | o | 0.67 | 0/1905 | 0.75 | 0/2583 |
| 14 | R | 0.45 | 0/227 | 0.59 | 0/313 |
| 14 | r | 0.42 | 0/227 | 0.60 | 0/313 |
| 15 | T | 0.78 | 0/257 | 0.68 | 0/349 |
| 15 | t | 0.76 | 0/255 | 0.71 | 0/346 |
| 16 | U | 0.62 | 0/785 | 0.71 | 0/1064 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | u | 0.68 | 0/785 | 0.74 | 0/1064 |
| 17 | V | 0.63 | 0/1085 | 0.75 | 1/1473 (0.1%) |
| 17 | v | 0.60 | 0/1085 | 0.68 | 0/1473 |
| 18 | X | 0.56 | 0/284 | 0.64 | 0/384 |
| 18 | x | 0.46 | 0/289 | 0.58 | 0/391 |
| 19 | Y | 0.46 | 0/197 | 0.63 | 0/264 |
| 19 | y | 0.41 | 0/219 | 0.57 | 0/294 |
| 20 | Z | 0.51 | 0/490 | 0.61 | 0/669 |
| 20 | z | 0.45 | 0/488 | 0.53 | 0/666 |
| All | All | 0.61 | 1/44035 (0.0%) | 0.67 | 6/59934 (0.0%) |

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

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

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7 | H | 41 | PHE | CB-CG | -5.10 | 1.42 | 1.51 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | b | 98 | LEU | CA-CB-CG | 5.97 | 129.04 | 115.30 |
| 17 | V | 63 | THR | C-N-CD | -5.92 | 107.59 | 120.60 |
| 2 | B | 15 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | A | 131 | TRP | CA-CB-CG | -5.18 | 103.86 | 113.70 |
| 2 | b | 334 | ASP | CB-CG-OD1 | 5.09 | 122.89 | 118.30 |
| 3 | C | 315 | MET | CG-SD-CE | -5.02 | 92.17 | 100.20 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | A | 397/344 (115%) | 390 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | a | 397/344 (115%) | 388 (98%) | 8 (2%) | 1 (0%) | 37 | 37 |
| 2 | B | 508/510 (100%) | 500 (98%) | 8 (2%) | 0 | 100 | 100 |
| 2 | b | 503/510 (99%) | 492 (98%) | 11 (2%) | 0 | 100 | 100 |
| 3 | C | 454/461 (98%) | 440 (97%) | 13 (3%) | 1 (0%) | 44 | 45 |
| 3 | c | 463/461 (100%) | 448 (97%) | 14 (3%) | 1 (0%) | 44 | 45 |
| 4 | D | 340/352 (97%) | 331 (97%) | 9 (3%) | 0 | 100 | 100 |
| 4 | d | 341/352 (97%) | 332 (97%) | 9 (3%) | 0 | 100 | 100 |
| 5 | E | 81/84 (96%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 5 | e | 80/84 (95%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 6 | F | 32/45 (71%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 32/45 (71%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 7 | H | 63/66 (96%) | 59 (94%) | 3 (5%) | 1 (2%) | 8 | 4 |
| 7 | h | 61/66 (92%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 8 | I | 34/38 (90%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | i | 34/38 (90%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | J | 34/40 (85%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | j | 34/40 (85%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/46 (76%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 10 | k | 35/46 (76%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |

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Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 11 | l | 34/37 (92%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 31/36 (86%) | 31 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 30/36 (83%) | 28 (93%) | 2 (7%) | 0 | 100 | 100 |
| 13 | O | 243/272 (89%) | 227 (93%) | 13 (5%) | 3 (1%) | 11 | 7 |
| 13 | o | 242/272 (89%) | 231 (96%) | 8 (3%) | 3 (1%) | 11 | 7 |
| 14 | R | 26/41 (63%) | 26 (100%) | 0 | 0 | 100 | 100 |
| 14 | r | 26/41 (63%) | 26 (100%) | 0 | 0 | 100 | 100 |
| 15 | T | 28/32 (88%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 15 | t | 28/32 (88%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 16 | U | 95/134 (71%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 16 | u | 95/134 (71%) | 90 (95%) | 4 (4%) | 1 (1%) | 12 | 8 |
| 17 | V | 135/163 (83%) | 129 (96%) | 5 (4%) | 1 (1%) | 19 | 16 |
| 17 | v | 135/163 (83%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 18 | X | 36/41 (88%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 18 | x | 37/41 (90%) | 37 (100%) | 0 | 0 | 100 | 100 |
| 19 | Y | 25/46 (54%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 19 | y | 28/46 (61%) | 26 (93%) | 2 (7%) | 0 | 100 | 100 |
| 20 | Z | 60/62 (97%) | 57 (95%) | 3 (5%) | 0 | 100 | 100 |
| 20 | z | 60/62 (97%) | 57 (95%) | 3 (5%) | 0 | 100 | 100 |
| All | All | 5387/5700 (94%) | 5225 (97%) | 150 (3%) | 12 (0%) | 44 | 45 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 416 | SER |
| 13 | O | 59 | LYS |
| 17 | V | 64 | PRO |
| 3 | c | 416 | SER |
| 13 | O | 62 | GLU |
| 16 | u | 53 | ALA |
| 13 | o | 61 | GLN |
| 13 | O | 26 | ALA |
| 13 | o | 58 | ASN |
| 7 | H | 12 | ARG |
| 1 | a | 259 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | o | 56 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1 | A | 324/280 (116%) | 319 (98%) | 5 (2%) | 60 | 67 |
| 1 | a | 323/280 (115%) | 310 (96%) | 13 (4%) | 27 | 28 |
| 2 | B | 408/407 (100%) | 400 (98%) | 8 (2%) | 50 | 57 |
| 2 | b | 402/407 (99%) | 391 (97%) | 11 (3%) | 40 | 44 |
| 3 | C | 356/362 (98%) | 350 (98%) | 6 (2%) | 56 | 63 |
| 3 | c | 364/362 (101%) | 350 (96%) | 14 (4%) | 28 | 30 |
| 4 | D | 277/283 (98%) | 275 (99%) | 2 (1%) | 81 | 87 |
| 4 | d | 278/283 (98%) | 269 (97%) | 9 (3%) | 34 | 37 |
| 5 | E | 72/73 (99%) | 69 (96%) | 3 (4%) | 25 | 26 |
| 5 | e | 71/73 (97%) | 69 (97%) | 2 (3%) | 38 | 43 |
| 6 | F | 28/39 (72%) | 28 (100%) | 0 | 100 | 100 |
| 6 | f | 28/39 (72%) | 24 (86%) | 4 (14%) | 2 | 1 |
| 7 | H | 54/55 (98%) | 52 (96%) | 2 (4%) | 29 | 31 |
| 7 | h | 53/55 (96%) | 49 (92%) | 4 (8%) | 11 | 9 |
| 8 | I | 32/34 (94%) | 30 (94%) | 2 (6%) | 15 | 13 |
| 8 | i | 32/34 (94%) | 31 (97%) | 1 (3%) | 35 | 39 |
| 9 | J | 24/28 (86%) | 24 (100%) | 0 | 100 | 100 |
| 9 | j | 24/28 (86%) | 23 (96%) | 1 (4%) | 25 | 26 |
| 10 | K | 30/37 (81%) | 28 (93%) | 2 (7%) | 13 | 11 |
| 10 | k | 30/37 (81%) | 28 (93%) | 2 (7%) | 13 | 11 |
| 11 | L | 35/35 (100%) | 33 (94%) | 2 (6%) | 17 | 15 |
| 11 | l | 34/35 (97%) | 31 (91%) | 3 (9%) | 8 | 5 |
| 12 | M | 28/32 (88%) | 27 (96%) | 1 (4%) | 30 | 32 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 12 | m | 28/32 (88%) | 25 (89%) | 3 (11%) | 5 | 3 |
| 13 | O | 206/228 (90%) | 198 (96%) | 8 (4%) | 27 | 29 |
| 13 | o | 207/228 (91%) | 201 (97%) | 6 (3%) | 37 | 41 |
| 14 | R | 22/33 (67%) | 19 (86%) | 3 (14%) | 3 | 1 |
| 14 | r | 22/33 (67%) | 20 (91%) | 2 (9%) | 7 | 5 |
| 15 | T | 26/28 (93%) | 25 (96%) | 1 (4%) | 28 | 30 |
| 15 | t | 25/28 (89%) | 25 (100%) | 0 | 100 | 100 |
| 16 | U | 84/112 (75%) | 82 (98%) | 2 (2%) | 44 | 49 |
| 16 | u | 84/112 (75%) | 82 (98%) | 2 (2%) | 44 | 49 |
| 17 | V | 117/138 (85%) | 114 (97%) | 3 (3%) | 41 | 46 |
| 17 | v | 117/138 (85%) | 113 (97%) | 4 (3%) | 32 | 35 |
| 18 | X | 31/34 (91%) | 31 (100%) | 0 | 100 | 100 |
| 18 | x | 31/34 (91%) | 29 (94%) | 2 (6%) | 14 | 12 |
| 19 | Y | 19/37 (51%) | 17 (90%) | 2 (10%) | 5 | 3 |
| 19 | y | 22/37 (60%) | 21 (96%) | 1 (4%) | 23 | 24 |
| 20 | Z | 52/52 (100%) | 43 (83%) | 9 (17%) | 1 | 1 |
| 20 | z | 51/52 (98%) | 46 (90%) | 5 (10%) | 6 | 4 |
| All | All | 4451/4654 (96%) | 4301 (97%) | 150 (3%) | 32 | 35 |

All (150) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 12 | ASN |
| 1 | A | 16 | ARG |
| 1 | A | 134 | SER |
| 1 | A | 205 | VAL |
| 1 | A | 229 | GLU |
| 2 | B | 127 | ARG |
| 2 | B | 240 | SER |
| 2 | B | 246 | PHE |
| 2 | B | 282 | GLN |
| 2 | B | 362 | PHE |
| 2 | B | 371 | THR |
| 2 | B | 472 | ARG |
| 2 | B | 476 | ARG |
| 3 | C | 104 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 3 | C | 130 | VAL |
| 3 | C | 141 | GLU |
| 3 | C | 240 | ILE |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 4 | D | 43 | LEU |
| 4 | D | 180 | ARG |
| 5 | E | 22[A] | ILE |
| 5 | E | 22[B] | ILE |
| 5 | E | 81 | GLU |
| 7 | H | 49 | TYR |
| 7 | H | 56 | ASP |
| 8 | I | 4 | LEU |
| 8 | I | 6 | ILE |
| 10 | K | 10 | LYS |
| 10 | K | 13 | GLU |
| 11 | L | 9 | PRO |
| 11 | L | 10 | VAL |
| 12 | M | 25 | LEU |
| 13 | O | 6 | THR |
| 13 | O | 18 | LYS |
| 13 | O | 64 | GLU |
| 13 | O | 78 | LEU |
| 13 | O | 107 | THR |
| 13 | O | 118 | LEU |
| 13 | O | 194 | LYS |
| 13 | O | 214 | THR |
| 14 | R | 13 | LEU |
| 14 | R | 21 | ARG |
| 14 | R | 22 | ASN |
| 15 | T | 25 | GLU |
| 16 | U | 61 | VAL |
| 16 | U | 67 | LEU |
| 17 | V | 3 | LEU |
| 17 | V | 31 | ARG |
| 17 | V | 86 | GLN |
| 19 | Y | 34 | MET |
| 19 | Y | 41 | VAL |
| 20 | Z | 7 | LEU |
| 20 | Z | 15 | LEU |
| 20 | Z | 17 | PHE |
| 20 | Z | 31 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 20 | Z | 32 | ASP |
| 20 | Z | 35 | ARG |
| 20 | Z | 38 | GLN |
| 20 | Z | 46 | LEU |
| 20 | Z | 50 | LEU |
| 1 | a | 16 | ARG |
| 1 | a | 28 | LEU |
| 1 | a | 42 | LEU |
| 1 | a | 121 | LEU |
| 1 | a | 159[A] | LEU |
| 1 | a | 159[B] | LEU |
| 1 | a | 200 | LEU |
| 1 | a | 223 | LEU |
| 1 | a | 229 | GLU |
| 1 | a | 238 | LYS |
| 1 | a | 243 | GLU |
| 1 | a | 245 | THR |
| 1 | a | 288 | LEU |
| 2 | b | 83 | GLU |
| 2 | b | 98 | LEU |
| 2 | b | 149 | LEU |
| 2 | b | 236 | THR |
| 2 | b | 246 | PHE |
| 2 | b | 357 | ARG |
| 2 | b | 362 | PHE |
| 2 | b | 444 | ARG |
| 2 | b | 492 | GLU |
| 2 | b | 505 | ARG |
| 2 | b | 506 | ARG |
| 3 | c | 24 | THR |
| 3 | c | 26 | ARG |
| 3 | c | 29 | GLU |
| 3 | c | 72 | LEU |
| 3 | c | 124 | VAL |
| 3 | c | 125 | LEU |
| 3 | c | 165 | LEU |
| 3 | c | 240 | ILE |
| 3 | c | 279 | LEU |
| 3 | c | 289 | PHE |
| 3 | c | 315 | MET |
| 3 | c | 413[A] | GLU |
| 3 | c | 413[B] | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | c | 418 | ASN |
| 4 | d | 180 | ARG |
| 4 | d | 182 | LEU |
| 4 | d | 230 | SER |
| 4 | d | 233 | ARG |
| 4 | d | 259 | ILE |
| 4 | d | 291 | LEU |
| 4 | d | 293 | LEU |
| 4 | d | 307 | GLU |
| 4 | d | 321 | LEU |
| 5 | e | 4 | THR |
| 5 | e | 66 | VAL |
| 6 | f | 15 | ILE |
| 6 | f | 23 | VAL |
| 6 | f | 25 | THR |
| 6 | f | 28 | VAL |
| 7 | h | 7 | LEU |
| 7 | h | 27 | THR |
| 7 | h | 38 | PHE |
| 7 | h | 49 | TYR |
| 8 | i | 2 | GLU |
| 9 | j | 7 | ARG |
| 10 | k | 10 | LYS |
| 10 | k | 30 | VAL |
| 11 | l | 7 | ARG |
| 11 | l | 21 | LEU |
| 11 | l | 30 | LEU |
| 12 | m | 2 | GLU |
| 12 | m | 13 | LEU |
| 12 | m | 16 | LEU |
| 13 | o | 34 | SER |
| 13 | o | 49 | THR |
| 13 | o | 60 | ARG |
| 13 | o | 118 | LEU |
| 13 | o | 143 | LYS |
| 13 | o | 207 | ARG |
| 14 | r | 3 | TRP |
| 14 | r | 9 | LEU |
| 16 | u | 23 | GLU |
| 16 | u | 80 | GLU |
| 17 | v | 52 | LEU |
| 17 | v | 107 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | v | 110 | LYS |
| 17 | v | 128 | ASP |
| 18 | x | 2 | THR |
| 18 | x | 15 | LEU |
| 19 | y | 19 | ILE |
| 20 | z | 1 | MET |
| 20 | z | 27 | TYR |
| 20 | z | 31 | GLN |
| 20 | z | 40 | ILE |
| 20 | z | 46 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 61 | HIS |
| 7 | H | 59 | ASN |
| 13 | O | 36 | GLN |
| 13 | O | 88 | ASN |
| 17 | V | 86 | GLN |
| 20 | Z | 38 | GLN |
| 2 | b | 179 | GLN |
| 2 | b | 490 | GLN |
| 5 | e | 74 | GLN |
| 13 | o | 61 | GLN |
| 20 | z | 31 | 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 | 0.91 | 0 | 8,9,11 | 0.99 | 0 |
| 8 | FME | I | 1 | 8 | 8,9,10 | 0.97 | 1 (12%) | 8,9,11 | 1.34 | 1 (12%) |
| 12 | FME | m | 1 | 12 | 8,9,10 | 1.07 | 1 (12%) | 8,9,11 | 1.14 | 0 |
| 15 | FME | t | 1 | 15 | 8,9,10 | 1.69 | 1 (12%) | 8,9,11 | 0.95 | 0 |
| 8 | FME | i | 1 | 8 | 8,9,10 | 1.01 | 1 (12%) | 8,9,11 | 1.36 | 1 (12%) |
| 15 | FME | T | 1 | 15 | 8,9,10 | 1.13 | 1 (12%) | 8,9,11 | 1.07 | 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 | - | 1/7/9/11 | - |
| 8 | FME | I | 1 | 8 | - | 1/7/9/11 | - |
| 12 | FME | m | 1 | 12 | - | 0/7/9/11 | - |
| 15 | FME | t | 1 | 15 | - | 1/7/9/11 | - |
| 8 | FME | i | 1 | 8 | - | 4/7/9/11 | - |
| 15 | FME | T | 1 | 15 | - | 1/7/9/11 | - |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15 | t | 1 | FME | CA-N | -4.26 | 1.40 | 1.46 |
| 12 | m | 1 | FME | CA-N | -2.33 | 1.43 | 1.46 |
| 15 | T | 1 | FME | CA-N | -2.28 | 1.43 | 1.46 |
| 8 | I | 1 | FME | CA-N | -2.10 | 1.43 | 1.46 |
| 8 | i | 1 | FME | CA-N | -2.08 | 1.43 | 1.46 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | i | 1 | FME | C-CA-N | 2.57 | 114.46 | 109.50 |
| 8 | I | 1 | FME | CA-N-CN | -2.47 | 119.02 | 122.82 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 8 | i | 1 | FME | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 8 | i | 1 | FME | C-CA-CB-CG |
| 15 | T | 1 | FME | CB-CG-SD-CE |
| 15 | t | 1 | FME | CB-CG-SD-CE |
| 8 | i | 1 | FME | CA-CB-CG-SD |
| 8 | i | 1 | FME | CB-CG-SD-CE |
| 8 | I | 1 | FME | C-CA-CB-CG |
| 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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 |
| 22 | CLA | b | 612 | - | 63,73,73 | 1.38 | 7 (11%) | 74,113,113 | 1.56 | 11 (14%) |
| 29 | DGD | c | 517 | - | 63,63,67 | 1.10 | 6 (9%) | 77,77,81 | 1.35 | 7 (9%) |
| 32 | STE | H | 103 | - | 17,17,19 | 0.59 | 0 | 16,16,19 | 0.59 | 0 |
| 27 | LMG | c | 523 | - | 49,49,55 | 1.04 | 3 (6%) | 57,57,63 | 1.28 | 7 (12%) |
| 22 | CLA | b | 610 | 37 | 63,73,73 | 1.34 | 9 (14%) | 74,113,113 | 1.45 | 14 (18%) |
| 29 | DGD | A | 414 | - | 67,67,67 | 1.39 | 7 (10%) | 81,81,81 | 1.48 | 11 (13%) |
| 29 | DGD | a | 412 | - | 43,43,67 | 1.15 | 3 (6%) | 45,45,81 | 1.47 | 7 (15%) |
| 24 | BCR | b | 618 | - | 41,41,41 | 1.37 | 4 (9%) | 56,56,56 | 1.22 | 5 (8%) |
| 32 | STE | d | 413 | - | 16,16,19 | 0.76 | 0 | 16,16,19 | 1.13 | 1 (6%) |
| 32 | STE | D | 411 | - | 19,19,19 | 0.67 | 1 (5%) | 19,19,19 | 1.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | SQD | a | 410 | - | 52,54,54 | 0.94 | 4 (7%) | 62,65,65 | 2.02 | 13 (20%) |
| 33 | LHG | l | 101 | - | 48,48,48 | 0.87 | 1 (2%) | 51,54,54 | 1.16 | 5 (9%) |
| 33 | LHG | B | 622 | - | 48,48,48 | 1.05 | 4 (8%) | 51,54,54 | 1.42 | 6 (11%) |
| 22 | CLA | b | 615 | - | 63,73,73 | 1.51 | 11 (17%) | 74,113,113 | 1.45 | 10 (13%) |
| 24 | BCR | B | 619 | - | 41,41,41 | 1.13 | 3 (7%) | 56,56,56 | 1.39 | 4 (7%) |
| 23 | PHO | d | 401 | - | 50,69,69 | 1.05 | 4 (8%) | 48,99,99 | 1.26 | 5 (10%) |
| 32 | STE | l | 102 | - | 17,17,19 | 0.47 | 0 | 16,16,19 | 0.80 | 0 |
| 22 | CLA | B | 608 | - | 63,73,73 | 1.37 | 7 (11%) | 74,113,113 | 1.68 | 10 (13%) |
| 31 | OEX | a | 416[A] | 3,37,1 | 0,15,15 | - | - | - | - | - |
| 22 | CLA | A | 402 | - | 63,73,73 | 1.62 | 7 (11%) | 74,113,113 | 1.51 | 10 (13%) |
| 22 | CLA | b | 616 | - | 58,68,73 | 1.35 | 6 (10%) | 68,107,113 | 1.74 | 10 (14%) |
| 24 | BCR | c | 516 | - | 41,41,41 | 1.13 | 2 (4%) | 56,56,56 | 1.20 | 7 (12%) |
| 24 | BCR | K | 101 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.39 | 9 (16%) |
| 22 | CLA | b | 607 | 37 | 63,73,73 | 1.58 | 9 (14%) | 74,113,113 | 1.31 | 9 (12%) |
| 28 | SQD | F | 101 | - | 34,36,54 | 1.01 | 3 (8%) | 42,45,65 | 1.84 | 9 (21%) |
| 24 | BCR | B | 618 | - | 41,41,41 | 1.27 | 4 (9%) | 56,56,56 | 1.19 | 9 (16%) |
| 22 | CLA | B | 612 | - | 63,73,73 | 1.37 | 7 (11%) | 74,113,113 | 1.51 | 9 (12%) |
| 22 | CLA | c | 508 | - | 62,72,73 | 1.50 | 8 (12%) | 72,111,113 | 1.58 | 12 (16%) |
| 22 | CLA | c | 511 | 3 | 63,73,73 | 1.78 | 6 (9%) | 74,113,113 | 1.53 | 7 (9%) |
| 24 | BCR | c | 514 | - | 41,41,41 | 1.24 | 2 (4%) | 56,56,56 | 1.32 | 8 (14%) |
| 32 | STE | I | 101 | - | 14,14,19 | 0.64 | 0 | 13,13,19 | 0.40 | 0 |
| 32 | STE | b | 623 | - | 15,15,19 | 0.94 | 1 (6%) | 15,15,19 | 0.94 | 1 (6%) |
| 31 | OEX | A | 416[A] | 3,37,1 | 0,15,15 | - | - | - | - | - |
| 33 | LHG | e | 101 | - | 41,41,48 | 0.88 | 1 (2%) | 44,47,54 | 1.29 | 4 (9%) |
| 27 | LMG | d | 412 | - | 44,44,55 | 1.23 | 6 (13%) | 52,52,63 | 1.39 | 8 (15%) |
| 33 | LHG | D | 409 | - | 46,46,48 | 1.13 | 3 (6%) | 49,52,54 | 1.14 | 3 (6%) |
| 32 | STE | T | 103 | - | 14,14,19 | 0.44 | 0 | 13,13,19 | 0.89 | 0 |
| 22 | CLA | A | 410 | 37 | 63,73,73 | 1.43 | 6 (9%) | 74,113,113 | 1.34 | 7 (9%) |
| 22 | CLA | c | 502 | - | 63,73,73 | 1.30 | 8 (12%) | 74,113,113 | 1.46 | 11 (14%) |
| 22 | CLA | c | 510 | - | 63,73,73 | 1.51 | 11 (17%) | 74,113,113 | 1.53 | 8 (10%) |
| 24 | BCR | C | 514 | - | 41,41,41 | 1.25 | 4 (9%) | 56,56,56 | 1.30 | 6 (10%) |
| 33 | LHG | L | 102 | - | 48,48,48 | 1.02 | 2 (4%) | 51,54,54 | 1.25 | 2 (3%) |
| 22 | CLA | A | 405 | - | 52,62,73 | 1.63 | 9 (17%) | 60,99,113 | 1.68 | 11 (18%) |
| 28 | SQD | f | 102 | - | 39,41,54 | 1.18 | 4 (10%) | 49,52,65 | 1.76 | 11 (22%) |
| 22 | CLA | B | 605 | - | 63,73,73 | 1.52 | 10 (15%) | 74,113,113 | 1.35 | 4 (5%) |
| 32 | STE | b | 625 | - | 9,9,19 | 0.64 | 0 | 8,8,19 | 0.48 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 27 | LMG | c | 520 | - | 37,37,55 | 1.25 | 5 (13%) | 45,45,63 | 1.31 | 6 (13%) |
| 29 | DGD | C | 516 | - | 63,63,67 | 1.36 | 11 (17%) | 77,77,81 | 1.40 | 10 (12%) |
| 22 | CLA | d | 403 | - | 63,73,73 | 1.38 | 7 (11%) | 74,113,113 | 1.30 | 6 (8%) |
| 24 | BCR | C | 515 | - | 41,41,41 | 1.21 | 5 (12%) | 56,56,56 | 1.13 | 4 (7%) |
| 24 | BCR | b | 619 | - | 41,41,41 | 1.21 | 2 (4%) | 56,56,56 | 1.42 | 11 (19%) |
| 22 | CLA | d | 405 | - | 63,73,73 | 1.23 | 9 (14%) | 74,113,113 | 1.34 | 5 (6%) |
| 22 | CLA | D | 403 | - | 63,73,73 | 1.61 | 8 (12%) | 74,113,113 | 1.38 | 10 (13%) |
| 22 | CLA | b | 604 | - | 63,73,73 | 1.18 | 7 (11%) | 74,113,113 | 1.65 | 12 (16%) |
| 27 | LMG | d | 411 | - | 21,21,55 | 0.83 | 0 | 20,20,63 | 1.21 | 1 (5%) |
| 22 | CLA | C | 508 | - | 63,73,73 | 1.54 | 9 (14%) | 74,113,113 | 1.51 | 7 (9%) |
| 24 | BCR | T | 101 | - | 41,41,41 | 1.34 | 4 (9%) | 56,56,56 | 1.27 | 6 (10%) |
| 22 | CLA | B | 603 | - | 63,73,73 | 1.50 | 12 (19%) | 74,113,113 | 1.50 | 15 (20%) |
| 33 | LHG | d | 410 | - | 38,38,48 | 0.89 | 3 (7%) | 41,44,54 | 1.15 | 3 (7%) |
| 24 | BCR | k | 101 | - | 41,41,41 | 1.12 | 5 (12%) | 56,56,56 | 1.13 | 3 (5%) |
| 27 | LMG | B | 621 | - | 26,26,55 | 0.96 | 1 (3%) | 26,26,63 | 1.14 | 1 (3%) |
| 22 | CLA | C | 501 | - | 63,73,73 | 1.36 | 10 (15%) | 74,113,113 | 1.58 | 8 (10%) |
| 22 | CLA | B | 614 | - | 63,73,73 | 1.60 | 8 (12%) | 74,113,113 | 1.29 | 10 (13%) |
| 26 | PL9 | D | 406 | - | 55,55,55 | 1.51 | 5 (9%) | 68,69,69 | 1.60 | 15 (22%) |
| 27 | LMG | b | 620 | - | 51,51,55 | 1.14 | 6 (11%) | 59,59,63 | 1.51 | 11 (18%) |
| 22 | CLA | a | 403 | 37 | 63,73,73 | 1.49 | 6 (9%) | 74,113,113 | 1.61 | 12 (16%) |
| 24 | BCR | a | 405 | - | 41,41,41 | 1.17 | 4 (9%) | 56,56,56 | 1.43 | 8 (14%) |
| 32 | STE | B | 626 | - | 15,15,19 | 0.49 | 0 | 14,14,19 | 0.73 | 0 |
| 22 | CLA | a | 402 | - | 63,73,73 | 1.63 | 8 (12%) | 74,113,113 | 1.48 | 11 (14%) |
| 22 | CLA | c | 512 | - | 63,73,73 | 1.36 | 10 (15%) | 74,113,113 | 1.49 | 8 (10%) |
| 24 | BCR | Y | 101 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.21 | 4 (7%) |
| 32 | STE | t | 102 | - | 13,13,19 | 0.71 | 0 | 13,13,19 | 1.15 | 1 (7%) |
| 32 | STE | C | 520 | - | 11,11,19 | 0.74 | 0 | 11,11,19 | 1.54 | 2 (18%) |
| 22 | CLA | A | 403 | 37 | 63,73,73 | 1.48 | 9 (14%) | 74,113,113 | 1.28 | 11 (14%) |
| 22 | CLA | C | 505 | - | 63,73,73 | 1.58 | 6 (9%) | 74,113,113 | 1.38 | 6 (8%) |
| 27 | LMG | A | 411 | - | 48,48,55 | 0.99 | 3 (6%) | 56,56,63 | 1.32 | 7 (12%) |
| 28 | SQD | A | 412 | - | 50,52,54 | 1.02 | 4 (8%) | 60,63,65 | 2.04 | 12 (20%) |
| 30 | OEY | A | 415[B] | 3,37,1 | 0,16,16 | - | - | - | - | - |
| 32 | STE | m | 101 | - | 11,11,19 | 0.70 | 0 | 11,11,19 | 1.69 | 2 (18%) |
| 22 | CLA | b | 605 | - | 63,73,73 | 1.32 | 8 (12%) | 74,113,113 | 1.50 | 16 (21%) |
| 22 | CLA | c | 513 | - | 63,73,73 | 1.39 | 8 (12%) | 74,113,113 | 1.44 | 11 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 33 | LHG | d | 408 | - | 48,48,48 | 1.06 | 4 (8%) | 51,54,54 | 1.47 | 8 (15%) |
| 32 | STE | B | 625 | - | 17,17,19 | 0.65 | 0 | 17,17,19 | 0.99 | 0 |
| 27 | LMG | D | 410 | - | 31,31,55 | 1.18 | 3 (9%) | 33,33,63 | 1.11 | 2 (6%) |
| 24 | BCR | t | 101 | - | 41,41,41 | 1.17 | 4 (9%) | 56,56,56 | 1.48 | 9 (16%) |
| 22 | CLA | b | 603 | - | 63,73,73 | 1.43 | 10 (15%) | 74,113,113 | 1.51 | 9 (12%) |
| 32 | STE | j | 101 | - | 11,11,19 | 0.84 | 0 | 11,11,19 | 1.65 | 3 (27%) |
| 28 | SQD | a | 411 | - | 35,35,54 | 1.13 | 2 (5%) | 37,37,65 | 1.19 | 5 (13%) |
| 22 | CLA | C | 507 | 37 | 63,73,73 | 1.38 | 6 (9%) | 74,113,113 | 1.72 | 11 (14%) |
| 23 | PHO | D | 401 | - | 50,69,69 | 1.11 | 6 (12%) | 48,99,99 | 1.38 | 7 (14%) |
| 33 | LHG | d | 409 | - | 48,48,48 | 0.78 | 2 (4%) | 51,54,54 | 1.15 | 3 (5%) |
| 22 | CLA | C | 512 | - | 63,73,73 | 1.67 | 11 (17%) | 74,113,113 | 1.40 | 10 (13%) |
| 22 | CLA | b | 609 | - | 63,73,73 | 1.26 | 9 (14%) | 74,113,113 | 1.41 | 7 (9%) |
| 35 | HEM | f | 101 | 5,6 | 42,50,50 | 1.50 | 5 (11%) | 46,82,82 | 1.52 | 7 (15%) |
| 22 | CLA | B | 606 | - | 63,73,73 | 1.56 | 8 (12%) | 74,113,113 | 1.45 | 13 (17%) |
| 24 | BCR | B | 617 | - | 41,41,41 | 1.21 | 3 (7%) | 56,56,56 | 1.26 | 6 (10%) |
| 22 | CLA | B | 613 | - | 63,73,73 | 1.35 | 8 (12%) | 74,113,113 | 1.57 | 10 (13%) |
| 30 | OEY | a | 415[B] | 3,37,1 | 0,16,16 | - | - | - | - | - |
| 28 | SQD | B | 623 | - | 52,54,54 | 1.00 | 2 (3%) | 62,65,65 | 1.82 | 11 (17%) |
| 22 | CLA | C | 513 | - | 63,73,73 | 1.39 | 7 (11%) | 74,113,113 | 1.56 | 10 (13%) |
| 22 | CLA | C | 504 | 37 | 57,67,73 | 1.28 | 5 (8%) | 66,105,113 | 1.32 | 7 (10%) |
| 22 | CLA | B | 607 | 37 | 63,73,73 | 1.64 | 10 (15%) | 74,113,113 | 1.58 | 7 (9%) |
| 32 | STE | J | 101 | - | 11,11,19 | 0.69 | 0 | 11,11,19 | 1.39 | 1 (9%) |
| 22 | CLA | c | 507 | 37 | 63,73,73 | 1.37 | 8 (12%) | 74,113,113 | 1.23 | 8 (10%) |
| 22 | CLA | c | 506 | - | 63,73,73 | 1.40 | 10 (15%) | 74,113,113 | 1.41 | 8 (10%) |
| 29 | DGD | c | 518 | - | 63,63,67 | 1.31 | 9 (14%) | 77,77,81 | 1.52 | 9 (11%) |
| 27 | LMG | D | 407 | - | 51,51,55 | 1.18 | 4 (7%) | 59,59,63 | 1.34 | 9 (15%) |
| 32 | STE | c | 521 | - | 19,19,19 | 0.79 | 1 (5%) | 19,19,19 | 0.94 | 0 |
| 24 | BCR | h | 101 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.30 | 9 (16%) |
| 34 | BCT | a | 408 | 21 | 3,3,3 | 1.10 | 0 | 2,3,3 | 3.45 | 2 (100%) |
| 33 | LHG | D | 408 | - | 48,48,48 | 1.00 | 5 (10%) | 51,54,54 | 1.29 | 5 (9%) |
| 28 | SQD | A | 413 | - | 38,38,54 | 1.04 | 3 (7%) | 40,40,65 | 1.45 | 6 (15%) |
| 32 | STE | b | 624 | - | 19,19,19 | 0.87 | 0 | 19,19,19 | 0.86 | 1 (5%) |
| 26 | PL9 | d | 407 | - | 55,55,55 | 1.44 | 6 (10%) | 68,69,69 | 1.81 | 16 (23%) |
| 22 | CLA | b | 614 | - | 63,73,73 | 1.49 | 9 (14%) | 74,113,113 | 1.39 | 11 (14%) |
| 32 | STE | a | 414 | - | 11,11,19 | 0.78 | 0 | 11,11,19 | 1.13 | 1 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | BCR | H | 101 | - | 41,41,41 | 1.16 | 1 (2%) | 56,56,56 | 1.28 | 8 (14%) |
| 24 | BCR | b | 617 | - | 41,41,41 | 1.10 | 3 (7%) | 56,56,56 | 1.46 | 11 (19%) |
| 34 | BCT | D | 402 | 21 | 3,3,3 | 1.02 | 0 | 2,3,3 | 3.66 | 2 (100%) |
| 22 | CLA | C | 503 | - | 63,73,73 | 1.67 | 7 (11%) | 74,113,113 | 1.51 | 11 (14%) |
| 27 | LMG | M | 101 | - | 51,51,55 | 1.11 | 5 (9%) | 59,59,63 | 1.41 | 7 (11%) |
| 32 | STE | b | 621 | - | 19,19,19 | 0.71 | 0 | 19,19,19 | 0.90 | 0 |
| 22 | CLA | c | 504 | 37 | 58,68,73 | 1.38 | 6 (10%) | 68,107,113 | 1.50 | 5 (7%) |
| 22 | CLA | c | 503 | - | 63,73,73 | 1.48 | 9 (14%) | 74,113,113 | 1.47 | 8 (10%) |
| 35 | HEM | E | 101 | 5,6 | 42,50,50 | 1.57 | 6 (14%) | 46,82,82 | 1.33 | 6 (13%) |
| 22 | CLA | d | 404 | 37 | 63,73,73 | 1.66 | 5 (7%) | 74,113,113 | 1.59 | 10 (13%) |
| 32 | STE | M | 102 | - | 14,14,19 | 0.84 | 0 | 14,14,19 | 1.06 | 0 |
| 24 | BCR | d | 406 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.31 | 6 (10%) |
| 32 | STE | M | 103 | - | 9,9,19 | 0.53 | 0 | 8,8,19 | 0.61 | 0 |
| 33 | LHG | E | 102 | - | 48,48,48 | 0.88 | 3 (6%) | 51,54,54 | 1.20 | 3 (5%) |
| 22 | CLA | b | 601 | 37 | 63,73,73 | 1.52 | 6 (9%) | 74,113,113 | 1.61 | 8 (10%) |
| 22 | CLA | b | 606 | - | 63,73,73 | 1.43 | 7 (11%) | 74,113,113 | 1.71 | 9 (12%) |
| 22 | CLA | C | 510 | - | 63,73,73 | 1.34 | 6 (9%) | 74,113,113 | 1.36 | 9 (12%) |
| 29 | DGD | H | 102 | - | 63,63,67 | 1.40 | 9 (14%) | 77,77,81 | 1.43 | 8 (10%) |
| 22 | CLA | b | 613 | - | 63,73,73 | 1.59 | 10 (15%) | 74,113,113 | 1.56 | 12 (16%) |
| 22 | CLA | C | 502 | - | 63,73,73 | 1.33 | 7 (11%) | 74,113,113 | 1.19 | 3 (4%) |
| 27 | LMG | c | 522 | - | 48,48,55 | 1.20 | 6 (12%) | 56,56,63 | 1.37 | 8 (14%) |
| 22 | CLA | C | 506 | - | 63,73,73 | 1.50 | 8 (12%) | 74,113,113 | 1.45 | 7 (9%) |
| 22 | CLA | B | 604 | - | 63,73,73 | 1.53 | 6 (9%) | 74,113,113 | 1.81 | 13 (17%) |
| 36 | HEC | V | 201 | 17 | 32,50,50 | 2.01 | 3 (9%) | 30,82,82 | 2.68 | 7 (23%) |
| 26 | PL9 | A | 409 | - | 55,55,55 | 1.14 | 5 (9%) | 68,69,69 | 1.57 | 13 (19%) |
| 22 | CLA | C | 511 | 3 | 63,73,73 | 1.54 | 7 (11%) | 74,113,113 | 1.34 | 7 (9%) |
| 24 | BCR | D | 405 | - | 41,41,41 | 1.22 | 3 (7%) | 56,56,56 | 1.16 | 6 (10%) |
| 22 | CLA | D | 404 | - | 63,73,73 | 1.40 | 9 (14%) | 74,113,113 | 1.62 | 7 (9%) |
| 32 | STE | T | 102 | - | 15,15,19 | 0.53 | 0 | 14,14,19 | 0.70 | 0 |
| 26 | PL9 | a | 409 | - | 55,55,55 | 0.94 | 2 (3%) | 68,69,69 | 1.66 | 16 (23%) |
| 22 | CLA | B | 610 | 37 | 63,73,73 | 1.45 | 5 (7%) | 74,113,113 | 1.53 | 12 (16%) |
| 22 | CLA | B | 616 | - | 58,68,73 | 1.54 | 8 (13%) | 68,107,113 | 1.83 | 9 (13%) |
| 22 | CLA | B | 609 | - | 63,73,73 | 1.21 | 6 (9%) | 74,113,113 | 1.31 | 9 (12%) |
| 32 | STE | C | 522 | - | 11,11,19 | 0.59 | 0 | 11,11,19 | 1.65 | 3 (27%) |
| 23 | PHO | d | 402 | - | 50,69,69 | 1.05 | 4 (8%) | 48,99,99 | 1.54 | 7 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | B | 615 | - | 63,73,73 | 1.59 | 7 (11%) | 74,113,113 | 1.50 | 9 (12%) |
| 22 | CLA | a | 404 | - | 63,73,73 | 1.58 | 10 (15%) | 74,113,113 | 1.33 | 9 (12%) |
| 29 | DGD | c | 519 | - | 63,63,67 | 1.40 | 9 (14%) | 77,77,81 | 1.43 | 12 (15%) |
| 32 | STE | B | 627 | - | 11,11,19 | 1.05 | 1 (9%) | 11,11,19 | 0.71 | 0 |
| 22 | CLA | B | 611 | - | 63,73,73 | 1.33 | 6 (9%) | 74,113,113 | 1.52 | 14 (18%) |
| 36 | HEC | v | 201 | 17 | 32,50,50 | 2.12 | 5 (15%) | 30,82,82 | 2.30 | 6 (20%) |
| 22 | CLA | b | 611 | - | 63,73,73 | 1.48 | 9 (14%) | 74,113,113 | 1.48 | 8 (10%) |
| 24 | BCR | c | 515 | - | 41,41,41 | 1.26 | 3 (7%) | 56,56,56 | 1.41 | 9 (16%) |
| 32 | STE | c | 524 | - | 11,11,19 | 0.75 | 0 | 11,11,19 | 1.20 | 1 (9%) |
| 22 | CLA | c | 501 | - | 63,73,73 | 1.27 | 8 (12%) | 74,113,113 | 1.52 | 12 (16%) |
| 24 | BCR | A | 406 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.46 | 10 (17%) |
| 22 | CLA | b | 602 | - | 63,73,73 | 1.19 | 8 (12%) | 74,113,113 | 1.57 | 10 (13%) |
| 32 | STE | B | 620 | - | 16,16,19 | 0.71 | 0 | 16,16,19 | 1.05 | 1 (6%) |
| 22 | CLA | b | 608 | - | 63,73,73 | 1.44 | 6 (9%) | 74,113,113 | 1.57 | 11 (14%) |
| 29 | DGD | h | 102 | - | 63,63,67 | 1.29 | 11 (17%) | 77,77,81 | 1.54 | 13 (16%) |
| 32 | STE | E | 103 | - | 11,11,19 | 0.98 | 0 | 11,11,19 | 0.83 | 0 |
| 28 | SQD | L | 101 | - | 47,49,54 | 0.99 | 3 (6%) | 57,60,65 | 2.25 | 16 (28%) |
| 22 | CLA | B | 602 | - | 63,73,73 | 1.28 | 8 (12%) | 74,113,113 | 1.70 | 10 (13%) |
| 27 | LMG | C | 519 | - | 48,48,55 | 1.19 | 7 (14%) | 56,56,63 | 1.43 | 7 (12%) |
| 22 | CLA | C | 509 | - | 63,73,73 | 1.52 | 11 (17%) | 74,113,113 | 1.57 | 12 (16%) |
| 27 | LMG | b | 622 | - | 55,55,55 | 1.04 | 7 (12%) | 63,63,63 | 1.44 | 7 (11%) |
| 29 | DGD | C | 517 | - | 63,63,67 | 1.40 | 7 (11%) | 77,77,81 | 1.55 | 14 (18%) |
| 32 | STE | C | 521 | - | 15,15,19 | 0.57 | 0 | 14,14,19 | 0.51 | 0 |
| 22 | CLA | c | 509 | - | 63,73,73 | 1.48 | 7 (11%) | 74,113,113 | 1.78 | 10 (13%) |
| 32 | STE | x | 101 | - | 19,19,19 | 0.82 | 0 | 19,19,19 | 0.65 | 0 |
| 32 | STE | a | 413 | - | 9,9,19 | 0.69 | 0 | 8,8,19 | 0.42 | 0 |
| 32 | STE | B | 624 | - | 11,11,19 | 0.86 | 0 | 11,11,19 | 0.96 | 1 (9%) |
| 22 | CLA | B | 601 | 37 | 63,73,73 | 1.70 | 9 (14%) | 74,113,113 | 1.47 | 7 (9%) |
| 23 | PHO | A | 404 | - | 50,69,69 | 1.10 | 5 (10%) | 48,99,99 | 1.52 | 10 (20%) |
| 29 | DGD | C | 518 | - | 63,63,67 | 1.17 | 10 (15%) | 77,77,81 | 1.36 | 9 (11%) |
| 22 | CLA | c | 505 | - | 63,73,73 | 1.23 | 6 (9%) | 74,113,113 | 1.36 | 9 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | b | 612 | - | 1/1/20/20 | 6/37/115/115 | - |
| 29 | DGD | c | 517 | - | - | 27/51/91/95 | 0/2/2/2 |
| 32 | STE | H | 103 | - | - | 6/15/15/17 | - |
| 27 | LMG | c | 523 | - | - | 23/44/64/70 | 0/1/1/1 |
| 22 | CLA | b | 610 | 37 | 1/1/20/20 | 3/37/115/115 | - |
| 29 | DGD | A | 414 | - | - | 25/55/95/95 | 0/2/2/2 |
| 29 | DGD | a | 412 | - | - | 27/45/45/95 | - |
| 24 | BCR | b | 618 | - | - | 7/29/63/63 | 0/2/2/2 |
| 32 | STE | d | 413 | - | - | 11/14/14/17 | - |
| 32 | STE | D | 411 | - | - | 12/17/17/17 | - |
| 28 | SQD | a | 410 | - | - | 20/49/69/69 | 0/1/1/1 |
| 33 | LHG | l | 101 | - | - | 26/53/53/53 | - |
| 33 | LHG | B | 622 | - | - | 18/53/53/53 | - |
| 22 | CLA | b | 615 | - | 1/1/20/20 | 11/37/115/115 | - |
| 24 | BCR | B | 619 | - | - | 1/29/63/63 | 0/2/2/2 |
| 23 | PHO | d | 401 | - | - | 3/37/103/103 | 0/5/6/6 |
| 32 | STE | l | 102 | - | - | 9/15/15/17 | - |
| 22 | CLA | B | 608 | - | 1/1/20/20 | 3/37/115/115 | - |
| 22 | CLA | A | 402 | - | 1/1/20/20 | 5/37/115/115 | - |
| 22 | CLA | b | 616 | - | 1/1/19/20 | 6/31/109/115 | - |
| 24 | BCR | c | 516 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | BCR | K | 101 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | b | 607 | 37 | 1/1/20/20 | 15/37/115/115 | - |
| 28 | SQD | F | 101 | - | - | 10/28/48/69 | 0/1/1/1 |
| 24 | BCR | B | 618 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 612 | - | 1/1/20/20 | 10/37/115/115 | - |
| 22 | CLA | c | 511 | 3 | 1/1/20/20 | 11/37/115/115 | - |
| 22 | CLA | c | 508 | - | - | 5/36/114/115 | - |
| 24 | BCR | c | 514 | - | - | 9/29/63/63 | 0/2/2/2 |
| 32 | STE | I | 101 | - | - | 8/12/12/17 | - |
| 32 | STE | b | 623 | - | - | 6/13/13/17 | - |
| 33 | LHG | e | 101 | - | - | 22/46/46/53 | - |
| 27 | LMG | d | 412 | - | - | 11/39/59/70 | 0/1/1/1 |
| 33 | LHG | D | 409 | - | - | 16/51/51/53 | - |
| 32 | STE | T | 103 | - | - | 7/12/12/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | A | 410 | 37 | 1/1/20/20 | 9/37/115/115 | - |
| 22 | CLA | c | 502 | - | 1/1/20/20 | 9/37/115/115 | - |
| 22 | CLA | c | 510 | - | 1/1/20/20 | 14/37/115/115 | - |
| 24 | BCR | C | 514 | - | - | 6/29/63/63 | 0/2/2/2 |
| 33 | LHG | L | 102 | - | - | 20/53/53/53 | - |
| 22 | CLA | A | 405 | - | 1/1/17/20 | 3/24/102/115 | - |
| 28 | SQD | f | 102 | - | - | 11/36/56/69 | 0/1/1/1 |
| 22 | CLA | B | 605 | - | 1/1/20/20 | 9/37/115/115 | - |
| 32 | STE | b | 625 | - | - | 5/7/7/17 | - |
| 27 | LMG | c | 520 | - | - | 8/31/51/70 | 0/1/1/1 |
| 29 | DGD | C | 516 | - | - | 21/51/91/95 | 0/2/2/2 |
| 22 | CLA | d | 403 | - | - | 9/37/115/115 | - |
| 24 | BCR | C | 515 | - | - | 13/29/63/63 | 0/2/2/2 |
| 24 | BCR | b | 619 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | d | 405 | - | 1/1/20/20 | 10/37/115/115 | - |
| 22 | CLA | D | 403 | - | 1/1/20/20 | 5/37/115/115 | - |
| 22 | CLA | b | 604 | - | 1/1/20/20 | 8/37/115/115 | - |
| 27 | LMG | d | 411 | - | - | 10/17/17/70 | - |
| 22 | CLA | C | 508 | - | - | 7/37/115/115 | - |
| 24 | BCR | T | 101 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 603 | - | 1/1/20/20 | 11/37/115/115 | - |
| 33 | LHG | d | 410 | - | - | 13/43/43/53 | - |
| 24 | BCR | k | 101 | - | - | 9/29/63/63 | 0/2/2/2 |
| 27 | LMG | B | 621 | - | - | 14/22/22/70 | - |
| 22 | CLA | C | 501 | - | 1/1/20/20 | 4/37/115/115 | - |
| 22 | CLA | B | 614 | - | 1/1/20/20 | 12/37/115/115 | - |
| 26 | PL9 | D | 406 | - | - | 7/53/73/73 | 0/1/1/1 |
| 27 | LMG | b | 620 | - | - | 14/46/66/70 | 0/1/1/1 |
| 22 | CLA | a | 403 | 37 | - | 9/37/115/115 | - |
| 24 | BCR | a | 405 | - | - | 4/29/63/63 | 0/2/2/2 |
| 32 | STE | B | 626 | - | - | 6/13/13/17 | - |
| 22 | CLA | a | 402 | - | 1/1/20/20 | 6/37/115/115 | - |
| 22 | CLA | c | 512 | - | 1/1/20/20 | 20/37/115/115 | - |
| 24 | BCR | Y | 101 | - | - | 8/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | STE | t | 102 | - | - | 4/11/11/17 | - |
| 32 | STE | C | 520 | - | - | 5/9/9/17 | - |
| 22 | CLA | A | 403 | 37 | - | 11/37/115/115 | - |
| 22 | CLA | C | 505 | - | 1/1/20/20 | 18/37/115/115 | - |
| 27 | LMG | A | 411 | - | - | 23/43/63/70 | 0/1/1/1 |
| 28 | SQD | A | 412 | - | - | 15/47/67/69 | 0/1/1/1 |
| 32 | STE | m | 101 | - | - | 5/9/9/17 | - |
| 22 | CLA | b | 605 | - | 1/1/20/20 | 8/37/115/115 | - |
| 22 | CLA | c | 513 | - | 1/1/20/20 | 6/37/115/115 | - |
| 33 | LHG | d | 408 | - | - | 24/53/53/53 | - |
| 32 | STE | B | 625 | - | - | 11/15/15/17 | - |
| 27 | LMG | D | 410 | - | - | 17/33/33/70 | - |
| 24 | BCR | t | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 22 | CLA | b | 603 | - | 1/1/20/20 | 4/37/115/115 | - |
| 32 | STE | j | 101 | - | - | 3/9/9/17 | - |
| 28 | SQD | a | 411 | - | - | 17/37/37/69 | - |
| 22 | CLA | C | 507 | 37 | 1/1/20/20 | 6/37/115/115 | - |
| 23 | PHO | D | 401 | - | - | 1/37/103/103 | 0/5/6/6 |
| 33 | LHG | d | 409 | - | - | 17/53/53/53 | - |
| 22 | CLA | C | 512 | - | 1/1/20/20 | 12/37/115/115 | - |
| 22 | CLA | b | 609 | - | 1/1/20/20 | 8/37/115/115 | - |
| 35 | HEM | f | 101 | 5,6 | - | 4/12/54/54 | - |
| 22 | CLA | B | 606 | - | 1/1/20/20 | 9/37/115/115 | - |
| 24 | BCR | B | 617 | - | - | 2/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 613 | - | 1/1/20/20 | 11/37/115/115 | - |
| 28 | SQD | B | 623 | - | - | 24/49/69/69 | 0/1/1/1 |
| 22 | CLA | C | 513 | - | 1/1/20/20 | 16/37/115/115 | - |
| 22 | CLA | C | 504 | 37 | 1/1/18/20 | 6/30/108/115 | - |
| 22 | CLA | B | 607 | 37 | 1/1/20/20 | 11/37/115/115 | - |
| 32 | STE | J | 101 | - | - | 2/9/9/17 | - |
| 22 | CLA | c | 507 | 37 | 1/1/20/20 | 8/37/115/115 | - |
| 22 | CLA | c | 506 | - | 1/1/20/20 | 11/37/115/115 | - |
| 29 | DGD | c | 518 | - | - | 21/51/91/95 | 0/2/2/2 |
| 27 | LMG | D | 407 | - | - | 17/46/66/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | STE | c | 521 | - | - | 10/17/17/17 | - |
| 24 | BCR | h | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 33 | LHG | D | 408 | - | - | 26/53/53/53 | - |
| 28 | SQD | A | 413 | - | - | 13/39/39/69 | - |
| 32 | STE | b | 624 | - | - | 8/17/17/17 | - |
| 26 | PL9 | d | 407 | - | - | 12/53/73/73 | 0/1/1/1 |
| 22 | CLA | b | 614 | - | 1/1/20/20 | 15/37/115/115 | - |
| 32 | STE | a | 414 | - | - | 7/9/9/17 | - |
| 24 | BCR | H | 101 | - | - | 7/29/63/63 | 0/2/2/2 |
| 24 | BCR | b | 617 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 503 | - | 1/1/20/20 | 6/37/115/115 | - |
| 27 | LMG | M | 101 | - | - | 24/46/66/70 | 0/1/1/1 |
| 32 | STE | b | 621 | - | - | 12/17/17/17 | - |
| 22 | CLA | c | 504 | 37 | 1/1/19/20 | 4/31/109/115 | - |
| 22 | CLA | c | 503 | - | 1/1/20/20 | 8/37/115/115 | - |
| 35 | HEM | E | 101 | 5,6 | - | 2/12/54/54 | - |
| 22 | CLA | d | 404 | 37 | 1/1/20/20 | 6/37/115/115 | - |
| 32 | STE | M | 102 | - | - | 4/12/12/17 | - |
| 24 | BCR | d | 406 | - | - | 7/29/63/63 | 0/2/2/2 |
| 32 | STE | M | 103 | - | - | 2/7/7/17 | - |
| 33 | LHG | E | 102 | - | - | 24/53/53/53 | - |
| 22 | CLA | b | 601 | 37 | 1/1/20/20 | 13/37/115/115 | - |
| 22 | CLA | b | 606 | - | 1/1/20/20 | 13/37/115/115 | - |
| 22 | CLA | C | 510 | - | 1/1/20/20 | 10/37/115/115 | - |
| 29 | DGD | H | 102 | - | - | 22/51/91/95 | 0/2/2/2 |
| 22 | CLA | b | 613 | - | 1/1/20/20 | 4/37/115/115 | - |
| 22 | CLA | C | 502 | - | 1/1/20/20 | 8/37/115/115 | - |
| 27 | LMG | c | 522 | - | - | 24/43/63/70 | 0/1/1/1 |
| 22 | CLA | C | 506 | - | 1/1/20/20 | 11/37/115/115 | - |
| 22 | CLA | B | 604 | - | 1/1/20/20 | 13/37/115/115 | - |
| 36 | HEC | V | 201 | 17 | - | 2/10/54/54 | - |
| 26 | PL9 | A | 409 | - | - | 22/53/73/73 | 0/1/1/1 |
| 22 | CLA | C | 511 | 3 | 1/1/20/20 | 6/37/115/115 | - |
| 24 | BCR | D | 405 | - | - | 5/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | D | 404 | - | - | 8/37/115/115 | - |
| 32 | STE | T | 102 | - | - | 5/13/13/17 | - |
| 26 | PL9 | a | 409 | - | - | 18/53/73/73 | 0/1/1/1 |
| 22 | CLA | B | 610 | 37 | 1/1/20/20 | 6/37/115/115 | - |
| 22 | CLA | B | 616 | - | 1/1/19/20 | 10/31/109/115 | - |
| 22 | CLA | B | 609 | - | - | 4/37/115/115 | - |
| 32 | STE | C | 522 | - | - | 4/9/9/17 | - |
| 23 | PHO | d | 402 | - | - | 8/37/103/103 | 0/5/6/6 |
| 22 | CLA | B | 615 | - | 1/1/20/20 | 7/37/115/115 | - |
| 22 | CLA | a | 404 | - | 1/1/20/20 | 8/37/115/115 | - |
| 29 | DGD | c | 519 | - | - | 19/51/91/95 | 0/2/2/2 |
| 32 | STE | B | 627 | - | - | 4/9/9/17 | - |
| 22 | CLA | B | 611 | - | 1/1/20/20 | 7/37/115/115 | - |
| 36 | HEC | v | 201 | 17 | - | 2/10/54/54 | - |
| 22 | CLA | b | 611 | - | 1/1/20/20 | 6/37/115/115 | - |
| 24 | BCR | c | 515 | - | - | 3/29/63/63 | 0/2/2/2 |
| 32 | STE | c | 524 | - | - | 5/9/9/17 | - |
| 22 | CLA | c | 501 | - | 1/1/20/20 | 3/37/115/115 | - |
| 24 | BCR | A | 406 | - | - | 3/29/63/63 | 0/2/2/2 |
| 22 | CLA | b | 602 | - | - | 11/37/115/115 | - |
| 32 | STE | B | 620 | - | - | 8/14/14/17 | - |
| 22 | CLA | b | 608 | - | 1/1/20/20 | 9/37/115/115 | - |
| 29 | DGD | h | 102 | - | - | 15/51/91/95 | 0/2/2/2 |
| 32 | STE | E | 103 | - | - | 6/9/9/17 | - |
| 28 | SQD | L | 101 | - | - | 22/44/64/69 | 0/1/1/1 |
| 22 | CLA | B | 602 | - | - | 9/37/115/115 | - |
| 27 | LMG | C | 519 | - | - | 19/43/63/70 | 0/1/1/1 |
| 22 | CLA | C | 509 | - | 1/1/20/20 | 14/37/115/115 | - |
| 27 | LMG | b | 622 | - | - | 29/50/70/70 | 0/1/1/1 |
| 29 | DGD | C | 517 | - | - | 19/51/91/95 | 0/2/2/2 |
| 32 | STE | C | 521 | - | - | 5/13/13/17 | - |
| 22 | CLA | c | 509 | - | 1/1/20/20 | 10/37/115/115 | - |
| 32 | STE | x | 101 | - | - | 9/17/17/17 | - |
| 32 | STE | a | 413 | - | - | 3/7/7/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | STE | B | 624 | - | - | 6/9/9/17 | - |
| 22 | CLA | B | 601 | 37 | 1/1/20/20 | 15/37/115/115 | - |
| 23 | PHO | A | 404 | - | - | 4/37/103/103 | 0/5/6/6 |
| 29 | DGD | C | 518 | - | - | 12/51/91/95 | 0/2/2/2 |
| 22 | CLA | c | 505 | - | 1/1/20/20 | 9/37/115/115 | - |

All (871) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 511 | CLA | CHB-C4A | 8.66 | 1.41 | 1.33 |
| 22 | A | 402 | CLA | CHB-C4A | 8.24 | 1.40 | 1.33 |
| 22 | d | 404 | CLA | CHB-C4A | 7.83 | 1.40 | 1.33 |
| 22 | D | 403 | CLA | CHB-C4A | 7.75 | 1.40 | 1.33 |
| 22 | B | 607 | CLA | CHB-C4A | 7.39 | 1.39 | 1.33 |
| 22 | B | 606 | CLA | CHB-C4A | 7.19 | 1.39 | 1.33 |
| 22 | b | 608 | CLA | CHB-C4A | 7.16 | 1.39 | 1.33 |
| 22 | c | 503 | CLA | CHB-C4A | 7.14 | 1.39 | 1.33 |
| 22 | B | 615 | CLA | CHB-C4A | 7.12 | 1.39 | 1.33 |
| 22 | C | 505 | CLA | CHB-C4A | 7.00 | 1.39 | 1.33 |
| 22 | a | 402 | CLA | CHB-C4A | 6.97 | 1.39 | 1.33 |
| 22 | B | 604 | CLA | CHB-C4A | 6.88 | 1.39 | 1.33 |
| 36 | V | 201 | HEC | C2B-C3B | -6.82 | 1.33 | 1.40 |
| 22 | c | 508 | CLA | CHB-C4A | 6.78 | 1.39 | 1.33 |
| 22 | B | 605 | CLA | CHB-C4A | 6.78 | 1.39 | 1.33 |
| 22 | c | 510 | CLA | CHB-C4A | 6.69 | 1.39 | 1.33 |
| 22 | A | 410 | CLA | CHB-C4A | 6.65 | 1.39 | 1.33 |
| 36 | v | 201 | HEC | C2B-C3B | -6.64 | 1.33 | 1.40 |
| 22 | c | 509 | CLA | CHB-C4A | 6.63 | 1.39 | 1.33 |
| 22 | B | 601 | CLA | MG-NA | 6.52 | 2.21 | 2.06 |
| 22 | C | 503 | CLA | MG-NA | 6.50 | 2.21 | 2.06 |
| 22 | B | 614 | CLA | CHB-C4A | 6.50 | 1.39 | 1.33 |
| 22 | a | 404 | CLA | CHB-C4A | 6.47 | 1.39 | 1.33 |
| 22 | C | 512 | CLA | CHB-C4A | 6.45 | 1.39 | 1.33 |
| 22 | b | 601 | CLA | CHB-C4A | 6.41 | 1.39 | 1.33 |
| 22 | C | 507 | CLA | CHB-C4A | 6.37 | 1.39 | 1.33 |
| 22 | c | 511 | CLA | MG-NA | 6.35 | 2.21 | 2.06 |
| 26 | D | 406 | PL9 | C6-C1 | -6.32 | 1.37 | 1.48 |
| 22 | C | 513 | CLA | CHB-C4A | 6.29 | 1.38 | 1.33 |
| 22 | B | 610 | CLA | CHB-C4A | 6.21 | 1.38 | 1.33 |
| 22 | A | 405 | CLA | MG-ND | -6.06 | 1.93 | 2.05 |
| 22 | C | 505 | CLA | MG-NA | 6.05 | 2.20 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | C | 506 | CLA | MG-ND | -6.02 | 1.93 | 2.05 |
| 22 | B | 616 | CLA | CHB-C4A | 5.98 | 1.38 | 1.33 |
| 22 | b | 605 | CLA | CHB-C4A | 5.98 | 1.38 | 1.33 |
| 22 | C | 508 | CLA | CHB-C4A | 5.93 | 1.38 | 1.33 |
| 22 | d | 404 | CLA | MG-NA | 5.89 | 2.20 | 2.06 |
| 22 | b | 612 | CLA | MG-ND | -5.89 | 1.94 | 2.05 |
| 22 | b | 616 | CLA | CHB-C4A | 5.83 | 1.38 | 1.33 |
| 22 | B | 616 | CLA | MG-NA | 5.82 | 2.20 | 2.06 |
| 22 | b | 614 | CLA | CHB-C4A | 5.81 | 1.38 | 1.33 |
| 22 | C | 503 | CLA | CHB-C4A | 5.80 | 1.38 | 1.33 |
| 22 | b | 611 | CLA | CHB-C4A | 5.76 | 1.38 | 1.33 |
| 22 | B | 611 | CLA | CHB-C4A | 5.74 | 1.38 | 1.33 |
| 22 | b | 613 | CLA | MG-NA | 5.73 | 2.19 | 2.06 |
| 22 | C | 511 | CLA | CHB-C4A | 5.72 | 1.38 | 1.33 |
| 35 | E | 101 | HEM | C3C-C2C | -5.68 | 1.32 | 1.40 |
| 22 | C | 510 | CLA | CHB-C4A | 5.67 | 1.38 | 1.33 |
| 22 | c | 507 | CLA | CHB-C4A | 5.62 | 1.38 | 1.33 |
| 22 | C | 511 | CLA | MG-NA | 5.62 | 2.19 | 2.06 |
| 22 | B | 612 | CLA | CHB-C4A | 5.61 | 1.38 | 1.33 |
| 22 | B | 601 | CLA | CHB-C4A | 5.60 | 1.38 | 1.33 |
| 22 | c | 505 | CLA | CHB-C4A | 5.50 | 1.38 | 1.33 |
| 22 | b | 606 | CLA | CHB-C4A | 5.41 | 1.38 | 1.33 |
| 22 | b | 610 | CLA | CHB-C4A | 5.38 | 1.38 | 1.33 |
| 22 | C | 509 | CLA | CHB-C4A | 5.36 | 1.38 | 1.33 |
| 22 | b | 603 | CLA | CHB-C4A | 5.35 | 1.38 | 1.33 |
| 22 | b | 615 | CLA | MG-ND | -5.31 | 1.95 | 2.05 |
| 22 | C | 512 | CLA | MG-NA | 5.30 | 2.18 | 2.06 |
| 22 | b | 607 | CLA | CHB-C4A | 5.29 | 1.38 | 1.33 |
| 22 | B | 604 | CLA | MG-NC | 5.25 | 2.18 | 2.06 |
| 29 | H | 102 | DGD | O5D-C1E | 5.18 | 1.48 | 1.40 |
| 24 | b | 618 | BCR | C30-C25 | -5.17 | 1.47 | 1.53 |
| 22 | b | 613 | CLA | CHB-C4A | 5.16 | 1.37 | 1.33 |
| 36 | V | 201 | HEC | C3C-C2C | -5.14 | 1.35 | 1.40 |
| 22 | B | 615 | CLA | MG-NA | 5.14 | 2.18 | 2.06 |
| 22 | b | 611 | CLA | MG-NA | 5.13 | 2.18 | 2.06 |
| 22 | c | 506 | CLA | MG-ND | -5.13 | 1.95 | 2.05 |
| 22 | C | 508 | CLA | MG-NA | 5.08 | 2.18 | 2.06 |
| 22 | a | 403 | CLA | MG-ND | -5.06 | 1.95 | 2.05 |
| 24 | B | 618 | BCR | C30-C25 | -5.03 | 1.47 | 1.53 |
| 22 | c | 509 | CLA | MG-ND | 5.01 | 2.15 | 2.05 |
| 22 | C | 506 | CLA | CHB-C4A | 4.97 | 1.37 | 1.33 |
| 22 | B | 603 | CLA | CHB-C4A | 4.92 | 1.37 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | a | 403 | CLA | CHB-C4A | 4.91 | 1.37 | 1.33 |
| 22 | A | 402 | CLA | MG-NA | 4.90 | 2.17 | 2.06 |
| 22 | c | 513 | CLA | MG-ND | -4.86 | 1.96 | 2.05 |
| 22 | C | 503 | CLA | MG-ND | 4.85 | 2.15 | 2.05 |
| 22 | c | 513 | CLA | CHB-C4A | 4.85 | 1.37 | 1.33 |
| 36 | v | 201 | HEC | C3D-C2D | 4.84 | 1.52 | 1.37 |
| 22 | C | 502 | CLA | CHB-C4A | 4.81 | 1.37 | 1.33 |
| 36 | v | 201 | HEC | C3C-C2C | -4.81 | 1.35 | 1.40 |
| 22 | b | 607 | CLA | MG-NA | 4.80 | 2.17 | 2.06 |
| 29 | A | 414 | DGD | O5D-C6D | -4.77 | 1.35 | 1.43 |
| 22 | b | 606 | CLA | MG-NA | 4.75 | 2.17 | 2.06 |
| 22 | c | 512 | CLA | CHB-C4A | 4.75 | 1.37 | 1.33 |
| 26 | D | 406 | PL9 | C52-C5 | -4.74 | 1.41 | 1.50 |
| 22 | B | 603 | CLA | MG-ND | 4.69 | 2.15 | 2.05 |
| 22 | c | 501 | CLA | CHB-C4A | 4.68 | 1.37 | 1.33 |
| 22 | a | 404 | CLA | MG-ND | -4.67 | 1.96 | 2.05 |
| 22 | c | 506 | CLA | CHB-C4A | 4.67 | 1.37 | 1.33 |
| 22 | A | 405 | CLA | CHB-C4A | 4.65 | 1.37 | 1.33 |
| 22 | C | 501 | CLA | MG-ND | -4.63 | 1.96 | 2.05 |
| 22 | c | 504 | CLA | MG-ND | -4.61 | 1.96 | 2.05 |
| 22 | B | 614 | CLA | MG-ND | -4.60 | 1.96 | 2.05 |
| 22 | B | 610 | CLA | C3B-C2B | -4.59 | 1.34 | 1.40 |
| 29 | C | 517 | DGD | O3G-C3G | -4.58 | 1.35 | 1.43 |
| 22 | B | 608 | CLA | CHB-C4A | 4.53 | 1.37 | 1.33 |
| 29 | c | 519 | DGD | C6D-C5D | 4.51 | 1.65 | 1.51 |
| 22 | B | 609 | CLA | CHB-C4A | 4.50 | 1.37 | 1.33 |
| 22 | b | 615 | CLA | CHB-C4A | 4.48 | 1.37 | 1.33 |
| 24 | T | 101 | BCR | C1-C6 | -4.47 | 1.48 | 1.53 |
| 29 | C | 517 | DGD | C4D-C3D | 4.46 | 1.63 | 1.52 |
| 26 | d | 407 | PL9 | C6-C1 | -4.44 | 1.41 | 1.48 |
| 22 | B | 613 | CLA | CHB-C4A | 4.42 | 1.37 | 1.33 |
| 22 | D | 404 | CLA | MG-NA | 4.41 | 2.16 | 2.06 |
| 22 | B | 607 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 24 | C | 514 | BCR | C1-C6 | -4.38 | 1.48 | 1.53 |
| 22 | b | 601 | CLA | MG-NA | 4.38 | 2.16 | 2.06 |
| 22 | d | 403 | CLA | CHB-C4A | 4.35 | 1.37 | 1.33 |
| 22 | B | 607 | CLA | MG-NA | 4.35 | 2.16 | 2.06 |
| 26 | d | 407 | PL9 | C3-C4 | -4.34 | 1.42 | 1.49 |
| 24 | b | 619 | BCR | C30-C25 | -4.31 | 1.48 | 1.53 |
| 22 | C | 512 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 27 | D | 407 | LMG | C4-C5 | 4.26 | 1.62 | 1.53 |
| 24 | T | 101 | BCR | C30-C25 | -4.26 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | D | 404 | CLA | CHB-C4A | 4.22 | 1.37 | 1.33 |
| 29 | a | 412 | DGD | O1G-C1A | 4.21 | 1.45 | 1.33 |
| 35 | f | 101 | HEM | C3C-C2C | -4.18 | 1.34 | 1.40 |
| 22 | c | 502 | CLA | CHB-C4A | 4.17 | 1.36 | 1.33 |
| 28 | B | 623 | SQD | O47-C7 | 4.15 | 1.46 | 1.34 |
| 22 | a | 402 | CLA | C1D-ND | 4.14 | 1.43 | 1.37 |
| 29 | A | 414 | DGD | C3E-C2E | 4.14 | 1.63 | 1.52 |
| 24 | c | 514 | BCR | C1-C6 | -4.13 | 1.48 | 1.53 |
| 22 | A | 405 | CLA | MG-NA | -4.12 | 1.96 | 2.06 |
| 22 | B | 610 | CLA | CMB-C2B | -4.12 | 1.43 | 1.51 |
| 27 | D | 410 | LMG | C7-C8 | 4.09 | 1.60 | 1.51 |
| 22 | b | 607 | CLA | C3B-C2B | -4.08 | 1.34 | 1.40 |
| 22 | C | 504 | CLA | CHB-C4A | 4.08 | 1.36 | 1.33 |
| 22 | a | 402 | CLA | MG-NC | 4.08 | 2.15 | 2.06 |
| 22 | D | 403 | CLA | MG-NA | 4.07 | 2.15 | 2.06 |
| 24 | H | 101 | BCR | C30-C25 | -4.07 | 1.48 | 1.53 |
| 22 | b | 604 | CLA | CHB-C4A | 4.06 | 1.36 | 1.33 |
| 24 | A | 406 | BCR | C1-C6 | -4.06 | 1.48 | 1.53 |
| 22 | C | 511 | CLA | MG-NC | -4.02 | 1.96 | 2.06 |
| 22 | c | 511 | CLA | CHC-C1C | 4.01 | 1.44 | 1.34 |
| 22 | a | 403 | CLA | C1D-ND | 4.00 | 1.43 | 1.37 |
| 36 | V | 201 | HEC | C3D-C2D | 3.99 | 1.49 | 1.37 |
| 22 | B | 608 | CLA | MG-NA | 3.98 | 2.15 | 2.06 |
| 24 | K | 101 | BCR | C30-C25 | -3.98 | 1.48 | 1.53 |
| 22 | A | 403 | CLA | C1D-ND | 3.97 | 1.43 | 1.37 |
| 22 | C | 509 | CLA | MG-ND | 3.97 | 2.13 | 2.05 |
| 22 | B | 601 | CLA | C3B-C2B | -3.97 | 1.35 | 1.40 |
| 33 | B | 622 | LHG | O7-C5 | -3.95 | 1.37 | 1.46 |
| 24 | D | 405 | BCR | C30-C25 | -3.94 | 1.48 | 1.53 |
| 22 | B | 610 | CLA | CHC-C1C | 3.92 | 1.44 | 1.34 |
| 22 | B | 613 | CLA | MG-NA | 3.90 | 2.15 | 2.06 |
| 24 | c | 515 | BCR | C1-C6 | -3.87 | 1.48 | 1.53 |
| 22 | b | 607 | CLA | MG-ND | -3.84 | 1.98 | 2.05 |
| 24 | c | 514 | BCR | C30-C25 | -3.84 | 1.48 | 1.53 |
| 22 | b | 601 | CLA | C1D-ND | 3.83 | 1.42 | 1.37 |
| 22 | b | 608 | CLA | CHC-C1C | 3.83 | 1.44 | 1.34 |
| 22 | B | 611 | CLA | CHC-C1C | 3.82 | 1.44 | 1.34 |
| 22 | C | 505 | CLA | CHC-C1C | 3.81 | 1.44 | 1.34 |
| 28 | L | 101 | SQD | O48-C23 | 3.81 | 1.44 | 1.33 |
| 22 | c | 504 | CLA | CHB-C4A | 3.80 | 1.36 | 1.33 |
| 22 | d | 403 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |
| 22 | b | 602 | CLA | CHB-C4A | 3.80 | 1.36 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | b | 609 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 22 | B | 606 | CLA | MG-NA | 3.79 | 2.15 | 2.06 |
| 22 | d | 405 | CLA | CHB-C4A | 3.79 | 1.36 | 1.33 |
| 22 | A | 403 | CLA | C3B-C2B | -3.78 | 1.35 | 1.40 |
| 22 | C | 513 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 22 | c | 502 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 22 | A | 410 | CLA | CHC-C1C | 3.76 | 1.43 | 1.34 |
| 22 | C | 501 | CLA | CHB-C4A | 3.74 | 1.36 | 1.33 |
| 23 | d | 402 | PHO | CAC-C3C | -3.74 | 1.45 | 1.52 |
| 24 | D | 405 | BCR | C1-C6 | -3.74 | 1.49 | 1.53 |
| 24 | B | 617 | BCR | C1-C6 | -3.73 | 1.49 | 1.53 |
| 22 | B | 606 | CLA | C3B-C2B | -3.72 | 1.35 | 1.40 |
| 27 | C | 519 | LMG | C4-C5 | 3.71 | 1.60 | 1.53 |
| 33 | D | 409 | LHG | O8-C6 | -3.70 | 1.36 | 1.45 |
| 22 | b | 609 | CLA | CHB-C4A | 3.70 | 1.36 | 1.33 |
| 27 | c | 523 | LMG | C4-C5 | 3.70 | 1.60 | 1.53 |
| 29 | c | 519 | DGD | O6D-C5D | -3.69 | 1.35 | 1.44 |
| 22 | A | 403 | CLA | CHB-C4A | 3.69 | 1.36 | 1.33 |
| 24 | B | 619 | BCR | C1-C6 | -3.69 | 1.49 | 1.53 |
| 22 | C | 512 | CLA | CHC-C1C | 3.67 | 1.43 | 1.34 |
| 29 | c | 519 | DGD | C4E-C5E | -3.67 | 1.45 | 1.53 |
| 24 | d | 406 | BCR | C30-C25 | -3.67 | 1.49 | 1.53 |
| 24 | b | 618 | BCR | C1-C6 | -3.66 | 1.49 | 1.53 |
| 22 | b | 604 | CLA | CHC-C1C | 3.65 | 1.43 | 1.34 |
| 22 | b | 612 | CLA | CHB-C4A | 3.63 | 1.36 | 1.33 |
| 22 | c | 507 | CLA | C3B-C2B | -3.63 | 1.35 | 1.40 |
| 22 | b | 615 | CLA | MG-NA | 3.62 | 2.14 | 2.06 |
| 27 | c | 522 | LMG | O1-C1 | 3.62 | 1.46 | 1.40 |
| 22 | b | 610 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 22 | B | 601 | CLA | MG-ND | -3.62 | 1.98 | 2.05 |
| 28 | a | 411 | SQD | O47-C7 | 3.61 | 1.44 | 1.34 |
| 22 | B | 602 | CLA | CHB-C4A | 3.58 | 1.36 | 1.33 |
| 26 | d | 407 | PL9 | C46-C44 | -3.58 | 1.43 | 1.51 |
| 24 | C | 515 | BCR | C30-C25 | -3.57 | 1.49 | 1.53 |
| 22 | d | 403 | CLA | MG-NA | 3.55 | 2.14 | 2.06 |
| 22 | b | 601 | CLA | CHC-C1C | 3.55 | 1.43 | 1.34 |
| 22 | b | 603 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 22 | B | 603 | CLA | CHC-C1C | 3.54 | 1.43 | 1.34 |
| 28 | A | 413 | SQD | O48-C23 | 3.53 | 1.43 | 1.33 |
| 22 | B | 614 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 22 | c | 508 | CLA | MG-ND | 3.53 | 2.12 | 2.05 |
| 22 | A | 402 | CLA | CHC-C1C | 3.52 | 1.43 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | c | 518 | DGD | O3E-C3E | -3.52 | 1.34 | 1.43 |
| 24 | c | 515 | BCR | C30-C25 | -3.52 | 1.49 | 1.53 |
| 29 | a | 412 | DGD | O2G-C1B | 3.51 | 1.44 | 1.34 |
| 22 | C | 509 | CLA | MG-NA | 3.51 | 2.14 | 2.06 |
| 22 | C | 510 | CLA | MG-NA | 3.51 | 2.14 | 2.06 |
| 22 | B | 606 | CLA | CHC-C1C | 3.50 | 1.43 | 1.34 |
| 29 | C | 516 | DGD | O2E-C2E | -3.50 | 1.34 | 1.43 |
| 22 | B | 602 | CLA | CHC-C1C | 3.49 | 1.43 | 1.34 |
| 22 | A | 403 | CLA | MG-NA | 3.49 | 2.14 | 2.06 |
| 22 | c | 505 | CLA | CHC-C1C | 3.48 | 1.43 | 1.34 |
| 22 | b | 615 | CLA | CMB-C2B | -3.48 | 1.44 | 1.51 |
| 22 | b | 614 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 24 | c | 516 | BCR | C30-C25 | -3.47 | 1.49 | 1.53 |
| 24 | h | 101 | BCR | C30-C25 | -3.47 | 1.49 | 1.53 |
| 22 | b | 613 | CLA | MG-ND | -3.47 | 1.98 | 2.05 |
| 22 | C | 506 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 29 | h | 102 | DGD | O2G-C2G | -3.46 | 1.38 | 1.46 |
| 22 | b | 605 | CLA | CHC-C1C | 3.46 | 1.43 | 1.34 |
| 22 | B | 615 | CLA | CHC-C1C | 3.45 | 1.43 | 1.34 |
| 28 | f | 102 | SQD | O47-C7 | 3.45 | 1.44 | 1.34 |
| 22 | b | 613 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 22 | b | 614 | CLA | MG-ND | -3.43 | 1.99 | 2.05 |
| 22 | c | 504 | CLA | CHC-C1C | 3.43 | 1.43 | 1.34 |
| 29 | C | 516 | DGD | O3E-C3E | -3.43 | 1.34 | 1.43 |
| 22 | b | 610 | CLA | C3B-C2B | -3.42 | 1.35 | 1.40 |
| 22 | A | 403 | CLA | MG-ND | -3.42 | 1.99 | 2.05 |
| 24 | b | 617 | BCR | C1-C6 | -3.41 | 1.49 | 1.53 |
| 22 | B | 614 | CLA | CHC-C1C | 3.41 | 1.43 | 1.34 |
| 28 | f | 102 | SQD | O48-C23 | 3.41 | 1.43 | 1.33 |
| 29 | A | 414 | DGD | C4E-C5E | 3.41 | 1.60 | 1.53 |
| 22 | c | 510 | CLA | CMB-C2B | -3.41 | 1.44 | 1.51 |
| 22 | B | 612 | CLA | MG-ND | -3.40 | 1.99 | 2.05 |
| 24 | B | 617 | BCR | C30-C25 | -3.39 | 1.49 | 1.53 |
| 22 | d | 404 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 22 | C | 510 | CLA | CHC-C1C | 3.38 | 1.42 | 1.34 |
| 22 | B | 603 | CLA | CMC-C2C | -3.38 | 1.43 | 1.50 |
| 22 | C | 507 | CLA | CHC-C1C | 3.38 | 1.42 | 1.34 |
| 22 | c | 504 | CLA | MG-NC | 3.36 | 2.14 | 2.06 |
| 23 | D | 401 | PHO | CHA-CBD | -3.35 | 1.48 | 1.52 |
| 22 | C | 502 | CLA | C3B-C2B | -3.35 | 1.35 | 1.40 |
| 22 | b | 613 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 22 | c | 508 | CLA | CHC-C1C | 3.34 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 513 | CLA | CHC-C1C | 3.34 | 1.42 | 1.34 |
| 29 | C | 518 | DGD | O2G-C2G | -3.34 | 1.38 | 1.46 |
| 22 | C | 508 | CLA | CHC-C1C | 3.34 | 1.42 | 1.34 |
| 22 | b | 606 | CLA | CHC-C1C | 3.34 | 1.42 | 1.34 |
| 28 | a | 411 | SQD | O48-C23 | 3.34 | 1.43 | 1.33 |
| 26 | D | 406 | PL9 | C11-C9 | -3.33 | 1.44 | 1.51 |
| 22 | B | 601 | CLA | CHC-C1C | 3.33 | 1.42 | 1.34 |
| 33 | L | 102 | LHG | O8-C23 | 3.33 | 1.43 | 1.33 |
| 27 | b | 620 | LMG | C4-C3 | 3.31 | 1.60 | 1.52 |
| 22 | B | 612 | CLA | C1D-ND | 3.31 | 1.42 | 1.37 |
| 22 | B | 605 | CLA | CHC-C1C | 3.31 | 1.42 | 1.34 |
| 29 | H | 102 | DGD | C4D-C5D | 3.31 | 1.60 | 1.53 |
| 29 | h | 102 | DGD | C4D-C3D | 3.30 | 1.60 | 1.52 |
| 29 | A | 414 | DGD | C6E-C5E | 3.30 | 1.62 | 1.51 |
| 22 | d | 404 | CLA | CMB-C2B | -3.29 | 1.45 | 1.51 |
| 22 | C | 504 | CLA | CHC-C1C | 3.29 | 1.42 | 1.34 |
| 22 | B | 601 | CLA | C1D-ND | 3.28 | 1.42 | 1.37 |
| 22 | C | 503 | CLA | CHC-C1C | 3.28 | 1.42 | 1.34 |
| 22 | c | 512 | CLA | CHC-C1C | 3.28 | 1.42 | 1.34 |
| 22 | B | 604 | CLA | CHC-C1C | 3.27 | 1.42 | 1.34 |
| 22 | B | 609 | CLA | CMD-C2D | -3.27 | 1.44 | 1.50 |
| 22 | D | 404 | CLA | C1D-ND | 3.26 | 1.42 | 1.37 |
| 22 | B | 614 | CLA | C3B-C2B | -3.25 | 1.36 | 1.40 |
| 24 | Y | 101 | BCR | C1-C6 | -3.25 | 1.49 | 1.53 |
| 27 | d | 412 | LMG | O1-C7 | -3.24 | 1.38 | 1.43 |
| 29 | A | 414 | DGD | C4D-C5D | 3.24 | 1.59 | 1.53 |
| 22 | B | 601 | CLA | CMB-C2B | -3.24 | 1.45 | 1.51 |
| 22 | b | 612 | CLA | CMB-C2B | -3.22 | 1.45 | 1.51 |
| 22 | C | 513 | CLA | CHC-C1C | 3.22 | 1.42 | 1.34 |
| 22 | a | 402 | CLA | MG-ND | -3.21 | 1.99 | 2.05 |
| 22 | d | 403 | CLA | CHC-C1C | 3.21 | 1.42 | 1.34 |
| 22 | C | 508 | CLA | C1D-ND | 3.21 | 1.42 | 1.37 |
| 22 | c | 510 | CLA | C1D-ND | 3.21 | 1.42 | 1.37 |
| 24 | k | 101 | BCR | C30-C25 | -3.21 | 1.49 | 1.53 |
| 22 | C | 509 | CLA | CHC-C1C | 3.20 | 1.42 | 1.34 |
| 24 | b | 619 | BCR | C1-C6 | -3.20 | 1.49 | 1.53 |
| 22 | A | 405 | CLA | C1D-ND | 3.19 | 1.42 | 1.37 |
| 22 | B | 603 | CLA | C3B-C2B | -3.19 | 1.36 | 1.40 |
| 28 | L | 101 | SQD | O47-C7 | 3.19 | 1.43 | 1.34 |
| 23 | d | 401 | PHO | O2D-CGD | 3.17 | 1.41 | 1.33 |
| 22 | A | 410 | CLA | C1D-ND | 3.17 | 1.42 | 1.37 |
| 22 | b | 614 | CLA | MG-NA | 3.16 | 2.13 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | a | 404 | CLA | C3B-C2B | -3.16 | 1.36 | 1.40 |
| 22 | C | 502 | CLA | CHC-C1C | 3.15 | 1.42 | 1.34 |
| 22 | B | 609 | CLA | C3B-C2B | -3.15 | 1.36 | 1.40 |
| 26 | d | 407 | PL9 | C53-C6 | -3.15 | 1.44 | 1.50 |
| 33 | d | 408 | LHG | O7-C5 | -3.14 | 1.39 | 1.46 |
| 22 | a | 403 | CLA | CHC-C1C | 3.14 | 1.42 | 1.34 |
| 22 | b | 604 | CLA | C1D-ND | 3.14 | 1.42 | 1.37 |
| 27 | b | 620 | LMG | C4-C5 | 3.13 | 1.59 | 1.53 |
| 22 | C | 511 | CLA | CMB-C2B | -3.13 | 1.45 | 1.51 |
| 24 | d | 406 | BCR | C1-C6 | -3.13 | 1.49 | 1.53 |
| 22 | B | 615 | CLA | CMB-C2B | -3.13 | 1.45 | 1.51 |
| 29 | c | 518 | DGD | O2E-C2E | -3.13 | 1.35 | 1.43 |
| 22 | d | 403 | CLA | CMB-C2B | -3.12 | 1.45 | 1.51 |
| 22 | D | 403 | CLA | CMD-C2D | -3.12 | 1.44 | 1.50 |
| 22 | c | 511 | CLA | C1D-ND | 3.12 | 1.42 | 1.37 |
| 22 | a | 402 | CLA | CHC-C1C | 3.12 | 1.42 | 1.34 |
| 22 | B | 613 | CLA | MG-ND | -3.12 | 1.99 | 2.05 |
| 22 | C | 506 | CLA | CHC-C1C | 3.12 | 1.42 | 1.34 |
| 22 | b | 602 | CLA | CHC-C1C | 3.12 | 1.42 | 1.34 |
| 29 | C | 517 | DGD | O3D-C3D | -3.12 | 1.35 | 1.43 |
| 27 | c | 520 | LMG | O1-C1 | 3.12 | 1.45 | 1.40 |
| 24 | b | 617 | BCR | C30-C25 | -3.11 | 1.49 | 1.53 |
| 22 | b | 608 | CLA | CMB-C2B | -3.11 | 1.45 | 1.51 |
| 22 | b | 614 | CLA | CMC-C2C | -3.11 | 1.44 | 1.50 |
| 22 | B | 605 | CLA | C3B-C2B | -3.10 | 1.36 | 1.40 |
| 22 | d | 405 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 26 | a | 409 | PL9 | C53-C6 | -3.09 | 1.44 | 1.50 |
| 22 | b | 611 | CLA | CHC-C1C | 3.09 | 1.42 | 1.34 |
| 27 | A | 411 | LMG | C4-C3 | 3.09 | 1.60 | 1.52 |
| 22 | c | 512 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 33 | D | 408 | LHG | P-O3 | 3.08 | 1.71 | 1.59 |
| 22 | C | 512 | CLA | MG-NC | -3.08 | 1.99 | 2.06 |
| 33 | D | 409 | LHG | P-O6 | 3.07 | 1.71 | 1.59 |
| 29 | A | 414 | DGD | C1E-C2E | 3.07 | 1.61 | 1.52 |
| 29 | A | 414 | DGD | O5D-C1E | 3.07 | 1.45 | 1.40 |
| 35 | f | 101 | HEM | C3C-CAC | 3.07 | 1.54 | 1.47 |
| 22 | C | 511 | CLA | CHC-C1C | 3.07 | 1.42 | 1.34 |
| 22 | B | 609 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 22 | C | 503 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 29 | C | 517 | DGD | O5D-C6D | -3.06 | 1.38 | 1.43 |
| 22 | b | 615 | CLA | CMD-C2D | -3.06 | 1.44 | 1.50 |
| 22 | c | 512 | CLA | MG-NA | 3.06 | 2.13 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 606 | CLA | MG-ND | 3.05 | 2.11 | 2.05 |
| 22 | a | 404 | CLA | CMC-C2C | -3.05 | 1.44 | 1.50 |
| 22 | B | 616 | CLA | C1D-ND | 3.05 | 1.41 | 1.37 |
| 29 | c | 517 | DGD | C4E-C3E | 3.05 | 1.60 | 1.52 |
| 33 | E | 102 | LHG | P-O6 | 3.05 | 1.71 | 1.59 |
| 22 | D | 404 | CLA | CMC-C2C | -3.04 | 1.44 | 1.50 |
| 22 | B | 605 | CLA | C1C-NC | -3.03 | 1.33 | 1.37 |
| 27 | B | 621 | LMG | O7-C10 | 3.03 | 1.40 | 1.30 |
| 29 | h | 102 | DGD | O2D-C2D | -3.03 | 1.35 | 1.43 |
| 22 | c | 507 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 22 | b | 607 | CLA | CHC-C1C | 3.02 | 1.42 | 1.34 |
| 22 | a | 402 | CLA | CMB-C2B | -3.02 | 1.45 | 1.51 |
| 22 | C | 507 | CLA | C3B-C2B | -3.02 | 1.36 | 1.40 |
| 22 | B | 606 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 22 | c | 513 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 22 | b | 607 | CLA | CMD-C2D | -3.01 | 1.44 | 1.50 |
| 22 | C | 509 | CLA | C1D-ND | 3.00 | 1.41 | 1.37 |
| 27 | M | 101 | LMG | O7-C8 | -3.00 | 1.39 | 1.46 |
| 35 | E | 101 | HEM | CAB-C3B | 3.00 | 1.55 | 1.47 |
| 22 | B | 615 | CLA | C1D-ND | 3.00 | 1.41 | 1.37 |
| 28 | A | 413 | SQD | O47-C45 | -3.00 | 1.42 | 1.47 |
| 22 | c | 503 | CLA | MG-NA | 3.00 | 2.13 | 2.06 |
| 22 | A | 403 | CLA | CHC-C1C | 2.99 | 1.41 | 1.34 |
| 22 | B | 602 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 22 | a | 404 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 22 | C | 505 | CLA | C1D-ND | 2.99 | 1.41 | 1.37 |
| 22 | c | 505 | CLA | C3B-C2B | -2.98 | 1.36 | 1.40 |
| 22 | c | 501 | CLA | C3B-C2B | -2.98 | 1.36 | 1.40 |
| 27 | c | 520 | LMG | C4-C5 | 2.98 | 1.59 | 1.53 |
| 29 | H | 102 | DGD | O2D-C2D | -2.98 | 1.35 | 1.43 |
| 22 | C | 508 | CLA | MG-ND | -2.98 | 1.99 | 2.05 |
| 22 | B | 611 | CLA | CMD-C2D | -2.98 | 1.44 | 1.50 |
| 22 | D | 403 | CLA | CHC-C1C | 2.97 | 1.41 | 1.34 |
| 29 | c | 518 | DGD | C1E-C2E | 2.97 | 1.61 | 1.52 |
| 22 | B | 608 | CLA | CMD-C2D | -2.97 | 1.44 | 1.50 |
| 33 | d | 408 | LHG | C24-C23 | 2.97 | 1.59 | 1.50 |
| 22 | a | 402 | CLA | MG-NA | 2.97 | 2.13 | 2.06 |
| 22 | b | 615 | CLA | CHC-C1C | 2.97 | 1.41 | 1.34 |
| 22 | c | 501 | CLA | CHC-C1C | 2.96 | 1.41 | 1.34 |
| 22 | D | 404 | CLA | CMB-C2B | -2.96 | 1.45 | 1.51 |
| 28 | A | 412 | SQD | O2-C2 | -2.96 | 1.35 | 1.43 |
| 22 | c | 501 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 509 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |
| 24 | K | 101 | BCR | C1-C6 | -2.96 | 1.50 | 1.53 |
| 22 | c | 510 | CLA | CHC-C1C | 2.96 | 1.41 | 1.34 |
| 22 | b | 611 | CLA | CMD-C2D | -2.95 | 1.44 | 1.50 |
| 29 | c | 518 | DGD | C4D-C3D | 2.95 | 1.60 | 1.52 |
| 28 | F | 101 | SQD | O48-C23 | 2.95 | 1.42 | 1.33 |
| 22 | B | 612 | CLA | CHC-C1C | 2.94 | 1.41 | 1.34 |
| 27 | c | 522 | LMG | C3-C2 | 2.94 | 1.60 | 1.52 |
| 28 | B | 623 | SQD | O48-C23 | 2.94 | 1.41 | 1.33 |
| 22 | A | 403 | CLA | CMD-C2D | -2.94 | 1.44 | 1.50 |
| 33 | B | 622 | LHG | C24-C23 | 2.94 | 1.59 | 1.50 |
| 27 | d | 412 | LMG | C4-C5 | 2.93 | 1.59 | 1.53 |
| 22 | c | 503 | CLA | C1D-ND | 2.93 | 1.41 | 1.37 |
| 22 | B | 605 | CLA | CMC-C2C | -2.92 | 1.44 | 1.50 |
| 22 | B | 607 | CLA | CHC-C1C | 2.92 | 1.41 | 1.34 |
| 22 | d | 405 | CLA | CHC-C1C | 2.92 | 1.41 | 1.34 |
| 22 | B | 608 | CLA | C1D-ND | 2.92 | 1.41 | 1.37 |
| 22 | d | 405 | CLA | CMB-C2B | -2.91 | 1.45 | 1.51 |
| 22 | B | 614 | CLA | CMB-C2B | -2.91 | 1.45 | 1.51 |
| 24 | a | 405 | BCR | C30-C25 | -2.91 | 1.50 | 1.53 |
| 22 | c | 501 | CLA | CMB-C2B | -2.91 | 1.45 | 1.51 |
| 29 | c | 519 | DGD | O2G-C2G | -2.89 | 1.39 | 1.46 |
| 22 | C | 507 | CLA | MG-NA | 2.89 | 2.13 | 2.06 |
| 27 | d | 412 | LMG | O8-C9 | -2.89 | 1.38 | 1.45 |
| 22 | B | 607 | CLA | MG-NC | 2.88 | 2.13 | 2.06 |
| 26 | A | 409 | PL9 | C21-C19 | 2.88 | 1.57 | 1.51 |
| 22 | B | 608 | CLA | CHC-C1C | 2.88 | 1.41 | 1.34 |
| 28 | A | 413 | SQD | O47-C7 | 2.88 | 1.42 | 1.34 |
| 29 | C | 516 | DGD | C4D-C3D | 2.87 | 1.59 | 1.52 |
| 28 | A | 412 | SQD | O48-C23 | 2.87 | 1.41 | 1.33 |
| 22 | c | 508 | CLA | CMB-C2B | -2.87 | 1.45 | 1.51 |
| 22 | b | 613 | CLA | CAA-C2A | -2.87 | 1.48 | 1.54 |
| 22 | c | 513 | CLA | MG-NC | 2.86 | 2.13 | 2.06 |
| 22 | c | 506 | CLA | CHC-C1C | 2.86 | 1.41 | 1.34 |
| 27 | D | 407 | LMG | O2-C2 | -2.85 | 1.35 | 1.43 |
| 22 | c | 509 | CLA | CHC-C1C | 2.85 | 1.41 | 1.34 |
| 22 | B | 613 | CLA | CMD-C2D | -2.85 | 1.44 | 1.50 |
| 22 | B | 612 | CLA | MG-NA | 2.85 | 2.13 | 2.06 |
| 22 | c | 502 | CLA | CMD-C2D | -2.84 | 1.44 | 1.50 |
| 22 | C | 501 | CLA | MG-NA | 2.84 | 2.13 | 2.06 |
| 22 | C | 503 | CLA | CMB-C2B | -2.83 | 1.46 | 1.51 |
| 27 | b | 620 | LMG | O6-C1 | 2.83 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | a | 403 | CLA | CMB-C2B | -2.83 | 1.46 | 1.51 |
| 22 | c | 503 | CLA | CHC-C1C | 2.83 | 1.41 | 1.34 |
| 22 | c | 502 | CLA | CMB-C2B | -2.83 | 1.46 | 1.51 |
| 29 | h | 102 | DGD | C4E-C5E | 2.83 | 1.59 | 1.53 |
| 22 | c | 512 | CLA | CMB-C2B | -2.82 | 1.46 | 1.51 |
| 22 | b | 616 | CLA | C1D-ND | 2.82 | 1.41 | 1.37 |
| 29 | C | 516 | DGD | C4E-C3E | 2.81 | 1.59 | 1.52 |
| 22 | C | 509 | CLA | CMB-C2B | -2.81 | 1.46 | 1.51 |
| 22 | C | 513 | CLA | CMC-C2C | -2.81 | 1.45 | 1.50 |
| 22 | B | 614 | CLA | MG-NA | 2.81 | 2.12 | 2.06 |
| 29 | c | 518 | DGD | C6E-C5E | 2.81 | 1.61 | 1.51 |
| 27 | C | 519 | LMG | O1-C7 | -2.80 | 1.38 | 1.43 |
| 22 | B | 602 | CLA | C1D-ND | 2.79 | 1.41 | 1.37 |
| 22 | b | 614 | CLA | CHC-C1C | 2.79 | 1.41 | 1.34 |
| 22 | B | 613 | CLA | CHC-C1C | 2.79 | 1.41 | 1.34 |
| 33 | L | 102 | LHG | P-O6 | 2.79 | 1.70 | 1.59 |
| 22 | D | 403 | CLA | C1D-ND | 2.79 | 1.41 | 1.37 |
| 22 | b | 603 | CLA | CMB-C2B | -2.79 | 1.46 | 1.51 |
| 24 | Y | 101 | BCR | C30-C25 | -2.78 | 1.50 | 1.53 |
| 22 | b | 607 | CLA | CMB-C2B | -2.78 | 1.46 | 1.51 |
| 22 | B | 611 | CLA | C1D-ND | 2.77 | 1.41 | 1.37 |
| 22 | c | 507 | CLA | MG-NA | 2.77 | 2.12 | 2.06 |
| 27 | M | 101 | LMG | O4-C4 | -2.77 | 1.36 | 1.43 |
| 35 | f | 101 | HEM | C3B-C2B | -2.77 | 1.31 | 1.37 |
| 22 | B | 605 | CLA | MG-ND | -2.77 | 2.00 | 2.05 |
| 22 | b | 609 | CLA | CMB-C2B | -2.77 | 1.46 | 1.51 |
| 22 | c | 512 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 22 | c | 502 | CLA | CHC-C1C | 2.76 | 1.41 | 1.34 |
| 22 | b | 606 | CLA | C1D-ND | 2.76 | 1.41 | 1.37 |
| 22 | c | 513 | CLA | CMB-C2B | -2.76 | 1.46 | 1.51 |
| 22 | A | 402 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 22 | b | 607 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 33 | l | 101 | LHG | P-O6 | 2.75 | 1.70 | 1.59 |
| 22 | c | 503 | CLA | CMB-C2B | -2.75 | 1.46 | 1.51 |
| 29 | c | 518 | DGD | O5D-C1E | 2.75 | 1.44 | 1.40 |
| 22 | C | 506 | CLA | C3B-C2B | -2.74 | 1.36 | 1.40 |
| 22 | B | 606 | CLA | CMB-C2B | -2.74 | 1.46 | 1.51 |
| 24 | k | 101 | BCR | C1-C6 | -2.74 | 1.50 | 1.53 |
| 24 | t | 101 | BCR | C27-C26 | -2.74 | 1.45 | 1.51 |
| 22 | c | 507 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 29 | c | 518 | DGD | O3G-C1D | -2.73 | 1.35 | 1.40 |
| 22 | b | 615 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 506 | CLA | CMC-C2C | -2.72 | 1.45 | 1.50 |
| 22 | a | 402 | CLA | CMC-C2C | -2.72 | 1.45 | 1.50 |
| 27 | b | 620 | LMG | O7-C8 | -2.72 | 1.40 | 1.46 |
| 23 | A | 404 | PHO | CHA-CBD | -2.71 | 1.49 | 1.52 |
| 22 | a | 404 | CLA | C1C-NC | -2.71 | 1.33 | 1.37 |
| 27 | c | 522 | LMG | C4-C3 | 2.71 | 1.59 | 1.52 |
| 22 | b | 612 | CLA | C1D-ND | 2.71 | 1.41 | 1.37 |
| 33 | d | 410 | LHG | P-O6 | 2.71 | 1.70 | 1.59 |
| 22 | C | 504 | CLA | C1D-ND | 2.71 | 1.41 | 1.37 |
| 24 | C | 514 | BCR | C36-C18 | -2.70 | 1.45 | 1.50 |
| 23 | D | 401 | PHO | CAC-C3C | -2.70 | 1.47 | 1.52 |
| 22 | b | 614 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 28 | f | 102 | SQD | O2-C2 | -2.69 | 1.36 | 1.43 |
| 22 | D | 404 | CLA | CMD-C2D | -2.69 | 1.45 | 1.50 |
| 27 | c | 523 | LMG | O1-C7 | -2.69 | 1.39 | 1.43 |
| 29 | c | 518 | DGD | O3D-C3D | -2.69 | 1.36 | 1.43 |
| 22 | B | 608 | CLA | CMB-C2B | -2.69 | 1.46 | 1.51 |
| 22 | D | 403 | CLA | CAA-C2A | -2.68 | 1.49 | 1.54 |
| 29 | C | 518 | DGD | O6D-C5D | -2.68 | 1.37 | 1.44 |
| 22 | c | 502 | CLA | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 22 | b | 602 | CLA | CMD-C2D | -2.68 | 1.45 | 1.50 |
| 26 | A | 409 | PL9 | C7-C3 | -2.68 | 1.47 | 1.51 |
| 29 | c | 519 | DGD | O5D-C1E | 2.67 | 1.44 | 1.40 |
| 22 | c | 509 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 24 | t | 101 | BCR | C30-C25 | -2.67 | 1.50 | 1.53 |
| 22 | C | 512 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 22 | C | 501 | CLA | CHC-C1C | 2.66 | 1.41 | 1.34 |
| 35 | E | 101 | HEM | C3C-C4C | 2.66 | 1.45 | 1.41 |
| 22 | B | 607 | CLA | CAC-C3C | -2.65 | 1.44 | 1.51 |
| 24 | c | 516 | BCR | C1-C6 | -2.65 | 1.50 | 1.53 |
| 24 | B | 617 | BCR | C33-C5 | -2.65 | 1.46 | 1.50 |
| 22 | d | 404 | CLA | CHC-C1C | 2.65 | 1.41 | 1.34 |
| 22 | b | 604 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 23 | d | 402 | PHO | CMC-C2C | -2.65 | 1.45 | 1.51 |
| 22 | C | 512 | CLA | C1D-ND | 2.65 | 1.41 | 1.37 |
| 27 | c | 520 | LMG | C3-C2 | 2.65 | 1.59 | 1.52 |
| 22 | A | 405 | CLA | CMD-C2D | -2.64 | 1.45 | 1.50 |
| 22 | b | 611 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 22 | C | 506 | CLA | CMC-C2C | -2.64 | 1.45 | 1.50 |
| 22 | a | 403 | CLA | CMC-C2C | -2.63 | 1.45 | 1.50 |
| 22 | c | 508 | CLA | CMC-C2C | -2.63 | 1.45 | 1.50 |
| 22 | b | 603 | CLA | MG-NA | 2.63 | 2.12 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | a | 404 | CLA | C4B-CHC | -2.63 | 1.33 | 1.41 |
| 24 | A | 406 | BCR | C33-C5 | -2.62 | 1.46 | 1.50 |
| 22 | D | 403 | CLA | C1C-NC | -2.62 | 1.33 | 1.37 |
| 28 | a | 410 | SQD | O48-C23 | 2.62 | 1.41 | 1.33 |
| 22 | C | 507 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 27 | D | 407 | LMG | O1-C1 | 2.62 | 1.44 | 1.40 |
| 22 | c | 509 | CLA | MG-NC | 2.61 | 2.12 | 2.06 |
| 22 | C | 502 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 22 | c | 510 | CLA | CMD-C2D | -2.61 | 1.45 | 1.50 |
| 22 | c | 504 | CLA | CMD-C2D | -2.61 | 1.45 | 1.50 |
| 23 | A | 404 | PHO | CMC-C2C | -2.61 | 1.45 | 1.51 |
| 22 | B | 611 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 24 | B | 619 | BCR | C30-C25 | -2.60 | 1.50 | 1.53 |
| 22 | c | 506 | CLA | CMD-C2D | -2.60 | 1.45 | 1.50 |
| 22 | B | 602 | CLA | CMD-C2D | -2.60 | 1.45 | 1.50 |
| 24 | a | 405 | BCR | C1-C6 | -2.60 | 1.50 | 1.53 |
| 24 | T | 101 | BCR | C38-C26 | -2.60 | 1.46 | 1.50 |
| 22 | B | 603 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 22 | C | 509 | CLA | MG-NC | -2.59 | 2.00 | 2.06 |
| 28 | F | 101 | SQD | O2-C2 | -2.59 | 1.36 | 1.43 |
| 27 | b | 622 | LMG | C7-C8 | 2.58 | 1.58 | 1.50 |
| 28 | a | 410 | SQD | O2-C2 | -2.58 | 1.36 | 1.43 |
| 22 | C | 506 | CLA | MG-NA | 2.58 | 2.12 | 2.06 |
| 24 | C | 515 | BCR | C27-C26 | -2.58 | 1.46 | 1.51 |
| 22 | C | 509 | CLA | CMD-C2D | -2.58 | 1.45 | 1.50 |
| 22 | B | 612 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 27 | M | 101 | LMG | C4-C5 | 2.58 | 1.58 | 1.53 |
| 22 | C | 502 | CLA | MG-NA | 2.57 | 2.12 | 2.06 |
| 22 | c | 502 | CLA | C4B-CHC | -2.57 | 1.33 | 1.41 |
| 22 | b | 605 | CLA | CMD-C2D | -2.57 | 1.45 | 1.50 |
| 28 | a | 410 | SQD | O47-C7 | 2.57 | 1.41 | 1.34 |
| 27 | C | 519 | LMG | O8-C9 | -2.57 | 1.39 | 1.45 |
| 24 | C | 514 | BCR | C33-C5 | -2.57 | 1.46 | 1.50 |
| 22 | c | 510 | CLA | MG-ND | -2.57 | 2.00 | 2.05 |
| 22 | b | 613 | CLA | CMD-C2D | -2.56 | 1.45 | 1.50 |
| 22 | c | 510 | CLA | MG-NC | 2.56 | 2.12 | 2.06 |
| 22 | B | 605 | CLA | CMD-C2D | -2.56 | 1.45 | 1.50 |
| 22 | b | 603 | CLA | CHC-C1C | 2.56 | 1.40 | 1.34 |
| 29 | C | 516 | DGD | C2B-C1B | -2.56 | 1.43 | 1.50 |
| 22 | c | 506 | CLA | C1D-ND | 2.56 | 1.41 | 1.37 |
| 22 | C | 513 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 23 | D | 401 | PHO | CMC-C2C | -2.56 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | C | 505 | CLA | MG-NC | -2.55 | 2.00 | 2.06 |
| 22 | c | 508 | CLA | CMD-C2D | -2.55 | 1.45 | 1.50 |
| 33 | e | 101 | LHG | P-O6 | 2.55 | 1.69 | 1.59 |
| 33 | B | 622 | LHG | P-O6 | 2.55 | 1.69 | 1.59 |
| 27 | c | 520 | LMG | O7-C10 | 2.55 | 1.40 | 1.35 |
| 22 | C | 513 | CLA | MG-NA | 2.54 | 2.12 | 2.06 |
| 22 | b | 613 | CLA | CMC-C2C | -2.53 | 1.45 | 1.50 |
| 22 | b | 609 | CLA | CHC-C1C | 2.53 | 1.40 | 1.34 |
| 22 | b | 612 | CLA | CHC-C1C | 2.53 | 1.40 | 1.34 |
| 22 | B | 605 | CLA | O2D-CED | -2.53 | 1.39 | 1.45 |
| 22 | b | 606 | CLA | C3B-C2B | -2.52 | 1.37 | 1.40 |
| 27 | c | 522 | LMG | C9-C8 | 2.52 | 1.58 | 1.50 |
| 29 | C | 516 | DGD | O2G-C2G | -2.52 | 1.40 | 1.46 |
| 24 | b | 617 | BCR | C33-C5 | -2.52 | 1.46 | 1.50 |
| 22 | b | 609 | CLA | CMD-C2D | -2.51 | 1.45 | 1.50 |
| 28 | A | 412 | SQD | O47-C7 | 2.51 | 1.41 | 1.34 |
| 23 | d | 401 | PHO | C3B-C2B | -2.51 | 1.37 | 1.40 |
| 29 | c | 519 | DGD | C1D-C2D | 2.51 | 1.59 | 1.52 |
| 22 | C | 501 | CLA | C1D-ND | 2.51 | 1.41 | 1.37 |
| 22 | b | 605 | CLA | MG-ND | 2.51 | 2.10 | 2.05 |
| 22 | b | 604 | CLA | CMC-C2C | -2.50 | 1.45 | 1.50 |
| 29 | H | 102 | DGD | C3E-C2E | 2.50 | 1.58 | 1.52 |
| 29 | c | 517 | DGD | O2G-C2G | -2.50 | 1.40 | 1.46 |
| 22 | b | 601 | CLA | O2A-CGA | 2.50 | 1.40 | 1.33 |
| 23 | A | 404 | PHO | CAC-C3C | -2.50 | 1.47 | 1.52 |
| 22 | b | 609 | CLA | C1D-ND | 2.50 | 1.41 | 1.37 |
| 29 | C | 517 | DGD | O2G-C2G | -2.49 | 1.40 | 1.46 |
| 22 | a | 404 | CLA | CMD-C2D | -2.49 | 1.45 | 1.50 |
| 22 | b | 616 | CLA | CHC-C1C | 2.49 | 1.40 | 1.34 |
| 22 | c | 508 | CLA | C1D-ND | 2.48 | 1.41 | 1.37 |
| 22 | C | 507 | CLA | C1D-ND | 2.48 | 1.41 | 1.37 |
| 29 | C | 518 | DGD | O1G-C1G | -2.48 | 1.39 | 1.45 |
| 22 | b | 610 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 22 | B | 607 | CLA | CMC-C2C | -2.48 | 1.45 | 1.50 |
| 22 | c | 510 | CLA | C3B-C2B | -2.48 | 1.37 | 1.40 |
| 22 | B | 605 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 27 | b | 622 | LMG | C3-C2 | 2.47 | 1.58 | 1.52 |
| 22 | b | 602 | CLA | C1D-ND | 2.46 | 1.41 | 1.37 |
| 22 | d | 405 | CLA | MG-ND | -2.46 | 2.00 | 2.05 |
| 22 | b | 616 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 22 | B | 616 | CLA | CHC-C1C | 2.46 | 1.40 | 1.34 |
| 22 | B | 603 | CLA | CMA-C3A | -2.45 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | b | 610 | CLA | CMD-C2D | -2.45 | 1.45 | 1.50 |
| 22 | C | 502 | CLA | MG-ND | -2.45 | 2.00 | 2.05 |
| 22 | b | 606 | CLA | MG-ND | 2.45 | 2.10 | 2.05 |
| 22 | b | 612 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |
| 22 | B | 615 | CLA | C3B-C2B | -2.45 | 1.37 | 1.40 |
| 27 | d | 412 | LMG | O7-C8 | -2.44 | 1.40 | 1.46 |
| 33 | D | 409 | LHG | C3-C2 | 2.44 | 1.59 | 1.51 |
| 22 | B | 616 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 27 | b | 620 | LMG | O1-C7 | -2.44 | 1.39 | 1.43 |
| 22 | b | 603 | CLA | C4B-CHC | -2.44 | 1.34 | 1.41 |
| 29 | H | 102 | DGD | C1E-C2E | 2.44 | 1.59 | 1.52 |
| 29 | c | 517 | DGD | C4D-C3D | 2.43 | 1.58 | 1.52 |
| 22 | B | 604 | CLA | C1D-ND | 2.43 | 1.41 | 1.37 |
| 29 | C | 517 | DGD | C4D-C5D | 2.43 | 1.58 | 1.53 |
| 27 | M | 101 | LMG | C9-C8 | 2.43 | 1.58 | 1.50 |
| 22 | C | 508 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 22 | D | 403 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 29 | C | 516 | DGD | C2A-C1A | -2.43 | 1.43 | 1.50 |
| 29 | C | 516 | DGD | O1G-C1G | -2.43 | 1.39 | 1.45 |
| 22 | B | 603 | CLA | MG-NC | -2.42 | 2.00 | 2.06 |
| 22 | c | 502 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 22 | B | 609 | CLA | C4B-CHC | -2.42 | 1.34 | 1.41 |
| 35 | E | 101 | HEM | C3C-CAC | 2.41 | 1.53 | 1.47 |
| 22 | a | 404 | CLA | O1D-CGD | 2.41 | 1.27 | 1.21 |
| 24 | t | 101 | BCR | C1-C6 | -2.41 | 1.50 | 1.53 |
| 22 | D | 404 | CLA | CHC-C1C | 2.41 | 1.40 | 1.34 |
| 22 | B | 603 | CLA | MG-NA | 2.41 | 2.12 | 2.06 |
| 23 | D | 401 | PHO | CMB-C2B | -2.41 | 1.45 | 1.51 |
| 26 | d | 407 | PL9 | C41-C39 | -2.41 | 1.46 | 1.51 |
| 29 | c | 519 | DGD | C2A-C1A | -2.41 | 1.43 | 1.50 |
| 24 | c | 515 | BCR | C33-C5 | -2.40 | 1.47 | 1.50 |
| 22 | C | 512 | CLA | CMD-C2D | -2.40 | 1.45 | 1.50 |
| 29 | C | 518 | DGD | O3G-C3G | -2.40 | 1.39 | 1.43 |
| 22 | b | 601 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 22 | b | 602 | CLA | MG-NC | -2.40 | 2.00 | 2.06 |
| 22 | b | 602 | CLA | C4B-CHC | -2.40 | 1.34 | 1.41 |
| 22 | B | 602 | CLA | CMC-C2C | -2.40 | 1.45 | 1.50 |
| 24 | C | 515 | BCR | C1-C6 | -2.40 | 1.50 | 1.53 |
| 22 | c | 511 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 22 | C | 501 | CLA | CMC-C2C | -2.39 | 1.45 | 1.50 |
| 22 | B | 607 | CLA | C3B-C2B | -2.39 | 1.37 | 1.40 |
| 22 | c | 501 | CLA | CMC-C2C | -2.39 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | b | 605 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 29 | h | 102 | DGD | C2A-C1A | -2.39 | 1.43 | 1.50 |
| 22 | C | 510 | CLA | C1D-ND | 2.38 | 1.41 | 1.37 |
| 24 | B | 618 | BCR | C33-C5 | -2.38 | 1.47 | 1.50 |
| 22 | B | 615 | CLA | CAC-C3C | -2.38 | 1.45 | 1.51 |
| 33 | D | 408 | LHG | O8-C6 | -2.38 | 1.39 | 1.45 |
| 33 | D | 408 | LHG | P-O4 | -2.38 | 1.44 | 1.55 |
| 22 | b | 611 | CLA | MG-NC | -2.37 | 2.00 | 2.06 |
| 29 | a | 412 | DGD | C1G-C2G | 2.37 | 1.58 | 1.50 |
| 23 | d | 401 | PHO | CBD-CGD | -2.37 | 1.49 | 1.52 |
| 22 | B | 602 | CLA | MG-NA | 2.37 | 2.11 | 2.06 |
| 24 | B | 618 | BCR | C1-C6 | -2.37 | 1.50 | 1.53 |
| 22 | c | 506 | CLA | C4B-CHC | -2.37 | 1.34 | 1.41 |
| 22 | c | 506 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 28 | a | 410 | SQD | O4-C4 | -2.37 | 1.37 | 1.43 |
| 35 | f | 101 | HEM | CAB-C3B | 2.37 | 1.53 | 1.47 |
| 29 | h | 102 | DGD | O5D-C6D | -2.37 | 1.39 | 1.43 |
| 24 | T | 101 | BCR | C27-C26 | -2.37 | 1.46 | 1.51 |
| 22 | b | 611 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 22 | A | 403 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 22 | C | 503 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 28 | L | 101 | SQD | O2-C2 | -2.36 | 1.37 | 1.43 |
| 22 | B | 603 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 27 | D | 410 | LMG | C9-C8 | 2.35 | 1.58 | 1.50 |
| 22 | C | 511 | CLA | C4B-CHC | -2.35 | 1.34 | 1.41 |
| 32 | b | 623 | STE | C2-C1 | 2.35 | 1.56 | 1.50 |
| 22 | d | 403 | CLA | CMD-C2D | -2.35 | 1.46 | 1.50 |
| 29 | H | 102 | DGD | C6D-C5D | 2.34 | 1.58 | 1.51 |
| 27 | b | 622 | LMG | O1-C7 | -2.34 | 1.39 | 1.43 |
| 32 | B | 627 | STE | O1-C1 | 2.34 | 1.29 | 1.22 |
| 24 | b | 618 | BCR | C33-C5 | -2.34 | 1.47 | 1.50 |
| 22 | C | 501 | CLA | C3B-C2B | -2.34 | 1.37 | 1.40 |
| 29 | H | 102 | DGD | C1G-C2G | 2.33 | 1.58 | 1.50 |
| 22 | c | 507 | CLA | CHC-C1C | 2.33 | 1.40 | 1.34 |
| 22 | c | 512 | CLA | CMC-C2C | -2.33 | 1.46 | 1.50 |
| 29 | h | 102 | DGD | C1E-C2E | 2.33 | 1.59 | 1.52 |
| 24 | C | 514 | BCR | C30-C25 | -2.33 | 1.50 | 1.53 |
| 22 | B | 616 | CLA | CMC-C2C | -2.33 | 1.46 | 1.50 |
| 22 | C | 501 | CLA | CMD-C2D | -2.32 | 1.46 | 1.50 |
| 29 | C | 516 | DGD | O5D-C6D | -2.32 | 1.39 | 1.43 |
| 22 | b | 607 | CLA | CMC-C2C | -2.32 | 1.46 | 1.50 |
| 22 | b | 615 | CLA | CMC-C2C | -2.31 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 510 | CLA | CMC-C2C | -2.31 | 1.46 | 1.50 |
| 22 | c | 503 | CLA | CMC-C2C | -2.31 | 1.46 | 1.50 |
| 22 | c | 505 | CLA | CMC-C2C | -2.31 | 1.46 | 1.50 |
| 28 | f | 102 | SQD | O3-C3 | -2.31 | 1.37 | 1.43 |
| 27 | d | 412 | LMG | O3-C3 | -2.31 | 1.37 | 1.43 |
| 22 | c | 507 | CLA | CMC-C2C | -2.30 | 1.46 | 1.50 |
| 29 | h | 102 | DGD | C4E-C3E | 2.30 | 1.58 | 1.52 |
| 22 | B | 612 | CLA | C4B-CHC | -2.30 | 1.34 | 1.41 |
| 22 | B | 604 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 35 | f | 101 | HEM | C3C-C4C | 2.30 | 1.44 | 1.41 |
| 22 | C | 501 | CLA | CMB-C2B | -2.30 | 1.47 | 1.51 |
| 22 | B | 601 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 24 | B | 618 | BCR | C36-C18 | -2.29 | 1.46 | 1.50 |
| 22 | A | 403 | CLA | CAA-C2A | -2.28 | 1.49 | 1.54 |
| 29 | c | 517 | DGD | O3G-C3G | -2.28 | 1.39 | 1.43 |
| 22 | c | 501 | CLA | C4B-CHC | -2.28 | 1.34 | 1.41 |
| 23 | d | 402 | PHO | CMD-C2D | -2.28 | 1.46 | 1.51 |
| 22 | B | 607 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 33 | D | 408 | LHG | P-O6 | 2.28 | 1.68 | 1.59 |
| 22 | c | 506 | CLA | CAC-C3C | -2.28 | 1.45 | 1.51 |
| 27 | A | 411 | LMG | C4-C5 | 2.28 | 1.57 | 1.53 |
| 22 | c | 503 | CLA | O2D-CGD | 2.28 | 1.38 | 1.33 |
| 22 | C | 501 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 22 | A | 405 | CLA | CMB-C2B | -2.27 | 1.47 | 1.51 |
| 29 | c | 518 | DGD | O6D-C5D | -2.27 | 1.38 | 1.44 |
| 22 | B | 609 | CLA | CHC-C1C | 2.27 | 1.40 | 1.34 |
| 22 | d | 405 | CLA | O2D-CGD | 2.27 | 1.38 | 1.33 |
| 33 | E | 102 | LHG | O8-C23 | 2.27 | 1.40 | 1.33 |
| 26 | D | 406 | PL9 | C21-C19 | -2.26 | 1.46 | 1.51 |
| 22 | b | 615 | CLA | C1D-ND | 2.26 | 1.40 | 1.37 |
| 28 | F | 101 | SQD | O3-C3 | -2.26 | 1.37 | 1.43 |
| 27 | C | 519 | LMG | O1-C1 | 2.26 | 1.44 | 1.40 |
| 22 | b | 611 | CLA | CMB-C2B | -2.26 | 1.47 | 1.51 |
| 22 | A | 402 | CLA | CMB-C2B | -2.26 | 1.47 | 1.51 |
| 22 | B | 613 | CLA | C1D-ND | 2.25 | 1.40 | 1.37 |
| 29 | c | 519 | DGD | O4E-C4E | -2.25 | 1.37 | 1.43 |
| 22 | b | 602 | CLA | CAC-C3C | -2.25 | 1.45 | 1.51 |
| 22 | b | 610 | CLA | C4B-CHC | -2.25 | 1.34 | 1.41 |
| 24 | k | 101 | BCR | C36-C18 | -2.25 | 1.46 | 1.50 |
| 22 | c | 504 | CLA | CMB-C2B | -2.25 | 1.47 | 1.51 |
| 22 | C | 512 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 33 | d | 410 | LHG | O8-C23 | 2.24 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | C | 518 | DGD | O4D-C4D | -2.24 | 1.37 | 1.43 |
| 27 | b | 622 | LMG | C1-C2 | 2.24 | 1.59 | 1.52 |
| 24 | t | 101 | BCR | C38-C26 | -2.23 | 1.47 | 1.50 |
| 22 | b | 608 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 22 | B | 602 | CLA | MG-ND | -2.23 | 2.01 | 2.05 |
| 22 | c | 506 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 33 | D | 408 | LHG | C8-C7 | -2.23 | 1.44 | 1.50 |
| 22 | b | 614 | CLA | O2D-CED | -2.23 | 1.40 | 1.45 |
| 22 | B | 611 | CLA | MG-NA | 2.23 | 2.11 | 2.06 |
| 22 | b | 603 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 36 | v | 201 | HEC | C1D-CHD | -2.23 | 1.34 | 1.41 |
| 22 | A | 405 | CLA | C4B-CHC | -2.22 | 1.34 | 1.41 |
| 29 | h | 102 | DGD | O4D-C4D | -2.22 | 1.37 | 1.43 |
| 29 | C | 517 | DGD | C1E-C2E | 2.22 | 1.59 | 1.52 |
| 22 | b | 605 | CLA | MG-NA | 2.22 | 2.11 | 2.06 |
| 24 | a | 405 | BCR | C35-C13 | -2.22 | 1.46 | 1.50 |
| 22 | B | 608 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 27 | C | 519 | LMG | O7-C8 | -2.21 | 1.41 | 1.46 |
| 22 | c | 512 | CLA | C1D-C2D | 2.21 | 1.49 | 1.45 |
| 22 | D | 404 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 22 | d | 405 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 22 | B | 616 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 23 | D | 401 | PHO | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 22 | b | 616 | CLA | O2D-CED | -2.20 | 1.40 | 1.45 |
| 22 | C | 504 | CLA | MG-ND | -2.20 | 2.01 | 2.05 |
| 24 | a | 405 | BCR | C38-C26 | -2.20 | 1.47 | 1.50 |
| 22 | C | 510 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 27 | c | 522 | LMG | C1-C2 | 2.19 | 1.58 | 1.52 |
| 22 | C | 502 | CLA | C1D-ND | 2.19 | 1.40 | 1.37 |
| 22 | a | 404 | CLA | CHC-C1C | 2.19 | 1.40 | 1.34 |
| 22 | c | 511 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 22 | B | 601 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 22 | D | 404 | CLA | C4B-CHC | -2.19 | 1.34 | 1.41 |
| 23 | A | 404 | PHO | CMD-C2D | -2.19 | 1.46 | 1.51 |
| 22 | b | 613 | CLA | CHC-C1C | 2.18 | 1.39 | 1.34 |
| 22 | b | 610 | CLA | C3D-C4D | 2.18 | 1.49 | 1.44 |
| 22 | b | 609 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 24 | C | 515 | BCR | C38-C26 | -2.18 | 1.47 | 1.50 |
| 29 | c | 519 | DGD | O3G-C1D | 2.18 | 1.43 | 1.40 |
| 27 | c | 520 | LMG | C1-C2 | 2.18 | 1.58 | 1.52 |
| 27 | C | 519 | LMG | C6-C5 | 2.17 | 1.59 | 1.51 |
| 22 | B | 613 | CLA | C5-C3 | -2.17 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | c | 513 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 27 | d | 412 | LMG | C7-C8 | 2.16 | 1.57 | 1.50 |
| 22 | b | 606 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 27 | b | 620 | LMG | C1-C2 | 2.16 | 1.58 | 1.52 |
| 26 | d | 407 | PL9 | C43-C44 | -2.16 | 1.28 | 1.33 |
| 22 | C | 504 | CLA | CAC-C3C | -2.16 | 1.45 | 1.51 |
| 22 | b | 603 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 22 | C | 508 | CLA | C1D-C2D | 2.16 | 1.49 | 1.45 |
| 22 | C | 506 | CLA | C3D-C4D | 2.15 | 1.49 | 1.44 |
| 29 | h | 102 | DGD | O2G-C1B | 2.15 | 1.40 | 1.34 |
| 22 | C | 509 | CLA | O2D-CED | -2.15 | 1.40 | 1.45 |
| 22 | b | 610 | CLA | CHC-C1C | 2.15 | 1.39 | 1.34 |
| 22 | b | 609 | CLA | C4B-CHC | -2.15 | 1.35 | 1.41 |
| 23 | d | 402 | PHO | CAA-C2A | -2.15 | 1.49 | 1.54 |
| 22 | c | 501 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 22 | C | 509 | CLA | O2A-CGA | 2.14 | 1.39 | 1.33 |
| 22 | b | 610 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 29 | H | 102 | DGD | O1G-C1G | -2.13 | 1.40 | 1.45 |
| 29 | h | 102 | DGD | O2E-C2E | -2.13 | 1.37 | 1.43 |
| 26 | D | 406 | PL9 | C3-C4 | -2.13 | 1.46 | 1.49 |
| 22 | A | 402 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 27 | M | 101 | LMG | C4-C3 | 2.13 | 1.57 | 1.52 |
| 29 | C | 516 | DGD | O5D-C1E | 2.13 | 1.43 | 1.40 |
| 26 | a | 409 | PL9 | C25-C24 | -2.13 | 1.45 | 1.50 |
| 22 | C | 509 | CLA | O2D-CGD | 2.13 | 1.38 | 1.33 |
| 33 | E | 102 | LHG | C24-C23 | 2.12 | 1.56 | 1.50 |
| 22 | A | 410 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 27 | b | 622 | LMG | O6-C1 | 2.12 | 1.47 | 1.41 |
| 22 | c | 503 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 22 | c | 503 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 22 | C | 510 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 22 | c | 505 | CLA | CMB-C2B | -2.12 | 1.47 | 1.51 |
| 29 | C | 518 | DGD | C2A-C1A | -2.12 | 1.44 | 1.50 |
| 22 | b | 602 | CLA | C1A-CHA | -2.12 | 1.34 | 1.43 |
| 33 | d | 409 | LHG | O7-C5 | -2.12 | 1.41 | 1.46 |
| 27 | c | 523 | LMG | O6-C5 | -2.12 | 1.39 | 1.44 |
| 22 | b | 608 | CLA | C3C-C2C | 2.12 | 1.41 | 1.36 |
| 28 | A | 412 | SQD | O47-C45 | -2.11 | 1.41 | 1.46 |
| 27 | b | 622 | LMG | O1-C1 | 2.11 | 1.43 | 1.40 |
| 24 | h | 101 | BCR | C1-C6 | -2.11 | 1.51 | 1.53 |
| 22 | b | 612 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 22 | b | 603 | CLA | MG-NC | -2.11 | 2.01 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 610 | CLA | C1A-CHA | -2.10 | 1.34 | 1.43 |
| 22 | c | 505 | CLA | C1D-ND | 2.10 | 1.40 | 1.37 |
| 22 | b | 608 | CLA | MG-NA | 2.10 | 2.11 | 2.06 |
| 29 | H | 102 | DGD | O2G-C2G | -2.10 | 1.41 | 1.46 |
| 36 | v | 201 | HEC | O1D-CGD | 2.10 | 1.29 | 1.22 |
| 22 | b | 615 | CLA | C4B-CHC | -2.10 | 1.35 | 1.41 |
| 29 | C | 518 | DGD | O5D-C6D | -2.10 | 1.40 | 1.43 |
| 22 | C | 512 | CLA | C5-C3 | -2.10 | 1.47 | 1.51 |
| 29 | C | 518 | DGD | O5D-C1E | 2.09 | 1.43 | 1.40 |
| 29 | c | 517 | DGD | O5D-C1E | 2.09 | 1.43 | 1.40 |
| 22 | C | 508 | CLA | C3D-C4D | 2.09 | 1.48 | 1.44 |
| 26 | A | 409 | PL9 | C37-C38 | 2.09 | 1.56 | 1.50 |
| 24 | B | 619 | BCR | C31-C1 | -2.09 | 1.49 | 1.53 |
| 24 | D | 405 | BCR | C27-C26 | -2.09 | 1.47 | 1.51 |
| 33 | B | 622 | LHG | P-O4 | -2.09 | 1.45 | 1.55 |
| 27 | C | 519 | LMG | C1-C2 | 2.09 | 1.58 | 1.52 |
| 29 | C | 518 | DGD | C3B-C2B | -2.09 | 1.44 | 1.52 |
| 22 | c | 509 | CLA | C4B-CHC | -2.08 | 1.35 | 1.41 |
| 22 | b | 615 | CLA | MG-NC | -2.08 | 2.01 | 2.06 |
| 24 | b | 618 | BCR | C36-C18 | -2.08 | 1.46 | 1.50 |
| 22 | b | 611 | CLA | C4B-CHC | -2.08 | 1.35 | 1.41 |
| 22 | b | 605 | CLA | C4B-CHC | -2.08 | 1.35 | 1.41 |
| 32 | D | 411 | STE | O1-C1 | 2.08 | 1.28 | 1.22 |
| 22 | A | 410 | CLA | C1D-C2D | 2.08 | 1.49 | 1.45 |
| 22 | c | 510 | CLA | CAA-C2A | -2.07 | 1.50 | 1.54 |
| 35 | E | 101 | HEM | CHC-C4B | -2.07 | 1.35 | 1.40 |
| 22 | b | 603 | CLA | C3D-C4D | 2.07 | 1.48 | 1.44 |
| 22 | c | 512 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 27 | c | 522 | LMG | O1-C7 | -2.07 | 1.40 | 1.43 |
| 22 | B | 603 | CLA | C1A-CHA | -2.06 | 1.34 | 1.43 |
| 29 | C | 518 | DGD | C6D-C5D | 2.06 | 1.57 | 1.51 |
| 22 | C | 511 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 33 | d | 408 | LHG | O6-C4 | -2.06 | 1.36 | 1.44 |
| 22 | b | 616 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 33 | d | 409 | LHG | O6-C4 | -2.06 | 1.36 | 1.44 |
| 22 | C | 505 | CLA | C4B-CHC | -2.06 | 1.35 | 1.41 |
| 22 | B | 613 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 22 | B | 607 | CLA | CMB-C2B | -2.06 | 1.47 | 1.51 |
| 22 | b | 604 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 22 | C | 508 | CLA | CAC-C3C | -2.05 | 1.45 | 1.51 |
| 24 | k | 101 | BCR | C33-C5 | -2.05 | 1.47 | 1.50 |
| 27 | b | 622 | LMG | C4-C5 | 2.05 | 1.57 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | C | 512 | CLA | C1D-C2D | 2.04 | 1.49 | 1.45 |
| 22 | C | 513 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |
| 23 | A | 404 | PHO | CBD-CGD | -2.04 | 1.49 | 1.52 |
| 22 | B | 606 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 22 | B | 604 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 24 | k | 101 | BCR | C38-C26 | -2.04 | 1.47 | 1.50 |
| 22 | c | 508 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |
| 27 | A | 411 | LMG | C1-C2 | 2.03 | 1.58 | 1.52 |
| 27 | D | 410 | LMG | O8-C28 | 2.03 | 1.39 | 1.33 |
| 32 | c | 521 | STE | C2-C1 | 2.03 | 1.55 | 1.50 |
| 22 | b | 604 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 23 | d | 401 | PHO | C1C-NC | -2.03 | 1.32 | 1.38 |
| 22 | d | 405 | CLA | O1D-CGD | 2.03 | 1.26 | 1.21 |
| 22 | d | 405 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 26 | A | 409 | PL9 | C41-C39 | 2.03 | 1.55 | 1.51 |
| 22 | A | 402 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 22 | B | 614 | CLA | C1A-CHA | -2.03 | 1.34 | 1.43 |
| 35 | E | 101 | HEM | C3D-C2D | -2.03 | 1.32 | 1.36 |
| 29 | c | 517 | DGD | O3E-C3E | -2.03 | 1.37 | 1.43 |
| 22 | c | 510 | CLA | C5-C3 | -2.03 | 1.47 | 1.51 |
| 22 | d | 403 | CLA | C4B-CHC | -2.03 | 1.35 | 1.41 |
| 22 | b | 613 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 22 | B | 605 | CLA | C4B-CHC | -2.02 | 1.35 | 1.41 |
| 22 | A | 410 | CLA | O2D-CED | -2.02 | 1.40 | 1.45 |
| 33 | d | 410 | LHG | C6-C5 | 2.02 | 1.57 | 1.50 |
| 22 | c | 513 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 22 | c | 507 | CLA | C4B-CHC | -2.02 | 1.35 | 1.41 |
| 23 | D | 401 | PHO | CMD-C2D | -2.01 | 1.46 | 1.51 |
| 26 | A | 409 | PL9 | C25-C24 | -2.01 | 1.45 | 1.50 |
| 22 | c | 512 | CLA | C3D-C4D | 2.01 | 1.48 | 1.44 |
| 22 | b | 605 | CLA | MG-NC | -2.01 | 2.01 | 2.06 |
| 22 | A | 405 | CLA | CHC-C1C | 2.01 | 1.39 | 1.34 |
| 22 | b | 609 | CLA | C1A-CHA | -2.01 | 1.34 | 1.43 |
| 29 | C | 516 | DGD | C3E-C2E | 2.01 | 1.57 | 1.52 |
| 24 | C | 515 | BCR | C33-C5 | -2.01 | 1.47 | 1.50 |
| 27 | D | 407 | LMG | C7-C8 | 2.01 | 1.57 | 1.50 |
| 22 | B | 603 | CLA | O2D-CGD | 2.00 | 1.38 | 1.33 |
| 33 | d | 408 | LHG | P-O6 | 2.00 | 1.67 | 1.59 |
| 22 | A | 405 | CLA | CAC-C3C | -2.00 | 1.46 | 1.51 |
| 22 | B | 616 | CLA | CMB-C2B | -2.00 | 1.47 | 1.51 |
| 22 | b | 614 | CLA | C1A-CHA | -2.00 | 1.34 | 1.43 |

All (1264) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | c | 509 | CLA | C4A-NA-C1A | 9.84 | 111.17 | 106.68 |
| 28 | L | 101 | SQD | O6-C1-C2 | 9.53 | 122.74 | 108.27 |
| 22 | c | 511 | CLA | C4A-NA-C1A | 9.36 | 110.95 | 106.68 |
| 22 | B | 616 | CLA | C4A-NA-C1A | 9.28 | 110.91 | 106.68 |
| 22 | C | 507 | CLA | C4A-NA-C1A | 9.25 | 110.90 | 106.68 |
| 22 | B | 607 | CLA | C4A-NA-C1A | 8.80 | 110.69 | 106.68 |
| 22 | C | 501 | CLA | C4A-NA-C1A | 8.69 | 110.64 | 106.68 |
| 28 | a | 410 | SQD | O6-C1-C2 | 8.62 | 121.37 | 108.27 |
| 22 | B | 601 | CLA | C4A-NA-C1A | 8.45 | 110.53 | 106.68 |
| 36 | V | 201 | HEC | CBB-CAB-C3B | -8.41 | 107.80 | 127.49 |
| 22 | b | 601 | CLA | C4A-NA-C1A | 8.37 | 110.50 | 106.68 |
| 28 | A | 412 | SQD | O6-C1-C2 | 8.29 | 120.86 | 108.27 |
| 22 | B | 604 | CLA | C4A-NA-C1A | 8.27 | 110.45 | 106.68 |
| 22 | B | 615 | CLA | C4A-NA-C1A | 7.71 | 110.20 | 106.68 |
| 22 | b | 606 | CLA | C4A-NA-C1A | 7.49 | 110.09 | 106.68 |
| 36 | v | 201 | HEC | CBB-CAB-C3B | -7.36 | 110.27 | 127.49 |
| 22 | C | 506 | CLA | C4A-NA-C1A | 7.08 | 109.91 | 106.68 |
| 22 | c | 503 | CLA | C4A-NA-C1A | 7.08 | 109.91 | 106.68 |
| 22 | b | 604 | CLA | C4A-NA-C1A | 6.96 | 109.85 | 106.68 |
| 28 | B | 623 | SQD | O6-C1-C2 | 6.95 | 118.82 | 108.27 |
| 22 | b | 616 | CLA | CMB-C2B-C1B | -6.89 | 118.36 | 128.46 |
| 36 | V | 201 | HEC | CBC-CAC-C3C | -6.76 | 111.66 | 127.49 |
| 22 | C | 513 | CLA | C4A-NA-C1A | 6.73 | 109.75 | 106.68 |
| 22 | d | 404 | CLA | C4A-NA-C1A | 6.32 | 109.56 | 106.68 |
| 22 | c | 508 | CLA | C4A-NA-C1A | 6.31 | 109.56 | 106.68 |
| 22 | c | 512 | CLA | C4A-NA-C1A | 6.29 | 109.55 | 106.68 |
| 22 | D | 404 | CLA | C4A-NA-C1A | 6.28 | 109.54 | 106.68 |
| 36 | v | 201 | HEC | CBC-CAC-C3C | -6.27 | 112.81 | 127.49 |
| 22 | D | 404 | CLA | CMB-C2B-C1B | -6.26 | 119.28 | 128.46 |
| 26 | D | 406 | PL9 | C7-C3-C4 | 6.23 | 122.04 | 116.91 |
| 22 | C | 508 | CLA | C4A-NA-C1A | 6.22 | 109.52 | 106.68 |
| 22 | C | 503 | CLA | C4A-NA-C1A | 6.22 | 109.52 | 106.68 |
| 22 | b | 612 | CLA | CMB-C2B-C1B | -6.18 | 119.41 | 128.46 |
| 22 | B | 602 | CLA | C4A-NA-C1A | 6.12 | 109.47 | 106.68 |
| 22 | B | 602 | CLA | CMB-C2B-C1B | -5.94 | 119.75 | 128.46 |
| 22 | c | 501 | CLA | C4A-NA-C1A | 5.82 | 109.33 | 106.68 |
| 22 | C | 509 | CLA | CMB-C2B-C1B | -5.81 | 119.94 | 128.46 |
| 22 | B | 608 | CLA | O2D-CGD-O1D | -5.74 | 112.67 | 123.85 |
| 22 | b | 616 | CLA | CMB-C2B-C3B | 5.71 | 136.09 | 124.68 |
| 22 | b | 608 | CLA | CMB-C2B-C1B | -5.70 | 120.10 | 128.46 |
| 22 | a | 403 | CLA | CMB-C2B-C1B | -5.70 | 120.11 | 128.46 |
| 22 | c | 504 | CLA | C4A-NA-C1A | 5.55 | 109.21 | 106.68 |
| 22 | b | 613 | CLA | C4A-NA-C1A | 5.54 | 109.21 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 402 | CLA | C4A-NA-C1A | 5.53 | 109.20 | 106.68 |
| 28 | L | 101 | SQD | O7-S-C6 | 5.43 | 114.86 | 106.76 |
| 22 | d | 405 | CLA | CMB-C2B-C1B | -5.41 | 120.52 | 128.46 |
| 22 | c | 504 | CLA | CMB-C2B-C1B | -5.40 | 120.54 | 128.46 |
| 22 | c | 513 | CLA | CMB-C2B-C1B | -5.38 | 120.57 | 128.46 |
| 22 | B | 608 | CLA | CMB-C2B-C1B | -5.33 | 120.64 | 128.46 |
| 22 | B | 613 | CLA | CMB-C2B-C1B | -5.33 | 120.65 | 128.46 |
| 22 | C | 511 | CLA | C4A-NA-C1A | 5.32 | 109.11 | 106.68 |
| 22 | b | 606 | CLA | CMB-C2B-C1B | -5.32 | 120.67 | 128.46 |
| 22 | c | 510 | CLA | C4A-NA-C1A | 5.32 | 109.10 | 106.68 |
| 22 | B | 608 | CLA | C4A-NA-C1A | 5.30 | 109.10 | 106.68 |
| 26 | d | 407 | PL9 | C7-C3-C4 | 5.26 | 121.24 | 116.91 |
| 22 | A | 405 | CLA | CMB-C2B-C1B | -5.23 | 120.79 | 128.46 |
| 22 | c | 505 | CLA | C4A-NA-C1A | 5.21 | 109.06 | 106.68 |
| 22 | b | 609 | CLA | CMB-C2B-C1B | -5.18 | 120.86 | 128.46 |
| 22 | a | 402 | CLA | CMB-C2B-C1B | -5.16 | 120.89 | 128.46 |
| 22 | c | 501 | CLA | O2D-CGD-O1D | -5.16 | 113.80 | 123.85 |
| 22 | b | 615 | CLA | C4A-NA-C1A | 5.16 | 109.03 | 106.68 |
| 22 | b | 603 | CLA | C4A-NA-C1A | 5.14 | 109.02 | 106.68 |
| 22 | c | 508 | CLA | CMB-C2B-C1B | -5.12 | 120.96 | 128.46 |
| 26 | d | 407 | PL9 | C40-C39-C41 | 5.09 | 124.06 | 115.23 |
| 22 | C | 509 | CLA | C4A-NA-C1A | 5.08 | 109.00 | 106.68 |
| 22 | B | 604 | CLA | CMB-C2B-C1B | -5.08 | 121.01 | 128.46 |
| 22 | a | 403 | CLA | C4A-NA-C1A | 5.06 | 108.99 | 106.68 |
| 22 | B | 606 | CLA | C4A-NA-C1A | 5.05 | 108.98 | 106.68 |
| 26 | a | 409 | PL9 | C7-C3-C4 | 5.05 | 121.07 | 116.91 |
| 22 | B | 612 | CLA | CMB-C2B-C1B | -5.04 | 121.07 | 128.46 |
| 22 | B | 610 | CLA | O2D-CGD-O1D | -5.04 | 114.04 | 123.85 |
| 22 | C | 508 | CLA | CMB-C2B-C1B | -5.03 | 121.09 | 128.46 |
| 28 | a | 410 | SQD | C1-O5-C5 | -5.03 | 103.90 | 113.72 |
| 22 | C | 505 | CLA | C4A-NA-C1A | 5.00 | 108.96 | 106.68 |
| 22 | c | 506 | CLA | C4A-NA-C1A | 4.98 | 108.95 | 106.68 |
| 22 | B | 612 | CLA | C4A-NA-C1A | 4.95 | 108.94 | 106.68 |
| 22 | b | 615 | CLA | CMB-C2B-C1B | -4.94 | 121.22 | 128.46 |
| 22 | a | 402 | CLA | C4A-NA-C1A | 4.91 | 108.92 | 106.68 |
| 28 | A | 412 | SQD | O8-S-C6 | 4.90 | 115.43 | 105.97 |
| 22 | c | 510 | CLA | CMB-C2B-C1B | -4.90 | 121.28 | 128.46 |
| 36 | V | 201 | HEC | CMC-C2C-C1C | -4.85 | 121.35 | 128.46 |
| 22 | b | 611 | CLA | C4A-NA-C1A | 4.85 | 108.89 | 106.68 |
| 22 | b | 602 | CLA | CMB-C2B-C1B | -4.84 | 121.36 | 128.46 |
| 22 | B | 612 | CLA | CMB-C2B-C3B | 4.84 | 134.35 | 124.68 |
| 26 | A | 409 | PL9 | C7-C3-C4 | 4.81 | 120.87 | 116.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | D | 404 | CLA | O2D-CGD-O1D | -4.77 | 114.56 | 123.85 |
| 22 | A | 402 | CLA | CMB-C2B-C1B | -4.77 | 121.47 | 128.46 |
| 22 | c | 502 | CLA | C4A-NA-C1A | 4.73 | 108.84 | 106.68 |
| 33 | L | 102 | LHG | O4-P-O5 | 4.70 | 134.32 | 112.44 |
| 23 | A | 404 | PHO | O2D-CGD-CBD | 4.70 | 116.11 | 110.95 |
| 28 | F | 101 | SQD | O6-C1-C2 | 4.69 | 115.40 | 108.27 |
| 22 | b | 613 | CLA | CMB-C2B-C1B | -4.67 | 121.61 | 128.46 |
| 22 | d | 403 | CLA | CMB-C2B-C1B | -4.66 | 121.62 | 128.46 |
| 22 | B | 605 | CLA | C4A-NA-C1A | 4.64 | 108.80 | 106.68 |
| 34 | D | 402 | BCT | O2-C-O1 | 4.63 | 131.53 | 119.68 |
| 22 | C | 511 | CLA | CMB-C2B-C1B | -4.61 | 121.69 | 128.46 |
| 28 | F | 101 | SQD | O9-S-C6 | 4.61 | 113.65 | 106.76 |
| 22 | C | 510 | CLA | CMB-C2B-C1B | -4.60 | 121.72 | 128.46 |
| 22 | c | 513 | CLA | C4A-NA-C1A | 4.58 | 108.77 | 106.68 |
| 22 | C | 510 | CLA | C4A-NA-C1A | 4.57 | 108.77 | 106.68 |
| 22 | C | 509 | CLA | CMB-C2B-C3B | 4.57 | 133.82 | 124.68 |
| 29 | H | 102 | DGD | O3G-C3G-C2G | -4.56 | 99.72 | 110.82 |
| 22 | c | 506 | CLA | CMB-C2B-C1B | -4.56 | 121.78 | 128.46 |
| 28 | A | 412 | SQD | O7-S-C6 | 4.55 | 113.55 | 106.76 |
| 22 | B | 602 | CLA | O2D-CGD-CBD | 4.55 | 119.19 | 111.23 |
| 29 | A | 414 | DGD | C4E-C3E-C2E | -4.55 | 102.85 | 110.83 |
| 26 | A | 409 | PL9 | C20-C19-C21 | 4.54 | 123.12 | 115.23 |
| 22 | B | 611 | CLA | CMB-C2B-C1B | -4.54 | 121.81 | 128.46 |
| 22 | b | 602 | CLA | C4A-NA-C1A | 4.53 | 108.75 | 106.68 |
| 22 | c | 509 | CLA | CMB-C2B-C1B | -4.50 | 121.86 | 128.46 |
| 33 | e | 101 | LHG | O4-P-O5 | 4.48 | 133.31 | 112.44 |
| 22 | c | 512 | CLA | C1-C2-C3 | -4.47 | 118.87 | 126.20 |
| 27 | b | 622 | LMG | C1-O6-C5 | -4.47 | 105.00 | 113.72 |
| 22 | d | 405 | CLA | CMB-C2B-C3B | 4.46 | 133.60 | 124.68 |
| 22 | b | 608 | CLA | C4A-NA-C1A | 4.46 | 108.71 | 106.68 |
| 24 | b | 617 | BCR | C2-C1-C6 | 4.44 | 116.89 | 110.44 |
| 22 | D | 403 | CLA | C4A-NA-C1A | 4.44 | 108.70 | 106.68 |
| 22 | b | 614 | CLA | C4A-NA-C1A | 4.43 | 108.70 | 106.68 |
| 22 | B | 602 | CLA | CMB-C2B-C3B | 4.43 | 133.54 | 124.68 |
| 28 | B | 623 | SQD | O47-C7-C8 | 4.43 | 121.07 | 111.48 |
| 22 | D | 404 | CLA | CMB-C2B-C3B | 4.42 | 133.53 | 124.68 |
| 22 | c | 510 | CLA | O2D-CGD-O1D | -4.41 | 115.26 | 123.85 |
| 29 | a | 412 | DGD | O3G-C3G-C2G | -4.40 | 100.46 | 111.77 |
| 22 | C | 513 | CLA | C4-C3-C5 | 4.37 | 122.82 | 115.23 |
| 24 | B | 619 | BCR | C2-C1-C6 | 4.36 | 116.77 | 110.44 |
| 22 | b | 616 | CLA | C4A-NA-C1A | 4.36 | 108.67 | 106.68 |
| 23 | d | 402 | PHO | O1D-CGD-CBD | 4.35 | 131.32 | 124.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36 | V | 201 | HEC | CBD-CAD-C3D | -4.35 | 105.22 | 112.54 |
| 22 | A | 410 | CLA | CMB-C2B-C1B | -4.35 | 122.08 | 128.46 |
| 28 | B | 623 | SQD | O7-S-C6 | 4.35 | 113.25 | 106.76 |
| 33 | d | 408 | LHG | O8-C23-O10 | -4.34 | 112.77 | 123.63 |
| 28 | f | 102 | SQD | O7-S-C6 | 4.33 | 113.22 | 106.76 |
| 29 | h | 102 | DGD | O3G-C3G-C2G | -4.32 | 100.31 | 110.82 |
| 22 | c | 503 | CLA | CMB-C2B-C1B | -4.31 | 122.14 | 128.46 |
| 33 | E | 102 | LHG | O4-P-O5 | 4.31 | 132.50 | 112.44 |
| 28 | A | 412 | SQD | C1-C2-C3 | -4.31 | 100.95 | 110.01 |
| 33 | B | 622 | LHG | O4-P-O5 | 4.30 | 132.43 | 112.44 |
| 22 | B | 608 | CLA | O2D-CGD-CBD | 4.29 | 118.74 | 111.23 |
| 33 | d | 408 | LHG | O4-P-O5 | 4.27 | 132.31 | 112.44 |
| 32 | m | 101 | STE | O2-C1-C2 | 4.27 | 127.49 | 114.00 |
| 22 | B | 609 | CLA | C4A-NA-C1A | 4.26 | 108.62 | 106.68 |
| 22 | C | 507 | CLA | O2D-CGD-O1D | -4.26 | 115.55 | 123.85 |
| 23 | d | 402 | PHO | O2D-CGD-O1D | -4.26 | 115.56 | 123.85 |
| 33 | d | 410 | LHG | O4-P-O5 | 4.25 | 132.22 | 112.44 |
| 22 | C | 505 | CLA | CMB-C2B-C1B | -4.25 | 122.23 | 128.46 |
| 35 | f | 101 | HEM | CBA-CAA-C2A | -4.25 | 105.39 | 112.54 |
| 22 | b | 605 | CLA | CMB-C2B-C1B | -4.24 | 122.24 | 128.46 |
| 22 | B | 613 | CLA | C1-C2-C3 | -4.24 | 119.25 | 126.20 |
| 22 | b | 611 | CLA | O2D-CGD-O1D | -4.24 | 115.60 | 123.85 |
| 22 | b | 608 | CLA | CMB-C2B-C3B | 4.22 | 133.11 | 124.68 |
| 22 | C | 506 | CLA | CMB-C2B-C1B | -4.18 | 122.33 | 128.46 |
| 22 | B | 616 | CLA | CMB-C2B-C1B | -4.17 | 122.35 | 128.46 |
| 26 | d | 407 | PL9 | C42-C43-C44 | -4.16 | 118.09 | 127.62 |
| 22 | b | 614 | CLA | CMB-C2B-C1B | -4.16 | 122.36 | 128.46 |
| 22 | B | 613 | CLA | CMB-C2B-C3B | 4.16 | 132.99 | 124.68 |
| 22 | b | 606 | CLA | O2D-CGD-O1D | -4.16 | 115.76 | 123.85 |
| 28 | F | 101 | SQD | O8-S-C6 | 4.16 | 114.00 | 105.97 |
| 29 | C | 517 | DGD | O3G-C3G-C2G | -4.15 | 100.72 | 110.82 |
| 22 | B | 610 | CLA | C4A-NA-C1A | 4.15 | 108.57 | 106.68 |
| 22 | B | 605 | CLA | O1D-CGD-CBD | 4.13 | 132.66 | 124.52 |
| 22 | A | 410 | CLA | C4A-NA-C1A | 4.12 | 108.56 | 106.68 |
| 22 | b | 612 | CLA | CMB-C2B-C3B | 4.10 | 132.88 | 124.68 |
| 22 | A | 405 | CLA | O2D-CGD-O1D | -4.10 | 115.87 | 123.85 |
| 22 | d | 404 | CLA | CMB-C2B-C1B | -4.08 | 122.47 | 128.46 |
| 22 | A | 410 | CLA | CMB-C2B-C3B | 4.07 | 132.82 | 124.68 |
| 33 | D | 408 | LHG | O4-P-O5 | 4.07 | 131.37 | 112.44 |
| 22 | C | 512 | CLA | C4A-NA-C1A | 4.06 | 108.53 | 106.68 |
| 28 | L | 101 | SQD | O48-C23-C24 | 4.06 | 124.20 | 111.83 |
| 22 | c | 509 | CLA | O2A-CGA-O1A | -4.05 | 113.49 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | A | 404 | PHO | CMB-C2B-C3B | 4.05 | 132.78 | 124.68 |
| 22 | B | 608 | CLA | CMB-C2B-C3B | 4.05 | 132.78 | 124.68 |
| 34 | a | 408 | BCT | O2-C-O1 | 4.04 | 130.02 | 119.68 |
| 22 | d | 404 | CLA | O2D-CGD-CBD | 4.04 | 118.29 | 111.23 |
| 26 | a | 409 | PL9 | C7-C3-C2 | -4.04 | 118.63 | 123.39 |
| 22 | B | 607 | CLA | CMB-C2B-C1B | -4.03 | 122.55 | 128.46 |
| 28 | A | 412 | SQD | O9-S-O7 | -4.03 | 100.73 | 113.82 |
| 22 | B | 611 | CLA | O2D-CGD-O1D | -4.02 | 116.03 | 123.85 |
| 22 | c | 502 | CLA | CMB-C2B-C1B | -4.01 | 122.58 | 128.46 |
| 22 | A | 405 | CLA | CMB-C2B-C3B | 4.01 | 132.70 | 124.68 |
| 29 | c | 519 | DGD | O3G-C3G-C2G | -4.00 | 101.08 | 110.82 |
| 33 | d | 409 | LHG | O4-P-O5 | 3.99 | 131.00 | 112.44 |
| 22 | b | 602 | CLA | CMB-C2B-C3B | 3.98 | 132.64 | 124.68 |
| 22 | c | 504 | CLA | CMB-C2B-C3B | 3.98 | 132.64 | 124.68 |
| 22 | a | 403 | CLA | CMB-C2B-C3B | 3.98 | 132.64 | 124.68 |
| 32 | j | 101 | STE | O2-C1-C2 | 3.98 | 126.58 | 114.00 |
| 22 | b | 604 | CLA | CHB-C4A-NA | 3.97 | 130.12 | 124.40 |
| 24 | T | 101 | BCR | C27-C26-C25 | 3.96 | 128.06 | 122.70 |
| 22 | C | 504 | CLA | CMB-C2B-C1B | -3.95 | 122.67 | 128.46 |
| 22 | b | 604 | CLA | C1-C2-C3 | -3.95 | 119.73 | 126.20 |
| 22 | b | 606 | CLA | CMB-C2B-C3B | 3.93 | 132.55 | 124.68 |
| 28 | f | 102 | SQD | O6-C1-C2 | 3.93 | 114.25 | 108.27 |
| 22 | c | 508 | CLA | CMB-C2B-C3B | 3.93 | 132.53 | 124.68 |
| 28 | f | 102 | SQD | O9-S-O7 | -3.92 | 101.07 | 113.82 |
| 22 | b | 607 | CLA | C4A-NA-C1A | 3.92 | 108.47 | 106.68 |
| 28 | A | 412 | SQD | O47-C7-O49 | -3.92 | 114.54 | 123.70 |
| 22 | B | 604 | CLA | O2D-CGD-O1D | -3.91 | 116.24 | 123.85 |
| 22 | b | 601 | CLA | CHB-C4A-NA | 3.90 | 130.03 | 124.40 |
| 22 | a | 402 | CLA | CMB-C2B-C3B | 3.90 | 132.47 | 124.68 |
| 24 | C | 514 | BCR | C36-C18-C17 | -3.90 | 116.50 | 122.82 |
| 22 | c | 513 | CLA | CMB-C2B-C3B | 3.89 | 132.46 | 124.68 |
| 28 | a | 410 | SQD | C1-C2-C3 | -3.89 | 101.83 | 110.01 |
| 22 | C | 510 | CLA | CMB-C2B-C3B | 3.88 | 132.44 | 124.68 |
| 29 | c | 518 | DGD | O3G-C3G-C2G | -3.88 | 101.39 | 110.82 |
| 22 | b | 612 | CLA | O2D-CGD-O1D | -3.88 | 116.30 | 123.85 |
| 22 | b | 605 | CLA | C4-C3-C5 | 3.87 | 121.94 | 115.23 |
| 22 | c | 502 | CLA | O2D-CGD-O1D | -3.87 | 116.32 | 123.85 |
| 22 | d | 403 | CLA | CMB-C2B-C3B | 3.87 | 132.41 | 124.68 |
| 22 | A | 402 | CLA | CMB-C2B-C3B | 3.87 | 132.41 | 124.68 |
| 22 | C | 502 | CLA | C4A-NA-C1A | 3.86 | 108.44 | 106.68 |
| 33 | D | 409 | LHG | O4-P-O5 | 3.86 | 130.39 | 112.44 |
| 29 | C | 518 | DGD | O3G-C3G-C2G | -3.85 | 101.45 | 110.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | d | 411 | LMG | O7-C10-O9 | -3.84 | 113.46 | 123.33 |
| 29 | C | 517 | DGD | O5D-C6D-C5D | -3.84 | 100.77 | 109.42 |
| 22 | c | 510 | CLA | CMB-C2B-C3B | 3.83 | 132.34 | 124.68 |
| 28 | A | 413 | SQD | O48-C23-C24 | 3.82 | 123.48 | 111.83 |
| 22 | b | 603 | CLA | CMB-C2B-C1B | -3.82 | 122.86 | 128.46 |
| 22 | B | 604 | CLA | CMB-C2B-C3B | 3.81 | 132.30 | 124.68 |
| 22 | A | 405 | CLA | C1B-CHB-C4A | -3.80 | 122.79 | 130.04 |
| 22 | B | 616 | CLA | CMB-C2B-C3B | 3.80 | 132.27 | 124.68 |
| 22 | B | 613 | CLA | C4A-NA-C1A | 3.79 | 108.41 | 106.68 |
| 22 | b | 610 | CLA | C1B-CHB-C4A | -3.79 | 122.80 | 130.04 |
| 24 | b | 618 | BCR | C36-C18-C17 | -3.79 | 116.68 | 122.82 |
| 33 | l | 101 | LHG | O4-P-O5 | 3.78 | 130.04 | 112.44 |
| 33 | B | 622 | LHG | O8-C23-C24 | 3.77 | 123.33 | 111.83 |
| 28 | a | 410 | SQD | O9-S-O7 | -3.77 | 101.57 | 113.82 |
| 22 | b | 610 | CLA | CAC-C3C-C4C | 3.77 | 129.69 | 124.79 |
| 28 | a | 410 | SQD | O7-S-C6 | 3.76 | 112.36 | 106.76 |
| 36 | v | 201 | HEC | CMC-C2C-C1C | -3.76 | 122.95 | 128.46 |
| 22 | b | 602 | CLA | CHB-C4A-NA | 3.75 | 129.82 | 124.40 |
| 24 | B | 617 | BCR | C2-C1-C6 | 3.75 | 115.88 | 110.44 |
| 22 | B | 610 | CLA | CHB-C4A-NA | 3.74 | 129.81 | 124.40 |
| 22 | b | 616 | CLA | O2D-CGD-O1D | -3.72 | 116.61 | 123.85 |
| 22 | b | 607 | CLA | CMB-C2B-C1B | -3.71 | 123.02 | 128.46 |
| 36 | v | 201 | HEC | CMB-C2B-C1B | -3.71 | 123.03 | 128.46 |
| 29 | h | 102 | DGD | O3E-C3E-C2E | -3.70 | 101.65 | 110.38 |
| 22 | B | 605 | CLA | O2D-CGD-O1D | -3.69 | 116.67 | 123.85 |
| 22 | a | 404 | CLA | CMB-C2B-C1B | -3.69 | 123.05 | 128.46 |
| 22 | b | 609 | CLA | CMB-C2B-C3B | 3.69 | 132.05 | 124.68 |
| 29 | C | 516 | DGD | O3G-C3G-C2G | -3.68 | 101.87 | 110.82 |
| 29 | C | 518 | DGD | O3G-C1D-C2D | -3.68 | 102.69 | 108.27 |
| 22 | B | 611 | CLA | CMB-C2B-C3B | 3.65 | 131.98 | 124.68 |
| 29 | C | 516 | DGD | O1G-C1A-C2A | -3.65 | 100.71 | 111.83 |
| 22 | D | 403 | CLA | CMB-C2B-C1B | -3.64 | 123.12 | 128.46 |
| 36 | V | 201 | HEC | CMC-C2C-C3C | 3.64 | 130.10 | 125.82 |
| 28 | f | 102 | SQD | O5-C5-C4 | 3.62 | 116.22 | 109.70 |
| 24 | a | 405 | BCR | C39-C30-C25 | -3.62 | 104.57 | 110.24 |
| 22 | b | 603 | CLA | O2D-CGD-O1D | -3.61 | 116.82 | 123.85 |
| 22 | b | 604 | CLA | CMB-C2B-C1B | -3.61 | 123.17 | 128.46 |
| 26 | a | 409 | PL9 | C35-C34-C36 | 3.60 | 121.47 | 115.23 |
| 28 | B | 623 | SQD | O9-S-O7 | -3.59 | 102.13 | 113.82 |
| 22 | b | 613 | CLA | C1-C2-C3 | -3.59 | 120.31 | 126.20 |
| 29 | C | 517 | DGD | O2D-C2D-C1D | -3.59 | 101.51 | 110.08 |
| 33 | d | 408 | LHG | O8-C23-C24 | 3.59 | 122.77 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28 | A | 413 | SQD | C45-O47-C7 | 3.58 | 122.95 | 117.78 |
| 22 | D | 403 | CLA | O2D-CGD-O1D | -3.58 | 116.88 | 123.85 |
| 22 | c | 501 | CLA | O2D-CGD-CBD | 3.58 | 117.48 | 111.23 |
| 23 | D | 401 | PHO | O1D-CGD-CBD | 3.57 | 130.13 | 124.72 |
| 22 | c | 502 | CLA | C1B-CHB-C4A | -3.57 | 123.24 | 130.04 |
| 22 | C | 503 | CLA | CMB-C2B-C1B | -3.56 | 123.24 | 128.46 |
| 22 | C | 507 | CLA | CMB-C2B-C1B | -3.56 | 123.25 | 128.46 |
| 23 | D | 401 | PHO | CMB-C2B-C3B | 3.56 | 131.79 | 124.68 |
| 22 | C | 508 | CLA | CMB-C2B-C3B | 3.55 | 131.78 | 124.68 |
| 24 | c | 515 | BCR | C2-C1-C6 | 3.55 | 115.59 | 110.44 |
| 22 | B | 602 | CLA | O2D-CGD-O1D | -3.55 | 116.95 | 123.85 |
| 24 | d | 406 | BCR | C38-C26-C25 | -3.54 | 120.62 | 124.48 |
| 22 | b | 602 | CLA | O2D-CGD-CBD | 3.54 | 117.42 | 111.23 |
| 22 | B | 610 | CLA | C1B-CHB-C4A | -3.54 | 123.28 | 130.04 |
| 22 | C | 513 | CLA | CMB-C2B-C1B | -3.54 | 123.27 | 128.46 |
| 28 | B | 623 | SQD | O48-C23-C24 | 3.54 | 122.63 | 111.83 |
| 24 | T | 101 | BCR | C7-C8-C9 | -3.53 | 121.02 | 126.23 |
| 28 | L | 101 | SQD | O9-S-C6 | 3.53 | 112.02 | 106.76 |
| 22 | B | 610 | CLA | O2D-CGD-CBD | 3.52 | 117.38 | 111.23 |
| 22 | b | 616 | CLA | C1B-CHB-C4A | -3.52 | 123.33 | 130.04 |
| 27 | b | 620 | LMG | O1-C1-C2 | -3.51 | 102.94 | 108.27 |
| 23 | d | 402 | PHO | CMC-C2C-C3C | 3.50 | 131.54 | 124.94 |
| 22 | c | 506 | CLA | CMB-C2B-C3B | 3.49 | 131.67 | 124.68 |
| 29 | A | 414 | DGD | O3G-C3G-C2G | -3.49 | 102.32 | 110.82 |
| 28 | L | 101 | SQD | O5-C1-C2 | -3.49 | 103.19 | 110.37 |
| 22 | a | 404 | CLA | C4A-NA-C1A | 3.49 | 108.27 | 106.68 |
| 26 | d | 407 | PL9 | C37-C38-C39 | -3.49 | 119.64 | 127.62 |
| 22 | A | 402 | CLA | CHB-C4A-NA | 3.48 | 129.42 | 124.40 |
| 27 | C | 519 | LMG | O2-C2-C1 | -3.47 | 101.81 | 110.08 |
| 24 | K | 101 | BCR | C15-C16-C17 | -3.46 | 116.44 | 123.52 |
| 22 | c | 509 | CLA | CMB-C2B-C3B | 3.46 | 131.59 | 124.68 |
| 28 | B | 623 | SQD | C3-C4-C5 | 3.45 | 116.50 | 110.23 |
| 22 | c | 508 | CLA | CHB-C4A-NA | 3.45 | 129.38 | 124.40 |
| 22 | C | 504 | CLA | C4-C3-C5 | 3.45 | 121.21 | 115.23 |
| 22 | B | 604 | CLA | CHB-C4A-NA | 3.44 | 129.37 | 124.40 |
| 22 | b | 603 | CLA | CHD-C1D-ND | -3.44 | 119.97 | 124.80 |
| 22 | B | 614 | CLA | C1B-CHB-C4A | -3.43 | 123.49 | 130.04 |
| 27 | C | 519 | LMG | O1-C1-C2 | -3.43 | 103.06 | 108.27 |
| 28 | A | 413 | SQD | O47-C7-C8 | 3.43 | 118.90 | 111.48 |
| 22 | d | 404 | CLA | O2D-CGD-O1D | -3.43 | 117.18 | 123.85 |
| 28 | a | 410 | SQD | O48-C23-C24 | 3.42 | 122.26 | 111.83 |
| 28 | A | 412 | SQD | C1-O5-C5 | -3.42 | 107.05 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | c | 517 | DGD | O3G-C1D-C2D | -3.42 | 103.08 | 108.27 |
| 23 | d | 402 | PHO | C1-C2-C3 | -3.42 | 120.60 | 126.20 |
| 22 | c | 513 | CLA | O2D-CGD-O1D | -3.41 | 117.21 | 123.85 |
| 22 | C | 512 | CLA | CHB-C4A-NA | 3.41 | 129.32 | 124.40 |
| 22 | B | 603 | CLA | C4-C3-C5 | 3.41 | 121.14 | 115.23 |
| 22 | c | 512 | CLA | O2D-CGD-O1D | -3.40 | 117.22 | 123.85 |
| 26 | A | 409 | PL9 | C36-C34-C33 | -3.40 | 113.53 | 121.17 |
| 22 | c | 501 | CLA | CMB-C2B-C1B | -3.40 | 123.47 | 128.46 |
| 29 | c | 518 | DGD | O2D-C2D-C1D | -3.40 | 101.97 | 110.08 |
| 28 | a | 410 | SQD | C3-C4-C5 | 3.40 | 116.39 | 110.23 |
| 24 | C | 514 | BCR | C2-C1-C6 | 3.40 | 115.37 | 110.44 |
| 22 | b | 601 | CLA | CMB-C2B-C1B | -3.39 | 123.49 | 128.46 |
| 22 | B | 606 | CLA | CMB-C2B-C1B | -3.38 | 123.51 | 128.46 |
| 22 | C | 501 | CLA | CMB-C2B-C1B | -3.38 | 123.51 | 128.46 |
| 22 | b | 612 | CLA | C1B-CHB-C4A | -3.37 | 123.61 | 130.04 |
| 22 | B | 612 | CLA | O2D-CGD-O1D | -3.37 | 117.29 | 123.85 |
| 24 | d | 406 | BCR | C27-C26-C25 | 3.37 | 127.26 | 122.70 |
| 28 | L | 101 | SQD | C1-C2-C3 | -3.37 | 102.93 | 110.01 |
| 29 | c | 517 | DGD | O3G-C3G-C2G | -3.36 | 102.65 | 110.82 |
| 27 | d | 412 | LMG | O2-C2-C1 | -3.36 | 102.08 | 110.08 |
| 28 | L | 101 | SQD | O9-S-O7 | -3.34 | 102.94 | 113.82 |
| 22 | B | 614 | CLA | CMB-C2B-C1B | -3.33 | 123.57 | 128.46 |
| 22 | C | 505 | CLA | CMB-C2B-C3B | 3.33 | 131.34 | 124.68 |
| 24 | a | 405 | BCR | C2-C1-C6 | 3.33 | 115.27 | 110.44 |
| 29 | H | 102 | DGD | C3E-C4E-C5E | -3.33 | 104.20 | 110.23 |
| 29 | C | 517 | DGD | O4D-C4D-C3D | 3.33 | 118.21 | 110.38 |
| 22 | b | 604 | CLA | C11-C12-C13 | -3.32 | 104.91 | 115.97 |
| 26 | d | 407 | PL9 | C36-C34-C33 | -3.32 | 113.71 | 121.17 |
| 22 | d | 403 | CLA | C4A-NA-C1A | 3.32 | 108.19 | 106.68 |
| 24 | b | 617 | BCR | C38-C26-C25 | -3.32 | 120.86 | 124.48 |
| 35 | f | 101 | HEM | C3B-C2B-C1B | 3.32 | 108.90 | 106.41 |
| 24 | a | 405 | BCR | C40-C30-C25 | 3.32 | 115.44 | 110.24 |
| 22 | C | 506 | CLA | CMB-C2B-C3B | 3.31 | 131.31 | 124.68 |
| 22 | B | 613 | CLA | CAC-C3C-C4C | 3.31 | 129.10 | 124.79 |
| 22 | A | 403 | CLA | CMB-C2B-C1B | -3.31 | 123.61 | 128.46 |
| 22 | B | 606 | CLA | C6-C5-C3 | -3.30 | 105.42 | 113.47 |
| 29 | C | 517 | DGD | C3D-C4D-C5D | -3.30 | 104.24 | 110.23 |
| 27 | b | 620 | LMG | O1-C7-C8 | -3.30 | 102.79 | 110.82 |
| 22 | B | 616 | CLA | O2D-CGD-O1D | -3.29 | 117.44 | 123.85 |
| 32 | C | 520 | STE | C3-C2-C1 | -3.29 | 105.92 | 114.51 |
| 29 | c | 518 | DGD | C3D-C4D-C5D | -3.28 | 104.28 | 110.23 |
| 22 | b | 611 | CLA | CMB-C2B-C1B | -3.27 | 123.66 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 612 | CLA | O1D-CGD-CBD | 3.27 | 130.97 | 124.52 |
| 22 | b | 611 | CLA | O2D-CGD-CBD | 3.27 | 116.95 | 111.23 |
| 22 | a | 403 | CLA | C1B-CHB-C4A | -3.27 | 123.80 | 130.04 |
| 27 | b | 620 | LMG | O3-C3-C2 | -3.26 | 102.70 | 110.38 |
| 27 | c | 523 | LMG | C1-O6-C5 | -3.25 | 107.37 | 113.72 |
| 22 | B | 615 | CLA | CHB-C4A-NA | 3.25 | 129.09 | 124.40 |
| 27 | M | 101 | LMG | C1-O6-C5 | -3.25 | 107.38 | 113.72 |
| 26 | d | 407 | PL9 | C22-C23-C24 | -3.25 | 120.19 | 127.62 |
| 26 | A | 409 | PL9 | C40-C39-C38 | -3.24 | 115.30 | 123.63 |
| 24 | D | 405 | BCR | C2-C1-C6 | 3.24 | 115.14 | 110.44 |
| 22 | b | 603 | CLA | C1B-CHB-C4A | -3.24 | 123.87 | 130.04 |
| 22 | a | 404 | CLA | CHB-C4A-NA | 3.24 | 129.07 | 124.40 |
| 22 | b | 613 | CLA | CMB-C2B-C3B | 3.23 | 131.15 | 124.68 |
| 22 | B | 611 | CLA | O2D-CGD-CBD | 3.23 | 116.88 | 111.23 |
| 22 | D | 404 | CLA | O2D-CGD-CBD | 3.23 | 116.87 | 111.23 |
| 22 | B | 610 | CLA | O2A-CGA-O1A | -3.23 | 115.56 | 123.63 |
| 23 | d | 401 | PHO | CMB-C2B-C3B | 3.23 | 131.13 | 124.68 |
| 22 | b | 608 | CLA | CHB-C4A-NA | 3.22 | 129.05 | 124.40 |
| 22 | b | 614 | CLA | C1B-CHB-C4A | -3.22 | 123.89 | 130.04 |
| 29 | C | 516 | DGD | O3E-C3E-C2E | -3.22 | 102.78 | 110.38 |
| 26 | a | 409 | PL9 | C40-C39-C41 | 3.22 | 120.82 | 115.23 |
| 24 | b | 619 | BCR | C12-C13-C14 | -3.22 | 113.95 | 119.01 |
| 24 | K | 101 | BCR | C11-C10-C9 | -3.22 | 122.77 | 127.28 |
| 22 | c | 507 | CLA | O2D-CGD-O1D | -3.22 | 117.59 | 123.85 |
| 24 | c | 515 | BCR | C15-C16-C17 | -3.21 | 116.95 | 123.52 |
| 26 | A | 409 | PL9 | C22-C23-C24 | -3.20 | 120.29 | 127.62 |
| 22 | C | 507 | CLA | CHB-C4A-NA | 3.20 | 129.02 | 124.40 |
| 22 | C | 513 | CLA | O2A-CGA-O1A | -3.20 | 115.63 | 123.63 |
| 22 | A | 405 | CLA | O2D-CGD-CBD | 3.20 | 116.82 | 111.23 |
| 27 | D | 407 | LMG | C3-C4-C5 | -3.19 | 104.44 | 110.23 |
| 22 | C | 512 | CLA | CMB-C2B-C1B | -3.19 | 123.78 | 128.46 |
| 22 | A | 410 | CLA | CHB-C4A-NA | 3.18 | 128.99 | 124.40 |
| 22 | B | 614 | CLA | O2D-CGD-O1D | -3.18 | 117.67 | 123.85 |
| 28 | L | 101 | SQD | C3-C4-C5 | 3.17 | 115.97 | 110.23 |
| 27 | b | 622 | LMG | O2-C2-C1 | -3.16 | 102.54 | 110.08 |
| 24 | t | 101 | BCR | C1-C6-C5 | -3.15 | 118.33 | 122.64 |
| 22 | B | 607 | CLA | CMB-C2B-C3B | 3.15 | 130.98 | 124.68 |
| 22 | B | 612 | CLA | C11-C12-C13 | -3.14 | 105.52 | 115.97 |
| 22 | B | 602 | CLA | CHB-C4A-NA | 3.14 | 128.93 | 124.40 |
| 22 | a | 403 | CLA | CHB-C4A-NA | 3.14 | 128.93 | 124.40 |
| 22 | B | 615 | CLA | O2D-CGD-O1D | -3.14 | 117.74 | 123.85 |
| 22 | a | 403 | CLA | CAC-C3C-C4C | 3.13 | 128.87 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 603 | CLA | CMB-C2B-C3B | 3.13 | 130.94 | 124.68 |
| 24 | c | 515 | BCR | C27-C26-C25 | 3.13 | 126.94 | 122.70 |
| 22 | C | 508 | CLA | O2D-CGD-O1D | -3.13 | 117.75 | 123.85 |
| 27 | M | 101 | LMG | C1-C2-C3 | -3.13 | 103.43 | 110.01 |
| 26 | D | 406 | PL9 | C7-C3-C2 | -3.13 | 119.70 | 123.39 |
| 27 | b | 622 | LMG | C3-C4-C5 | -3.13 | 104.56 | 110.23 |
| 22 | b | 616 | CLA | CHB-C4A-NA | 3.12 | 128.91 | 124.40 |
| 28 | F | 101 | SQD | O48-C23-O10 | -3.12 | 115.82 | 123.63 |
| 22 | b | 602 | CLA | O2D-CGD-O1D | -3.12 | 117.78 | 123.85 |
| 24 | d | 406 | BCR | C16-C15-C14 | -3.12 | 117.14 | 123.52 |
| 22 | D | 403 | CLA | O2D-CGD-CBD | 3.12 | 116.68 | 111.23 |
| 28 | L | 101 | SQD | O5-C5-C4 | 3.12 | 115.31 | 109.70 |
| 22 | B | 603 | CLA | CHD-C4C-NC | 3.11 | 129.06 | 124.23 |
| 24 | b | 619 | BCR | C36-C18-C17 | -3.11 | 117.77 | 122.82 |
| 22 | B | 611 | CLA | C1-C2-C3 | -3.11 | 121.10 | 126.20 |
| 22 | C | 511 | CLA | CMB-C2B-C3B | 3.11 | 130.90 | 124.68 |
| 26 | D | 406 | PL9 | C12-C13-C14 | -3.11 | 120.51 | 127.62 |
| 22 | C | 509 | CLA | CHB-C4A-NA | 3.10 | 128.88 | 124.40 |
| 36 | V | 201 | HEC | C1D-C2D-C3D | -3.10 | 104.84 | 107.00 |
| 29 | C | 517 | DGD | O5D-C1E-C2E | 3.10 | 112.98 | 108.27 |
| 22 | b | 613 | CLA | O2D-CGD-CBD | 3.10 | 116.64 | 111.23 |
| 26 | a | 409 | PL9 | C22-C23-C24 | -3.09 | 120.55 | 127.62 |
| 28 | f | 102 | SQD | C45-O47-C7 | 3.09 | 125.19 | 117.80 |
| 22 | B | 616 | CLA | CAA-CBA-CGA | -3.08 | 104.45 | 113.21 |
| 28 | A | 412 | SQD | O47-C7-C8 | 3.08 | 118.15 | 111.48 |
| 24 | b | 618 | BCR | C8-C7-C6 | -3.08 | 118.76 | 127.00 |
| 22 | d | 405 | CLA | C1B-CHB-C4A | -3.08 | 124.16 | 130.04 |
| 22 | b | 615 | CLA | O2D-CGD-O1D | -3.07 | 117.86 | 123.85 |
| 22 | D | 403 | CLA | C1B-CHB-C4A | -3.07 | 124.18 | 130.04 |
| 22 | b | 601 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 35 | f | 101 | HEM | CBD-CAD-C3D | -3.07 | 104.05 | 112.53 |
| 36 | V | 201 | HEC | CMB-C2B-C1B | -3.07 | 123.96 | 128.46 |
| 22 | C | 513 | CLA | O2D-CGD-O1D | -3.07 | 117.88 | 123.85 |
| 22 | b | 610 | CLA | CHB-C4A-NA | 3.06 | 128.82 | 124.40 |
| 22 | A | 402 | CLA | O1D-CGD-CBD | 3.06 | 130.55 | 124.52 |
| 22 | b | 610 | CLA | CMB-C2B-C1B | -3.06 | 123.98 | 128.46 |
| 22 | C | 510 | CLA | O2D-CGD-O1D | -3.06 | 117.90 | 123.85 |
| 22 | c | 502 | CLA | CMB-C2B-C3B | 3.05 | 130.79 | 124.68 |
| 23 | d | 401 | PHO | OBD-CAD-CBD | -3.05 | 121.35 | 125.82 |
| 22 | b | 602 | CLA | C1B-CHB-C4A | -3.04 | 124.24 | 130.04 |
| 27 | d | 412 | LMG | C3-C4-C5 | -3.04 | 104.72 | 110.23 |
| 26 | A | 409 | PL9 | C7-C3-C2 | -3.04 | 119.81 | 123.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32 | C | 522 | STE | C4-C3-C2 | -3.04 | 101.97 | 113.13 |
| 22 | B | 601 | CLA | O2D-CGD-O1D | -3.03 | 117.94 | 123.85 |
| 33 | E | 102 | LHG | O8-C23-C24 | 3.03 | 121.06 | 111.83 |
| 22 | C | 506 | CLA | O1D-CGD-CBD | 3.02 | 130.48 | 124.52 |
| 22 | C | 507 | CLA | CMB-C2B-C3B | 3.02 | 130.72 | 124.68 |
| 26 | a | 409 | PL9 | C36-C34-C33 | -3.02 | 114.39 | 121.17 |
| 28 | a | 410 | SQD | O47-C7-O49 | -3.02 | 116.65 | 123.70 |
| 22 | B | 613 | CLA | O2A-CGA-O1A | -3.02 | 116.08 | 123.63 |
| 22 | c | 512 | CLA | CHB-C4A-NA | 3.02 | 128.76 | 124.40 |
| 22 | b | 602 | CLA | C1-C2-C3 | -3.02 | 121.26 | 126.20 |
| 28 | F | 101 | SQD | O48-C23-C24 | 3.01 | 121.03 | 111.83 |
| 27 | b | 622 | LMG | O7-C10-O9 | -3.01 | 116.66 | 123.70 |
| 33 | D | 408 | LHG | O8-C23-O10 | -3.01 | 116.10 | 123.63 |
| 28 | A | 412 | SQD | O48-C23-O10 | -3.01 | 116.11 | 123.63 |
| 22 | B | 602 | CLA | C16-C15-C13 | -3.01 | 105.97 | 115.97 |
| 28 | L | 101 | SQD | O2-C2-C1 | 3.00 | 117.23 | 110.08 |
| 28 | F | 101 | SQD | C44-O6-C1 | 3.00 | 118.81 | 113.68 |
| 24 | B | 619 | BCR | C29-C30-C25 | 3.00 | 114.80 | 110.44 |
| 35 | E | 101 | HEM | CBD-CAD-C3D | -3.00 | 104.25 | 112.53 |
| 24 | A | 406 | BCR | C37-C22-C21 | -3.00 | 117.96 | 122.82 |
| 26 | d | 407 | PL9 | C7-C3-C2 | -3.00 | 119.86 | 123.39 |
| 24 | c | 516 | BCR | C2-C1-C6 | 3.00 | 114.79 | 110.44 |
| 24 | B | 618 | BCR | C2-C1-C6 | 2.99 | 114.79 | 110.44 |
| 24 | k | 101 | BCR | C27-C26-C25 | 2.99 | 126.75 | 122.70 |
| 22 | c | 505 | CLA | O2D-CGD-O1D | -2.99 | 118.03 | 123.85 |
| 27 | c | 522 | LMG | O1-C1-C2 | -2.99 | 103.74 | 108.27 |
| 28 | a | 411 | SQD | O48-C23-O10 | -2.98 | 116.17 | 123.63 |
| 24 | Y | 101 | BCR | C27-C26-C25 | 2.98 | 126.73 | 122.70 |
| 24 | C | 514 | BCR | C15-C16-C17 | -2.98 | 117.42 | 123.52 |
| 24 | A | 406 | BCR | C27-C26-C25 | 2.98 | 126.73 | 122.70 |
| 33 | D | 408 | LHG | C18-C17-C16 | -2.98 | 99.32 | 114.37 |
| 22 | b | 609 | CLA | C1B-CHB-C4A | -2.97 | 124.37 | 130.04 |
| 22 | A | 403 | CLA | C1B-CHB-C4A | -2.97 | 124.37 | 130.04 |
| 22 | c | 503 | CLA | CMB-C2B-C3B | 2.97 | 130.62 | 124.68 |
| 29 | C | 518 | DGD | CDB-CCB-CBB | -2.97 | 99.35 | 114.37 |
| 24 | D | 405 | BCR | C27-C26-C25 | 2.97 | 126.72 | 122.70 |
| 22 | c | 510 | CLA | O1D-CGD-CBD | 2.97 | 130.37 | 124.52 |
| 22 | c | 506 | CLA | C1B-CHB-C4A | -2.97 | 124.38 | 130.04 |
| 28 | f | 102 | SQD | C1-C2-C3 | -2.96 | 103.77 | 110.01 |
| 29 | h | 102 | DGD | O2D-C2D-C1D | -2.96 | 103.02 | 110.08 |
| 22 | C | 504 | CLA | O2A-CGA-O1A | -2.95 | 116.25 | 123.63 |
| 22 | b | 606 | CLA | CHB-C4A-NA | 2.95 | 128.65 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 607 | CLA | C4-C3-C5 | 2.94 | 120.34 | 115.23 |
| 22 | b | 604 | CLA | O2D-CGD-O1D | -2.94 | 118.12 | 123.85 |
| 29 | h | 102 | DGD | C4D-C3D-C2D | -2.94 | 105.67 | 110.83 |
| 26 | a | 409 | PL9 | C20-C19-C21 | 2.93 | 120.32 | 115.23 |
| 22 | b | 610 | CLA | CMB-C2B-C3B | 2.93 | 130.55 | 124.68 |
| 27 | C | 519 | LMG | O1-C7-C8 | -2.93 | 103.68 | 110.82 |
| 22 | C | 501 | CLA | O2D-CGD-O1D | -2.93 | 118.14 | 123.85 |
| 22 | C | 503 | CLA | CHD-C1D-ND | -2.93 | 120.68 | 124.80 |
| 27 | b | 622 | LMG | O8-C28-O10 | -2.93 | 116.30 | 123.63 |
| 29 | a | 412 | DGD | C5B-C4B-C3B | -2.93 | 99.56 | 114.37 |
| 24 | h | 101 | BCR | C15-C16-C17 | -2.93 | 117.53 | 123.52 |
| 22 | c | 511 | CLA | O2D-CGD-O1D | -2.92 | 118.16 | 123.85 |
| 22 | c | 509 | CLA | CHB-C4A-NA | 2.92 | 128.61 | 124.40 |
| 27 | d | 412 | LMG | O6-C1-O1 | -2.92 | 103.15 | 110.04 |
| 22 | a | 402 | CLA | O1D-CGD-CBD | 2.91 | 130.27 | 124.52 |
| 22 | b | 615 | CLA | CMB-C2B-C3B | 2.91 | 130.51 | 124.68 |
| 22 | C | 507 | CLA | O1D-CGD-CBD | 2.91 | 130.26 | 124.52 |
| 24 | H | 101 | BCR | C16-C15-C14 | -2.91 | 117.56 | 123.52 |
| 22 | C | 509 | CLA | C1-C2-C3 | -2.91 | 121.43 | 126.20 |
| 22 | c | 507 | CLA | C4A-NA-C1A | 2.90 | 108.00 | 106.68 |
| 29 | c | 518 | DGD | O4D-C4D-C3D | 2.90 | 117.20 | 110.38 |
| 22 | a | 402 | CLA | C1B-CHB-C4A | -2.90 | 124.52 | 130.04 |
| 22 | b | 616 | CLA | CHD-C1D-ND | -2.90 | 120.73 | 124.80 |
| 22 | D | 404 | CLA | C1B-CHB-C4A | -2.89 | 124.52 | 130.04 |
| 22 | C | 508 | CLA | CHD-C1D-ND | -2.89 | 120.73 | 124.80 |
| 23 | D | 401 | PHO | C1-C2-C3 | -2.89 | 121.46 | 126.20 |
| 22 | b | 605 | CLA | CMB-C2B-C3B | 2.89 | 130.46 | 124.68 |
| 24 | K | 101 | BCR | C38-C26-C25 | -2.89 | 121.33 | 124.48 |
| 22 | c | 511 | CLA | CMB-C2B-C1B | -2.89 | 124.23 | 128.46 |
| 33 | d | 410 | LHG | O8-C23-C24 | 2.89 | 120.63 | 111.83 |
| 22 | B | 609 | CLA | CMB-C2B-C1B | -2.89 | 124.23 | 128.46 |
| 28 | L | 101 | SQD | O8-S-O7 | -2.89 | 104.18 | 111.40 |
| 22 | b | 612 | CLA | C1-C2-C3 | -2.88 | 121.47 | 126.20 |
| 29 | H | 102 | DGD | C1D-C2D-C3D | -2.86 | 103.99 | 110.01 |
| 32 | J | 101 | STE | C3-C2-C1 | -2.86 | 107.04 | 114.51 |
| 22 | C | 512 | CLA | C1-C2-C3 | -2.86 | 121.51 | 126.20 |
| 22 | b | 608 | CLA | O2D-CGD-CBD | 2.85 | 116.22 | 111.23 |
| 22 | B | 604 | CLA | C2D-C1D-ND | -2.85 | 107.30 | 110.13 |
| 22 | A | 402 | CLA | C7-C6-C5 | -2.85 | 105.66 | 113.26 |
| 29 | H | 102 | DGD | O2D-C2D-C1D | -2.85 | 103.28 | 110.08 |
| 22 | c | 505 | CLA | CHB-C4A-NA | 2.85 | 128.51 | 124.40 |
| 27 | c | 522 | LMG | O7-C10-O9 | -2.84 | 117.06 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | c | 514 | BCR | C2-C1-C6 | 2.84 | 114.57 | 110.44 |
| 22 | C | 502 | CLA | O2D-CGD-O1D | -2.84 | 118.32 | 123.85 |
| 22 | b | 610 | CLA | C1-C2-C3 | -2.84 | 121.54 | 126.20 |
| 22 | C | 508 | CLA | O2D-CGD-CBD | 2.84 | 116.19 | 111.23 |
| 29 | a | 412 | DGD | C1G-C2G-C3G | -2.84 | 105.25 | 111.80 |
| 26 | D | 406 | PL9 | C22-C23-C24 | -2.83 | 121.14 | 127.62 |
| 26 | D | 406 | PL9 | C7-C8-C9 | -2.83 | 121.95 | 126.83 |
| 24 | b | 619 | BCR | C38-C26-C25 | -2.83 | 121.40 | 124.48 |
| 22 | c | 502 | CLA | CHD-C1D-ND | -2.82 | 120.83 | 124.80 |
| 27 | c | 520 | LMG | C9-C8-C7 | -2.82 | 105.22 | 111.78 |
| 22 | b | 610 | CLA | CAA-CBA-CGA | -2.82 | 105.21 | 113.21 |
| 22 | b | 607 | CLA | CMB-C2B-C3B | 2.82 | 130.31 | 124.68 |
| 22 | c | 506 | CLA | CHB-C4A-NA | 2.81 | 128.46 | 124.40 |
| 22 | b | 602 | CLA | C11-C12-C13 | -2.81 | 106.63 | 115.97 |
| 22 | c | 509 | CLA | O2D-CGD-O1D | -2.81 | 118.38 | 123.85 |
| 22 | B | 603 | CLA | CMB-C2B-C3B | 2.81 | 130.29 | 124.68 |
| 22 | C | 510 | CLA | C1B-CHB-C4A | -2.81 | 124.69 | 130.04 |
| 22 | B | 601 | CLA | C4-C3-C5 | 2.81 | 120.10 | 115.23 |
| 32 | d | 413 | STE | O2-C1-C2 | 2.81 | 122.87 | 114.00 |
| 27 | b | 620 | LMG | O7-C10-O9 | -2.80 | 117.15 | 123.70 |
| 24 | A | 406 | BCR | C15-C16-C17 | -2.80 | 117.79 | 123.52 |
| 22 | b | 609 | CLA | O2D-CGD-O1D | -2.80 | 118.40 | 123.85 |
| 24 | H | 101 | BCR | C2-C1-C6 | 2.79 | 114.50 | 110.44 |
| 22 | b | 609 | CLA | O1D-CGD-CBD | 2.79 | 130.03 | 124.52 |
| 29 | A | 414 | DGD | O5D-C6D-C5D | -2.79 | 103.12 | 109.42 |
| 24 | t | 101 | BCR | C36-C18-C19 | 2.79 | 122.35 | 118.09 |
| 22 | B | 614 | CLA | C4-C3-C5 | 2.78 | 120.06 | 115.23 |
| 32 | m | 101 | STE | O1-C1-C2 | -2.78 | 114.27 | 123.09 |
| 22 | C | 513 | CLA | CMB-C2B-C3B | 2.78 | 130.24 | 124.68 |
| 22 | B | 604 | CLA | C1D-ND-C4D | 2.78 | 108.26 | 106.31 |
| 22 | B | 603 | CLA | C4A-NA-C1A | 2.77 | 107.94 | 106.68 |
| 22 | a | 402 | CLA | O2D-CGD-O1D | -2.77 | 118.45 | 123.85 |
| 29 | H | 102 | DGD | C1E-O6E-C5E | 2.77 | 119.13 | 113.72 |
| 22 | b | 609 | CLA | CHB-C4A-NA | 2.77 | 128.40 | 124.40 |
| 24 | c | 515 | BCR | C38-C26-C25 | -2.77 | 121.46 | 124.48 |
| 22 | b | 605 | CLA | O2A-CGA-O1A | -2.77 | 116.71 | 123.63 |
| 28 | L | 101 | SQD | O10-C23-C24 | -2.76 | 112.97 | 123.78 |
| 22 | b | 608 | CLA | O2D-CGD-O1D | -2.76 | 118.47 | 123.85 |
| 28 | B | 623 | SQD | O8-S-C6 | 2.76 | 111.31 | 105.97 |
| 29 | c | 518 | DGD | O6D-C1D-O3G | -2.76 | 103.52 | 110.04 |
| 22 | b | 613 | CLA | CHB-C4A-NA | 2.76 | 128.38 | 124.40 |
| 22 | A | 402 | CLA | C1B-CHB-C4A | -2.76 | 124.78 | 130.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 513 | CLA | CHB-C4A-NA | 2.75 | 128.37 | 124.40 |
| 28 | a | 411 | SQD | O49-C7-C8 | -2.75 | 113.03 | 123.78 |
| 22 | c | 507 | CLA | C1B-CHB-C4A | -2.75 | 124.80 | 130.04 |
| 24 | c | 514 | BCR | C15-C14-C13 | -2.75 | 123.43 | 127.28 |
| 27 | d | 412 | LMG | O1-C1-C2 | -2.75 | 104.10 | 108.27 |
| 22 | D | 403 | CLA | CHB-C4A-NA | 2.74 | 128.36 | 124.40 |
| 22 | B | 613 | CLA | C4-C3-C5 | 2.74 | 119.99 | 115.23 |
| 28 | A | 412 | SQD | O5-C1-O6 | 2.74 | 116.52 | 110.04 |
| 24 | c | 514 | BCR | C15-C16-C17 | -2.74 | 117.92 | 123.52 |
| 22 | A | 405 | CLA | CHD-C1D-ND | -2.73 | 120.96 | 124.80 |
| 26 | a | 409 | PL9 | O2-C1-C2 | -2.73 | 115.61 | 121.83 |
| 22 | B | 611 | CLA | C4A-NA-C1A | 2.73 | 107.92 | 106.68 |
| 29 | C | 516 | DGD | O6D-C1D-O3G | -2.73 | 103.60 | 110.04 |
| 27 | c | 523 | LMG | O6-C1-O1 | -2.72 | 103.61 | 110.04 |
| 34 | a | 408 | BCT | O3-C-O1 | -2.72 | 112.71 | 119.68 |
| 22 | a | 404 | CLA | CMB-C2B-C3B | 2.72 | 130.12 | 124.68 |
| 22 | A | 403 | CLA | O2D-CGD-O1D | -2.72 | 118.55 | 123.85 |
| 22 | c | 508 | CLA | O2D-CGD-O1D | -2.72 | 118.55 | 123.85 |
| 22 | b | 614 | CLA | O2D-CGD-O1D | -2.72 | 118.56 | 123.85 |
| 22 | d | 404 | CLA | CMB-C2B-C3B | 2.72 | 130.11 | 124.68 |
| 22 | d | 404 | CLA | CHB-C4A-NA | 2.72 | 128.32 | 124.40 |
| 22 | c | 504 | CLA | O2A-CGA-O1A | -2.72 | 116.83 | 123.63 |
| 22 | b | 615 | CLA | C1B-CHB-C4A | -2.72 | 124.86 | 130.04 |
| 28 | a | 410 | SQD | O9-S-C6 | 2.71 | 110.81 | 106.76 |
| 23 | d | 402 | PHO | CMB-C2B-C3B | 2.71 | 130.11 | 124.68 |
| 22 | b | 615 | CLA | CHB-C4A-NA | 2.71 | 128.31 | 124.40 |
| 26 | d | 407 | PL9 | C8-C7-C3 | 2.71 | 119.04 | 112.03 |
| 22 | c | 505 | CLA | O2D-CGD-CBD | 2.71 | 115.97 | 111.23 |
| 22 | c | 507 | CLA | O2A-CGA-O1A | -2.71 | 116.85 | 123.63 |
| 22 | c | 502 | CLA | O1D-CGD-CBD | 2.71 | 129.86 | 124.52 |
| 22 | C | 501 | CLA | O2A-CGA-O1A | -2.71 | 116.86 | 123.63 |
| 22 | B | 615 | CLA | O2D-CGD-CBD | 2.71 | 115.96 | 111.23 |
| 26 | D | 406 | PL9 | C20-C19-C21 | 2.70 | 119.92 | 115.23 |
| 24 | c | 516 | BCR | C27-C26-C25 | 2.70 | 126.36 | 122.70 |
| 24 | a | 405 | BCR | C37-C22-C23 | 2.70 | 122.22 | 118.09 |
| 27 | b | 620 | LMG | C38-C37-C36 | -2.70 | 100.72 | 114.37 |
| 24 | Y | 101 | BCR | C37-C22-C21 | -2.69 | 118.45 | 122.82 |
| 27 | M | 101 | LMG | C38-C37-C36 | -2.69 | 100.77 | 114.37 |
| 22 | B | 614 | CLA | CHB-C4A-NA | 2.69 | 128.28 | 124.40 |
| 22 | C | 503 | CLA | C7-C6-C5 | -2.69 | 106.10 | 113.26 |
| 22 | c | 513 | CLA | CHB-C4A-NA | 2.68 | 128.27 | 124.40 |
| 24 | b | 619 | BCR | C2-C1-C6 | 2.68 | 114.33 | 110.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | a | 409 | PL9 | C37-C38-C39 | -2.68 | 121.49 | 127.62 |
| 22 | B | 603 | CLA | C5-C3-C2 | -2.68 | 115.16 | 121.17 |
| 22 | B | 610 | CLA | CMA-C3A-C4A | -2.68 | 104.58 | 111.77 |
| 33 | l | 101 | LHG | O8-C23-O10 | -2.68 | 116.94 | 123.63 |
| 22 | b | 605 | CLA | O2D-CGD-O1D | -2.68 | 118.64 | 123.85 |
| 32 | C | 520 | STE | O2-C1-C2 | 2.67 | 122.45 | 114.00 |
| 24 | B | 618 | BCR | C3-C4-C5 | -2.67 | 109.29 | 114.06 |
| 22 | b | 601 | CLA | CMB-C2B-C3B | 2.67 | 130.01 | 124.68 |
| 22 | b | 612 | CLA | CHB-C4A-NA | 2.67 | 128.25 | 124.40 |
| 33 | B | 622 | LHG | O8-C23-O10 | -2.67 | 116.96 | 123.63 |
| 29 | A | 414 | DGD | C3E-C4E-C5E | -2.67 | 105.40 | 110.23 |
| 22 | C | 503 | CLA | C4D-CHA-C1A | 2.67 | 124.42 | 121.24 |
| 27 | D | 407 | LMG | O6-C1-O1 | -2.66 | 103.75 | 110.04 |
| 27 | D | 407 | LMG | O3-C3-C2 | -2.66 | 104.10 | 110.38 |
| 29 | C | 517 | DGD | C1D-O6D-C5D | -2.66 | 108.52 | 113.72 |
| 22 | A | 403 | CLA | CMB-C2B-C3B | 2.66 | 130.00 | 124.68 |
| 22 | B | 611 | CLA | CHD-C4C-NC | 2.66 | 128.35 | 124.23 |
| 33 | e | 101 | LHG | O8-C23-C24 | 2.66 | 119.94 | 111.83 |
| 22 | c | 511 | CLA | O2D-CGD-CBD | 2.66 | 115.88 | 111.23 |
| 29 | h | 102 | DGD | O2E-C2E-C3E | -2.66 | 104.11 | 110.38 |
| 22 | b | 614 | CLA | CAC-C3C-C4C | 2.66 | 128.25 | 124.79 |
| 22 | b | 605 | CLA | O1D-CGD-CBD | 2.66 | 129.75 | 124.52 |
| 24 | c | 515 | BCR | C36-C18-C17 | -2.65 | 118.52 | 122.82 |
| 22 | c | 501 | CLA | CHB-C4A-NA | 2.65 | 128.22 | 124.40 |
| 22 | c | 508 | CLA | C1B-CHB-C4A | -2.65 | 124.99 | 130.04 |
| 22 | a | 404 | CLA | C3D-C4D-ND | 2.65 | 114.29 | 109.99 |
| 22 | b | 605 | CLA | C4A-NA-C1A | 2.65 | 107.89 | 106.68 |
| 26 | D | 406 | PL9 | C30-C29-C31 | -2.64 | 110.64 | 115.23 |
| 24 | k | 101 | BCR | C38-C26-C25 | -2.64 | 121.60 | 124.48 |
| 36 | v | 201 | HEC | CBD-CAD-C3D | -2.64 | 108.10 | 112.54 |
| 22 | B | 609 | CLA | C1B-CHB-C4A | -2.64 | 125.01 | 130.04 |
| 22 | A | 405 | CLA | C2C-C1C-NC | 2.64 | 112.75 | 109.98 |
| 24 | K | 101 | BCR | C7-C8-C9 | -2.64 | 122.33 | 126.23 |
| 27 | b | 620 | LMG | O6-C1-O1 | -2.63 | 103.82 | 110.04 |
| 27 | b | 622 | LMG | O6-C5-C6 | 2.63 | 112.97 | 106.44 |
| 24 | b | 618 | BCR | C27-C26-C25 | 2.63 | 126.26 | 122.70 |
| 24 | h | 101 | BCR | C27-C26-C25 | 2.63 | 126.26 | 122.70 |
| 22 | C | 511 | CLA | O2D-CGD-O1D | -2.63 | 118.72 | 123.85 |
| 29 | A | 414 | DGD | CDB-CCB-CBB | -2.63 | 101.08 | 114.37 |
| 33 | d | 410 | LHG | C26-C25-C24 | 2.63 | 122.79 | 113.13 |
| 22 | b | 613 | CLA | O2D-CGD-O1D | -2.63 | 118.73 | 123.85 |
| 33 | D | 408 | LHG | C20-C19-C18 | -2.62 | 101.12 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 604 | CLA | CMB-C2B-C3B | 2.62 | 129.91 | 124.68 |
| 22 | a | 403 | CLA | CED-O2D-CGD | -2.62 | 109.98 | 115.92 |
| 23 | A | 404 | PHO | C1B-NB-C4B | 2.62 | 112.46 | 107.09 |
| 32 | b | 624 | STE | C3-C2-C1 | -2.61 | 107.69 | 114.51 |
| 22 | B | 603 | CLA | CHD-C1D-ND | -2.61 | 121.13 | 124.80 |
| 26 | d | 407 | PL9 | C7-C8-C9 | -2.61 | 122.34 | 126.83 |
| 22 | B | 609 | CLA | CMB-C2B-C3B | 2.61 | 129.89 | 124.68 |
| 22 | b | 608 | CLA | C11-C10-C8 | -2.60 | 107.32 | 115.97 |
| 22 | d | 404 | CLA | CMC-C2C-C1C | 2.60 | 129.09 | 125.03 |
| 28 | A | 412 | SQD | O5-C1-C2 | -2.60 | 105.03 | 110.37 |
| 22 | C | 504 | CLA | CMB-C2B-C3B | 2.60 | 129.87 | 124.68 |
| 22 | c | 512 | CLA | CMB-C2B-C1B | -2.59 | 124.66 | 128.46 |
| 23 | D | 401 | PHO | O2D-CGD-O1D | -2.59 | 118.81 | 123.85 |
| 24 | b | 617 | BCR | C29-C30-C25 | 2.59 | 114.20 | 110.44 |
| 28 | F | 101 | SQD | C1-C2-C3 | -2.59 | 104.57 | 110.01 |
| 22 | B | 612 | CLA | O1D-CGD-CBD | 2.59 | 129.62 | 124.52 |
| 22 | d | 403 | CLA | C1B-CHB-C4A | -2.59 | 125.11 | 130.04 |
| 22 | B | 604 | CLA | CGD-CBD-CAD | -2.58 | 102.48 | 110.85 |
| 22 | b | 607 | CLA | C1B-CHB-C4A | -2.58 | 125.11 | 130.04 |
| 28 | a | 411 | SQD | O48-C23-C24 | 2.58 | 119.70 | 111.83 |
| 22 | c | 510 | CLA | C1B-CHB-C4A | -2.58 | 125.13 | 130.04 |
| 22 | B | 603 | CLA | CMB-C2B-C1B | -2.58 | 124.68 | 128.46 |
| 22 | a | 402 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 22 | c | 513 | CLA | CAC-C3C-C4C | 2.57 | 128.14 | 124.79 |
| 22 | C | 512 | CLA | CHD-C1D-ND | -2.57 | 121.18 | 124.80 |
| 22 | b | 608 | CLA | C1B-CHB-C4A | -2.57 | 125.14 | 130.04 |
| 27 | D | 407 | LMG | O4-C4-C5 | 2.57 | 115.65 | 109.32 |
| 29 | C | 516 | DGD | C3G-C2G-C1G | -2.57 | 105.80 | 111.78 |
| 26 | A | 409 | PL9 | O1-C4-C3 | -2.56 | 118.03 | 120.73 |
| 22 | c | 501 | CLA | O2A-CGA-O1A | -2.56 | 117.22 | 123.63 |
| 27 | M | 101 | LMG | O8-C28-O10 | -2.56 | 117.22 | 123.63 |
| 22 | c | 508 | CLA | C1-C2-C3 | -2.56 | 122.00 | 126.20 |
| 22 | B | 602 | CLA | C1B-CHB-C4A | -2.56 | 125.16 | 130.04 |
| 22 | C | 501 | CLA | O2D-CGD-CBD | 2.56 | 115.70 | 111.23 |
| 23 | D | 401 | PHO | C1A-C2A-C3A | -2.56 | 100.41 | 102.84 |
| 22 | c | 505 | CLA | CMB-C2B-C1B | -2.56 | 124.71 | 128.46 |
| 29 | c | 519 | DGD | O6D-C1D-O3G | -2.55 | 104.01 | 110.04 |
| 23 | A | 404 | PHO | CMA-C3A-C2A | -2.55 | 104.28 | 114.13 |
| 26 | a | 409 | PL9 | C27-C28-C29 | -2.55 | 121.79 | 127.62 |
| 22 | c | 503 | CLA | C4-C3-C5 | 2.55 | 119.65 | 115.23 |
| 26 | d | 407 | PL9 | C50-C49-C48 | -2.55 | 115.00 | 122.66 |
| 22 | B | 616 | CLA | C1B-CHB-C4A | -2.55 | 125.18 | 130.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 601 | CLA | C1B-CHB-C4A | -2.55 | 125.18 | 130.04 |
| 24 | d | 406 | BCR | C24-C23-C22 | -2.54 | 122.47 | 126.23 |
| 28 | B | 623 | SQD | O5-C5-C4 | 2.54 | 114.28 | 109.70 |
| 22 | B | 615 | CLA | C1B-CHB-C4A | -2.54 | 125.19 | 130.04 |
| 22 | b | 611 | CLA | CHD-C1D-ND | -2.54 | 121.22 | 124.80 |
| 24 | a | 405 | BCR | C29-C30-C25 | 2.54 | 114.13 | 110.44 |
| 22 | B | 603 | CLA | CHD-C1D-C2D | 2.54 | 130.78 | 125.49 |
| 22 | b | 614 | CLA | CMB-C2B-C3B | 2.54 | 129.76 | 124.68 |
| 24 | C | 514 | BCR | C37-C22-C21 | -2.54 | 118.70 | 122.82 |
| 27 | D | 407 | LMG | C38-C37-C36 | -2.54 | 101.53 | 114.37 |
| 24 | b | 617 | BCR | C27-C26-C25 | 2.54 | 126.14 | 122.70 |
| 22 | B | 613 | CLA | CHB-C4A-NA | 2.54 | 128.06 | 124.40 |
| 26 | d | 407 | PL9 | C20-C19-C21 | 2.54 | 119.63 | 115.23 |
| 28 | A | 413 | SQD | O48-C46-C45 | 2.54 | 115.57 | 108.35 |
| 22 | B | 611 | CLA | CHB-C4A-NA | 2.53 | 128.06 | 124.40 |
| 22 | B | 604 | CLA | C11-C10-C8 | -2.53 | 107.55 | 115.97 |
| 22 | c | 506 | CLA | CBC-CAC-C3C | -2.53 | 105.56 | 112.42 |
| 29 | c | 518 | DGD | C1D-C2D-C3D | -2.53 | 104.69 | 110.01 |
| 28 | f | 102 | SQD | O48-C23-C24 | 2.53 | 119.54 | 111.83 |
| 33 | D | 409 | LHG | O8-C6-C5 | -2.53 | 101.11 | 108.40 |
| 22 | C | 511 | CLA | CHB-C4A-NA | 2.53 | 128.04 | 124.40 |
| 22 | b | 608 | CLA | C3B-C4B-NB | -2.52 | 105.95 | 109.21 |
| 22 | c | 507 | CLA | CMB-C2B-C1B | -2.52 | 124.76 | 128.46 |
| 22 | B | 615 | CLA | CMB-C2B-C1B | -2.52 | 124.76 | 128.46 |
| 27 | c | 522 | LMG | C9-C8-C7 | -2.52 | 105.91 | 111.78 |
| 26 | D | 406 | PL9 | C42-C43-C44 | -2.52 | 121.86 | 127.62 |
| 22 | C | 512 | CLA | C1B-CHB-C4A | -2.52 | 125.23 | 130.04 |
| 22 | B | 606 | CLA | CHD-C4C-NC | 2.51 | 128.13 | 124.23 |
| 22 | B | 609 | CLA | O2A-CGA-O1A | -2.51 | 117.35 | 123.63 |
| 22 | b | 615 | CLA | CHC-C1C-NC | 2.51 | 128.09 | 124.31 |
| 22 | C | 501 | CLA | C1B-CHB-C4A | -2.51 | 125.25 | 130.04 |
| 22 | b | 606 | CLA | C1B-CHB-C4A | -2.51 | 125.26 | 130.04 |
| 27 | M | 101 | LMG | O7-C10-O9 | -2.51 | 117.84 | 123.70 |
| 29 | A | 414 | DGD | C5B-C4B-C3B | -2.51 | 101.70 | 114.37 |
| 29 | h | 102 | DGD | C1D-O6D-C5D | -2.51 | 108.83 | 113.72 |
| 22 | B | 611 | CLA | C14-C13-C15 | -2.50 | 102.35 | 111.27 |
| 22 | a | 403 | CLA | O2D-CGD-O1D | -2.50 | 118.97 | 123.85 |
| 23 | A | 404 | PHO | C1A-C2A-C3A | -2.50 | 100.46 | 102.84 |
| 35 | E | 101 | HEM | O2D-CGD-CBD | 2.50 | 121.91 | 114.00 |
| 29 | A | 414 | DGD | C1D-C2D-C3D | -2.50 | 104.75 | 110.01 |
| 23 | A | 404 | PHO | C1-C2-C3 | -2.50 | 122.10 | 126.20 |
| 28 | a | 410 | SQD | O47-C7-C8 | 2.50 | 116.88 | 111.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 606 | CLA | C4-C3-C5 | 2.50 | 119.56 | 115.23 |
| 22 | c | 509 | CLA | CHD-C1D-ND | -2.49 | 121.29 | 124.80 |
| 24 | b | 619 | BCR | C36-C18-C19 | 2.49 | 121.90 | 118.09 |
| 33 | d | 409 | LHG | O8-C23-C24 | 2.49 | 119.43 | 111.83 |
| 22 | b | 613 | CLA | CHA-C1A-NA | -2.49 | 120.75 | 126.39 |
| 22 | C | 503 | CLA | CMB-C2B-C3B | 2.49 | 129.66 | 124.68 |
| 23 | A | 404 | PHO | C16-C17-C18 | -2.49 | 104.84 | 115.94 |
| 24 | A | 406 | BCR | C16-C15-C14 | -2.49 | 118.43 | 123.52 |
| 22 | b | 612 | CLA | C11-C12-C13 | -2.48 | 107.71 | 115.97 |
| 22 | B | 612 | CLA | O2A-CGA-O1A | -2.48 | 117.41 | 123.63 |
| 24 | t | 101 | BCR | C4-C5-C6 | 2.48 | 126.06 | 122.70 |
| 22 | B | 612 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 26 | A | 409 | PL9 | C12-C13-C14 | -2.48 | 121.94 | 127.62 |
| 24 | B | 618 | BCR | C15-C16-C17 | -2.48 | 118.45 | 123.52 |
| 22 | b | 610 | CLA | O2D-CGD-O1D | -2.48 | 119.03 | 123.85 |
| 29 | C | 517 | DGD | CDB-CCB-CBB | -2.47 | 101.87 | 114.37 |
| 22 | C | 509 | CLA | C1B-CHB-C4A | -2.47 | 125.32 | 130.04 |
| 29 | C | 518 | DGD | C3G-C2G-C1G | -2.47 | 106.02 | 111.78 |
| 33 | d | 409 | LHG | C18-C17-C16 | -2.47 | 101.87 | 114.37 |
| 28 | A | 413 | SQD | O47-C45-C44 | 2.47 | 113.50 | 107.96 |
| 22 | D | 403 | CLA | CMB-C2B-C3B | 2.47 | 129.62 | 124.68 |
| 22 | A | 410 | CLA | O2D-CGD-O1D | -2.47 | 119.04 | 123.85 |
| 22 | c | 510 | CLA | C1-C2-C3 | -2.47 | 122.15 | 126.20 |
| 22 | b | 614 | CLA | O2A-CGA-O1A | -2.47 | 117.46 | 123.63 |
| 29 | h | 102 | DGD | C4E-C3E-C2E | -2.46 | 106.51 | 110.83 |
| 23 | d | 402 | PHO | O2A-CGA-O1A | -2.46 | 117.47 | 123.63 |
| 24 | c | 516 | BCR | C24-C23-C22 | -2.46 | 122.59 | 126.23 |
| 22 | B | 614 | CLA | O1D-CGD-CBD | 2.46 | 129.37 | 124.52 |
| 22 | B | 610 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 22 | B | 609 | CLA | C2C-C1C-NC | 2.46 | 112.56 | 109.98 |
| 22 | b | 603 | CLA | CHD-C1D-C2D | 2.46 | 130.59 | 125.49 |
| 28 | f | 102 | SQD | O5-C1-O6 | 2.45 | 115.84 | 110.04 |
| 22 | c | 513 | CLA | C11-C12-C13 | -2.45 | 107.81 | 115.97 |
| 28 | B | 623 | SQD | O48-C23-O10 | -2.45 | 117.49 | 123.63 |
| 22 | d | 404 | CLA | C1B-CHB-C4A | -2.45 | 125.36 | 130.04 |
| 24 | B | 619 | BCR | C1-C6-C5 | -2.45 | 119.29 | 122.64 |
| 27 | c | 522 | LMG | O2-C2-C1 | -2.45 | 104.23 | 110.08 |
| 27 | A | 411 | LMG | O1-C7-C8 | -2.45 | 104.86 | 110.82 |
| 27 | c | 523 | LMG | C9-C8-C7 | -2.45 | 106.07 | 111.78 |
| 22 | a | 403 | CLA | O2D-CGD-CBD | 2.45 | 115.51 | 111.23 |
| 22 | B | 614 | CLA | C4A-NA-C1A | 2.45 | 107.80 | 106.68 |
| 24 | B | 617 | BCR | C38-C26-C25 | -2.45 | 121.81 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 604 | CLA | O2D-CGD-CBD | 2.45 | 115.50 | 111.23 |
| 36 | v | 201 | HEC | C1D-C2D-C3D | -2.44 | 105.30 | 107.00 |
| 22 | d | 403 | CLA | O2D-CGD-O1D | -2.44 | 119.09 | 123.85 |
| 24 | t | 101 | BCR | C19-C18-C17 | -2.44 | 115.17 | 119.01 |
| 23 | D | 401 | PHO | CMC-C2C-C3C | 2.44 | 129.55 | 124.94 |
| 24 | c | 514 | BCR | C20-C21-C22 | -2.44 | 123.85 | 127.28 |
| 23 | d | 401 | PHO | C1-C2-C3 | -2.44 | 122.20 | 126.20 |
| 28 | f | 102 | SQD | O5-C1-C2 | -2.44 | 105.36 | 110.37 |
| 24 | c | 515 | BCR | C7-C8-C9 | -2.44 | 122.63 | 126.23 |
| 35 | E | 101 | HEM | CHC-C4B-NB | 2.44 | 127.06 | 124.44 |
| 22 | C | 509 | CLA | CED-O2D-CGD | 2.43 | 121.44 | 115.92 |
| 23 | D | 401 | PHO | C1B-NB-C4B | 2.43 | 112.08 | 107.09 |
| 22 | A | 403 | CLA | C4A-NA-C1A | 2.43 | 107.79 | 106.68 |
| 24 | H | 101 | BCR | C27-C26-C25 | 2.43 | 125.99 | 122.70 |
| 22 | A | 403 | CLA | CED-O2D-CGD | -2.43 | 110.41 | 115.92 |
| 24 | h | 101 | BCR | C2-C1-C6 | 2.43 | 113.97 | 110.44 |
| 24 | A | 406 | BCR | C11-C10-C9 | -2.43 | 123.88 | 127.28 |
| 22 | C | 505 | CLA | C1B-CHB-C4A | -2.43 | 125.41 | 130.04 |
| 22 | B | 605 | CLA | C1B-CHB-C4A | -2.42 | 125.42 | 130.04 |
| 22 | B | 603 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 27 | c | 522 | LMG | O3-C3-C2 | -2.42 | 104.66 | 110.38 |
| 22 | A | 402 | CLA | C6-C5-C3 | 2.42 | 119.36 | 113.47 |
| 27 | b | 620 | LMG | C1-O6-C5 | -2.42 | 109.00 | 113.72 |
| 22 | B | 616 | CLA | O1D-CGD-CBD | 2.42 | 129.29 | 124.52 |
| 22 | b | 604 | CLA | O1D-CGD-CBD | 2.42 | 129.28 | 124.52 |
| 27 | b | 620 | LMG | C9-C8-C7 | -2.41 | 106.16 | 111.78 |
| 22 | c | 504 | CLA | O2D-CGD-O1D | -2.41 | 119.15 | 123.85 |
| 22 | B | 606 | CLA | CMB-C2B-C3B | 2.41 | 129.50 | 124.68 |
| 24 | c | 516 | BCR | C38-C26-C25 | -2.41 | 121.85 | 124.48 |
| 22 | B | 613 | CLA | CHA-C1A-NA | -2.41 | 120.93 | 126.39 |
| 28 | L | 101 | SQD | O47-C45-C46 | 2.41 | 116.98 | 108.34 |
| 24 | H | 101 | BCR | C29-C30-C25 | 2.41 | 113.94 | 110.44 |
| 24 | a | 405 | BCR | C27-C26-C25 | 2.41 | 125.96 | 122.70 |
| 22 | C | 512 | CLA | CAA-CBA-CGA | -2.41 | 106.38 | 113.21 |
| 24 | T | 101 | BCR | C4-C5-C6 | 2.41 | 125.95 | 122.70 |
| 22 | a | 404 | CLA | O2A-CGA-O1A | -2.40 | 117.62 | 123.63 |
| 23 | A | 404 | PHO | CMC-C2C-C3C | 2.40 | 129.47 | 124.94 |
| 33 | L | 102 | LHG | O8-C23-O10 | -2.40 | 117.63 | 123.63 |
| 22 | D | 403 | CLA | C1-C2-C3 | -2.40 | 122.27 | 126.20 |
| 24 | C | 515 | BCR | C27-C26-C25 | 2.40 | 125.94 | 122.70 |
| 22 | b | 605 | CLA | C1-C2-C3 | -2.40 | 122.27 | 126.20 |
| 29 | c | 519 | DGD | CDB-CCB-CBB | -2.40 | 102.26 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | t | 101 | BCR | C28-C27-C26 | -2.40 | 109.78 | 114.06 |
| 29 | a | 412 | DGD | C7B-C6B-C5B | -2.39 | 102.26 | 114.37 |
| 27 | A | 411 | LMG | O3-C3-C2 | -2.39 | 104.74 | 110.38 |
| 22 | c | 508 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 22 | c | 510 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 22 | a | 402 | CLA | CAC-C3C-C4C | 2.39 | 127.90 | 124.79 |
| 22 | B | 609 | CLA | CAC-C3C-C4C | 2.39 | 127.90 | 124.79 |
| 35 | E | 101 | HEM | CBA-CAA-C2A | -2.39 | 108.52 | 112.54 |
| 24 | B | 617 | BCR | C3-C4-C5 | -2.39 | 109.80 | 114.06 |
| 32 | b | 623 | STE | O2-C1-C2 | 2.39 | 121.54 | 114.00 |
| 22 | b | 614 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |
| 29 | H | 102 | DGD | C3G-C2G-C1G | -2.38 | 106.23 | 111.78 |
| 33 | B | 622 | LHG | C18-C17-C16 | -2.38 | 102.34 | 114.37 |
| 28 | a | 410 | SQD | O8-S-O9 | -2.38 | 105.45 | 111.40 |
| 33 | l | 101 | LHG | O10-C23-C24 | -2.38 | 114.49 | 123.78 |
| 22 | c | 508 | CLA | CHD-C1D-C2D | 2.37 | 130.43 | 125.49 |
| 22 | A | 402 | CLA | O2D-CGD-O1D | -2.37 | 119.23 | 123.85 |
| 24 | h | 101 | BCR | C37-C22-C23 | 2.37 | 121.71 | 118.09 |
| 27 | c | 523 | LMG | O8-C28-O10 | -2.37 | 117.70 | 123.63 |
| 22 | c | 506 | CLA | C1-O2A-CGA | 2.37 | 122.39 | 116.65 |
| 26 | D | 406 | PL9 | C32-C33-C34 | -2.37 | 122.20 | 127.62 |
| 29 | H | 102 | DGD | CAB-C9B-C8B | -2.37 | 102.39 | 114.37 |
| 22 | c | 509 | CLA | C11-C10-C8 | -2.37 | 108.09 | 115.97 |
| 29 | c | 518 | DGD | CDB-CCB-CBB | -2.37 | 102.39 | 114.37 |
| 22 | C | 507 | CLA | O2A-CGA-O1A | -2.37 | 117.70 | 123.63 |
| 22 | C | 512 | CLA | CMB-C2B-C3B | 2.37 | 129.41 | 124.68 |
| 24 | t | 101 | BCR | C15-C16-C17 | -2.37 | 118.68 | 123.52 |
| 24 | t | 101 | BCR | C27-C26-C25 | 2.37 | 125.90 | 122.70 |
| 22 | b | 606 | CLA | O1D-CGD-CBD | 2.36 | 129.18 | 124.52 |
| 24 | b | 617 | BCR | C23-C22-C21 | -2.36 | 115.29 | 119.01 |
| 27 | C | 519 | LMG | C38-C37-C36 | -2.36 | 102.42 | 114.37 |
| 28 | a | 410 | SQD | O8-S-C6 | 2.36 | 110.53 | 105.97 |
| 27 | c | 523 | LMG | O1-C7-C8 | -2.36 | 105.07 | 110.82 |
| 24 | a | 405 | BCR | C37-C22-C21 | -2.36 | 118.99 | 122.82 |
| 24 | K | 101 | BCR | C2-C1-C6 | 2.36 | 113.87 | 110.44 |
| 22 | B | 603 | CLA | OBD-CAD-C3D | 2.36 | 133.94 | 128.42 |
| 24 | c | 515 | BCR | C37-C22-C23 | 2.36 | 121.69 | 118.09 |
| 22 | C | 510 | CLA | O2D-CGD-CBD | 2.36 | 115.36 | 111.23 |
| 22 | B | 602 | CLA | O2A-CGA-O1A | -2.36 | 117.72 | 123.63 |
| 24 | D | 405 | BCR | C7-C8-C9 | -2.36 | 122.74 | 126.23 |
| 26 | D | 406 | PL9 | C35-C34-C36 | 2.36 | 119.32 | 115.23 |
| 24 | t | 101 | BCR | C16-C17-C18 | -2.35 | 123.98 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | a | 409 | PL9 | O2-C1-C6 | 2.35 | 124.22 | 120.48 |
| 22 | C | 512 | CLA | O2D-CGD-O1D | -2.35 | 119.27 | 123.85 |
| 26 | a | 409 | PL9 | C40-C39-C38 | -2.35 | 117.59 | 123.63 |
| 24 | A | 406 | BCR | C38-C26-C25 | -2.35 | 121.92 | 124.48 |
| 22 | b | 613 | CLA | C16-C15-C13 | -2.35 | 108.16 | 115.97 |
| 29 | c | 519 | DGD | C6B-C5B-C4B | -2.34 | 102.52 | 114.37 |
| 22 | b | 616 | CLA | CGD-CBD-CAD | -2.34 | 103.26 | 110.85 |
| 29 | A | 414 | DGD | O6D-C1D-O3G | -2.34 | 104.51 | 110.04 |
| 22 | C | 506 | CLA | C1-C2-C3 | -2.34 | 122.36 | 126.20 |
| 22 | b | 614 | CLA | O2D-CGD-CBD | 2.34 | 115.32 | 111.23 |
| 29 | C | 518 | DGD | C4D-C3D-C2D | -2.34 | 106.72 | 110.83 |
| 22 | b | 603 | CLA | O2D-CGD-CBD | 2.34 | 115.32 | 111.23 |
| 22 | A | 405 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 22 | c | 502 | CLA | C1-C2-C3 | -2.34 | 122.37 | 126.20 |
| 23 | d | 402 | PHO | C1B-NB-C4B | 2.33 | 111.89 | 107.09 |
| 22 | b | 614 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 29 | c | 519 | DGD | C6D-O5D-C1E | 2.33 | 118.80 | 113.80 |
| 26 | a | 409 | PL9 | O1-C4-C3 | -2.33 | 118.27 | 120.73 |
| 24 | b | 619 | BCR | C27-C26-C25 | 2.33 | 125.86 | 122.70 |
| 22 | C | 505 | CLA | O2A-CGA-O1A | -2.33 | 117.80 | 123.63 |
| 22 | b | 610 | CLA | O2A-CGA-O1A | -2.33 | 117.80 | 123.63 |
| 33 | d | 408 | LHG | C5-O7-C7 | -2.33 | 112.22 | 117.80 |
| 22 | b | 605 | CLA | CHD-C4C-NC | 2.33 | 127.84 | 124.23 |
| 22 | C | 504 | CLA | CHA-C1A-NA | -2.32 | 121.13 | 126.39 |
| 22 | c | 513 | CLA | O1D-CGD-CBD | 2.32 | 129.10 | 124.52 |
| 33 | l | 101 | LHG | C20-C19-C18 | -2.32 | 102.62 | 114.37 |
| 22 | C | 513 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 26 | D | 406 | PL9 | C36-C34-C33 | -2.32 | 115.95 | 121.17 |
| 23 | d | 401 | PHO | CMA-C3A-C4A | -2.32 | 109.61 | 114.61 |
| 22 | b | 607 | CLA | CED-O2D-CGD | 2.32 | 121.18 | 115.92 |
| 28 | F | 101 | SQD | O9-S-O7 | -2.32 | 106.28 | 113.82 |
| 24 | b | 619 | BCR | C29-C30-C25 | 2.32 | 113.81 | 110.44 |
| 28 | a | 411 | SQD | O47-C7-C8 | 2.32 | 116.50 | 111.48 |
| 24 | B | 619 | BCR | C15-C16-C17 | -2.32 | 118.77 | 123.52 |
| 24 | c | 514 | BCR | C27-C26-C25 | 2.32 | 125.84 | 122.70 |
| 29 | A | 414 | DGD | C3G-C2G-C1G | -2.32 | 106.38 | 111.78 |
| 22 | C | 512 | CLA | O2A-CGA-O1A | -2.32 | 117.83 | 123.63 |
| 22 | b | 608 | CLA | C1-C2-C3 | -2.32 | 122.40 | 126.20 |
| 28 | a | 411 | SQD | O6-C44-C45 | -2.32 | 105.82 | 111.77 |
| 22 | B | 606 | CLA | O2D-CGD-CBD | 2.31 | 115.28 | 111.23 |
| 29 | C | 517 | DGD | C6D-O5D-C1E | 2.31 | 118.76 | 113.80 |
| 29 | C | 517 | DGD | CAB-C9B-C8B | -2.31 | 102.68 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 612 | CLA | CAC-C3C-C4C | 2.31 | 127.80 | 124.79 |
| 22 | c | 513 | CLA | O2A-CGA-O1A | -2.31 | 117.85 | 123.63 |
| 22 | c | 511 | CLA | CHB-C4A-NA | 2.31 | 127.73 | 124.40 |
| 22 | B | 607 | CLA | C2A-C1A-CHA | 2.31 | 127.88 | 123.87 |
| 24 | b | 619 | BCR | C16-C15-C14 | -2.31 | 118.79 | 123.52 |
| 32 | C | 522 | STE | O1-C1-C2 | -2.31 | 115.78 | 123.09 |
| 22 | B | 604 | CLA | C6-C7-C8 | -2.31 | 108.30 | 115.97 |
| 29 | C | 517 | DGD | C1D-C2D-C3D | -2.31 | 105.16 | 110.01 |
| 29 | c | 519 | DGD | O5D-C1E-C2E | 2.31 | 111.77 | 108.27 |
| 22 | c | 502 | CLA | O2A-CGA-O1A | -2.31 | 117.86 | 123.63 |
| 22 | b | 613 | CLA | O2A-CGA-O1A | -2.30 | 117.86 | 123.63 |
| 22 | B | 611 | CLA | C9-C8-C10 | -2.30 | 103.06 | 111.27 |
| 29 | h | 102 | DGD | CDB-CCB-CBB | -2.30 | 102.72 | 114.37 |
| 27 | c | 522 | LMG | C6-C5-C4 | -2.30 | 107.36 | 113.02 |
| 28 | B | 623 | SQD | C1-C2-C3 | -2.30 | 105.17 | 110.01 |
| 34 | D | 402 | BCT | O3-C-O1 | -2.30 | 113.79 | 119.68 |
| 22 | b | 615 | CLA | O2A-CGA-O1A | -2.30 | 117.87 | 123.63 |
| 22 | A | 402 | CLA | CAA-CBA-CGA | -2.30 | 106.67 | 113.21 |
| 35 | f | 101 | HEM | CHB-C1B-NB | 2.30 | 127.22 | 124.37 |
| 24 | b | 619 | BCR | C37-C22-C21 | -2.30 | 119.09 | 122.82 |
| 22 | B | 606 | CLA | CGD-CBD-CAD | -2.30 | 103.41 | 110.85 |
| 22 | c | 507 | CLA | CMB-C2B-C3B | 2.29 | 129.27 | 124.68 |
| 22 | B | 610 | CLA | C11-C10-C8 | -2.29 | 108.34 | 115.97 |
| 29 | C | 517 | DGD | C7B-C6B-C5B | -2.29 | 102.79 | 114.37 |
| 29 | C | 516 | DGD | C4E-C3E-C2E | -2.29 | 106.81 | 110.83 |
| 26 | a | 409 | PL9 | C25-C24-C26 | 2.29 | 119.20 | 115.23 |
| 22 | C | 501 | CLA | OBD-CAD-C3D | 2.29 | 133.76 | 128.42 |
| 22 | B | 603 | CLA | O2A-CGA-O1A | -2.28 | 117.91 | 123.63 |
| 26 | D | 406 | PL9 | C37-C38-C39 | -2.28 | 122.40 | 127.62 |
| 27 | A | 411 | LMG | C12-C11-C10 | -2.28 | 105.33 | 113.69 |
| 22 | b | 612 | CLA | C4A-NA-C1A | 2.28 | 107.72 | 106.68 |
| 22 | c | 507 | CLA | CHA-C1A-NA | -2.28 | 121.23 | 126.39 |
| 22 | D | 403 | CLA | O2A-CGA-O1A | -2.28 | 117.93 | 123.63 |
| 24 | b | 619 | BCR | C15-C16-C17 | -2.28 | 118.86 | 123.52 |
| 23 | A | 404 | PHO | O2D-CGD-O1D | -2.28 | 119.41 | 123.85 |
| 27 | C | 519 | LMG | C6-C5-C4 | -2.28 | 107.43 | 113.02 |
| 22 | b | 604 | CLA | C4D-C3D-CAD | -2.28 | 105.63 | 108.11 |
| 33 | d | 408 | LHG | C11-C10-C9 | -2.28 | 102.86 | 114.37 |
| 29 | a | 412 | DGD | CFB-CEB-CDB | -2.28 | 102.87 | 114.37 |
| 29 | c | 519 | DGD | O1G-C1G-C2G | -2.27 | 101.84 | 108.40 |
| 22 | B | 602 | CLA | C11-C12-C13 | -2.27 | 108.40 | 115.97 |
| 32 | j | 101 | STE | O1-C1-C2 | -2.27 | 115.88 | 123.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 611 | CLA | CHB-C4A-NA | 2.27 | 127.68 | 124.40 |
| 29 | c | 519 | DGD | O2D-C2D-C1D | -2.27 | 104.66 | 110.08 |
| 22 | a | 402 | CLA | C4-C3-C5 | 2.27 | 119.17 | 115.23 |
| 22 | b | 607 | CLA | CHB-C4A-NA | 2.27 | 127.68 | 124.40 |
| 22 | d | 403 | CLA | C1C-C2C-C3C | -2.27 | 104.59 | 106.98 |
| 24 | A | 406 | BCR | C2-C1-C6 | 2.27 | 113.73 | 110.44 |
| 22 | A | 405 | CLA | C4A-NA-C1A | 2.27 | 107.71 | 106.68 |
| 29 | C | 516 | DGD | C9B-C8B-C7B | -2.27 | 102.90 | 114.37 |
| 29 | H | 102 | DGD | CDB-CCB-CBB | -2.27 | 102.90 | 114.37 |
| 22 | b | 612 | CLA | CED-O2D-CGD | -2.27 | 110.77 | 115.92 |
| 22 | c | 513 | CLA | C1B-CHB-C4A | -2.27 | 125.72 | 130.04 |
| 22 | B | 613 | CLA | C1B-CHB-C4A | -2.27 | 125.72 | 130.04 |
| 28 | A | 413 | SQD | O48-C23-O10 | -2.27 | 117.96 | 123.63 |
| 22 | C | 509 | CLA | C2A-C3A-C4A | 2.27 | 105.53 | 101.87 |
| 22 | c | 503 | CLA | C5-C3-C2 | -2.26 | 116.08 | 121.17 |
| 22 | b | 605 | CLA | CHD-C1D-C2D | 2.26 | 130.19 | 125.49 |
| 22 | c | 507 | CLA | O1D-CGD-CBD | 2.26 | 128.98 | 124.52 |
| 22 | B | 610 | CLA | CMB-C2B-C1B | -2.26 | 125.14 | 128.46 |
| 22 | C | 508 | CLA | CHD-C4C-NC | 2.26 | 127.74 | 124.23 |
| 22 | B | 616 | CLA | CHA-C4D-ND | 2.26 | 137.21 | 132.55 |
| 22 | B | 614 | CLA | C1-C2-C3 | -2.26 | 122.49 | 126.20 |
| 22 | b | 606 | CLA | CHD-C4C-NC | 2.26 | 127.73 | 124.23 |
| 22 | b | 605 | CLA | CHA-C1A-NA | -2.26 | 121.28 | 126.39 |
| 28 | L | 101 | SQD | O8-S-C6 | 2.26 | 110.33 | 105.97 |
| 24 | Y | 101 | BCR | C15-C16-C17 | -2.25 | 118.91 | 123.52 |
| 29 | h | 102 | DGD | C7B-C6B-C5B | -2.25 | 102.97 | 114.37 |
| 24 | c | 515 | BCR | C8-C9-C10 | 2.25 | 122.55 | 119.01 |
| 29 | C | 518 | DGD | CBB-CAB-C9B | -2.25 | 102.98 | 114.37 |
| 26 | d | 407 | PL9 | C27-C28-C29 | -2.25 | 122.47 | 127.62 |
| 32 | j | 101 | STE | O2-C1-O1 | -2.25 | 117.54 | 123.33 |
| 22 | B | 606 | CLA | O2A-CGA-O1A | -2.25 | 118.00 | 123.63 |
| 24 | T | 101 | BCR | C1-C6-C5 | -2.25 | 119.56 | 122.64 |
| 26 | d | 407 | PL9 | C12-C13-C14 | -2.25 | 122.48 | 127.62 |
| 28 | a | 410 | SQD | O48-C23-O10 | -2.25 | 118.01 | 123.63 |
| 26 | a | 409 | PL9 | C7-C8-C9 | -2.25 | 122.96 | 126.83 |
| 24 | H | 101 | BCR | C37-C22-C21 | -2.24 | 119.18 | 122.82 |
| 22 | B | 610 | CLA | C1-C2-C3 | -2.24 | 122.52 | 126.20 |
| 22 | B | 614 | CLA | CHD-C4C-NC | 2.24 | 127.71 | 124.23 |
| 27 | D | 407 | LMG | O1-C1-C2 | -2.24 | 104.87 | 108.27 |
| 24 | B | 618 | BCR | C38-C26-C25 | -2.24 | 122.04 | 124.48 |
| 26 | A | 409 | PL9 | C20-C19-C18 | -2.24 | 117.88 | 123.63 |
| 24 | B | 617 | BCR | C29-C30-C25 | 2.24 | 113.69 | 110.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | c | 502 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 22 | B | 609 | CLA | O2D-CGD-O1D | -2.24 | 119.50 | 123.85 |
| 24 | c | 516 | BCR | C15-C16-C17 | -2.23 | 118.95 | 123.52 |
| 22 | C | 503 | CLA | C1B-CHB-C4A | -2.23 | 125.78 | 130.04 |
| 33 | e | 101 | LHG | C11-C10-C9 | -2.23 | 103.08 | 114.37 |
| 24 | b | 617 | BCR | C24-C23-C22 | -2.23 | 122.93 | 126.23 |
| 24 | B | 618 | BCR | C27-C26-C25 | 2.23 | 125.72 | 122.70 |
| 22 | b | 611 | CLA | CHD-C1D-C2D | 2.23 | 130.12 | 125.49 |
| 29 | a | 412 | DGD | CDB-CCB-CBB | -2.23 | 103.10 | 114.37 |
| 22 | C | 507 | CLA | C4-C3-C5 | 2.23 | 119.09 | 115.23 |
| 22 | d | 404 | CLA | C1C-C2C-C3C | -2.23 | 104.64 | 106.98 |
| 29 | h | 102 | DGD | O3E-C3E-C4E | 2.23 | 115.63 | 110.38 |
| 24 | b | 617 | BCR | C37-C22-C21 | -2.23 | 119.21 | 122.82 |
| 27 | c | 522 | LMG | O6-C1-O1 | -2.22 | 104.79 | 110.04 |
| 24 | b | 617 | BCR | C8-C7-C6 | -2.22 | 121.06 | 127.00 |
| 22 | C | 503 | CLA | CHD-C4C-NC | 2.22 | 127.68 | 124.23 |
| 33 | B | 622 | LHG | C20-C19-C18 | -2.22 | 103.14 | 114.37 |
| 28 | f | 102 | SQD | O47-C7-O49 | -2.22 | 118.51 | 123.70 |
| 29 | c | 517 | DGD | C4E-C3E-C2E | -2.22 | 106.94 | 110.83 |
| 24 | A | 406 | BCR | C34-C9-C8 | -2.22 | 114.70 | 118.09 |
| 24 | C | 515 | BCR | C37-C22-C21 | -2.22 | 119.22 | 122.82 |
| 22 | B | 615 | CLA | C2A-C3A-C4A | 2.22 | 105.45 | 101.87 |
| 22 | B | 604 | CLA | O2A-CGA-O1A | -2.22 | 118.08 | 123.63 |
| 24 | d | 406 | BCR | C2-C1-C6 | 2.22 | 113.66 | 110.44 |
| 24 | B | 617 | BCR | C37-C22-C23 | 2.22 | 121.47 | 118.09 |
| 24 | T | 101 | BCR | C38-C26-C27 | -2.22 | 108.87 | 113.60 |
| 22 | a | 403 | CLA | CMA-C3A-C4A | -2.22 | 105.82 | 111.77 |
| 22 | B | 611 | CLA | C5-C3-C2 | 2.22 | 126.14 | 121.17 |
| 22 | C | 504 | CLA | CHD-C1D-ND | -2.22 | 121.69 | 124.80 |
| 26 | d | 407 | PL9 | C32-C33-C34 | -2.21 | 122.56 | 127.62 |
| 22 | b | 610 | CLA | O1D-CGD-CBD | 2.21 | 128.88 | 124.52 |
| 22 | B | 607 | CLA | C1B-CHB-C4A | -2.21 | 125.83 | 130.04 |
| 33 | l | 101 | LHG | O8-C23-C24 | 2.21 | 118.57 | 111.83 |
| 22 | B | 608 | CLA | CHB-C4A-NA | 2.21 | 127.58 | 124.40 |
| 27 | b | 620 | LMG | O8-C28-O10 | -2.21 | 118.11 | 123.63 |
| 22 | b | 608 | CLA | C4-C3-C5 | 2.21 | 119.06 | 115.23 |
| 29 | c | 519 | DGD | C8B-C7B-C6B | -2.20 | 103.23 | 114.37 |
| 27 | d | 412 | LMG | C40-C39-C38 | -2.20 | 103.23 | 114.37 |
| 22 | C | 513 | CLA | O1D-CGD-CBD | 2.20 | 128.86 | 124.52 |
| 27 | M | 101 | LMG | O3-C3-C2 | -2.20 | 105.18 | 110.38 |
| 22 | a | 404 | CLA | C1-O2A-CGA | -2.20 | 111.32 | 116.65 |
| 32 | C | 522 | STE | C6-C5-C4 | -2.20 | 103.24 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | E | 102 | LHG | C18-C17-C16 | -2.20 | 103.25 | 114.37 |
| 22 | c | 512 | CLA | CHD-C1D-ND | -2.20 | 121.71 | 124.80 |
| 24 | h | 101 | BCR | C36-C18-C19 | 2.20 | 121.45 | 118.09 |
| 22 | b | 613 | CLA | C2A-C1A-CHA | 2.20 | 127.68 | 123.87 |
| 22 | A | 410 | CLA | CHD-C1D-ND | -2.20 | 121.71 | 124.80 |
| 22 | B | 608 | CLA | C11-C12-C13 | -2.20 | 108.67 | 115.97 |
| 22 | C | 511 | CLA | CHD-C1D-ND | -2.20 | 121.71 | 124.80 |
| 22 | C | 506 | CLA | CHB-C4A-NA | 2.20 | 127.57 | 124.40 |
| 24 | c | 514 | BCR | C33-C5-C6 | -2.20 | 122.09 | 124.48 |
| 22 | b | 605 | CLA | C16-C15-C13 | -2.20 | 108.67 | 115.97 |
| 22 | D | 403 | CLA | C4-C3-C5 | 2.19 | 119.04 | 115.23 |
| 24 | K | 101 | BCR | C31-C1-C6 | 2.19 | 113.69 | 110.24 |
| 29 | c | 517 | DGD | O2G-C1B-C2B | -2.19 | 106.74 | 111.48 |
| 29 | h | 102 | DGD | O6E-C1E-O5D | -2.19 | 104.86 | 110.04 |
| 27 | c | 520 | LMG | O6-C1-O1 | -2.19 | 104.86 | 110.04 |
| 22 | C | 507 | CLA | C1-C2-C3 | -2.19 | 122.61 | 126.20 |
| 29 | A | 414 | DGD | C8B-C7B-C6B | -2.19 | 103.29 | 114.37 |
| 29 | C | 517 | DGD | O6D-C1D-O3G | -2.19 | 104.87 | 110.04 |
| 27 | C | 519 | LMG | O7-C10-O9 | -2.19 | 118.58 | 123.70 |
| 22 | c | 503 | CLA | C11-C12-C13 | -2.19 | 108.69 | 115.97 |
| 22 | b | 609 | CLA | CHA-C1A-NA | -2.19 | 121.43 | 126.39 |
| 27 | c | 520 | LMG | C40-C39-C38 | -2.19 | 103.30 | 114.37 |
| 33 | e | 101 | LHG | O8-C23-O10 | -2.19 | 118.16 | 123.63 |
| 22 | b | 614 | CLA | C4-C3-C5 | 2.19 | 119.03 | 115.23 |
| 28 | L | 101 | SQD | O47-C7-C8 | 2.19 | 116.21 | 111.48 |
| 24 | b | 617 | BCR | C36-C18-C17 | -2.18 | 119.28 | 122.82 |
| 22 | A | 405 | CLA | C1C-C2C-C3C | -2.18 | 104.68 | 106.98 |
| 22 | B | 601 | CLA | O2A-CGA-O1A | -2.18 | 118.17 | 123.63 |
| 22 | A | 403 | CLA | C1-C2-C3 | -2.18 | 122.63 | 126.20 |
| 28 | L | 101 | SQD | C45-O47-C7 | 2.18 | 123.01 | 117.80 |
| 35 | f | 101 | HEM | CAB-C3B-C2B | -2.18 | 121.36 | 128.43 |
| 29 | C | 518 | DGD | C7B-C6B-C5B | -2.18 | 103.37 | 114.37 |
| 24 | c | 514 | BCR | C36-C18-C17 | -2.17 | 119.30 | 122.82 |
| 22 | c | 509 | CLA | C1B-CHB-C4A | -2.17 | 125.90 | 130.04 |
| 22 | b | 605 | CLA | C2D-C1D-ND | -2.17 | 107.98 | 110.13 |
| 23 | d | 401 | PHO | O2A-CGA-O1A | -2.17 | 118.20 | 123.63 |
| 22 | b | 610 | CLA | C11-C12-C13 | -2.17 | 108.75 | 115.97 |
| 22 | c | 506 | CLA | C4-C3-C2 | -2.17 | 118.06 | 123.63 |
| 22 | C | 509 | CLA | CHD-C4C-NC | 2.17 | 127.59 | 124.23 |
| 22 | B | 611 | CLA | C7-C6-C5 | -2.17 | 107.49 | 113.26 |
| 22 | B | 609 | CLA | CAA-CBA-CGA | -2.16 | 107.06 | 113.21 |
| 22 | c | 513 | CLA | C1-C2-C3 | -2.16 | 122.65 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | c | 503 | CLA | CHB-C4A-NA | 2.16 | 127.52 | 124.40 |
| 22 | b | 602 | CLA | CHC-C1C-NC | 2.16 | 127.57 | 124.31 |
| 22 | a | 403 | CLA | O2A-CGA-O1A | -2.16 | 118.22 | 123.63 |
| 22 | b | 616 | CLA | O1D-CGD-CBD | 2.16 | 128.78 | 124.52 |
| 22 | B | 614 | CLA | CMB-C2B-C3B | 2.16 | 129.00 | 124.68 |
| 22 | B | 607 | CLA | CHA-C1A-NA | -2.16 | 121.50 | 126.39 |
| 22 | b | 601 | CLA | CHD-C1D-ND | -2.16 | 121.77 | 124.80 |
| 24 | h | 101 | BCR | C7-C8-C9 | -2.16 | 123.04 | 126.23 |
| 29 | c | 517 | DGD | C4A-C3A-C2A | -2.16 | 105.20 | 113.13 |
| 22 | c | 512 | CLA | O2A-CGA-O1A | -2.16 | 118.23 | 123.63 |
| 24 | D | 405 | BCR | C3-C4-C5 | -2.16 | 110.21 | 114.06 |
| 32 | B | 624 | STE | C4-C3-C2 | -2.15 | 105.21 | 113.13 |
| 29 | A | 414 | DGD | C6E-C5E-C4E | 2.15 | 118.31 | 113.02 |
| 24 | H | 101 | BCR | C16-C17-C18 | -2.15 | 124.26 | 127.28 |
| 22 | b | 615 | CLA | O2D-CGD-CBD | 2.15 | 115.00 | 111.23 |
| 29 | C | 516 | DGD | CDB-CCB-CBB | -2.15 | 103.48 | 114.37 |
| 22 | C | 510 | CLA | O2A-CGA-O1A | -2.15 | 118.25 | 123.63 |
| 27 | A | 411 | LMG | O6-C1-O1 | -2.15 | 104.96 | 110.04 |
| 22 | B | 612 | CLA | C1B-CHB-C4A | -2.15 | 125.94 | 130.04 |
| 24 | t | 101 | BCR | C7-C8-C9 | -2.15 | 123.06 | 126.23 |
| 24 | b | 619 | BCR | C11-C10-C9 | -2.15 | 124.27 | 127.28 |
| 22 | B | 604 | CLA | C2A-C3A-C4A | 2.15 | 105.34 | 101.87 |
| 24 | B | 618 | BCR | C7-C8-C9 | -2.15 | 123.06 | 126.23 |
| 22 | c | 505 | CLA | CMB-C2B-C3B | 2.15 | 128.97 | 124.68 |
| 24 | b | 617 | BCR | C11-C10-C9 | -2.15 | 124.27 | 127.28 |
| 32 | c | 524 | STE | O2-C1-C2 | 2.14 | 120.78 | 114.00 |
| 22 | a | 402 | CLA | O2A-CGA-O1A | -2.14 | 118.26 | 123.63 |
| 22 | B | 606 | CLA | C1B-CHB-C4A | -2.14 | 125.95 | 130.04 |
| 22 | C | 502 | CLA | CHA-C1A-NA | -2.14 | 121.54 | 126.39 |
| 29 | h | 102 | DGD | C1D-C2D-C3D | -2.14 | 105.50 | 110.01 |
| 22 | C | 509 | CLA | CHD-C1D-ND | -2.14 | 121.79 | 124.80 |
| 22 | b | 607 | CLA | O1A-CGA-CBA | 2.14 | 132.16 | 123.78 |
| 22 | b | 610 | CLA | CBC-CAC-C3C | 2.14 | 118.22 | 112.42 |
| 22 | b | 610 | CLA | CHD-C1D-ND | -2.14 | 121.79 | 124.80 |
| 22 | B | 606 | CLA | O2D-CGD-O1D | -2.14 | 119.69 | 123.85 |
| 22 | B | 603 | CLA | C2D-C1D-ND | -2.14 | 108.01 | 110.13 |
| 29 | c | 518 | DGD | O5D-C1E-C2E | 2.14 | 111.52 | 108.27 |
| 32 | t | 102 | STE | O2-C1-C2 | 2.14 | 120.75 | 114.00 |
| 22 | b | 606 | CLA | O2A-CGA-O1A | -2.14 | 118.28 | 123.63 |
| 29 | C | 518 | DGD | O3E-C3E-C2E | -2.13 | 105.34 | 110.38 |
| 24 | B | 618 | BCR | C37-C22-C21 | -2.13 | 119.36 | 122.82 |
| 22 | c | 505 | CLA | O2A-CGA-O1A | -2.13 | 118.30 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 603 | CLA | C1B-CHB-C4A | -2.13 | 125.98 | 130.04 |
| 22 | C | 501 | CLA | CMB-C2B-C3B | 2.13 | 128.94 | 124.68 |
| 22 | B | 608 | CLA | C1C-C2C-C3C | -2.13 | 104.74 | 106.98 |
| 22 | A | 403 | CLA | C1-O2A-CGA | 2.13 | 121.80 | 116.65 |
| 35 | f | 101 | HEM | CHC-C4B-C3B | 2.13 | 127.83 | 124.57 |
| 22 | C | 509 | CLA | C1-O2A-CGA | 2.13 | 121.80 | 116.65 |
| 22 | b | 610 | CLA | CHC-C1C-C2C | -2.13 | 120.92 | 126.94 |
| 33 | d | 408 | LHG | O8-C6-C5 | -2.13 | 102.27 | 108.40 |
| 35 | f | 101 | HEM | CMC-C2C-C3C | 2.13 | 128.93 | 124.68 |
| 24 | B | 617 | BCR | C15-C16-C17 | -2.12 | 119.17 | 123.52 |
| 33 | B | 622 | LHG | C11-C10-C9 | -2.12 | 103.64 | 114.37 |
| 29 | c | 519 | DGD | O5D-C6D-C5D | -2.12 | 104.64 | 109.42 |
| 29 | C | 517 | DGD | O6E-C1E-O5D | -2.12 | 105.03 | 110.04 |
| 29 | c | 519 | DGD | O1G-C1A-O1A | -2.12 | 118.32 | 123.63 |
| 22 | B | 615 | CLA | C6-C7-C8 | -2.12 | 108.92 | 115.97 |
| 22 | c | 511 | CLA | O1A-CGA-CBA | 2.12 | 132.07 | 123.78 |
| 22 | b | 605 | CLA | CHD-C1D-ND | -2.12 | 121.82 | 124.80 |
| 24 | C | 514 | BCR | C27-C26-C25 | 2.12 | 125.56 | 122.70 |
| 27 | c | 520 | LMG | C6-C5-C4 | -2.11 | 107.83 | 113.02 |
| 27 | b | 620 | LMG | C22-C21-C20 | -2.11 | 103.69 | 114.37 |
| 24 | h | 101 | BCR | C36-C18-C17 | -2.11 | 119.39 | 122.82 |
| 32 | a | 414 | STE | C3-C2-C1 | -2.11 | 109.00 | 114.51 |
| 26 | d | 407 | PL9 | O1-C4-C3 | -2.11 | 118.50 | 120.73 |
| 22 | C | 503 | CLA | C1-C2-C3 | 2.11 | 129.66 | 126.20 |
| 22 | c | 501 | CLA | O1D-CGD-CBD | 2.11 | 128.68 | 124.52 |
| 22 | c | 502 | CLA | CHD-C1D-C2D | 2.11 | 129.88 | 125.49 |
| 27 | D | 407 | LMG | O1-C7-C8 | -2.11 | 105.68 | 110.82 |
| 24 | H | 101 | BCR | C38-C26-C25 | -2.11 | 122.18 | 124.48 |
| 26 | a | 409 | PL9 | C32-C33-C34 | -2.11 | 122.79 | 127.62 |
| 22 | b | 616 | CLA | O2A-CGA-O1A | -2.11 | 118.35 | 123.63 |
| 22 | C | 505 | CLA | C6-C7-C8 | -2.11 | 108.96 | 115.97 |
| 29 | c | 517 | DGD | CDB-CCB-CBB | -2.11 | 103.71 | 114.37 |
| 27 | d | 412 | LMG | O3-C3-C2 | -2.11 | 105.41 | 110.38 |
| 24 | K | 101 | BCR | C27-C26-C25 | 2.11 | 125.55 | 122.70 |
| 22 | a | 404 | CLA | CHA-C1A-NA | -2.11 | 121.62 | 126.39 |
| 27 | c | 520 | LMG | O2-C2-C1 | -2.10 | 105.06 | 110.08 |
| 22 | A | 410 | CLA | CED-O2D-CGD | -2.10 | 111.14 | 115.92 |
| 24 | D | 405 | BCR | C24-C23-C22 | -2.10 | 123.12 | 126.23 |
| 22 | c | 501 | CLA | C1-C2-C3 | -2.10 | 122.75 | 126.20 |
| 22 | C | 503 | CLA | C3A-C2A-C1A | 2.10 | 104.49 | 101.34 |
| 22 | d | 405 | CLA | CHA-C1A-NA | -2.10 | 121.64 | 126.39 |
| 22 | b | 615 | CLA | CHC-C1C-C2C | -2.10 | 121.00 | 126.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 613 | CLA | C1B-CHB-C4A | -2.10 | 126.04 | 130.04 |
| 24 | h | 101 | BCR | C37-C22-C21 | -2.10 | 119.42 | 122.82 |
| 22 | A | 403 | CLA | O2A-CGA-O1A | -2.10 | 118.38 | 123.63 |
| 24 | B | 618 | BCR | C29-C30-C25 | 2.10 | 113.48 | 110.44 |
| 24 | C | 515 | BCR | C3-C4-C5 | -2.09 | 110.32 | 114.06 |
| 27 | B | 621 | LMG | O7-C10-O9 | -2.09 | 117.95 | 123.33 |
| 22 | B | 606 | CLA | CHB-C4A-NA | 2.09 | 127.42 | 124.40 |
| 22 | c | 505 | CLA | C3B-C4B-NB | -2.09 | 106.50 | 109.21 |
| 27 | D | 410 | LMG | O8-C28-O10 | -2.09 | 118.39 | 123.63 |
| 22 | B | 603 | CLA | CHD-C4C-C3C | -2.09 | 121.72 | 124.77 |
| 22 | C | 507 | CLA | C2A-C1A-CHA | 2.09 | 127.50 | 123.87 |
| 22 | a | 403 | CLA | CHA-C1A-NA | -2.09 | 121.66 | 126.39 |
| 22 | C | 509 | CLA | C11-C12-C13 | -2.09 | 109.02 | 115.97 |
| 22 | c | 512 | CLA | O1D-CGD-CBD | 2.09 | 128.64 | 124.52 |
| 33 | d | 408 | LHG | C18-C17-C16 | -2.09 | 103.81 | 114.37 |
| 28 | B | 623 | SQD | C25-C24-C23 | -2.09 | 106.04 | 113.69 |
| 27 | D | 410 | LMG | C38-C37-C36 | -2.09 | 103.81 | 114.37 |
| 29 | c | 517 | DGD | O6D-C1D-O3G | -2.09 | 105.11 | 110.04 |
| 24 | C | 514 | BCR | C7-C8-C9 | -2.08 | 123.15 | 126.23 |
| 33 | d | 408 | LHG | C20-C19-C18 | -2.08 | 103.84 | 114.37 |
| 24 | T | 101 | BCR | C37-C22-C21 | -2.08 | 119.44 | 122.82 |
| 33 | D | 409 | LHG | O8-C23-O10 | -2.08 | 118.42 | 123.63 |
| 22 | c | 501 | CLA | CMB-C2B-C3B | 2.08 | 128.84 | 124.68 |
| 22 | c | 501 | CLA | CHD-C1D-ND | -2.08 | 121.88 | 124.80 |
| 22 | b | 604 | CLA | O2A-CGA-O1A | -2.08 | 118.42 | 123.63 |
| 35 | E | 101 | HEM | CHB-C1B-NB | 2.08 | 126.95 | 124.37 |
| 22 | b | 607 | CLA | C1-O2A-CGA | 2.08 | 121.68 | 116.65 |
| 27 | D | 407 | LMG | O2-C2-C1 | -2.08 | 105.13 | 110.08 |
| 22 | b | 603 | CLA | C11-C12-C13 | -2.08 | 109.06 | 115.97 |
| 22 | C | 503 | CLA | CHA-C1A-NA | -2.07 | 121.69 | 126.39 |
| 24 | Y | 101 | BCR | C16-C15-C14 | -2.07 | 119.28 | 123.52 |
| 22 | A | 405 | CLA | C4-C3-C5 | 2.07 | 118.82 | 115.23 |
| 22 | d | 405 | CLA | O2A-CGA-O1A | -2.07 | 118.45 | 123.63 |
| 28 | A | 412 | SQD | C3-C4-C5 | 2.07 | 113.98 | 110.23 |
| 22 | B | 608 | CLA | CHA-C1A-NA | -2.07 | 121.71 | 126.39 |
| 22 | B | 601 | CLA | O2D-CGD-CBD | 2.07 | 114.84 | 111.23 |
| 29 | a | 412 | DGD | CBB-CAB-C9B | -2.07 | 103.92 | 114.37 |
| 22 | C | 507 | CLA | C1B-CHB-C4A | -2.07 | 126.10 | 130.04 |
| 22 | C | 506 | CLA | O2D-CGD-O1D | -2.06 | 119.83 | 123.85 |
| 28 | f | 102 | SQD | O47-C7-C8 | 2.06 | 118.51 | 110.93 |
| 26 | A | 409 | PL9 | O2-C1-C2 | -2.06 | 117.14 | 121.83 |
| 22 | a | 402 | CLA | CHA-C4D-ND | 2.06 | 136.80 | 132.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 611 | CLA | CMB-C2B-C3B | 2.06 | 128.80 | 124.68 |
| 22 | c | 509 | CLA | C1-O2A-CGA | -2.06 | 111.66 | 116.65 |
| 22 | c | 511 | CLA | C11-C12-C13 | -2.06 | 109.12 | 115.97 |
| 22 | C | 511 | CLA | C1B-CHB-C4A | -2.06 | 126.11 | 130.04 |
| 22 | a | 404 | CLA | CAC-C3C-C4C | 2.06 | 127.47 | 124.79 |
| 24 | d | 406 | BCR | C30-C25-C26 | -2.06 | 119.82 | 122.64 |
| 24 | b | 618 | BCR | C15-C16-C17 | -2.06 | 119.31 | 123.52 |
| 22 | B | 611 | CLA | C4-C3-C2 | -2.06 | 118.34 | 123.63 |
| 27 | C | 519 | LMG | C40-C39-C38 | -2.06 | 103.97 | 114.37 |
| 26 | d | 407 | PL9 | C41-C39-C38 | -2.06 | 116.55 | 121.17 |
| 27 | A | 411 | LMG | C9-C8-C7 | -2.06 | 106.99 | 111.78 |
| 22 | b | 605 | CLA | O1A-CGA-CBA | 2.05 | 131.82 | 123.78 |
| 27 | c | 522 | LMG | C3-C4-C5 | -2.05 | 106.51 | 110.23 |
| 24 | b | 618 | BCR | C30-C25-C26 | -2.05 | 119.83 | 122.64 |
| 22 | A | 403 | CLA | CHA-C1A-NA | -2.05 | 121.74 | 126.39 |
| 22 | B | 603 | CLA | C3B-C4B-NB | -2.05 | 106.56 | 109.21 |
| 22 | b | 604 | CLA | CHC-C1C-NC | 2.05 | 127.40 | 124.31 |
| 27 | c | 520 | LMG | O8-C28-O10 | -2.05 | 118.50 | 123.63 |
| 22 | b | 607 | CLA | CHA-C1A-NA | -2.05 | 121.75 | 126.39 |
| 24 | A | 406 | BCR | C7-C8-C9 | -2.05 | 123.20 | 126.23 |
| 22 | D | 404 | CLA | O1D-CGD-CBD | 2.05 | 128.56 | 124.52 |
| 29 | C | 516 | DGD | O5D-C6D-C5D | -2.05 | 104.80 | 109.42 |
| 22 | B | 601 | CLA | CHA-C4D-ND | 2.05 | 136.78 | 132.55 |
| 27 | M | 101 | LMG | C22-C21-C20 | -2.05 | 104.01 | 114.37 |
| 22 | C | 510 | CLA | CHD-C1D-ND | -2.05 | 121.92 | 124.80 |
| 27 | b | 622 | LMG | C40-C39-C38 | -2.05 | 104.03 | 114.37 |
| 22 | c | 508 | CLA | CHD-C4C-NC | 2.04 | 127.40 | 124.23 |
| 22 | c | 503 | CLA | CHD-C1D-ND | -2.04 | 121.93 | 124.80 |
| 22 | c | 501 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 24 | B | 618 | BCR | C24-C23-C22 | -2.04 | 123.21 | 126.23 |
| 24 | c | 516 | BCR | C21-C20-C19 | -2.04 | 117.28 | 123.20 |
| 24 | b | 617 | BCR | C34-C9-C8 | -2.04 | 114.97 | 118.09 |
| 24 | c | 516 | BCR | C16-C15-C14 | -2.04 | 119.35 | 123.52 |
| 22 | C | 513 | CLA | C6-C5-C3 | 2.04 | 118.43 | 113.47 |
| 22 | B | 615 | CLA | O2A-CGA-O1A | -2.04 | 118.53 | 123.63 |
| 29 | c | 519 | DGD | O3G-C1D-C2D | -2.04 | 105.18 | 108.27 |
| 26 | D | 406 | PL9 | C50-C49-C48 | -2.04 | 116.54 | 122.66 |
| 22 | C | 510 | CLA | C7-C6-C5 | -2.04 | 107.83 | 113.26 |
| 22 | b | 601 | CLA | C1B-CHB-C4A | -2.04 | 126.16 | 130.04 |
| 22 | B | 610 | CLA | O1D-CGD-CBD | 2.03 | 128.53 | 124.52 |
| 22 | c | 508 | CLA | C7-C6-C5 | -2.03 | 107.84 | 113.26 |
| 35 | E | 101 | HEM | CHD-C1D-ND | 2.03 | 126.62 | 124.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | A | 411 | LMG | C1-O6-C5 | -2.03 | 109.75 | 113.72 |
| 22 | c | 501 | CLA | CHC-C1C-NC | 2.03 | 127.37 | 124.31 |
| 22 | B | 616 | CLA | C2C-C1C-NC | 2.03 | 112.12 | 109.98 |
| 33 | D | 408 | LHG | C11-C10-C9 | -2.03 | 104.10 | 114.37 |
| 22 | A | 403 | CLA | O1D-CGD-CBD | 2.03 | 128.53 | 124.52 |
| 27 | d | 412 | LMG | C7-O1-C1 | -2.03 | 109.44 | 113.80 |
| 24 | c | 515 | BCR | C1-C6-C5 | -2.03 | 119.86 | 122.64 |
| 26 | D | 406 | PL9 | C27-C28-C29 | -2.03 | 122.98 | 127.62 |
| 27 | b | 620 | LMG | C33-C32-C31 | -2.03 | 104.11 | 114.37 |
| 27 | D | 407 | LMG | O2-C2-C3 | -2.03 | 105.60 | 110.38 |
| 22 | c | 505 | CLA | C4D-C3D-CAD | -2.03 | 105.90 | 108.11 |
| 22 | B | 606 | CLA | CHD-C4C-C3C | -2.03 | 121.82 | 124.77 |
| 22 | b | 604 | CLA | C6-C7-C8 | -2.03 | 109.23 | 115.97 |
| 24 | a | 405 | BCR | C21-C20-C19 | -2.02 | 117.33 | 123.20 |
| 24 | D | 405 | BCR | C30-C25-C26 | -2.02 | 119.87 | 122.64 |
| 28 | F | 101 | SQD | O8-S-O9 | -2.02 | 106.33 | 111.40 |
| 29 | c | 518 | DGD | CCB-CBB-CAB | -2.02 | 104.14 | 114.37 |
| 22 | B | 608 | CLA | O1D-CGD-CBD | 2.02 | 128.51 | 124.52 |
| 24 | h | 101 | BCR | C15-C14-C13 | -2.02 | 124.44 | 127.28 |
| 29 | C | 516 | DGD | CAB-C9B-C8B | -2.02 | 104.15 | 114.37 |
| 27 | d | 412 | LMG | C1-C2-C3 | -2.02 | 105.76 | 110.01 |
| 26 | A | 409 | PL9 | C41-C39-C38 | -2.02 | 116.63 | 121.17 |
| 29 | C | 518 | DGD | O6D-C1D-O3G | -2.02 | 105.27 | 110.04 |
| 22 | b | 605 | CLA | C4-C3-C2 | -2.02 | 118.44 | 123.63 |
| 26 | A | 409 | PL9 | C42-C43-C44 | -2.02 | 123.00 | 127.62 |
| 22 | c | 508 | CLA | C2D-C1D-ND | -2.02 | 108.13 | 110.13 |
| 27 | c | 523 | LMG | C12-C11-C10 | -2.01 | 106.31 | 113.69 |
| 22 | C | 504 | CLA | C11-C10-C8 | -2.01 | 109.27 | 115.97 |
| 22 | B | 611 | CLA | CHD-C1D-ND | -2.01 | 121.97 | 124.80 |
| 29 | h | 102 | DGD | C3E-C4E-C5E | -2.01 | 106.58 | 110.23 |
| 32 | B | 620 | STE | O2-C1-C2 | 2.01 | 120.35 | 114.00 |
| 24 | C | 515 | BCR | C2-C1-C6 | 2.01 | 113.36 | 110.44 |
| 24 | K | 101 | BCR | C15-C14-C13 | -2.01 | 124.46 | 127.28 |
| 26 | A | 409 | PL9 | C27-C28-C29 | -2.01 | 123.02 | 127.62 |
| 22 | d | 404 | CLA | CGD-CBD-CAD | -2.01 | 104.34 | 110.85 |
| 26 | D | 406 | PL9 | O2-C1-C2 | -2.01 | 117.26 | 121.83 |
| 24 | k | 101 | BCR | C30-C25-C26 | -2.01 | 119.89 | 122.64 |
| 27 | c | 523 | LMG | O2-C2-C1 | -2.01 | 105.30 | 110.08 |
| 24 | c | 514 | BCR | C38-C26-C25 | -2.01 | 122.30 | 124.48 |
| 27 | A | 411 | LMG | C38-C37-C36 | -2.00 | 104.24 | 114.37 |
| 24 | A | 406 | BCR | C8-C7-C6 | -2.00 | 121.65 | 127.00 |
| 23 | A | 404 | PHO | OBD-CAD-CBD | -2.00 | 122.89 | 125.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | H | 101 | BCR | C1-C6-C5 | -2.00 | 119.90 | 122.64 |
| 24 | K | 101 | BCR | C36-C18-C17 | -2.00 | 119.57 | 122.82 |
| 22 | b | 601 | CLA | O1D-CGD-CBD | 2.00 | 128.46 | 124.52 |

All (61) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | A | 402 | CLA | ND |
| 22 | A | 405 | CLA | ND |
| 22 | A | 410 | CLA | ND |
| 22 | B | 601 | CLA | ND |
| 22 | B | 603 | CLA | ND |
| 22 | B | 604 | CLA | ND |
| 22 | B | 605 | CLA | ND |
| 22 | B | 606 | CLA | ND |
| 22 | B | 607 | CLA | ND |
| 22 | B | 608 | CLA | ND |
| 22 | B | 610 | CLA | ND |
| 22 | B | 611 | CLA | ND |
| 22 | B | 612 | CLA | ND |
| 22 | B | 613 | CLA | ND |
| 22 | B | 614 | CLA | ND |
| 22 | B | 615 | CLA | ND |
| 22 | B | 616 | CLA | ND |
| 22 | C | 501 | CLA | ND |
| 22 | C | 502 | CLA | ND |
| 22 | C | 503 | CLA | ND |
| 22 | C | 504 | CLA | ND |
| 22 | C | 505 | CLA | ND |
| 22 | C | 506 | CLA | ND |
| 22 | C | 507 | CLA | ND |
| 22 | C | 509 | CLA | ND |
| 22 | C | 510 | CLA | ND |
| 22 | C | 511 | CLA | ND |
| 22 | C | 512 | CLA | ND |
| 22 | C | 513 | CLA | ND |
| 22 | D | 403 | CLA | ND |
| 22 | a | 402 | CLA | ND |
| 22 | a | 404 | CLA | ND |
| 22 | b | 601 | CLA | ND |
| 22 | b | 603 | CLA | ND |
| 22 | b | 604 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | b | 605 | CLA | ND |
| 22 | b | 606 | CLA | ND |
| 22 | b | 607 | CLA | ND |
| 22 | b | 608 | CLA | ND |
| 22 | b | 609 | CLA | ND |
| 22 | b | 610 | CLA | ND |
| 22 | b | 611 | CLA | ND |
| 22 | b | 612 | CLA | ND |
| 22 | b | 613 | CLA | ND |
| 22 | b | 614 | CLA | ND |
| 22 | b | 615 | CLA | ND |
| 22 | b | 616 | CLA | ND |
| 22 | c | 501 | CLA | ND |
| 22 | c | 502 | CLA | ND |
| 22 | c | 503 | CLA | ND |
| 22 | c | 504 | CLA | ND |
| 22 | c | 505 | CLA | ND |
| 22 | c | 506 | CLA | ND |
| 22 | c | 507 | CLA | ND |
| 22 | c | 509 | CLA | ND |
| 22 | c | 510 | CLA | ND |
| 22 | c | 511 | CLA | ND |
| 22 | c | 512 | CLA | ND |
| 22 | c | 513 | CLA | ND |
| 22 | d | 404 | CLA | ND |
| 22 | d | 405 | CLA | ND |

All (1820) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 601 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 607 | CLA | C14-C13-C15-C16 |
| 22 | B | 614 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 507 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 508 | CLA | C12-C13-C15-C16 |
| 22 | C | 509 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 513 | CLA | C6-C7-C8-C9 |
| 22 | b | 614 | CLA | CAD-CBD-CGD-O1D |
| 22 | b | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 614 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | b | 616 | CLA | CHA-CBD-CGD-O1D |
| 22 | b | 616 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 509 | CLA | C6-C7-C8-C9 |
| 22 | c | 509 | CLA | C11-C12-C13-C14 |
| 24 | A | 406 | BCR | C17-C18-C19-C20 |
| 24 | B | 618 | BCR | C20-C21-C22-C37 |
| 24 | C | 514 | BCR | C20-C21-C22-C37 |
| 24 | C | 515 | BCR | C17-C18-C19-C20 |
| 24 | D | 405 | BCR | C22-C23-C24-C25 |
| 24 | D | 405 | BCR | C23-C24-C25-C26 |
| 24 | D | 405 | BCR | C23-C24-C25-C30 |
| 24 | K | 101 | BCR | C7-C8-C9-C34 |
| 24 | T | 101 | BCR | C1-C6-C7-C8 |
| 24 | T | 101 | BCR | C7-C8-C9-C10 |
| 24 | T | 101 | BCR | C36-C18-C19-C20 |
| 24 | T | 101 | BCR | C20-C21-C22-C37 |
| 24 | Y | 101 | BCR | C1-C6-C7-C8 |
| 24 | Y | 101 | BCR | C5-C6-C7-C8 |
| 24 | Y | 101 | BCR | C21-C22-C23-C24 |
| 24 | b | 617 | BCR | C20-C21-C22-C37 |
| 24 | c | 514 | BCR | C35-C13-C14-C15 |
| 24 | c | 514 | BCR | C16-C17-C18-C36 |
| 24 | d | 406 | BCR | C21-C22-C23-C24 |
| 24 | k | 101 | BCR | C7-C8-C9-C10 |
| 24 | k | 101 | BCR | C7-C8-C9-C34 |
| 24 | k | 101 | BCR | C17-C18-C19-C20 |
| 24 | t | 101 | BCR | C11-C10-C9-C34 |
| 24 | t | 101 | BCR | C36-C18-C19-C20 |
| 24 | t | 101 | BCR | C20-C21-C22-C37 |
| 26 | A | 409 | PL9 | C12-C13-C14-C15 |
| 26 | A | 409 | PL9 | C12-C13-C14-C16 |
| 26 | A | 409 | PL9 | C22-C23-C24-C25 |
| 26 | A | 409 | PL9 | C22-C23-C24-C26 |
| 26 | A | 409 | PL9 | C37-C38-C39-C40 |
| 26 | D | 406 | PL9 | C32-C33-C34-C36 |
| 26 | a | 409 | PL9 | C22-C23-C24-C25 |
| 26 | a | 409 | PL9 | C22-C23-C24-C26 |
| 26 | a | 409 | PL9 | C24-C26-C27-C28 |
| 26 | a | 409 | PL9 | C32-C33-C34-C36 |
| 26 | a | 409 | PL9 | C42-C43-C44-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | d | 407 | PL9 | C42-C43-C44-C45 |
| 27 | A | 411 | LMG | O6-C1-O1-C7 |
| 27 | A | 411 | LMG | O1-C7-C8-O7 |
| 27 | A | 411 | LMG | O9-C10-O7-C8 |
| 27 | c | 522 | LMG | O7-C8-C9-O8 |
| 27 | c | 522 | LMG | O9-C10-O7-C8 |
| 27 | c | 523 | LMG | O6-C1-O1-C7 |
| 28 | B | 623 | SQD | O5-C1-O6-C44 |
| 28 | B | 623 | SQD | O49-C7-O47-C45 |
| 28 | L | 101 | SQD | C8-C7-O47-C45 |
| 28 | L | 101 | SQD | O10-C23-O48-C46 |
| 28 | L | 101 | SQD | C24-C23-O48-C46 |
| 28 | a | 411 | SQD | C8-C7-O47-C45 |
| 28 | f | 102 | SQD | C2-C1-O6-C44 |
| 28 | f | 102 | SQD | O5-C1-O6-C44 |
| 29 | A | 414 | DGD | O1B-C1B-O2G-C2G |
| 29 | C | 517 | DGD | C2E-C1E-O5D-C6D |
| 33 | B | 622 | LHG | O1-C1-C2-C3 |
| 33 | B | 622 | LHG | C3-O3-P-O5 |
| 33 | B | 622 | LHG | C3-O3-P-O6 |
| 33 | D | 408 | LHG | C1-C2-C3-O3 |
| 33 | D | 408 | LHG | C3-O3-P-O5 |
| 33 | D | 408 | LHG | C3-O3-P-O6 |
| 33 | D | 408 | LHG | C4-O6-P-O4 |
| 33 | D | 409 | LHG | C4-O6-P-O4 |
| 33 | E | 102 | LHG | C3-O3-P-O5 |
| 33 | L | 102 | LHG | C3-O3-P-O4 |
| 33 | L | 102 | LHG | C4-O6-P-O4 |
| 33 | d | 408 | LHG | O1-C1-C2-C3 |
| 33 | d | 408 | LHG | C3-O3-P-O6 |
| 33 | d | 408 | LHG | C4-O6-P-O5 |
| 33 | d | 409 | LHG | O1-C1-C2-C3 |
| 33 | d | 409 | LHG | C3-O3-P-O4 |
| 33 | d | 409 | LHG | C3-O3-P-O6 |
| 33 | d | 409 | LHG | C4-O6-P-O4 |
| 33 | e | 101 | LHG | O1-C1-C2-O2 |
| 33 | e | 101 | LHG | O1-C1-C2-C3 |
| 33 | e | 101 | LHG | C3-O3-P-O4 |
| 33 | e | 101 | LHG | C3-O3-P-O6 |
| 33 | e | 101 | LHG | O10-C23-O8-C6 |
| 33 | l | 101 | LHG | C3-O3-P-O4 |
| 33 | l | 101 | LHG | C4-O6-P-O3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | l | 101 | LHG | C4-O6-P-O4 |
| 22 | b | 614 | CLA | O1D-CGD-O2D-CED |
| 22 | D | 404 | CLA | CBD-CGD-O2D-CED |
| 22 | b | 614 | CLA | CBD-CGD-O2D-CED |
| 23 | d | 402 | PHO | CBD-CGD-O2D-CED |
| 22 | B | 601 | CLA | O1A-CGA-O2A-C1 |
| 28 | f | 102 | SQD | O10-C23-O48-C46 |
| 33 | E | 102 | LHG | O10-C23-O8-C6 |
| 26 | d | 407 | PL9 | C47-C48-C49-C50 |
| 22 | B | 601 | CLA | CBA-CGA-O2A-C1 |
| 33 | e | 101 | LHG | C24-C23-O8-C6 |
| 27 | M | 101 | LMG | O10-C28-O8-C9 |
| 28 | F | 101 | SQD | O10-C23-O48-C46 |
| 28 | a | 411 | SQD | O10-C23-O48-C46 |
| 27 | b | 622 | LMG | O9-C10-O7-C8 |
| 28 | f | 102 | SQD | O49-C7-O47-C45 |
| 26 | d | 407 | PL9 | C47-C48-C49-C51 |
| 22 | b | 614 | CLA | C3-C5-C6-C7 |
| 28 | a | 411 | SQD | C24-C23-O48-C46 |
| 22 | c | 511 | CLA | CBD-CGD-O2D-CED |
| 22 | c | 512 | CLA | CBD-CGD-O2D-CED |
| 22 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 27 | A | 411 | LMG | C11-C10-O7-C8 |
| 27 | C | 519 | LMG | C11-C10-O7-C8 |
| 27 | D | 410 | LMG | C11-C10-O7-C8 |
| 28 | B | 623 | SQD | C8-C7-O47-C45 |
| 29 | A | 414 | DGD | C2B-C1B-O2G-C2G |
| 22 | A | 405 | CLA | C4-C3-C5-C6 |
| 22 | B | 603 | CLA | C4-C3-C5-C6 |
| 22 | C | 504 | CLA | C4-C3-C5-C6 |
| 22 | b | 614 | CLA | C4-C3-C5-C6 |
| 26 | A | 409 | PL9 | C20-C19-C21-C22 |
| 26 | a | 409 | PL9 | C20-C19-C21-C22 |
| 26 | d | 407 | PL9 | C40-C39-C41-C42 |
| 22 | C | 504 | CLA | C2-C3-C5-C6 |
| 26 | A | 409 | PL9 | C43-C44-C46-C47 |
| 22 | c | 509 | CLA | CBD-CGD-O2D-CED |
| 22 | D | 404 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 616 | CLA | C3-C5-C6-C7 |
| 22 | C | 513 | CLA | C3-C5-C6-C7 |
| 22 | b | 606 | CLA | C3-C5-C6-C7 |
| 22 | c | 510 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | c | 523 | LMG | C29-C28-O8-C9 |
| 28 | B | 623 | SQD | C24-C23-O48-C46 |
| 28 | f | 102 | SQD | C24-C23-O48-C46 |
| 33 | E | 102 | LHG | C24-C23-O8-C6 |
| 26 | A | 409 | PL9 | C32-C33-C34-C36 |
| 26 | A | 409 | PL9 | C37-C38-C39-C41 |
| 27 | A | 411 | LMG | O6-C5-C6-O5 |
| 26 | D | 406 | PL9 | C47-C48-C49-C51 |
| 22 | B | 605 | CLA | C3-C5-C6-C7 |
| 22 | b | 601 | CLA | CBD-CGD-O2D-CED |
| 33 | D | 408 | LHG | O2-C2-C3-O3 |
| 33 | e | 101 | LHG | O2-C2-C3-O3 |
| 22 | a | 404 | CLA | CBA-CGA-O2A-C1 |
| 28 | F | 101 | SQD | C24-C23-O48-C46 |
| 29 | c | 519 | DGD | O1A-C1A-O1G-C1G |
| 23 | d | 402 | PHO | O1D-CGD-O2D-CED |
| 28 | f | 102 | SQD | C8-C7-O47-C45 |
| 22 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 27 | A | 411 | LMG | C4-C5-C6-O5 |
| 26 | a | 409 | PL9 | C35-C34-C36-C37 |
| 22 | A | 405 | CLA | C2-C3-C5-C6 |
| 26 | A | 409 | PL9 | C18-C19-C21-C22 |
| 26 | A | 409 | PL9 | C38-C39-C41-C42 |
| 26 | a | 409 | PL9 | C33-C34-C36-C37 |
| 26 | d | 407 | PL9 | C38-C39-C41-C42 |
| 27 | c | 523 | LMG | O10-C28-O8-C9 |
| 27 | D | 410 | LMG | O9-C10-O7-C8 |
| 26 | A | 409 | PL9 | C19-C21-C22-C23 |
| 26 | A | 409 | PL9 | C24-C26-C27-C28 |
| 26 | a | 409 | PL9 | C44-C46-C47-C48 |
| 26 | d | 407 | PL9 | C44-C46-C47-C48 |
| 28 | B | 623 | SQD | O10-C23-O48-C46 |
| 29 | C | 517 | DGD | O6E-C1E-O5D-C6D |
| 22 | D | 403 | CLA | CBD-CGD-O2D-CED |
| 33 | l | 101 | LHG | C7-C8-C9-C10 |
| 26 | A | 409 | PL9 | C32-C33-C34-C35 |
| 26 | D | 406 | PL9 | C37-C38-C39-C40 |
| 22 | a | 404 | CLA | O1A-CGA-O2A-C1 |
| 26 | d | 407 | PL9 | C42-C43-C44-C46 |
| 22 | B | 603 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 511 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | b | 622 | LMG | C11-C10-O7-C8 |
| 33 | d | 408 | LHG | C1-C2-C3-O3 |
| 22 | C | 513 | CLA | CBA-CGA-O2A-C1 |
| 27 | C | 519 | LMG | C29-C28-O8-C9 |
| 27 | M | 101 | LMG | C29-C28-O8-C9 |
| 32 | b | 625 | STE | C3-C4-C5-C6 |
| 27 | c | 522 | LMG | C4-C5-C6-O5 |
| 22 | C | 513 | CLA | C4-C3-C5-C6 |
| 26 | A | 409 | PL9 | C45-C44-C46-C47 |
| 22 | B | 603 | CLA | C2-C3-C5-C6 |
| 22 | C | 513 | CLA | C2-C3-C5-C6 |
| 26 | a | 409 | PL9 | C38-C39-C41-C42 |
| 22 | B | 604 | CLA | C3-C5-C6-C7 |
| 22 | B | 606 | CLA | C11-C10-C8-C9 |
| 22 | B | 611 | CLA | C11-C12-C13-C14 |
| 22 | B | 613 | CLA | C11-C12-C13-C14 |
| 22 | B | 614 | CLA | C14-C13-C15-C16 |
| 22 | B | 616 | CLA | C11-C10-C8-C9 |
| 22 | C | 503 | CLA | C11-C10-C8-C9 |
| 22 | C | 509 | CLA | C11-C10-C8-C9 |
| 22 | C | 512 | CLA | C6-C7-C8-C9 |
| 22 | C | 512 | CLA | C11-C10-C8-C9 |
| 22 | b | 601 | CLA | C14-C13-C15-C16 |
| 22 | b | 605 | CLA | C11-C10-C8-C9 |
| 22 | b | 606 | CLA | C14-C13-C15-C16 |
| 22 | b | 607 | CLA | C11-C10-C8-C9 |
| 22 | b | 616 | CLA | C11-C10-C8-C9 |
| 22 | c | 502 | CLA | C6-C7-C8-C9 |
| 22 | c | 511 | CLA | C11-C10-C8-C9 |
| 22 | c | 511 | CLA | C14-C13-C15-C16 |
| 22 | c | 512 | CLA | C6-C7-C8-C9 |
| 29 | H | 102 | DGD | C4E-C5E-C6E-O5E |
| 33 | d | 408 | LHG | O2-C2-C3-O3 |
| 28 | F | 101 | SQD | C44-C45-C46-O48 |
| 32 | B | 624 | STE | C4-C5-C6-C7 |
| 24 | C | 515 | BCR | C36-C18-C19-C20 |
| 24 | C | 515 | BCR | C37-C22-C23-C24 |
| 24 | D | 405 | BCR | C37-C22-C23-C24 |
| 24 | H | 101 | BCR | C11-C12-C13-C35 |
| 24 | Y | 101 | BCR | C37-C22-C23-C24 |
| 24 | a | 405 | BCR | C36-C18-C19-C20 |
| 24 | b | 617 | BCR | C7-C8-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | b | 618 | BCR | C36-C18-C19-C20 |
| 24 | b | 619 | BCR | C11-C12-C13-C35 |
| 24 | b | 619 | BCR | C37-C22-C23-C24 |
| 24 | d | 406 | BCR | C7-C8-C9-C34 |
| 24 | d | 406 | BCR | C37-C22-C23-C24 |
| 24 | t | 101 | BCR | C7-C8-C9-C34 |
| 29 | c | 518 | DGD | C1A-C2A-C3A-C4A |
| 32 | D | 411 | STE | C1-C2-C3-C4 |
| 28 | L | 101 | SQD | O49-C7-O47-C45 |
| 28 | a | 411 | SQD | O49-C7-O47-C45 |
| 27 | c | 522 | LMG | O6-C5-C6-O5 |
| 29 | H | 102 | DGD | O6E-C5E-C6E-O5E |
| 28 | a | 410 | SQD | O6-C44-C45-O47 |
| 22 | C | 509 | CLA | C5-C6-C7-C8 |
| 22 | b | 603 | CLA | C5-C6-C7-C8 |
| 22 | b | 615 | CLA | C5-C6-C7-C8 |
| 22 | c | 506 | CLA | C2-C1-O2A-CGA |
| 22 | c | 512 | CLA | O1D-CGD-O2D-CED |
| 26 | a | 409 | PL9 | C47-C48-C49-C51 |
| 28 | A | 413 | SQD | C7-C8-C9-C10 |
| 33 | e | 101 | LHG | C23-C24-C25-C26 |
| 22 | c | 511 | CLA | O1D-CGD-O2D-CED |
| 22 | C | 513 | CLA | C12-C13-C15-C16 |
| 22 | b | 606 | CLA | C11-C10-C8-C7 |
| 22 | b | 615 | CLA | C11-C12-C13-C15 |
| 28 | a | 410 | SQD | C11-C12-C13-C14 |
| 22 | B | 603 | CLA | C8-C10-C11-C12 |
| 22 | C | 506 | CLA | C13-C15-C16-C17 |
| 22 | c | 505 | CLA | C5-C6-C7-C8 |
| 27 | c | 520 | LMG | C4-C5-C6-O5 |
| 28 | L | 101 | SQD | C23-C24-C25-C26 |
| 32 | d | 413 | STE | C1-C2-C3-C4 |
| 26 | A | 409 | PL9 | C34-C36-C37-C38 |
| 27 | c | 523 | LMG | C4-C5-C6-O5 |
| 22 | C | 509 | CLA | C3-C5-C6-C7 |
| 22 | c | 510 | CLA | C10-C11-C12-C13 |
| 22 | C | 505 | CLA | C2C-C3C-CAC-CBC |
| 27 | d | 412 | LMG | C28-C29-C30-C31 |
| 33 | d | 408 | LHG | C7-C8-C9-C10 |
| 22 | C | 509 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 410 | CLA | C13-C15-C16-C17 |
| 22 | B | 603 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 509 | CLA | C8-C10-C11-C12 |
| 22 | C | 510 | CLA | C13-C15-C16-C17 |
| 22 | C | 513 | CLA | C8-C10-C11-C12 |
| 22 | b | 602 | CLA | C13-C15-C16-C17 |
| 22 | B | 606 | CLA | C2A-CAA-CBA-CGA |
| 24 | C | 514 | BCR | C18-C19-C20-C21 |
| 24 | t | 101 | BCR | C10-C11-C12-C13 |
| 22 | A | 410 | CLA | C15-C16-C17-C18 |
| 22 | C | 513 | CLA | C5-C6-C7-C8 |
| 22 | a | 404 | CLA | C5-C6-C7-C8 |
| 22 | b | 605 | CLA | C5-C6-C7-C8 |
| 26 | D | 406 | PL9 | C47-C48-C49-C50 |
| 26 | a | 409 | PL9 | C47-C48-C49-C50 |
| 29 | A | 414 | DGD | O6E-C5E-C6E-O5E |
| 28 | a | 410 | SQD | C23-C24-C25-C26 |
| 29 | C | 516 | DGD | C1B-C2B-C3B-C4B |
| 29 | H | 102 | DGD | C1A-C2A-C3A-C4A |
| 29 | a | 412 | DGD | C1A-C2A-C3A-C4A |
| 32 | B | 620 | STE | C1-C2-C3-C4 |
| 22 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 22 | C | 513 | CLA | O1A-CGA-O2A-C1 |
| 27 | b | 622 | LMG | O10-C28-O8-C9 |
| 29 | C | 518 | DGD | O1A-C1A-O1G-C1G |
| 29 | a | 412 | DGD | O1A-C1A-O1G-C1G |
| 29 | A | 414 | DGD | C4E-C5E-C6E-O5E |
| 22 | B | 601 | CLA | C5-C6-C7-C8 |
| 22 | B | 607 | CLA | C5-C6-C7-C8 |
| 22 | B | 614 | CLA | C13-C15-C16-C17 |
| 22 | C | 503 | CLA | C5-C6-C7-C8 |
| 22 | C | 506 | CLA | C8-C10-C11-C12 |
| 22 | b | 603 | CLA | C13-C15-C16-C17 |
| 22 | b | 611 | CLA | C8-C10-C11-C12 |
| 22 | c | 503 | CLA | C5-C6-C7-C8 |
| 22 | c | 503 | CLA | C8-C10-C11-C12 |
| 22 | c | 506 | CLA | C8-C10-C11-C12 |
| 22 | c | 509 | CLA | C10-C11-C12-C13 |
| 33 | B | 622 | LHG | C28-C29-C30-C31 |
| 33 | B | 622 | LHG | O2-C2-C3-O3 |
| 23 | d | 401 | PHO | CBD-CGD-O2D-CED |
| 33 | d | 408 | LHG | C23-C24-C25-C26 |
| 22 | b | 605 | CLA | C10-C11-C12-C13 |
| 22 | b | 615 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | b | 616 | CLA | C5-C6-C7-C8 |
| 22 | b | 602 | CLA | C3-C5-C6-C7 |
| 22 | c | 509 | CLA | O1D-CGD-O2D-CED |
| 27 | D | 410 | LMG | C10-C11-C12-C13 |
| 22 | b | 601 | CLA | O1D-CGD-O2D-CED |
| 22 | b | 608 | CLA | C5-C6-C7-C8 |
| 22 | c | 510 | CLA | C15-C16-C17-C18 |
| 22 | c | 506 | CLA | CBA-CGA-O2A-C1 |
| 27 | c | 522 | LMG | C29-C28-O8-C9 |
| 22 | c | 506 | CLA | O1A-CGA-O2A-C1 |
| 32 | T | 102 | STE | C5-C6-C7-C8 |
| 22 | B | 601 | CLA | C15-C16-C17-C18 |
| 33 | B | 622 | LHG | C1-C2-C3-O3 |
| 33 | E | 102 | LHG | C1-C2-C3-O3 |
| 33 | e | 101 | LHG | C1-C2-C3-O3 |
| 22 | B | 604 | CLA | C13-C15-C16-C17 |
| 22 | B | 607 | CLA | C10-C11-C12-C13 |
| 22 | B | 607 | CLA | C13-C15-C16-C17 |
| 22 | B | 611 | CLA | C8-C10-C11-C12 |
| 22 | B | 613 | CLA | C8-C10-C11-C12 |
| 22 | B | 615 | CLA | C5-C6-C7-C8 |
| 22 | C | 513 | CLA | C13-C15-C16-C17 |
| 22 | C | 513 | CLA | C15-C16-C17-C18 |
| 22 | D | 404 | CLA | C10-C11-C12-C13 |
| 22 | b | 607 | CLA | C8-C10-C11-C12 |
| 22 | b | 613 | CLA | C13-C15-C16-C17 |
| 22 | c | 511 | CLA | C15-C16-C17-C18 |
| 22 | B | 605 | CLA | C13-C15-C16-C17 |
| 22 | b | 601 | CLA | C10-C11-C12-C13 |
| 22 | c | 511 | CLA | C13-C15-C16-C17 |
| 22 | c | 512 | CLA | C13-C15-C16-C17 |
| 22 | c | 506 | CLA | C13-C15-C16-C17 |
| 29 | c | 519 | DGD | C1A-C2A-C3A-C4A |
| 22 | b | 614 | CLA | C8-C10-C11-C12 |
| 22 | B | 608 | CLA | C3-C5-C6-C7 |
| 22 | b | 614 | CLA | C6-C7-C8-C9 |
| 27 | C | 519 | LMG | C2-C1-O1-C7 |
| 28 | B | 623 | SQD | C2-C1-O6-C44 |
| 28 | F | 101 | SQD | C2-C1-O6-C44 |
| 29 | c | 518 | DGD | C2E-C1E-O5D-C6D |
| 22 | d | 405 | CLA | C5-C6-C7-C8 |
| 27 | b | 620 | LMG | C29-C28-O8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | c | 519 | DGD | C2A-C1A-O1G-C1G |
| 24 | C | 515 | BCR | C20-C21-C22-C37 |
| 24 | K | 101 | BCR | C16-C17-C18-C36 |
| 24 | T | 101 | BCR | C11-C10-C9-C34 |
| 24 | T | 101 | BCR | C35-C13-C14-C15 |
| 24 | Y | 101 | BCR | C16-C17-C18-C36 |
| 24 | a | 405 | BCR | C35-C13-C14-C15 |
| 24 | b | 618 | BCR | C20-C21-C22-C37 |
| 24 | b | 619 | BCR | C35-C13-C14-C15 |
| 24 | b | 619 | BCR | C20-C21-C22-C37 |
| 24 | c | 515 | BCR | C16-C17-C18-C36 |
| 24 | h | 101 | BCR | C35-C13-C14-C15 |
| 24 | h | 101 | BCR | C20-C21-C22-C37 |
| 24 | k | 101 | BCR | C35-C13-C14-C15 |
| 24 | k | 101 | BCR | C16-C17-C18-C36 |
| 24 | t | 101 | BCR | C35-C13-C14-C15 |
| 22 | b | 607 | CLA | C10-C11-C12-C13 |
| 22 | c | 510 | CLA | C8-C10-C11-C12 |
| 24 | C | 514 | BCR | C36-C18-C19-C20 |
| 27 | c | 520 | LMG | O6-C5-C6-O5 |
| 33 | D | 408 | LHG | O1-C1-C2-C3 |
| 33 | d | 410 | LHG | O1-C1-C2-C3 |
| 28 | L | 101 | SQD | C46-C45-O47-C7 |
| 33 | d | 410 | LHG | C24-C25-C26-C27 |
| 22 | a | 403 | CLA | C16-C17-C18-C20 |
| 22 | b | 607 | CLA | C16-C17-C18-C19 |
| 22 | b | 607 | CLA | C16-C17-C18-C20 |
| 22 | B | 601 | CLA | C10-C11-C12-C13 |
| 24 | C | 514 | BCR | C16-C17-C18-C19 |
| 24 | C | 514 | BCR | C20-C21-C22-C23 |
| 24 | C | 515 | BCR | C12-C13-C14-C15 |
| 24 | K | 101 | BCR | C16-C17-C18-C19 |
| 24 | b | 617 | BCR | C12-C13-C14-C15 |
| 24 | b | 618 | BCR | C11-C10-C9-C8 |
| 24 | b | 618 | BCR | C20-C21-C22-C23 |
| 24 | c | 514 | BCR | C12-C13-C14-C15 |
| 24 | c | 514 | BCR | C16-C17-C18-C19 |
| 24 | d | 406 | BCR | C20-C21-C22-C23 |
| 24 | h | 101 | BCR | C11-C10-C9-C8 |
| 24 | h | 101 | BCR | C16-C17-C18-C19 |
| 24 | h | 101 | BCR | C20-C21-C22-C23 |
| 27 | C | 519 | LMG | O6-C1-O1-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | M | 101 | LMG | O6-C1-O1-C7 |
| 28 | F | 101 | SQD | O5-C1-O6-C44 |
| 28 | L | 101 | SQD | O5-C1-O6-C44 |
| 29 | c | 518 | DGD | O6E-C1E-O5D-C6D |
| 27 | b | 622 | LMG | C28-C29-C30-C31 |
| 22 | C | 512 | CLA | C13-C15-C16-C17 |
| 26 | a | 409 | PL9 | C18-C19-C21-C22 |
| 26 | d | 407 | PL9 | C33-C34-C36-C37 |
| 22 | D | 403 | CLA | O1D-CGD-O2D-CED |
| 22 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 22 | c | 512 | CLA | CBA-CGA-O2A-C1 |
| 29 | a | 412 | DGD | C2A-C1A-O1G-C1G |
| 22 | c | 509 | CLA | C8-C10-C11-C12 |
| 27 | M | 101 | LMG | C28-C29-C30-C31 |
| 22 | B | 602 | CLA | C16-C17-C18-C19 |
| 22 | B | 602 | CLA | C16-C17-C18-C20 |
| 22 | B | 604 | CLA | C16-C17-C18-C20 |
| 22 | C | 513 | CLA | C16-C17-C18-C19 |
| 22 | c | 511 | CLA | C16-C17-C18-C20 |
| 24 | K | 101 | BCR | C14-C15-C16-C17 |
| 24 | k | 101 | BCR | C14-C15-C16-C17 |
| 27 | B | 621 | LMG | C33-C34-C35-C36 |
| 27 | D | 410 | LMG | C14-C15-C16-C17 |
| 27 | M | 101 | LMG | C38-C39-C40-C41 |
| 27 | b | 620 | LMG | C39-C40-C41-C42 |
| 27 | c | 522 | LMG | C30-C31-C32-C33 |
| 28 | A | 413 | SQD | C12-C13-C14-C15 |
| 28 | a | 411 | SQD | C18-C19-C20-C21 |
| 32 | B | 626 | STE | C5-C6-C7-C8 |
| 32 | l | 102 | STE | C3-C4-C5-C6 |
| 33 | D | 409 | LHG | C34-C35-C36-C37 |
| 33 | d | 408 | LHG | C32-C33-C34-C35 |
| 33 | d | 409 | LHG | C12-C13-C14-C15 |
| 33 | d | 409 | LHG | C29-C30-C31-C32 |
| 33 | e | 101 | LHG | C27-C28-C29-C30 |
| 33 | l | 101 | LHG | C28-C29-C30-C31 |
| 22 | B | 616 | CLA | C5-C6-C7-C8 |
| 22 | D | 404 | CLA | C13-C15-C16-C17 |
| 22 | b | 601 | CLA | C13-C15-C16-C17 |
| 27 | c | 523 | LMG | C12-C13-C14-C15 |
| 29 | C | 516 | DGD | C5B-C6B-C7B-C8B |
| 32 | x | 101 | STE | C2-C3-C4-C5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | A | 414 | DGD | C2A-C1A-O1G-C1G |
| 27 | B | 621 | LMG | C32-C33-C34-C35 |
| 27 | b | 622 | LMG | C16-C17-C18-C19 |
| 27 | b | 622 | LMG | C23-C24-C25-C26 |
| 28 | A | 412 | SQD | C16-C17-C18-C19 |
| 28 | a | 411 | SQD | C10-C11-C12-C13 |
| 29 | C | 518 | DGD | C2B-C3B-C4B-C5B |
| 29 | a | 412 | DGD | C3A-C4A-C5A-C6A |
| 29 | c | 517 | DGD | C7A-C8A-C9A-CAA |
| 29 | c | 518 | DGD | CCA-CDA-CEA-CFA |
| 29 | c | 519 | DGD | CCA-CDA-CEA-CFA |
| 32 | H | 103 | STE | C5-C6-C7-C8 |
| 32 | T | 103 | STE | C5-C6-C7-C8 |
| 33 | L | 102 | LHG | C27-C28-C29-C30 |
| 33 | l | 101 | LHG | C24-C25-C26-C27 |
| 33 | B | 622 | LHG | O1-C1-C2-O2 |
| 33 | d | 408 | LHG | O1-C1-C2-O2 |
| 33 | d | 409 | LHG | O1-C1-C2-O2 |
| 27 | M | 101 | LMG | C12-C13-C14-C15 |
| 27 | M | 101 | LMG | C15-C16-C17-C18 |
| 27 | c | 522 | LMG | C36-C37-C38-C39 |
| 28 | a | 410 | SQD | C17-C18-C19-C20 |
| 28 | a | 411 | SQD | C11-C10-C9-C8 |
| 29 | a | 412 | DGD | C6A-C7A-C8A-C9A |
| 29 | c | 518 | DGD | C8A-C9A-CAA-CBA |
| 32 | I | 101 | STE | C4-C5-C6-C7 |
| 32 | I | 101 | STE | C10-C11-C12-C13 |
| 32 | a | 414 | STE | C5-C6-C7-C8 |
| 32 | x | 101 | STE | C3-C4-C5-C6 |
| 27 | C | 519 | LMG | C17-C18-C19-C20 |
| 27 | d | 411 | LMG | C34-C35-C36-C37 |
| 29 | H | 102 | DGD | C8B-C9B-CAB-CBB |
| 32 | H | 103 | STE | C11-C12-C13-C14 |
| 32 | x | 101 | STE | C12-C13-C14-C15 |
| 22 | a | 403 | CLA | C16-C17-C18-C19 |
| 22 | b | 606 | CLA | C2A-CAA-CBA-CGA |
| 27 | c | 522 | LMG | C33-C34-C35-C36 |
| 28 | B | 623 | SQD | C11-C12-C13-C14 |
| 29 | C | 517 | DGD | C6B-C7B-C8B-C9B |
| 33 | d | 410 | LHG | C33-C34-C35-C36 |
| 22 | b | 604 | CLA | C15-C16-C17-C18 |
| 22 | b | 615 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | a | 412 | DGD | C2B-C1B-O2G-C2G |
| 22 | B | 611 | CLA | C12-C13-C15-C16 |
| 27 | D | 407 | LMG | C31-C32-C33-C34 |
| 27 | M | 101 | LMG | C14-C15-C16-C17 |
| 27 | b | 622 | LMG | C11-C12-C13-C14 |
| 27 | c | 523 | LMG | C34-C35-C36-C37 |
| 28 | a | 410 | SQD | C34-C35-C36-C37 |
| 29 | h | 102 | DGD | C6B-C7B-C8B-C9B |
| 32 | B | 625 | STE | C5-C6-C7-C8 |
| 32 | B | 627 | STE | C5-C6-C7-C8 |
| 27 | D | 407 | LMG | C10-C11-C12-C13 |
| 32 | x | 101 | STE | C1-C2-C3-C4 |
| 22 | b | 615 | CLA | C13-C15-C16-C17 |
| 22 | c | 507 | CLA | C5-C6-C7-C8 |
| 29 | C | 517 | DGD | C9A-CAA-CBA-CCA |
| 32 | B | 620 | STE | C6-C7-C8-C9 |
| 22 | B | 607 | CLA | C4-C3-C5-C6 |
| 22 | c | 512 | CLA | C3A-C2A-CAA-CBA |
| 23 | d | 402 | PHO | C3A-C2A-CAA-CBA |
| 33 | d | 409 | LHG | C32-C33-C34-C35 |
| 33 | e | 101 | LHG | C14-C15-C16-C17 |
| 27 | d | 411 | LMG | C35-C36-C37-C38 |
| 29 | c | 517 | DGD | C4B-C5B-C6B-C7B |
| 22 | b | 615 | CLA | C16-C17-C18-C20 |
| 29 | C | 518 | DGD | C8A-C9A-CAA-CBA |
| 32 | B | 624 | STE | C2-C3-C4-C5 |
| 33 | L | 102 | LHG | C12-C13-C14-C15 |
| 27 | M | 101 | LMG | C37-C38-C39-C40 |
| 27 | c | 522 | LMG | C16-C17-C18-C19 |
| 28 | A | 412 | SQD | C10-C11-C12-C13 |
| 28 | F | 101 | SQD | C25-C26-C27-C28 |
| 29 | C | 516 | DGD | C4B-C5B-C6B-C7B |
| 32 | T | 102 | STE | C7-C8-C9-C10 |
| 32 | c | 521 | STE | C9-C10-C11-C12 |
| 33 | D | 408 | LHG | C10-C11-C12-C13 |
| 33 | E | 102 | LHG | C17-C18-C19-C20 |
| 28 | A | 412 | SQD | O6-C44-C45-C46 |
| 27 | D | 407 | LMG | C14-C15-C16-C17 |
| 27 | D | 410 | LMG | C34-C35-C36-C37 |
| 27 | b | 620 | LMG | C17-C18-C19-C20 |
| 28 | a | 411 | SQD | C11-C12-C13-C14 |
| 32 | J | 101 | STE | C3-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | M | 102 | STE | C9-C10-C11-C12 |
| 32 | c | 524 | STE | C5-C6-C7-C8 |
| 33 | e | 101 | LHG | C16-C17-C18-C19 |
| 22 | d | 405 | CLA | C10-C11-C12-C13 |
| 27 | A | 411 | LMG | C31-C32-C33-C34 |
| 27 | D | 407 | LMG | C17-C18-C19-C20 |
| 27 | c | 523 | LMG | C35-C36-C37-C38 |
| 27 | d | 411 | LMG | C31-C32-C33-C34 |
| 28 | A | 413 | SQD | C28-C29-C30-C31 |
| 28 | a | 410 | SQD | C13-C14-C15-C16 |
| 29 | A | 414 | DGD | C2B-C3B-C4B-C5B |
| 29 | A | 414 | DGD | C8B-C9B-CAB-CBB |
| 32 | B | 620 | STE | C9-C10-C11-C12 |
| 32 | a | 414 | STE | C4-C5-C6-C7 |
| 32 | m | 101 | STE | C5-C6-C7-C8 |
| 33 | B | 622 | LHG | C26-C27-C28-C29 |
| 33 | E | 102 | LHG | C27-C28-C29-C30 |
| 33 | E | 102 | LHG | C32-C33-C34-C35 |
| 33 | l | 101 | LHG | C16-C17-C18-C19 |
| 28 | B | 623 | SQD | C16-C17-C18-C19 |
| 29 | c | 519 | DGD | C8B-C9B-CAB-CBB |
| 29 | h | 102 | DGD | C5B-C6B-C7B-C8B |
| 28 | a | 410 | SQD | C29-C30-C31-C32 |
| 29 | c | 517 | DGD | C3B-C4B-C5B-C6B |
| 33 | d | 410 | LHG | C27-C28-C29-C30 |
| 28 | A | 413 | SQD | C18-C19-C20-C21 |
| 29 | C | 517 | DGD | C5A-C6A-C7A-C8A |
| 22 | A | 410 | CLA | C16-C17-C18-C20 |
| 22 | B | 605 | CLA | C16-C17-C18-C20 |
| 22 | B | 609 | CLA | C16-C17-C18-C20 |
| 22 | C | 513 | CLA | C16-C17-C18-C20 |
| 22 | c | 503 | CLA | C16-C17-C18-C20 |
| 22 | c | 511 | CLA | C16-C17-C18-C19 |
| 22 | c | 512 | CLA | O1A-CGA-O2A-C1 |
| 24 | H | 101 | BCR | C23-C24-C25-C26 |
| 24 | H | 101 | BCR | C23-C24-C25-C30 |
| 24 | T | 101 | BCR | C5-C6-C7-C8 |
| 24 | b | 617 | BCR | C1-C6-C7-C8 |
| 24 | k | 101 | BCR | C1-C6-C7-C8 |
| 24 | t | 101 | BCR | C1-C6-C7-C8 |
| 27 | d | 411 | LMG | C32-C33-C34-C35 |
| 29 | h | 102 | DGD | C3B-C4B-C5B-C6B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | E | 103 | STE | C3-C4-C5-C6 |
| 33 | E | 102 | LHG | C33-C34-C35-C36 |
| 22 | d | 404 | CLA | CBD-CGD-O2D-CED |
| 22 | a | 402 | CLA | C15-C16-C17-C18 |
| 22 | c | 503 | CLA | C15-C16-C17-C18 |
| 27 | C | 519 | LMG | C13-C14-C15-C16 |
| 29 | c | 519 | DGD | C9A-CAA-CBA-CCA |
| 32 | c | 521 | STE | C2-C3-C4-C5 |
| 33 | e | 101 | LHG | C11-C10-C9-C8 |
| 32 | b | 623 | STE | C6-C7-C8-C9 |
| 27 | c | 522 | LMG | C10-C11-C12-C13 |
| 29 | C | 516 | DGD | C1A-C2A-C3A-C4A |
| 29 | c | 518 | DGD | C1B-C2B-C3B-C4B |
| 29 | H | 102 | DGD | C6B-C7B-C8B-C9B |
| 29 | c | 517 | DGD | CBB-CCB-CDB-CEB |
| 29 | c | 518 | DGD | C4A-C5A-C6A-C7A |
| 33 | d | 409 | LHG | C34-C35-C36-C37 |
| 26 | A | 409 | PL9 | C4-C3-C7-C8 |
| 27 | c | 523 | LMG | C18-C19-C20-C21 |
| 28 | L | 101 | SQD | C11-C10-C9-C8 |
| 32 | C | 521 | STE | C7-C8-C9-C10 |
| 33 | D | 409 | LHG | C29-C30-C31-C32 |
| 33 | d | 408 | LHG | C11-C10-C9-C8 |
| 33 | l | 101 | LHG | C10-C11-C12-C13 |
| 22 | B | 614 | CLA | C4-C3-C5-C6 |
| 27 | c | 522 | LMG | C40-C41-C42-C43 |
| 27 | d | 411 | LMG | C36-C37-C38-C39 |
| 32 | C | 520 | STE | C3-C4-C5-C6 |
| 32 | b | 621 | STE | C6-C7-C8-C9 |
| 33 | E | 102 | LHG | C29-C30-C31-C32 |
| 24 | C | 515 | BCR | C18-C19-C20-C21 |
| 24 | H | 101 | BCR | C10-C11-C12-C13 |
| 24 | c | 514 | BCR | C18-C19-C20-C21 |
| 24 | d | 406 | BCR | C10-C11-C12-C13 |
| 22 | C | 509 | CLA | C13-C15-C16-C17 |
| 22 | B | 605 | CLA | C2-C3-C5-C6 |
| 22 | B | 607 | CLA | C2-C3-C5-C6 |
| 22 | B | 614 | CLA | C2-C3-C5-C6 |
| 22 | b | 605 | CLA | C2-C3-C5-C6 |
| 27 | b | 622 | LMG | C12-C13-C14-C15 |
| 27 | c | 522 | LMG | C31-C32-C33-C34 |
| 29 | c | 517 | DGD | C9B-CAB-CBB-CCB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | E | 102 | LHG | C25-C26-C27-C28 |
| 33 | L | 102 | LHG | C18-C19-C20-C21 |
| 33 | l | 101 | LHG | C23-C24-C25-C26 |
| 22 | A | 403 | CLA | C14-C13-C15-C16 |
| 27 | C | 519 | LMG | C31-C32-C33-C34 |
| 27 | c | 522 | LMG | C15-C16-C17-C18 |
| 28 | F | 101 | SQD | C26-C27-C28-C29 |
| 28 | f | 102 | SQD | C29-C30-C31-C32 |
| 29 | c | 517 | DGD | C4A-C5A-C6A-C7A |
| 29 | c | 517 | DGD | CCB-CDB-CEB-CFB |
| 32 | b | 624 | STE | C4-C5-C6-C7 |
| 27 | A | 411 | LMG | C14-C15-C16-C17 |
| 29 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 27 | B | 621 | LMG | C34-C35-C36-C37 |
| 27 | D | 407 | LMG | C15-C16-C17-C18 |
| 27 | d | 411 | LMG | C38-C39-C40-C41 |
| 28 | A | 413 | SQD | C30-C31-C32-C33 |
| 28 | a | 410 | SQD | C27-C28-C29-C30 |
| 29 | H | 102 | DGD | C6A-C7A-C8A-C9A |
| 32 | D | 411 | STE | C4-C5-C6-C7 |
| 32 | d | 413 | STE | C10-C11-C12-C13 |
| 33 | E | 102 | LHG | C11-C10-C9-C8 |
| 27 | c | 523 | LMG | O6-C5-C6-O5 |
| 27 | c | 523 | LMG | C2-C1-O1-C7 |
| 22 | c | 507 | CLA | C8-C10-C11-C12 |
| 29 | a | 412 | DGD | C8B-C9B-CAB-CBB |
| 29 | c | 517 | DGD | C8A-C9A-CAA-CBA |
| 29 | C | 516 | DGD | O6E-C5E-C6E-O5E |
| 27 | c | 520 | LMG | C38-C39-C40-C41 |
| 28 | B | 623 | SQD | C33-C34-C35-C36 |
| 29 | C | 516 | DGD | C3B-C4B-C5B-C6B |
| 29 | c | 517 | DGD | C6B-C7B-C8B-C9B |
| 32 | I | 101 | STE | C2-C3-C4-C5 |
| 32 | x | 101 | STE | C7-C8-C9-C10 |
| 27 | D | 407 | LMG | C38-C39-C40-C41 |
| 27 | c | 522 | LMG | C13-C14-C15-C16 |
| 29 | H | 102 | DGD | CAB-CBB-CCB-CDB |
| 32 | b | 621 | STE | C3-C4-C5-C6 |
| 32 | t | 102 | STE | C11-C10-C9-C8 |
| 33 | d | 410 | LHG | C26-C27-C28-C29 |
| 22 | B | 606 | CLA | C15-C16-C17-C18 |
| 28 | f | 102 | SQD | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | c | 522 | LMG | C11-C10-O7-C8 |
| 28 | L | 101 | SQD | C7-C8-C9-C10 |
| 33 | d | 410 | LHG | C23-C24-C25-C26 |
| 22 | b | 616 | CLA | C10-C11-C12-C13 |
| 29 | c | 517 | DGD | O1B-C1B-O2G-C2G |
| 27 | b | 622 | LMG | C13-C14-C15-C16 |
| 32 | x | 101 | STE | C5-C6-C7-C8 |
| 27 | d | 411 | LMG | C37-C38-C39-C40 |
| 22 | B | 607 | CLA | C8-C10-C11-C12 |
| 27 | D | 407 | LMG | C32-C33-C34-C35 |
| 29 | a | 412 | DGD | CEB-CFB-CGB-CHB |
| 26 | D | 406 | PL9 | C32-C33-C34-C35 |
| 32 | b | 621 | STE | C14-C15-C16-C17 |
| 33 | l | 101 | LHG | C33-C34-C35-C36 |
| 29 | C | 517 | DGD | CBA-CCA-CDA-CEA |
| 33 | E | 102 | LHG | C24-C25-C26-C27 |
| 22 | B | 605 | CLA | C16-C17-C18-C19 |
| 22 | B | 612 | CLA | C16-C17-C18-C20 |
| 22 | b | 615 | CLA | C16-C17-C18-C19 |
| 27 | c | 522 | LMG | C32-C33-C34-C35 |
| 29 | A | 414 | DGD | C2A-C3A-C4A-C5A |
| 32 | C | 522 | STE | C6-C7-C8-C9 |
| 32 | d | 413 | STE | C4-C5-C6-C7 |
| 33 | D | 408 | LHG | C30-C31-C32-C33 |
| 26 | D | 406 | PL9 | C30-C29-C31-C32 |
| 29 | C | 517 | DGD | C4B-C5B-C6B-C7B |
| 29 | c | 517 | DGD | CCA-CDA-CEA-CFA |
| 29 | c | 519 | DGD | CBA-CCA-CDA-CEA |
| 32 | d | 413 | STE | C11-C12-C13-C14 |
| 32 | x | 101 | STE | C4-C5-C6-C7 |
| 33 | d | 410 | LHG | C31-C32-C33-C34 |
| 27 | M | 101 | LMG | C13-C14-C15-C16 |
| 33 | E | 102 | LHG | C34-C35-C36-C37 |
| 22 | B | 606 | CLA | C13-C15-C16-C17 |
| 22 | C | 505 | CLA | C5-C6-C7-C8 |
| 33 | D | 409 | LHG | C13-C14-C15-C16 |
| 33 | L | 102 | LHG | C17-C18-C19-C20 |
| 29 | a | 412 | DGD | O1B-C1B-O2G-C2G |
| 33 | L | 102 | LHG | C30-C31-C32-C33 |
| 22 | B | 603 | CLA | C10-C11-C12-C13 |
| 22 | B | 606 | CLA | C5-C6-C7-C8 |
| 22 | C | 509 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 604 | CLA | C16-C17-C18-C19 |
| 27 | B | 621 | LMG | C11-C12-C13-C14 |
| 33 | D | 409 | LHG | C33-C34-C35-C36 |
| 27 | D | 410 | LMG | O10-C28-O8-C9 |
| 27 | M | 101 | LMG | C33-C34-C35-C36 |
| 29 | H | 102 | DGD | C8A-C9A-CAA-CBA |
| 29 | c | 517 | DGD | C5B-C6B-C7B-C8B |
| 29 | h | 102 | DGD | C9A-CAA-CBA-CCA |
| 33 | B | 622 | LHG | C12-C13-C14-C15 |
| 28 | A | 412 | SQD | C7-C8-C9-C10 |
| 32 | E | 103 | STE | C1-C2-C3-C4 |
| 22 | D | 403 | CLA | C15-C16-C17-C18 |
| 22 | b | 602 | CLA | C15-C16-C17-C18 |
| 29 | C | 518 | DGD | C4B-C5B-C6B-C7B |
| 29 | c | 518 | DGD | C2A-C3A-C4A-C5A |
| 27 | d | 412 | LMG | O6-C5-C6-O5 |
| 22 | C | 512 | CLA | C3-C5-C6-C7 |
| 28 | A | 412 | SQD | O6-C44-C45-O47 |
| 28 | a | 410 | SQD | O47-C45-C46-O48 |
| 27 | A | 411 | LMG | C29-C30-C31-C32 |
| 27 | b | 622 | LMG | C18-C19-C20-C21 |
| 27 | A | 411 | LMG | C37-C38-C39-C40 |
| 22 | c | 502 | CLA | C13-C15-C16-C17 |
| 27 | c | 522 | LMG | C38-C39-C40-C41 |
| 29 | c | 519 | DGD | C2A-C3A-C4A-C5A |
| 29 | c | 519 | DGD | C6A-C7A-C8A-C9A |
| 33 | D | 409 | LHG | C9-C10-C11-C12 |
| 27 | D | 407 | LMG | C36-C37-C38-C39 |
| 29 | a | 412 | DGD | C8A-C9A-CAA-CBA |
| 32 | a | 413 | STE | C5-C6-C7-C8 |
| 32 | c | 521 | STE | C11-C12-C13-C14 |
| 32 | j | 101 | STE | C4-C5-C6-C7 |
| 22 | A | 403 | CLA | C10-C11-C12-C13 |
| 22 | B | 615 | CLA | C13-C15-C16-C17 |
| 22 | C | 505 | CLA | C10-C11-C12-C13 |
| 32 | T | 103 | STE | C11-C12-C13-C14 |
| 32 | l | 102 | STE | C7-C8-C9-C10 |
| 33 | D | 409 | LHG | C27-C28-C29-C30 |
| 32 | B | 625 | STE | C2-C3-C4-C5 |
| 29 | c | 517 | DGD | O6D-C5D-C6D-O5D |
| 22 | C | 510 | CLA | C3-C5-C6-C7 |
| 28 | B | 623 | SQD | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | C | 516 | DGD | C9B-CAB-CBB-CCB |
| 29 | h | 102 | DGD | C2B-C3B-C4B-C5B |
| 33 | D | 409 | LHG | C11-C12-C13-C14 |
| 33 | L | 102 | LHG | C11-C12-C13-C14 |
| 28 | A | 412 | SQD | C11-C10-C9-C8 |
| 29 | a | 412 | DGD | C3B-C4B-C5B-C6B |
| 33 | D | 409 | LHG | C25-C26-C27-C28 |
| 33 | L | 102 | LHG | C32-C33-C34-C35 |
| 28 | B | 623 | SQD | C45-C46-O48-C23 |
| 27 | c | 522 | LMG | C11-C12-C13-C14 |
| 32 | B | 620 | STE | C11-C12-C13-C14 |
| 32 | l | 102 | STE | C13-C14-C15-C16 |
| 33 | l | 101 | LHG | C11-C12-C13-C14 |
| 27 | c | 520 | LMG | C31-C32-C33-C34 |
| 32 | T | 103 | STE | C6-C7-C8-C9 |
| 33 | D | 408 | LHG | C29-C30-C31-C32 |
| 33 | E | 102 | LHG | C13-C14-C15-C16 |
| 33 | d | 410 | LHG | O1-C1-C2-O2 |
| 29 | A | 414 | DGD | CCA-CDA-CEA-CFA |
| 22 | B | 604 | CLA | C1A-C2A-CAA-CBA |
| 22 | b | 601 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 512 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 513 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 512 | CLA | C8-C10-C11-C12 |
| 28 | f | 102 | SQD | C28-C29-C30-C31 |
| 32 | B | 620 | STE | C7-C8-C9-C10 |
| 22 | C | 505 | CLA | C4C-C3C-CAC-CBC |
| 27 | D | 410 | LMG | C16-C17-C18-C19 |
| 32 | B | 625 | STE | C12-C13-C14-C15 |
| 22 | C | 510 | CLA | C15-C16-C17-C18 |
| 22 | b | 609 | CLA | C13-C15-C16-C17 |
| 33 | e | 101 | LHG | O6-C4-C5-C6 |
| 27 | C | 519 | LMG | O9-C10-O7-C8 |
| 33 | e | 101 | LHG | O9-C7-O7-C5 |
| 27 | D | 407 | LMG | C12-C13-C14-C15 |
| 29 | A | 414 | DGD | CEA-CFA-CGA-CHA |
| 32 | a | 413 | STE | C2-C3-C4-C5 |
| 22 | b | 604 | CLA | C3-C5-C6-C7 |
| 22 | A | 403 | CLA | C6-C7-C8-C10 |
| 22 | B | 602 | CLA | C11-C12-C13-C15 |
| 22 | B | 604 | CLA | C12-C13-C15-C16 |
| 22 | B | 615 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 503 | CLA | C12-C13-C15-C16 |
| 22 | C | 505 | CLA | C12-C13-C15-C16 |
| 22 | C | 507 | CLA | C11-C10-C8-C7 |
| 22 | C | 511 | CLA | C6-C7-C8-C10 |
| 22 | b | 604 | CLA | C12-C13-C15-C16 |
| 22 | b | 606 | CLA | C12-C13-C15-C16 |
| 22 | b | 607 | CLA | C6-C7-C8-C10 |
| 22 | b | 608 | CLA | C11-C12-C13-C15 |
| 22 | b | 615 | CLA | C11-C10-C8-C7 |
| 22 | c | 504 | CLA | C11-C10-C8-C7 |
| 22 | c | 505 | CLA | C11-C10-C8-C7 |
| 22 | c | 506 | CLA | C11-C10-C8-C7 |
| 22 | c | 509 | CLA | C6-C7-C8-C10 |
| 29 | c | 517 | DGD | C8B-C9B-CAB-CBB |
| 32 | M | 102 | STE | C11-C10-C9-C8 |
| 27 | C | 519 | LMG | O10-C28-O8-C9 |
| 28 | L | 101 | SQD | C29-C30-C31-C32 |
| 29 | H | 102 | DGD | CCB-CDB-CEB-CFB |
| 29 | a | 412 | DGD | C4B-C5B-C6B-C7B |
| 28 | F | 101 | SQD | C30-C31-C32-C33 |
| 32 | I | 101 | STE | C7-C8-C9-C10 |
| 27 | c | 523 | LMG | C15-C16-C17-C18 |
| 32 | l | 102 | STE | C4-C5-C6-C7 |
| 22 | B | 601 | CLA | C8-C10-C11-C12 |
| 22 | C | 511 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 604 | CLA | C11-C12-C13-C14 |
| 22 | B | 605 | CLA | C11-C12-C13-C14 |
| 22 | B | 607 | CLA | C6-C7-C8-C9 |
| 22 | B | 608 | CLA | C6-C7-C8-C9 |
| 22 | B | 616 | CLA | C6-C7-C8-C9 |
| 22 | C | 507 | CLA | C11-C10-C8-C9 |
| 22 | C | 511 | CLA | C6-C7-C8-C9 |
| 22 | D | 404 | CLA | C6-C7-C8-C9 |
| 22 | b | 602 | CLA | C6-C7-C8-C9 |
| 22 | b | 607 | CLA | C6-C7-C8-C9 |
| 22 | b | 609 | CLA | C14-C13-C15-C16 |
| 22 | c | 504 | CLA | C11-C10-C8-C9 |
| 29 | A | 414 | DGD | CBB-CCB-CDB-CEB |
| 29 | C | 517 | DGD | C4A-C5A-C6A-C7A |
| 22 | c | 506 | CLA | C16-C17-C18-C20 |
| 32 | D | 411 | STE | C6-C7-C8-C9 |
| 28 | a | 410 | SQD | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | L | 102 | LHG | C31-C32-C33-C34 |
| 27 | M | 101 | LMG | C2-C1-O1-C7 |
| 27 | A | 411 | LMG | O1-C7-C8-C9 |
| 27 | M | 101 | LMG | C7-C8-C9-O8 |
| 27 | c | 522 | LMG | C7-C8-C9-O8 |
| 27 | c | 523 | LMG | C7-C8-C9-O8 |
| 28 | B | 623 | SQD | O6-C44-C45-C46 |
| 28 | a | 410 | SQD | C44-C45-C46-O48 |
| 28 | a | 411 | SQD | C44-C45-C46-O48 |
| 33 | E | 102 | LHG | C4-C5-C6-O8 |
| 27 | C | 519 | LMG | C30-C31-C32-C33 |
| 32 | T | 103 | STE | C9-C10-C11-C12 |
| 33 | e | 101 | LHG | C17-C18-C19-C20 |
| 22 | B | 605 | CLA | C8-C10-C11-C12 |
| 22 | B | 614 | CLA | C15-C16-C17-C18 |
| 22 | b | 601 | CLA | C15-C16-C17-C18 |
| 28 | B | 623 | SQD | C32-C33-C34-C35 |
| 29 | c | 519 | DGD | C8A-C9A-CAA-CBA |
| 32 | c | 524 | STE | C6-C7-C8-C9 |
| 27 | b | 622 | LMG | O6-C5-C6-O5 |
| 27 | C | 519 | LMG | C14-C15-C16-C17 |
| 27 | c | 522 | LMG | C34-C35-C36-C37 |
| 29 | H | 102 | DGD | CBA-CCA-CDA-CEA |
| 29 | h | 102 | DGD | CAB-CBB-CCB-CDB |
| 22 | C | 509 | CLA | O1D-CGD-O2D-CED |
| 29 | c | 517 | DGD | O6E-C5E-C6E-O5E |
| 33 | l | 101 | LHG | C25-C26-C27-C28 |
| 24 | b | 619 | BCR | C16-C17-C18-C36 |
| 27 | A | 411 | LMG | C38-C39-C40-C41 |
| 22 | C | 505 | CLA | C4-C3-C5-C6 |
| 22 | C | 505 | CLA | C2-C3-C5-C6 |
| 29 | c | 517 | DGD | C4D-C5D-C6D-O5D |
| 27 | d | 411 | LMG | C30-C31-C32-C33 |
| 28 | B | 623 | SQD | C12-C13-C14-C15 |
| 33 | L | 102 | LHG | C13-C14-C15-C16 |
| 27 | D | 407 | LMG | O6-C5-C6-O5 |
| 22 | b | 606 | CLA | C10-C11-C12-C13 |
| 22 | b | 606 | CLA | C15-C16-C17-C18 |
| 28 | a | 410 | SQD | C25-C26-C27-C28 |
| 29 | H | 102 | DGD | C5A-C6A-C7A-C8A |
| 29 | h | 102 | DGD | O6E-C5E-C6E-O5E |
| 27 | A | 411 | LMG | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | b | 621 | STE | C5-C6-C7-C8 |
| 22 | b | 601 | CLA | O2A-C1-C2-C3 |
| 27 | D | 410 | LMG | C9-C8-O7-C10 |
| 29 | a | 412 | DGD | C1G-C2G-O2G-C1B |
| 27 | b | 622 | LMG | C40-C41-C42-C43 |
| 29 | A | 414 | DGD | C5B-C6B-C7B-C8B |
| 32 | d | 413 | STE | C9-C10-C11-C12 |
| 32 | l | 102 | STE | C10-C11-C12-C13 |
| 29 | a | 412 | DGD | CBA-CCA-CDA-CEA |
| 32 | B | 625 | STE | C3-C4-C5-C6 |
| 32 | B | 626 | STE | C6-C7-C8-C9 |
| 32 | D | 411 | STE | C14-C15-C16-C17 |
| 22 | a | 402 | CLA | CBD-CGD-O2D-CED |
| 24 | b | 618 | BCR | C16-C17-C18-C19 |
| 33 | e | 101 | LHG | O6-C4-C5-O7 |
| 27 | b | 622 | LMG | C37-C38-C39-C40 |
| 28 | A | 412 | SQD | C12-C13-C14-C15 |
| 28 | A | 413 | SQD | C32-C33-C34-C35 |
| 29 | C | 518 | DGD | C8B-C9B-CAB-CBB |
| 22 | B | 604 | CLA | CBA-CGA-O2A-C1 |
| 32 | b | 625 | STE | C7-C8-C9-C10 |
| 32 | b | 621 | STE | C1-C2-C3-C4 |
| 32 | b | 623 | STE | C3-C4-C5-C6 |
| 27 | b | 622 | LMG | C38-C39-C40-C41 |
| 32 | D | 411 | STE | C7-C8-C9-C10 |
| 27 | c | 523 | LMG | C20-C21-C22-C23 |
| 32 | M | 103 | STE | C1-C2-C3-C4 |
| 28 | a | 411 | SQD | C15-C16-C17-C18 |
| 29 | C | 517 | DGD | C6A-C7A-C8A-C9A |
| 33 | D | 409 | LHG | C30-C31-C32-C33 |
| 22 | B | 614 | CLA | C16-C17-C18-C19 |
| 27 | B | 621 | LMG | C31-C32-C33-C34 |
| 27 | M | 101 | LMG | C35-C36-C37-C38 |
| 27 | b | 620 | LMG | C37-C38-C39-C40 |
| 27 | b | 622 | LMG | C33-C34-C35-C36 |
| 27 | c | 520 | LMG | C39-C40-C41-C42 |
| 29 | a | 412 | DGD | C4A-C5A-C6A-C7A |
| 32 | a | 414 | STE | C2-C3-C4-C5 |
| 32 | b | 624 | STE | C12-C13-C14-C15 |
| 32 | c | 521 | STE | C10-C11-C12-C13 |
| 33 | l | 101 | LHG | C14-C15-C16-C17 |
| 28 | f | 102 | SQD | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | B | 621 | LMG | C16-C17-C18-C19 |
| 27 | d | 412 | LMG | C30-C31-C32-C33 |
| 28 | B | 623 | SQD | C9-C10-C11-C12 |
| 32 | x | 101 | STE | C9-C10-C11-C12 |
| 27 | M | 101 | LMG | O7-C8-C9-O8 |
| 28 | B | 623 | SQD | O6-C44-C45-O47 |
| 29 | A | 414 | DGD | O2G-C2G-C3G-O3G |
| 29 | c | 519 | DGD | CDA-CEA-CFA-CGA |
| 27 | d | 412 | LMG | C36-C37-C38-C39 |
| 32 | t | 102 | STE | C6-C7-C8-C9 |
| 28 | A | 412 | SQD | C17-C18-C19-C20 |
| 29 | A | 414 | DGD | CFA-CGA-CHA-CIA |
| 32 | D | 411 | STE | C15-C16-C17-C18 |
| 32 | C | 520 | STE | C6-C7-C8-C9 |
| 32 | t | 102 | STE | C2-C3-C4-C5 |
| 33 | D | 408 | LHG | C11-C12-C13-C14 |
| 29 | H | 102 | DGD | O2G-C1B-C2B-C3B |
| 27 | M | 101 | LMG | C17-C18-C19-C20 |
| 28 | B | 623 | SQD | C31-C32-C33-C34 |
| 32 | b | 621 | STE | C13-C14-C15-C16 |
| 29 | c | 518 | DGD | CBA-CCA-CDA-CEA |
| 33 | d | 408 | LHG | C16-C17-C18-C19 |
| 22 | a | 404 | CLA | C10-C11-C12-C13 |
| 22 | b | 606 | CLA | C8-C10-C11-C12 |
| 27 | D | 410 | LMG | C15-C16-C17-C18 |
| 29 | c | 519 | DGD | C5B-C6B-C7B-C8B |
| 32 | C | 521 | STE | C5-C6-C7-C8 |
| 28 | A | 412 | SQD | C8-C7-O47-C45 |
| 28 | A | 412 | SQD | C27-C28-C29-C30 |
| 33 | D | 408 | LHG | C18-C19-C20-C21 |
| 33 | d | 409 | LHG | C14-C15-C16-C17 |
| 22 | b | 608 | CLA | C13-C15-C16-C17 |
| 23 | d | 401 | PHO | O1D-CGD-O2D-CED |
| 29 | A | 414 | DGD | CFB-CGB-CHB-CIB |
| 33 | d | 409 | LHG | C35-C36-C37-C38 |
| 32 | E | 103 | STE | C4-C5-C6-C7 |
| 22 | B | 610 | CLA | O1D-CGD-O2D-CED |
| 22 | b | 605 | CLA | C4-C3-C5-C6 |
| 26 | a | 409 | PL9 | C15-C14-C16-C17 |
| 23 | A | 404 | PHO | C2-C3-C5-C6 |
| 26 | d | 407 | PL9 | C13-C14-C16-C17 |
| 27 | c | 520 | LMG | C29-C28-O8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | b | 620 | LMG | C15-C16-C17-C18 |
| 33 | B | 622 | LHG | O9-C7-O7-C5 |
| 22 | A | 403 | CLA | C6-C7-C8-C9 |
| 22 | A | 403 | CLA | C11-C12-C13-C14 |
| 22 | B | 602 | CLA | C11-C12-C13-C14 |
| 22 | B | 604 | CLA | C14-C13-C15-C16 |
| 22 | C | 505 | CLA | C14-C13-C15-C16 |
| 22 | C | 510 | CLA | C11-C10-C8-C9 |
| 22 | b | 604 | CLA | C14-C13-C15-C16 |
| 22 | b | 606 | CLA | C11-C10-C8-C9 |
| 22 | b | 608 | CLA | C11-C12-C13-C14 |
| 22 | b | 615 | CLA | C11-C10-C8-C9 |
| 22 | b | 615 | CLA | C11-C12-C13-C14 |
| 22 | c | 505 | CLA | C11-C10-C8-C9 |
| 22 | c | 506 | CLA | C11-C10-C8-C9 |
| 33 | L | 102 | LHG | C15-C16-C17-C18 |
| 22 | b | 613 | CLA | C10-C11-C12-C13 |
| 28 | L | 101 | SQD | C16-C17-C18-C19 |
| 29 | c | 518 | DGD | C7B-C8B-C9B-CAB |
| 32 | B | 625 | STE | C10-C11-C12-C13 |
| 32 | T | 102 | STE | C12-C13-C14-C15 |
| 27 | D | 410 | LMG | C35-C36-C37-C38 |
| 27 | d | 412 | LMG | C37-C38-C39-C40 |
| 29 | a | 412 | DGD | CDA-CEA-CFA-CGA |
| 29 | a | 412 | DGD | CEA-CFA-CGA-CHA |
| 29 | C | 517 | DGD | C3A-C4A-C5A-C6A |
| 32 | b | 621 | STE | C7-C8-C9-C10 |
| 33 | d | 408 | LHG | C17-C18-C19-C20 |
| 29 | a | 412 | DGD | C7B-C8B-C9B-CAB |
| 22 | A | 403 | CLA | C11-C10-C8-C7 |
| 22 | A | 403 | CLA | C11-C12-C13-C15 |
| 22 | B | 604 | CLA | C11-C12-C13-C15 |
| 22 | B | 607 | CLA | C12-C13-C15-C16 |
| 22 | B | 608 | CLA | C6-C7-C8-C10 |
| 22 | B | 613 | CLA | C12-C13-C15-C16 |
| 22 | B | 614 | CLA | C12-C13-C15-C16 |
| 22 | C | 512 | CLA | C11-C10-C8-C7 |
| 22 | C | 512 | CLA | C11-C12-C13-C15 |
| 22 | C | 513 | CLA | C6-C7-C8-C10 |
| 22 | D | 404 | CLA | C6-C7-C8-C10 |
| 22 | b | 601 | CLA | C12-C13-C15-C16 |
| 22 | b | 602 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | b | 609 | CLA | C12-C13-C15-C16 |
| 22 | c | 507 | CLA | C11-C10-C8-C7 |
| 22 | c | 509 | CLA | C11-C12-C13-C15 |
| 22 | c | 511 | CLA | C12-C13-C15-C16 |
| 22 | b | 612 | CLA | C13-C15-C16-C17 |
| 22 | b | 614 | CLA | C13-C15-C16-C17 |
| 32 | m | 101 | STE | C1-C2-C3-C4 |
| 27 | b | 622 | LMG | C24-C25-C26-C27 |
| 29 | C | 517 | DGD | CDA-CEA-CFA-CGA |
| 33 | l | 101 | LHG | C31-C32-C33-C34 |
| 22 | c | 503 | CLA | C16-C17-C18-C19 |
| 27 | c | 520 | LMG | C35-C36-C37-C38 |
| 29 | C | 518 | DGD | CDA-CEA-CFA-CGA |
| 22 | C | 510 | CLA | C4-C3-C5-C6 |
| 22 | c | 505 | CLA | C4-C3-C5-C6 |
| 32 | H | 103 | STE | C15-C16-C17-C18 |
| 29 | C | 517 | DGD | CCB-CDB-CEB-CFB |
| 29 | a | 412 | DGD | CFA-CGA-CHA-CIA |
| 28 | B | 623 | SQD | C14-C15-C16-C17 |
| 28 | L | 101 | SQD | C12-C13-C14-C15 |
| 28 | L | 101 | SQD | C18-C19-C20-C21 |
| 32 | b | 624 | STE | C14-C15-C16-C17 |
| 33 | L | 102 | LHG | O10-C23-O8-C6 |
| 32 | T | 102 | STE | C15-C16-C17-C18 |
| 22 | B | 616 | CLA | CBA-CGA-O2A-C1 |
| 27 | D | 410 | LMG | C29-C28-O8-C9 |
| 27 | c | 523 | LMG | C31-C32-C33-C34 |
| 33 | d | 408 | LHG | C29-C30-C31-C32 |
| 24 | h | 101 | BCR | C15-C16-C17-C18 |
| 22 | b | 607 | CLA | C13-C15-C16-C17 |
| 27 | d | 412 | LMG | C14-C15-C16-C17 |
| 22 | B | 616 | CLA | O1A-CGA-O2A-C1 |
| 27 | A | 411 | LMG | C30-C31-C32-C33 |
| 28 | f | 102 | SQD | C34-C35-C36-C37 |
| 32 | a | 413 | STE | C4-C5-C6-C7 |
| 27 | d | 412 | LMG | C39-C40-C41-C42 |
| 28 | a | 411 | SQD | C14-C15-C16-C17 |
| 29 | a | 412 | DGD | C5A-C6A-C7A-C8A |
| 29 | c | 518 | DGD | CBB-CCB-CDB-CEB |
| 22 | c | 512 | CLA | C2A-CAA-CBA-CGA |
| 32 | B | 625 | STE | C13-C14-C15-C16 |
| 22 | B | 612 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | b | 620 | LMG | C31-C32-C33-C34 |
| 29 | a | 412 | DGD | C9A-CAA-CBA-CCA |
| 33 | d | 409 | LHG | C11-C12-C13-C14 |
| 27 | C | 519 | LMG | O1-C7-C8-C9 |
| 27 | M | 101 | LMG | O1-C7-C8-C9 |
| 28 | a | 410 | SQD | O6-C44-C45-C46 |
| 29 | A | 414 | DGD | C1G-C2G-C3G-O3G |
| 27 | c | 523 | LMG | C29-C30-C31-C32 |
| 27 | c | 523 | LMG | C38-C39-C40-C41 |
| 33 | d | 408 | LHG | C15-C16-C17-C18 |
| 32 | c | 521 | STE | C1-C2-C3-C4 |
| 33 | D | 408 | LHG | C15-C16-C17-C18 |
| 27 | D | 410 | LMG | C33-C34-C35-C36 |
| 27 | b | 622 | LMG | C31-C32-C33-C34 |
| 29 | a | 412 | DGD | CAB-CBB-CCB-CDB |
| 29 | c | 517 | DGD | C5A-C6A-C7A-C8A |
| 32 | b | 621 | STE | C12-C13-C14-C15 |
| 22 | b | 609 | CLA | C4-C3-C5-C6 |
| 23 | A | 404 | PHO | C4-C3-C5-C6 |
| 28 | A | 413 | SQD | C10-C11-C12-C13 |
| 29 | A | 414 | DGD | C7B-C8B-C9B-CAB |
| 29 | C | 517 | DGD | C8B-C9B-CAB-CBB |
| 33 | D | 408 | LHG | C32-C33-C34-C35 |
| 22 | b | 609 | CLA | C2-C3-C5-C6 |
| 27 | c | 522 | LMG | O10-C28-O8-C9 |
| 28 | a | 411 | SQD | C31-C32-C33-C34 |
| 22 | a | 403 | CLA | CBD-CGD-O2D-CED |
| 22 | a | 402 | CLA | C16-C17-C18-C20 |
| 22 | A | 402 | CLA | C15-C16-C17-C18 |
| 29 | c | 517 | DGD | CAB-CBB-CCB-CDB |
| 24 | C | 515 | BCR | C1-C6-C7-C8 |
| 24 | d | 406 | BCR | C23-C24-C25-C30 |
| 27 | b | 620 | LMG | C11-C10-O7-C8 |
| 27 | b | 620 | LMG | C20-C21-C22-C23 |
| 29 | C | 518 | DGD | CBB-CCB-CDB-CEB |
| 33 | D | 408 | LHG | C12-C13-C14-C15 |
| 32 | b | 621 | STE | C2-C3-C4-C5 |
| 32 | t | 102 | STE | C3-C4-C5-C6 |
| 29 | H | 102 | DGD | CDB-CEB-CFB-CGB |
| 27 | C | 519 | LMG | C32-C33-C34-C35 |
| 33 | d | 409 | LHG | C33-C34-C35-C36 |
| 22 | B | 612 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | b | 604 | CLA | C13-C15-C16-C17 |
| 27 | c | 523 | LMG | O7-C8-C9-O8 |
| 33 | d | 410 | LHG | C35-C36-C37-C38 |
| 32 | x | 101 | STE | C11-C10-C9-C8 |
| 29 | h | 102 | DGD | CDB-CEB-CFB-CGB |
| 32 | E | 103 | STE | C7-C8-C9-C10 |
| 33 | e | 101 | LHG | C28-C29-C30-C31 |
| 27 | c | 522 | LMG | C41-C42-C43-C44 |
| 32 | H | 103 | STE | C13-C14-C15-C16 |
| 33 | e | 101 | LHG | C11-C12-C13-C14 |
| 27 | c | 523 | LMG | C28-C29-C30-C31 |
| 32 | B | 627 | STE | C1-C2-C3-C4 |
| 32 | d | 413 | STE | C12-C13-C14-C15 |
| 22 | b | 602 | CLA | CBD-CGD-O2D-CED |
| 24 | T | 101 | BCR | C18-C19-C20-C21 |
| 22 | C | 510 | CLA | C2-C3-C5-C6 |
| 22 | c | 505 | CLA | C2-C3-C5-C6 |
| 26 | d | 407 | PL9 | C43-C44-C46-C47 |
| 27 | D | 407 | LMG | C22-C23-C24-C25 |
| 27 | A | 411 | LMG | C12-C13-C14-C15 |
| 33 | d | 408 | LHG | C14-C15-C16-C17 |
| 22 | A | 410 | CLA | C16-C17-C18-C19 |
| 22 | B | 609 | CLA | C16-C17-C18-C19 |
| 27 | A | 411 | LMG | C35-C36-C37-C38 |
| 28 | a | 411 | SQD | C12-C13-C14-C15 |
| 32 | D | 411 | STE | C12-C13-C14-C15 |
| 32 | j | 101 | STE | C5-C6-C7-C8 |
| 28 | A | 413 | SQD | C23-C24-C25-C26 |
| 28 | a | 410 | SQD | C15-C16-C17-C18 |
| 29 | C | 516 | DGD | O6D-C5D-C6D-O5D |
| 22 | B | 613 | CLA | C14-C13-C15-C16 |
| 22 | C | 503 | CLA | C14-C13-C15-C16 |
| 22 | C | 508 | CLA | C11-C10-C8-C9 |
| 22 | C | 512 | CLA | C11-C12-C13-C14 |
| 22 | a | 403 | CLA | C14-C13-C15-C16 |
| 28 | A | 413 | SQD | C14-C15-C16-C17 |
| 22 | B | 614 | CLA | C16-C17-C18-C20 |
| 22 | B | 603 | CLA | O1D-CGD-O2D-CED |
| 29 | a | 412 | DGD | C6B-C7B-C8B-C9B |
| 27 | M | 101 | LMG | C39-C40-C41-C42 |
| 27 | A | 411 | LMG | C11-C12-C13-C14 |
| 28 | L | 101 | SQD | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | H | 102 | DGD | C3B-C4B-C5B-C6B |
| 32 | M | 102 | STE | C10-C11-C12-C13 |
| 33 | E | 102 | LHG | O2-C2-C3-O3 |
| 22 | B | 612 | CLA | C10-C11-C12-C13 |
| 33 | D | 408 | LHG | O1-C1-C2-O2 |
| 22 | c | 502 | CLA | CBA-CGA-O2A-C1 |
| 22 | c | 506 | CLA | C16-C17-C18-C19 |
| 32 | j | 101 | STE | C7-C8-C9-C10 |
| 27 | C | 519 | LMG | C18-C19-C20-C21 |
| 33 | E | 102 | LHG | C10-C11-C12-C13 |
| 29 | h | 102 | DGD | C7A-C8A-C9A-CAA |
| 22 | c | 513 | CLA | C5-C6-C7-C8 |
| 22 | C | 505 | CLA | CBD-CGD-O2D-CED |
| 33 | l | 101 | LHG | C17-C18-C19-C20 |
| 24 | B | 617 | BCR | C35-C13-C14-C15 |
| 24 | B | 617 | BCR | C20-C21-C22-C37 |
| 24 | C | 515 | BCR | C35-C13-C14-C15 |
| 24 | C | 515 | BCR | C16-C17-C18-C36 |
| 24 | H | 101 | BCR | C11-C10-C9-C34 |
| 24 | H | 101 | BCR | C20-C21-C22-C37 |
| 24 | Y | 101 | BCR | C20-C21-C22-C37 |
| 24 | b | 617 | BCR | C11-C10-C9-C34 |
| 24 | b | 617 | BCR | C35-C13-C14-C15 |
| 24 | c | 515 | BCR | C20-C21-C22-C37 |
| 24 | h | 101 | BCR | C16-C17-C18-C36 |
| 22 | c | 502 | CLA | C3-C5-C6-C7 |
| 29 | c | 519 | DGD | C5A-C6A-C7A-C8A |
| 22 | B | 611 | CLA | C13-C15-C16-C17 |
| 33 | B | 622 | LHG | C9-C10-C11-C12 |
| 32 | B | 626 | STE | C4-C5-C6-C7 |
| 33 | l | 101 | LHG | C30-C31-C32-C33 |
| 22 | B | 616 | CLA | C6-C7-C8-C10 |
| 22 | C | 502 | CLA | C11-C12-C13-C15 |
| 22 | C | 503 | CLA | C11-C10-C8-C7 |
| 22 | C | 508 | CLA | C11-C10-C8-C7 |
| 22 | C | 509 | CLA | C11-C10-C8-C7 |
| 22 | C | 510 | CLA | C11-C10-C8-C7 |
| 22 | a | 404 | CLA | C12-C13-C15-C16 |
| 22 | b | 605 | CLA | C12-C13-C15-C16 |
| 22 | b | 607 | CLA | C11-C12-C13-C15 |
| 22 | c | 510 | CLA | C6-C7-C8-C10 |
| 22 | d | 405 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | B | 621 | LMG | C15-C16-C17-C18 |
| 29 | A | 414 | DGD | CDB-CEB-CFB-CGB |
| 33 | D | 409 | LHG | C11-C10-C9-C8 |
| 22 | C | 502 | CLA | C3-C5-C6-C7 |
| 22 | b | 609 | CLA | C15-C16-C17-C18 |
| 24 | D | 405 | BCR | C21-C22-C23-C24 |
| 24 | H | 101 | BCR | C7-C8-C9-C10 |
| 24 | T | 101 | BCR | C17-C18-C19-C20 |
| 33 | D | 409 | LHG | O10-C23-O8-C6 |
| 29 | C | 517 | DGD | C2G-C3G-O3G-C1D |
| 27 | D | 407 | LMG | C30-C31-C32-C33 |
| 27 | b | 622 | LMG | C10-C11-C12-C13 |
| 28 | B | 623 | SQD | C23-C24-C25-C26 |
| 28 | L | 101 | SQD | C19-C20-C21-C22 |
| 29 | A | 414 | DGD | C8A-C9A-CAA-CBA |
| 33 | L | 102 | LHG | O9-C7-O7-C5 |
| 22 | c | 512 | CLA | C4-C3-C5-C6 |
| 26 | d | 407 | PL9 | C15-C14-C16-C17 |
| 22 | c | 502 | CLA | O1A-CGA-O2A-C1 |
| 32 | m | 101 | STE | C3-C4-C5-C6 |
| 32 | B | 625 | STE | C4-C5-C6-C7 |
| 22 | C | 501 | CLA | CBD-CGD-O2D-CED |
| 29 | H | 102 | DGD | C4B-C5B-C6B-C7B |
| 22 | c | 508 | CLA | C8-C10-C11-C12 |
| 22 | B | 604 | CLA | O1A-CGA-O2A-C1 |
| 32 | T | 103 | STE | C13-C14-C15-C16 |
| 22 | B | 613 | CLA | C5-C6-C7-C8 |
| 22 | c | 509 | CLA | C13-C15-C16-C17 |
| 24 | k | 101 | BCR | C19-C20-C21-C22 |
| 32 | b | 624 | STE | C5-C6-C7-C8 |
| 22 | b | 612 | CLA | C16-C17-C18-C20 |
| 27 | D | 407 | LMG | C39-C40-C41-C42 |
| 33 | d | 409 | LHG | C15-C16-C17-C18 |
| 24 | t | 101 | BCR | C20-C21-C22-C23 |
| 28 | L | 101 | SQD | C26-C27-C28-C29 |
| 29 | a | 412 | DGD | C9B-CAB-CBB-CCB |
| 32 | C | 520 | STE | C4-C5-C6-C7 |
| 29 | c | 518 | DGD | O6D-C1D-O3G-C3G |
| 29 | a | 412 | DGD | C5B-C6B-C7B-C8B |
| 32 | T | 102 | STE | C6-C7-C8-C9 |
| 32 | c | 524 | STE | C7-C8-C9-C10 |
| 32 | b | 623 | STE | C1-C2-C3-C4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | c | 510 | CLA | C5-C6-C7-C8 |
| 22 | b | 609 | CLA | C16-C17-C18-C20 |
| 29 | c | 519 | DGD | CAB-CBB-CCB-CDB |
| 33 | d | 408 | LHG | C27-C28-C29-C30 |
| 22 | B | 612 | CLA | O1A-CGA-O2A-C1 |
| 29 | C | 516 | DGD | C4D-C5D-C6D-O5D |
| 27 | c | 523 | LMG | C13-C14-C15-C16 |
| 32 | C | 520 | STE | C5-C6-C7-C8 |
| 22 | C | 506 | CLA | C4-C3-C5-C6 |
| 32 | I | 101 | STE | C12-C13-C14-C15 |
| 28 | A | 412 | SQD | C14-C15-C16-C17 |
| 27 | C | 519 | LMG | O1-C7-C8-O7 |
| 27 | M | 101 | LMG | O1-C7-C8-O7 |
| 28 | a | 411 | SQD | O47-C45-C46-O48 |
| 29 | C | 516 | DGD | O1G-C1G-C2G-O2G |
| 22 | B | 614 | CLA | C6-C7-C8-C9 |
| 29 | c | 519 | DGD | C4A-C5A-C6A-C7A |
| 29 | c | 519 | DGD | C7B-C8B-C9B-CAB |
| 28 | L | 101 | SQD | C11-C12-C13-C14 |
| 22 | C | 508 | CLA | C5-C6-C7-C8 |
| 22 | c | 506 | CLA | C5-C6-C7-C8 |
| 23 | D | 401 | PHO | C2C-C3C-CAC-CBC |
| 32 | a | 414 | STE | C6-C7-C8-C9 |
| 32 | b | 625 | STE | C1-C2-C3-C4 |
| 22 | C | 505 | CLA | O1A-CGA-O2A-C1 |
| 27 | C | 519 | LMG | C15-C16-C17-C18 |
| 27 | A | 411 | LMG | C2-C1-O1-C7 |
| 29 | c | 517 | DGD | C2E-C1E-O5D-C6D |
| 22 | D | 404 | CLA | C16-C17-C18-C19 |
| 22 | b | 604 | CLA | C16-C17-C18-C19 |
| 27 | A | 411 | LMG | C17-C18-C19-C20 |
| 32 | C | 521 | STE | C4-C5-C6-C7 |
| 26 | a | 409 | PL9 | C25-C24-C26-C27 |
| 33 | E | 102 | LHG | O9-C7-O7-C5 |
| 22 | b | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | c | 503 | CLA | CBA-CGA-O2A-C1 |
| 32 | c | 524 | STE | C2-C3-C4-C5 |
| 22 | a | 402 | CLA | C16-C17-C18-C19 |
| 22 | c | 505 | CLA | C16-C17-C18-C20 |
| 22 | d | 404 | CLA | C16-C17-C18-C19 |
| 33 | D | 408 | LHG | C17-C18-C19-C20 |
| 27 | c | 522 | LMG | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | L | 102 | LHG | C19-C20-C21-C22 |
| 35 | f | 101 | HEM | C2A-CAA-CBA-CGA |
| 32 | B | 625 | STE | C7-C8-C9-C10 |
| 32 | d | 413 | STE | C6-C7-C8-C9 |
| 33 | E | 102 | LHG | C28-C29-C30-C31 |
| 22 | B | 606 | CLA | C10-C11-C12-C13 |
| 22 | D | 403 | CLA | C2C-C3C-CAC-CBC |
| 32 | B | 626 | STE | C3-C4-C5-C6 |
| 22 | C | 505 | CLA | CBA-CGA-O2A-C1 |
| 33 | l | 101 | LHG | C24-C23-O8-C6 |
| 32 | B | 620 | STE | C11-C10-C9-C8 |
| 22 | c | 502 | CLA | O1D-CGD-O2D-CED |
| 28 | F | 101 | SQD | C45-C44-O6-C1 |
| 27 | b | 620 | LMG | C14-C15-C16-C17 |
| 22 | B | 601 | CLA | C1A-C2A-CAA-CBA |
| 24 | K | 101 | BCR | C6-C7-C8-C9 |
| 22 | c | 512 | CLA | C2-C3-C5-C6 |
| 28 | a | 410 | SQD | C19-C20-C21-C22 |
| 24 | t | 101 | BCR | C17-C18-C19-C20 |
| 28 | A | 412 | SQD | C29-C30-C31-C32 |
| 32 | M | 102 | STE | C4-C5-C6-C7 |
| 33 | d | 410 | LHG | C30-C31-C32-C33 |
| 27 | b | 622 | LMG | C19-C20-C21-C22 |
| 29 | C | 518 | DGD | C3A-C4A-C5A-C6A |
| 22 | B | 602 | CLA | C12-C13-C15-C16 |
| 22 | B | 603 | CLA | C12-C13-C15-C16 |
| 22 | B | 613 | CLA | C6-C7-C8-C10 |
| 22 | B | 616 | CLA | C11-C10-C8-C7 |
| 22 | C | 505 | CLA | C6-C7-C8-C10 |
| 22 | C | 506 | CLA | C12-C13-C15-C16 |
| 22 | C | 509 | CLA | C12-C13-C15-C16 |
| 22 | b | 602 | CLA | C11-C12-C13-C15 |
| 22 | b | 603 | CLA | C11-C12-C13-C15 |
| 22 | b | 606 | CLA | C11-C12-C13-C15 |
| 22 | c | 505 | CLA | C6-C7-C8-C10 |
| 22 | c | 512 | CLA | C6-C7-C8-C10 |
| 22 | c | 512 | CLA | C12-C13-C15-C16 |
| 32 | I | 101 | STE | C11-C12-C13-C14 |
| 22 | b | 604 | CLA | C16-C17-C18-C20 |
| 22 | b | 608 | CLA | C16-C17-C18-C19 |
| 22 | b | 611 | CLA | C16-C17-C18-C20 |
| 22 | b | 612 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | d | 404 | CLA | C16-C17-C18-C20 |
| 29 | H | 102 | DGD | CDA-CEA-CFA-CGA |
| 32 | B | 620 | STE | C4-C5-C6-C7 |
| 32 | b | 624 | STE | C6-C7-C8-C9 |
| 33 | d | 408 | LHG | C18-C19-C20-C21 |
| 22 | C | 504 | CLA | C11-C12-C13-C14 |
| 33 | d | 409 | LHG | C17-C18-C19-C20 |
| 32 | l | 102 | STE | C1-C2-C3-C4 |
| 29 | C | 516 | DGD | CCB-CDB-CEB-CFB |
| 32 | B | 620 | STE | C10-C11-C12-C13 |
| 33 | D | 408 | LHG | C25-C26-C27-C28 |
| 22 | B | 601 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 610 | CLA | C16-C17-C18-C19 |
| 22 | a | 402 | CLA | O1D-CGD-O2D-CED |
| 33 | L | 102 | LHG | C10-C11-C12-C13 |
| 27 | A | 411 | LMG | C40-C41-C42-C43 |
| 22 | B | 613 | CLA | C6-C7-C8-C9 |
| 22 | a | 404 | CLA | C14-C13-C15-C16 |
| 22 | b | 601 | CLA | C6-C7-C8-C9 |
| 22 | b | 605 | CLA | C14-C13-C15-C16 |
| 22 | b | 607 | CLA | C11-C12-C13-C14 |
| 22 | c | 507 | CLA | C11-C10-C8-C9 |
| 22 | d | 405 | CLA | C11-C12-C13-C14 |
| 27 | c | 523 | LMG | C39-C40-C41-C42 |
| 29 | c | 518 | DGD | CCB-CDB-CEB-CFB |
| 22 | B | 601 | CLA | C16-C17-C18-C20 |
| 32 | H | 103 | STE | C10-C11-C12-C13 |
| 22 | B | 605 | CLA | C10-C11-C12-C13 |
| 27 | C | 519 | LMG | C16-C17-C18-C19 |
| 32 | a | 414 | STE | C1-C2-C3-C4 |
| 28 | L | 101 | SQD | O47-C45-C46-O48 |
| 32 | J | 101 | STE | C2-C3-C4-C5 |
| 33 | B | 622 | LHG | C4-C5-C6-O8 |
| 29 | c | 518 | DGD | C5B-C6B-C7B-C8B |
| 22 | A | 405 | CLA | C6-C7-C8-C9 |
| 29 | A | 414 | DGD | CBA-CCA-CDA-CEA |
| 33 | l | 101 | LHG | C32-C33-C34-C35 |
| 22 | C | 502 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 504 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 607 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 504 | CLA | CAD-CBD-CGD-O2D |
| 29 | c | 517 | DGD | CDB-CEB-CFB-CGB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 501 | CLA | C16-C17-C18-C20 |
| 22 | C | 506 | CLA | C16-C17-C18-C20 |
| 27 | b | 622 | LMG | C39-C40-C41-C42 |
| 29 | A | 414 | DGD | O1A-C1A-O1G-C1G |
| 27 | c | 522 | LMG | C29-C30-C31-C32 |
| 29 | a | 412 | DGD | CFB-CGB-CHB-CIB |
| 29 | C | 518 | DGD | C6A-C7A-C8A-C9A |
| 22 | C | 502 | CLA | CAD-CBD-CGD-O1D |
| 22 | C | 504 | CLA | CAD-CBD-CGD-O1D |
| 22 | C | 507 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 509 | CLA | CHA-CBD-CGD-O1D |
| 22 | b | 607 | CLA | CAD-CBD-CGD-O1D |
| 22 | c | 504 | CLA | CAD-CBD-CGD-O1D |
| 23 | d | 402 | PHO | CHA-CBD-CGD-O2D |
| 24 | a | 405 | BCR | C19-C20-C21-C22 |
| 28 | A | 413 | SQD | C46-C45-O47-C7 |
| 33 | D | 408 | LHG | C3-O3-P-O4 |
| 33 | D | 408 | LHG | C4-O6-P-O3 |
| 33 | L | 102 | LHG | C3-O3-P-O6 |
| 33 | d | 408 | LHG | C3-O3-P-O5 |
| 33 | d | 409 | LHG | C4-O6-P-O3 |
| 33 | l | 101 | LHG | C3-O3-P-O6 |
| 33 | l | 101 | LHG | C4-O6-P-O5 |
| 22 | c | 502 | CLA | CBD-CGD-O2D-CED |
| 27 | b | 622 | LMG | C34-C35-C36-C37 |
| 32 | E | 103 | STE | C5-C6-C7-C8 |
| 24 | C | 514 | BCR | C23-C24-C25-C30 |
| 33 | l | 101 | LHG | C27-C28-C29-C30 |
| 22 | C | 506 | CLA | C2-C3-C5-C6 |
| 26 | D | 406 | PL9 | C38-C39-C41-C42 |
| 32 | b | 623 | STE | C11-C10-C9-C8 |
| 32 | B | 624 | STE | C7-C8-C9-C10 |
| 27 | B | 621 | LMG | C29-C30-C31-C32 |
| 28 | B | 623 | SQD | C27-C28-C29-C30 |
| 32 | b | 623 | STE | C7-C8-C9-C10 |
| 22 | c | 509 | CLA | CAA-CBA-CGA-O2A |
| 32 | B | 625 | STE | C6-C7-C8-C9 |
| 33 | d | 409 | LHG | C31-C32-C33-C34 |
| 27 | C | 519 | LMG | C37-C38-C39-C40 |
| 29 | h | 102 | DGD | CBA-CCA-CDA-CEA |
| 26 | a | 409 | PL9 | C4-C3-C7-C8 |
| 28 | a | 410 | SQD | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 33 | D | 409 | LHG | O1-C1-C2-C3 |
| 27 | A | 411 | LMG | C9-C8-O7-C10 |
| 27 | b | 622 | LMG | C9-C8-O7-C10 |
| 28 | B | 623 | SQD | C46-C45-O47-C7 |
| 29 | C | 516 | DGD | O1G-C1A-C2A-C3A |
| 29 | c | 517 | DGD | C6A-C7A-C8A-C9A |
| 27 | c | 523 | LMG | C40-C41-C42-C43 |
| 32 | H | 103 | STE | C7-C8-C9-C10 |
| 22 | b | 614 | CLA | C16-C17-C18-C20 |
| 22 | A | 403 | CLA | C11-C10-C8-C9 |
| 22 | B | 615 | CLA | C11-C12-C13-C14 |
| 22 | C | 502 | CLA | C11-C12-C13-C14 |
| 22 | b | 602 | CLA | C11-C12-C13-C14 |
| 22 | c | 510 | CLA | C6-C7-C8-C9 |
| 22 | c | 512 | CLA | C11-C12-C13-C14 |
| 22 | B | 604 | CLA | C11-C10-C8-C7 |
| 22 | B | 606 | CLA | C11-C10-C8-C7 |
| 22 | a | 403 | CLA | C12-C13-C15-C16 |
| 22 | c | 512 | CLA | C11-C10-C8-C7 |
| 24 | B | 619 | BCR | C11-C10-C9-C8 |
| 27 | d | 412 | LMG | C11-C12-C13-C14 |
| 33 | L | 102 | LHG | C14-C15-C16-C17 |
| 27 | A | 411 | LMG | C13-C14-C15-C16 |
| 33 | l | 101 | LHG | C18-C19-C20-C21 |
| 27 | D | 410 | LMG | C31-C32-C33-C34 |
| 32 | l | 102 | STE | C12-C13-C14-C15 |
| 33 | l | 101 | LHG | C26-C27-C28-C29 |
| 27 | d | 412 | LMG | C10-C11-C12-C13 |
| 33 | d | 408 | LHG | C25-C26-C27-C28 |
| 22 | b | 608 | CLA | C2C-C3C-CAC-CBC |
| 32 | T | 103 | STE | C10-C11-C12-C13 |
| 26 | a | 409 | PL9 | C13-C14-C16-C17 |
| 29 | H | 102 | DGD | C9B-CAB-CBB-CCB |
| 33 | E | 102 | LHG | O7-C5-C6-O8 |
| 22 | c | 503 | CLA | O1A-CGA-O2A-C1 |
| 29 | H | 102 | DGD | C3A-C4A-C5A-C6A |
| 29 | C | 518 | DGD | C2A-C1A-O1G-C1G |
| 33 | d | 410 | LHG | C7-C8-C9-C10 |
| 33 | B | 622 | LHG | C19-C20-C21-C22 |
| 32 | l | 102 | STE | C15-C16-C17-C18 |
| 22 | B | 603 | CLA | C2A-CAA-CBA-CGA |
| 22 | c | 501 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 402 | CLA | C13-C15-C16-C17 |
| 22 | C | 509 | CLA | C2-C1-O2A-CGA |
| 22 | d | 405 | CLA | C4-C3-C5-C6 |
| 22 | A | 403 | CLA | C16-C17-C18-C20 |
| 27 | D | 407 | LMG | C34-C35-C36-C37 |
| 27 | b | 620 | LMG | C12-C13-C14-C15 |
| 27 | c | 523 | LMG | C11-C12-C13-C14 |
| 32 | m | 101 | STE | C6-C7-C8-C9 |
| 32 | b | 625 | STE | C4-C5-C6-C7 |
| 27 | D | 410 | LMG | C32-C33-C34-C35 |
| 32 | C | 522 | STE | C3-C4-C5-C6 |
| 24 | c | 514 | BCR | C17-C18-C19-C20 |
| 22 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 22 | C | 505 | CLA | C15-C16-C17-C18 |
| 29 | C | 516 | DGD | C5D-C6D-O5D-C1E |
| 29 | c | 518 | DGD | C5D-C6D-O5D-C1E |
| 22 | A | 402 | CLA | C4C-C3C-CAC-CBC |
| 22 | D | 404 | CLA | C16-C17-C18-C20 |
| 33 | d | 410 | LHG | C25-C26-C27-C28 |
| 28 | a | 411 | SQD | C30-C31-C32-C33 |
| 29 | h | 102 | DGD | C7B-C8B-C9B-CAB |
| 32 | D | 411 | STE | C2-C3-C4-C5 |
| 22 | B | 616 | CLA | C4-C3-C5-C6 |
| 29 | c | 518 | DGD | C5A-C6A-C7A-C8A |
| 32 | d | 413 | STE | C5-C6-C7-C8 |
| 29 | C | 516 | DGD | CDA-CEA-CFA-CGA |
| 22 | B | 615 | CLA | C16-C17-C18-C19 |
| 22 | c | 505 | CLA | C16-C17-C18-C19 |
| 22 | B | 602 | CLA | C14-C13-C15-C16 |
| 22 | C | 505 | CLA | C6-C7-C8-C9 |
| 22 | b | 603 | CLA | C11-C12-C13-C14 |
| 22 | c | 505 | CLA | C6-C7-C8-C9 |
| 33 | D | 409 | LHG | C2-C3-O3-P |
| 33 | d | 410 | LHG | C2-C3-O3-P |
| 33 | l | 101 | LHG | C11-C10-C9-C8 |
| 33 | d | 408 | LHG | C33-C34-C35-C36 |
| 22 | b | 609 | CLA | C16-C17-C18-C19 |
| 26 | A | 409 | PL9 | C15-C14-C16-C17 |
| 29 | C | 518 | DGD | CBA-CCA-CDA-CEA |
| 26 | A | 409 | PL9 | C13-C14-C16-C17 |
| 32 | c | 521 | STE | C7-C8-C9-C10 |
| 29 | c | 518 | DGD | C3B-C4B-C5B-C6B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | h | 102 | DGD | C5A-C6A-C7A-C8A |
| 29 | c | 518 | DGD | C8B-C9B-CAB-CBB |
| 32 | b | 623 | STE | C9-C10-C11-C12 |
| 22 | A | 410 | CLA | C11-C12-C13-C15 |
| 22 | C | 512 | CLA | C6-C7-C8-C10 |
| 22 | b | 606 | CLA | C6-C7-C8-C10 |
| 22 | d | 405 | CLA | C12-C13-C15-C16 |
| 22 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 32 | T | 103 | STE | C12-C13-C14-C15 |
| 27 | D | 410 | LMG | C29-C30-C31-C32 |
| 29 | C | 516 | DGD | C2A-C3A-C4A-C5A |
| 22 | a | 403 | CLA | O1D-CGD-O2D-CED |
| 22 | C | 508 | CLA | C16-C17-C18-C19 |
| 22 | A | 402 | CLA | C2C-C3C-CAC-CBC |
| 32 | b | 625 | STE | C5-C6-C7-C8 |
| 26 | d | 407 | PL9 | C32-C33-C34-C36 |
| 28 | B | 623 | SQD | C28-C29-C30-C31 |
| 29 | H | 102 | DGD | C2B-C3B-C4B-C5B |
| 24 | C | 515 | BCR | C11-C10-C9-C34 |
| 24 | b | 617 | BCR | C6-C7-C8-C9 |
| 29 | A | 414 | DGD | O6D-C1D-O3G-C3G |
| 27 | b | 620 | LMG | C33-C34-C35-C36 |
| 36 | v | 201 | HEC | CAD-CBD-CGD-O1D |
| 24 | B | 618 | BCR | C19-C20-C21-C22 |
| 22 | c | 511 | CLA | C8-C10-C11-C12 |
| 24 | B | 618 | BCR | C37-C22-C23-C24 |
| 24 | c | 515 | BCR | C7-C8-C9-C34 |
| 33 | E | 102 | LHG | C19-C20-C21-C22 |
| 22 | c | 512 | CLA | C5-C6-C7-C8 |
| 32 | M | 103 | STE | C4-C5-C6-C7 |
| 33 | E | 102 | LHG | C30-C31-C32-C33 |
| 29 | h | 102 | DGD | O2G-C1B-C2B-C3B |
| 22 | C | 502 | CLA | C16-C17-C18-C20 |
| 22 | b | 611 | CLA | C16-C17-C18-C19 |
| 22 | b | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 503 | CLA | C15-C16-C17-C18 |
| 27 | b | 622 | LMG | O1-C7-C8-C9 |
| 32 | m | 101 | STE | C4-C5-C6-C7 |
| 22 | B | 604 | CLA | C11-C10-C8-C9 |
| 22 | C | 501 | CLA | C14-C13-C15-C16 |
| 22 | C | 505 | CLA | C11-C10-C8-C9 |
| 22 | C | 506 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 509 | CLA | C14-C13-C15-C16 |
| 22 | C | 513 | CLA | C11-C10-C8-C9 |
| 22 | b | 606 | CLA | C6-C7-C8-C9 |
| 22 | c | 510 | CLA | C14-C13-C15-C16 |
| 22 | d | 403 | CLA | C6-C7-C8-C9 |
| 22 | d | 405 | CLA | C14-C13-C15-C16 |
| 27 | d | 412 | LMG | C15-C16-C17-C18 |
| 32 | C | 521 | STE | C14-C15-C16-C17 |
| 32 | D | 411 | STE | C11-C12-C13-C14 |
| 32 | c | 521 | STE | C3-C4-C5-C6 |
| 27 | c | 523 | LMG | C7-C8-O7-C10 |
| 22 | b | 614 | CLA | C10-C11-C12-C13 |
| 23 | d | 402 | PHO | C1A-C2A-CAA-CBA |
| 24 | c | 514 | BCR | C15-C16-C17-C18 |
| 32 | d | 413 | STE | O2-C1-C2-C3 |
| 27 | b | 622 | LMG | C29-C30-C31-C32 |
| 22 | B | 614 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 512 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 508 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 511 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 618 | BCR | C23-C24-C25-C30 |
| 24 | C | 515 | BCR | C5-C6-C7-C8 |
| 24 | b | 617 | BCR | C5-C6-C7-C8 |
| 24 | d | 406 | BCR | C23-C24-C25-C26 |
| 24 | h | 101 | BCR | C23-C24-C25-C26 |
| 24 | h | 101 | BCR | C23-C24-C25-C30 |
| 24 | k | 101 | BCR | C5-C6-C7-C8 |
| 32 | d | 413 | STE | O1-C1-C2-C3 |
| 29 | c | 518 | DGD | CDA-CEA-CFA-CGA |
| 27 | b | 622 | LMG | C29-C28-O8-C9 |
| 32 | C | 521 | STE | C9-C10-C11-C12 |
| 33 | D | 408 | LHG | C16-C17-C18-C19 |
| 22 | d | 403 | CLA | C16-C17-C18-C19 |
| 27 | d | 411 | LMG | O7-C10-C11-C12 |
| 32 | c | 521 | STE | O1-C1-C2-C3 |
| 36 | V | 201 | HEC | CAD-CBD-CGD-O2D |
| 36 | v | 201 | HEC | CAD-CBD-CGD-O2D |
| 22 | B | 605 | CLA | C4-C3-C5-C6 |
| 22 | c | 507 | CLA | C4-C3-C5-C6 |
| 27 | A | 411 | LMG | C28-C29-C30-C31 |
| 27 | B | 621 | LMG | O9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 32 | b | 621 | STE | O1-C1-C2-C3 |
| 35 | f | 101 | HEM | CAD-CBD-CGD-O1D |
| 22 | A | 410 | CLA | C6-C7-C8-C10 |
| 22 | B | 613 | CLA | C11-C12-C13-C15 |
| 22 | C | 505 | CLA | C11-C10-C8-C7 |
| 22 | C | 510 | CLA | C6-C7-C8-C10 |
| 22 | b | 616 | CLA | C11-C10-C8-C7 |
| 22 | c | 502 | CLA | C6-C7-C8-C10 |
| 22 | c | 512 | CLA | C11-C12-C13-C15 |
| 22 | B | 601 | CLA | C16-C17-C18-C19 |
| 22 | b | 614 | CLA | C16-C17-C18-C19 |
| 22 | d | 403 | CLA | C16-C17-C18-C20 |
| 33 | B | 622 | LHG | O7-C5-C6-O8 |
| 32 | D | 411 | STE | C13-C14-C15-C16 |
| 32 | b | 624 | STE | O1-C1-C2-C3 |
| 29 | A | 414 | DGD | O6D-C5D-C6D-O5D |
| 29 | C | 517 | DGD | C8A-C9A-CAA-CBA |
| 24 | h | 101 | BCR | C7-C8-C9-C34 |
| 22 | c | 506 | CLA | C4-C3-C5-C6 |
| 27 | B | 621 | LMG | C37-C38-C39-C40 |
| 22 | d | 403 | CLA | C5-C6-C7-C8 |
| 32 | B | 625 | STE | O2-C1-C2-C3 |
| 28 | A | 412 | SQD | C34-C35-C36-C37 |
| 33 | D | 409 | LHG | C17-C18-C19-C20 |
| 27 | B | 621 | LMG | C28-C29-C30-C31 |
| 32 | E | 103 | STE | C6-C7-C8-C9 |
| 33 | D | 408 | LHG | C11-C10-C9-C8 |
| 33 | B | 622 | LHG | C29-C30-C31-C32 |
| 22 | C | 502 | CLA | C4-C3-C5-C6 |
| 22 | C | 507 | CLA | C4-C3-C5-C6 |
| 22 | d | 403 | CLA | C4-C3-C5-C6 |
| 22 | B | 612 | CLA | C13-C15-C16-C17 |
| 22 | C | 510 | CLA | C8-C10-C11-C12 |
| 35 | f | 101 | HEM | CAD-CBD-CGD-O2D |
| 36 | V | 201 | HEC | CAD-CBD-CGD-O1D |
| 26 | a | 409 | PL9 | C23-C24-C26-C27 |
| 22 | b | 604 | CLA | C8-C10-C11-C12 |
| 22 | B | 602 | CLA | C15-C16-C17-C18 |
| 29 | H | 102 | DGD | O1A-C1A-O1G-C1G |
| 29 | C | 518 | DGD | C9A-CAA-CBA-CCA |
| 33 | d | 408 | LHG | C31-C32-C33-C34 |
| 27 | D | 410 | LMG | C7-C8-C9-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | C | 516 | DGD | O1G-C1G-C2G-C3G |
| 27 | B | 621 | LMG | O7-C10-C11-C12 |
| 32 | b | 621 | STE | O2-C1-C2-C3 |
| 32 | b | 624 | STE | O2-C1-C2-C3 |
| 32 | c | 521 | STE | O2-C1-C2-C3 |
| 33 | D | 409 | LHG | C12-C13-C14-C15 |
| 29 | C | 516 | DGD | C8A-C9A-CAA-CBA |
| 28 | A | 413 | SQD | C16-C17-C18-C19 |
| 32 | a | 414 | STE | C7-C8-C9-C10 |
| 22 | c | 510 | CLA | C4-C3-C5-C6 |
| 24 | C | 515 | BCR | C15-C16-C17-C18 |
| 24 | c | 516 | BCR | C13-C14-C15-C16 |
| 32 | c | 521 | STE | C4-C5-C6-C7 |
| 22 | d | 404 | CLA | O1D-CGD-O2D-CED |
| 22 | C | 506 | CLA | C16-C17-C18-C19 |
| 22 | d | 404 | CLA | C2C-C3C-CAC-CBC |
| 24 | a | 405 | BCR | C11-C10-C9-C34 |
| 22 | b | 608 | CLA | C4C-C3C-CAC-CBC |
| 22 | b | 610 | CLA | C10-C11-C12-C13 |
| 32 | B | 624 | STE | O2-C1-C2-C3 |
| 32 | B | 625 | STE | O1-C1-C2-C3 |
| 22 | B | 610 | CLA | C16-C17-C18-C20 |
| 22 | B | 611 | CLA | C16-C17-C18-C20 |
| 22 | B | 609 | CLA | C4-C3-C5-C6 |
| 27 | b | 622 | LMG | O1-C7-C8-O7 |
| 28 | L | 101 | SQD | O6-C44-C45-O47 |
| 29 | c | 517 | DGD | O1G-C1G-C2G-O2G |
| 35 | E | 101 | HEM | CAD-CBD-CGD-O1D |
| 22 | c | 510 | CLA | C2-C3-C5-C6 |
| 32 | B | 626 | STE | C11-C12-C13-C14 |
| 22 | b | 607 | CLA | C5-C6-C7-C8 |
| 22 | c | 501 | CLA | C11-C12-C13-C15 |
| 32 | B | 627 | STE | C2-C3-C4-C5 |
| 32 | C | 522 | STE | C7-C8-C9-C10 |
| 32 | B | 624 | STE | O1-C1-C2-C3 |
| 26 | A | 409 | PL9 | C44-C46-C47-C48 |
| 22 | A | 410 | CLA | C11-C12-C13-C14 |
| 22 | B | 603 | CLA | C14-C13-C15-C16 |
| 22 | b | 606 | CLA | C11-C12-C13-C14 |
| 27 | b | 620 | LMG | C18-C19-C20-C21 |
| 27 | b | 622 | LMG | C14-C15-C16-C17 |
| 22 | C | 501 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | d | 405 | CLA | C16-C17-C18-C19 |
| 33 | D | 408 | LHG | C35-C36-C37-C38 |
| 29 | H | 102 | DGD | C7B-C8B-C9B-CAB |
| 22 | C | 512 | CLA | C3A-C2A-CAA-CBA |
| 28 | B | 623 | SQD | C19-C20-C21-C22 |
| 22 | c | 507 | CLA | C2-C3-C5-C6 |
| 22 | d | 405 | CLA | C8-C10-C11-C12 |
| 32 | b | 624 | STE | C1-C2-C3-C4 |
| 27 | M | 101 | LMG | C9-C8-O7-C10 |
| 32 | b | 621 | STE | C4-C5-C6-C7 |
| 22 | a | 403 | CLA | C13-C15-C16-C17 |
| 27 | D | 410 | LMG | C11-C12-C13-C14 |
| 23 | d | 402 | PHO | C4C-C3C-CAC-CBC |
| 24 | c | 516 | BCR | C11-C10-C9-C8 |
| 22 | B | 607 | CLA | C15-C16-C17-C18 |
| 32 | d | 413 | STE | C11-C10-C9-C8 |
| 29 | c | 519 | DGD | C1B-C2B-C3B-C4B |
| 33 | B | 622 | LHG | C24-C23-O8-C6 |
| 32 | D | 411 | STE | O2-C1-C2-C3 |
| 28 | L | 101 | SQD | C44-C45-C46-O48 |
| 29 | c | 517 | DGD | C1G-C2G-C3G-O3G |
| 35 | f | 101 | HEM | C4B-C3B-CAB-CBB |
| 27 | d | 411 | LMG | O9-C10-C11-C12 |
| 27 | b | 620 | LMG | C32-C33-C34-C35 |
| 22 | C | 505 | CLA | O1D-CGD-O2D-CED |
| 22 | d | 405 | CLA | C2-C3-C5-C6 |
| 22 | A | 403 | CLA | C16-C17-C18-C19 |
| 28 | a | 410 | SQD | C14-C15-C16-C17 |
| 27 | M | 101 | LMG | C36-C37-C38-C39 |
| 33 | E | 102 | LHG | C16-C17-C18-C19 |
| 22 | b | 613 | CLA | CAA-CBA-CGA-O2A |
| 33 | D | 408 | LHG | C33-C34-C35-C36 |
| 33 | E | 102 | LHG | C35-C36-C37-C38 |
| 28 | A | 413 | SQD | C17-C18-C19-C20 |
| 22 | B | 601 | CLA | C6-C7-C8-C9 |
| 22 | B | 606 | CLA | C11-C12-C13-C14 |
| 22 | C | 506 | CLA | C14-C13-C15-C16 |
| 22 | C | 510 | CLA | C6-C7-C8-C9 |
| 22 | D | 403 | CLA | C11-C10-C8-C9 |
| 22 | b | 607 | CLA | C14-C13-C15-C16 |
| 33 | l | 101 | LHG | O7-C7-C8-C9 |
| 27 | D | 407 | LMG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | d | 402 | PHO | C2C-C3C-CAC-CBC |
| 22 | C | 507 | CLA | C5-C6-C7-C8 |
| 29 | c | 517 | DGD | O1G-C1A-C2A-C3A |
| 22 | C | 502 | CLA | C2-C3-C5-C6 |
| 22 | A | 403 | CLA | C12-C13-C15-C16 |
| 22 | B | 601 | CLA | C6-C7-C8-C10 |
| 22 | B | 601 | CLA | C11-C12-C13-C15 |
| 22 | B | 612 | CLA | C11-C10-C8-C7 |
| 22 | B | 615 | CLA | C12-C13-C15-C16 |
| 22 | C | 513 | CLA | C11-C10-C8-C7 |
| 22 | b | 605 | CLA | C11-C10-C8-C7 |
| 22 | b | 607 | CLA | C11-C10-C8-C7 |
| 22 | b | 608 | CLA | C11-C10-C8-C7 |
| 22 | b | 611 | CLA | C12-C13-C15-C16 |
| 22 | b | 614 | CLA | C11-C12-C13-C15 |
| 22 | c | 508 | CLA | C11-C10-C8-C7 |
| 22 | c | 510 | CLA | C12-C13-C15-C16 |
| 22 | d | 403 | CLA | C6-C7-C8-C10 |
| 29 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 24 | A | 406 | BCR | C1-C6-C7-C8 |
| 24 | A | 406 | BCR | C5-C6-C7-C8 |
| 24 | B | 618 | BCR | C23-C24-C25-C26 |
| 24 | C | 515 | BCR | C23-C24-C25-C30 |
| 24 | Y | 101 | BCR | C23-C24-C25-C30 |
| 24 | b | 618 | BCR | C23-C24-C25-C26 |
| 24 | b | 618 | BCR | C23-C24-C25-C30 |
| 24 | c | 514 | BCR | C1-C6-C7-C8 |
| 24 | c | 514 | BCR | C5-C6-C7-C8 |
| 24 | c | 516 | BCR | C23-C24-C25-C26 |
| 24 | c | 516 | BCR | C23-C24-C25-C30 |
| 24 | t | 101 | BCR | C5-C6-C7-C8 |
| 27 | d | 412 | LMG | C32-C33-C34-C35 |
| 32 | B | 626 | STE | C11-C10-C9-C8 |
| 22 | A | 402 | CLA | C2-C1-O2A-CGA |
| 22 | B | 613 | CLA | C2-C1-O2A-CGA |
| 22 | a | 402 | CLA | C2-C1-O2A-CGA |
| 22 | c | 513 | CLA | C2-C1-O2A-CGA |
| 22 | d | 403 | CLA | C2-C1-O2A-CGA |
| 33 | L | 102 | LHG | C9-C10-C11-C12 |
| 26 | A | 409 | PL9 | C9-C11-C12-C13 |
| 22 | B | 613 | CLA | C16-C17-C18-C19 |
| 22 | a | 404 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | F | 101 | SQD | C23-C24-C25-C26 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O2A |
| 22 | b | 612 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 609 | CLA | C2-C3-C5-C6 |
| 35 | E | 101 | HEM | CAD-CBD-CGD-O2D |
| 22 | C | 512 | CLA | C2A-CAA-CBA-CGA |
| 22 | b | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 508 | CLA | C8-C10-C11-C12 |
| 27 | b | 620 | LMG | O8-C28-C29-C30 |
| 22 | c | 508 | CLA | O1D-CGD-O2D-CED |
| 27 | M | 101 | LMG | C40-C41-C42-C43 |
| 32 | c | 524 | STE | C3-C4-C5-C6 |
| 22 | b | 601 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 616 | CLA | C2-C3-C5-C6 |
| 32 | C | 522 | STE | C4-C5-C6-C7 |
| 29 | c | 518 | DGD | CAB-CBB-CCB-CDB |
| 29 | c | 517 | DGD | C2A-C3A-C4A-C5A |
| 22 | b | 612 | CLA | C8-C10-C11-C12 |
| 29 | a | 412 | DGD | C7A-C8A-C9A-CAA |
| 22 | A | 410 | CLA | C6-C7-C8-C9 |
| 22 | B | 610 | CLA | C14-C13-C15-C16 |
| 22 | c | 501 | CLA | C11-C12-C13-C14 |
| 22 | c | 508 | CLA | C11-C10-C8-C9 |
| 27 | D | 407 | LMG | C37-C38-C39-C40 |
| 32 | C | 520 | STE | C1-C2-C3-C4 |
| 28 | A | 412 | SQD | O47-C7-C8-C9 |
| 33 | L | 102 | LHG | O7-C7-C8-C9 |
| 27 | c | 520 | LMG | C36-C37-C38-C39 |
| 27 | D | 407 | LMG | O10-C28-O8-C9 |
| 29 | C | 516 | DGD | C1G-C2G-C3G-O3G |
| 29 | C | 516 | DGD | O6E-C1E-O5D-C6D |
| 29 | C | 517 | DGD | O6D-C1D-O3G-C3G |
| 29 | A | 414 | DGD | O2G-C1B-C2B-C3B |
| 33 | e | 101 | LHG | C12-C13-C14-C15 |
| 27 | M | 101 | LMG | O6-C5-C6-O5 |
| 32 | l | 102 | STE | C9-C10-C11-C12 |
| 28 | a | 411 | SQD | C29-C30-C31-C32 |
| 28 | a | 410 | SQD | O47-C7-C8-C9 |
| 27 | b | 622 | LMG | C32-C33-C34-C35 |
| 28 | L | 101 | SQD | C25-C26-C27-C28 |
| 32 | B | 624 | STE | C3-C4-C5-C6 |
| 23 | A | 404 | PHO | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | b | 602 | CLA | C8-C10-C11-C12 |
| 32 | B | 627 | STE | C4-C5-C6-C7 |
| 22 | d | 403 | CLA | C2C-C3C-CAC-CBC |
| 28 | a | 410 | SQD | C5-C6-S-O7 |
| 33 | d | 408 | LHG | C35-C36-C37-C38 |
| 22 | C | 506 | CLA | C2-C1-O2A-CGA |
| 22 | b | 608 | CLA | C2-C1-O2A-CGA |
| 29 | c | 519 | DGD | C4B-C5B-C6B-C7B |
| 22 | B | 606 | CLA | C11-C12-C13-C15 |
| 22 | B | 611 | CLA | C11-C12-C13-C15 |
| 22 | C | 504 | CLA | C11-C10-C8-C7 |
| 22 | C | 506 | CLA | C6-C7-C8-C10 |
| 22 | a | 403 | CLA | C11-C10-C8-C7 |
| 22 | b | 614 | CLA | C6-C7-C8-C10 |
| 22 | d | 403 | CLA | C11-C12-C13-C15 |
| 22 | b | 615 | CLA | C8-C10-C11-C12 |
| 32 | D | 411 | STE | O1-C1-C2-C3 |
| 22 | C | 505 | CLA | C16-C17-C18-C19 |
| 29 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 33 | D | 408 | LHG | C13-C14-C15-C16 |
| 22 | c | 512 | CLA | C15-C16-C17-C18 |
| 28 | L | 101 | SQD | C14-C15-C16-C17 |
| 29 | h | 102 | DGD | O1B-C1B-C2B-C3B |
| 22 | c | 502 | CLA | C16-C17-C18-C19 |
| 29 | c | 519 | DGD | C2B-C3B-C4B-C5B |
| 27 | B | 621 | LMG | O10-C28-C29-C30 |
| 22 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 33 | D | 408 | LHG | O10-C23-O8-C6 |
| 22 | b | 611 | CLA | C10-C11-C12-C13 |
| 22 | c | 503 | CLA | C10-C11-C12-C13 |
| 22 | B | 602 | CLA | C3A-C2A-CAA-CBA |
| 32 | I | 101 | STE | C6-C7-C8-C9 |
| 27 | C | 519 | LMG | C36-C37-C38-C39 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 518 | DGD | O1A-C1A-C2A-C3A |
| 33 | e | 101 | LHG | O10-C23-C24-C25 |
| 22 | B | 611 | CLA | C6-C7-C8-C9 |
| 22 | B | 612 | CLA | C11-C10-C8-C9 |
| 22 | B | 615 | CLA | C14-C13-C15-C16 |
| 22 | C | 508 | CLA | C14-C13-C15-C16 |
| 22 | a | 403 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | c | 512 | CLA | C11-C10-C8-C9 |
| 22 | c | 512 | CLA | C14-C13-C15-C16 |
| 29 | C | 516 | DGD | CAA-CBA-CCA-CDA |
| 33 | B | 622 | LHG | O10-C23-O8-C6 |
| 22 | b | 602 | CLA | O1D-CGD-O2D-CED |
| 32 | I | 101 | STE | C5-C6-C7-C8 |
| 28 | a | 410 | SQD | C35-C36-C37-C38 |
| 22 | B | 603 | CLA | C13-C15-C16-C17 |
| 28 | B | 623 | SQD | O5-C5-C6-S |
| 29 | A | 414 | DGD | O1B-C1B-C2B-C3B |
| 22 | a | 404 | CLA | C15-C16-C17-C18 |
| 22 | b | 613 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 517 | DGD | O1B-C1B-C2B-C3B |
| 33 | l | 101 | LHG | O9-C7-C8-C9 |
| 33 | B | 622 | LHG | C35-C36-C37-C38 |
| 28 | A | 412 | SQD | C23-C24-C25-C26 |
| 23 | d | 402 | PHO | C5-C6-C7-C8 |
| 27 | M | 101 | LMG | C8-C7-O1-C1 |
| 27 | B | 621 | LMG | O8-C28-C29-C30 |
| 28 | A | 413 | SQD | O10-C23-C24-C25 |
| 33 | d | 408 | LHG | O8-C23-C24-C25 |
| 29 | H | 102 | DGD | C5B-C6B-C7B-C8B |
| 27 | b | 622 | LMG | O10-C28-C29-C30 |
| 28 | a | 411 | SQD | O10-C23-C24-C25 |
| 22 | d | 404 | CLA | C4C-C3C-CAC-CBC |
| 22 | B | 610 | CLA | C10-C11-C12-C13 |
| 24 | Y | 101 | BCR | C13-C14-C15-C16 |
| 22 | b | 601 | CLA | CAA-CBA-CGA-O1A |
| 22 | b | 612 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 410 | CLA | C4C-C3C-CAC-CBC |
| 22 | B | 607 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 513 | CLA | CAD-CBD-CGD-O2D |
| 23 | A | 404 | PHO | CAD-CBD-CGD-O2D |
| 23 | d | 401 | PHO | CAD-CBD-CGD-O2D |
| 29 | C | 516 | DGD | O1B-C1B-C2B-C3B |
| 33 | d | 408 | LHG | C10-C11-C12-C13 |
| 32 | a | 414 | STE | O2-C1-C2-C3 |
| 22 | b | 611 | CLA | C13-C15-C16-C17 |
| 33 | e | 101 | LHG | O8-C23-C24-C25 |
| 33 | D | 408 | LHG | C28-C29-C30-C31 |
| 26 | A | 409 | PL9 | C2-C3-C7-C8 |
| 29 | C | 517 | DGD | C9B-CAB-CBB-CCB |

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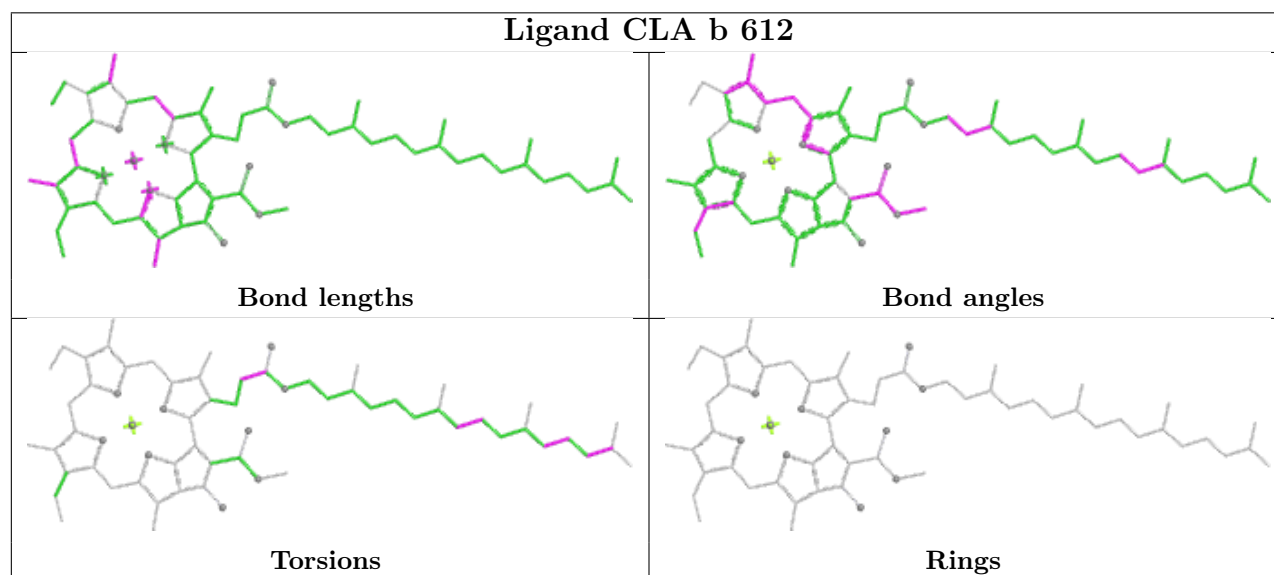
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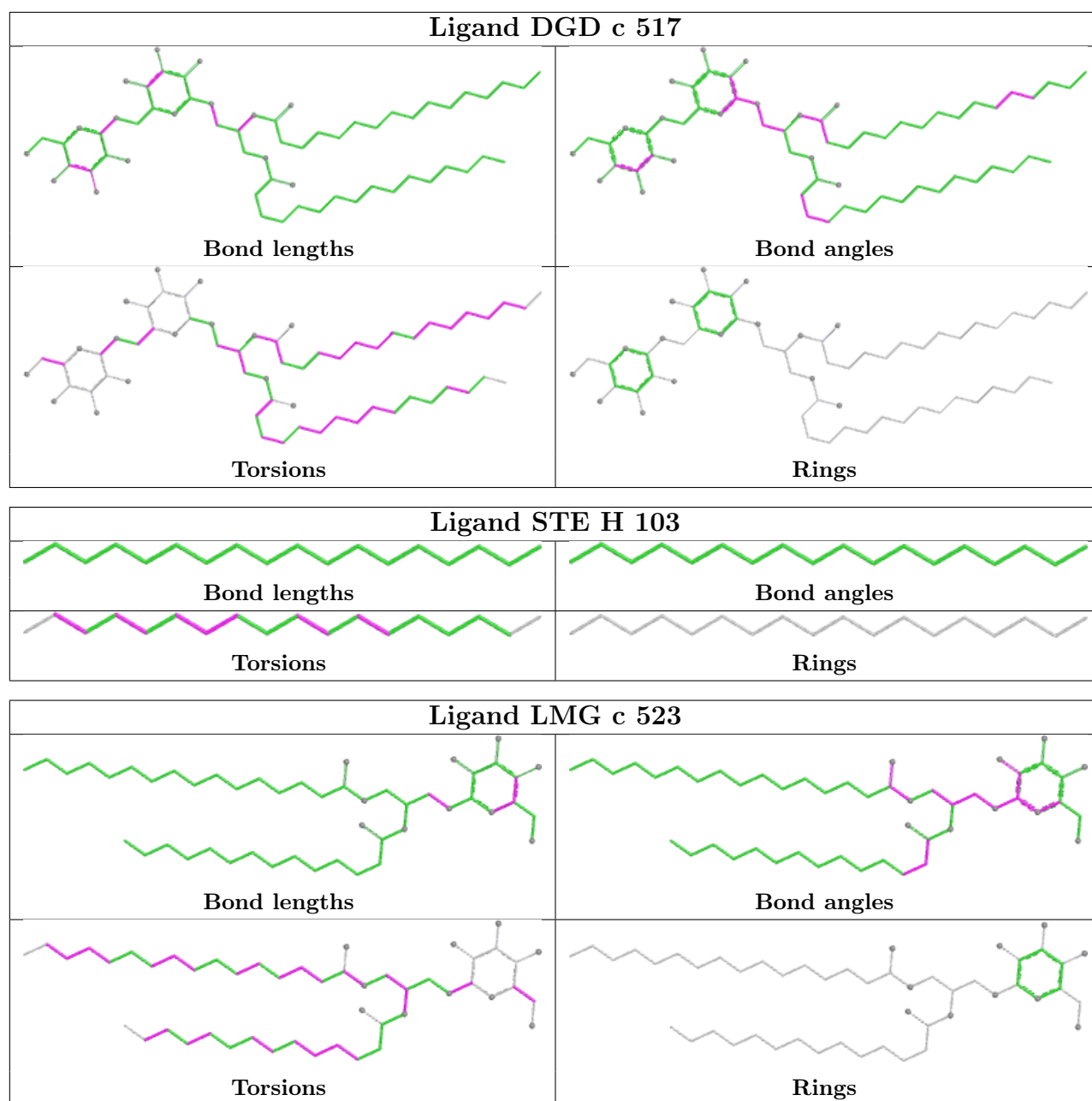
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | b | 610 | CLA | C13-C15-C16-C17 |
| 29 | C | 517 | DGD | C2B-C3B-C4B-C5B |

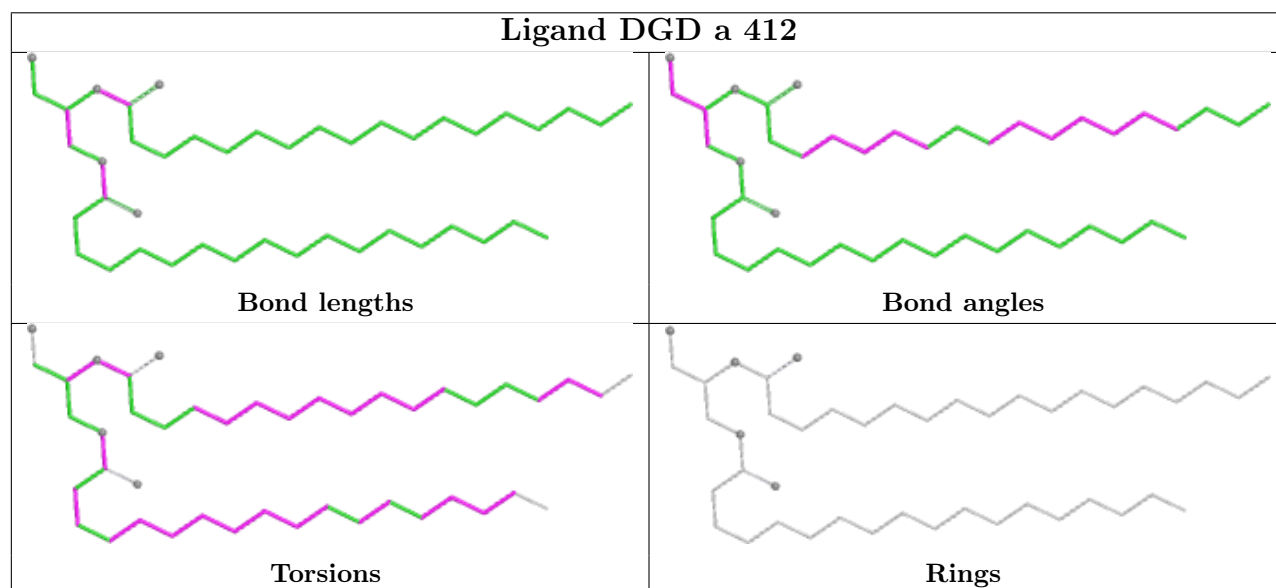
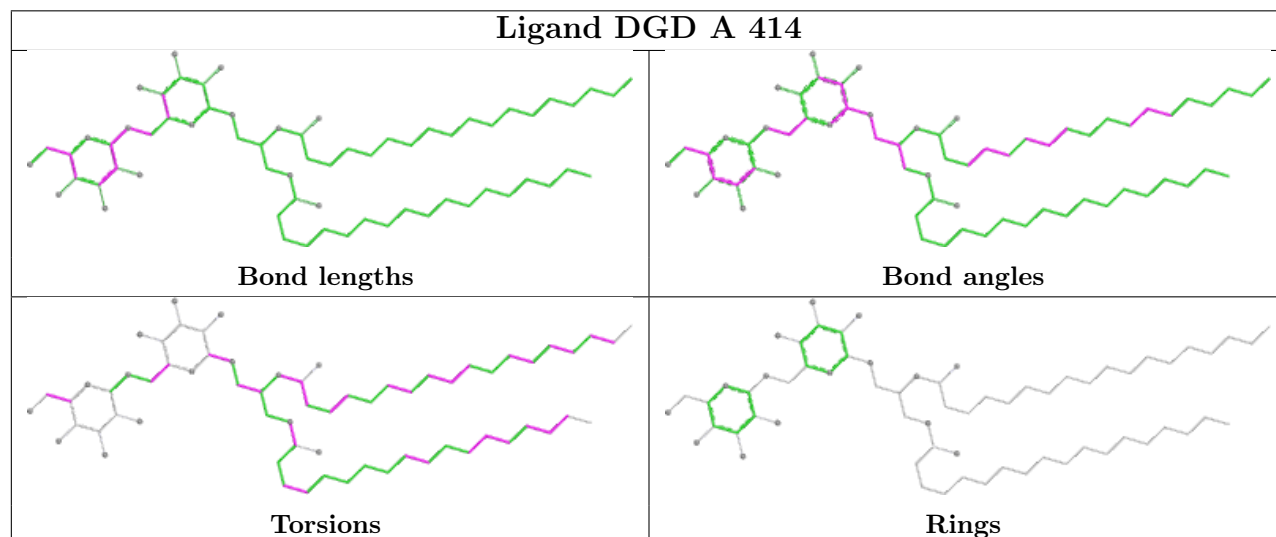
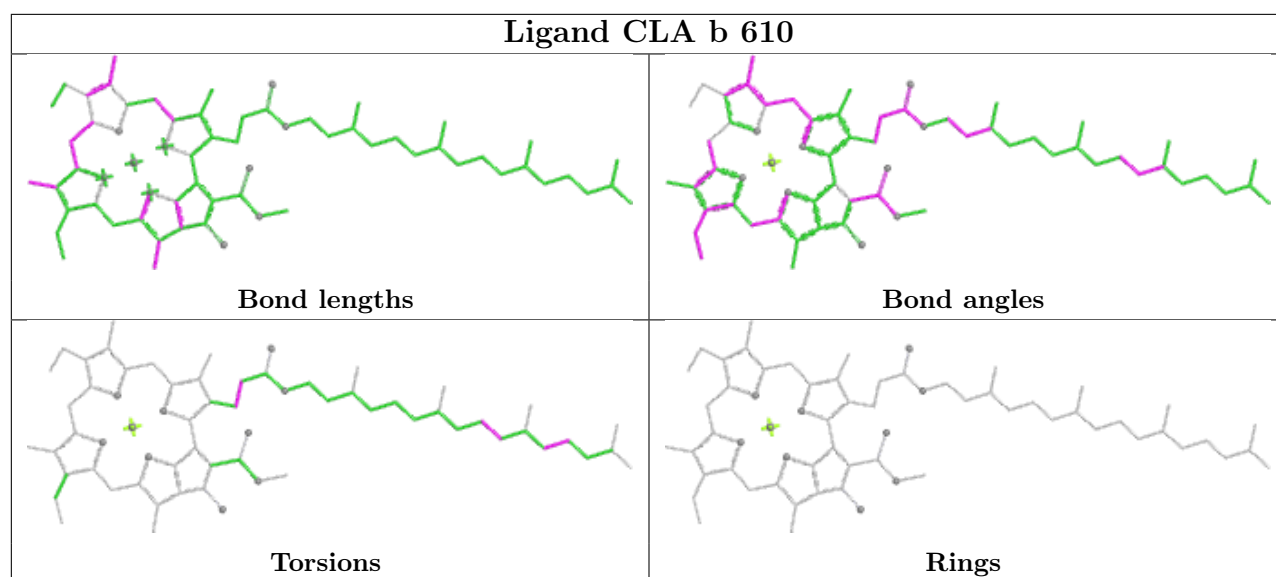
There are no ring outliers.

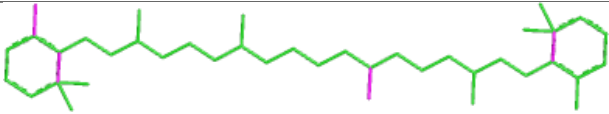
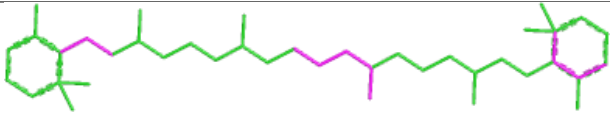
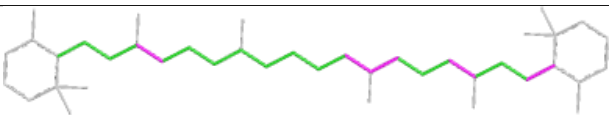
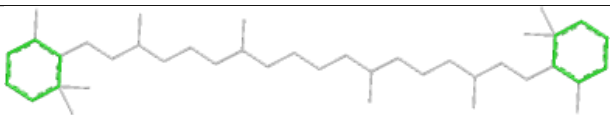
No monomer is involved in short contacts.



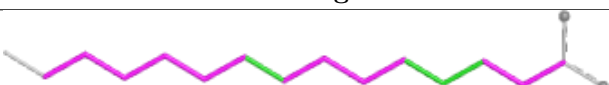
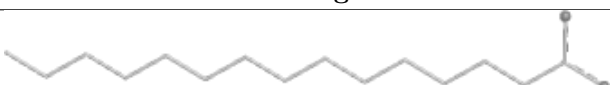
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

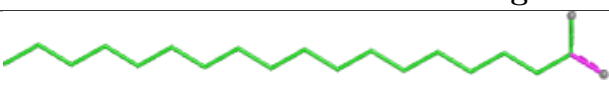
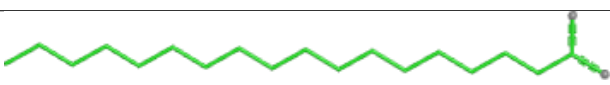
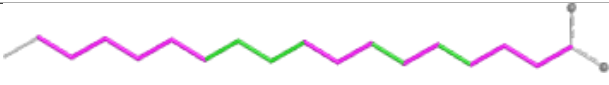
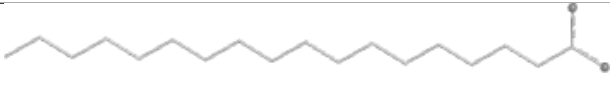


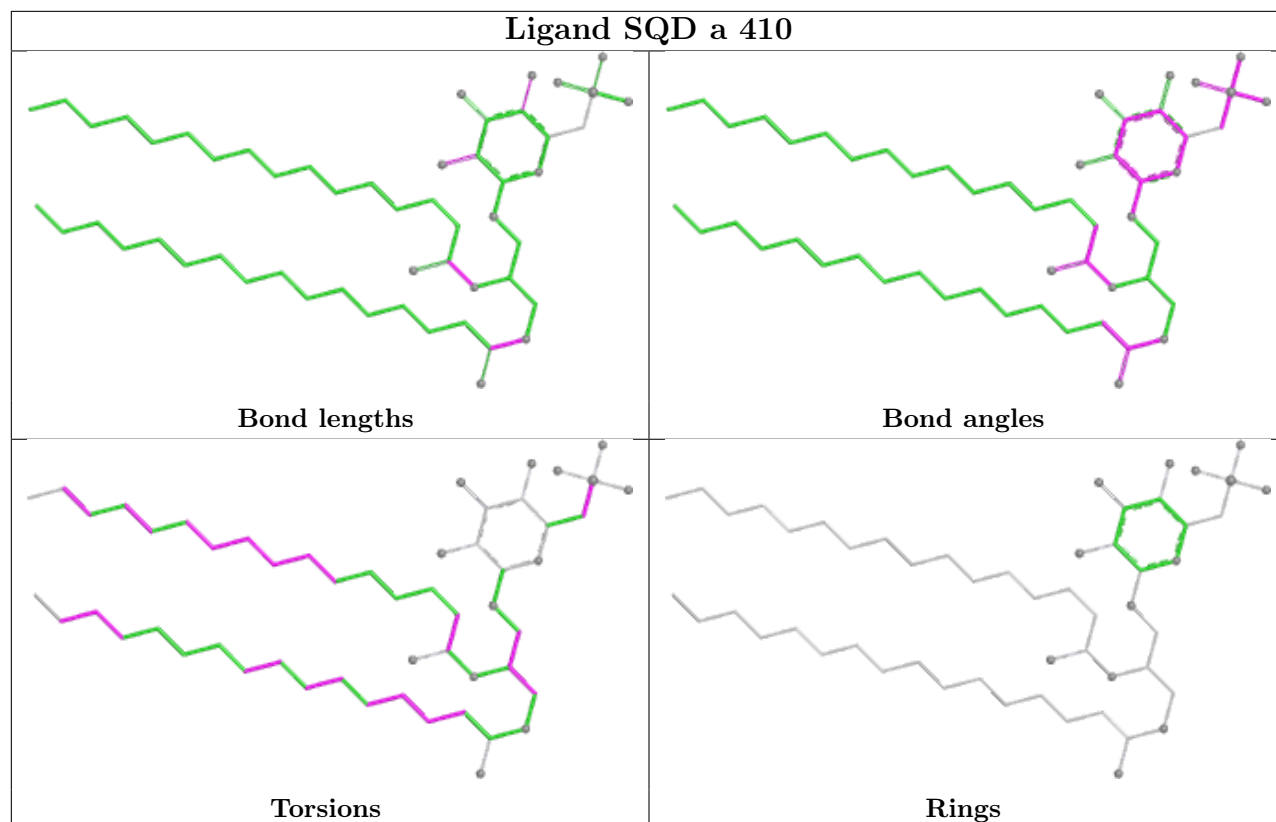


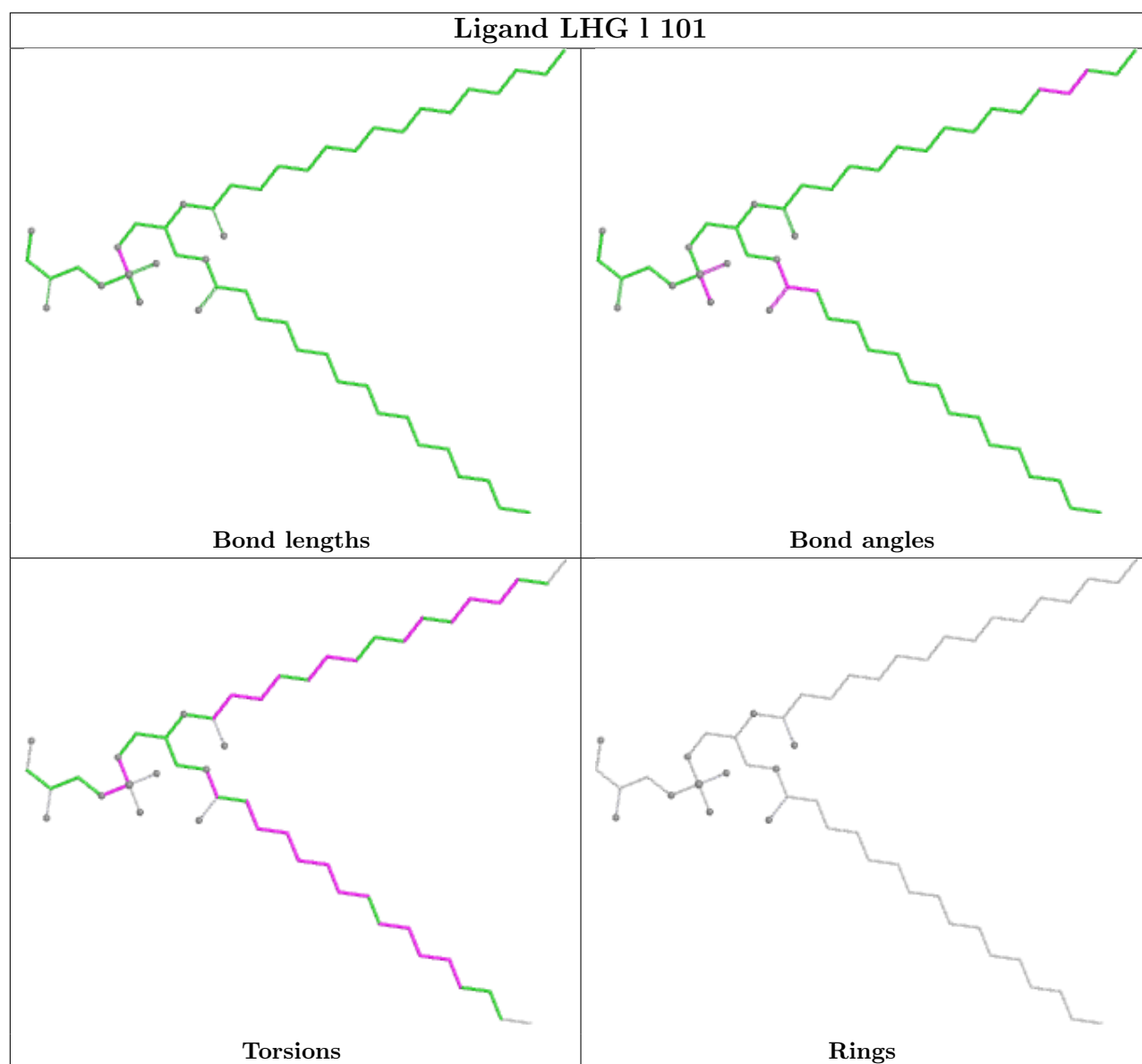


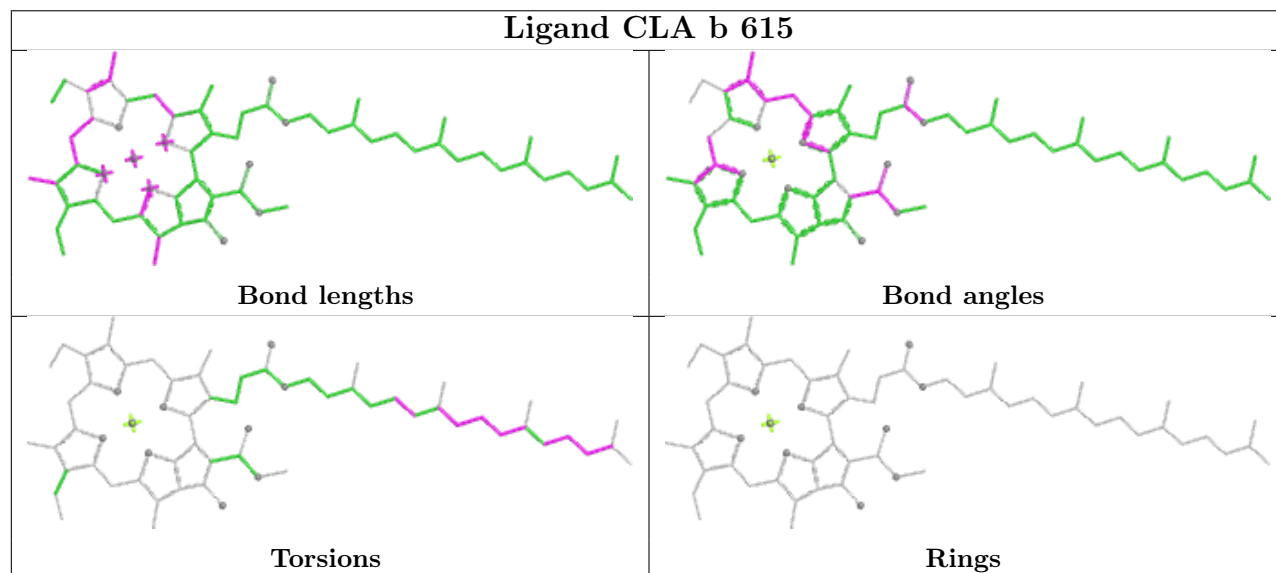
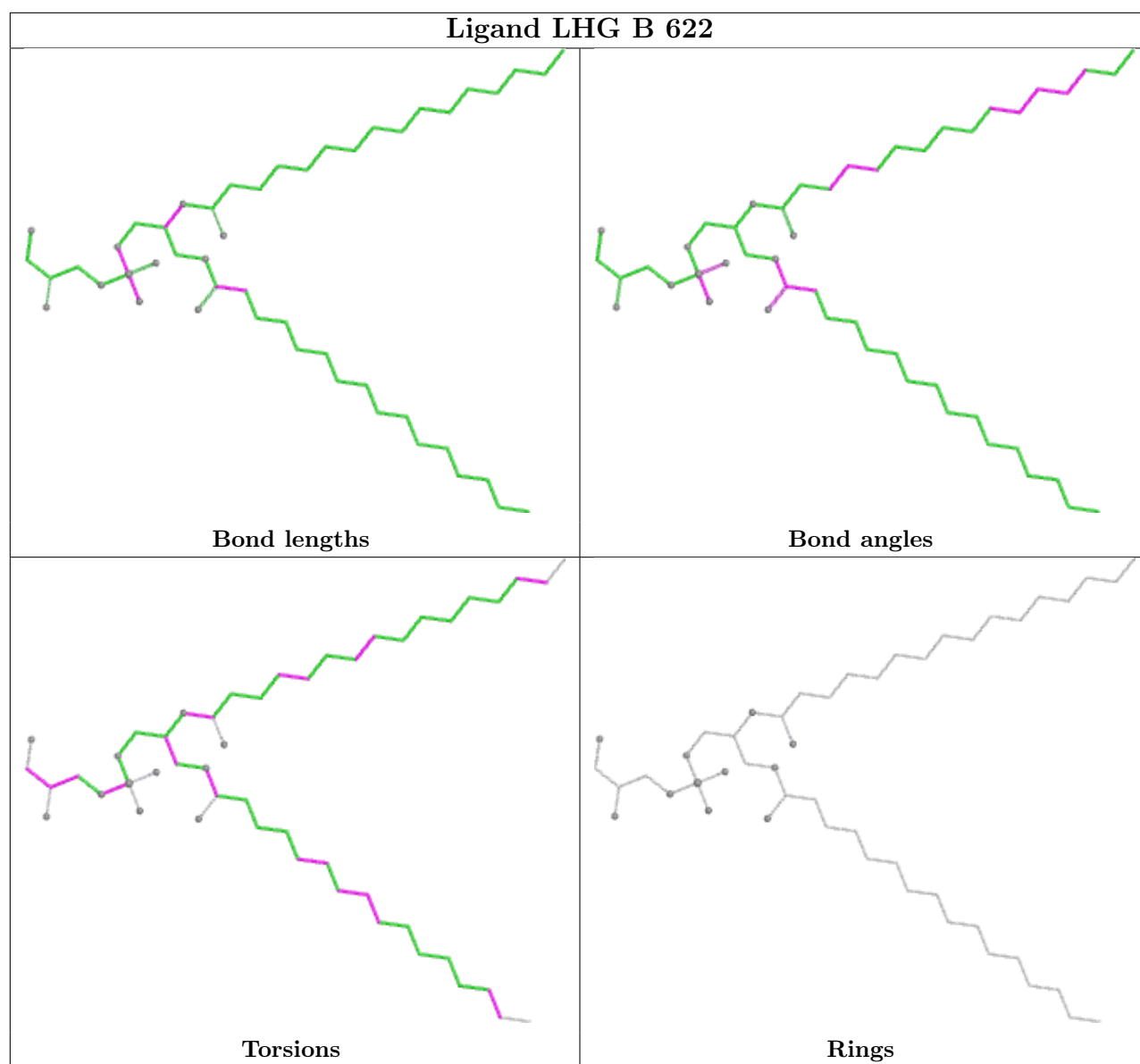
| Ligand BCR b 618 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

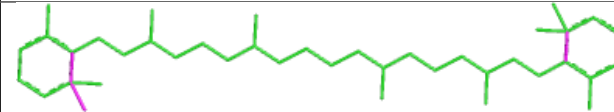
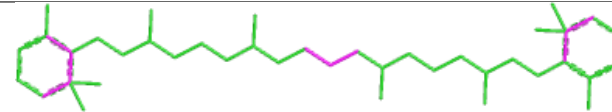
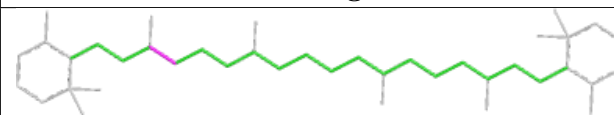
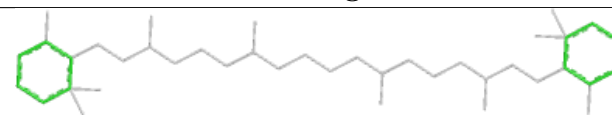
| Ligand STE d 413 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

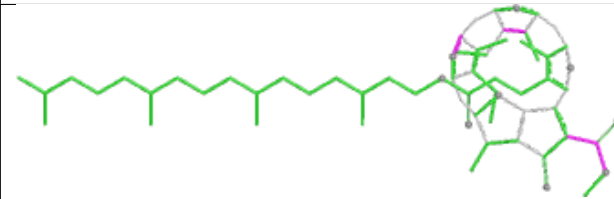
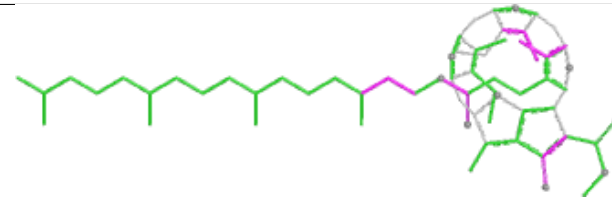
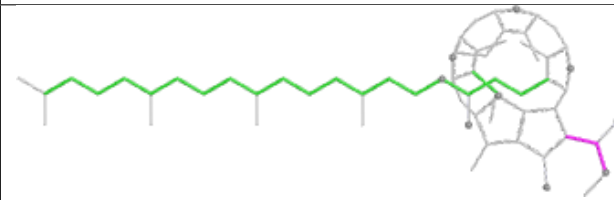
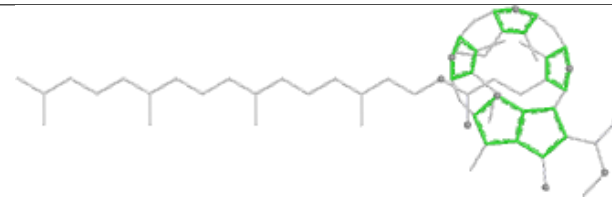
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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |







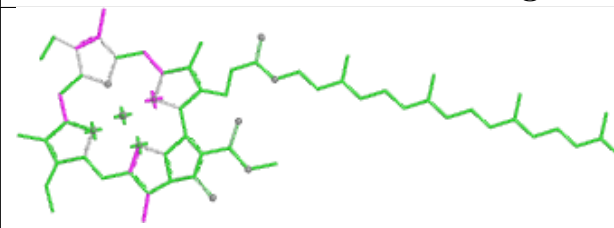
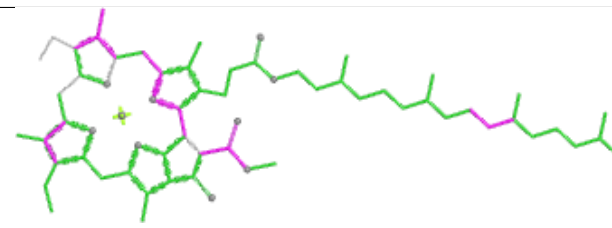
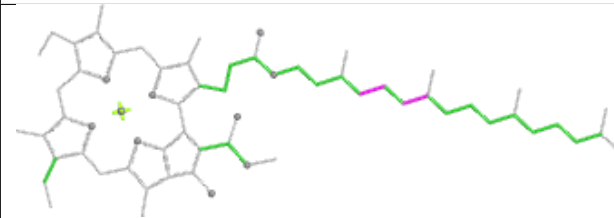
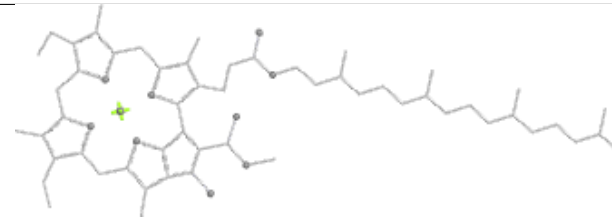


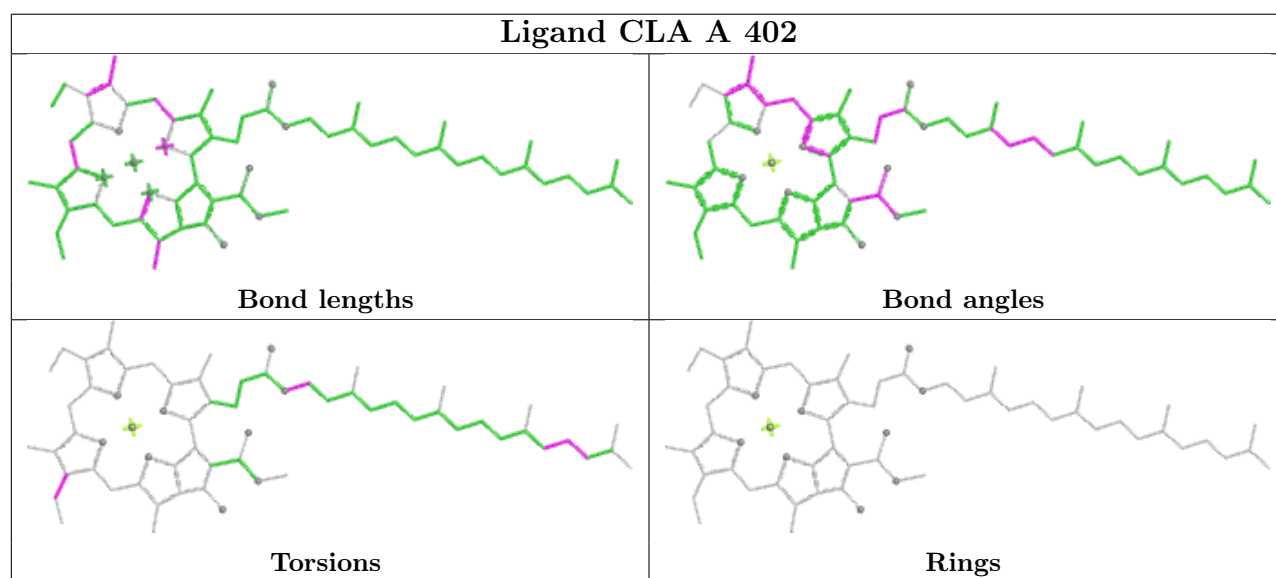
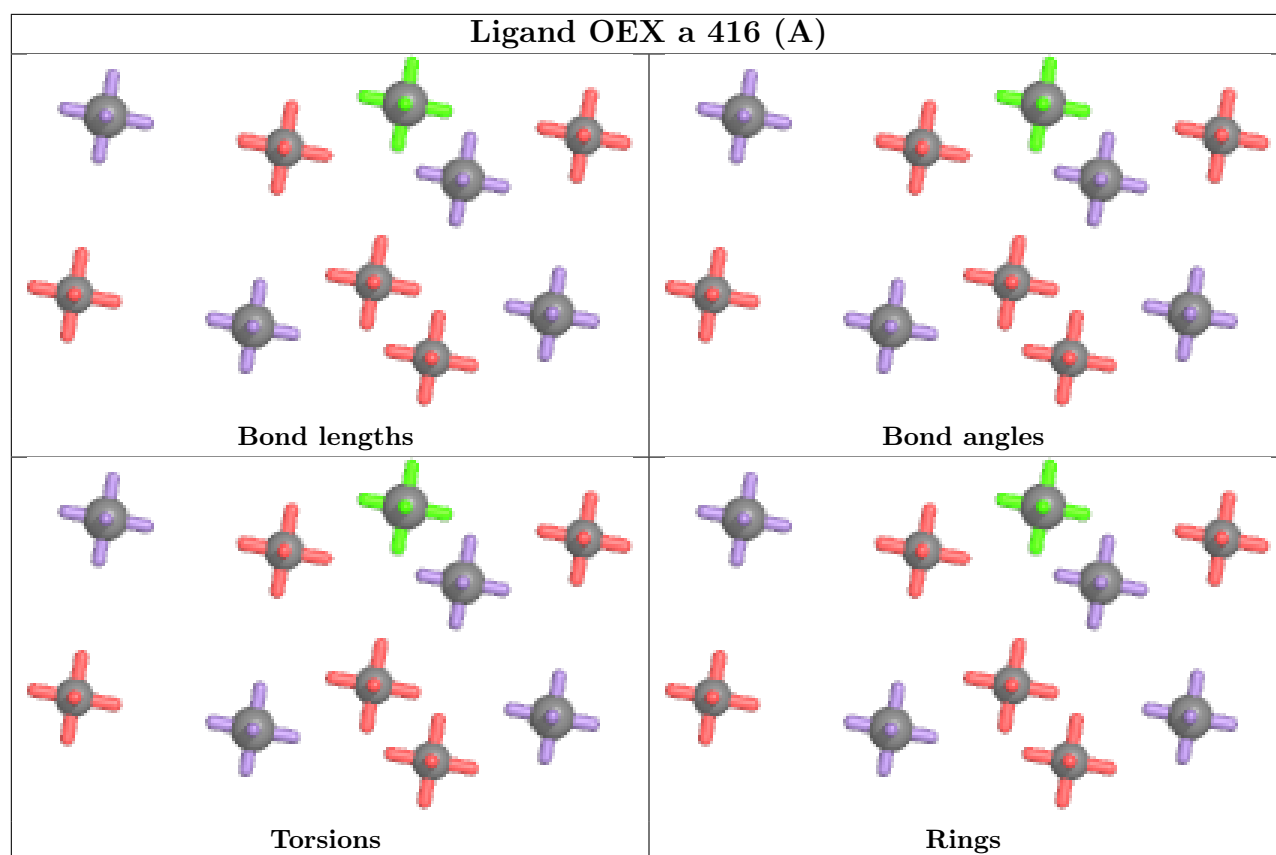


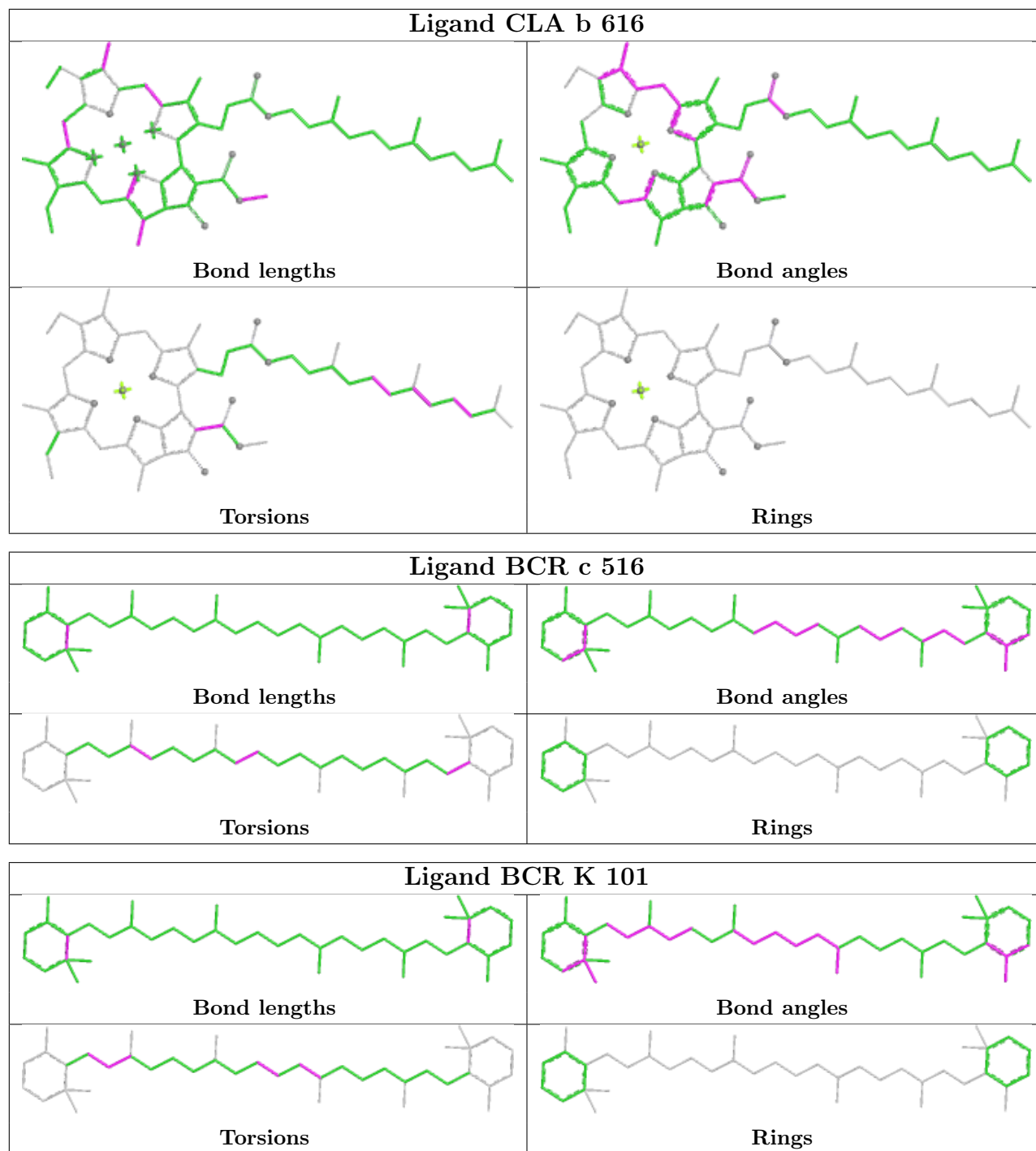
| Ligand BCR B 619 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

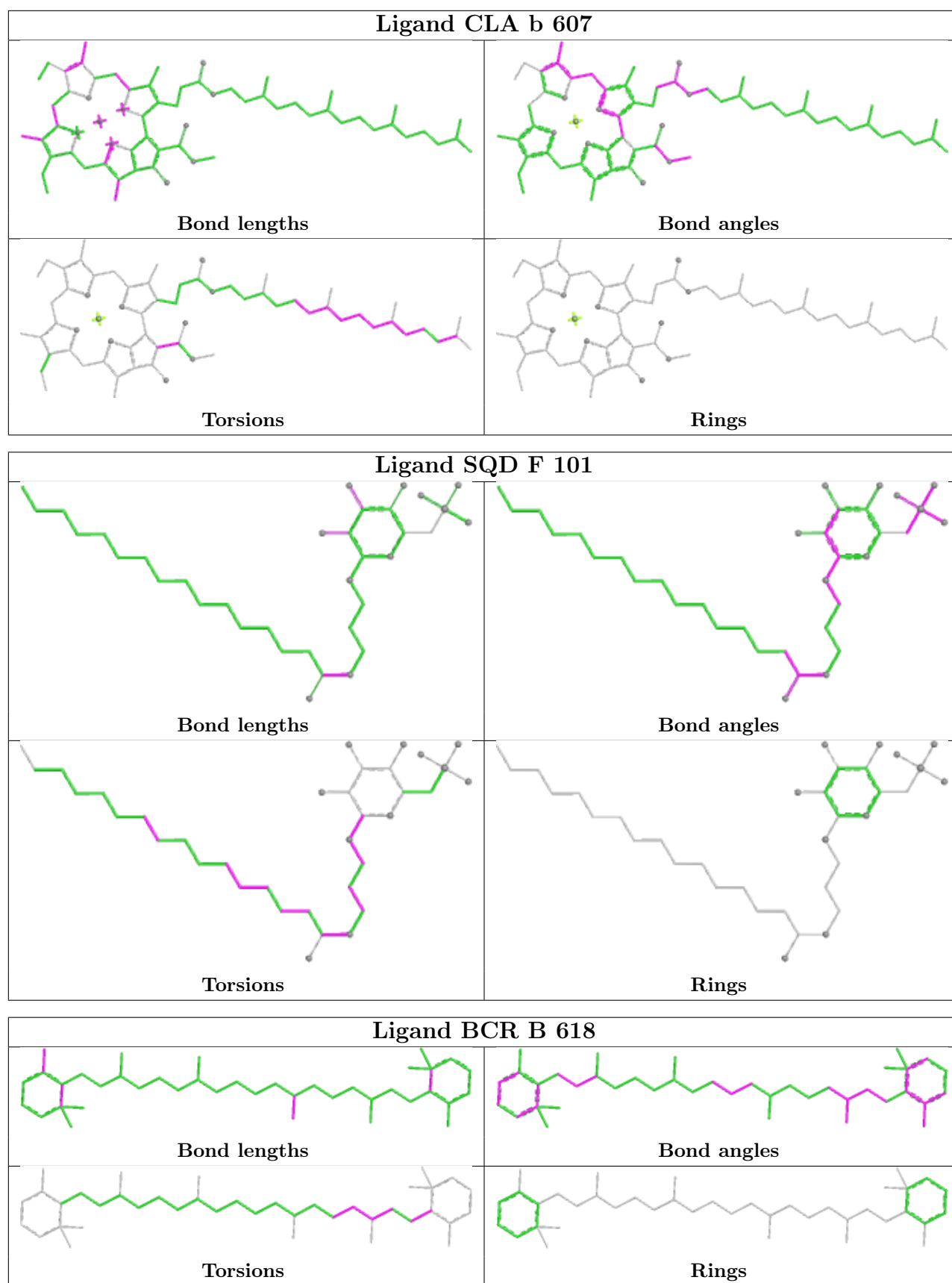
| Ligand PHO d 401 | |
|--|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

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

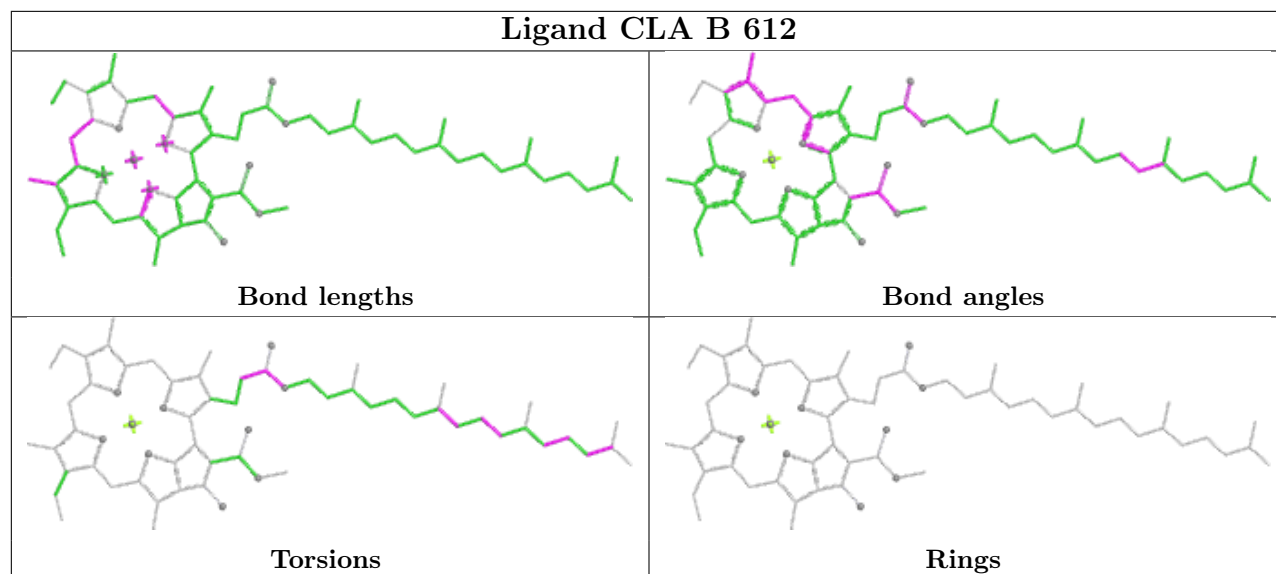
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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |



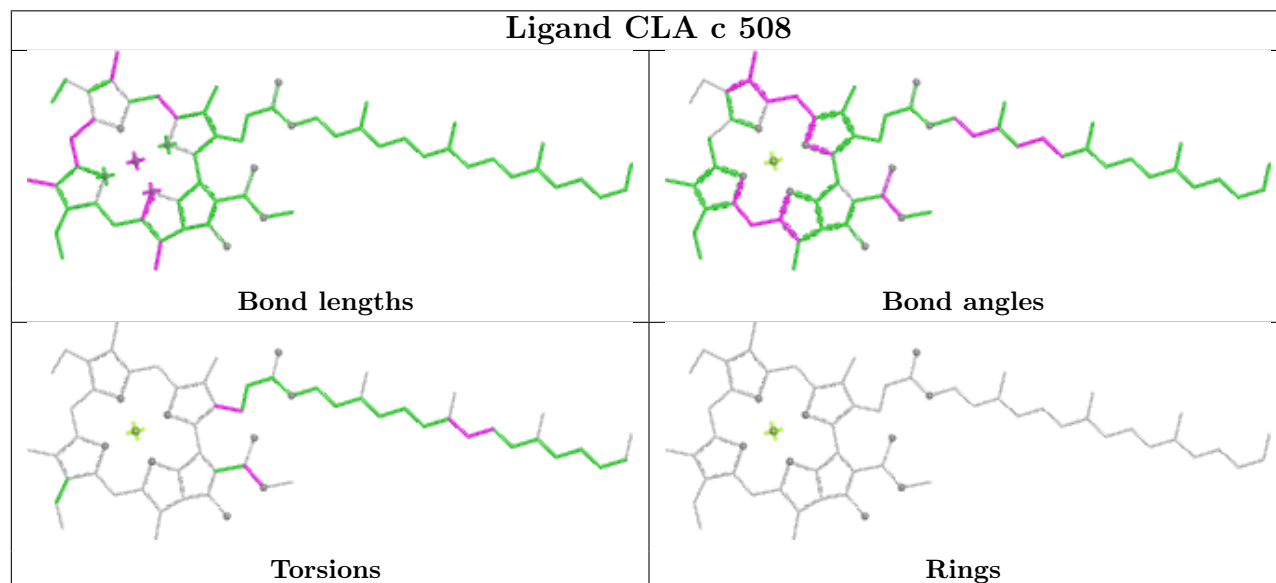




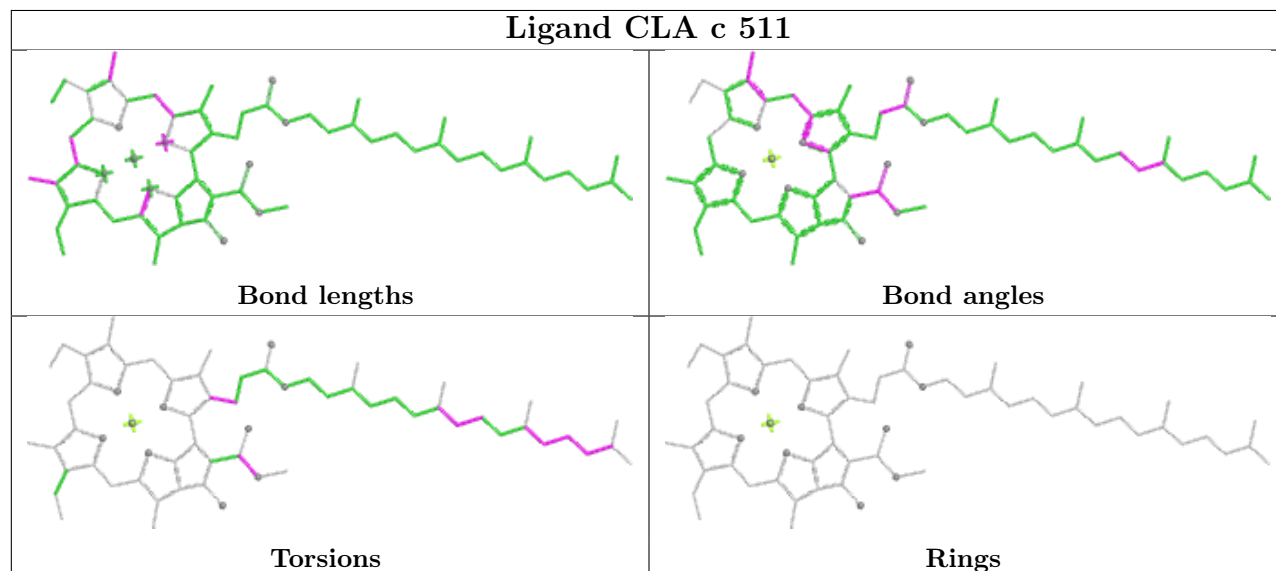
Ligand CLA B 612

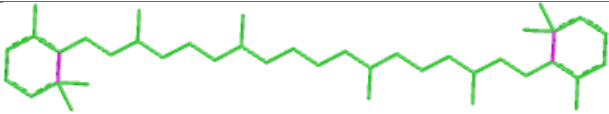
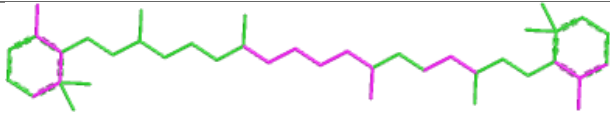
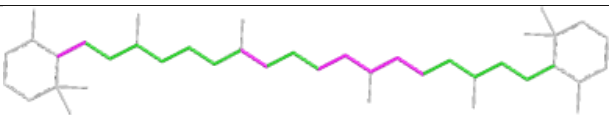
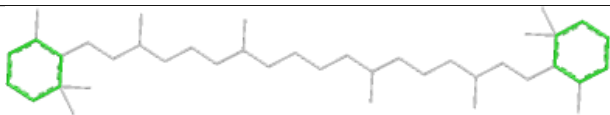






Ligand CLA c 508

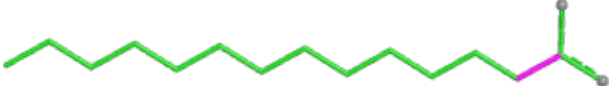
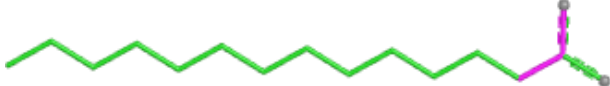




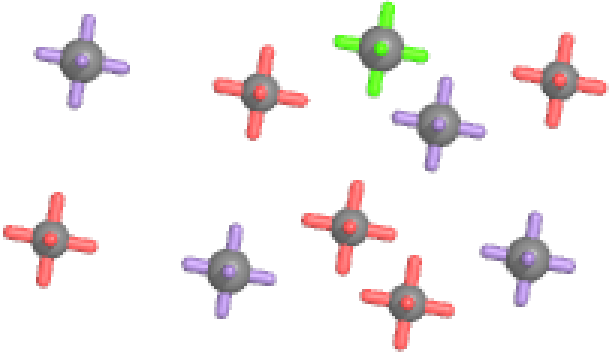
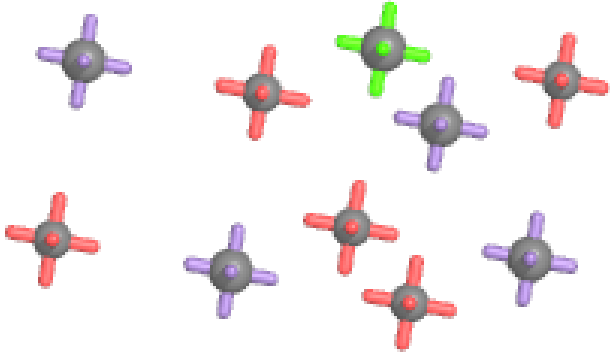
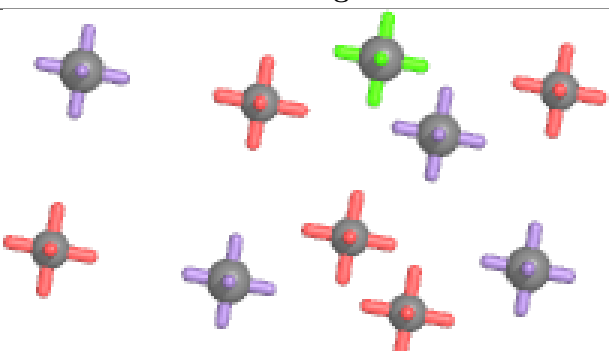
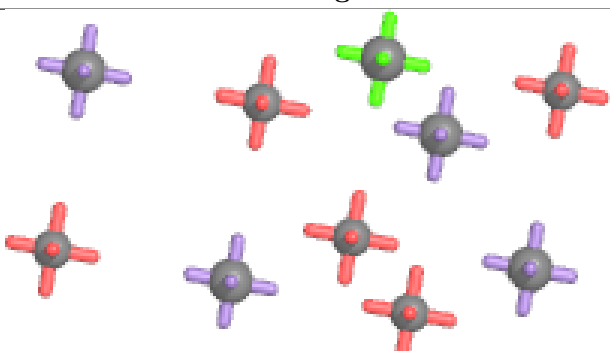
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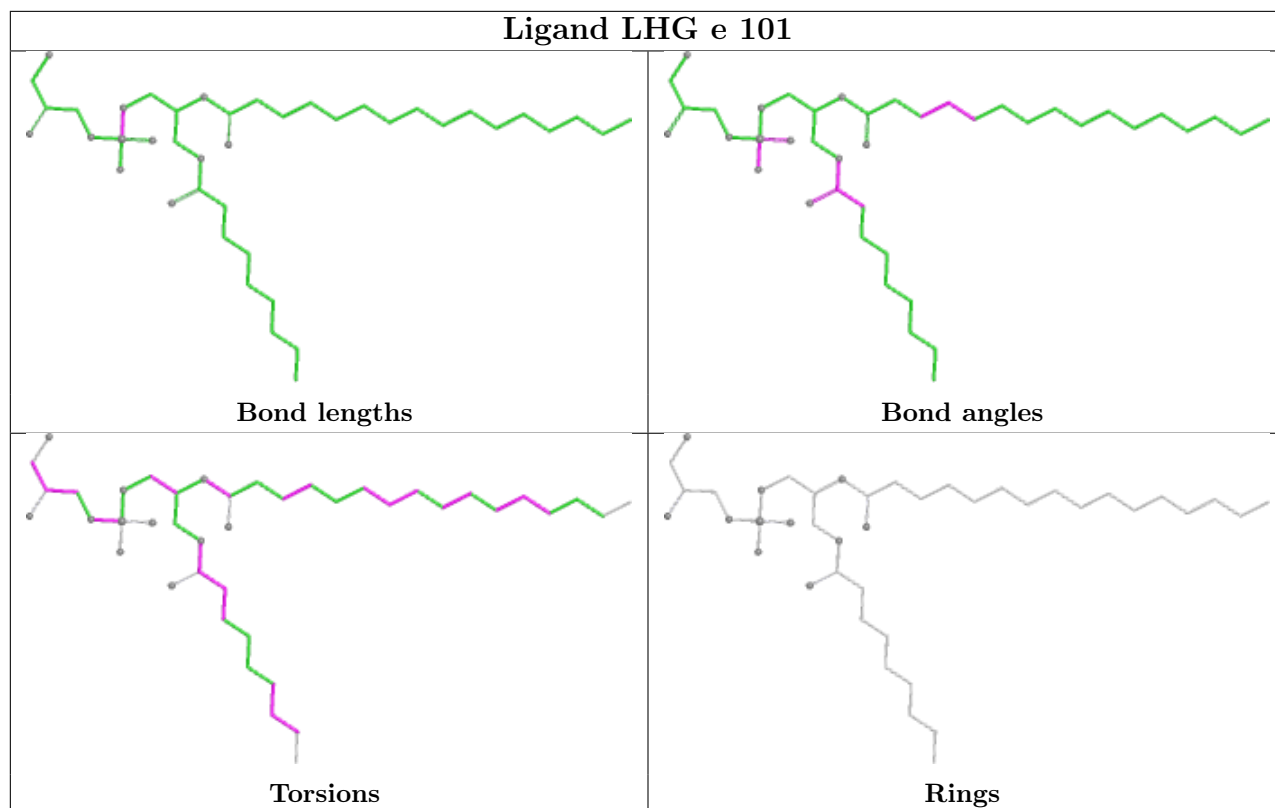
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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

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

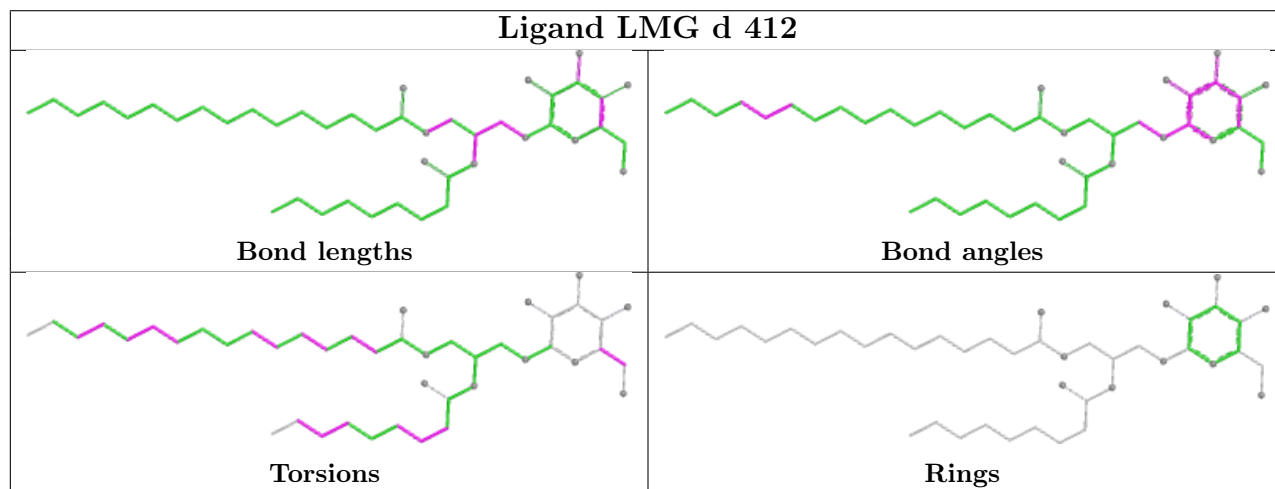
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|--|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

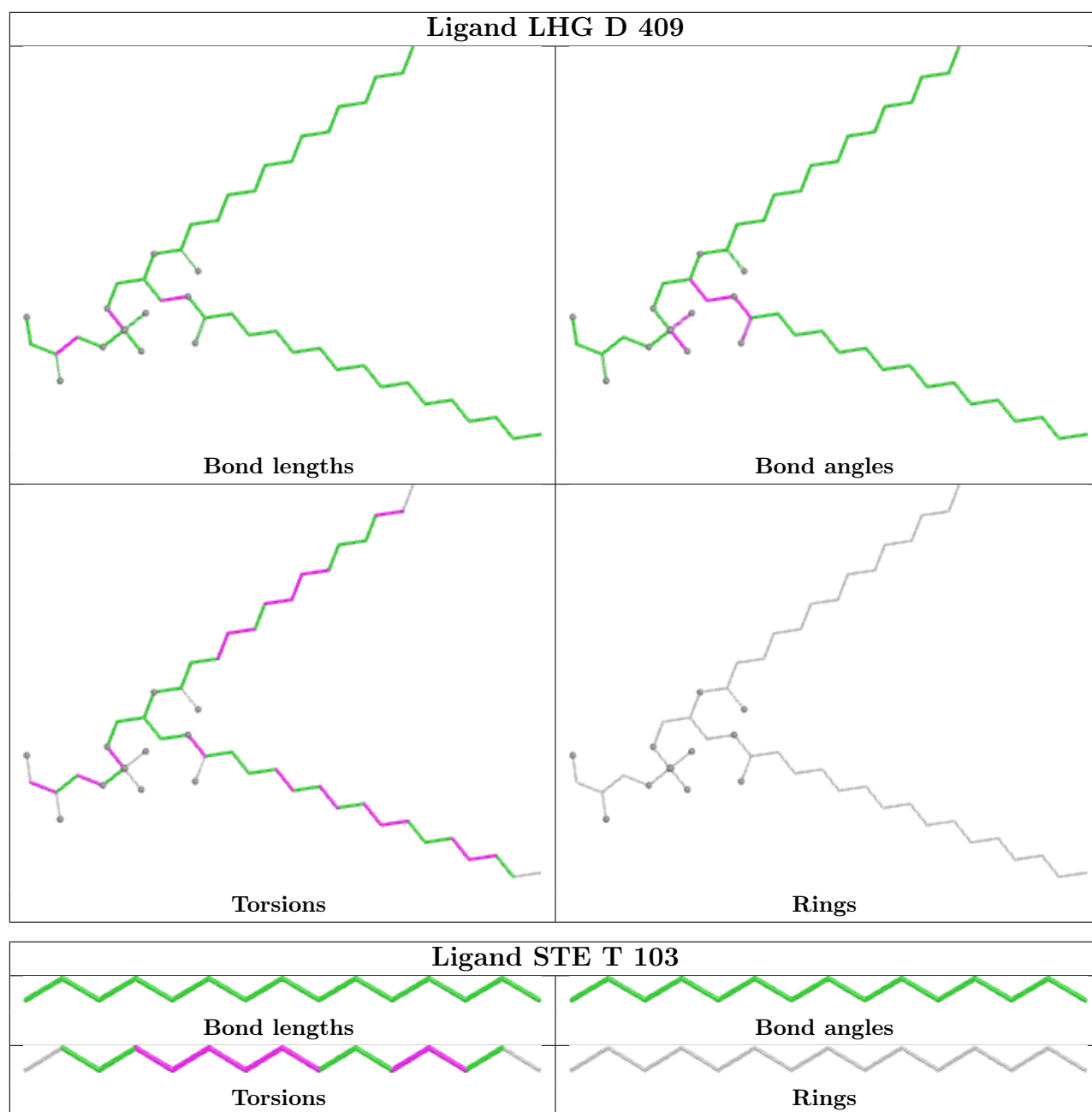
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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

Ligand LHG e 101

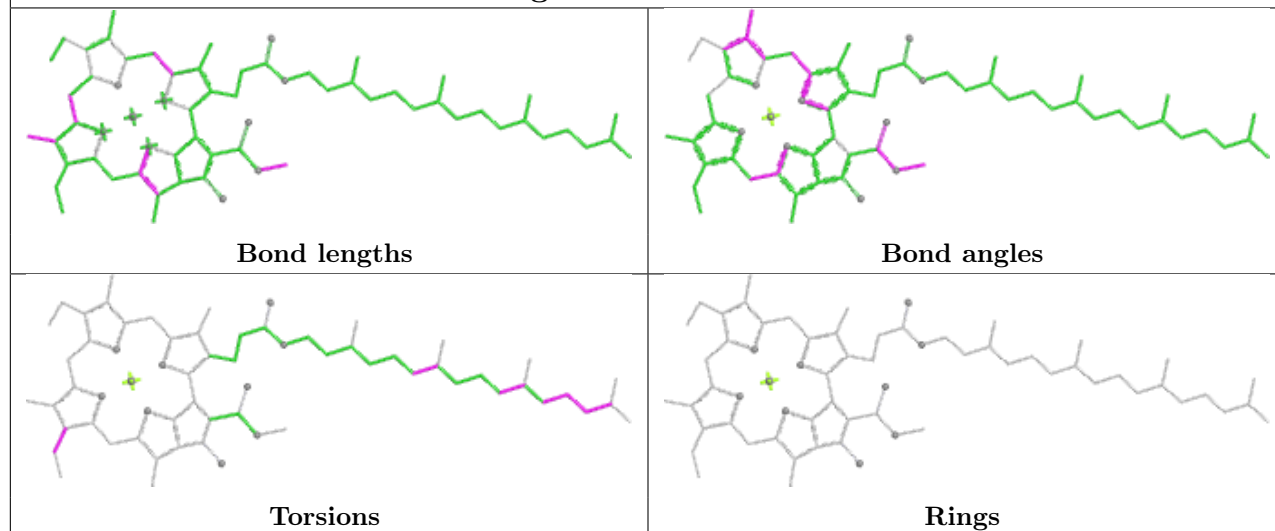


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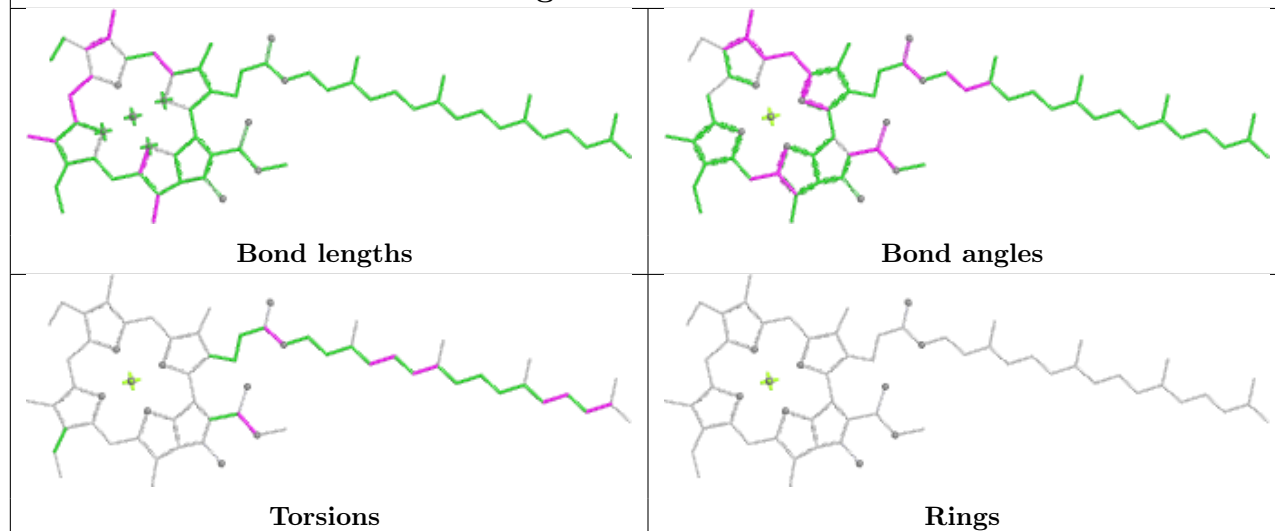




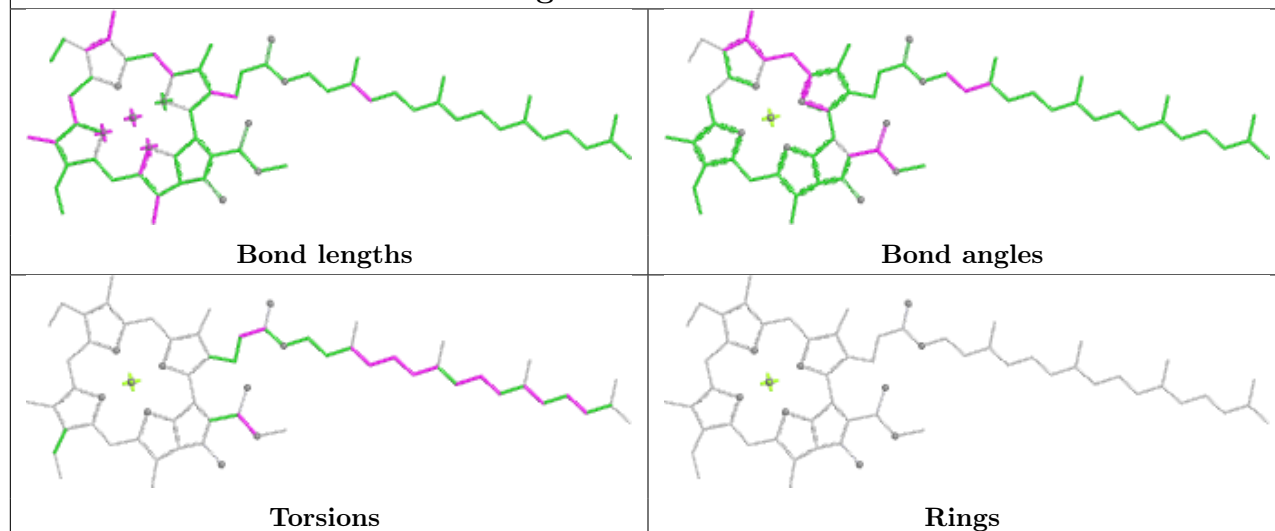
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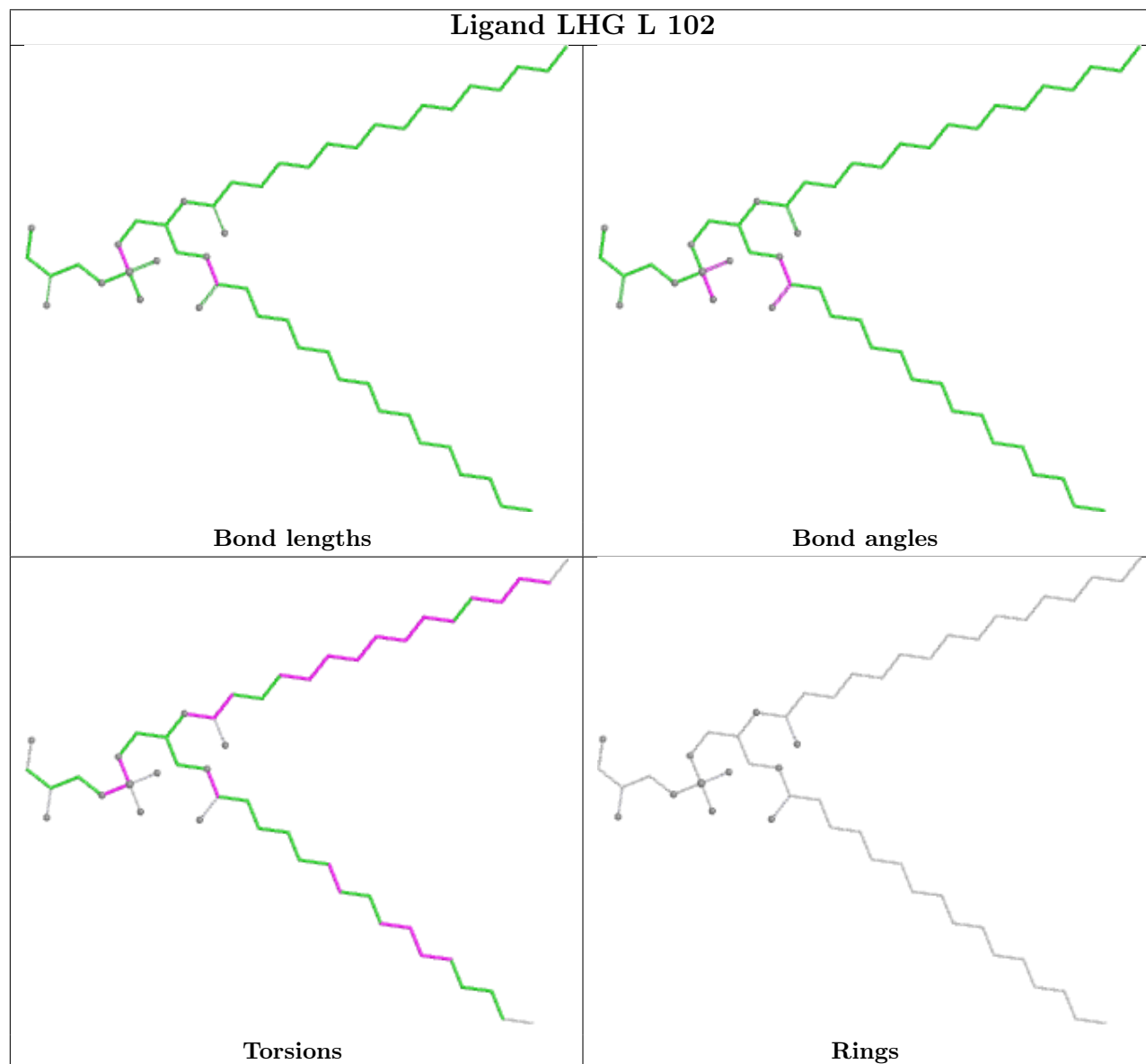
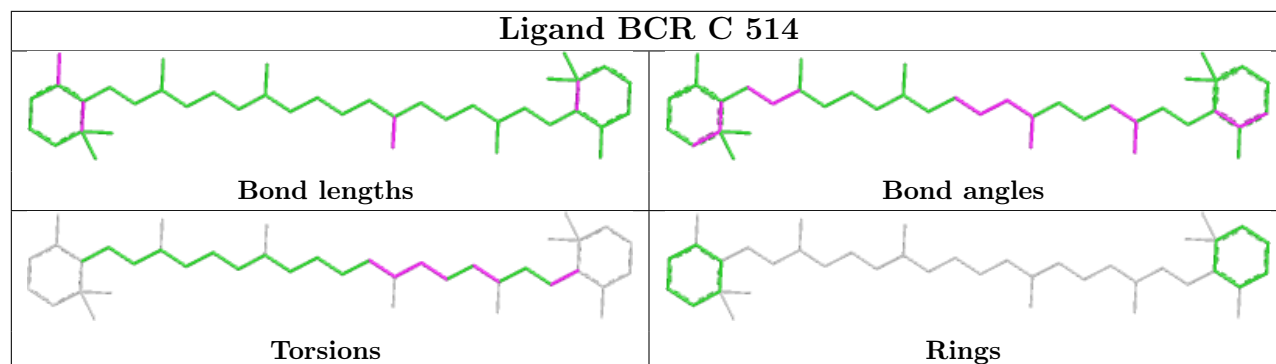


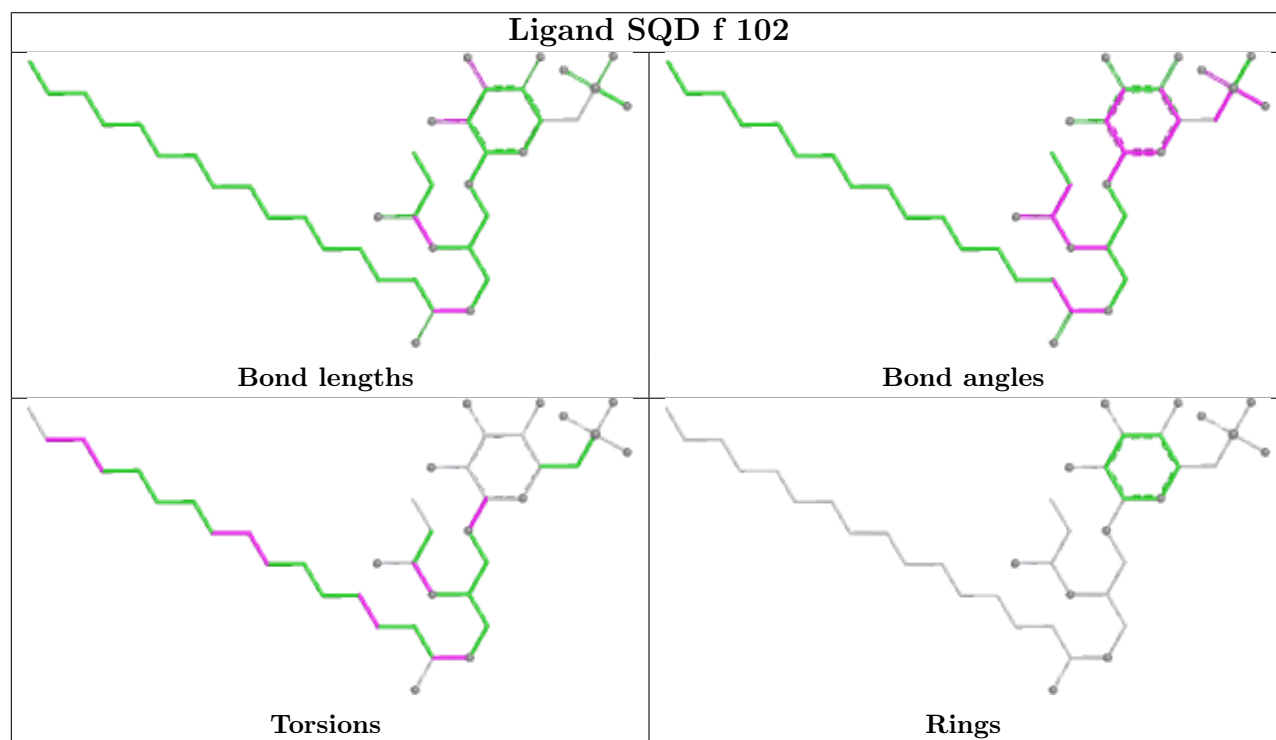
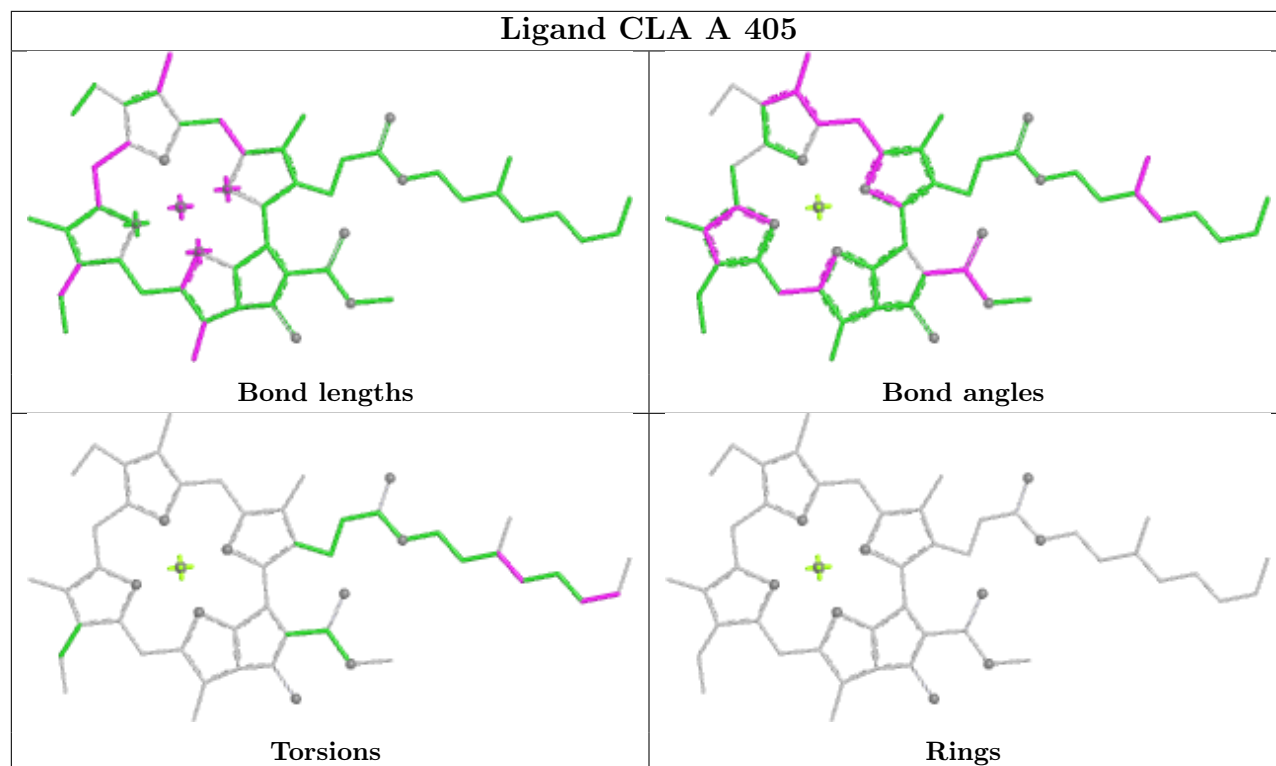
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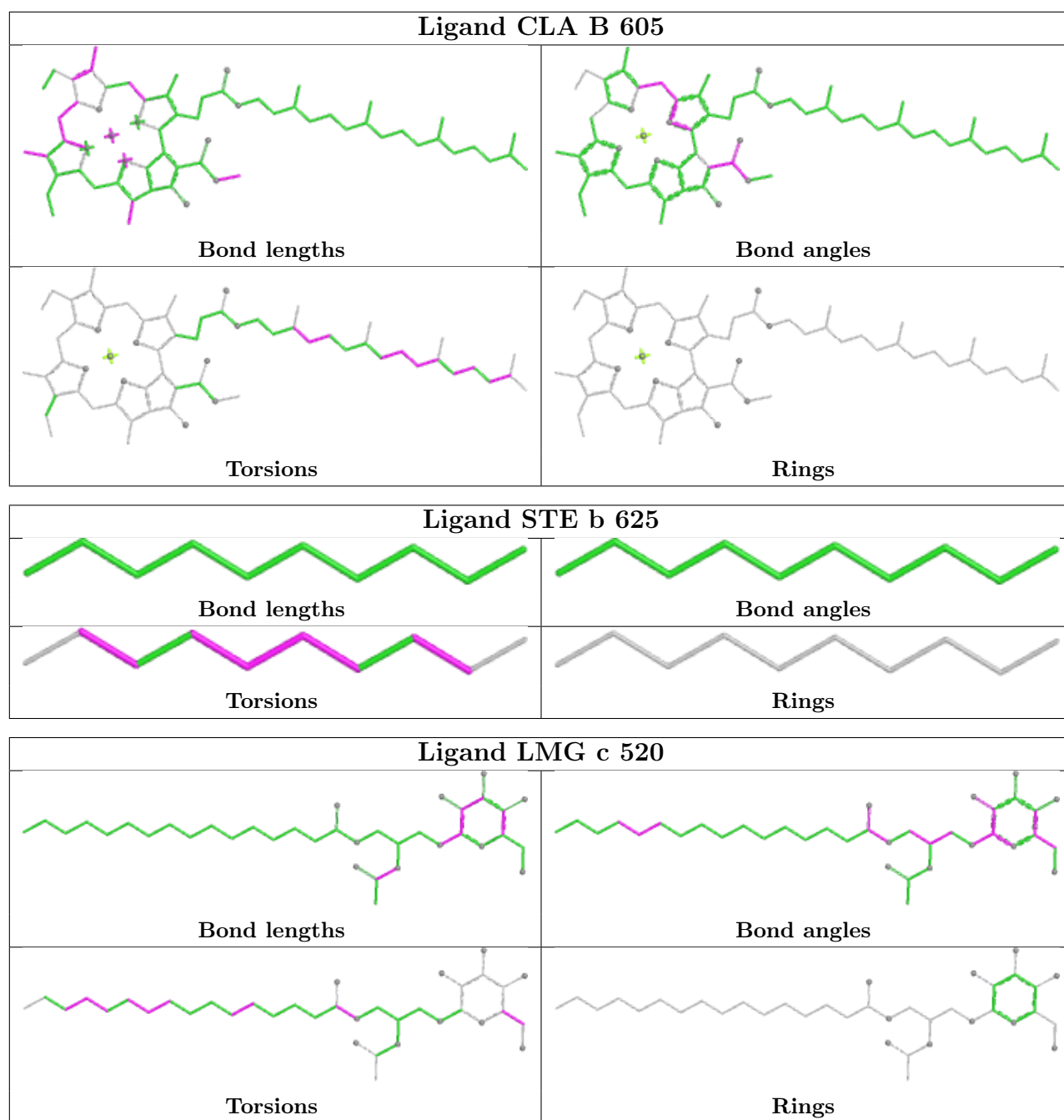


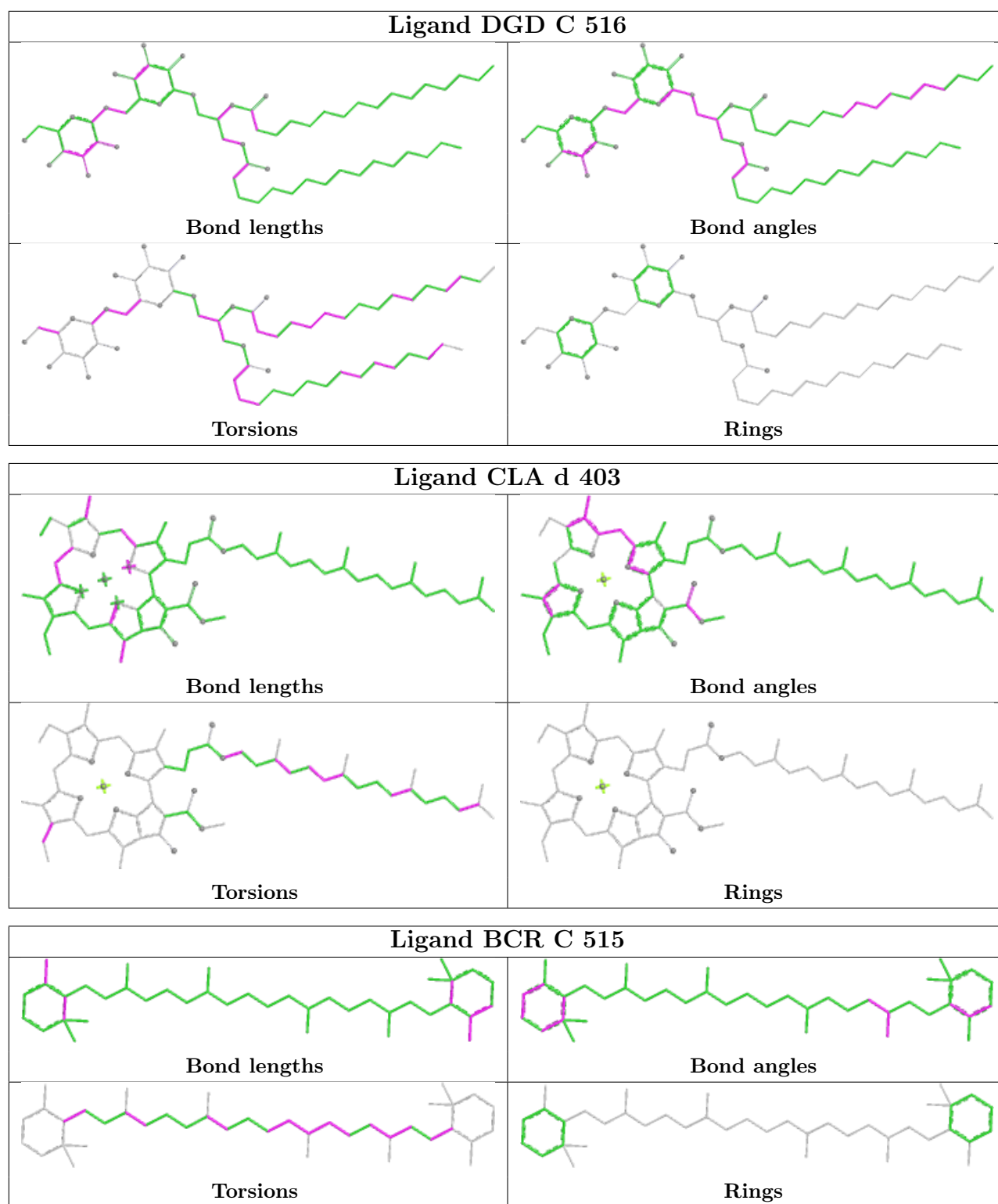
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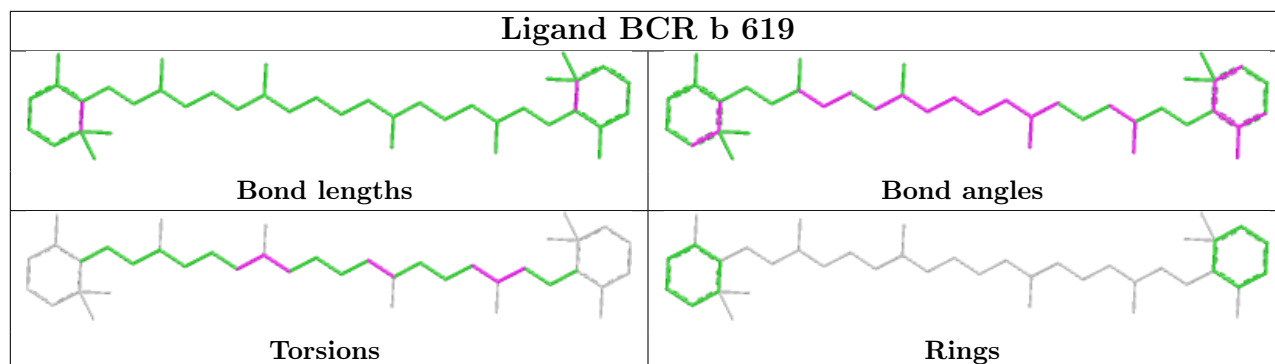




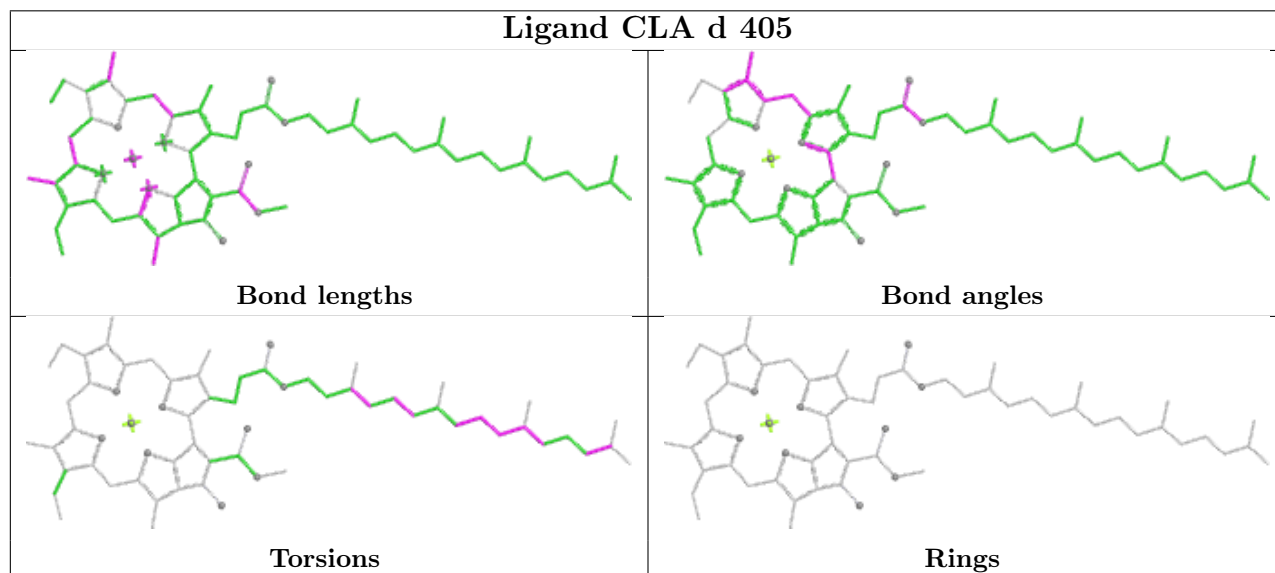




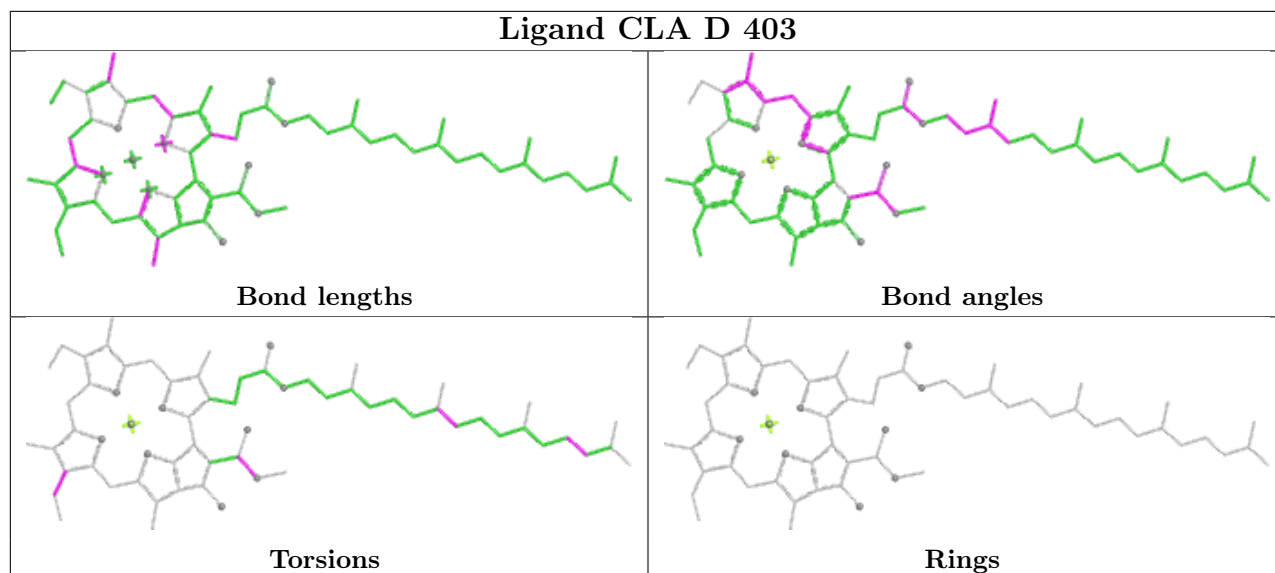
Ligand BCR b 619



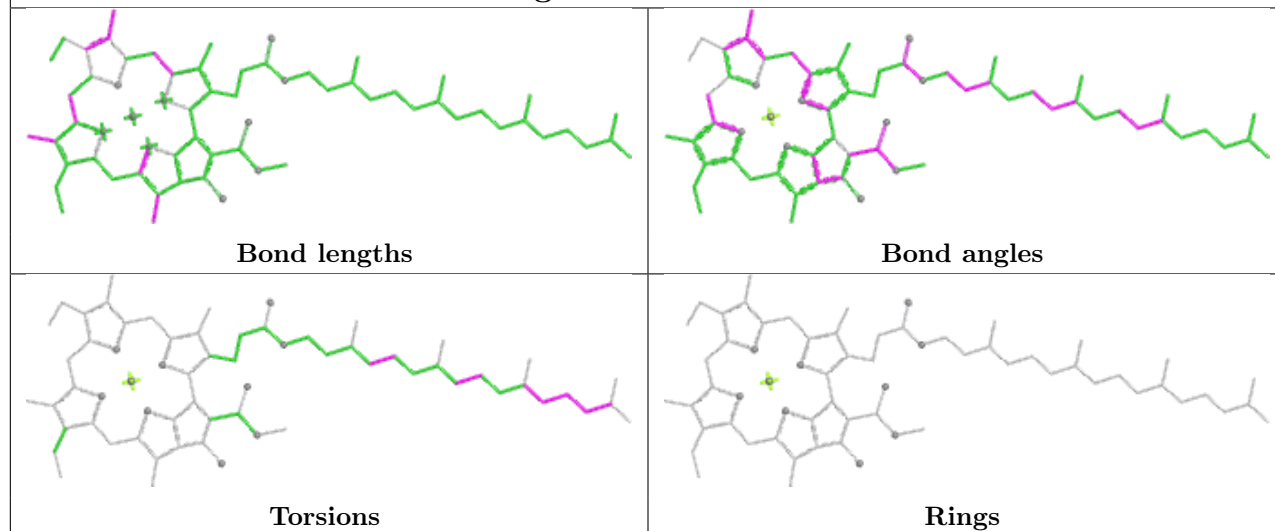
Ligand CLA d 405



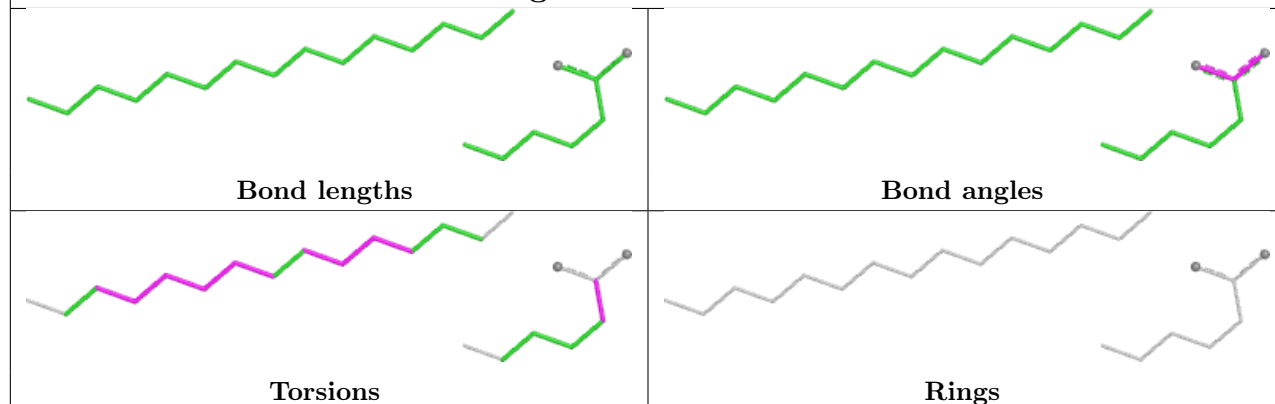
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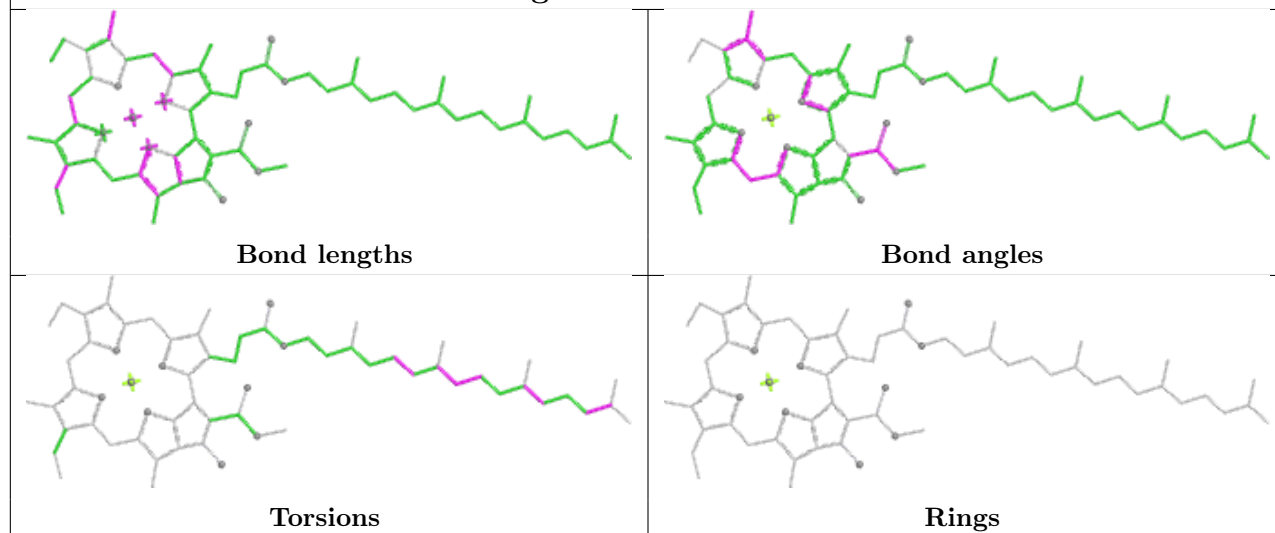
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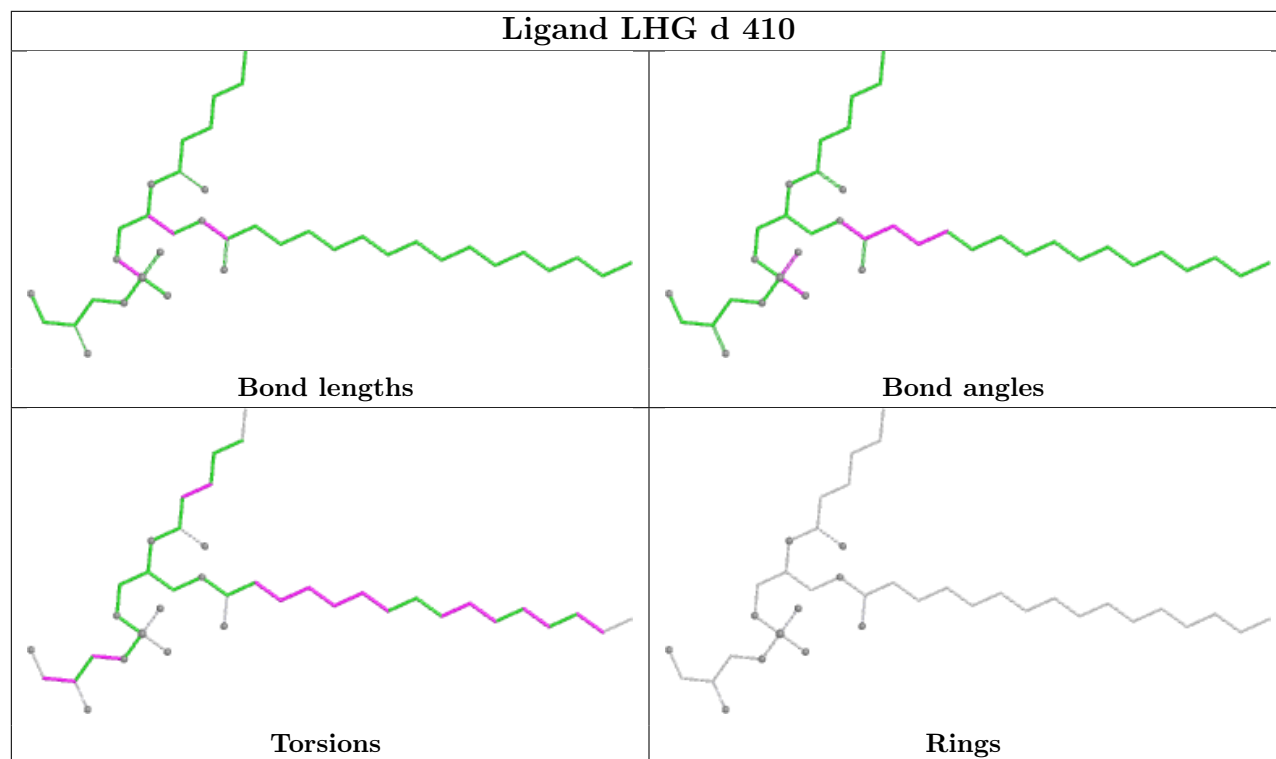
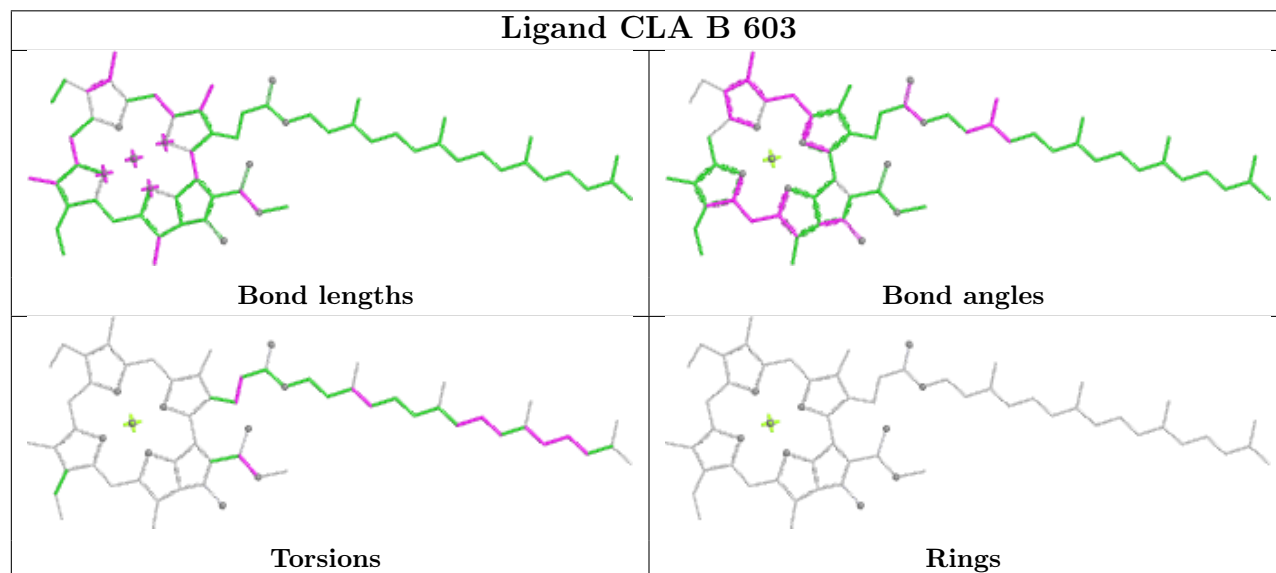
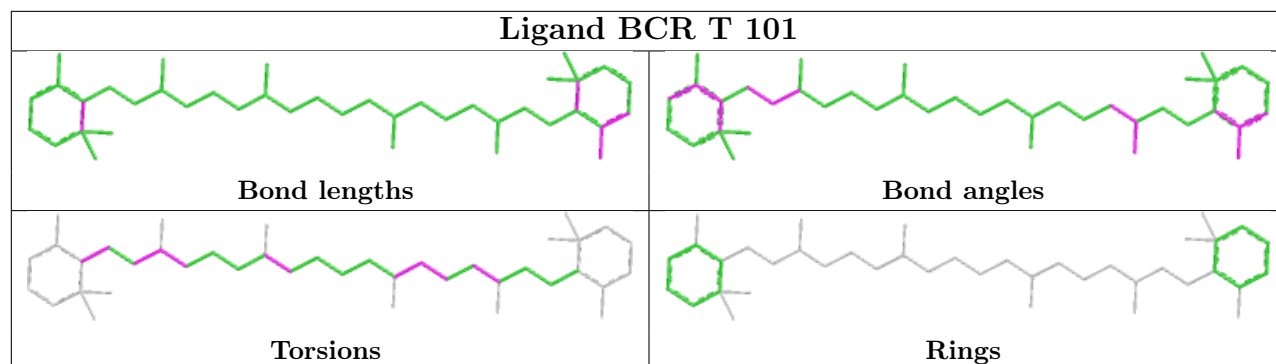


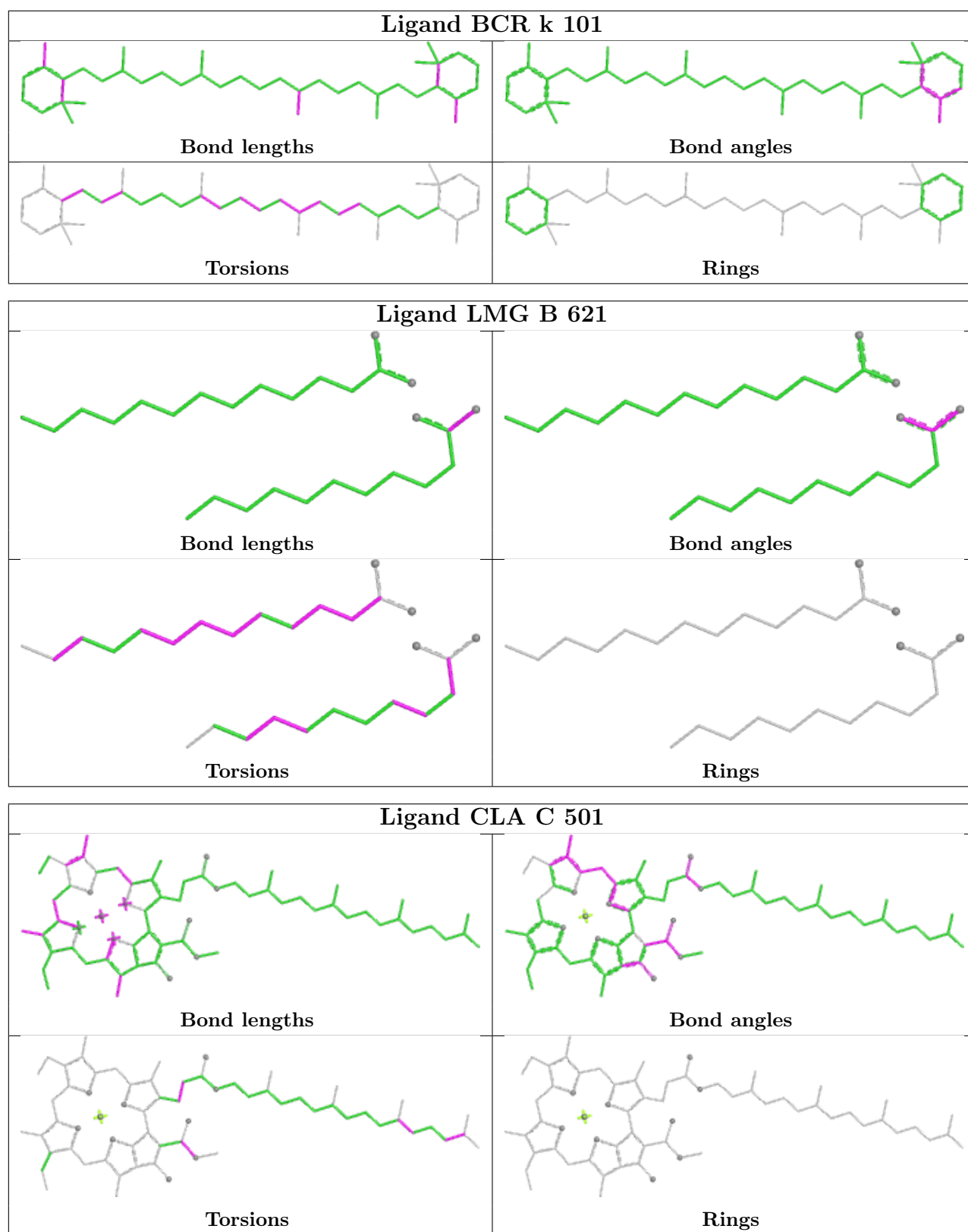
Ligand LMG d 411

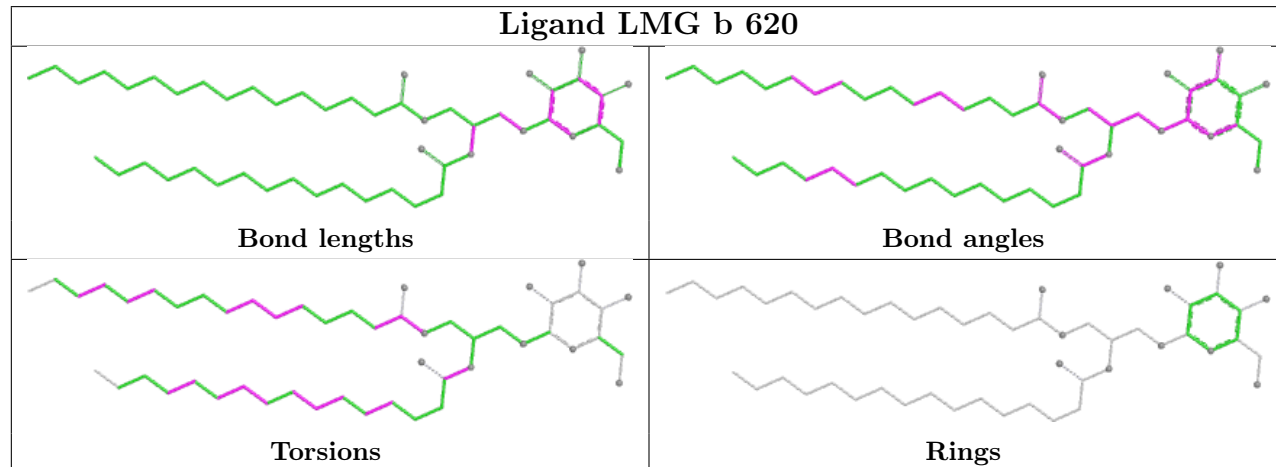
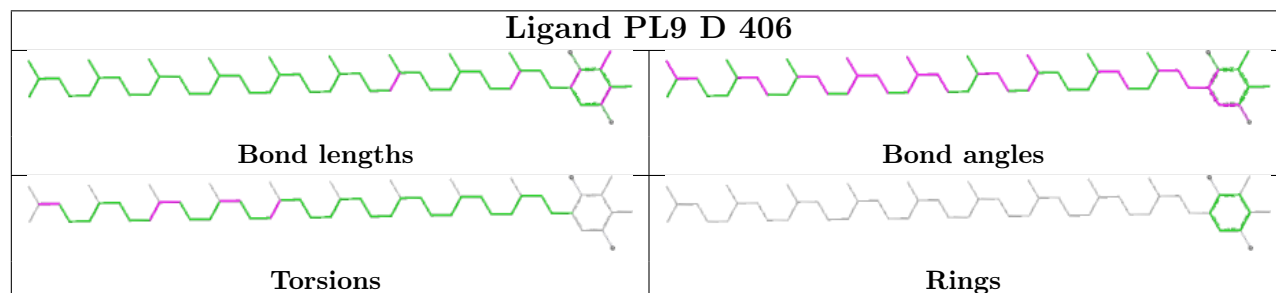
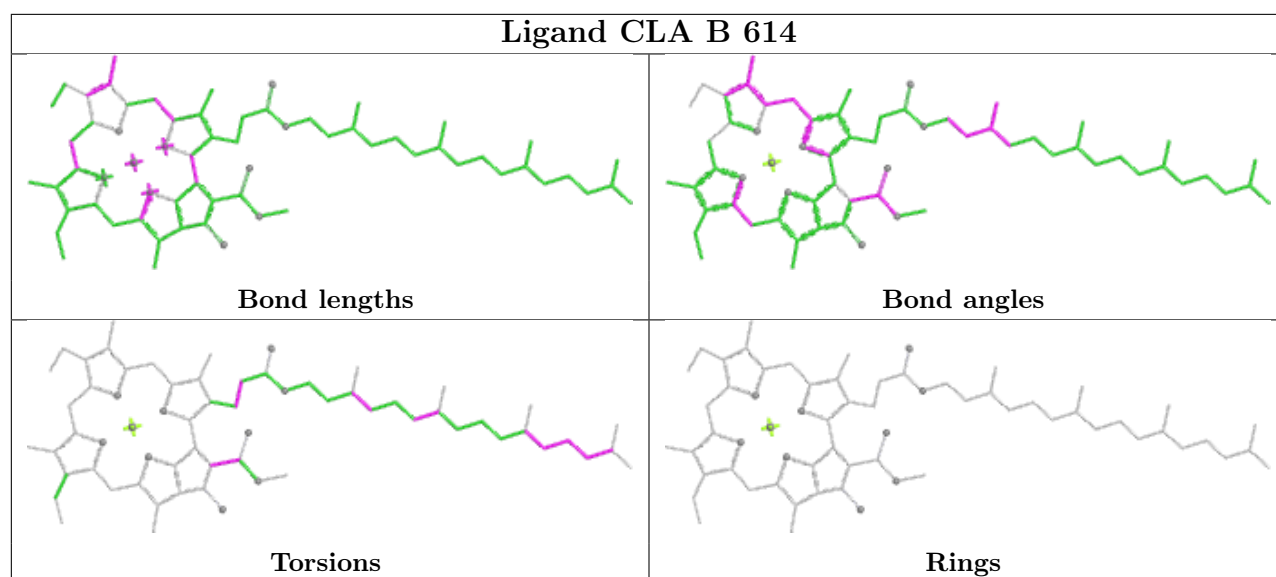


Ligand CLA C 508

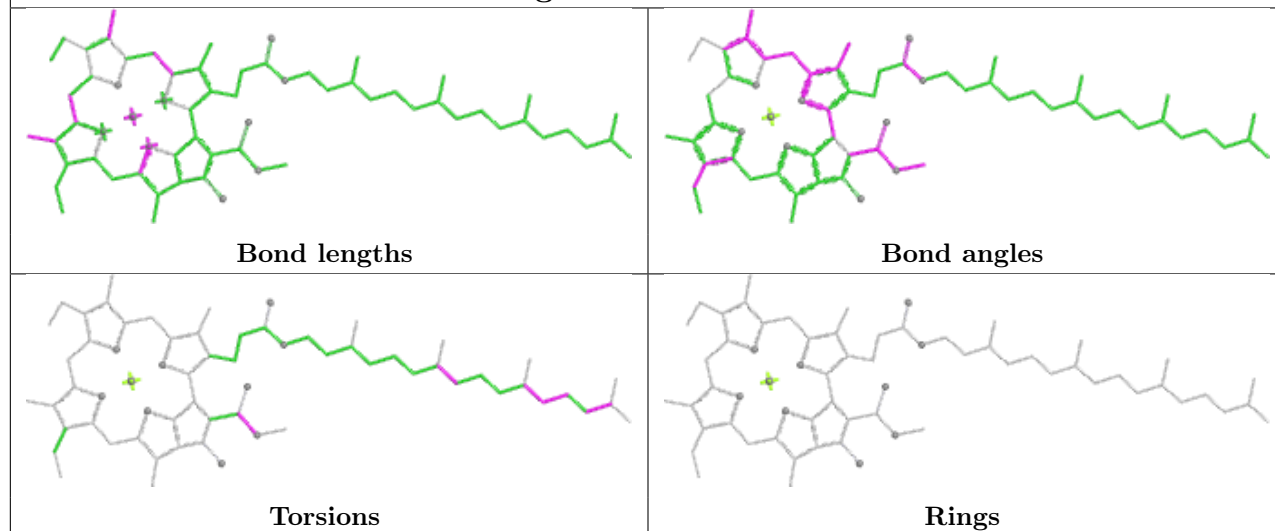




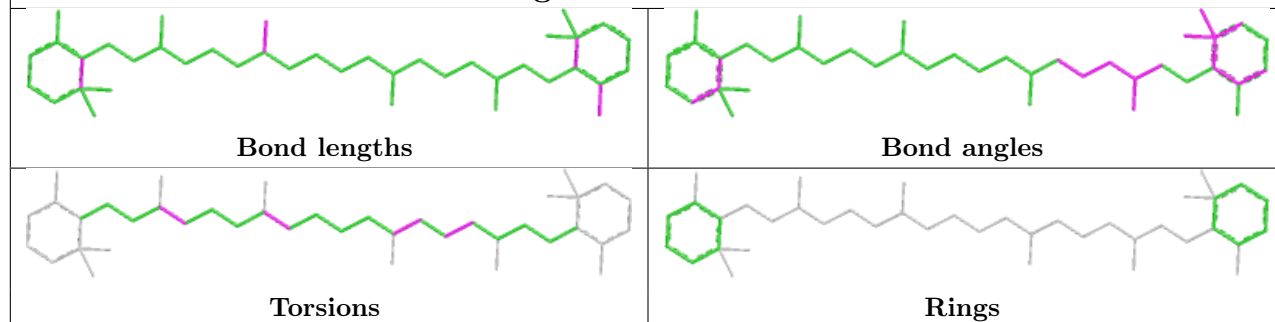




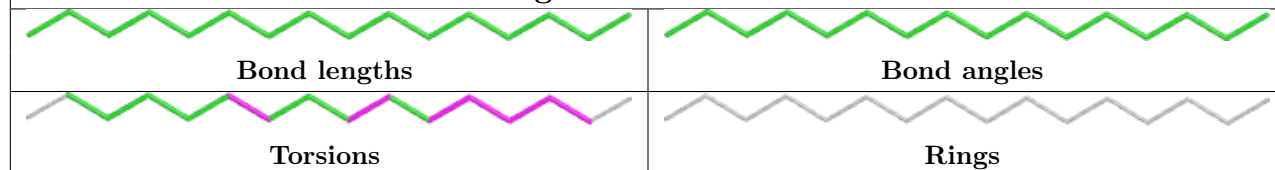
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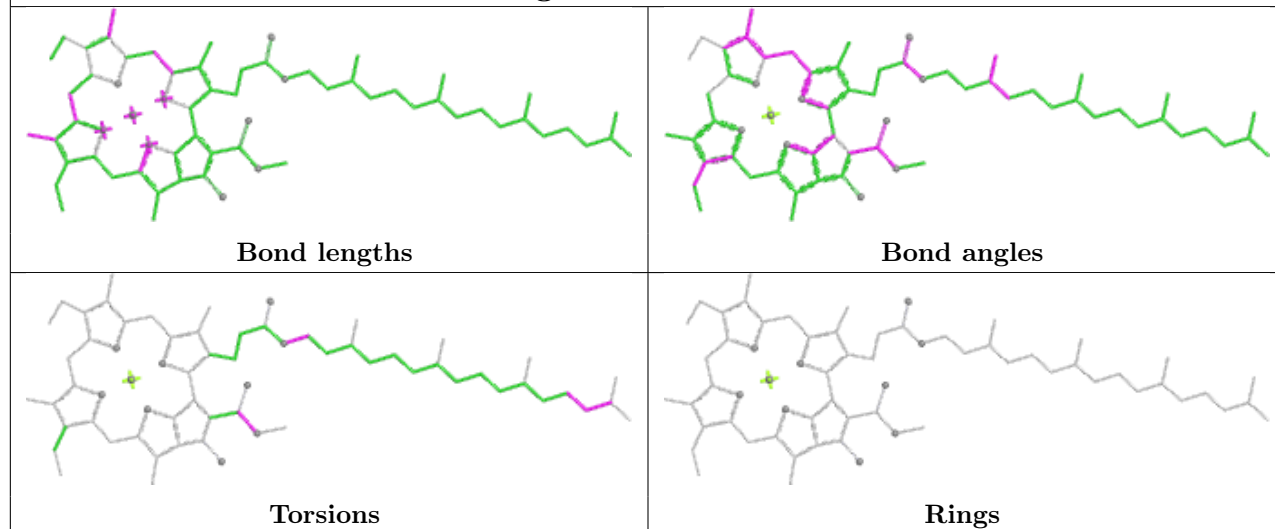
Ligand BCR a 405



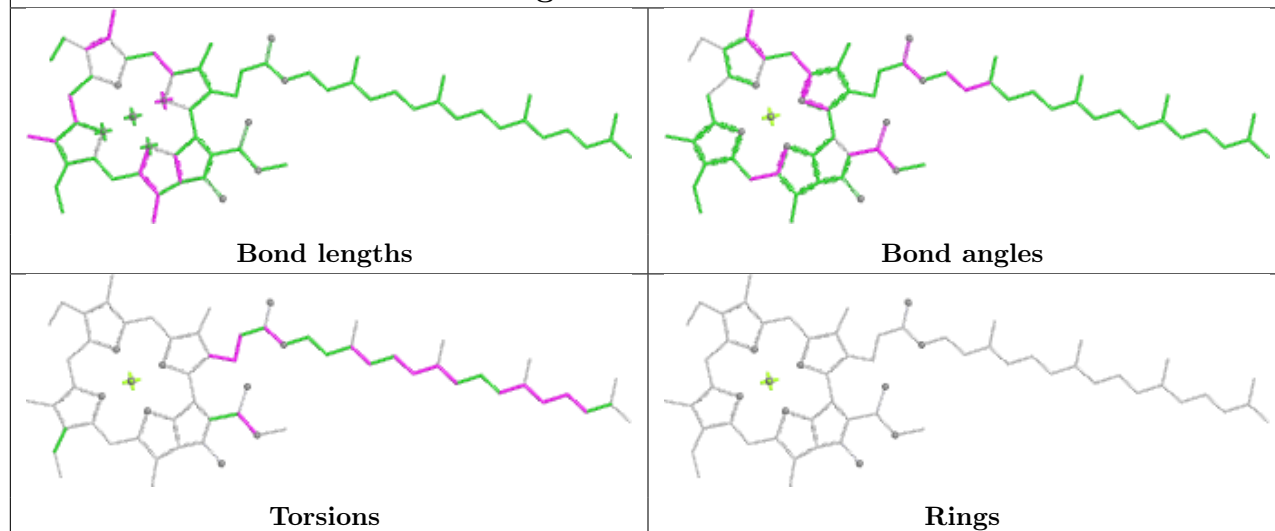
Ligand STE B 626



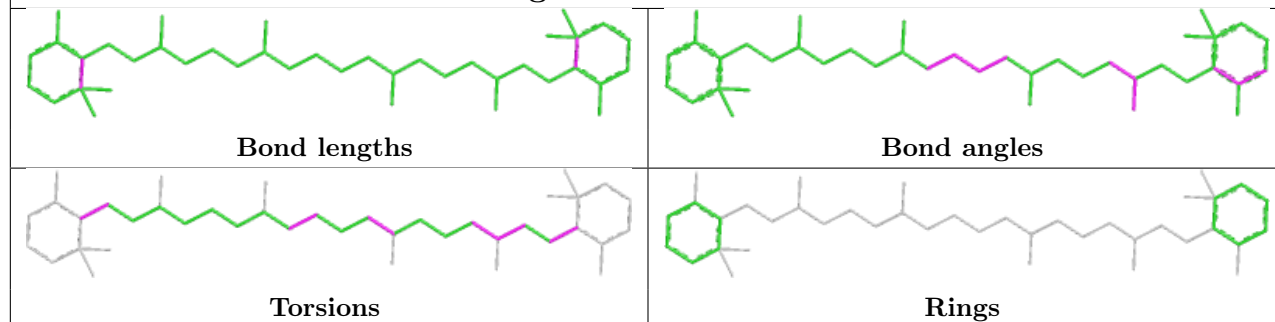
Ligand CLA a 402



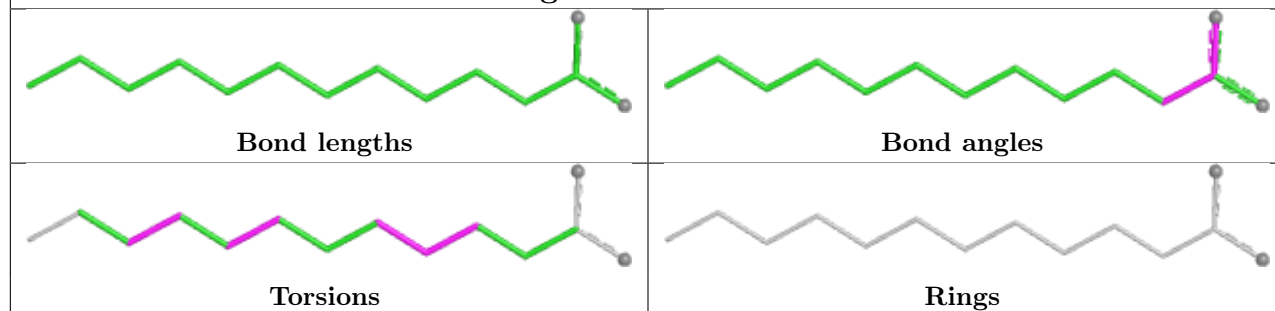
Ligand CLA c 512



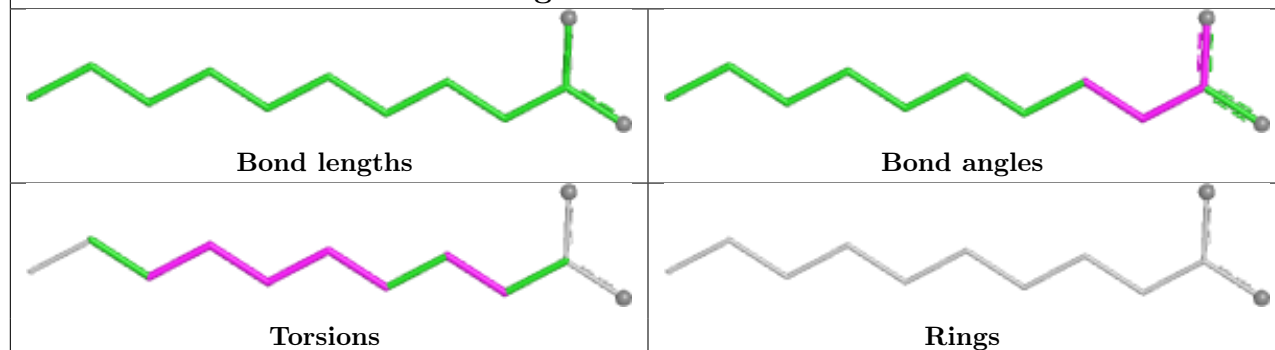
Ligand BCR Y 101



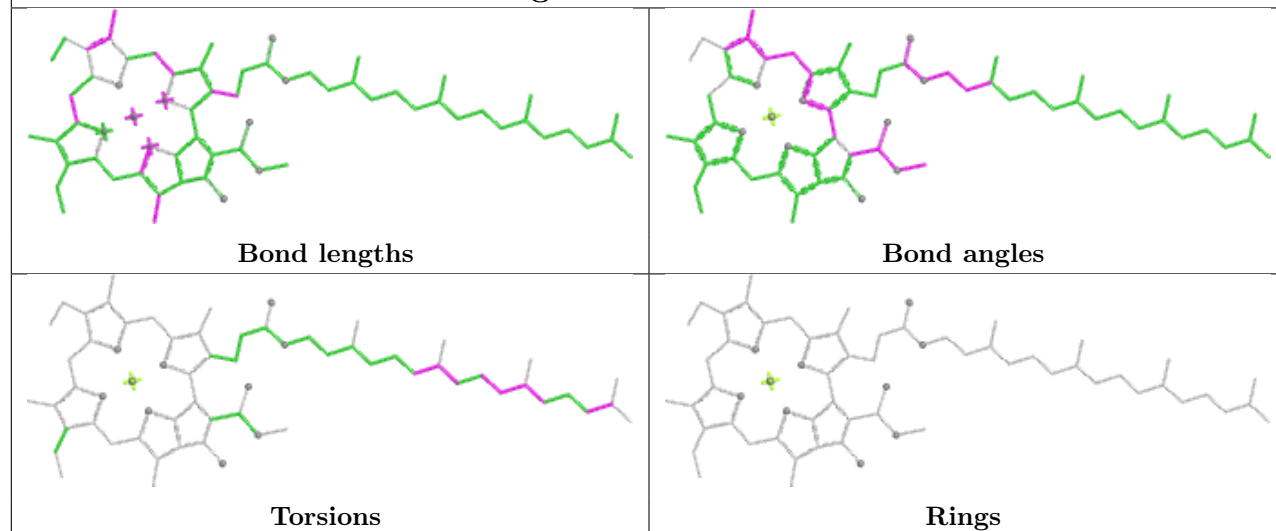
Ligand STE t 102



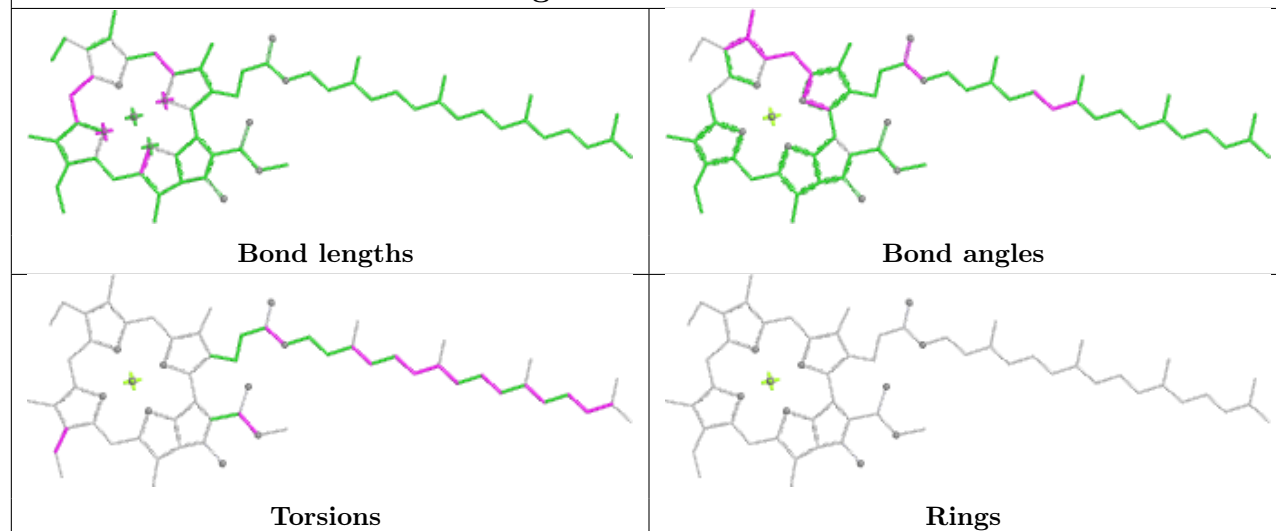
Ligand STE C 520



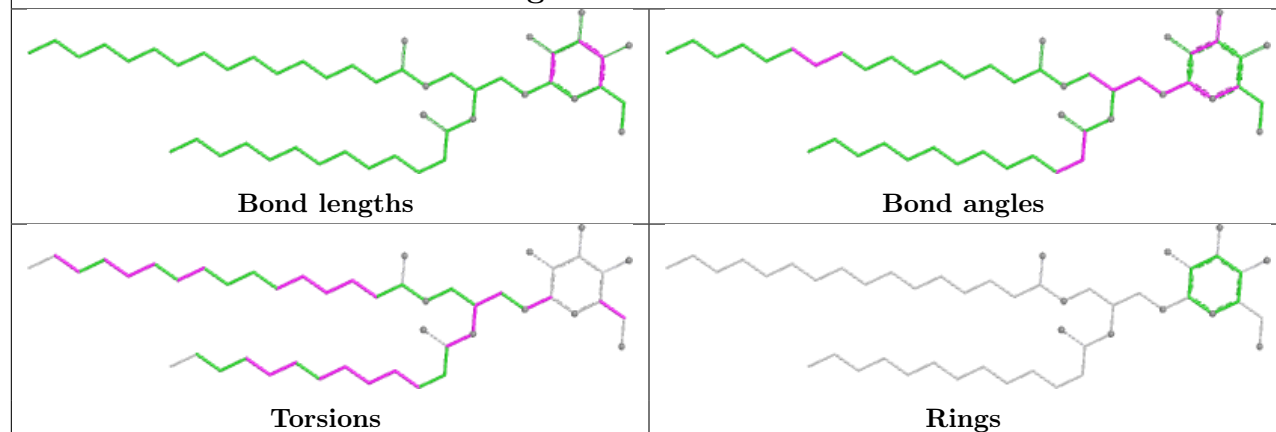
Ligand CLA A 403

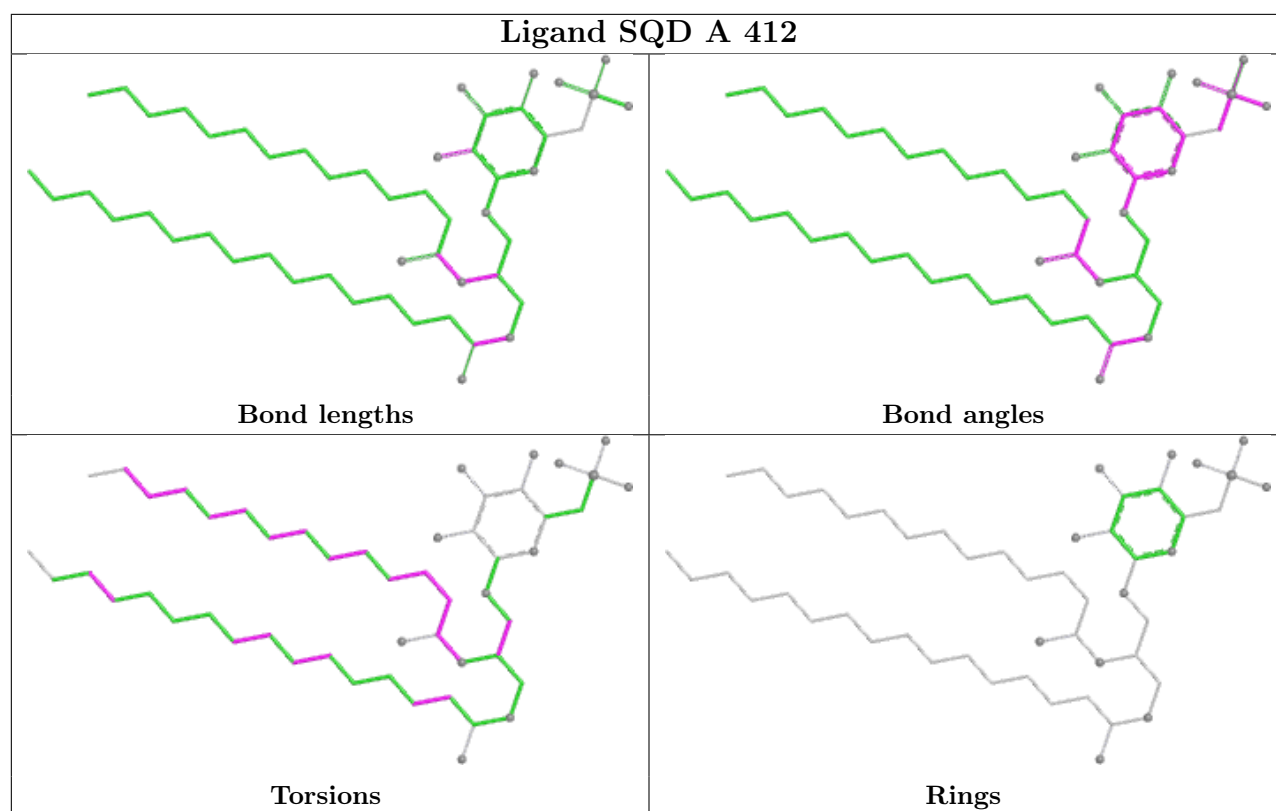


Ligand CLA C 505

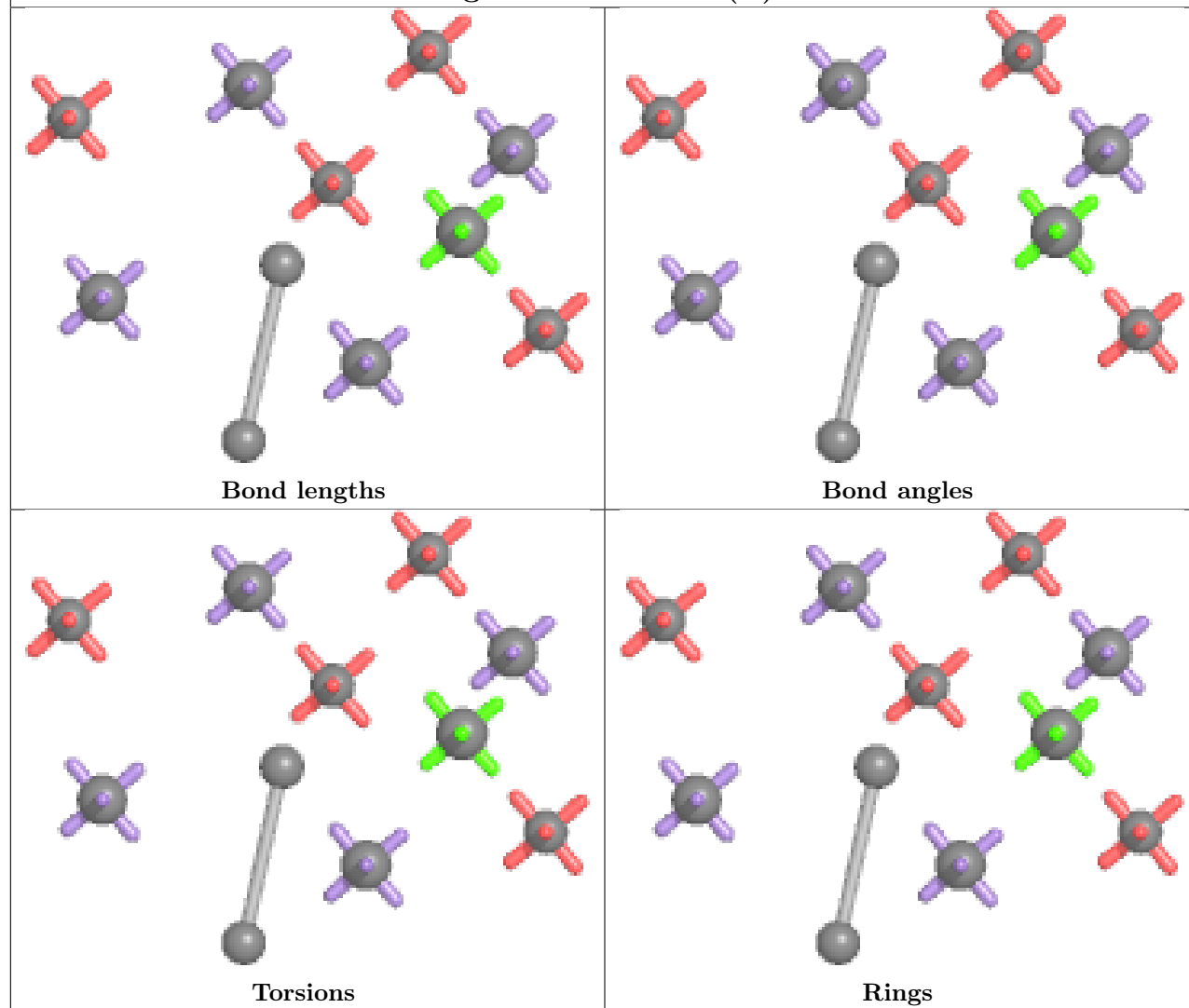


Ligand LMG A 411

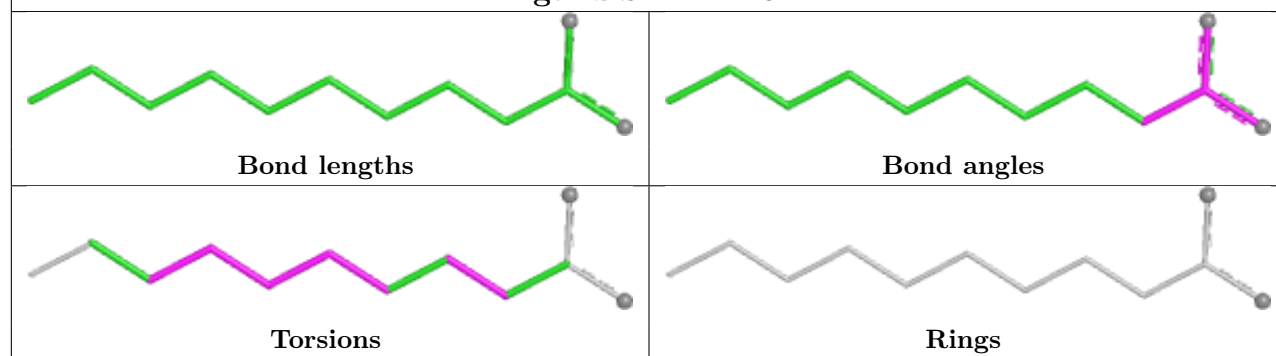


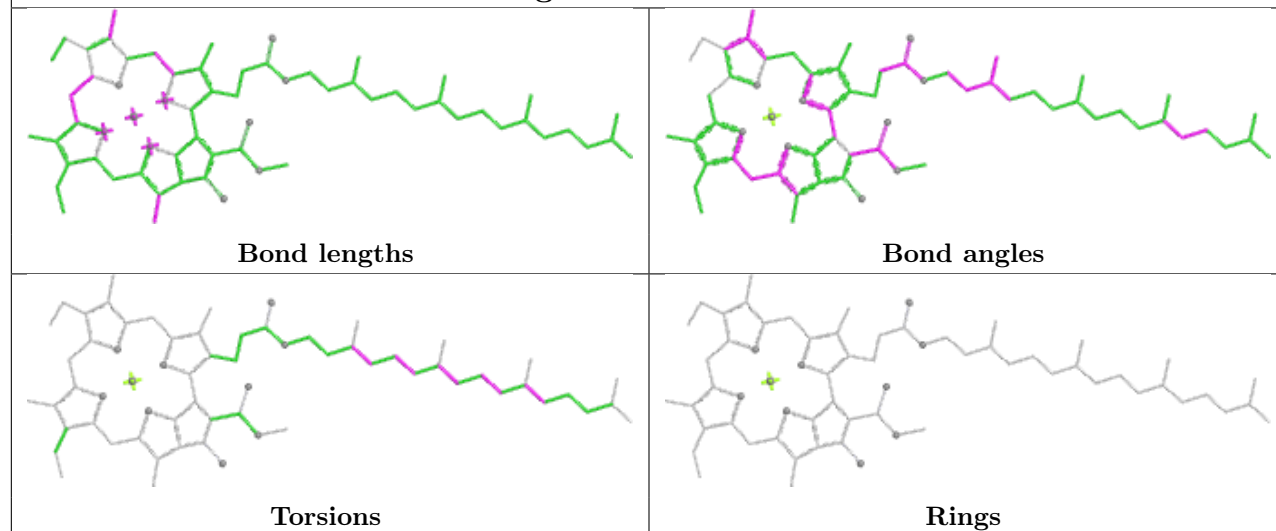
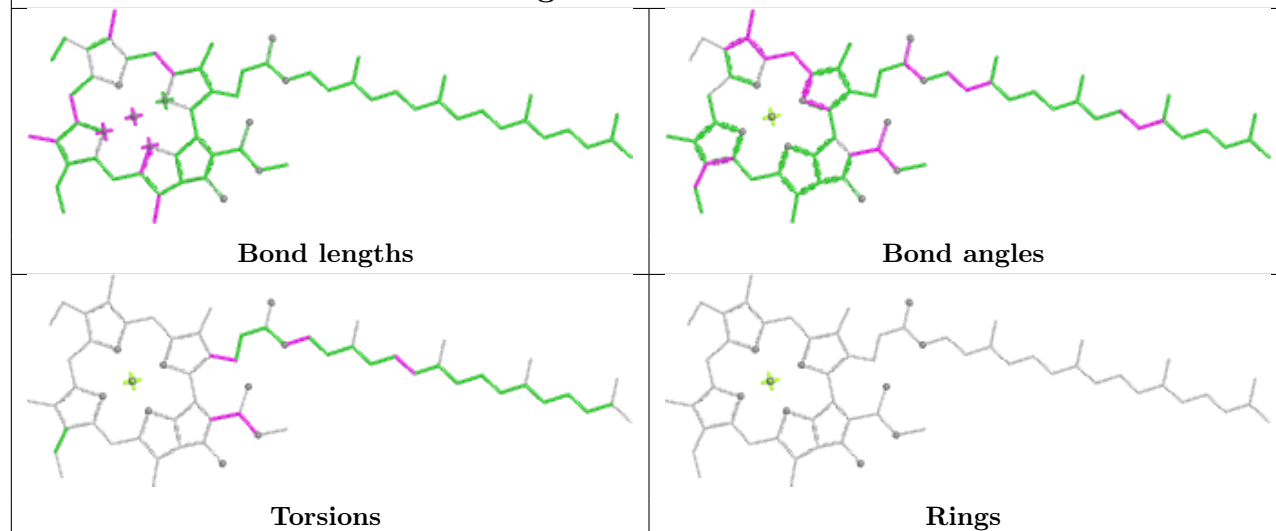


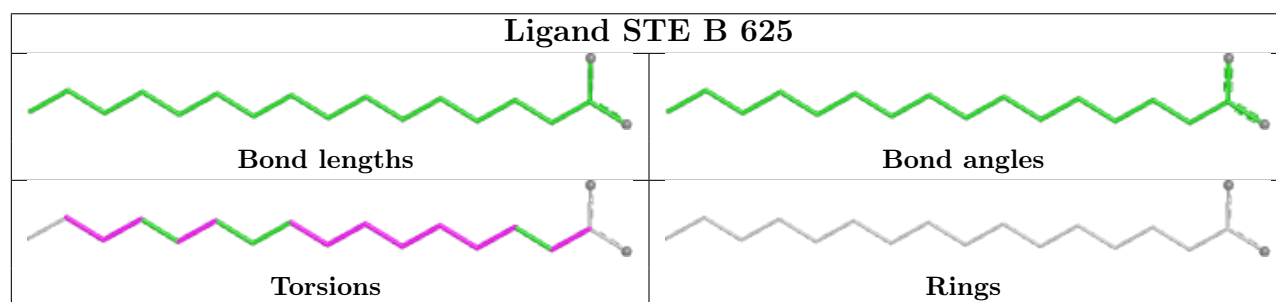
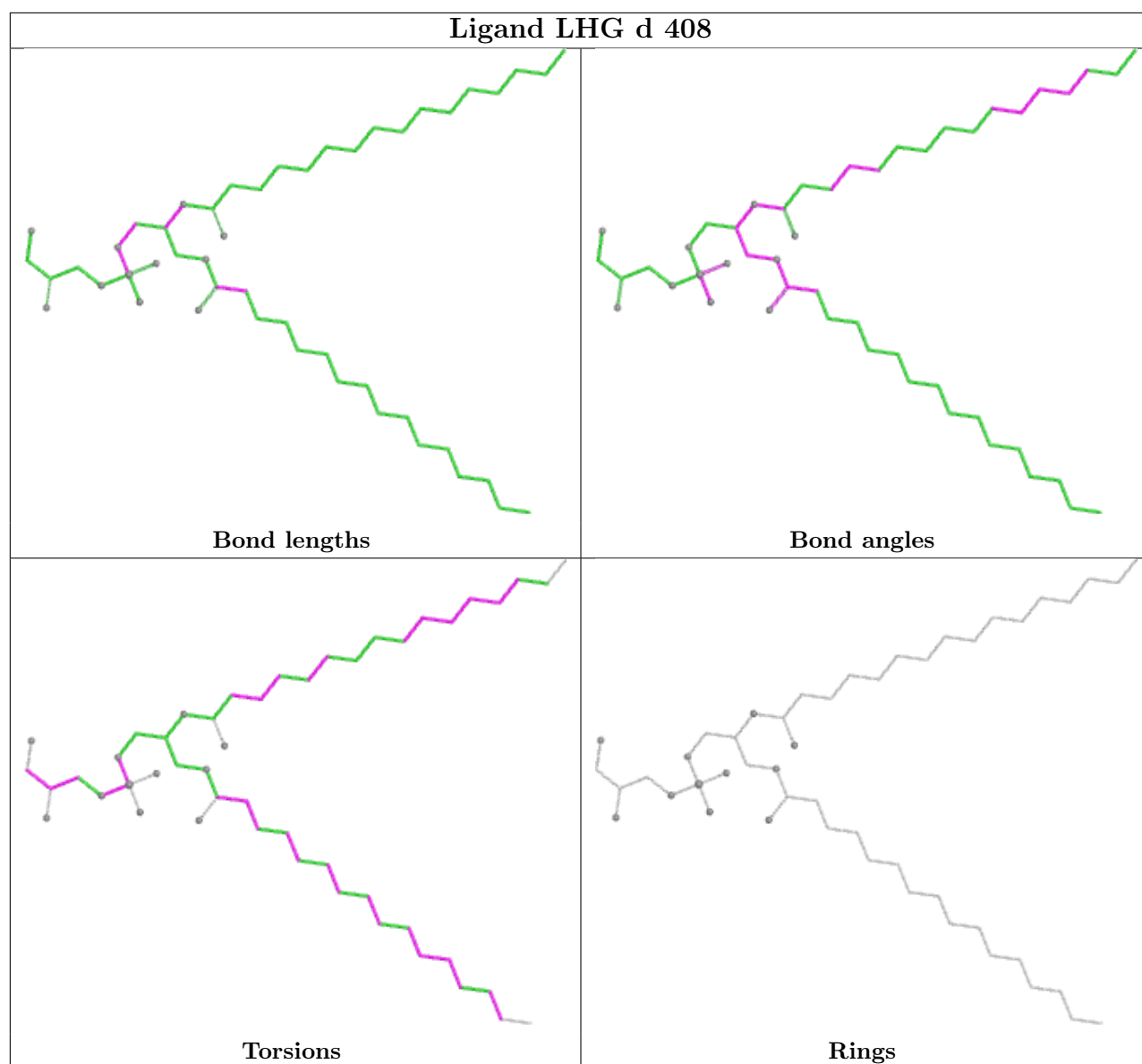
Ligand OEY A 415 (B)

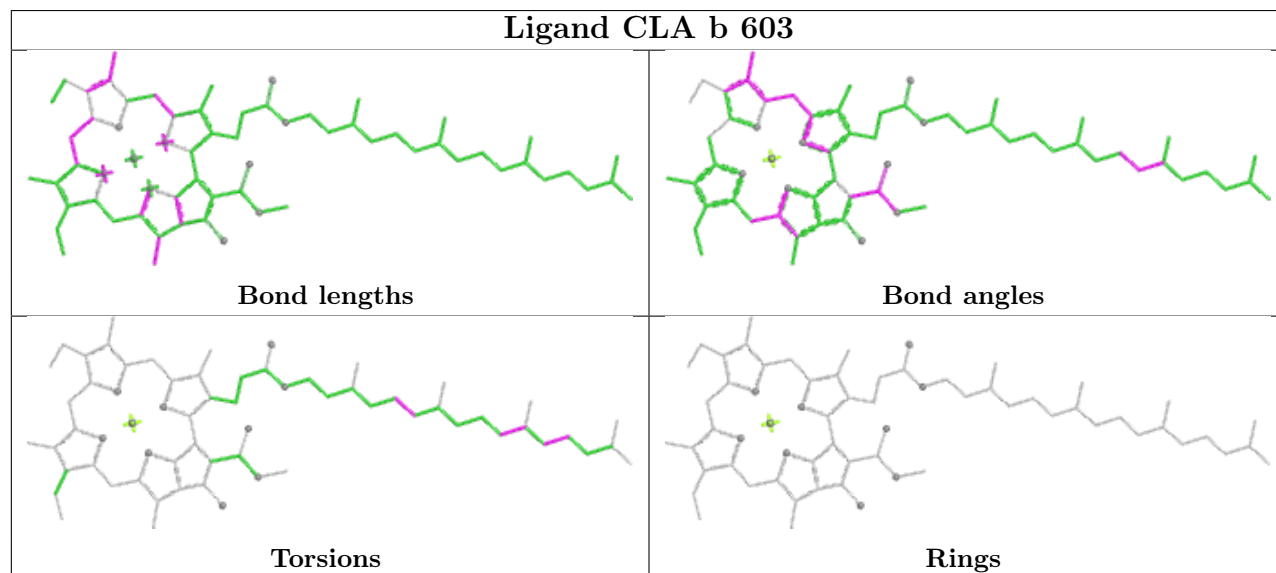
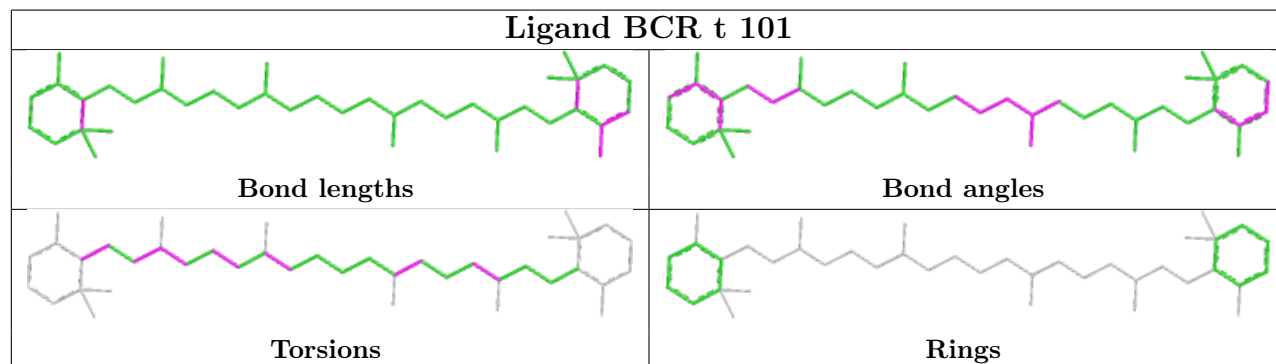
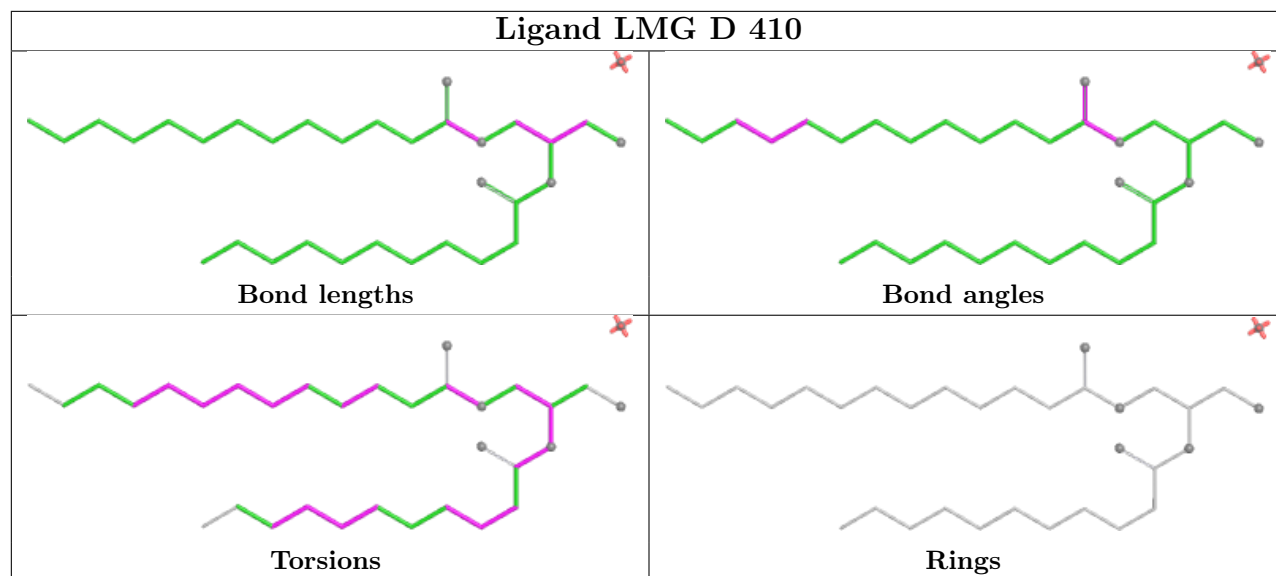


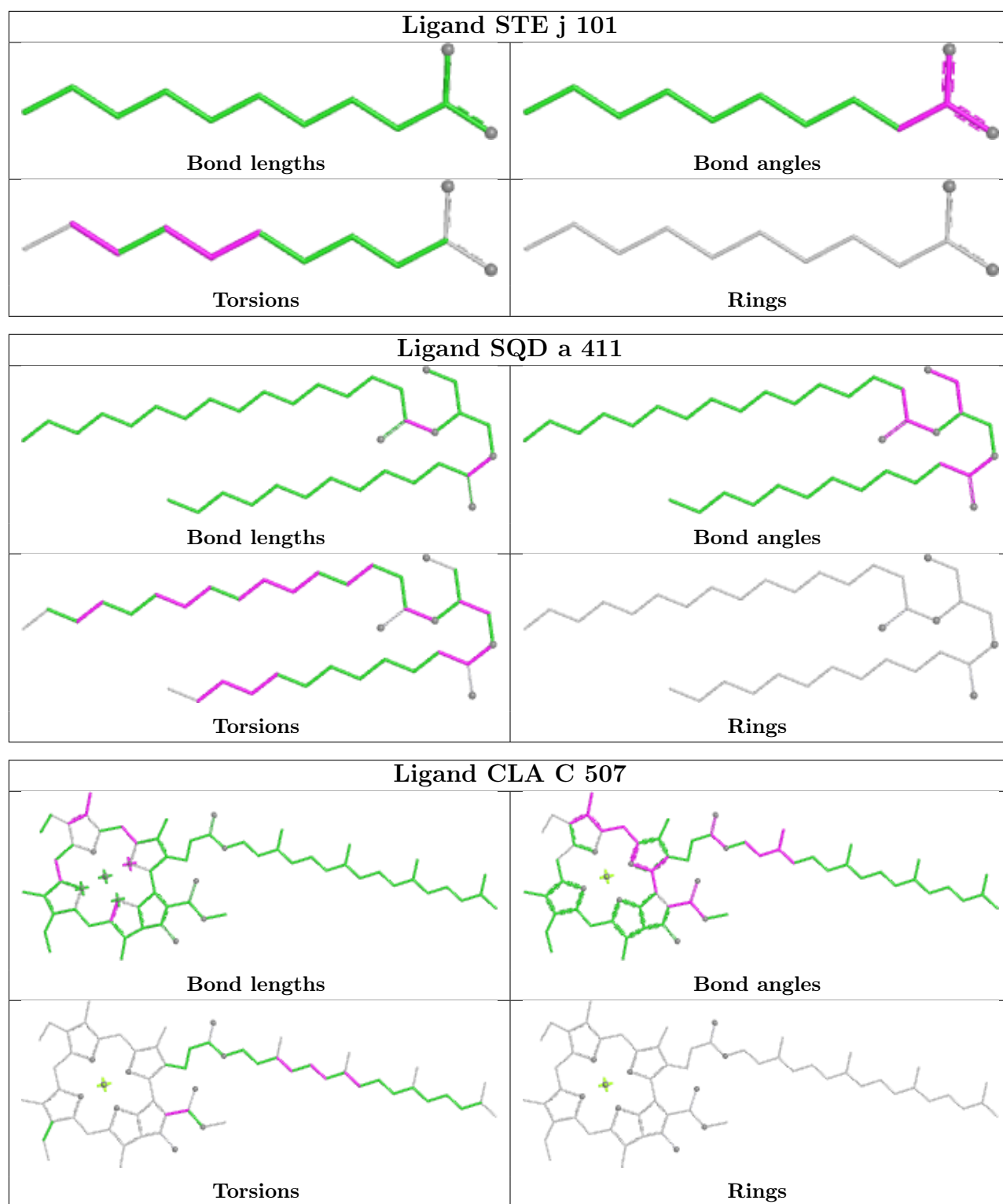
Ligand STE m 101

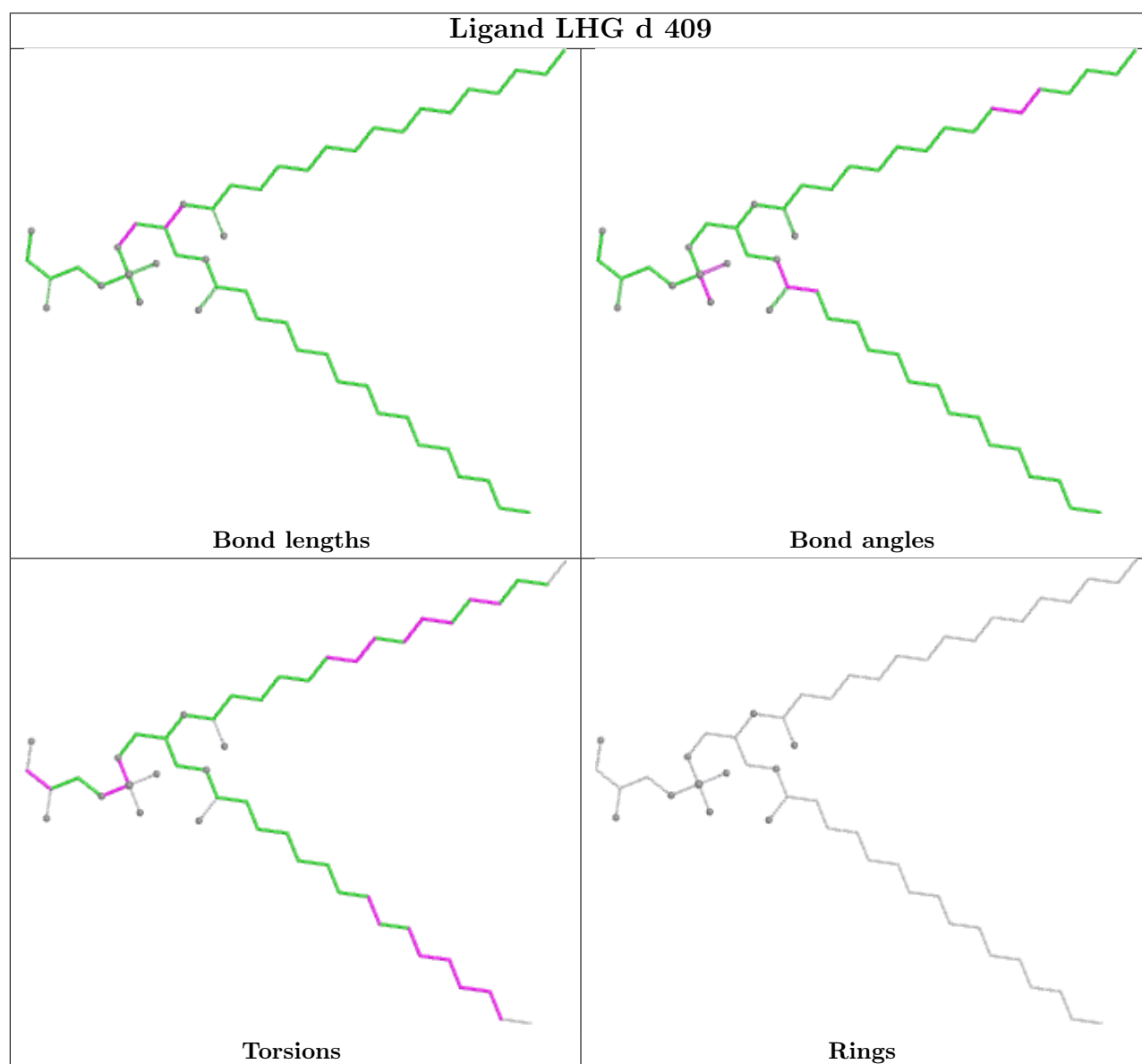
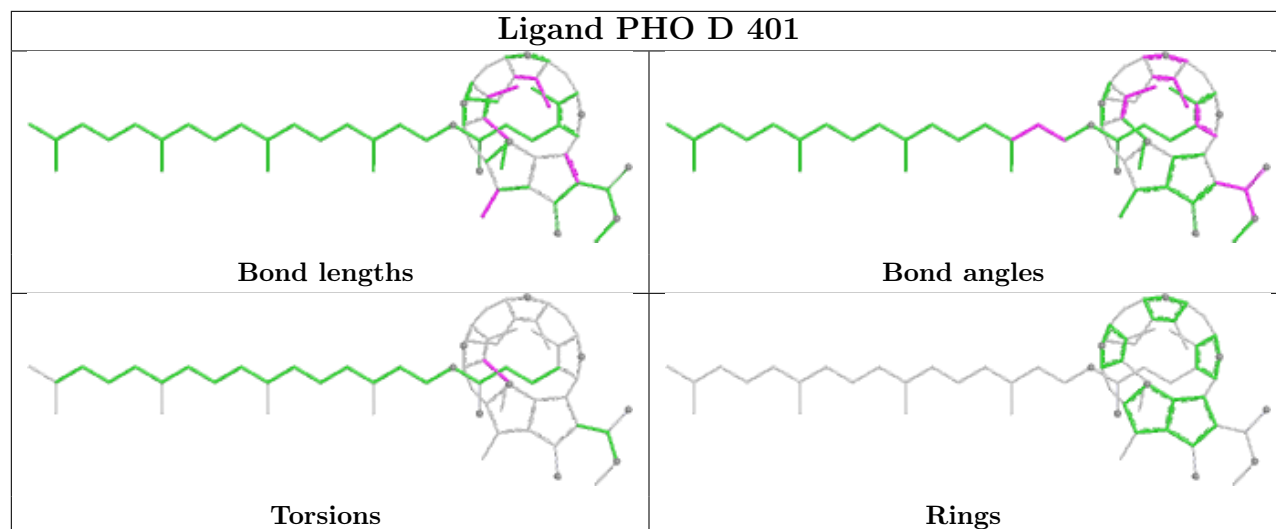


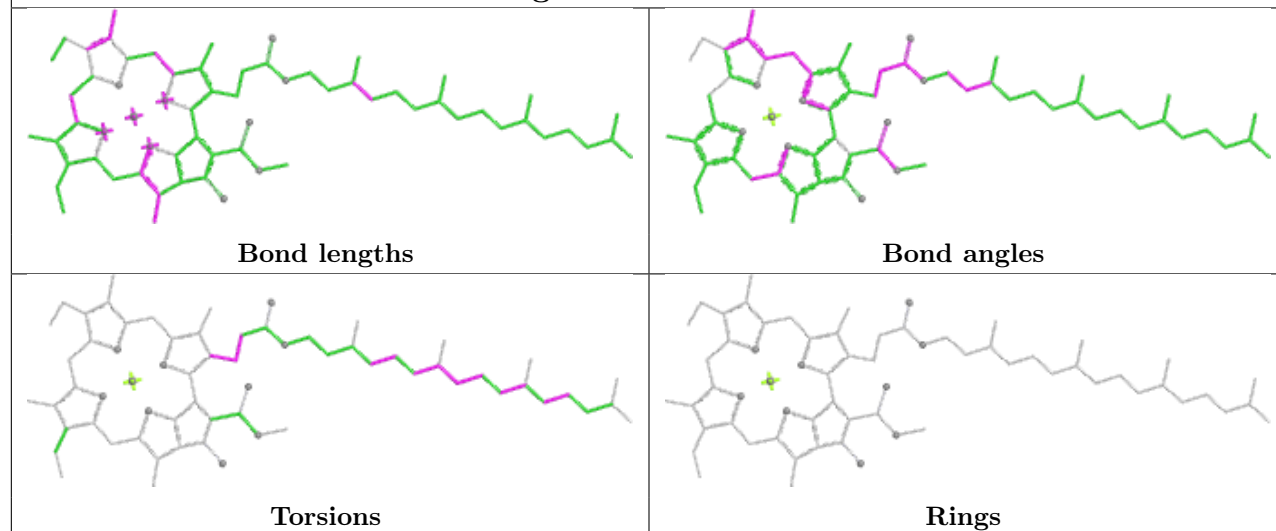
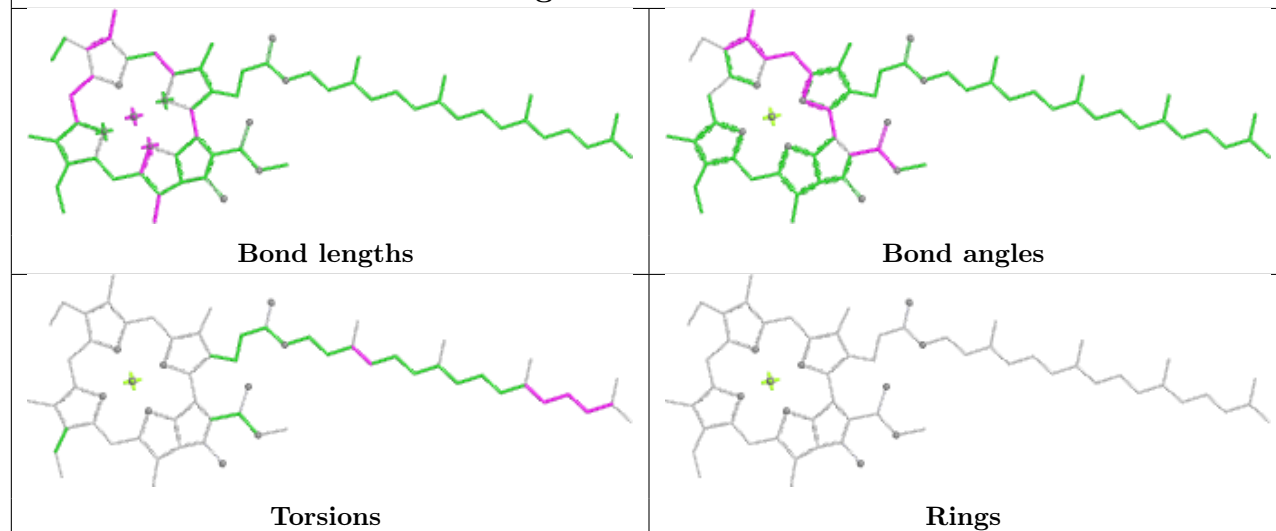
Ligand CLA b 605**Ligand CLA c 513**



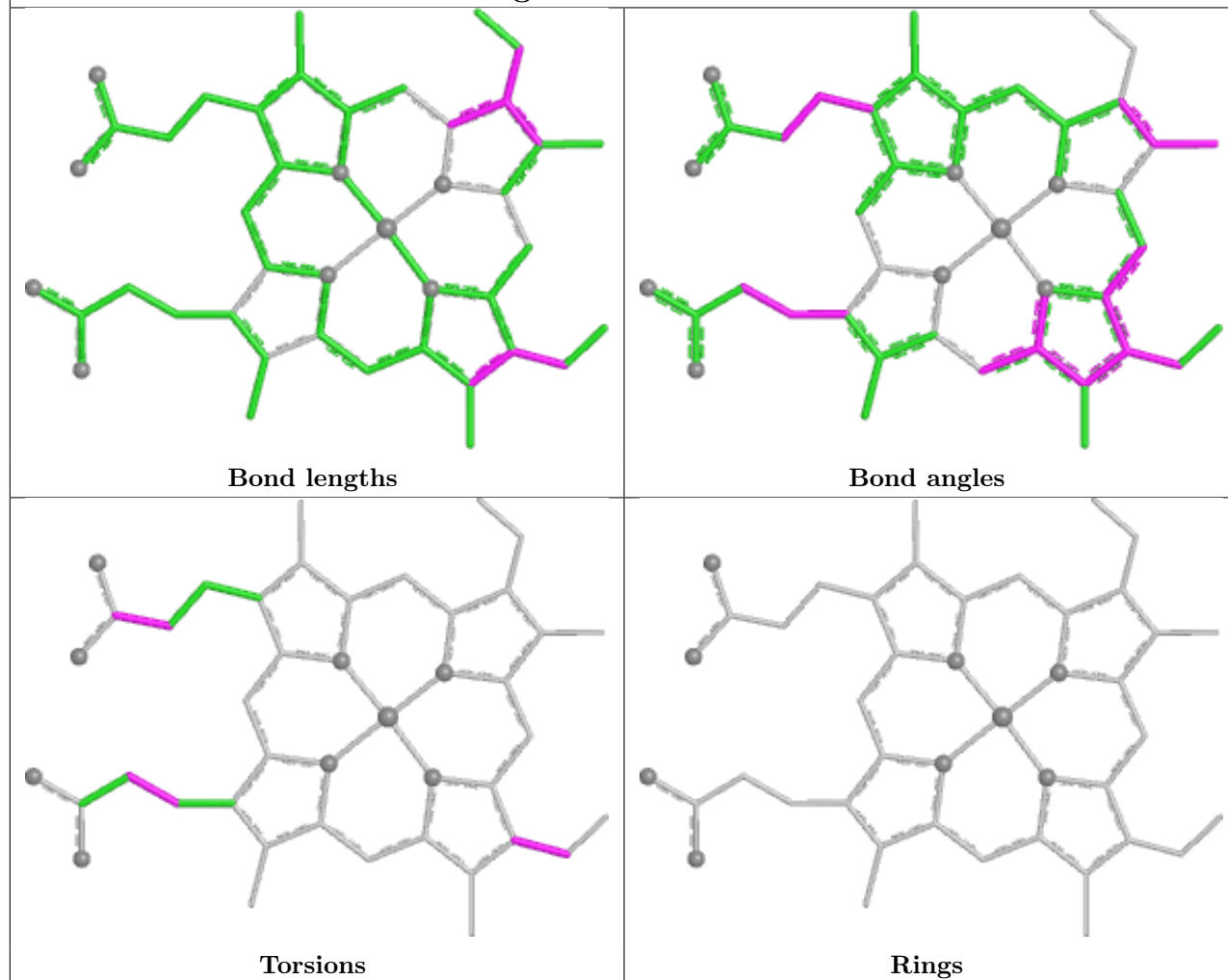




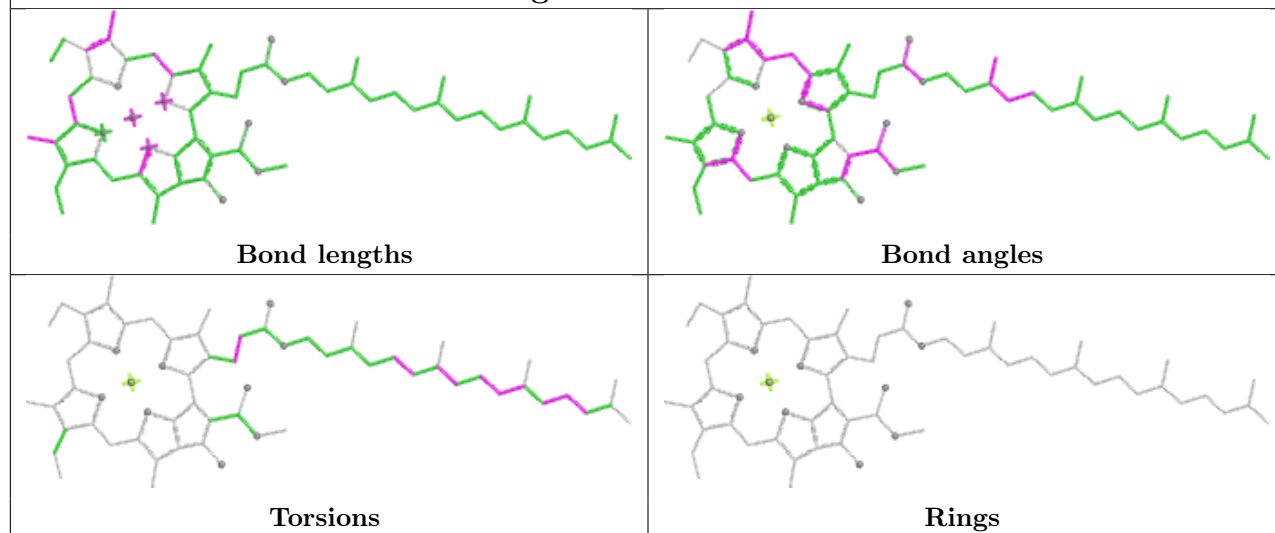


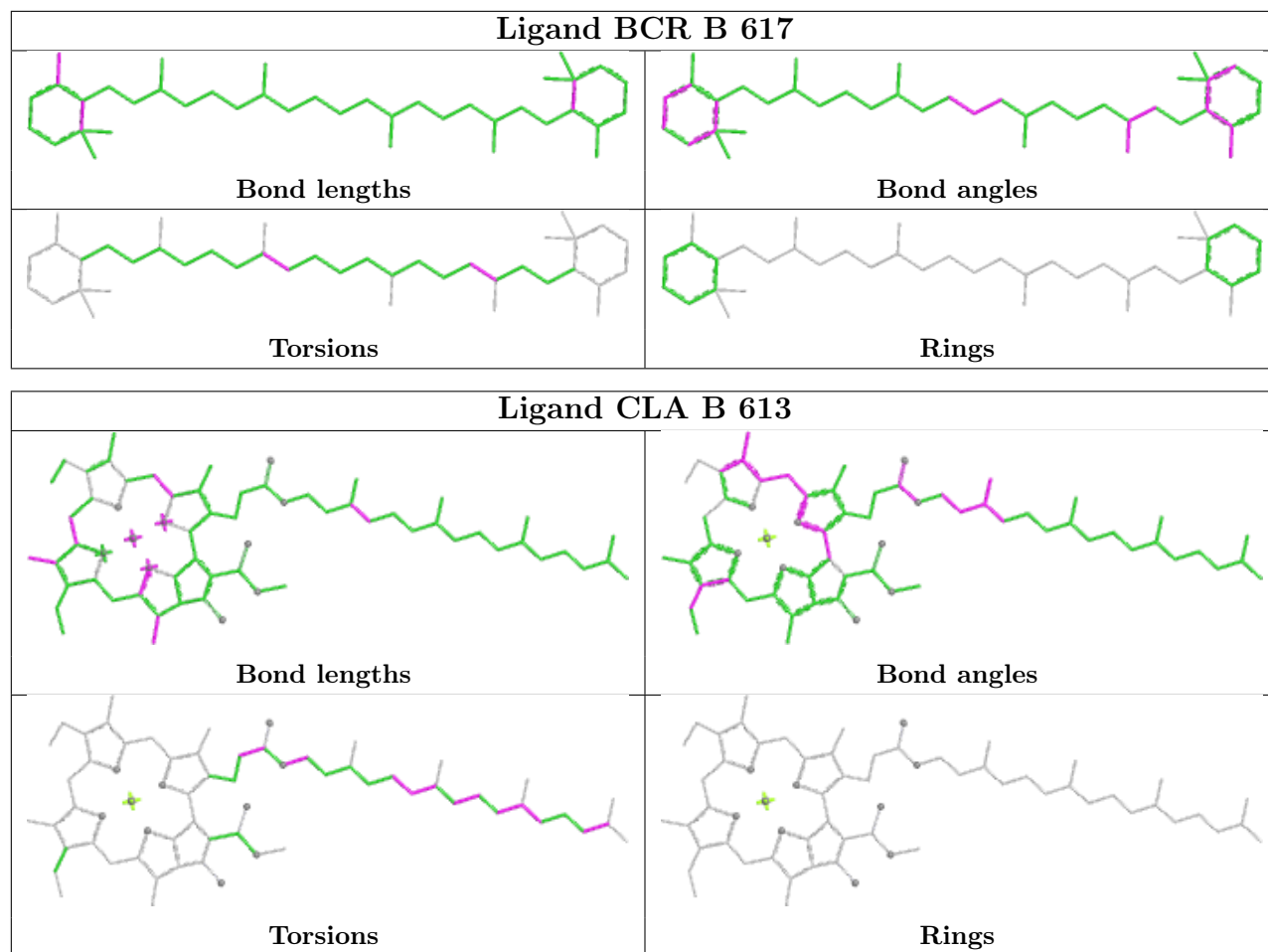
Ligand CLA C 512**Ligand CLA b 609**

Ligand HEM f 101

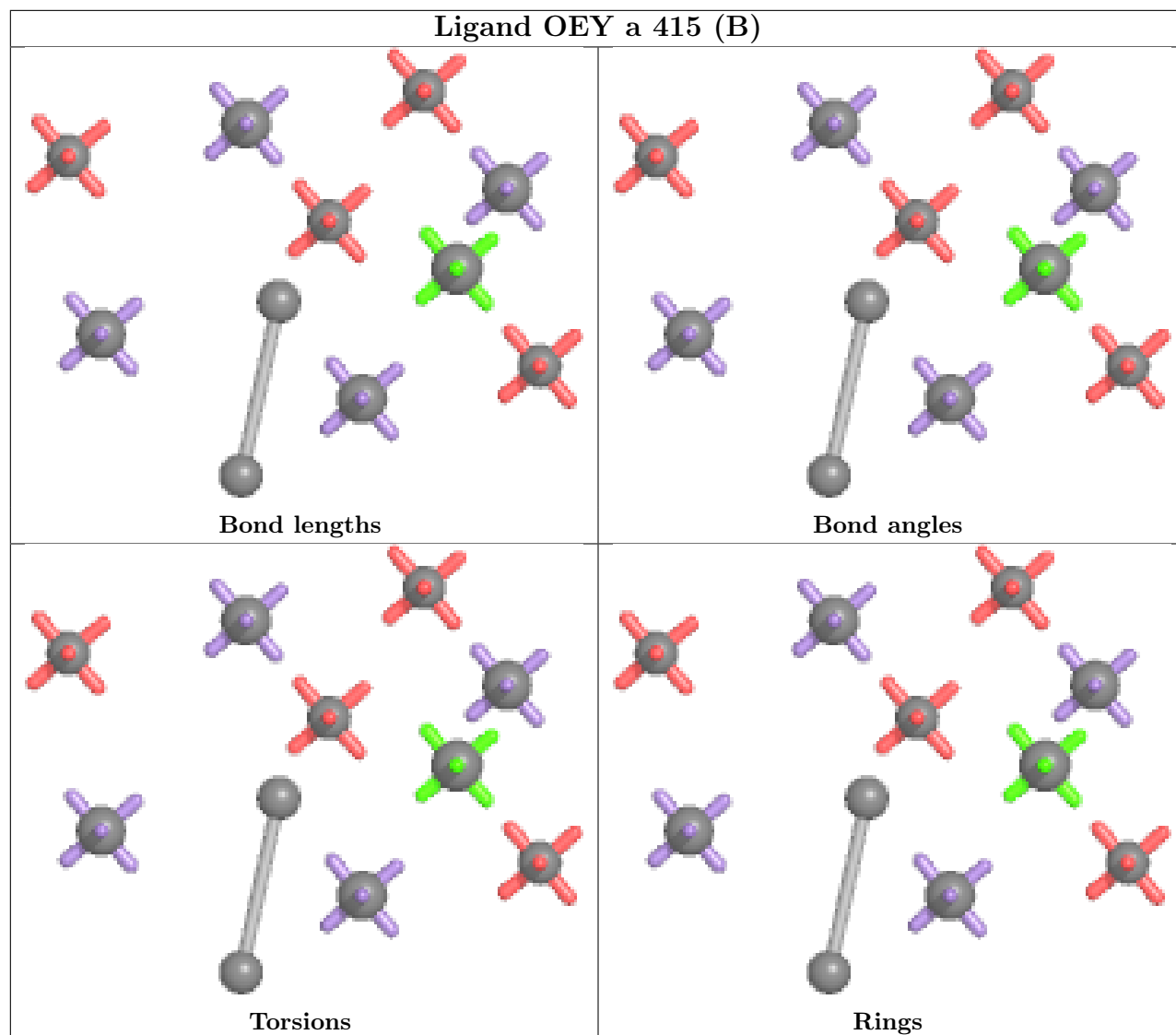


Ligand CLA B 606

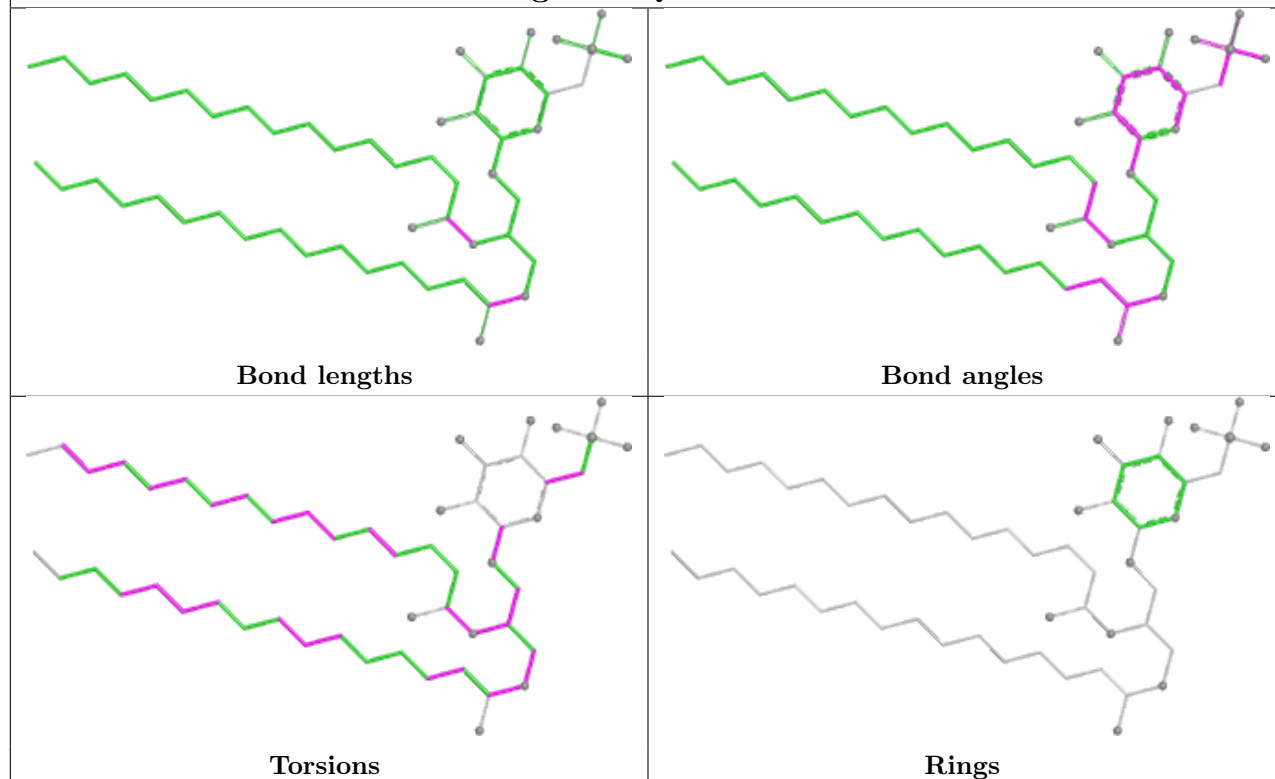




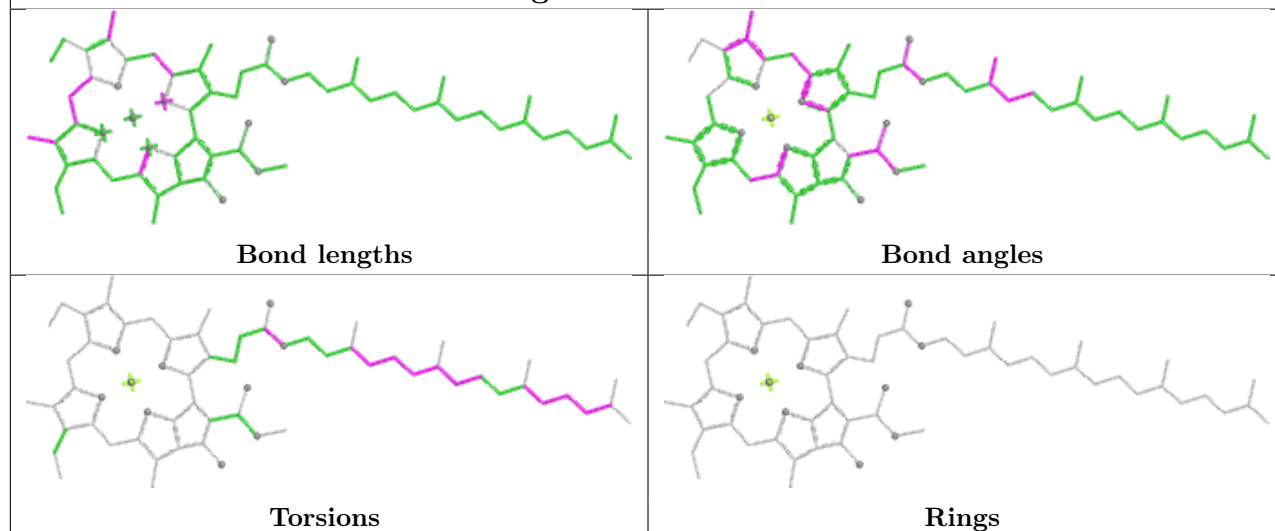
Ligand OEY a 415 (B)



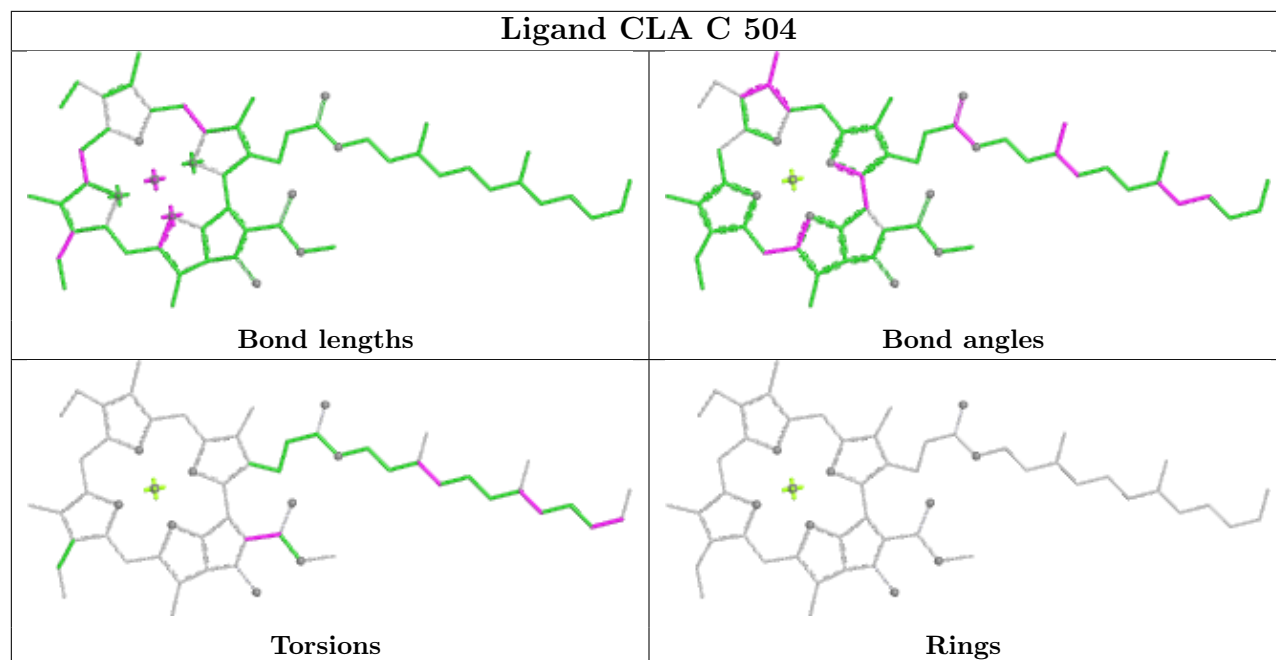
Ligand SQD B 623



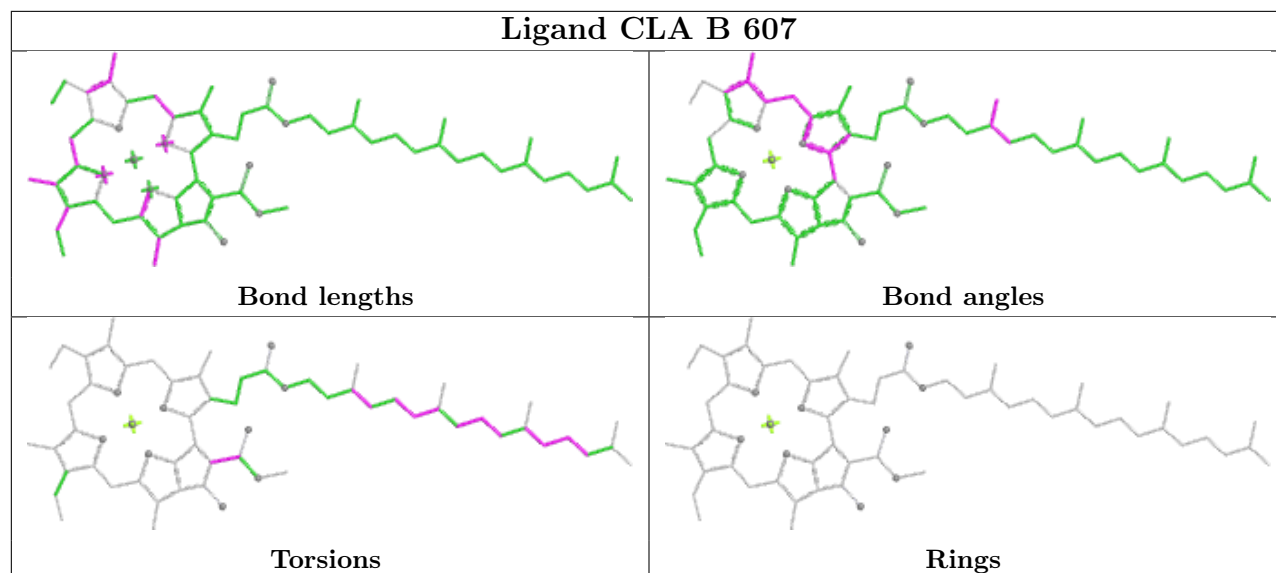
Ligand CLA C 513



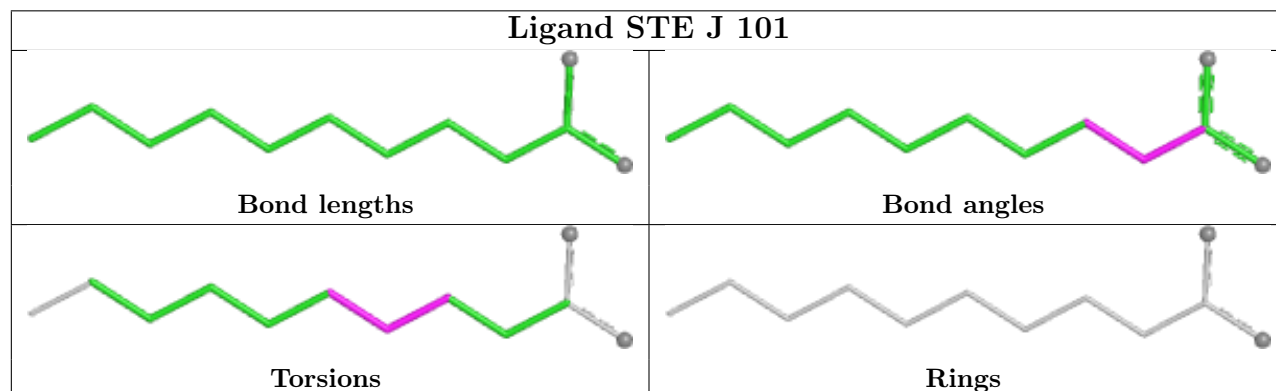
Ligand CLA C 504



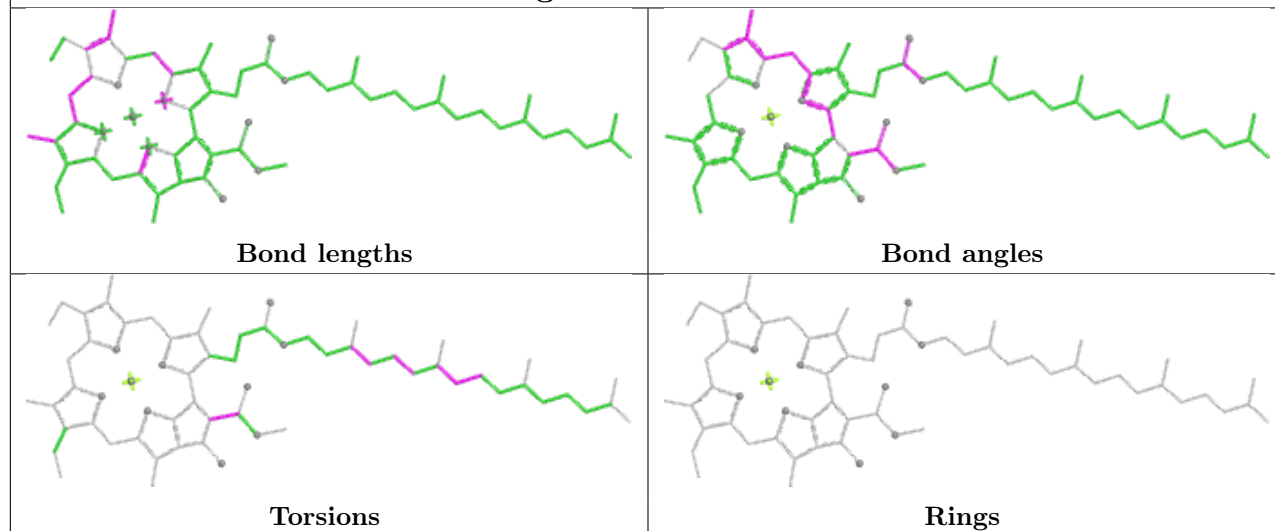
Ligand CLA B 607



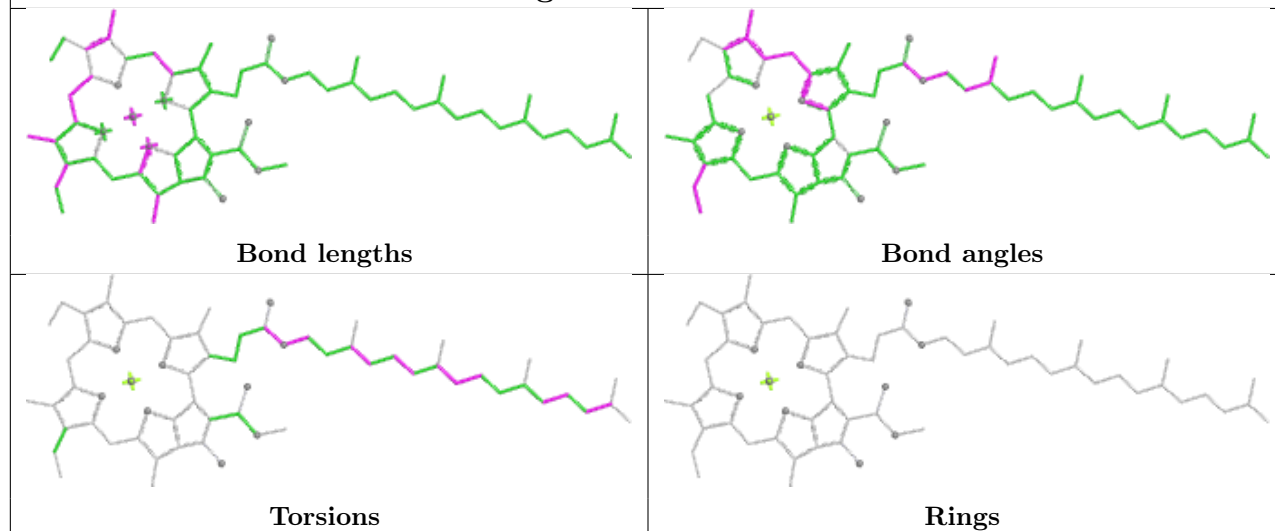
Ligand STE J 101



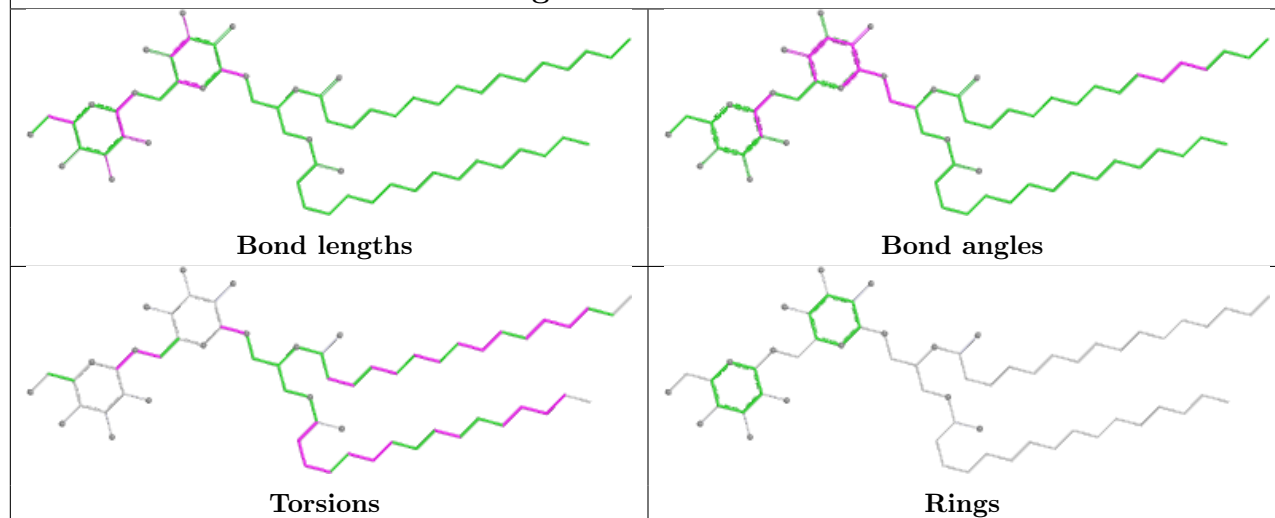
Ligand CLA c 507

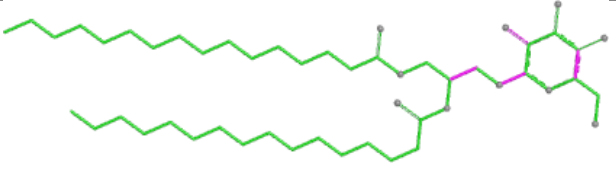
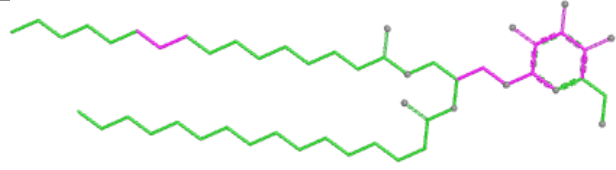
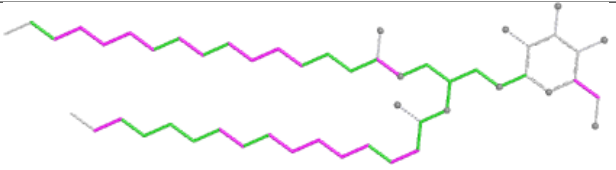
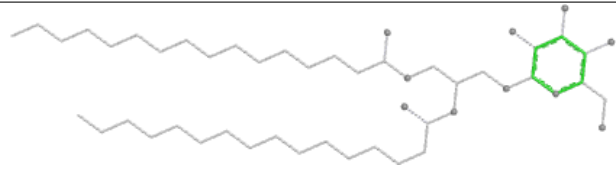


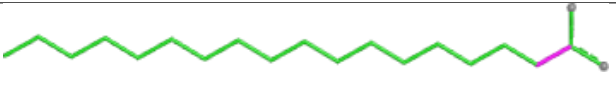
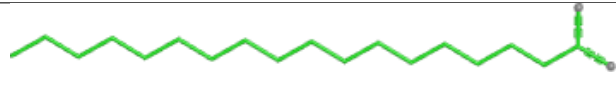


Ligand CLA c 506


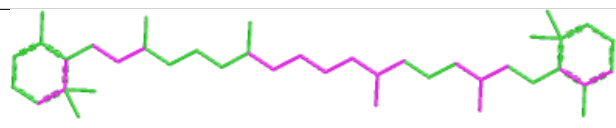
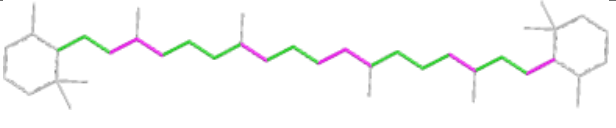
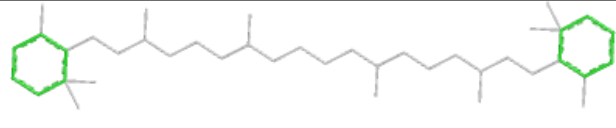


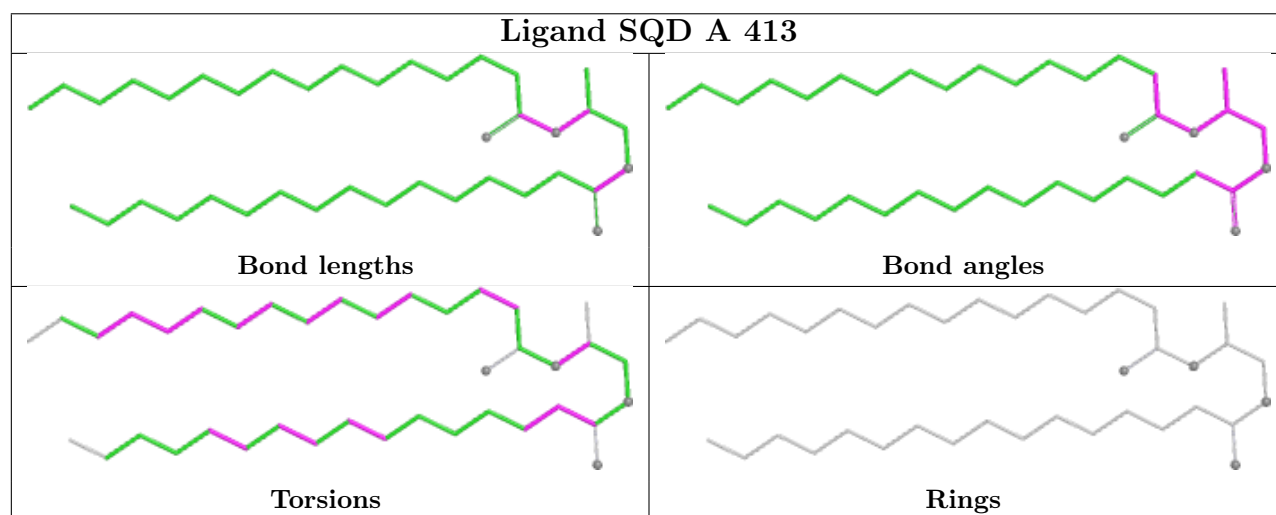
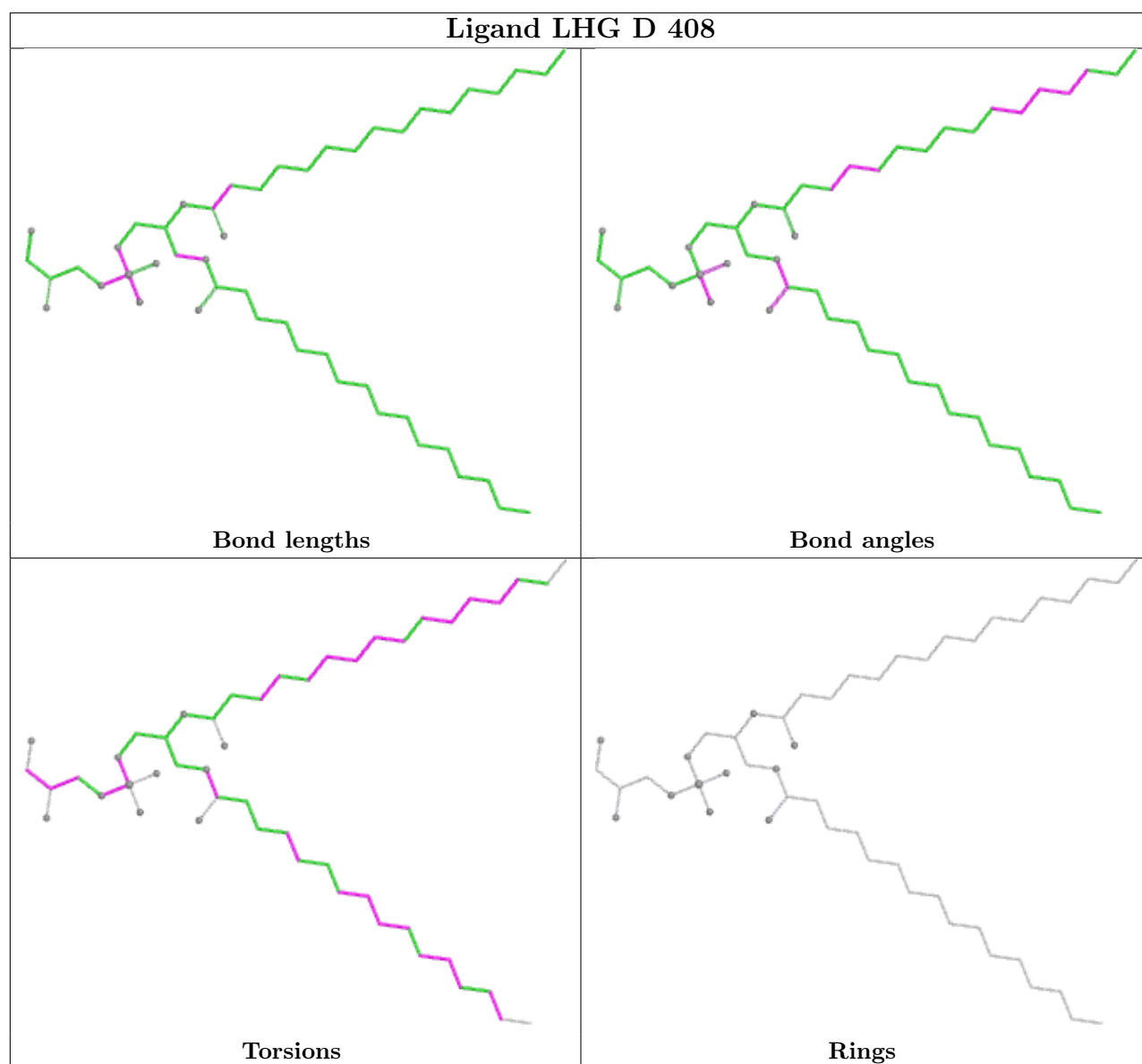
Ligand DGD c 518

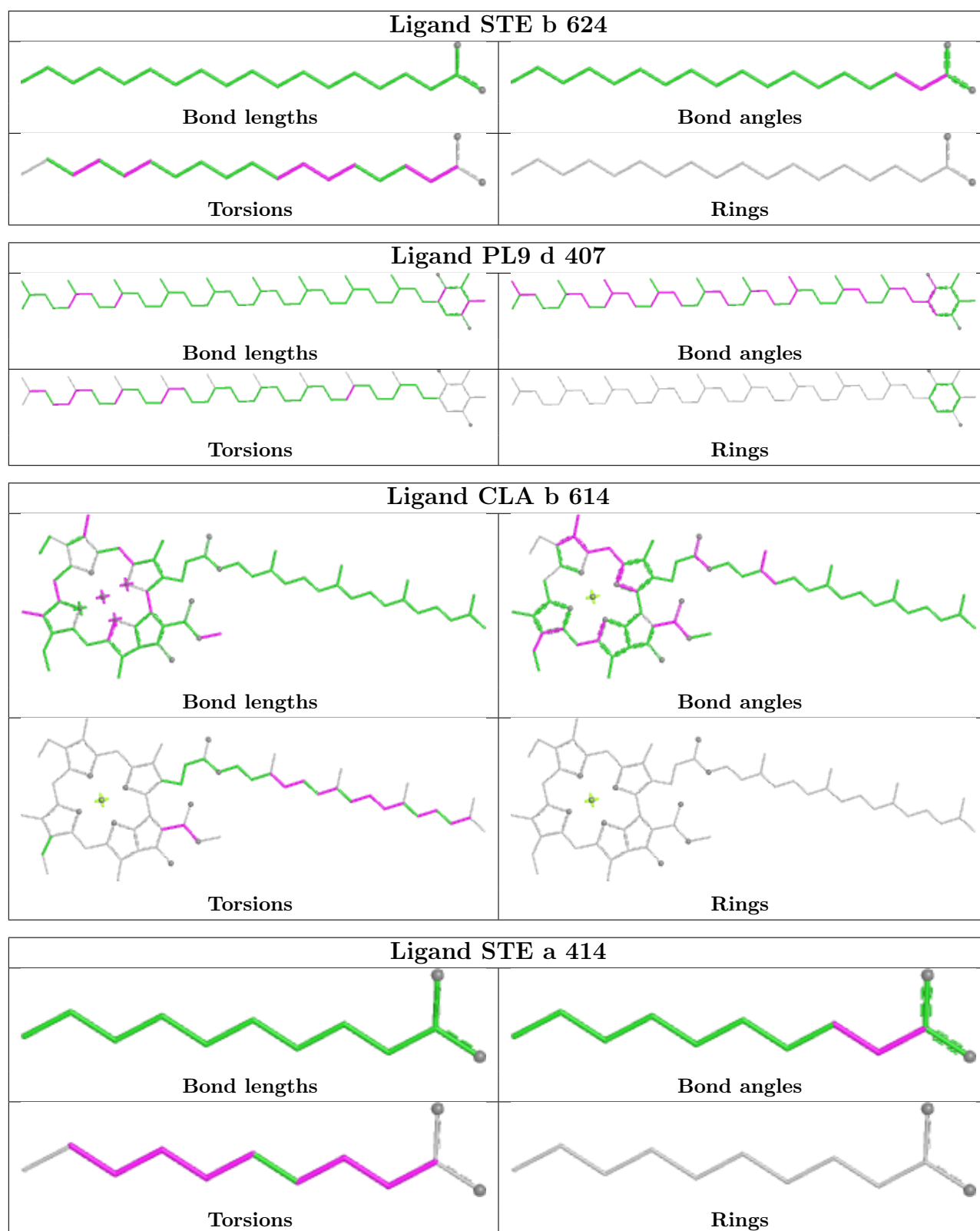


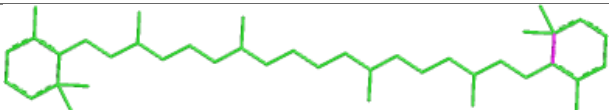
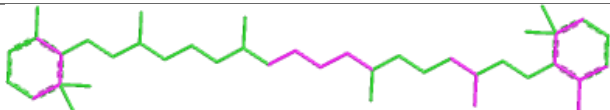
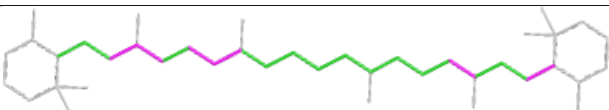
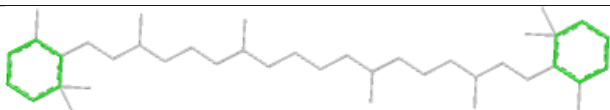
| Ligand LMG D 407 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |



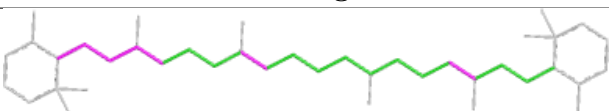
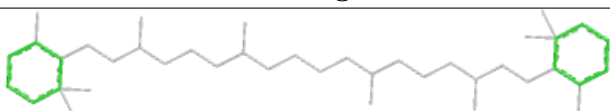
| Ligand STE c 521 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

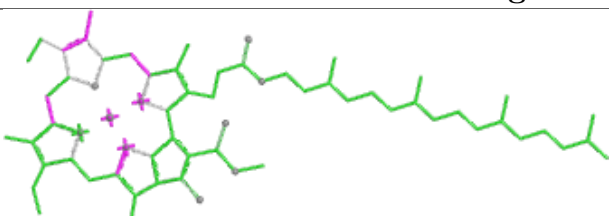
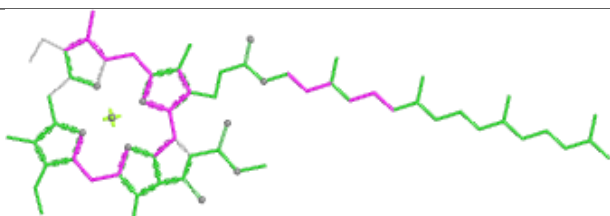
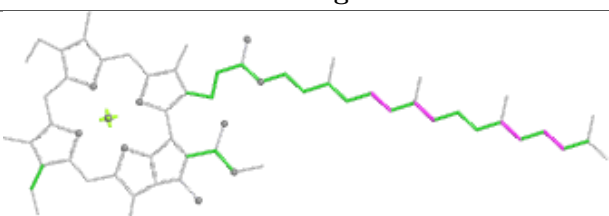
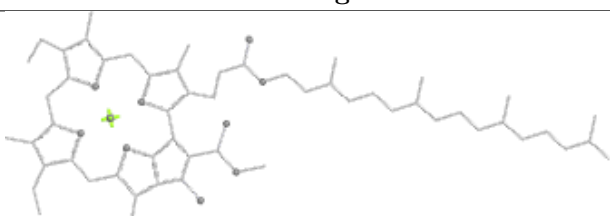
| Ligand BCR h 101 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

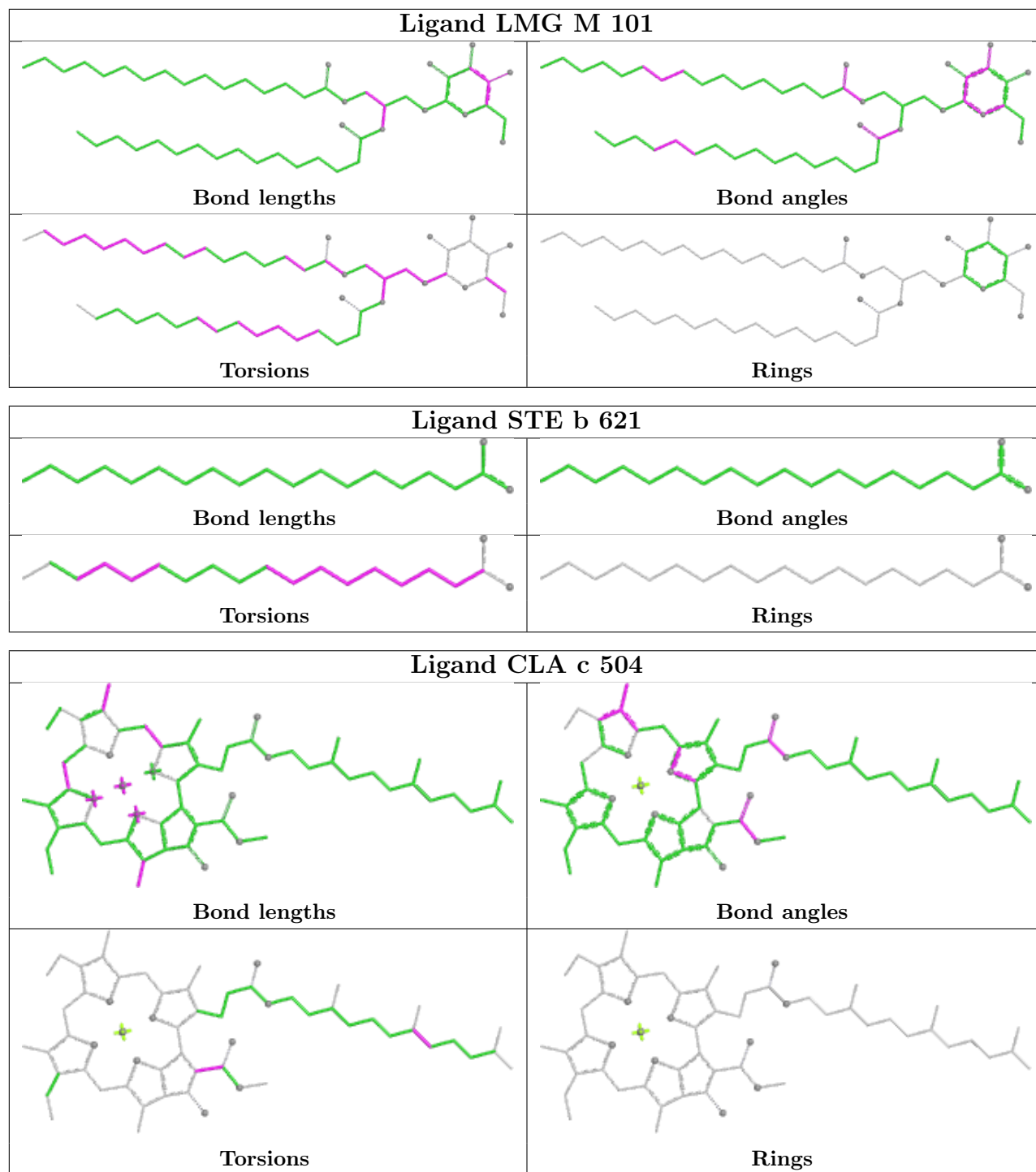




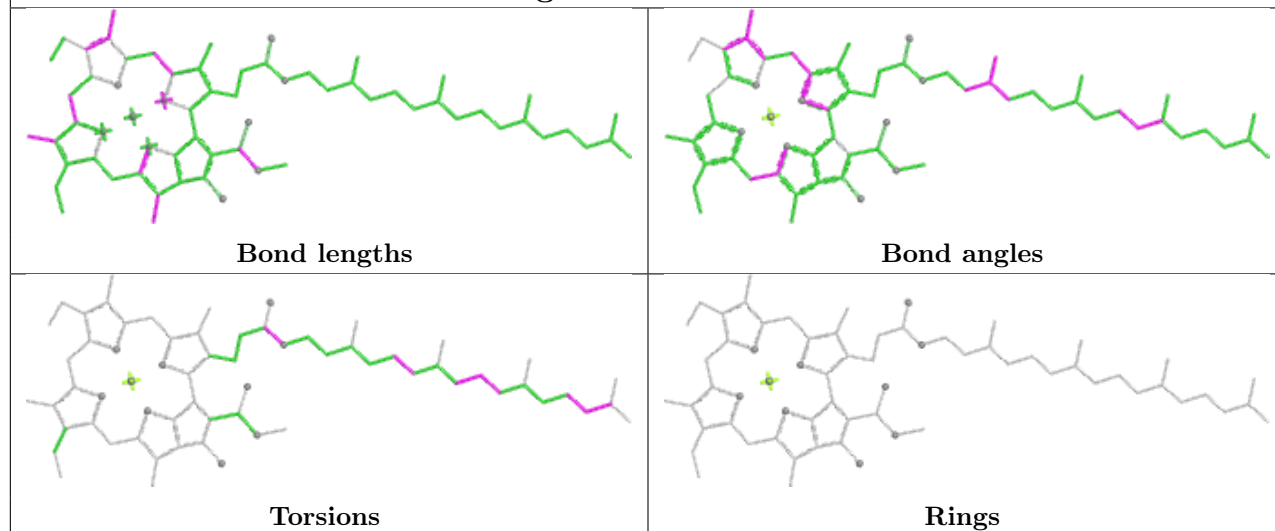
| Ligand BCR H 101 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand BCR b 617 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

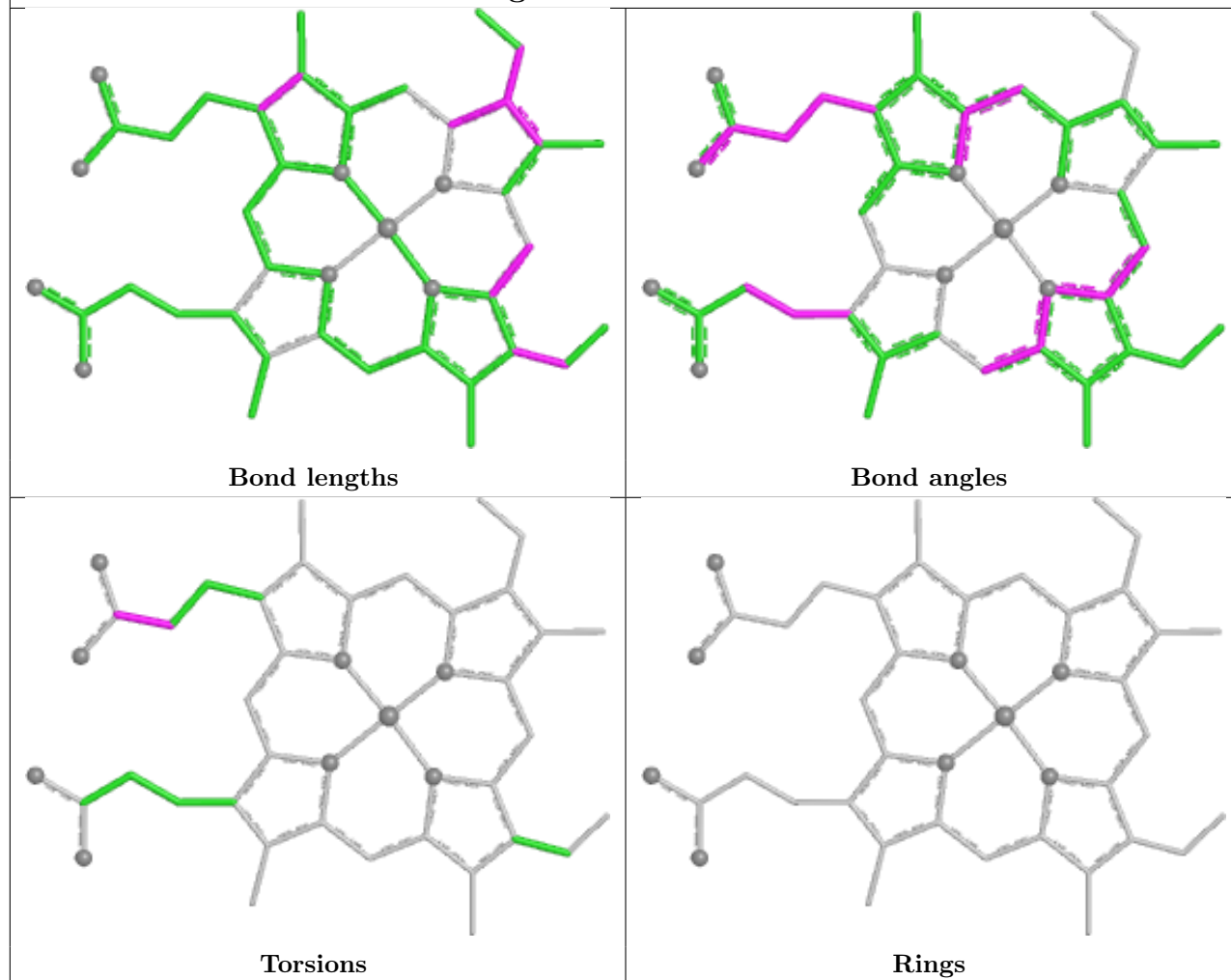
| Ligand CLA C 503 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

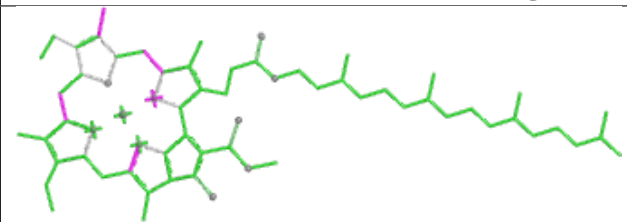
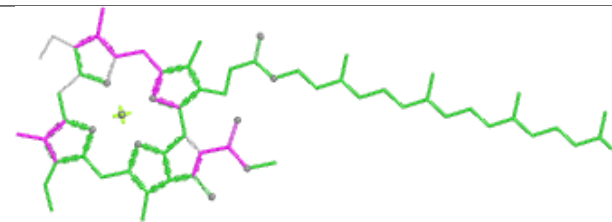
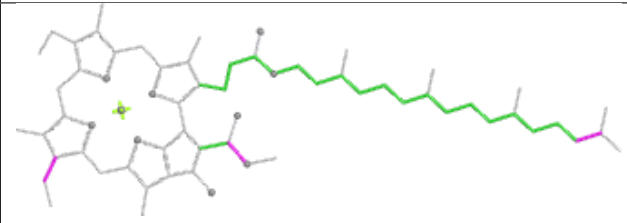
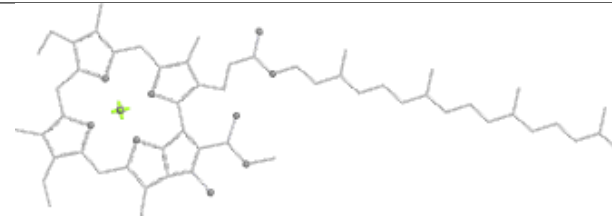





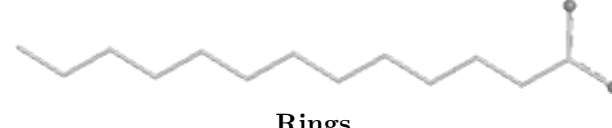
Ligand CLA c 503


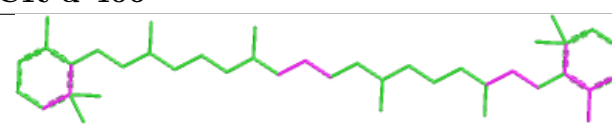
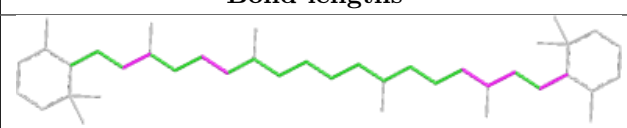
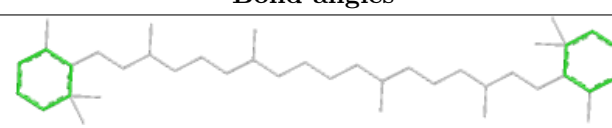




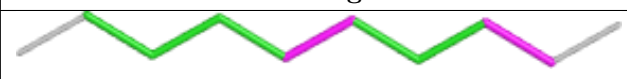

Ligand HEM E 101

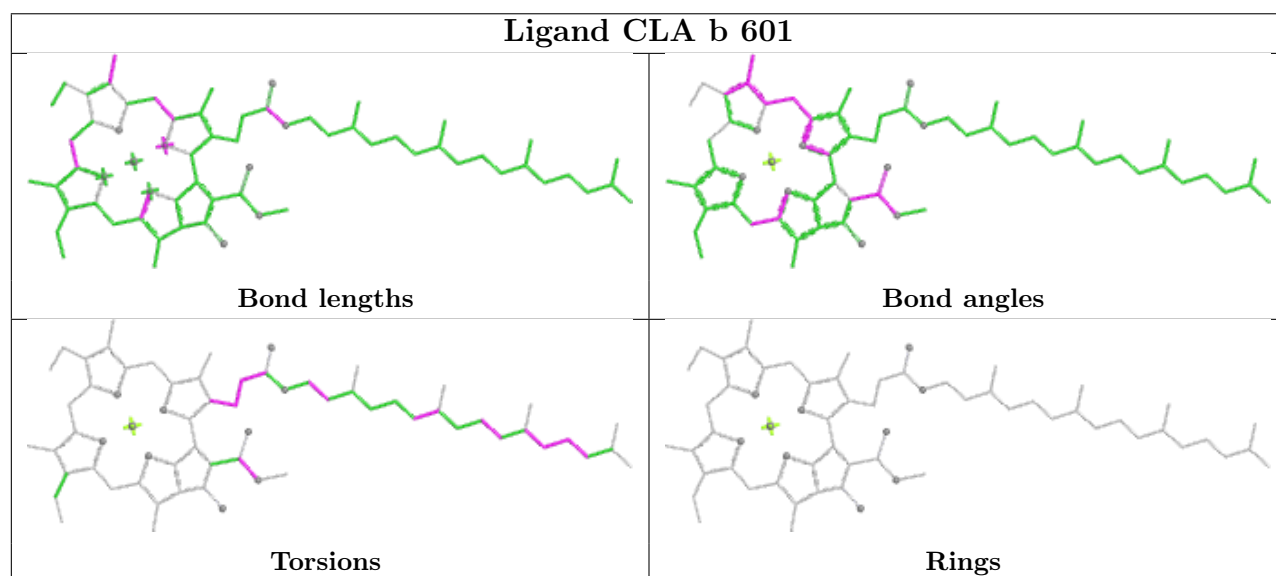
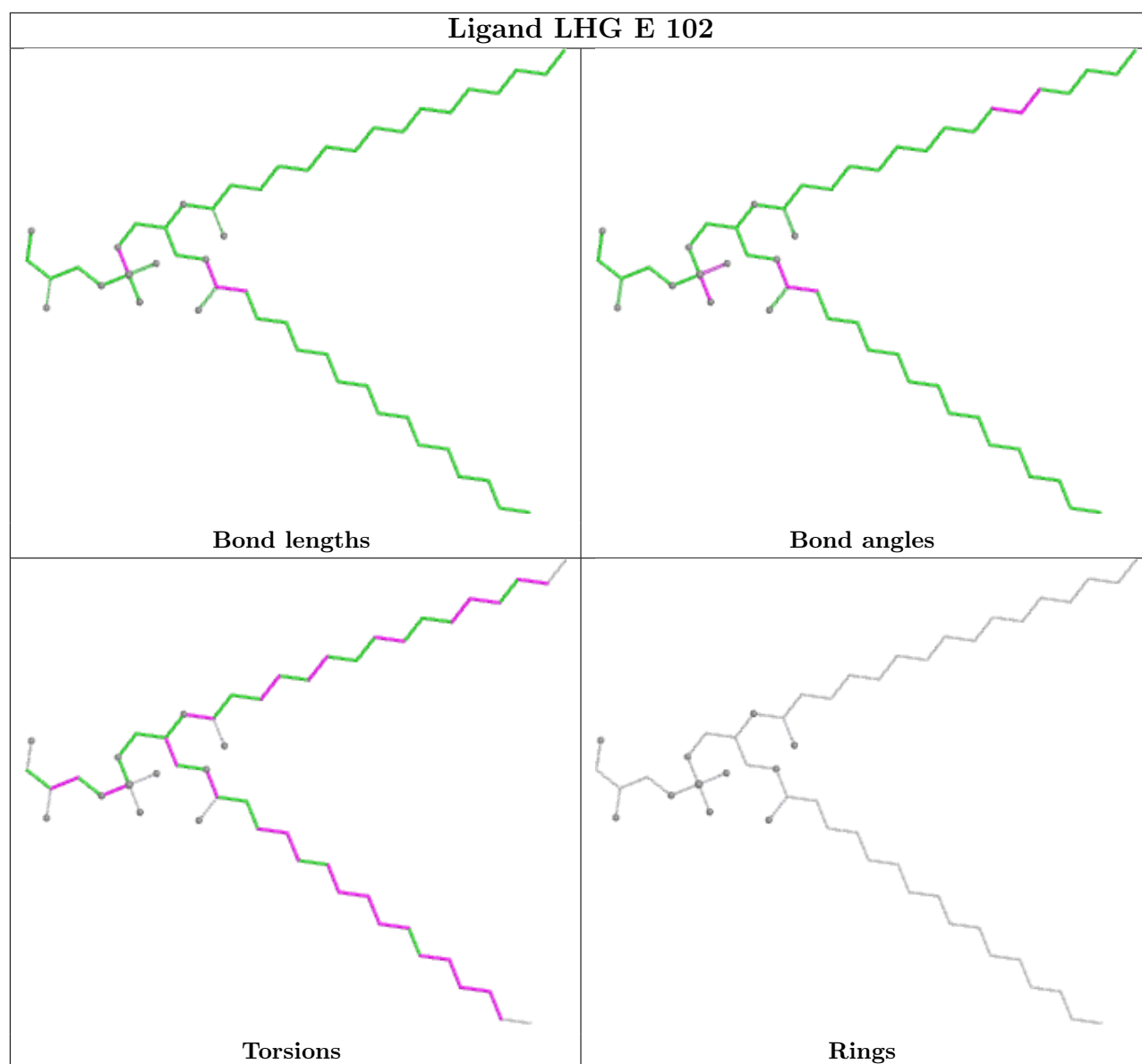


| Ligand CLA d 404 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

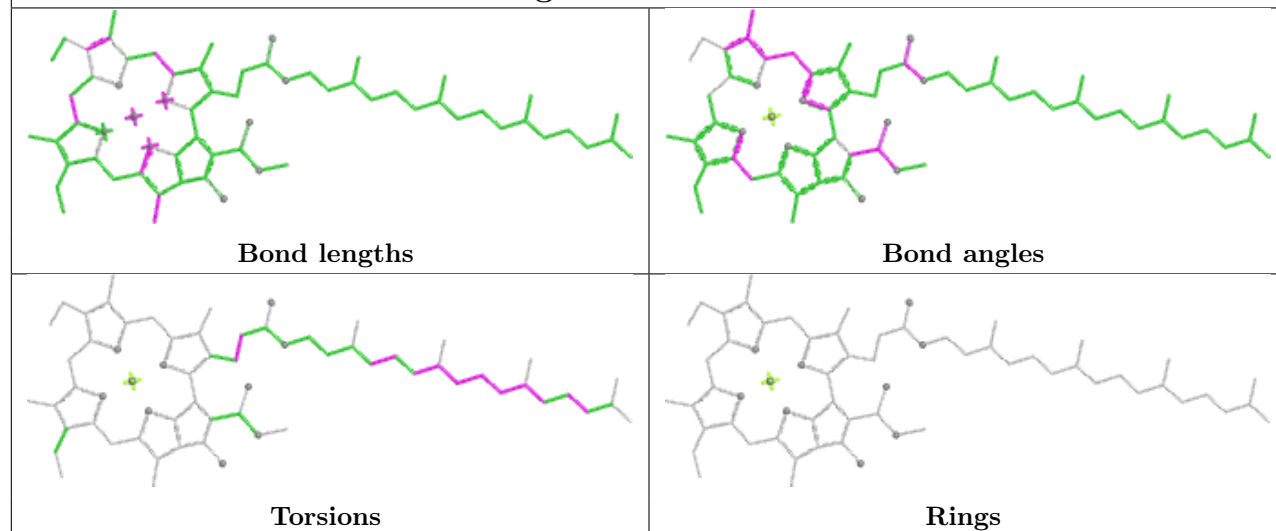
| Ligand STE M 102 | |
|--|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand BCR d 406 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

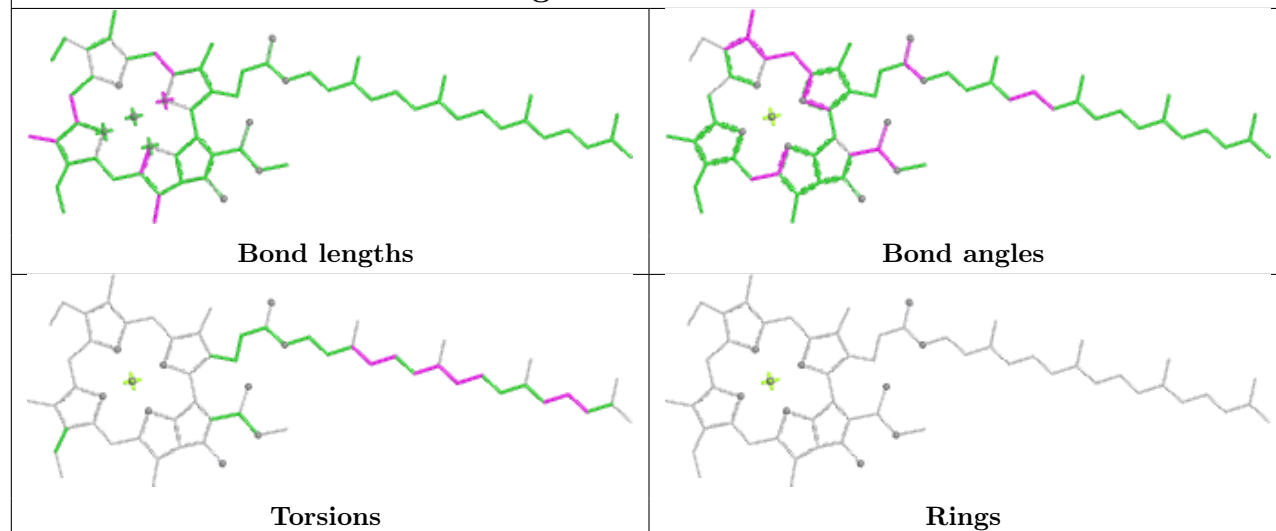
| Ligand STE M 103 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |



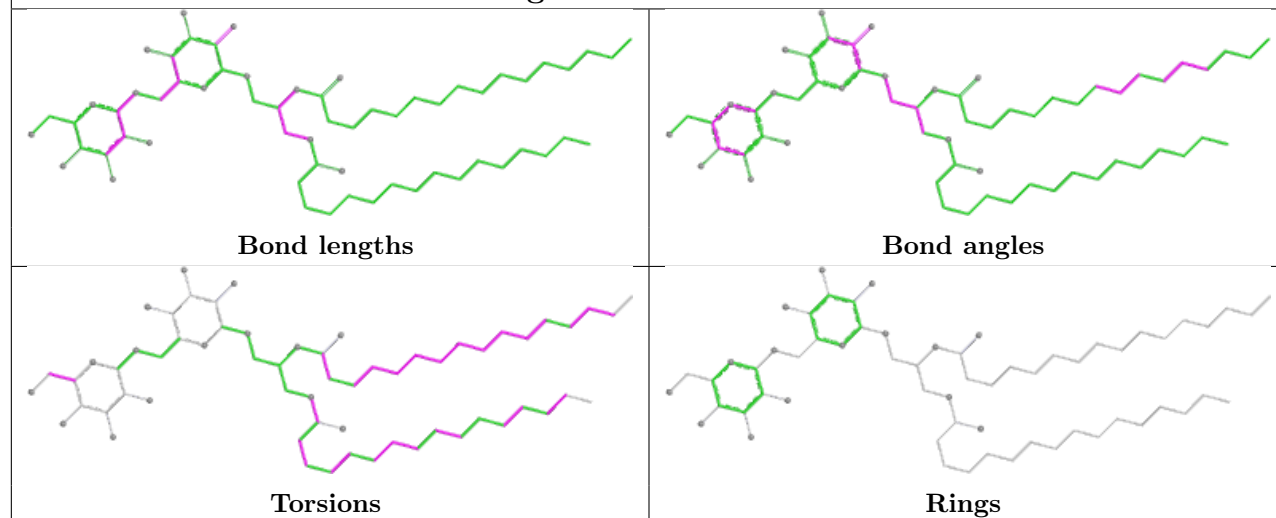
Ligand CLA b 606



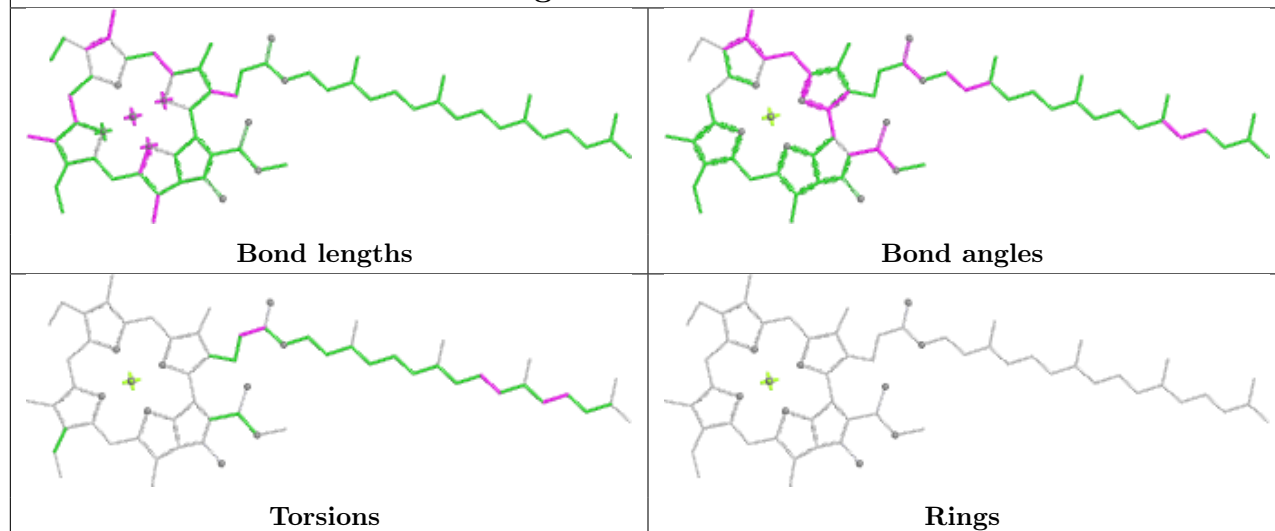
Ligand CLA C 510



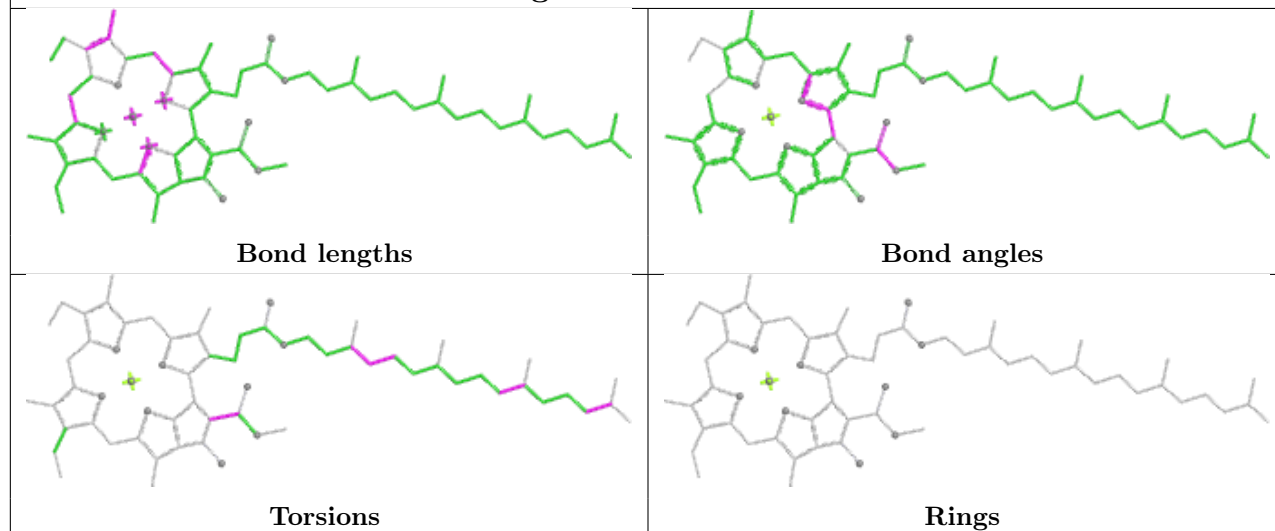
Ligand DGD H 102



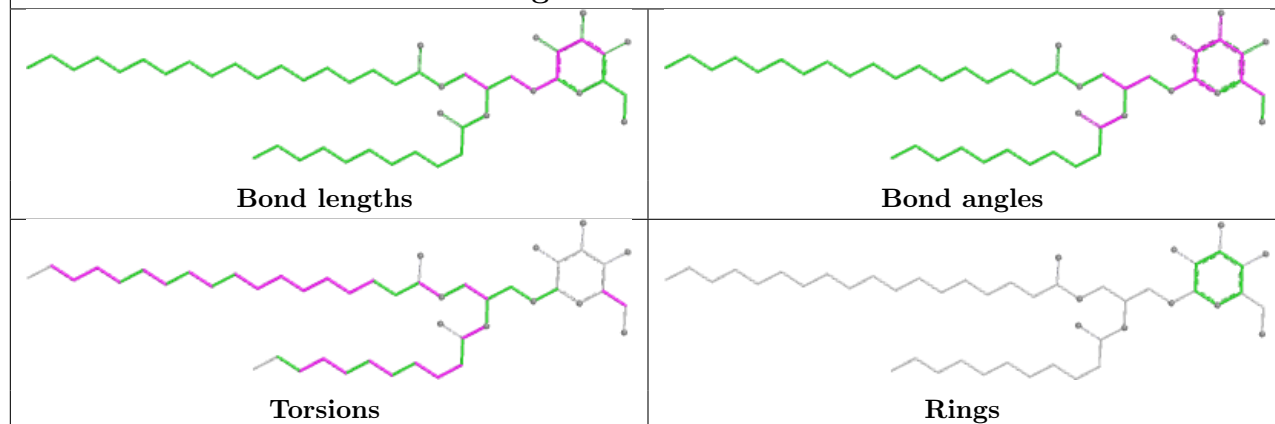
Ligand CLA b 613

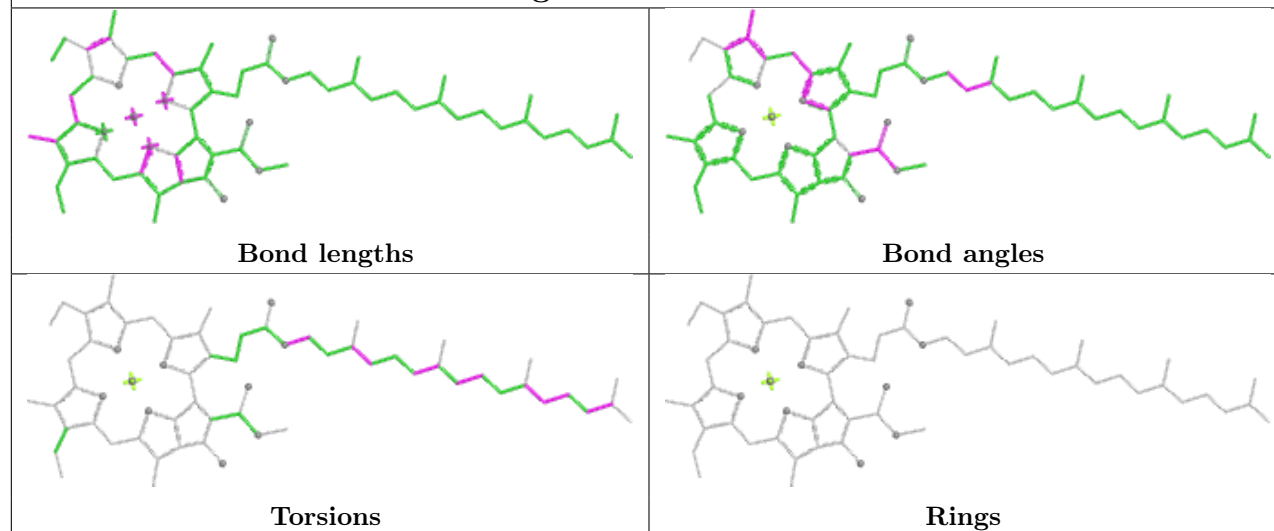
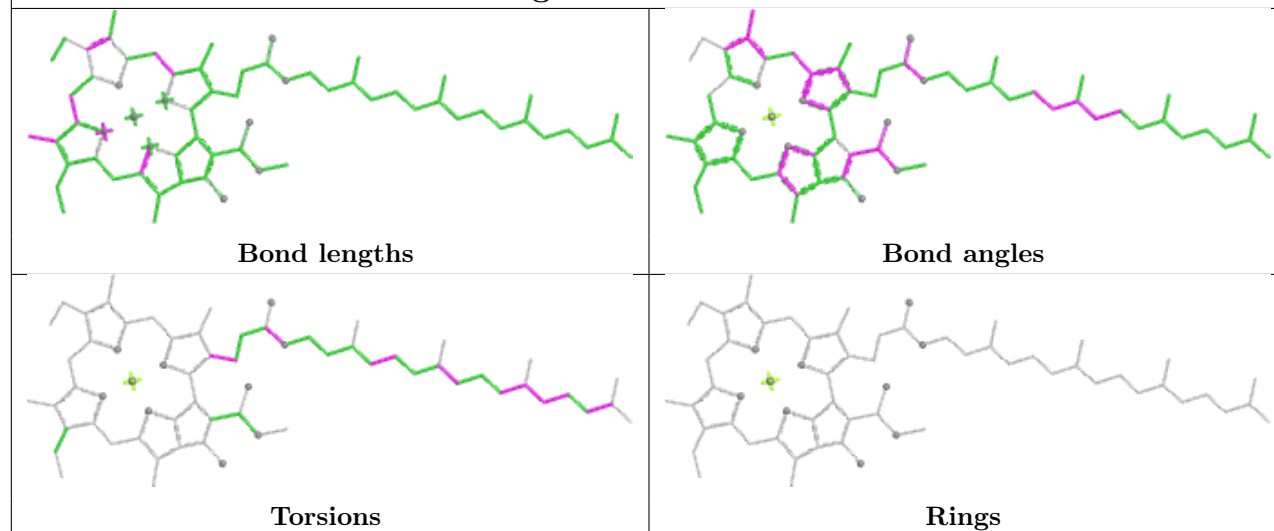


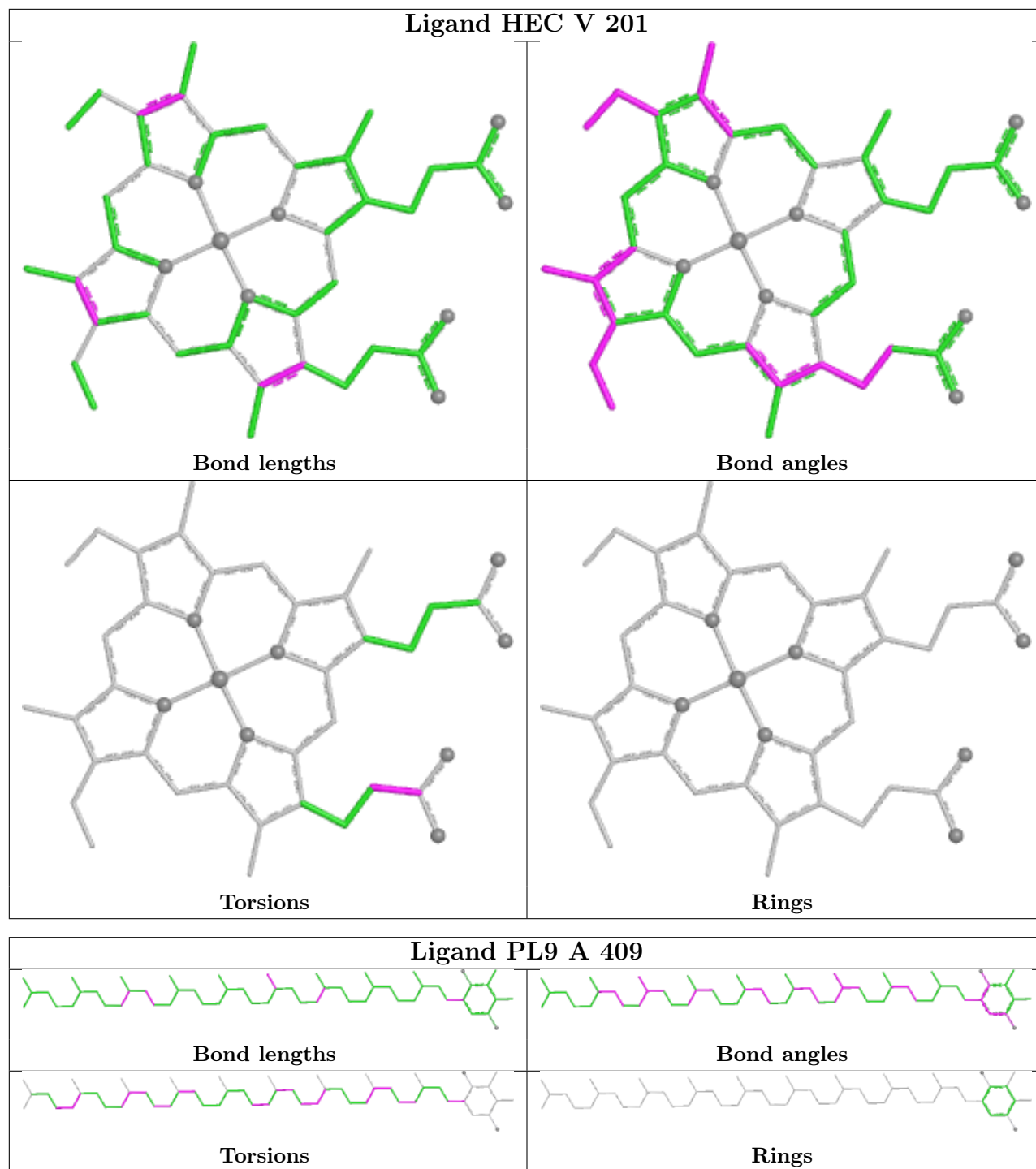
Ligand CLA C 502

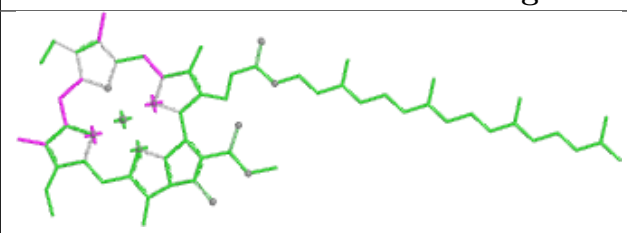
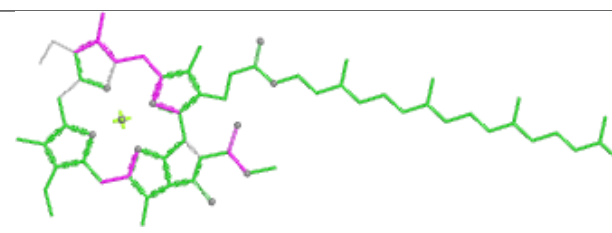
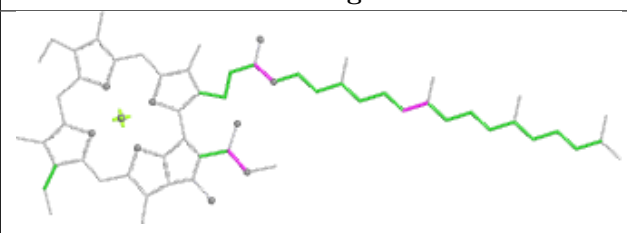
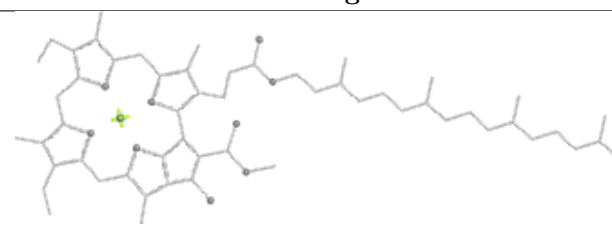




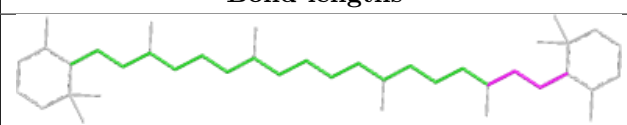
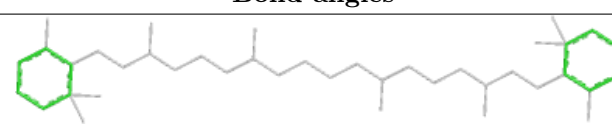
Ligand LMG c 522

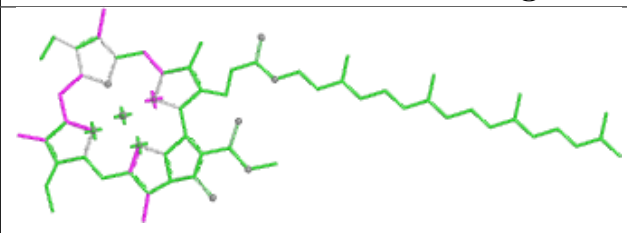
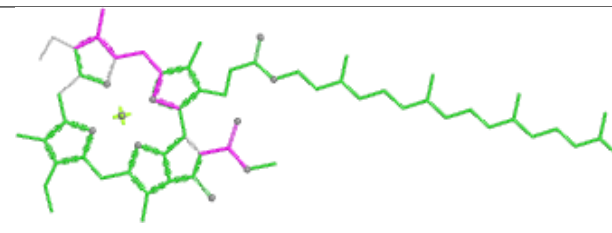
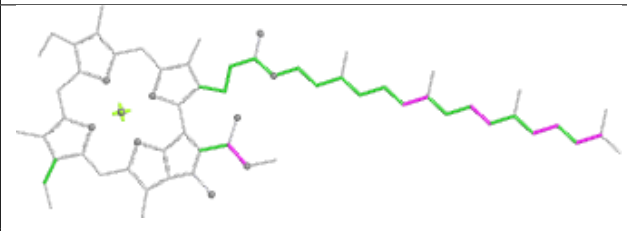
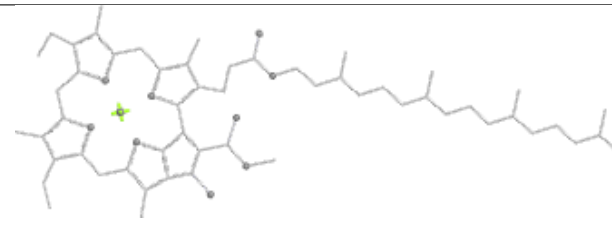




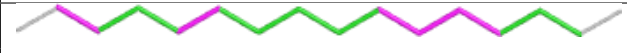

Ligand CLA C 506**Ligand CLA B 604**

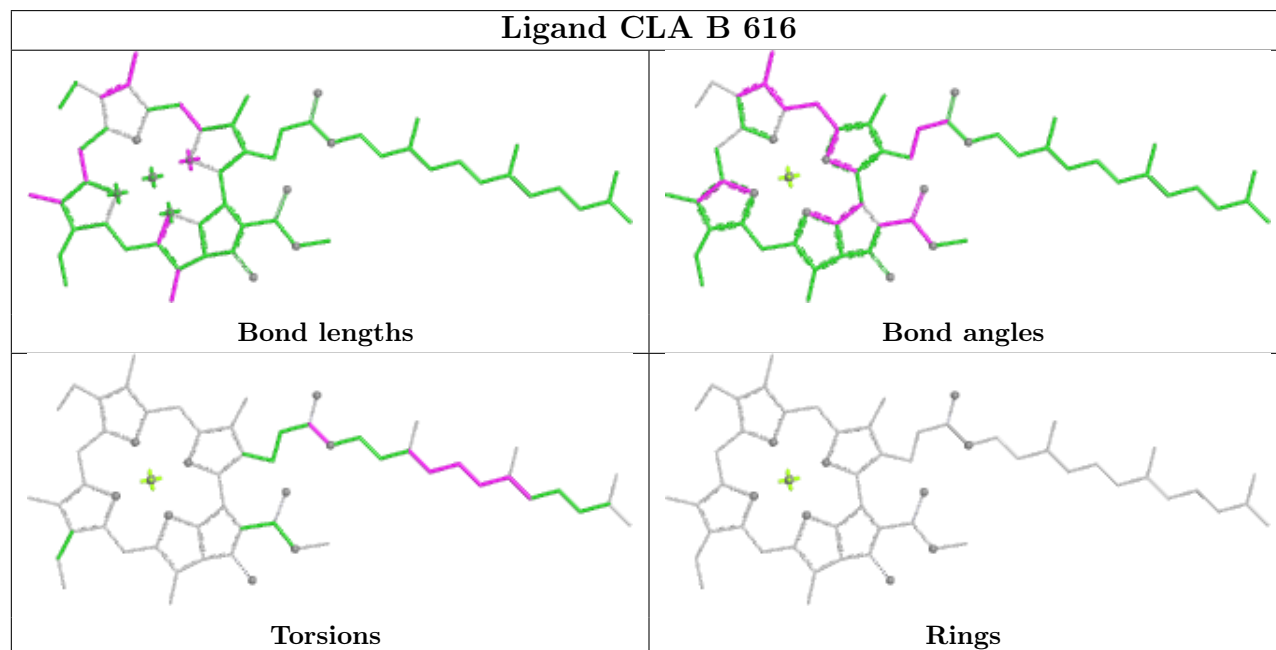
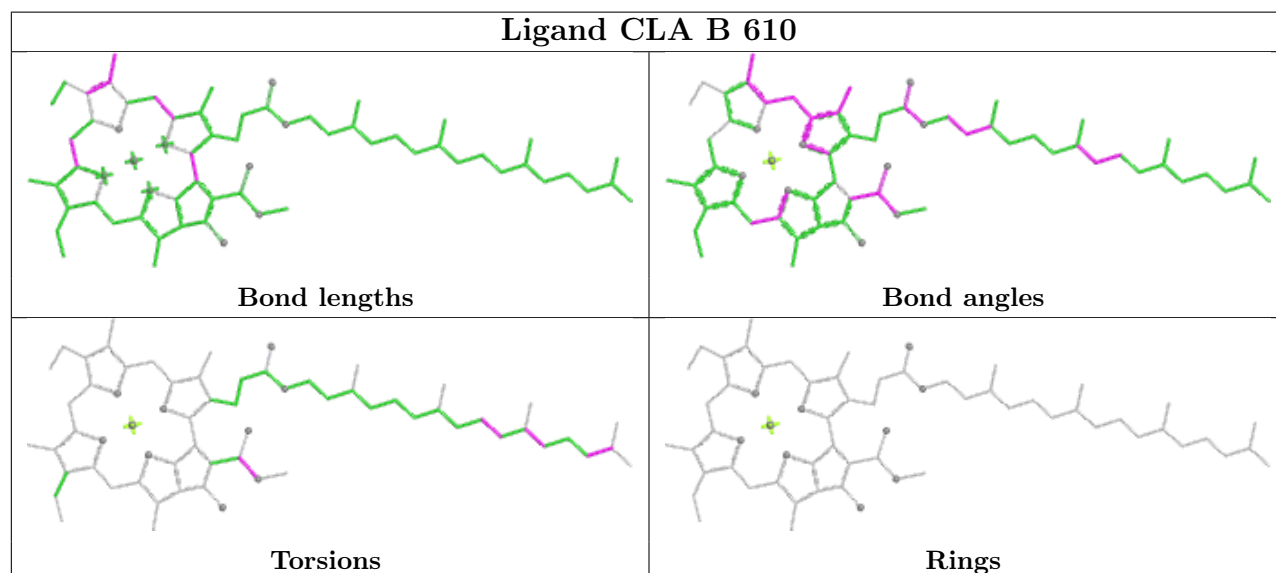
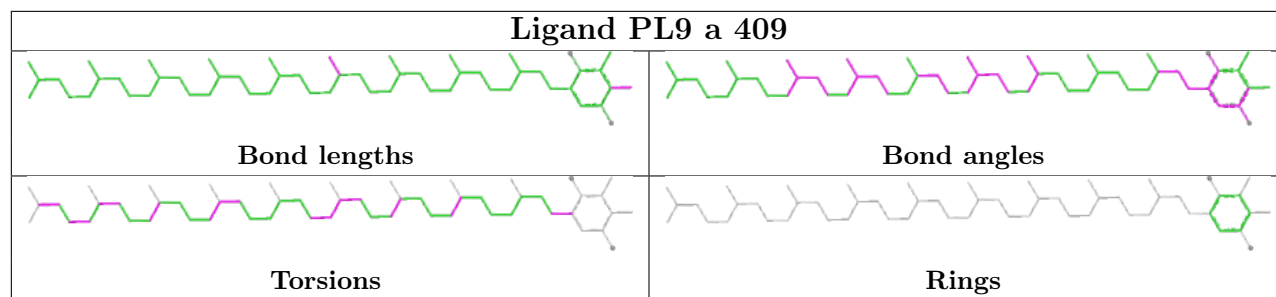


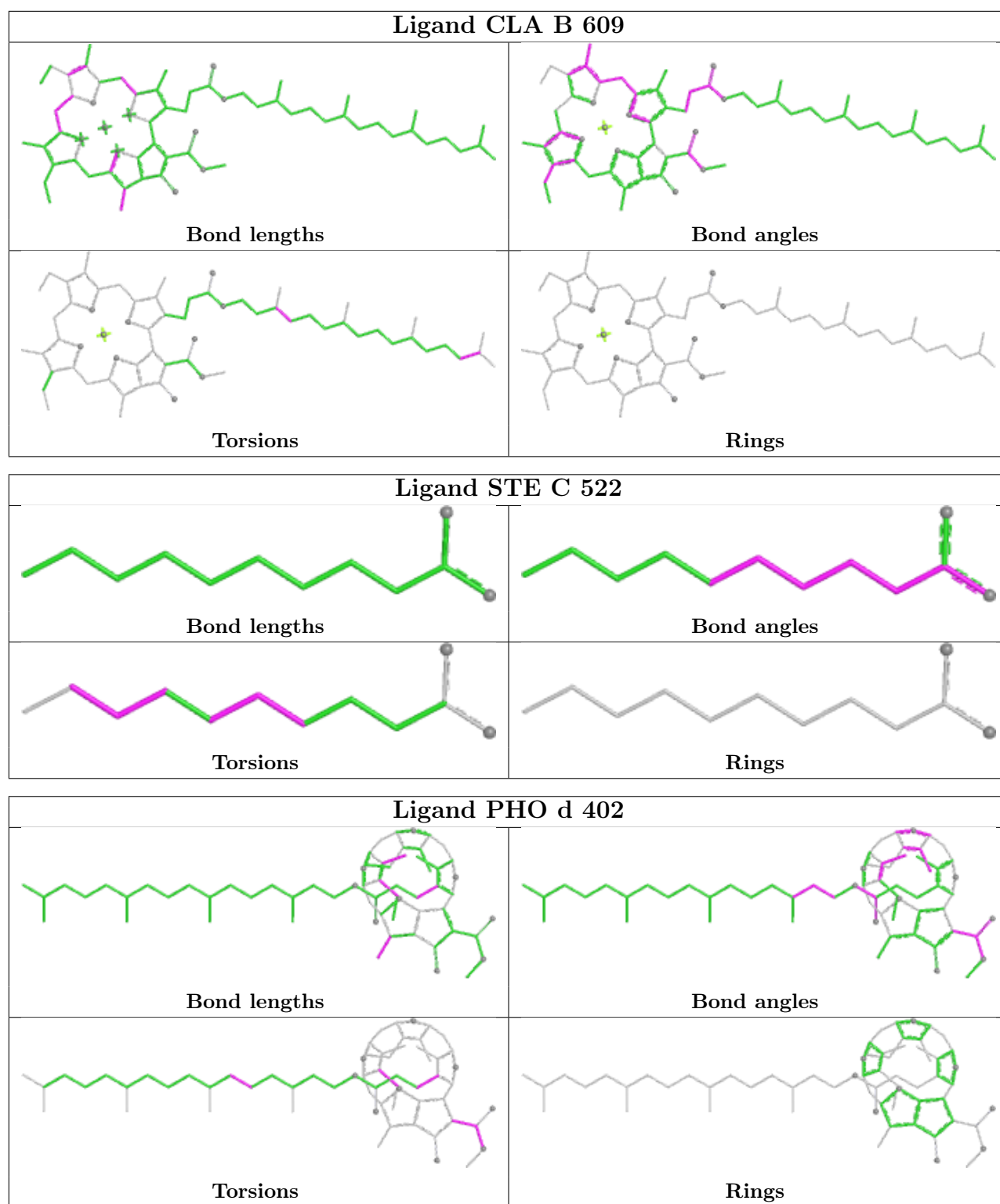
| Ligand CLA C 511 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

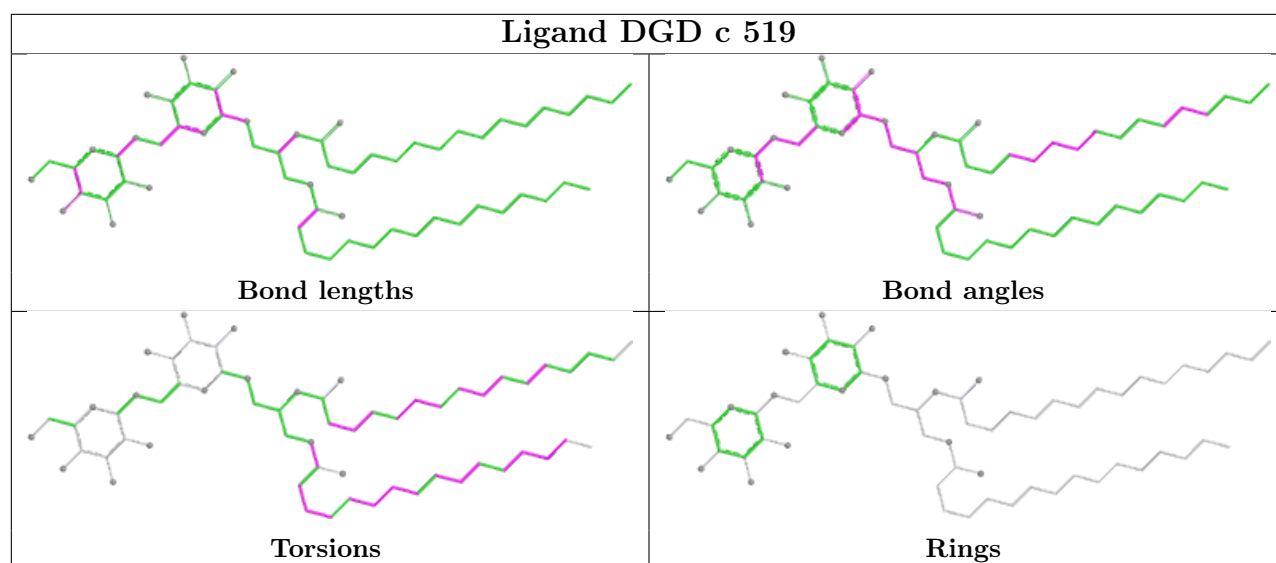
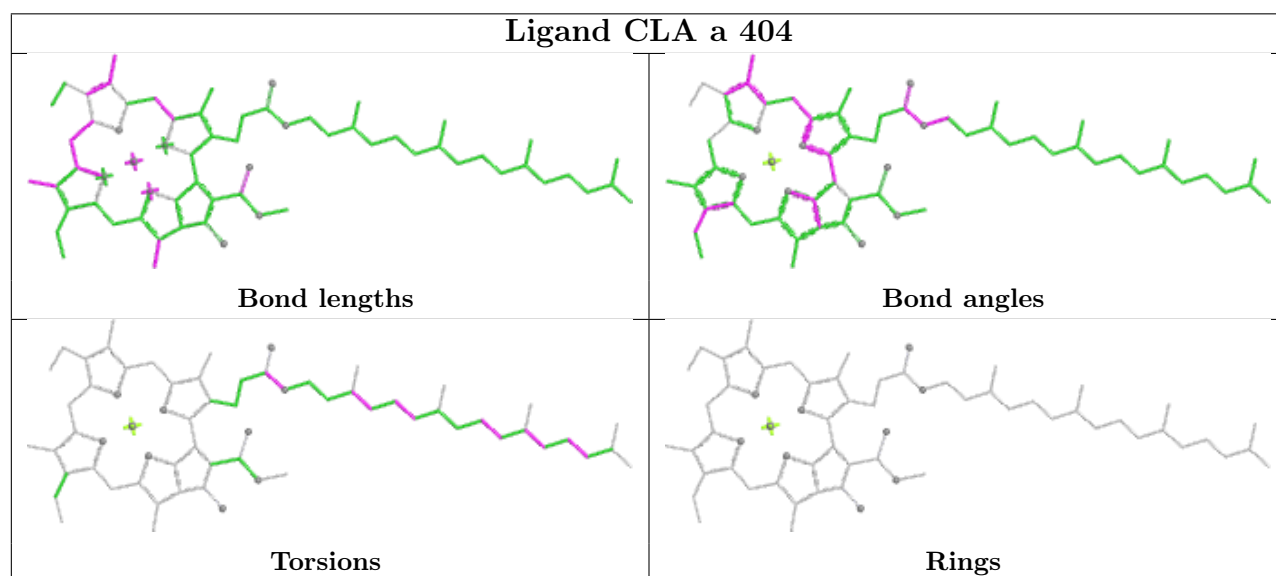
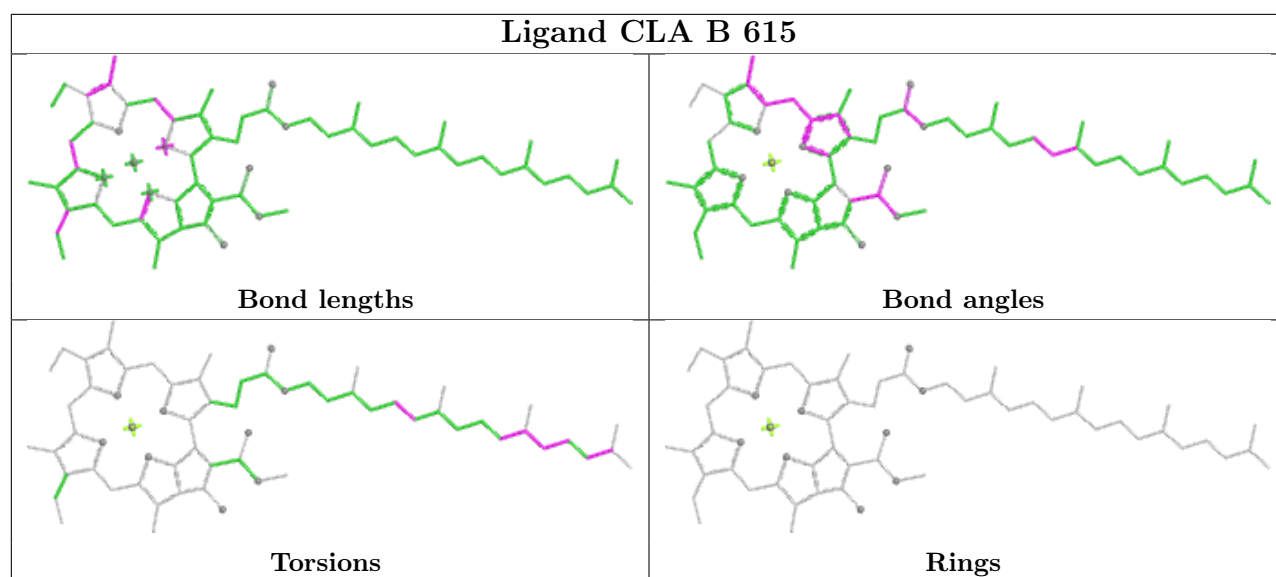
| Ligand BCR D 405 | |
|--|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

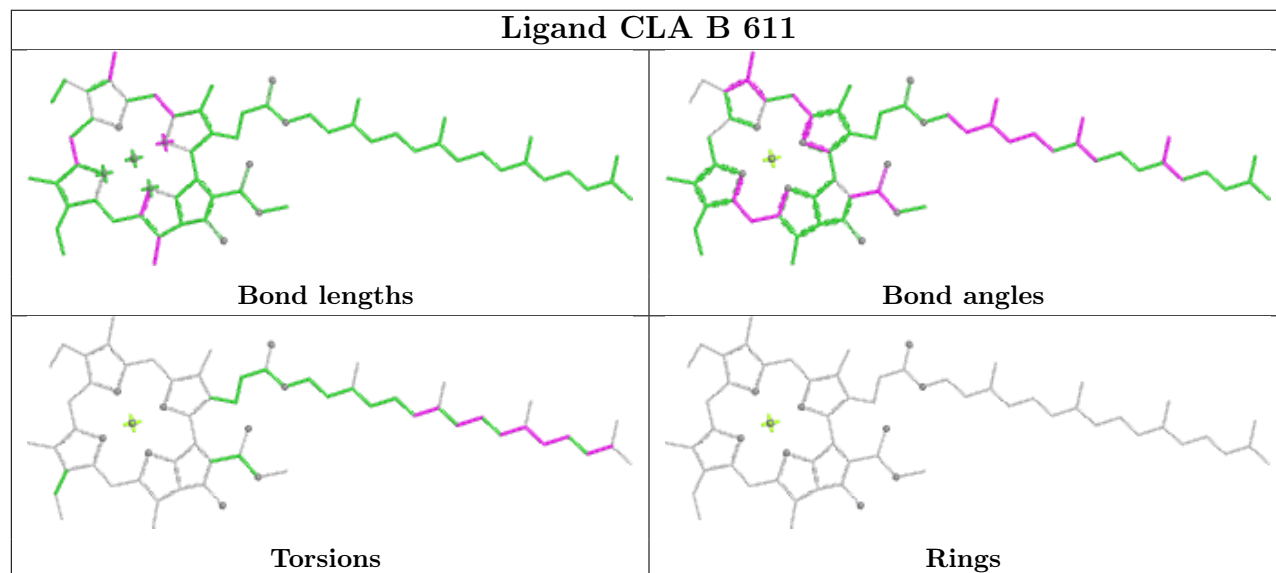
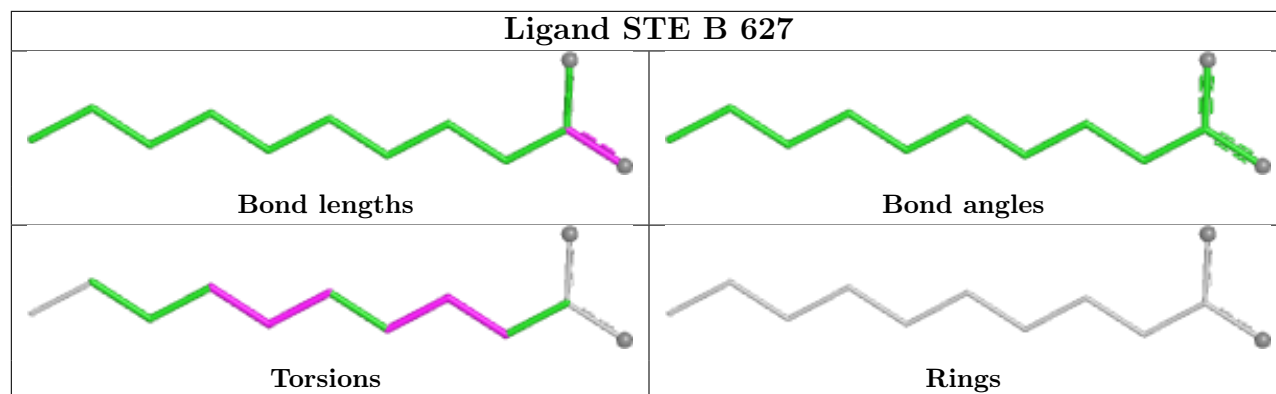
| Ligand CLA D 404 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

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

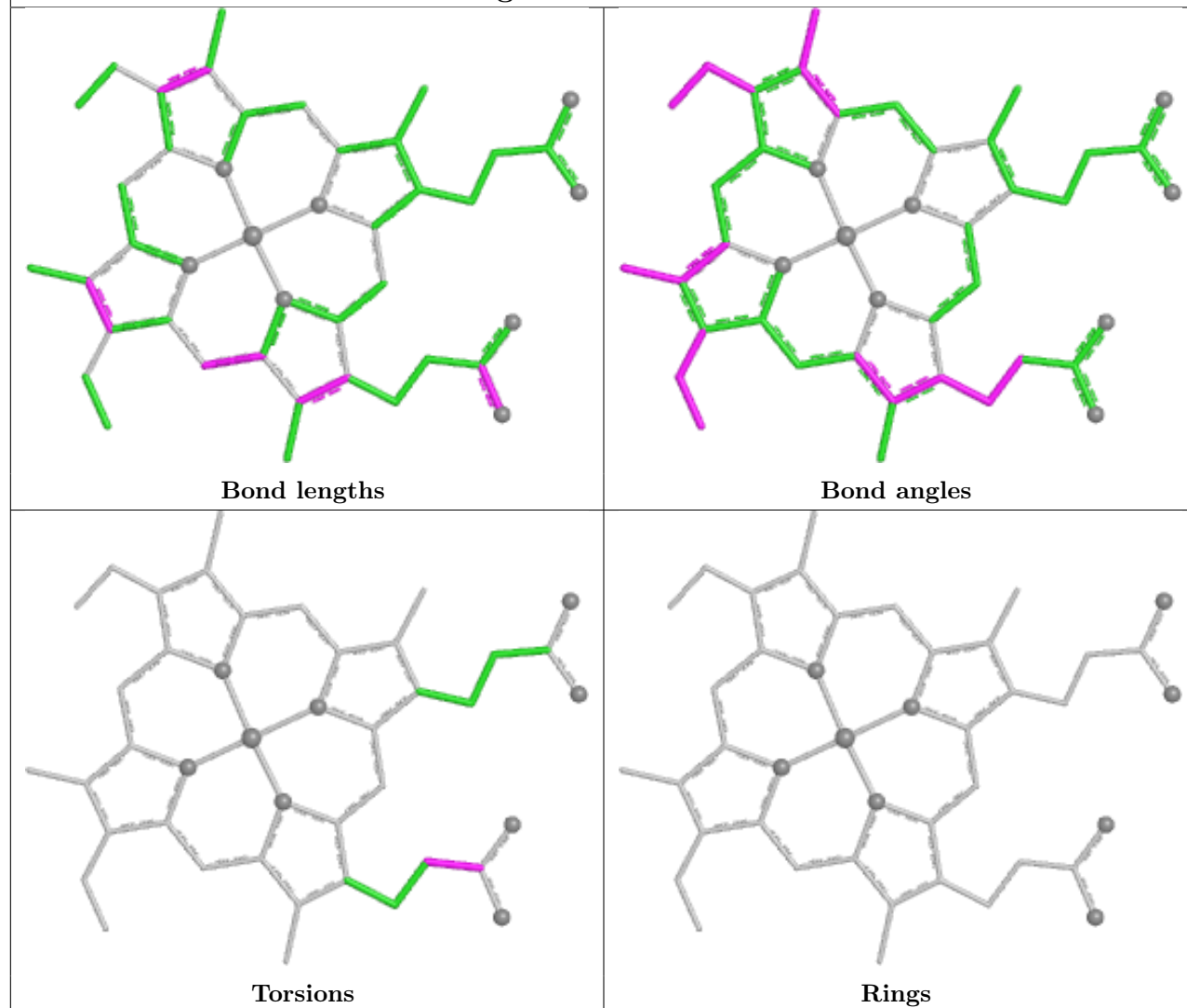




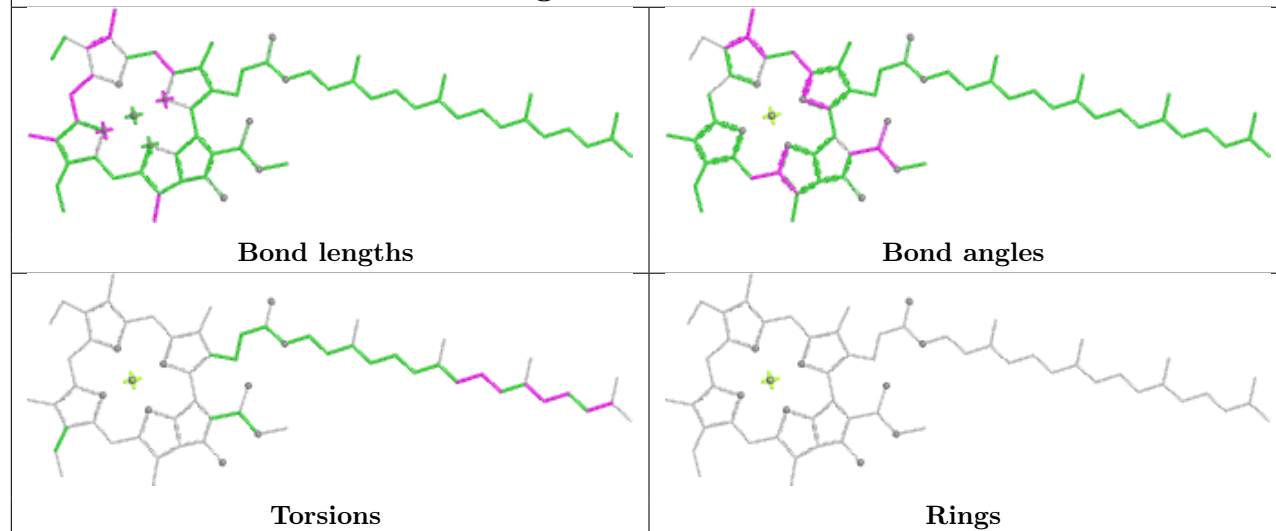




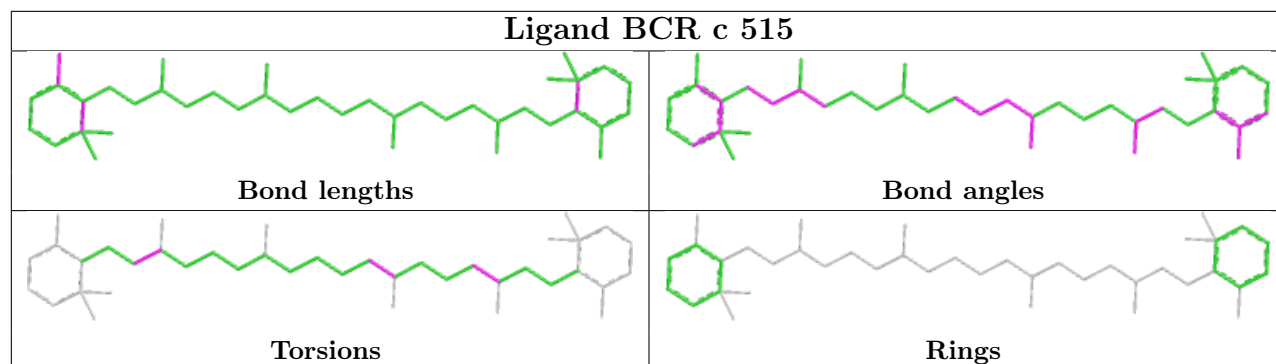
Ligand HEC v 201



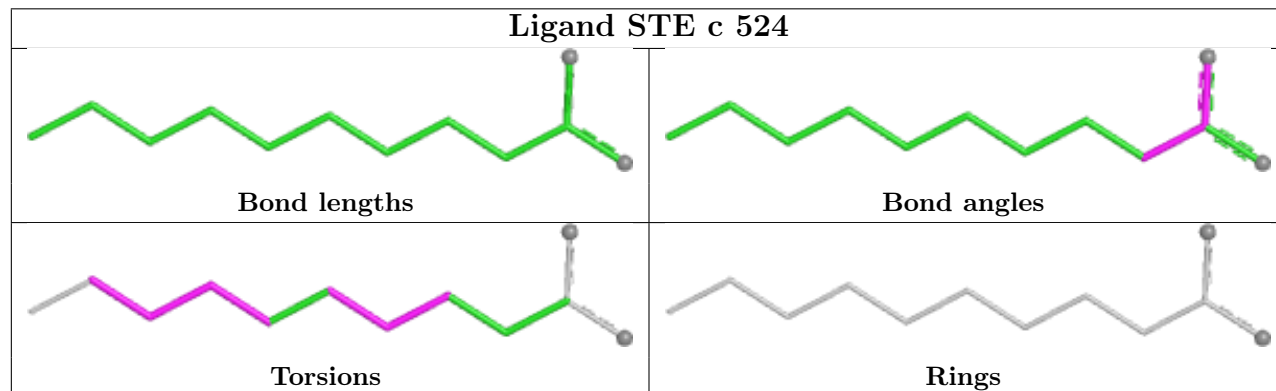
Ligand CLA b 611



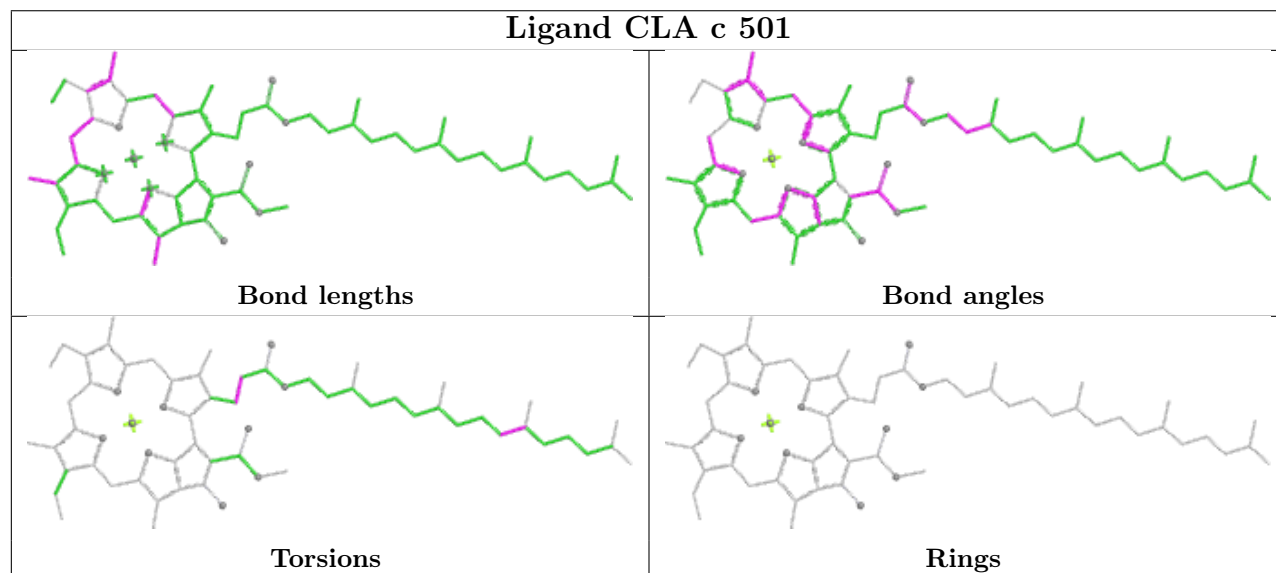
Ligand BCR c 515



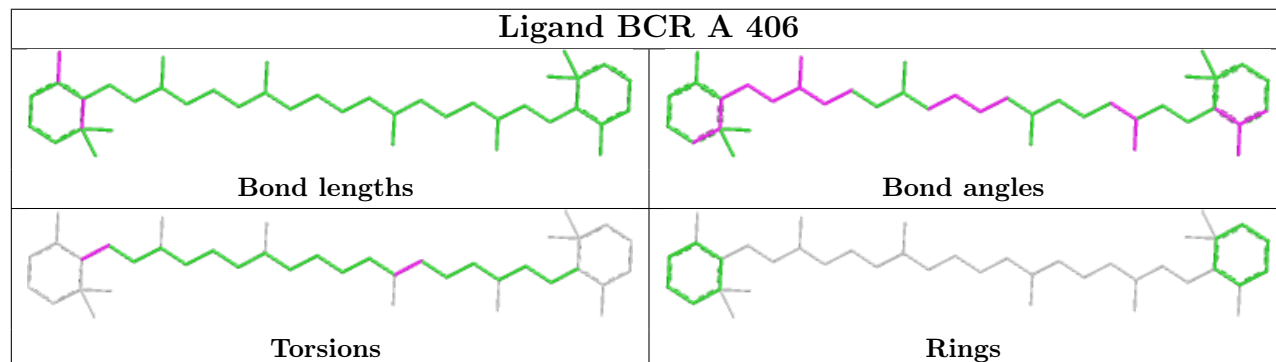
Ligand STE c 524



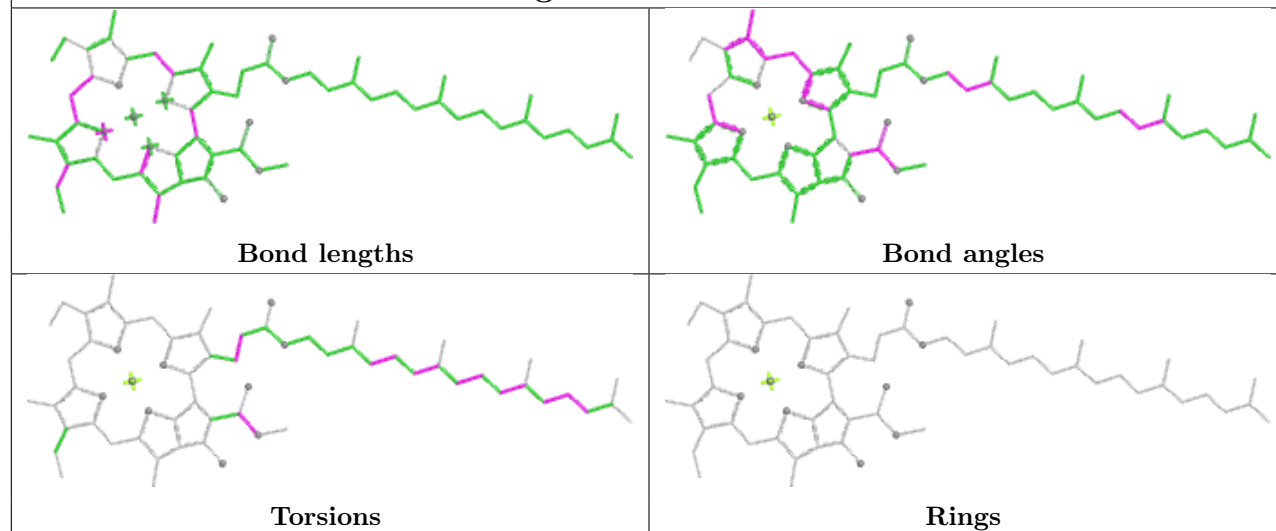
Ligand CLA c 501



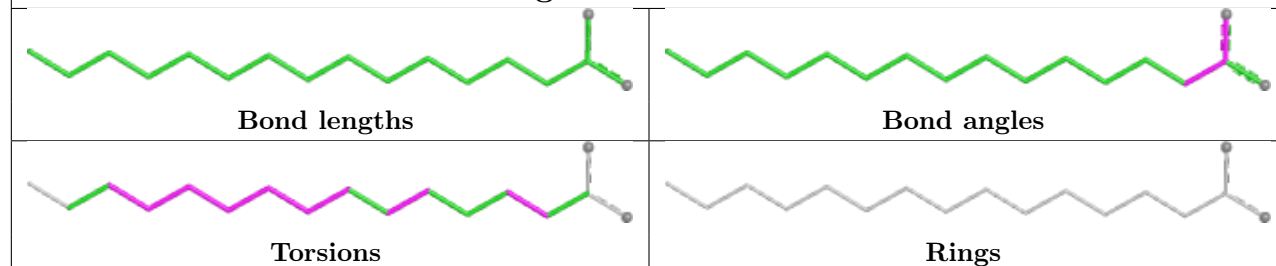
Ligand BCR A 406



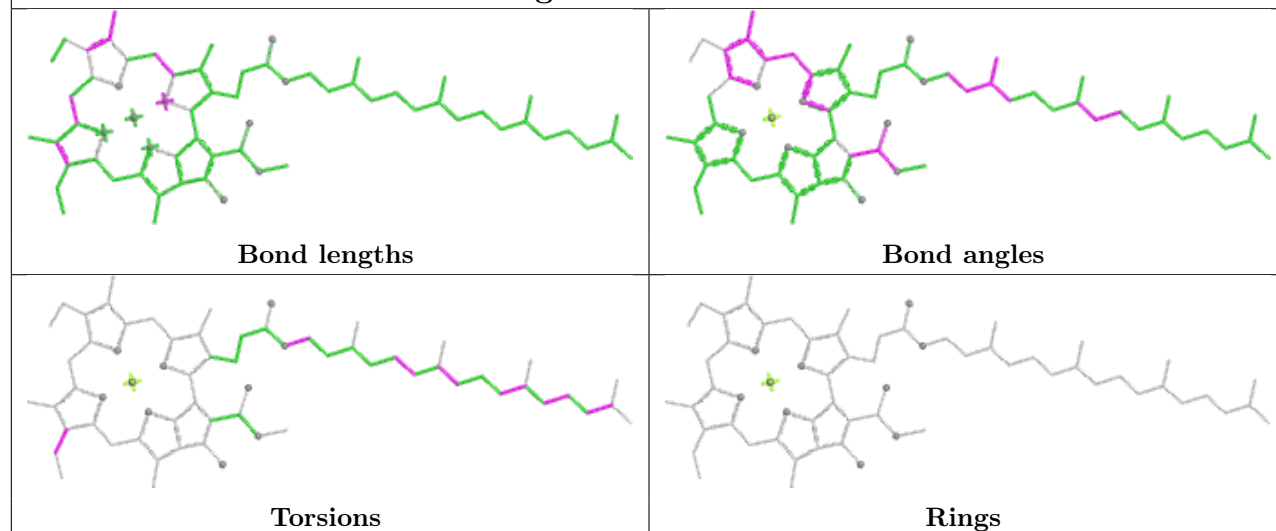
Ligand CLA b 602

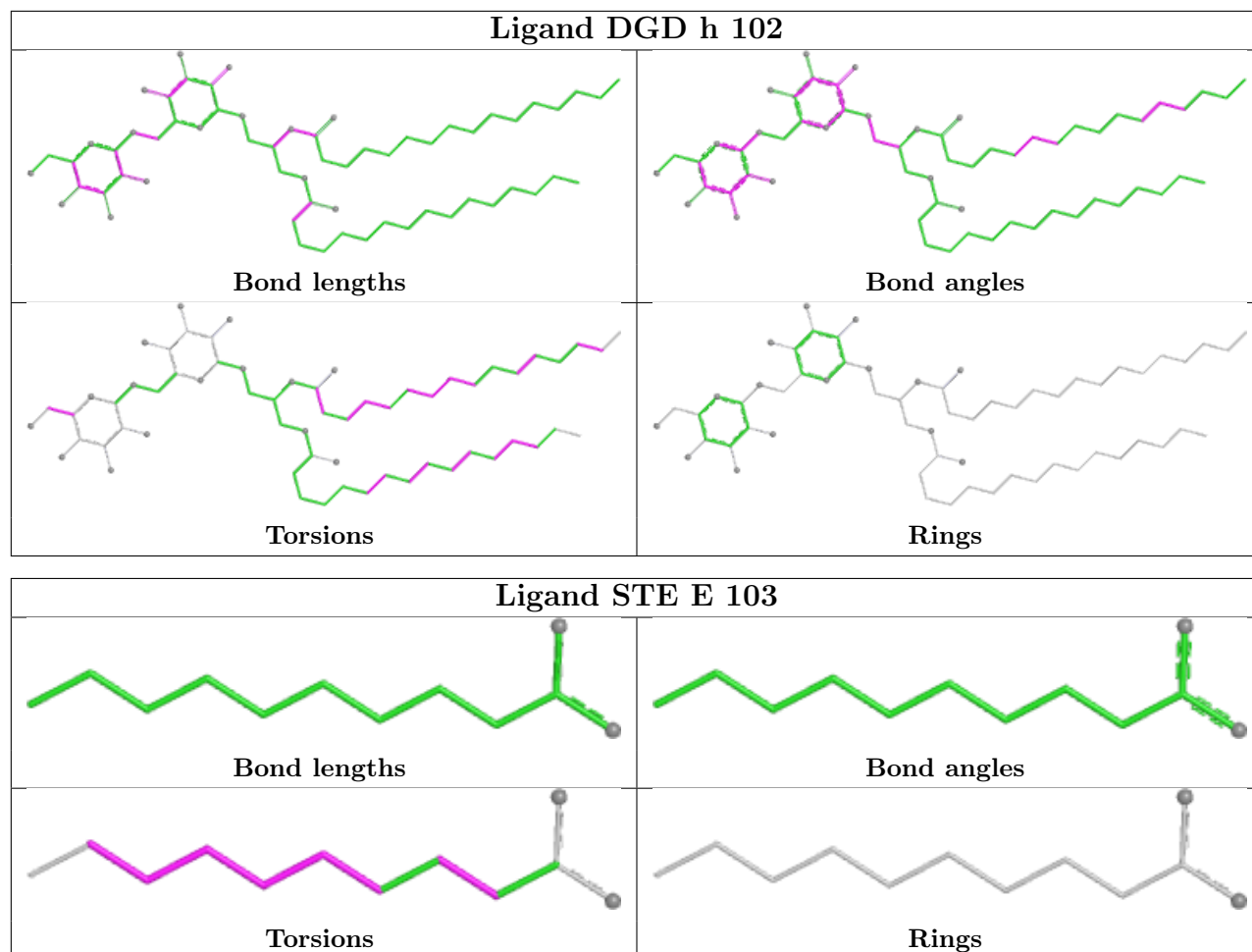


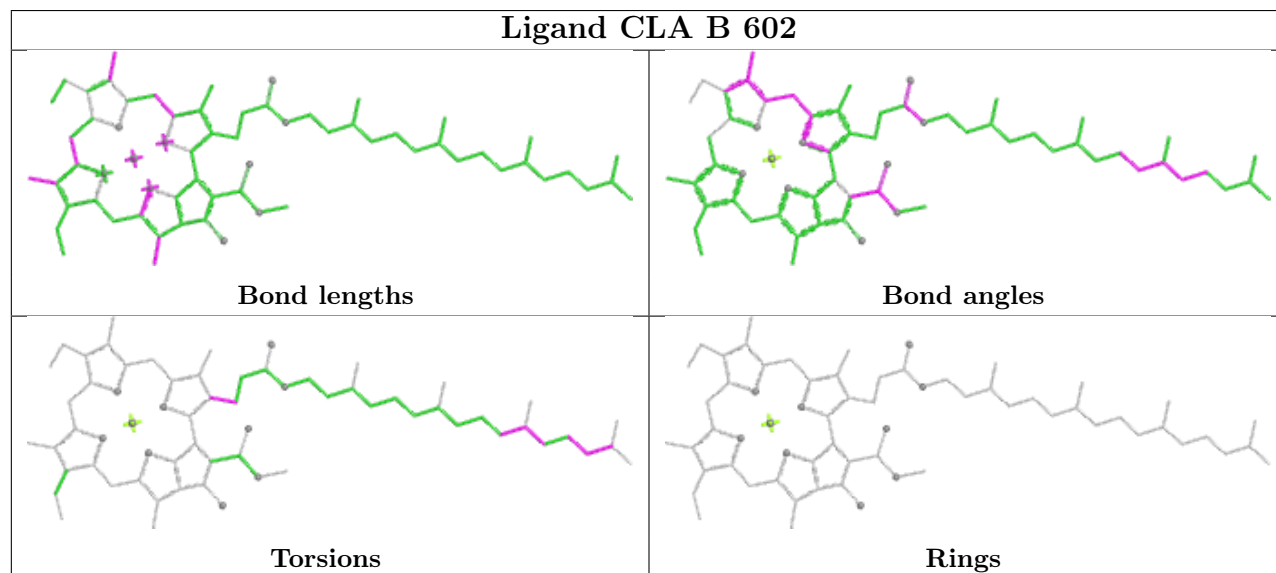
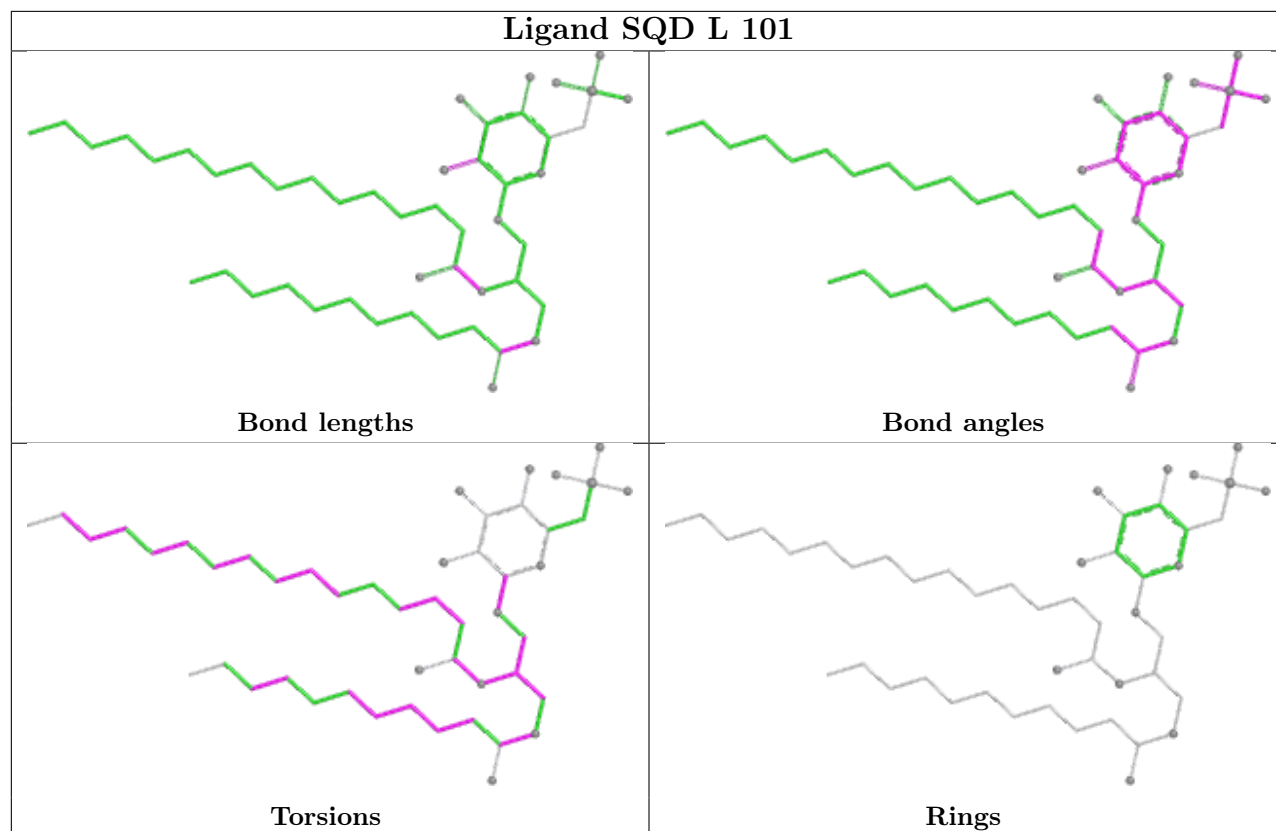
Ligand STE B 620

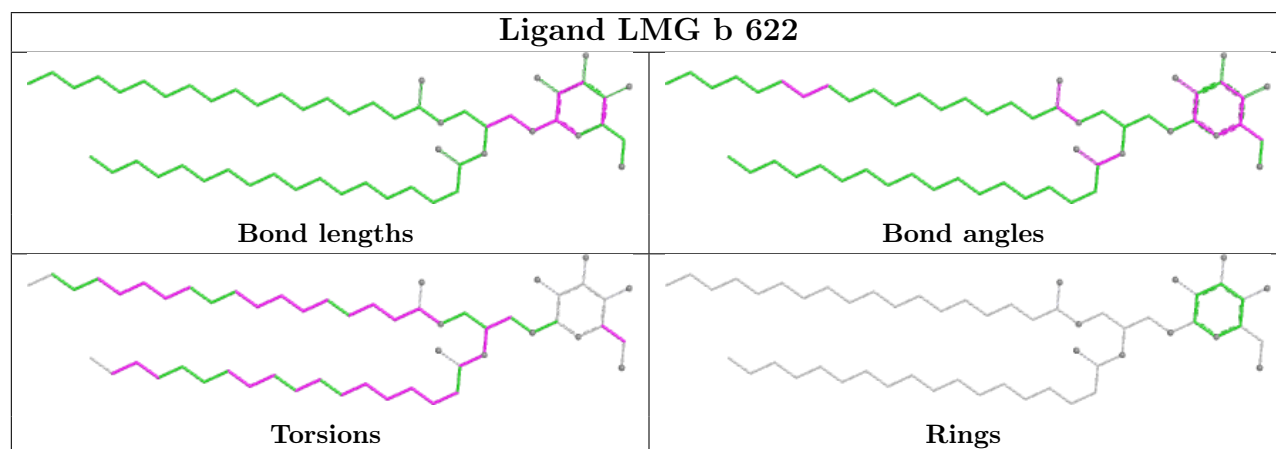
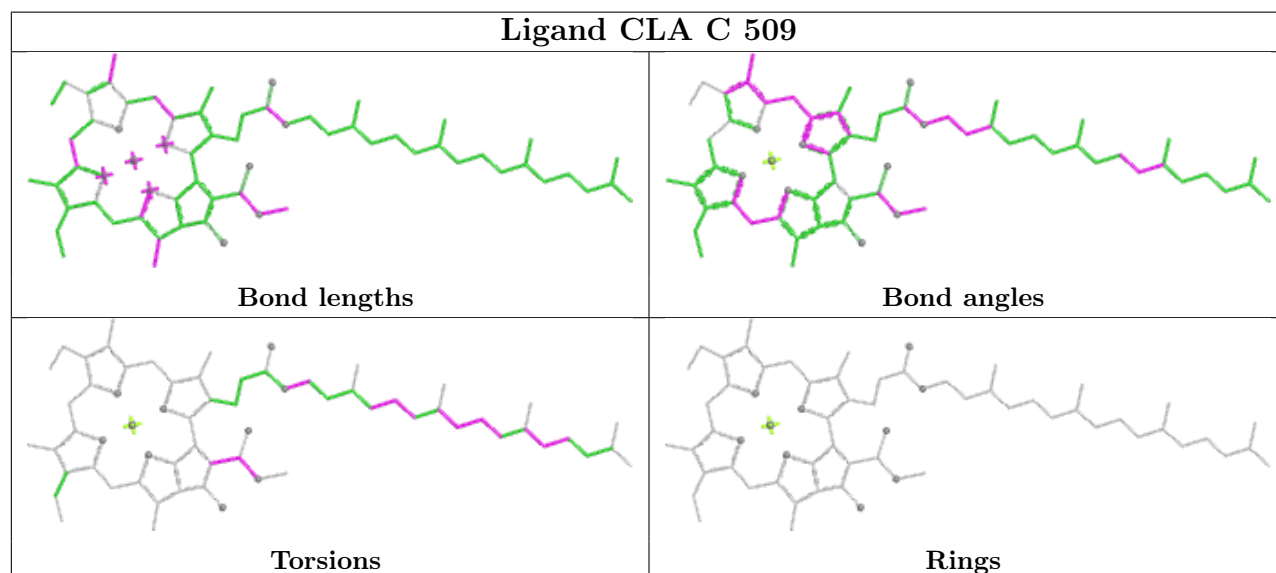
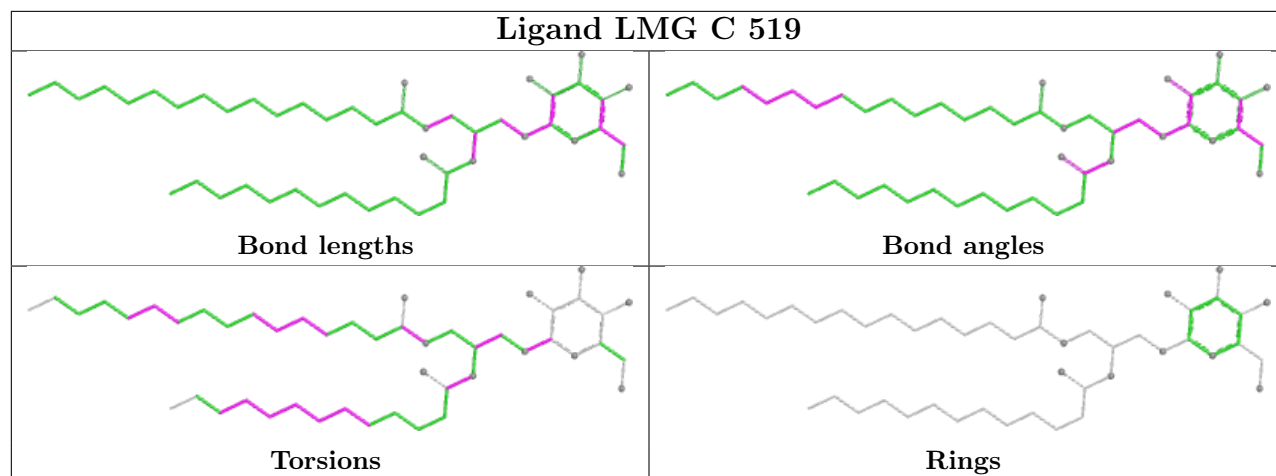


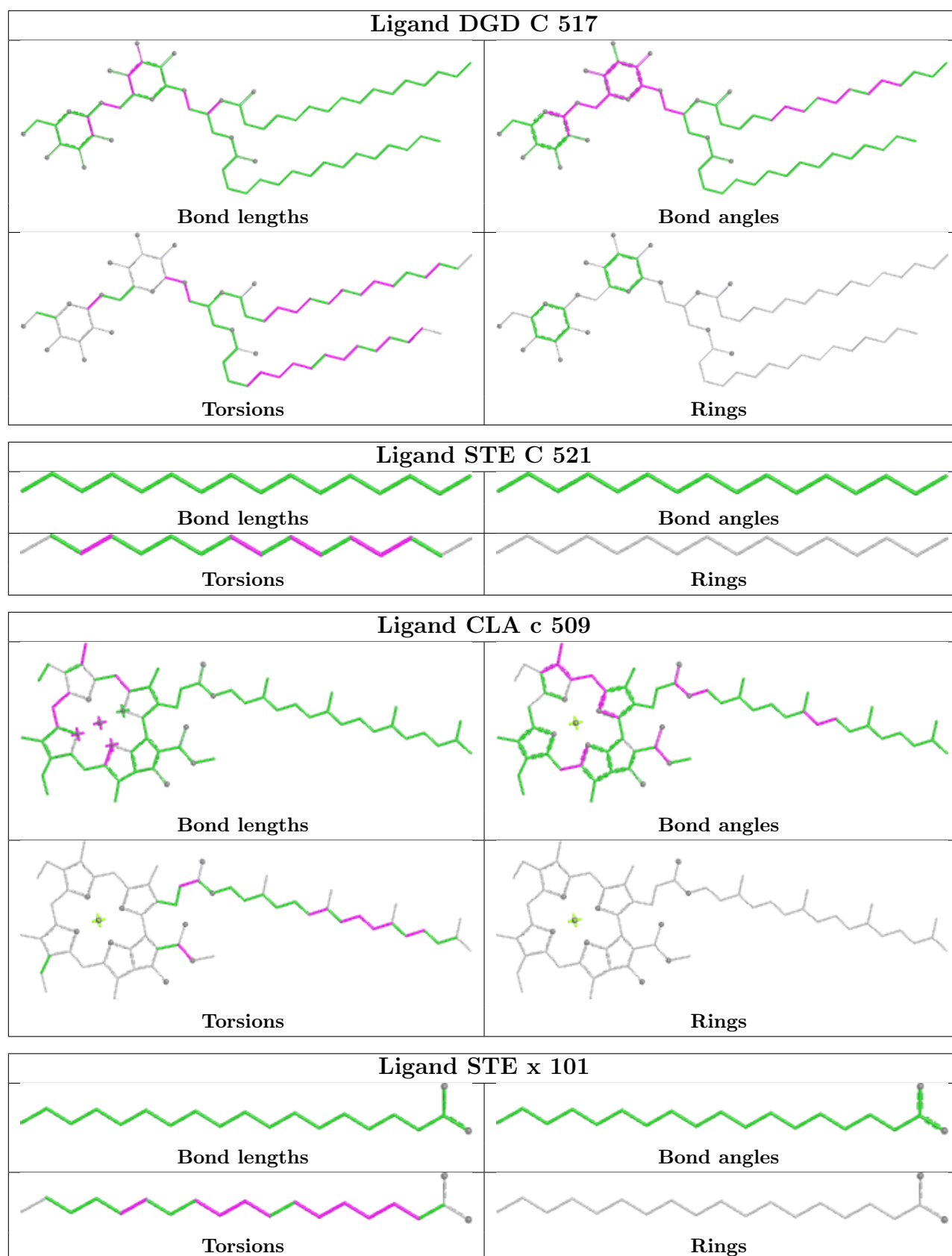
Ligand CLA b 608

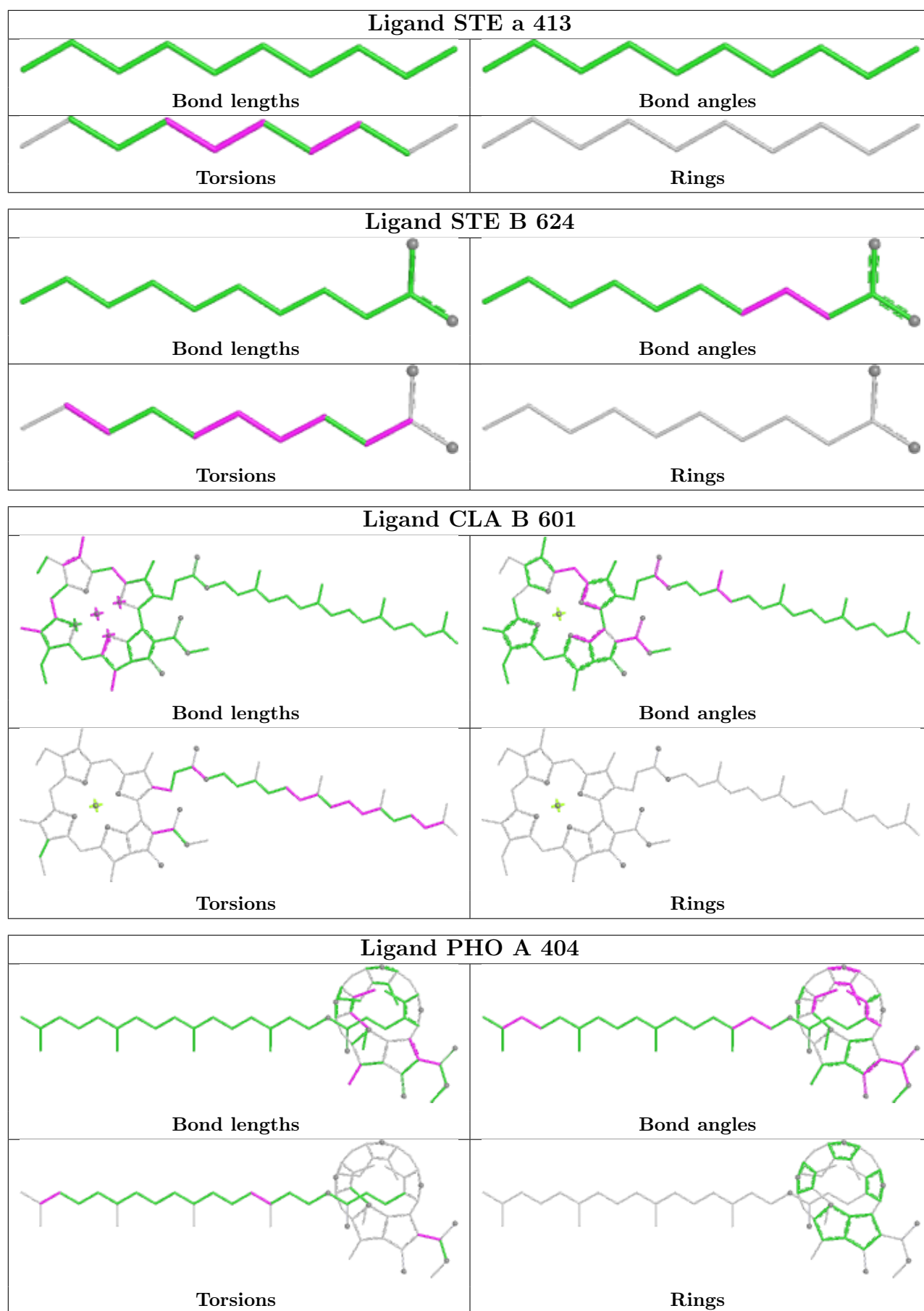


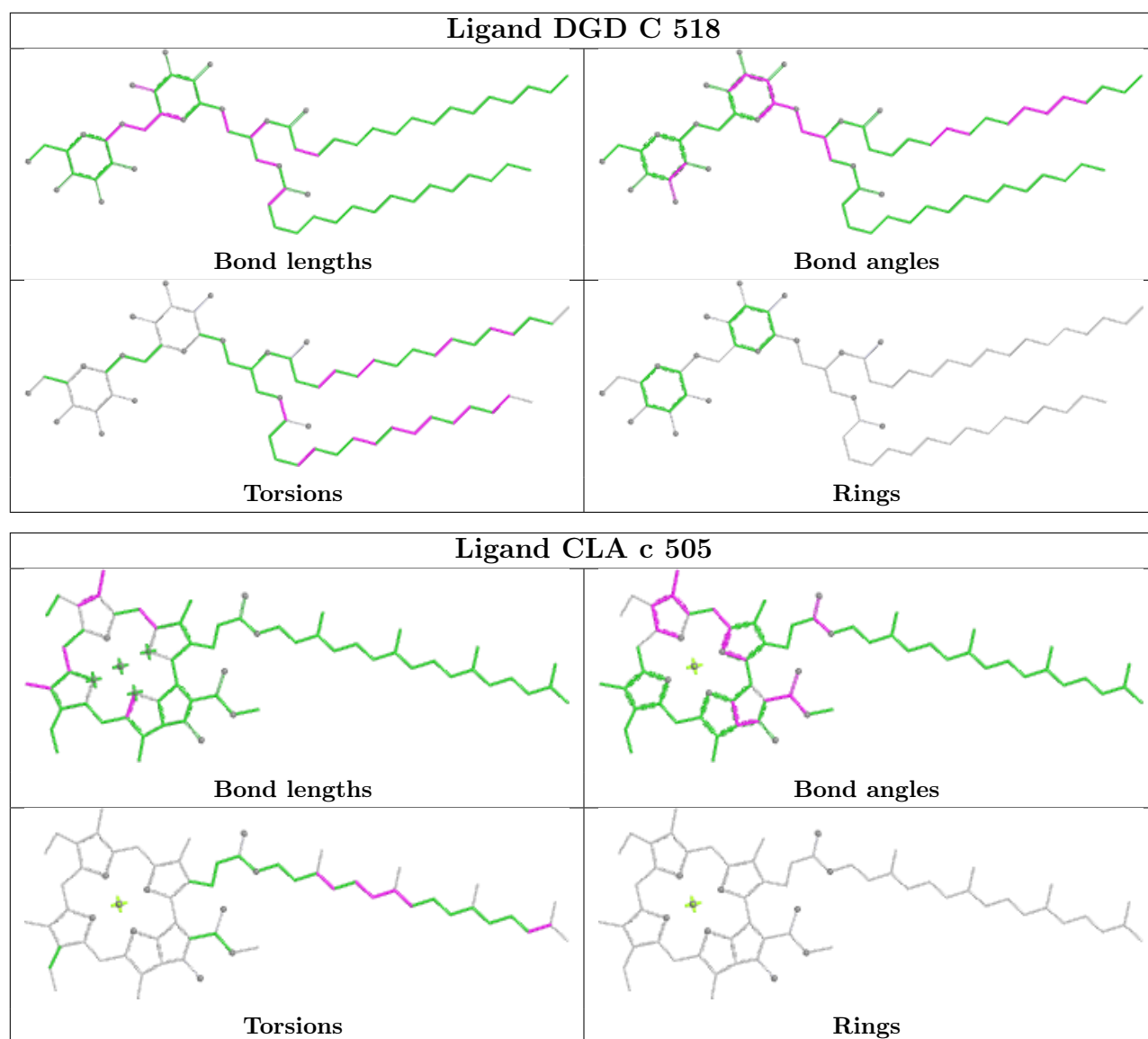












5.7 Other polymers [i](#)

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%) | -0.54 | 0 100 100 | 15, 35, 57, 92 | 64 (19%) |
| 1 | a | 334/344 (97%) | -0.41 | 3 (0%) 81 82 | 15, 37, 69, 86 | 64 (19%) |
| 2 | B | 505/510 (99%) | -0.49 | 1 (0%) 92 92 | 20, 40, 69, 101 | 4 (0%) |
| 2 | b | 505/510 (99%) | -0.34 | 4 (0%) 82 83 | 31, 43, 80, 129 | 0 |
| 3 | C | 442/461 (95%) | -0.43 | 0 100 100 | 17, 43, 61, 93 | 11 (2%) |
| 3 | c | 451/461 (97%) | -0.31 | 3 (0%) 84 85 | 17, 47, 70, 107 | 12 (2%) |
| 4 | D | 341/352 (96%) | -0.61 | 0 100 100 | 17, 37, 56, 88 | 2 (0%) |
| 4 | d | 341/352 (96%) | -0.44 | 0 100 100 | 18, 41, 67, 94 | 3 (0%) |
| 5 | E | 82/84 (97%) | 0.14 | 0 100 100 | 38, 61, 78, 93 | 1 (1%) |
| 5 | e | 82/84 (97%) | 0.20 | 1 (1%) 76 77 | 45, 69, 89, 94 | 0 |
| 6 | F | 34/45 (75%) | -0.20 | 0 100 100 | 46, 53, 77, 98 | 0 |
| 6 | f | 34/45 (75%) | 0.03 | 0 100 100 | 48, 57, 88, 102 | 0 |
| 7 | H | 65/66 (98%) | -0.30 | 2 (3%) 51 53 | 40, 49, 65, 83 | 0 |
| 7 | h | 63/66 (95%) | 0.04 | 1 (1%) 70 71 | 47, 59, 71, 79 | 0 |
| 8 | I | 35/38 (92%) | -0.45 | 0 100 100 | 38, 45, 79, 89 | 0 |
| 8 | i | 35/38 (92%) | -0.31 | 0 100 100 | 37, 47, 85, 91 | 0 |
| 9 | J | 36/40 (90%) | -0.20 | 0 100 100 | 41, 57, 83, 101 | 0 |
| 9 | j | 36/40 (90%) | 0.14 | 1 (2%) 55 57 | 46, 59, 95, 114 | 0 |
| 10 | K | 37/46 (80%) | -0.05 | 0 100 100 | 52, 61, 84, 88 | 0 |
| 10 | k | 37/46 (80%) | 0.12 | 0 100 100 | 51, 65, 80, 88 | 0 |
| 11 | L | 37/37 (100%) | -0.64 | 0 100 100 | 30, 37, 74, 77 | 0 |
| 11 | l | 36/37 (97%) | -0.65 | 0 100 100 | 28, 37, 79, 97 | 0 |
| 12 | M | 32/36 (88%) | -0.52 | 1 (3%) 51 53 | 31, 40, 68, 79 | 0 |
| 12 | m | 31/36 (86%) | -0.61 | 0 100 100 | 31, 41, 55, 77 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 13 | O | 244/272 (89%) | -0.27 | 2 (0%) 82 83 | 31, 49, 89, 147 | 1 (0%) |
| 13 | o | 244/272 (89%) | -0.30 | 1 (0%) 89 90 | 31, 48, 93, 137 | 0 |
| 14 | R | 28/41 (68%) | 0.72 | 0 100 100 | 68, 85, 99, 113 | 0 |
| 14 | r | 28/41 (68%) | 1.20 | 4 (14%) 7 8 | 82, 110, 127, 139 | 0 |
| 15 | T | 29/32 (90%) | -0.66 | 0 100 100 | 31, 37, 72, 80 | 0 |
| 15 | t | 29/32 (90%) | -0.50 | 1 (3%) 48 50 | 31, 38, 87, 95 | 0 |
| 16 | U | 97/134 (72%) | -0.27 | 0 100 100 | 36, 51, 77, 100 | 0 |
| 16 | u | 97/134 (72%) | -0.35 | 0 100 100 | 37, 47, 66, 89 | 0 |
| 17 | V | 137/163 (84%) | -0.42 | 0 100 100 | 34, 47, 63, 88 | 0 |
| 17 | v | 137/163 (84%) | -0.25 | 0 100 100 | 38, 54, 78, 93 | 0 |
| 18 | X | 38/41 (92%) | -0.15 | 0 100 100 | 47, 59, 84, 91 | 0 |
| 18 | x | 39/41 (95%) | 0.14 | 1 (2%) 57 59 | 58, 69, 100, 115 | 0 |
| 19 | Y | 27/46 (58%) | 0.77 | 2 (7%) 22 24 | 61, 83, 99, 111 | 0 |
| 19 | y | 30/46 (65%) | 0.54 | 0 100 100 | 70, 85, 101, 108 | 0 |
| 20 | Z | 62/62 (100%) | 0.60 | 2 (3%) 50 52 | 62, 79, 123, 138 | 0 |
| 20 | z | 62/62 (100%) | 0.59 | 3 (4%) 36 38 | 67, 83, 125, 138 | 0 |
| All | All | 5293/5700 (92%) | -0.32 | 33 (0%) 85 86 | 15, 45, 84, 147 | 162 (3%) |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15 | t | 30 | THR | 3.9 |
| 13 | O | 60 | ARG | 3.8 |
| 13 | o | 58 | ASN | 3.5 |
| 3 | c | 23 | ALA | 3.3 |
| 18 | x | 40 | SER | 3.1 |
| 13 | O | 59 | LYS | 3.1 |
| 19 | Y | 22 | LEU | 3.0 |
| 5 | e | 79 | PHE | 2.9 |
| 20 | Z | 62 | VAL | 2.9 |
| 20 | z | 33 | TRP | 2.8 |
| 9 | j | 6 | GLY | 2.7 |
| 7 | H | 65 | LEU | 2.7 |
| 7 | H | 41 | PHE | 2.6 |
| 19 | Y | 25 | ILE | 2.6 |
| 2 | b | 495 | PHE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 14 | r | 18 | TRP | 2.5 |
| 20 | z | 62 | VAL | 2.5 |
| 7 | h | 64 | ALA | 2.5 |
| 14 | r | 3 | TRP | 2.4 |
| 14 | r | 14 | LEU | 2.4 |
| 2 | b | 84 | THR | 2.3 |
| 1 | a | 250 | ALA | 2.3 |
| 3 | c | 24 | THR | 2.3 |
| 12 | M | 33 | GLN | 2.2 |
| 2 | b | 499 | VAL | 2.2 |
| 20 | z | 40 | ILE | 2.2 |
| 2 | B | 479[A] | PHE | 2.2 |
| 1 | a | 248 | ILE | 2.1 |
| 2 | b | 486 | LEU | 2.1 |
| 3 | c | 134 | ILE | 2.1 |
| 14 | r | 20 | VAL | 2.1 |
| 20 | Z | 33 | TRP | 2.0 |
| 1 | a | 249 | VAL | 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(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 15 | FME | t | 1 | 10/11 | 0.94 | 0.08 | 33,48,71,72 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.95 | 0.09 | 44,54,68,76 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.95 | 0.08 | 40,52,64,70 | 0 |
| 15 | FME | T | 1 | 10/11 | 0.96 | 0.07 | 29,52,69,69 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.96 | 0.08 | 41,51,64,67 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.97 | 0.08 | 33,50,72,82 | 0 |

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 32 | STE | H | 103 | 18/20 | 0.74 | 0.18 | 43,78,89,95 | 0 |
| 32 | STE | I | 101 | 15/20 | 0.77 | 0.18 | 38,59,77,81 | 0 |
| 32 | STE | b | 624 | 20/20 | 0.78 | 0.15 | 51,69,78,93 | 0 |
| 32 | STE | a | 413 | 10/20 | 0.79 | 0.16 | 37,66,75,80 | 0 |
| 32 | STE | b | 625 | 10/20 | 0.79 | 0.14 | 40,53,63,74 | 0 |
| 32 | STE | B | 626 | 16/20 | 0.80 | 0.15 | 39,72,94,94 | 0 |
| 27 | LMG | b | 622 | 55/55 | 0.80 | 0.16 | 53,80,98,112 | 0 |
| 33 | LHG | E | 102 | 49/49 | 0.80 | 0.14 | 55,87,113,120 | 0 |
| 26 | PL9 | A | 409 | 55/55 | 0.81 | 0.16 | 44,72,93,105 | 0 |
| 27 | LMG | c | 522 | 48/55 | 0.82 | 0.14 | 39,82,115,118 | 0 |
| 27 | LMG | d | 411 | 23/55 | 0.82 | 0.17 | 42,72,88,92 | 0 |
| 32 | STE | m | 101 | 12/20 | 0.82 | 0.16 | 48,64,76,82 | 0 |
| 32 | STE | x | 101 | 20/20 | 0.82 | 0.13 | 49,67,79,79 | 0 |
| 32 | STE | b | 623 | 16/20 | 0.82 | 0.16 | 50,68,83,94 | 0 |
| 32 | STE | c | 524 | 12/20 | 0.83 | 0.11 | 57,73,82,84 | 0 |
| 29 | DGD | a | 412 | 44/66 | 0.83 | 0.13 | 35,58,82,91 | 0 |
| 26 | PL9 | a | 409 | 55/55 | 0.83 | 0.16 | 42,76,96,107 | 0 |
| 32 | STE | E | 103 | 12/20 | 0.83 | 0.16 | 63,80,88,95 | 0 |
| 32 | STE | c | 521 | 20/20 | 0.84 | 0.12 | 44,63,94,107 | 0 |
| 32 | STE | T | 102 | 16/20 | 0.84 | 0.14 | 41,53,78,79 | 0 |
| 32 | STE | j | 101 | 12/20 | 0.84 | 0.12 | 48,62,70,79 | 0 |
| 33 | LHG | e | 101 | 42/49 | 0.84 | 0.13 | 56,93,112,132 | 0 |
| 29 | DGD | A | 414 | 66/66 | 0.85 | 0.11 | 47,67,82,90 | 0 |
| 28 | SQD | A | 413 | 39/54 | 0.85 | 0.13 | 43,66,94,100 | 0 |
| 28 | SQD | a | 411 | 36/54 | 0.85 | 0.13 | 32,65,86,91 | 0 |
| 32 | STE | J | 101 | 12/20 | 0.86 | 0.12 | 49,62,72,73 | 0 |
| 32 | STE | B | 627 | 12/20 | 0.86 | 0.14 | 53,66,83,86 | 0 |
| 32 | STE | C | 521 | 16/20 | 0.86 | 0.13 | 38,58,85,88 | 0 |
| 32 | STE | a | 414 | 12/20 | 0.86 | 0.12 | 54,67,77,79 | 0 |
| 27 | LMG | D | 410 | 33/55 | 0.86 | 0.13 | 41,58,86,90 | 0 |
| 22 | CLA | b | 601 | 65/65 | 0.86 | 0.11 | 53,72,92,96 | 0 |
| 27 | LMG | A | 411 | 48/55 | 0.86 | 0.11 | 43,65,84,101 | 0 |
| 32 | STE | B | 625 | 18/20 | 0.87 | 0.12 | 41,59,81,88 | 0 |
| 27 | LMG | B | 621 | 28/55 | 0.87 | 0.14 | 37,53,66,72 | 0 |
| 32 | STE | B | 620 | 17/20 | 0.87 | 0.11 | 39,59,71,80 | 0 |
| 32 | STE | T | 103 | 15/20 | 0.87 | 0.14 | 44,60,81,84 | 0 |
| 32 | STE | d | 413 | 17/20 | 0.88 | 0.14 | 48,62,75,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 32 | STE | M | 103 | 10/20 | 0.88 | 0.11 | 36,54,57,61 | 0 |
| 28 | SQD | F | 101 | 36/54 | 0.88 | 0.12 | 43,77,93,98 | 0 |
| 27 | LMG | c | 520 | 37/55 | 0.88 | 0.12 | 43,72,92,96 | 0 |
| 28 | SQD | f | 102 | 41/54 | 0.88 | 0.12 | 63,89,107,109 | 0 |
| 32 | STE | B | 624 | 12/20 | 0.88 | 0.10 | 37,56,70,74 | 0 |
| 32 | STE | l | 102 | 18/20 | 0.89 | 0.12 | 37,54,88,89 | 0 |
| 28 | SQD | B | 623 | 54/54 | 0.89 | 0.10 | 43,66,97,109 | 0 |
| 27 | LMG | b | 620 | 51/55 | 0.89 | 0.10 | 38,57,76,91 | 0 |
| 32 | STE | C | 520 | 12/20 | 0.89 | 0.12 | 43,57,68,70 | 0 |
| 27 | LMG | C | 519 | 48/55 | 0.89 | 0.12 | 49,74,93,98 | 0 |
| 27 | LMG | M | 101 | 51/55 | 0.90 | 0.09 | 33,53,76,92 | 0 |
| 32 | STE | b | 621 | 20/20 | 0.90 | 0.10 | 39,58,79,80 | 0 |
| 28 | SQD | L | 101 | 49/54 | 0.90 | 0.09 | 40,61,93,97 | 0 |
| 22 | CLA | B | 601 | 65/65 | 0.90 | 0.10 | 35,64,90,100 | 0 |
| 32 | STE | C | 522 | 12/20 | 0.90 | 0.10 | 34,45,58,64 | 0 |
| 24 | BCR | c | 514 | 40/40 | 0.90 | 0.10 | 47,64,79,81 | 0 |
| 24 | BCR | d | 406 | 40/40 | 0.90 | 0.11 | 40,57,98,114 | 0 |
| 22 | CLA | C | 513 | 65/65 | 0.91 | 0.10 | 45,68,103,112 | 0 |
| 32 | STE | D | 411 | 20/20 | 0.91 | 0.09 | 38,55,79,84 | 0 |
| 24 | BCR | K | 101 | 40/40 | 0.91 | 0.11 | 51,65,74,78 | 0 |
| 32 | STE | t | 102 | 14/20 | 0.91 | 0.10 | 35,55,65,68 | 0 |
| 24 | BCR | h | 101 | 40/40 | 0.91 | 0.10 | 43,60,79,91 | 0 |
| 27 | LMG | c | 523 | 49/55 | 0.91 | 0.10 | 35,62,83,99 | 0 |
| 24 | BCR | k | 101 | 40/40 | 0.91 | 0.10 | 45,67,78,80 | 0 |
| 28 | SQD | a | 410 | 54/54 | 0.92 | 0.10 | 44,67,96,99 | 0 |
| 22 | CLA | c | 512 | 65/65 | 0.92 | 0.10 | 47,64,99,104 | 0 |
| 24 | BCR | Y | 101 | 40/40 | 0.92 | 0.09 | 43,58,76,83 | 0 |
| 24 | BCR | b | 618 | 40/40 | 0.92 | 0.08 | 30,44,56,60 | 0 |
| 29 | DGD | C | 517 | 62/66 | 0.92 | 0.09 | 41,56,102,121 | 0 |
| 29 | DGD | H | 102 | 62/66 | 0.92 | 0.09 | 33,48,61,66 | 0 |
| 24 | BCR | B | 618 | 40/40 | 0.92 | 0.08 | 28,41,58,61 | 0 |
| 29 | DGD | h | 102 | 62/66 | 0.92 | 0.09 | 33,53,64,71 | 0 |
| 24 | BCR | D | 405 | 40/40 | 0.92 | 0.10 | 35,49,85,89 | 0 |
| 24 | BCR | H | 101 | 40/40 | 0.92 | 0.09 | 38,53,64,74 | 0 |
| 22 | CLA | c | 513 | 65/65 | 0.93 | 0.10 | 49,74,106,110 | 0 |
| 24 | BCR | c | 515 | 40/40 | 0.93 | 0.08 | 35,47,58,72 | 0 |
| 32 | STE | M | 102 | 15/20 | 0.93 | 0.09 | 37,50,66,69 | 0 |
| 22 | CLA | c | 508 | 64/65 | 0.93 | 0.09 | 37,50,94,112 | 0 |
| 27 | LMG | D | 407 | 51/55 | 0.93 | 0.10 | 31,60,86,92 | 0 |
| 28 | SQD | A | 412 | 52/54 | 0.93 | 0.09 | 33,66,94,99 | 0 |
| 24 | BCR | B | 619 | 40/40 | 0.93 | 0.08 | 33,45,59,61 | 0 |
| 24 | BCR | C | 514 | 40/40 | 0.93 | 0.09 | 32,43,56,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 29 | DGD | c | 518 | 62/66 | 0.93 | 0.09 | 35,58,94,103 | 0 |
| 24 | BCR | C | 515 | 40/40 | 0.93 | 0.11 | 45,60,78,81 | 0 |
| 24 | BCR | b | 619 | 40/40 | 0.93 | 0.08 | 35,52,70,70 | 0 |
| 34 | BCT | a | 408 | 4/4 | 0.93 | 0.10 | 35,40,48,58 | 0 |
| 27 | LMG | d | 412 | 44/55 | 0.94 | 0.09 | 37,58,89,92 | 0 |
| 22 | CLA | c | 509 | 65/65 | 0.94 | 0.09 | 37,53,70,75 | 0 |
| 22 | CLA | c | 510 | 65/65 | 0.94 | 0.08 | 36,53,67,73 | 0 |
| 29 | DGD | c | 519 | 62/66 | 0.94 | 0.08 | 31,57,86,101 | 0 |
| 24 | BCR | c | 516 | 40/40 | 0.94 | 0.11 | 45,60,71,79 | 0 |
| 22 | CLA | C | 503 | 65/65 | 0.94 | 0.07 | 36,47,59,62 | 0 |
| 22 | CLA | C | 511 | 65/65 | 0.94 | 0.09 | 36,57,71,76 | 0 |
| 24 | BCR | A | 406 | 40/40 | 0.94 | 0.07 | 28,38,49,52 | 0 |
| 24 | BCR | T | 101 | 40/40 | 0.94 | 0.07 | 29,44,58,62 | 0 |
| 24 | BCR | B | 617 | 40/40 | 0.94 | 0.07 | 30,45,60,65 | 0 |
| 22 | CLA | c | 506 | 65/65 | 0.94 | 0.09 | 36,53,94,101 | 0 |
| 33 | LHG | d | 408 | 49/49 | 0.94 | 0.10 | 30,55,77,83 | 0 |
| 33 | LHG | d | 410 | 39/49 | 0.94 | 0.08 | 34,50,72,74 | 0 |
| 29 | DGD | C | 516 | 62/66 | 0.94 | 0.09 | 25,48,84,91 | 0 |
| 22 | CLA | C | 512 | 65/65 | 0.94 | 0.09 | 35,61,88,97 | 0 |
| 22 | CLA | c | 502 | 65/65 | 0.95 | 0.07 | 34,49,69,75 | 0 |
| 22 | CLA | c | 503 | 65/65 | 0.95 | 0.08 | 35,48,61,64 | 0 |
| 24 | BCR | a | 405 | 40/40 | 0.95 | 0.06 | 25,36,52,56 | 0 |
| 24 | BCR | b | 617 | 40/40 | 0.95 | 0.07 | 29,43,52,56 | 0 |
| 22 | CLA | c | 504 | 60/65 | 0.95 | 0.07 | 35,50,87,88 | 0 |
| 22 | CLA | c | 505 | 65/65 | 0.95 | 0.08 | 28,45,71,75 | 0 |
| 22 | CLA | C | 505 | 65/65 | 0.95 | 0.08 | 22,44,72,75 | 0 |
| 22 | CLA | c | 507 | 65/65 | 0.95 | 0.08 | 30,49,61,66 | 0 |
| 22 | CLA | C | 506 | 65/65 | 0.95 | 0.09 | 29,49,89,94 | 0 |
| 22 | CLA | C | 508 | 65/65 | 0.95 | 0.08 | 32,46,104,115 | 0 |
| 22 | CLA | C | 509 | 65/65 | 0.95 | 0.09 | 32,50,65,74 | 0 |
| 22 | CLA | c | 511 | 65/65 | 0.95 | 0.09 | 43,60,78,82 | 0 |
| 24 | BCR | t | 101 | 40/40 | 0.95 | 0.06 | 27,39,55,58 | 0 |
| 22 | CLA | C | 510 | 65/65 | 0.95 | 0.07 | 34,49,66,74 | 0 |
| 29 | DGD | C | 518 | 62/66 | 0.95 | 0.08 | 33,54,82,91 | 0 |
| 26 | PL9 | D | 406 | 55/55 | 0.95 | 0.07 | 24,38,49,50 | 0 |
| 22 | CLA | B | 609 | 65/65 | 0.95 | 0.08 | 29,42,56,59 | 0 |
| 26 | PL9 | d | 407 | 55/55 | 0.95 | 0.07 | 27,38,45,52 | 0 |
| 22 | CLA | d | 405 | 65/65 | 0.95 | 0.09 | 32,53,93,101 | 0 |
| 22 | CLA | B | 615 | 65/65 | 0.95 | 0.07 | 29,42,67,77 | 0 |
| 22 | CLA | C | 502 | 65/65 | 0.95 | 0.07 | 35,47,60,68 | 0 |
| 22 | CLA | a | 403 | 65/65 | 0.95 | 0.09 | 30,45,99,107 | 0 |
| 22 | CLA | B | 606 | 65/65 | 0.95 | 0.07 | 28,41,71,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 33 | LHG | B | 622 | 49/49 | 0.95 | 0.09 | 28,48,68,77 | 0 |
| 33 | LHG | D | 409 | 47/49 | 0.95 | 0.09 | 29,53,82,99 | 0 |
| 22 | CLA | b | 606 | 65/65 | 0.95 | 0.08 | 29,45,77,78 | 0 |
| 33 | LHG | L | 102 | 49/49 | 0.95 | 0.07 | 30,44,59,74 | 0 |
| 22 | CLA | b | 608 | 65/65 | 0.95 | 0.07 | 34,48,64,68 | 0 |
| 22 | CLA | b | 614 | 65/65 | 0.95 | 0.08 | 25,44,78,85 | 0 |
| 22 | CLA | b | 615 | 65/65 | 0.95 | 0.07 | 31,45,61,65 | 0 |
| 33 | LHG | l | 101 | 49/49 | 0.95 | 0.07 | 34,48,59,67 | 0 |
| 22 | CLA | b | 616 | 60/65 | 0.95 | 0.09 | 34,48,89,91 | 0 |
| 22 | CLA | a | 402 | 65/65 | 0.96 | 0.06 | 24,35,48,62 | 0 |
| 22 | CLA | B | 602 | 65/65 | 0.96 | 0.07 | 27,40,62,65 | 0 |
| 22 | CLA | a | 404 | 65/65 | 0.96 | 0.08 | 21,40,80,85 | 0 |
| 22 | CLA | d | 403 | 65/65 | 0.96 | 0.07 | 23,40,60,68 | 0 |
| 22 | CLA | d | 404 | 65/65 | 0.96 | 0.06 | 24,35,46,50 | 0 |
| 22 | CLA | B | 616 | 60/65 | 0.96 | 0.09 | 28,45,84,100 | 0 |
| 23 | PHO | A | 404 | 64/64 | 0.96 | 0.05 | 20,31,40,48 | 0 |
| 23 | PHO | D | 401 | 64/64 | 0.96 | 0.06 | 25,37,45,53 | 0 |
| 23 | PHO | d | 401 | 64/64 | 0.96 | 0.06 | 23,35,43,48 | 0 |
| 23 | PHO | d | 402 | 64/64 | 0.96 | 0.06 | 32,43,54,63 | 0 |
| 22 | CLA | b | 602 | 65/65 | 0.96 | 0.08 | 31,46,65,71 | 0 |
| 22 | CLA | b | 603 | 65/65 | 0.96 | 0.07 | 24,40,71,79 | 0 |
| 22 | CLA | b | 604 | 65/65 | 0.96 | 0.07 | 24,39,80,93 | 0 |
| 22 | CLA | b | 605 | 65/65 | 0.96 | 0.07 | 24,39,54,60 | 0 |
| 22 | CLA | C | 501 | 65/65 | 0.96 | 0.07 | 26,41,54,58 | 0 |
| 22 | CLA | b | 607 | 65/65 | 0.96 | 0.07 | 21,40,65,77 | 0 |
| 22 | CLA | B | 604 | 65/65 | 0.96 | 0.07 | 26,38,75,80 | 0 |
| 22 | CLA | b | 609 | 65/65 | 0.96 | 0.08 | 32,50,71,77 | 0 |
| 22 | CLA | b | 610 | 65/65 | 0.96 | 0.08 | 28,42,53,58 | 0 |
| 22 | CLA | b | 611 | 65/65 | 0.96 | 0.07 | 27,39,57,66 | 0 |
| 22 | CLA | b | 612 | 65/65 | 0.96 | 0.07 | 26,39,54,63 | 0 |
| 22 | CLA | b | 613 | 65/65 | 0.96 | 0.07 | 26,40,76,83 | 0 |
| 22 | CLA | B | 605 | 65/65 | 0.96 | 0.07 | 24,35,49,54 | 0 |
| 22 | CLA | C | 504 | 59/65 | 0.96 | 0.07 | 32,47,85,92 | 0 |
| 22 | CLA | A | 403 | 65/65 | 0.96 | 0.09 | 26,40,103,112 | 0 |
| 22 | CLA | c | 501 | 65/65 | 0.96 | 0.07 | 31,44,54,62 | 0 |
| 22 | CLA | B | 608 | 65/65 | 0.96 | 0.06 | 22,39,59,65 | 0 |
| 22 | CLA | C | 507 | 65/65 | 0.96 | 0.07 | 27,45,60,65 | 0 |
| 33 | LHG | D | 408 | 49/49 | 0.96 | 0.07 | 26,44,56,63 | 0 |
| 29 | DGD | c | 517 | 62/66 | 0.96 | 0.07 | 25,46,77,83 | 0 |
| 22 | CLA | A | 402 | 65/65 | 0.96 | 0.06 | 21,32,46,56 | 0 |
| 22 | CLA | B | 610 | 65/65 | 0.96 | 0.07 | 23,35,47,51 | 0 |
| 22 | CLA | B | 611 | 65/65 | 0.96 | 0.07 | 23,35,50,56 | 0 |

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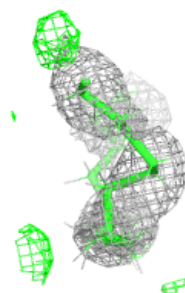
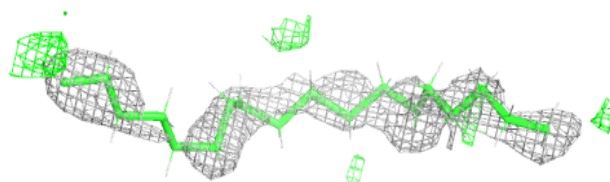
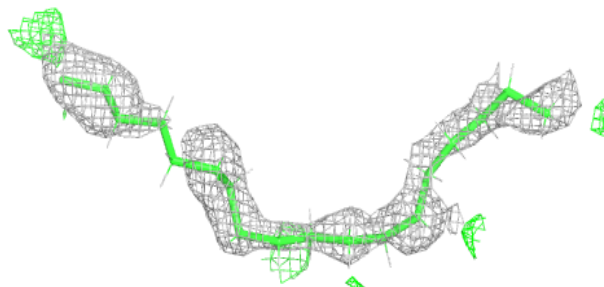
Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 33 | LHG | d | 409 | 49/49 | 0.96 | 0.07 | 30,49,61,71 | 0 |
| 22 | CLA | B | 612 | 65/65 | 0.96 | 0.07 | 25,36,50,55 | 0 |
| 22 | CLA | B | 613 | 65/65 | 0.96 | 0.07 | 21,35,71,75 | 0 |
| 22 | CLA | B | 614 | 65/65 | 0.96 | 0.08 | 26,43,77,92 | 0 |
| 34 | BCT | D | 402 | 4/4 | 0.96 | 0.09 | 32,33,37,44 | 0 |
| 22 | CLA | D | 404 | 65/65 | 0.96 | 0.08 | 27,47,106,117 | 0 |
| 22 | CLA | A | 410 | 65/65 | 0.97 | 0.06 | 20,32,52,58 | 0 |
| 22 | CLA | B | 607 | 65/65 | 0.97 | 0.07 | 17,37,68,76 | 0 |
| 22 | CLA | B | 603 | 65/65 | 0.97 | 0.06 | 24,38,63,64 | 0 |
| 22 | CLA | D | 403 | 65/65 | 0.97 | 0.06 | 22,32,59,60 | 0 |
| 35 | HEM | E | 101 | 43/43 | 0.97 | 0.08 | 42,57,75,75 | 0 |
| 35 | HEM | f | 101 | 43/43 | 0.97 | 0.09 | 46,64,89,90 | 0 |
| 22 | CLA | A | 405 | 54/65 | 0.98 | 0.06 | 20,34,68,73 | 0 |
| 25 | CL | a | 406 | 1/1 | 0.98 | 0.05 | 30,30,30,30 | 0 |
| 36 | HEC | V | 201 | 43/43 | 0.98 | 0.07 | 24,37,49,51 | 0 |
| 36 | HEC | v | 201 | 43/43 | 0.98 | 0.06 | 32,41,52,55 | 0 |
| 31 | OEX | a | 416[A] | 10/10 | 0.99 | 0.03 | 32,38,41,41 | 10 |
| 25 | CL | a | 407 | 1/1 | 0.99 | 0.08 | 33,33,33,33 | 0 |
| 25 | CL | A | 407 | 1/1 | 0.99 | 0.04 | 33,33,33,33 | 0 |
| 25 | CL | A | 408 | 1/1 | 0.99 | 0.07 | 32,32,32,32 | 0 |
| 21 | FE2 | a | 401 | 1/1 | 0.99 | 0.02 | 37,37,37,37 | 0 |
| 31 | OEX | A | 416[A] | 10/10 | 0.99 | 0.03 | 35,37,41,41 | 10 |
| 30 | OEY | A | 415[B] | 11/11 | 1.00 | 0.03 | 21,26,30,34 | 11 |
| 30 | OEY | a | 415[B] | 11/11 | 1.00 | 0.02 | 25,27,31,37 | 11 |
| 21 | FE2 | A | 401 | 1/1 | 1.00 | 0.02 | 33,33,33,33 | 0 |

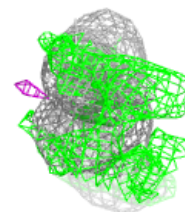
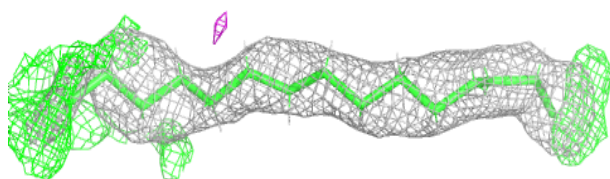
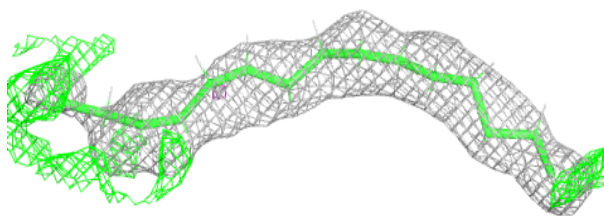
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

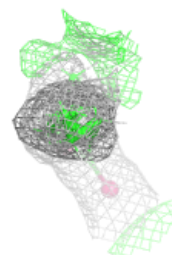
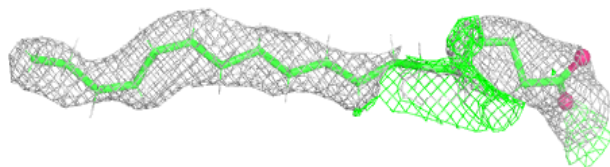
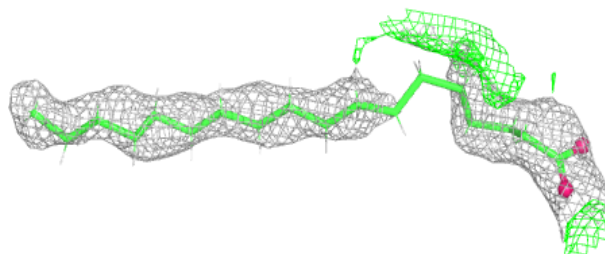
**Electron density around STE I 101:**

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

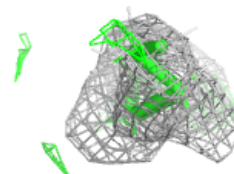
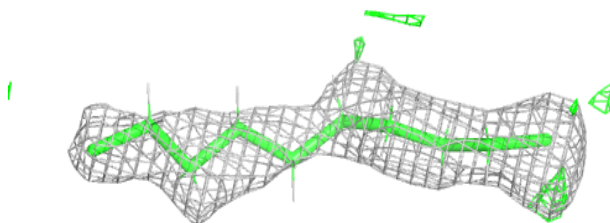
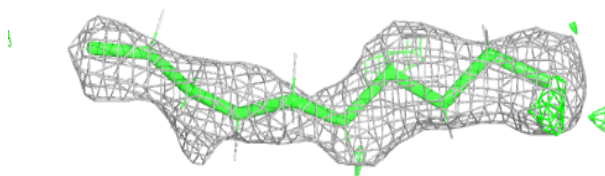


Electron density around STE b 624:

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

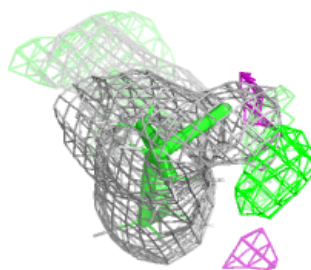
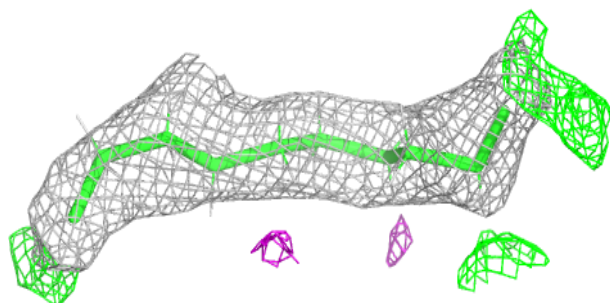
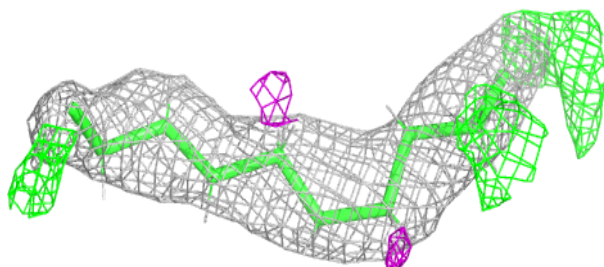
**Electron density around STE a 413:**

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

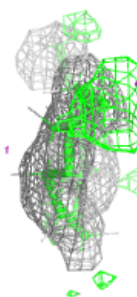
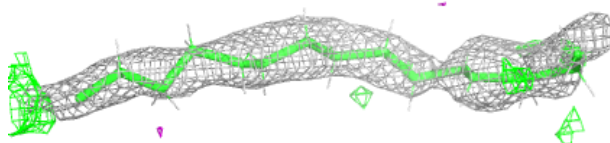


Electron density around STE b 625:

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

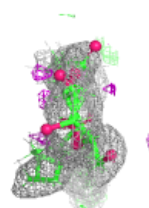
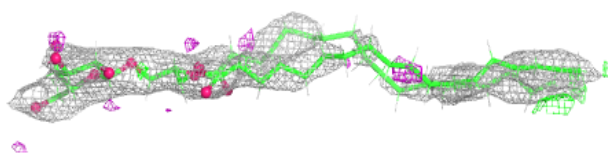
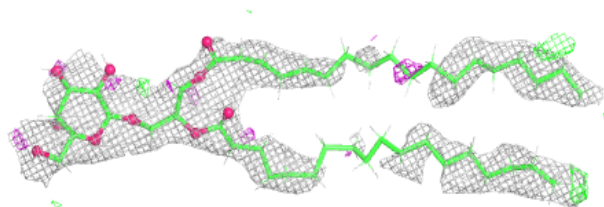
**Electron density around STE B 626:**

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



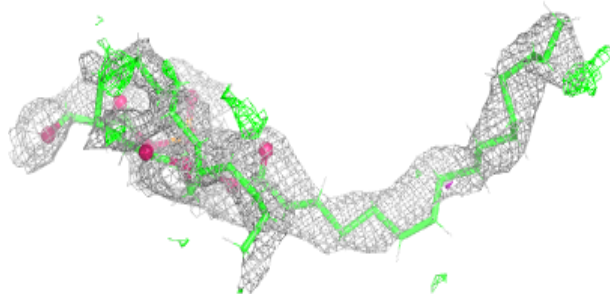
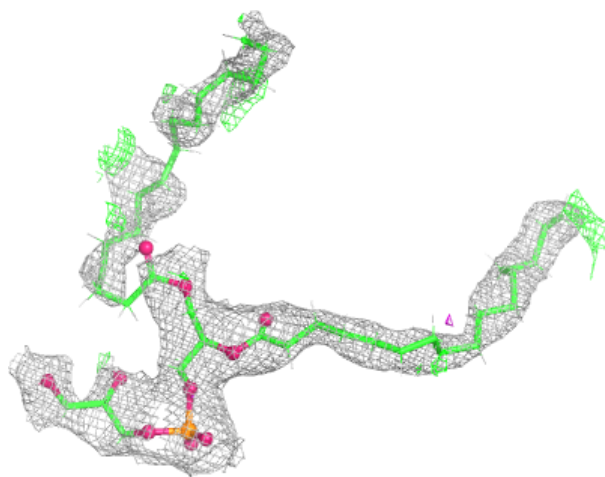
Electron density around LMG b 622:

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



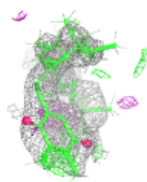
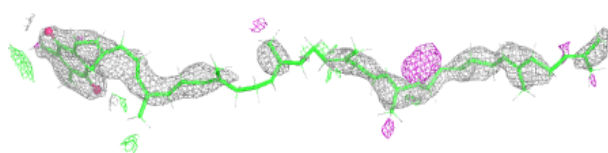
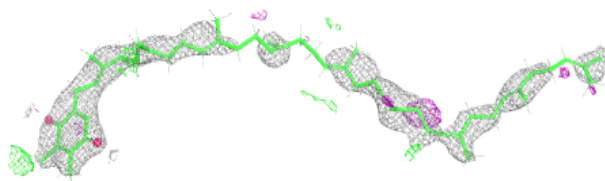
Electron density around LHG E 102:

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

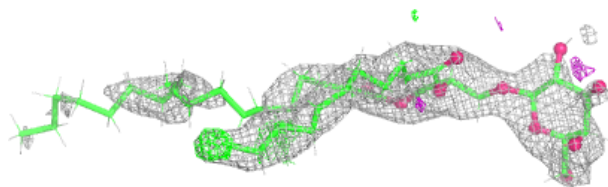


Electron density around PL9 A 409:

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

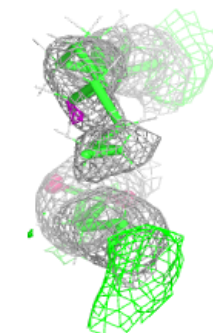
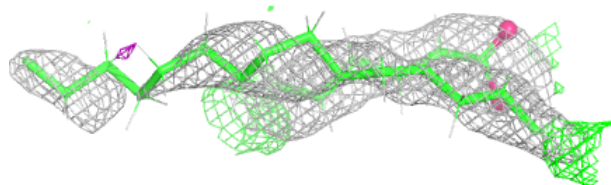
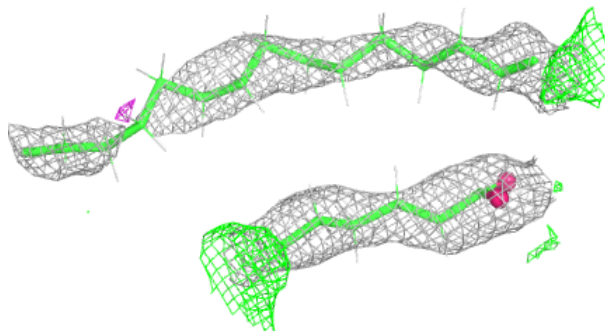
**Electron density around LMG c 522:**

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

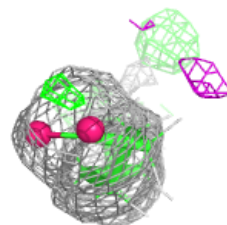
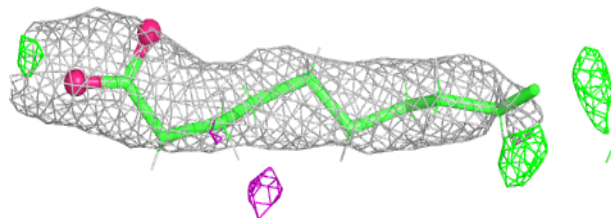
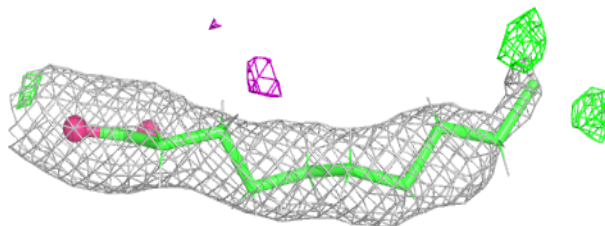


Electron density around LMG d 411:

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

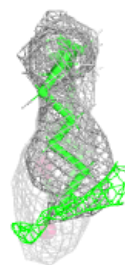
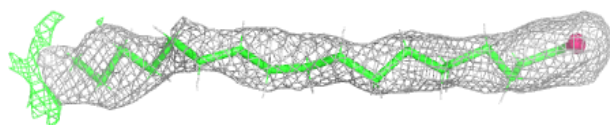
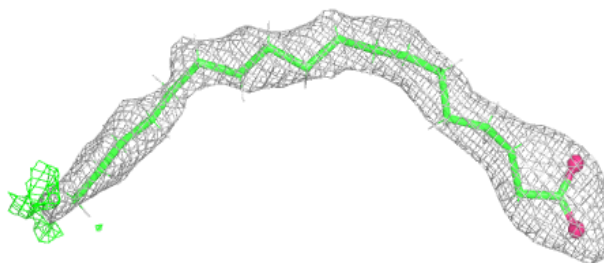
**Electron density around STE m 101:**

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

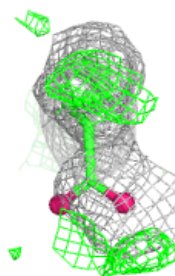
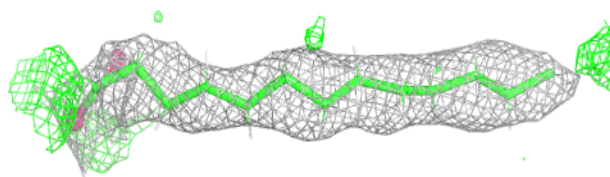
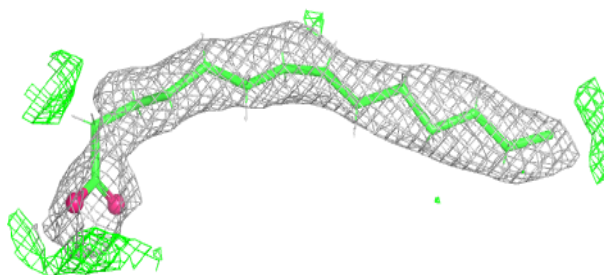


Electron density around STE x 101:

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

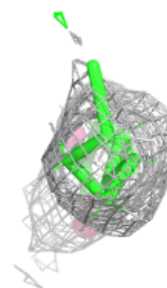
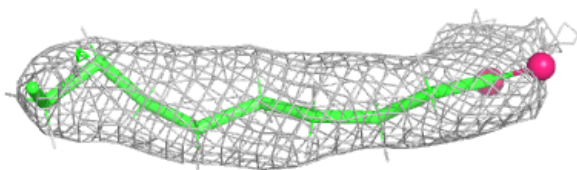
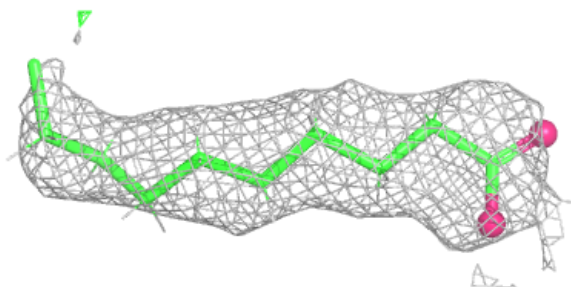
**Electron density around STE b 623:**

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

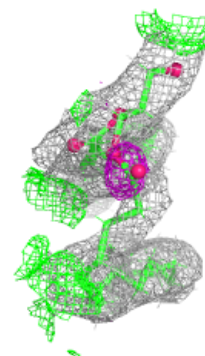
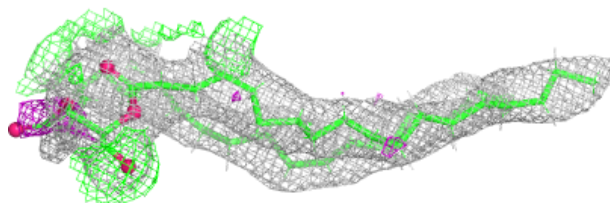
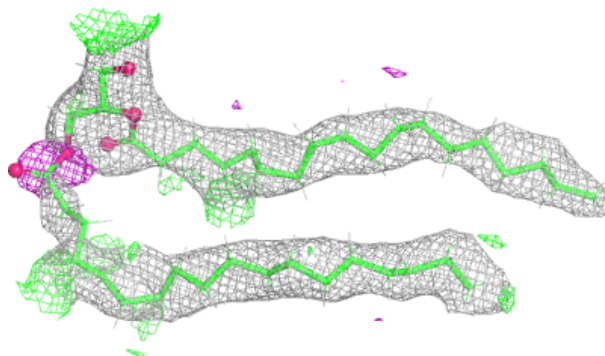


Electron density around STE c 524:

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

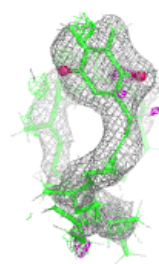
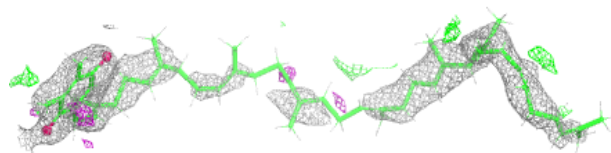
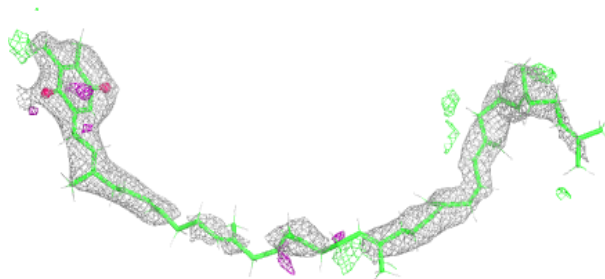
**Electron density around DGD a 412:**

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

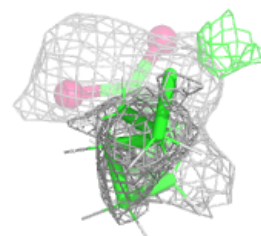
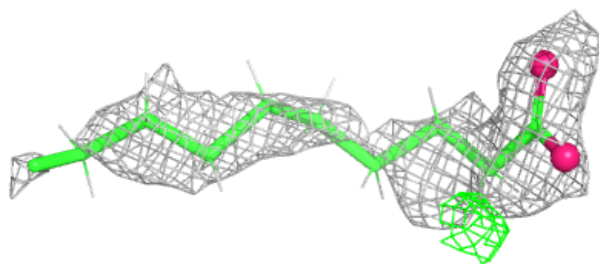
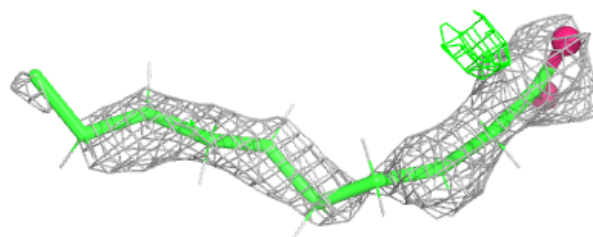


Electron density around PL9 a 409:

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

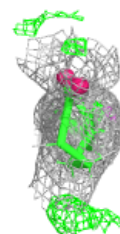
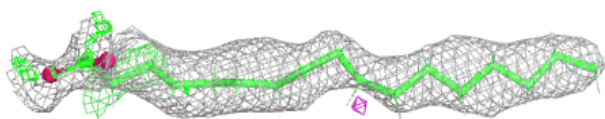
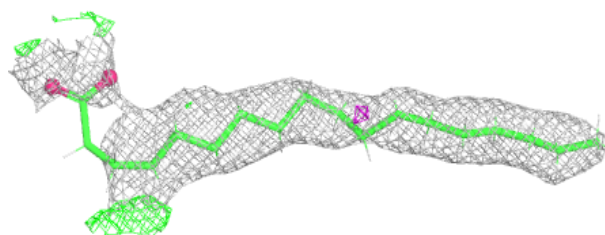
**Electron density around STE E 103:**

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

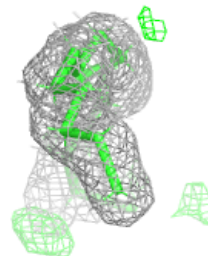
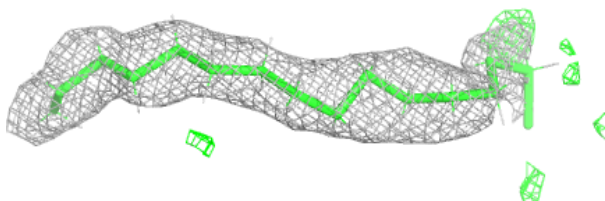
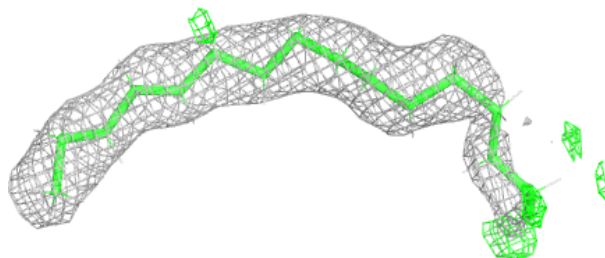


Electron density around STE c 521:

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

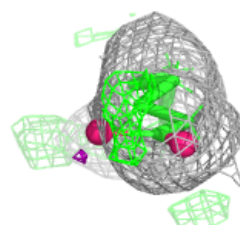
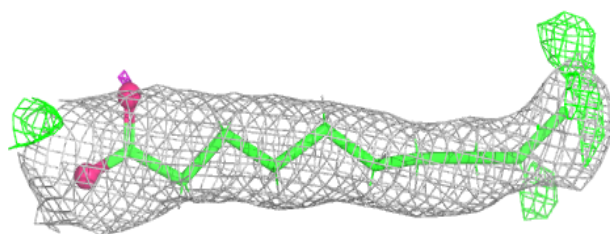
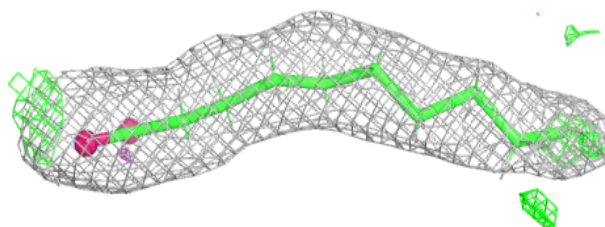
**Electron density around STE T 102:**

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

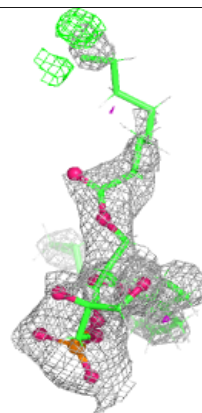
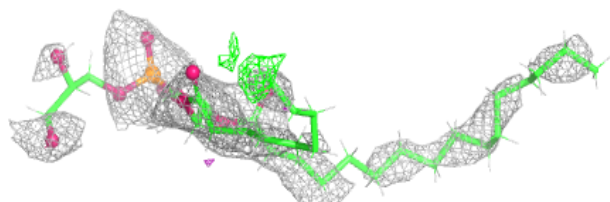
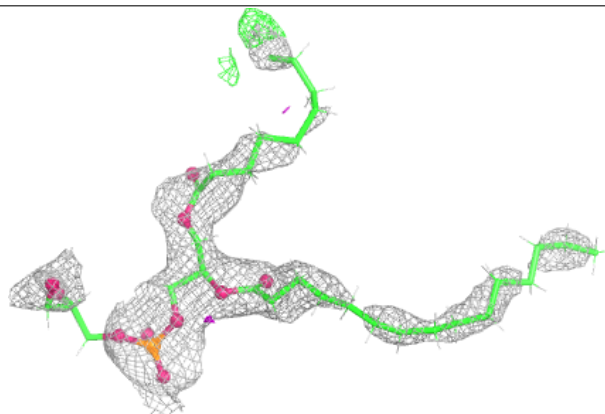


Electron density around STE j 101:

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

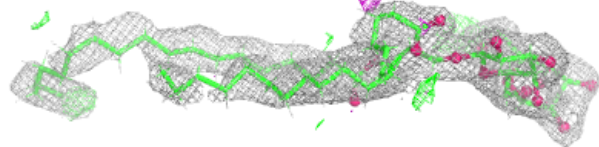
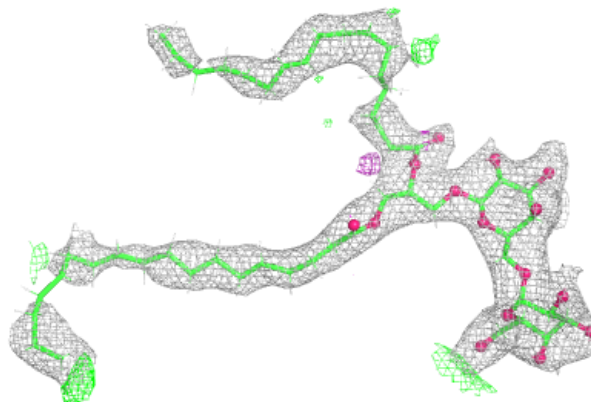
**Electron density around LHG e 101:**

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



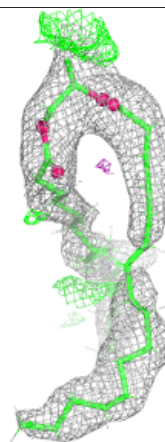
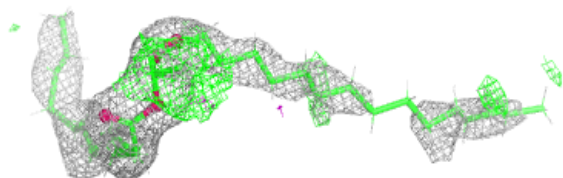
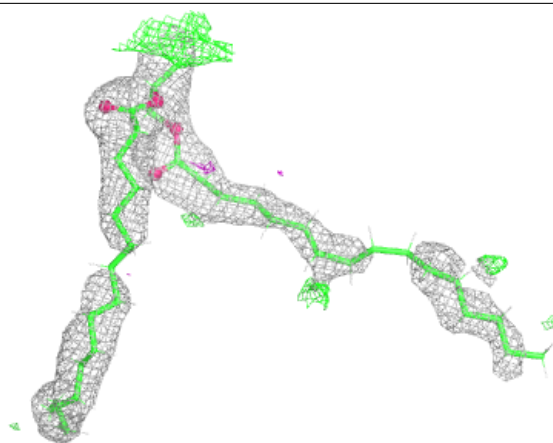
Electron density around DGD A 414:

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



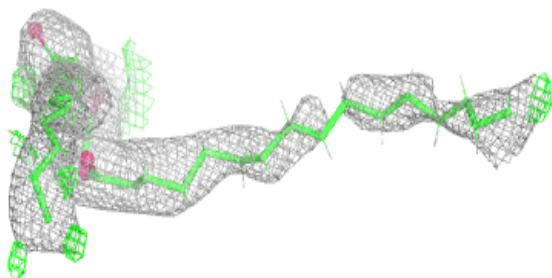
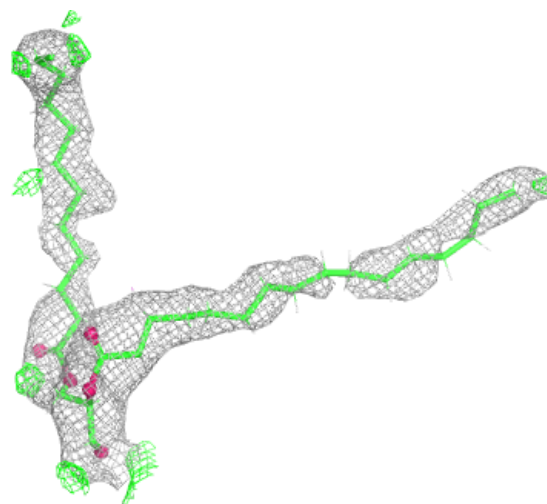
Electron density around SQD A 413:

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



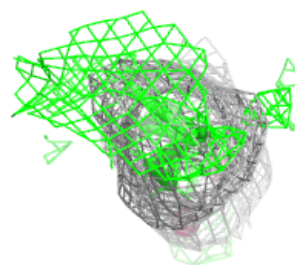
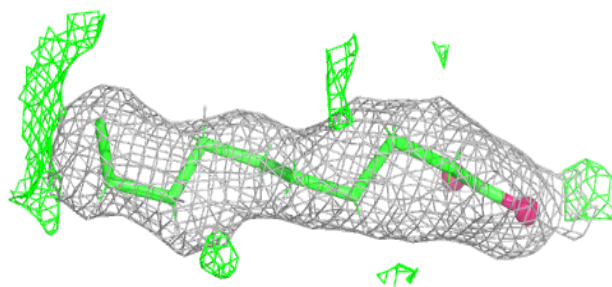
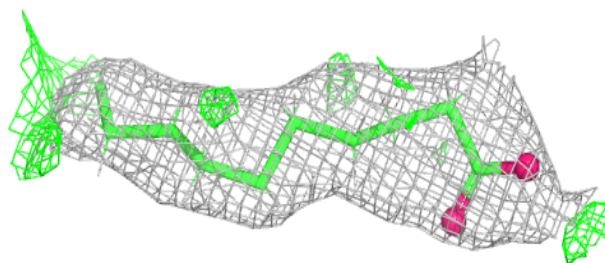
Electron density around SQD a 411:

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

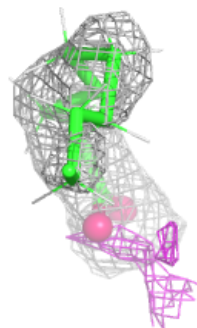
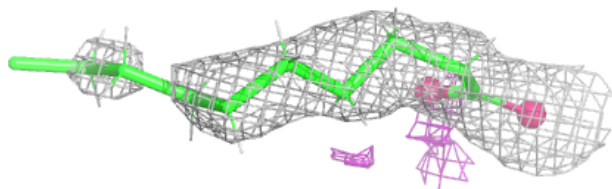
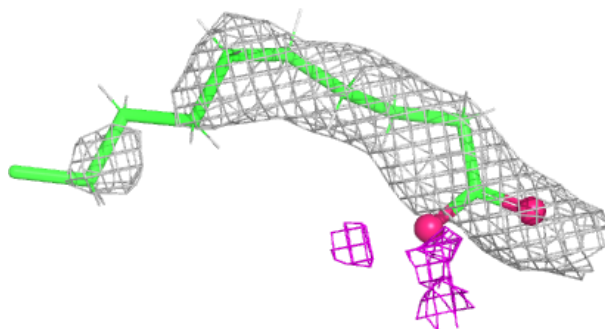


Electron density around STE J 101:

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

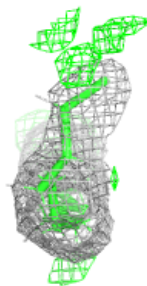
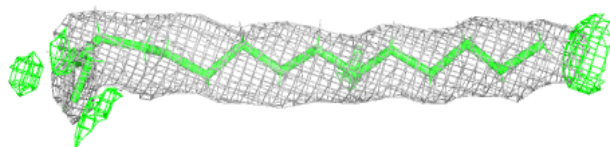
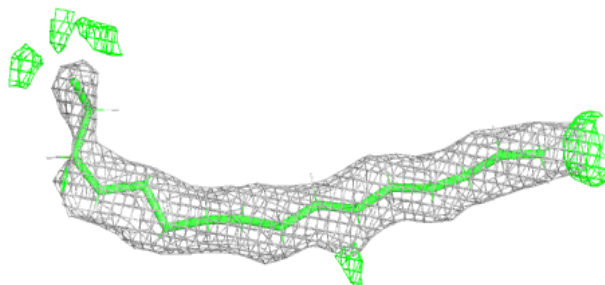
**Electron density around STE B 627:**

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

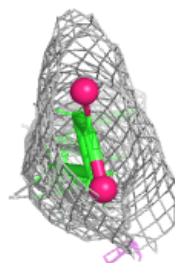
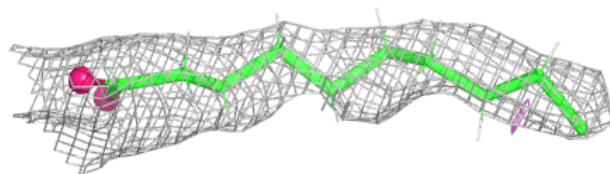
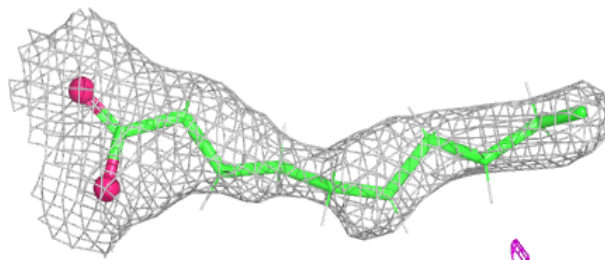


Electron density around STE C 521:

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

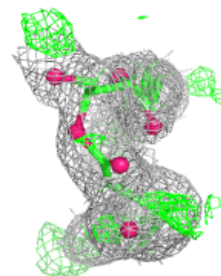
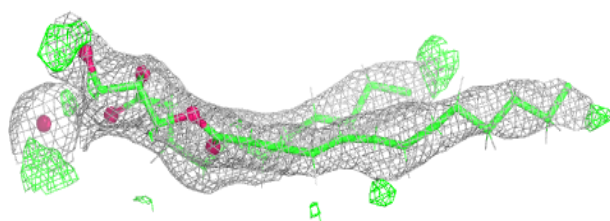
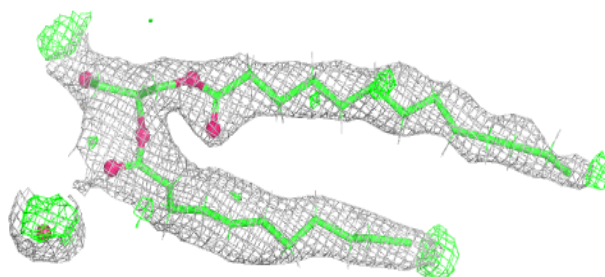
**Electron density around STE a 414:**

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

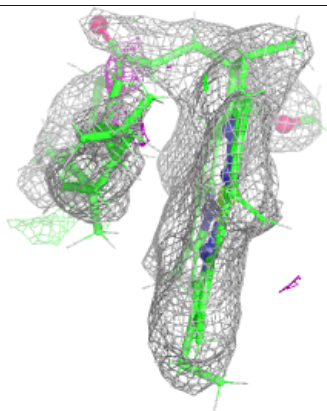
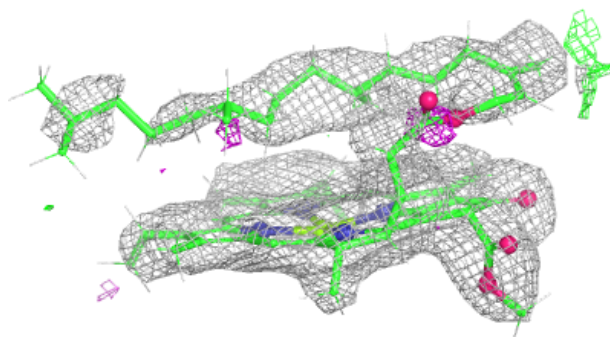
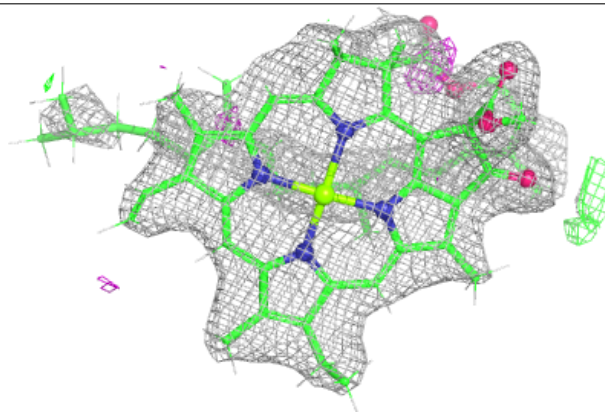


Electron density around LMG D 410:

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

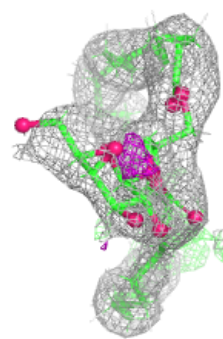
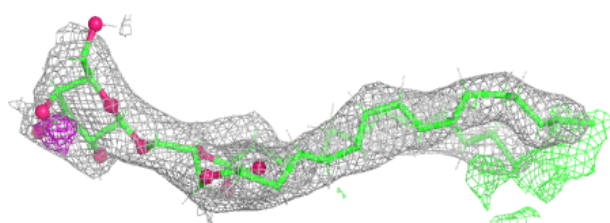
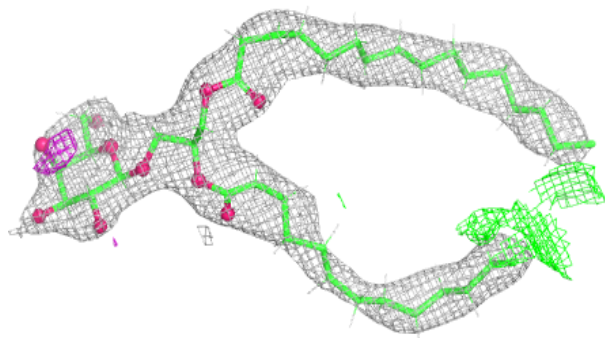
**Electron density around CLA b 601:**

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

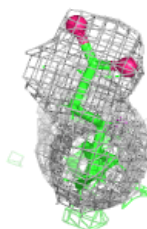
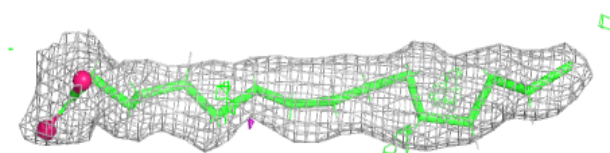
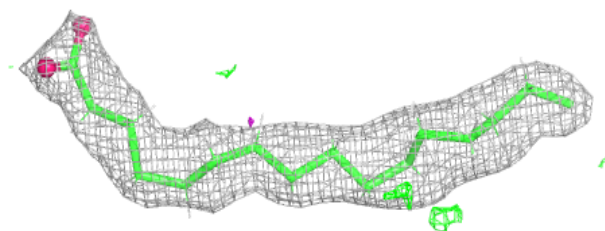


Electron density around LMG A 411:

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

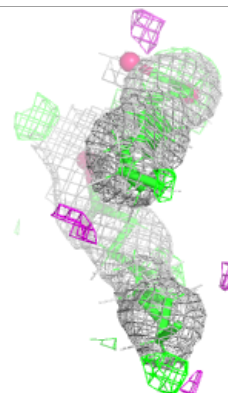
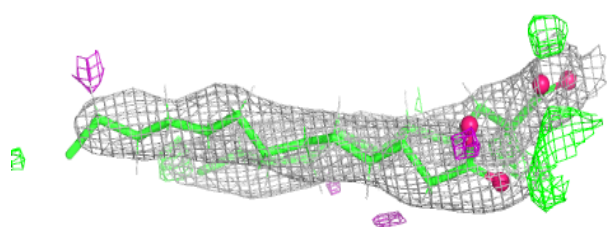
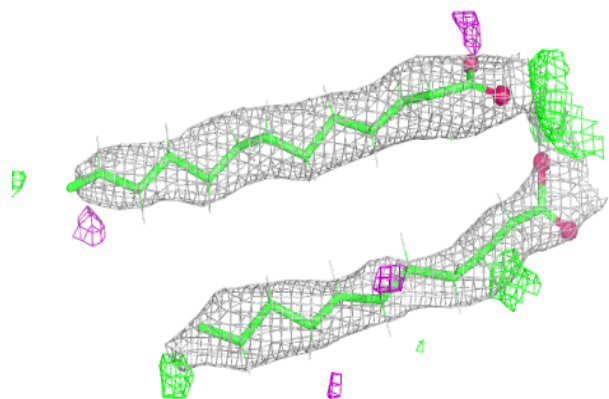
**Electron density around STE B 625:**

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

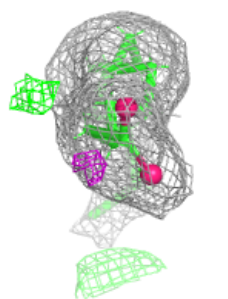
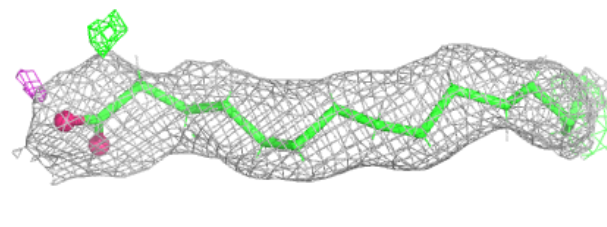
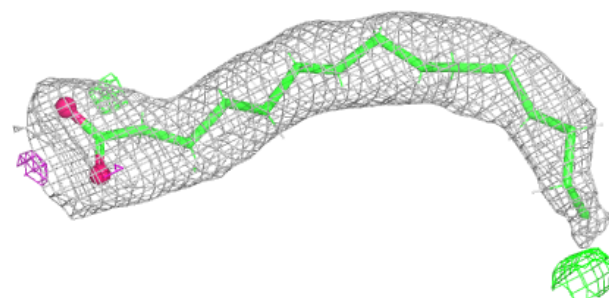


Electron density around LMG B 621:

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

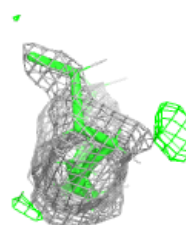
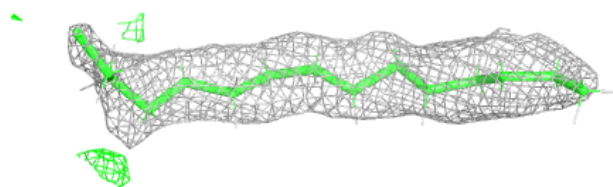
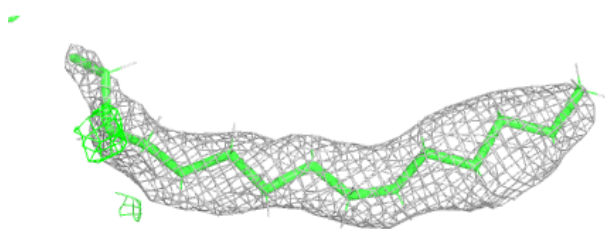
**Electron density around STE B 620:**

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

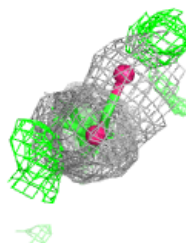
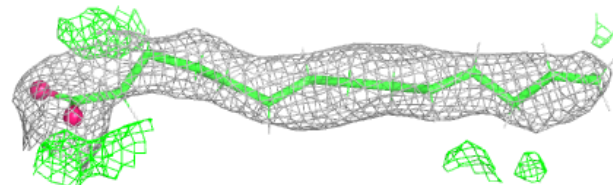
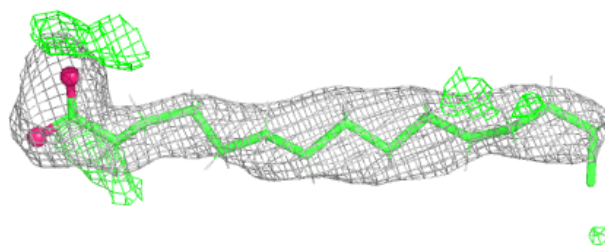


Electron density around STE T 103:

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

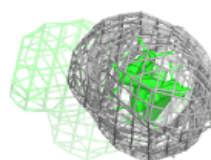
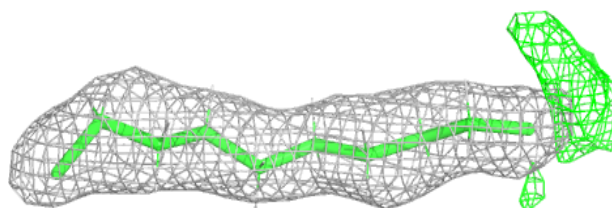
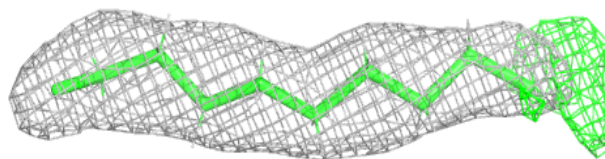
**Electron density around STE d 413:**

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

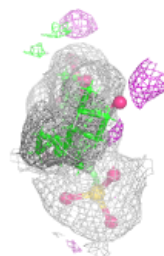
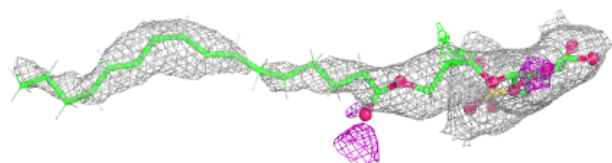
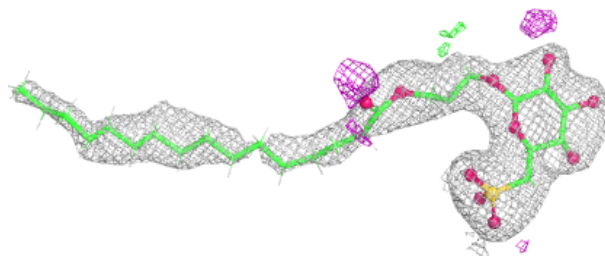


Electron density around STE M 103:

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

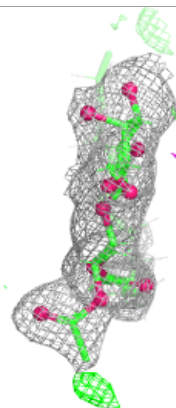
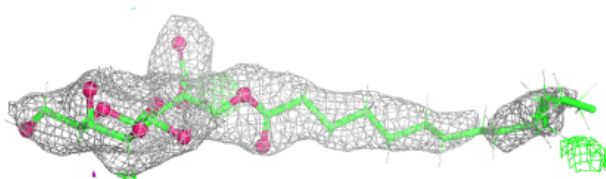
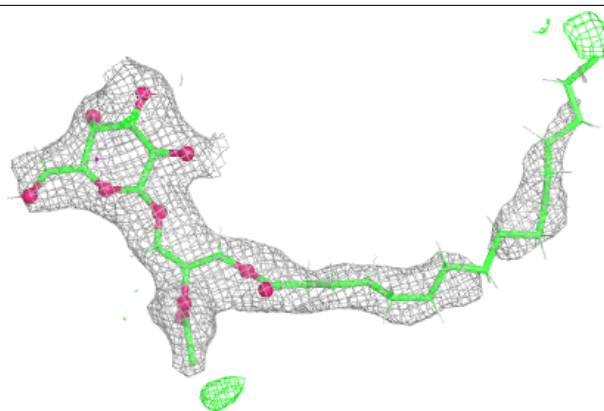
**Electron density around SQD F 101:**

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

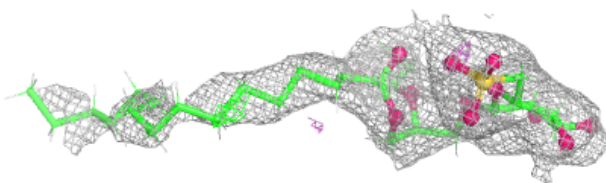
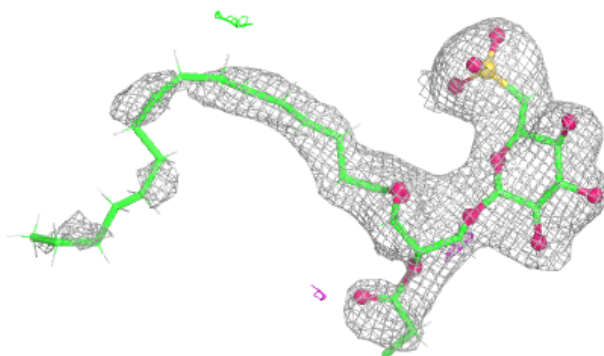


Electron density around LMG c 520:

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

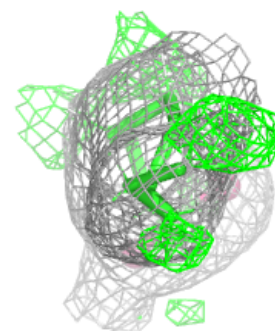
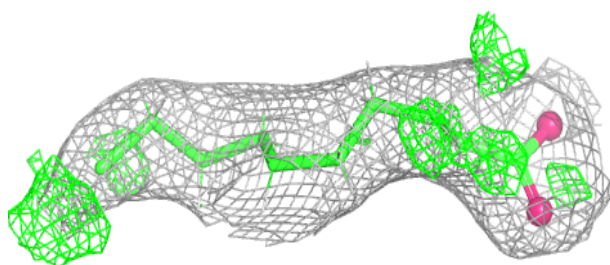
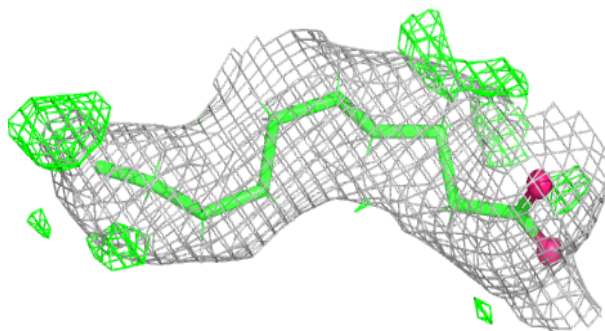
**Electron density around SQD f 102:**

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

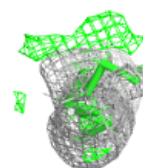
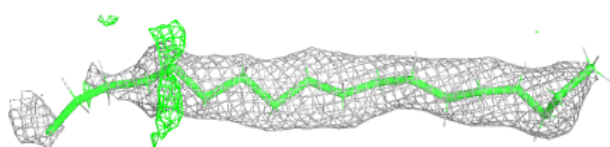
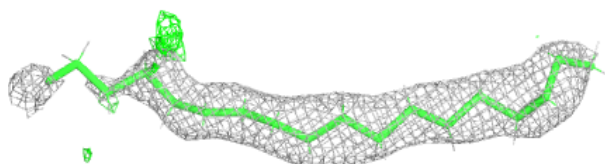


Electron density around STE B 624:

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

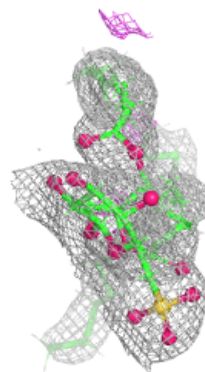
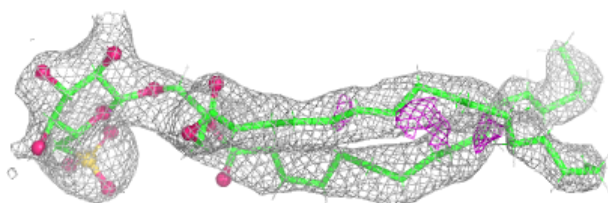
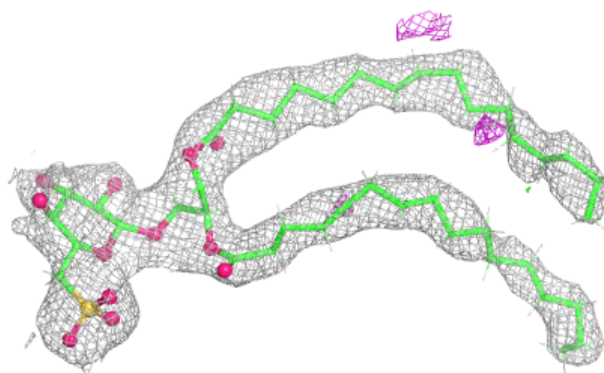
**Electron density around STE I 102:**

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

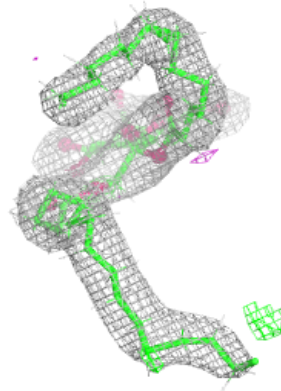
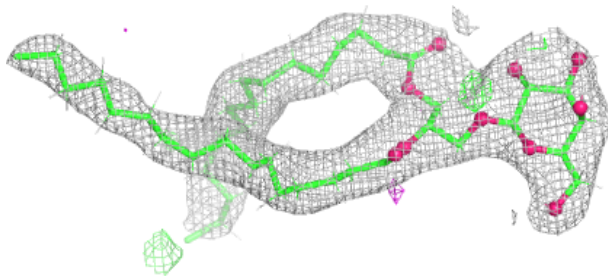
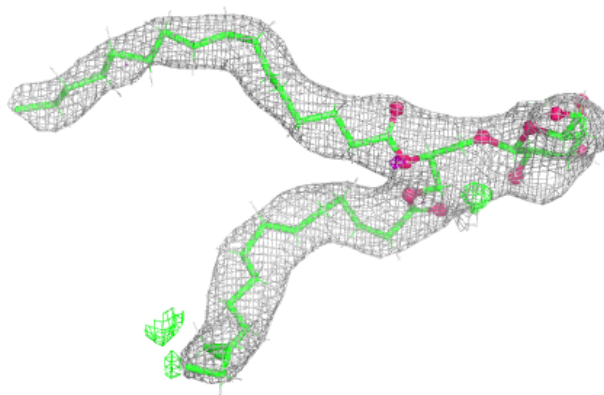


Electron density around SQD B 623:

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

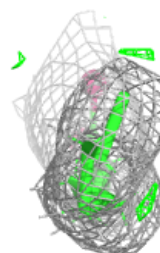
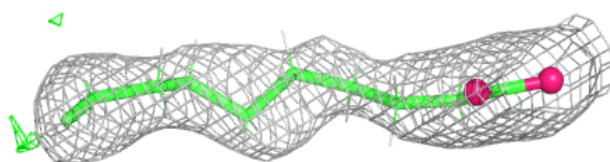
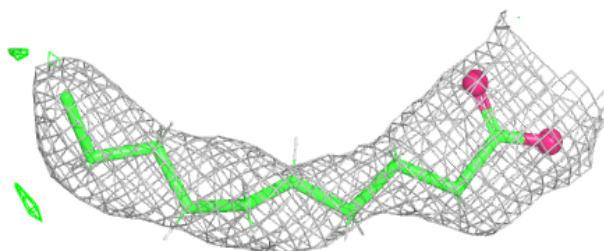
**Electron density around LMG b 620:**

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



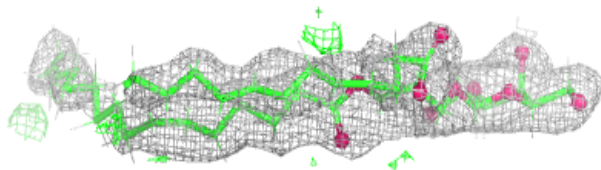
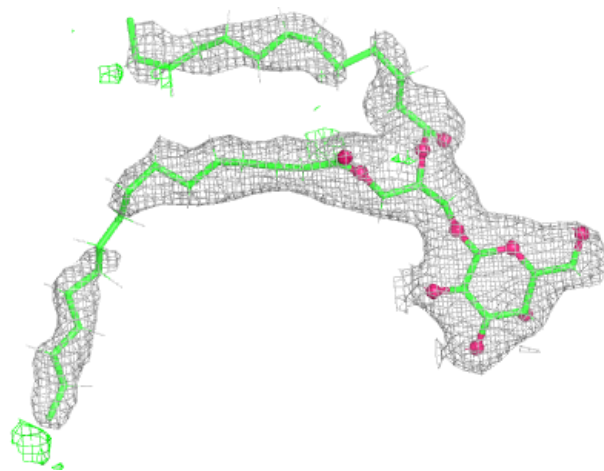
Electron density around STE C 520:

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



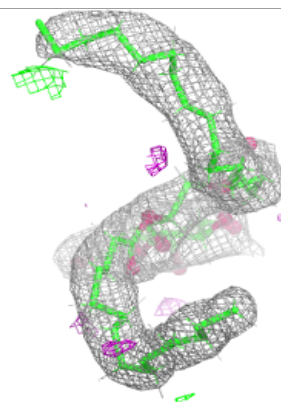
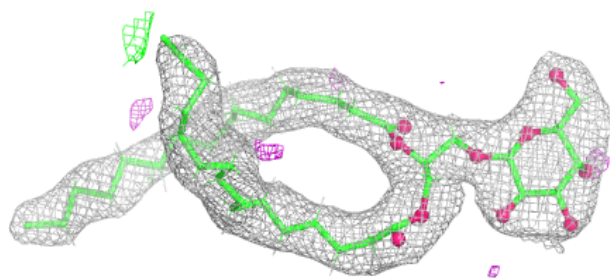
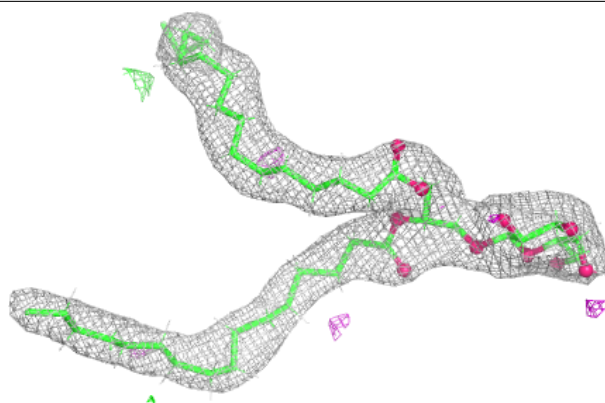
Electron density around LMG C 519:

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

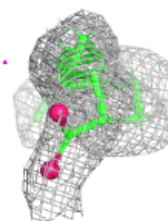
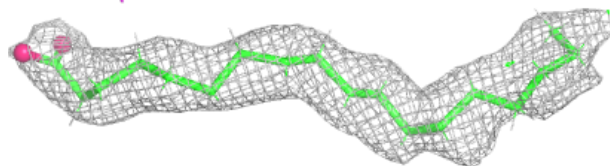
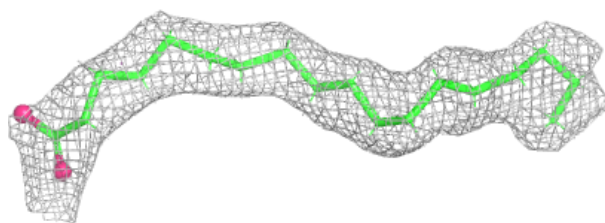


Electron density around LMG M 101:

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

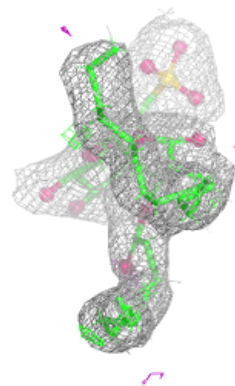
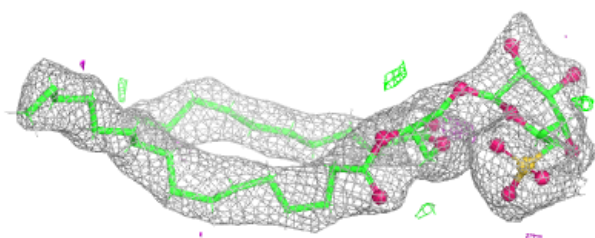
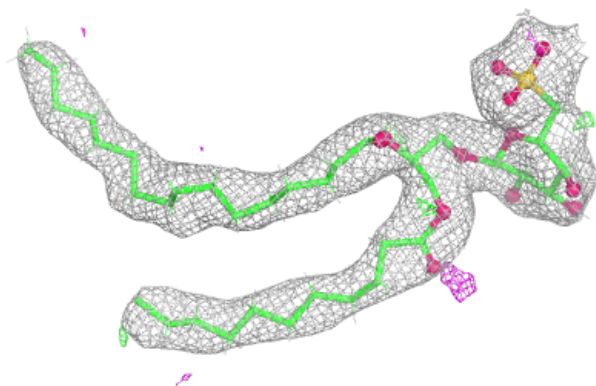
**Electron density around STE b 621:**

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

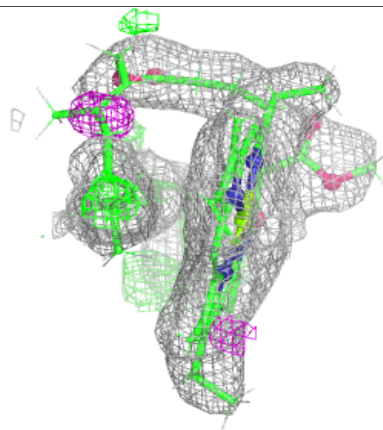
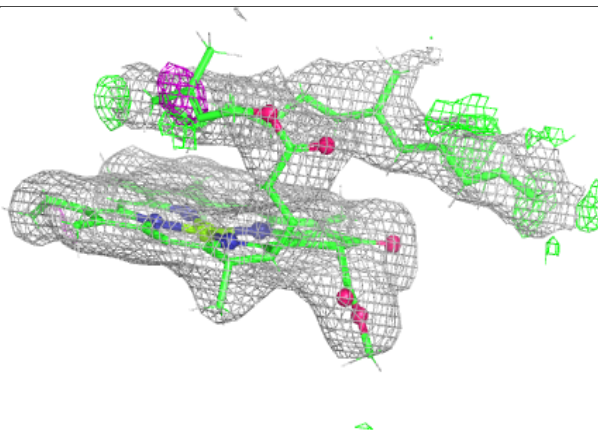
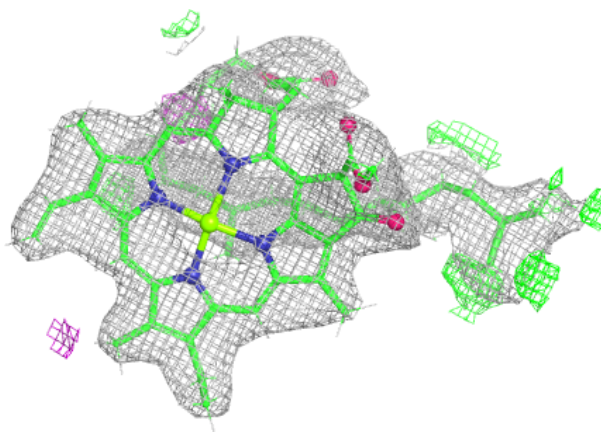


Electron density around SQD L 101:

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

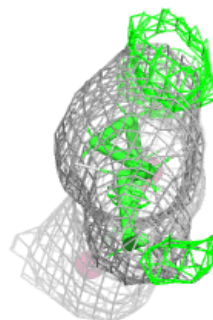
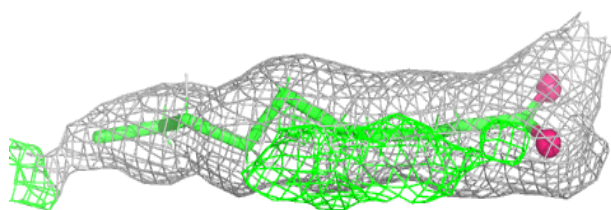
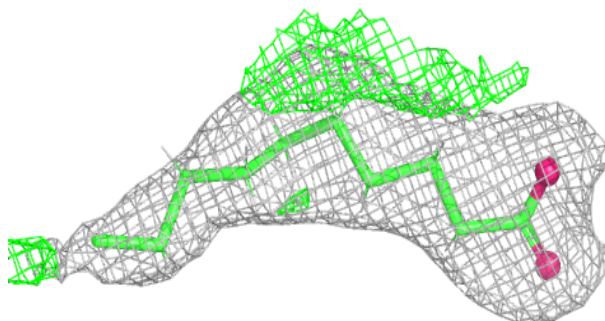
**Electron density around CLA B 601:**

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

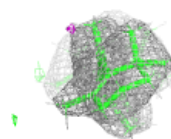
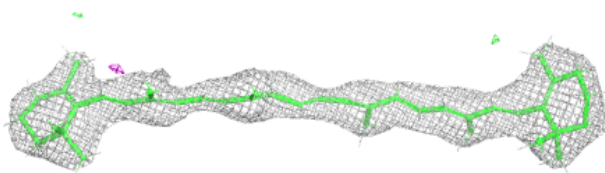
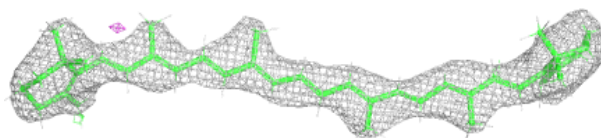


Electron density around STE C 522:

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

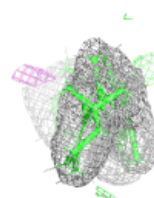
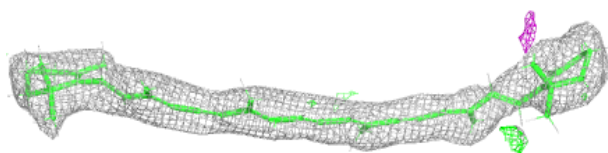
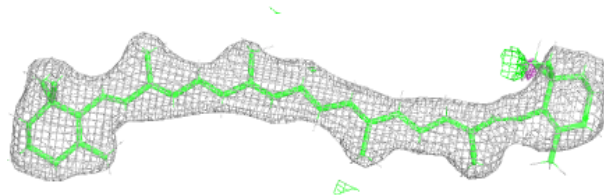
**Electron density around BCR c 514:**

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

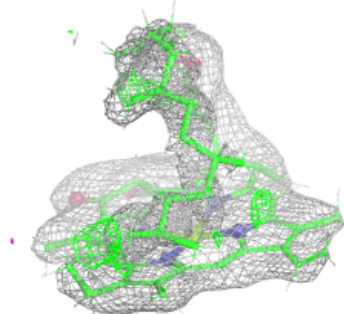
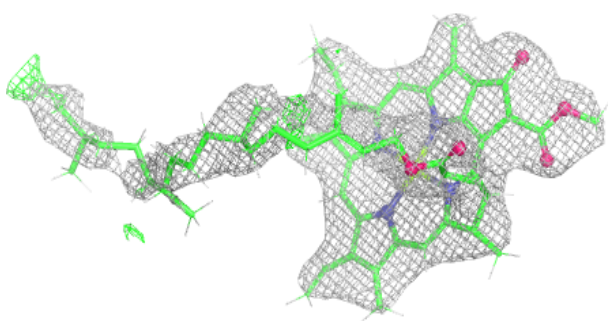
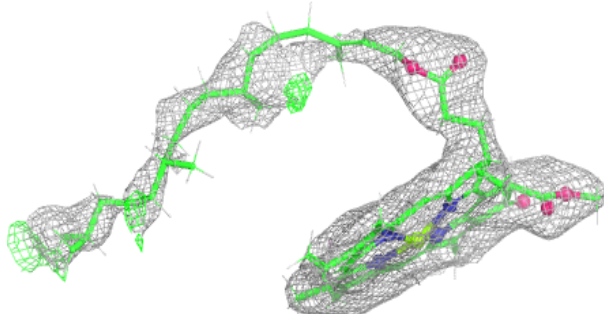


Electron density around BCR d 406:

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

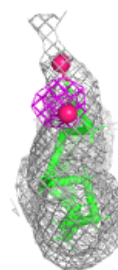
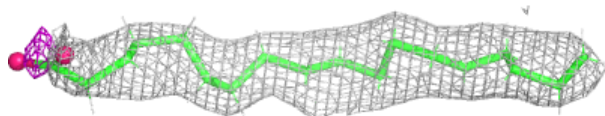
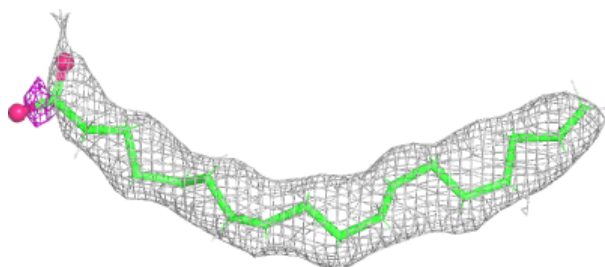
**Electron density around CLA C 513:**

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

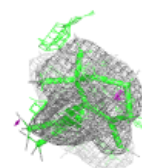
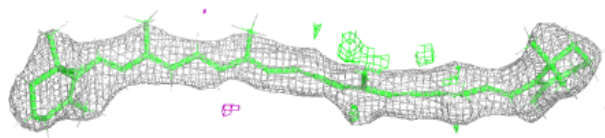
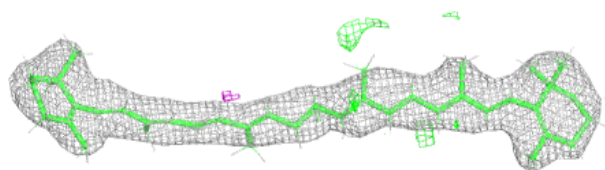


Electron density around STE D 411:

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

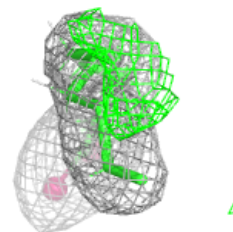
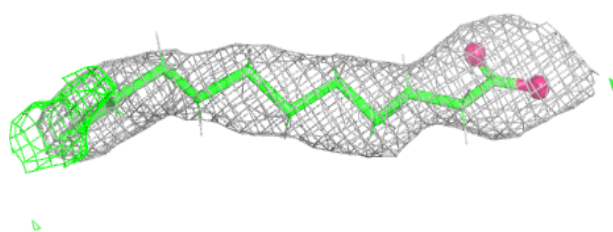
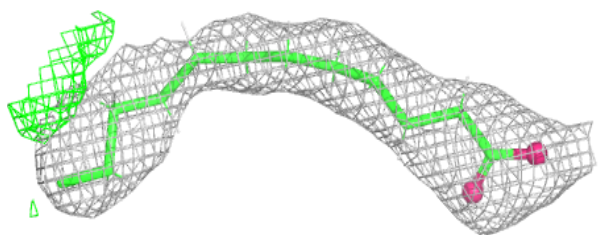
**Electron density around BCR K 101:**

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

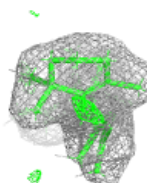
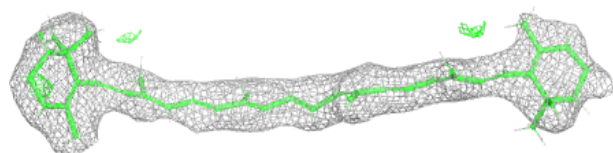
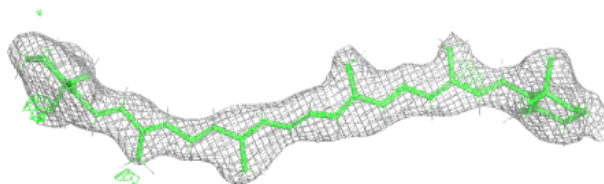


Electron density around STE t 102:

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

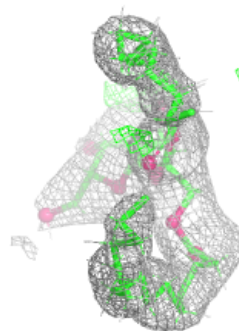
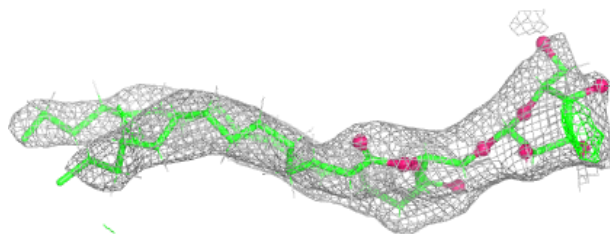
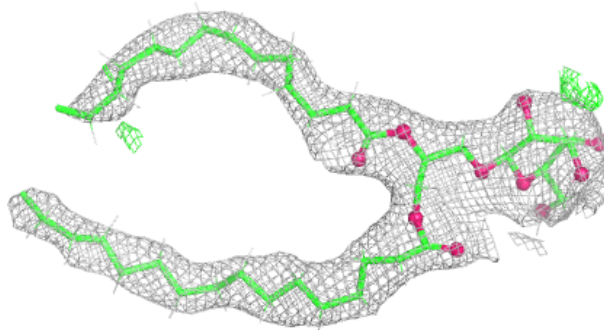
**Electron density around BCR h 101:**

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

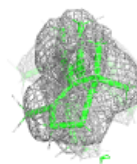
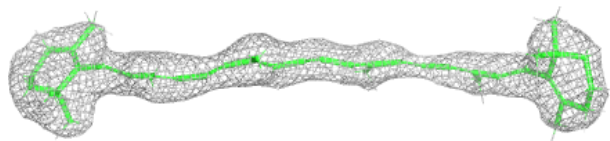


Electron density around LMG c 523:

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

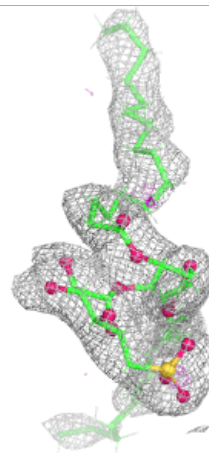
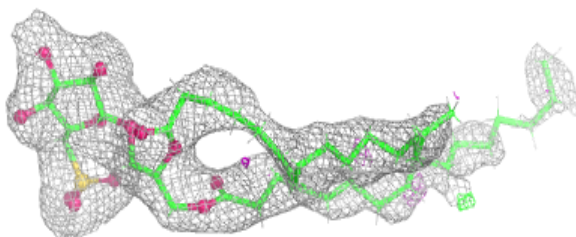
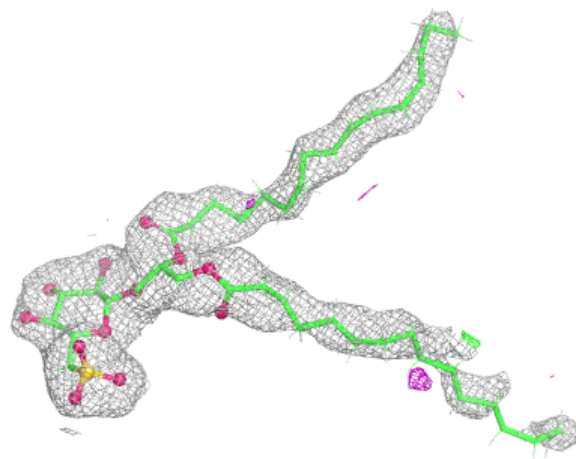
**Electron density around BCR k 101:**

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



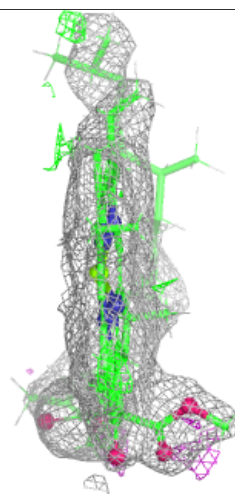
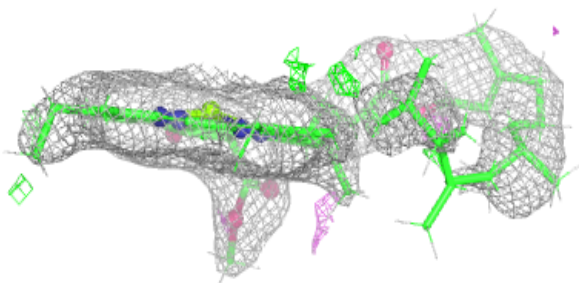
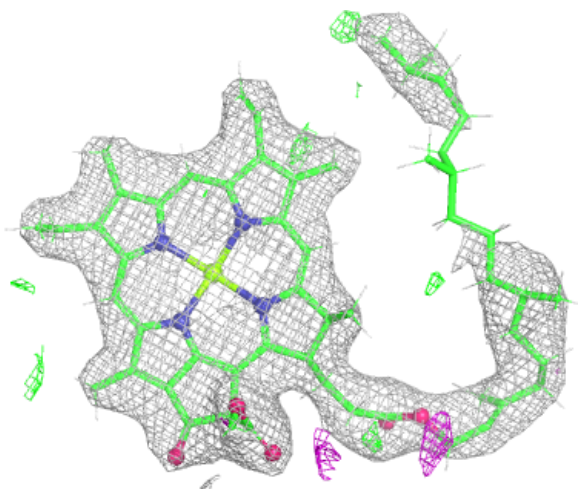
Electron density around SQD a 410:

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



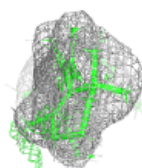
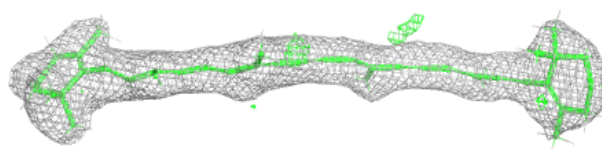
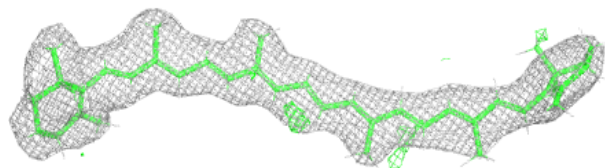
Electron density around CLA c 512:

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

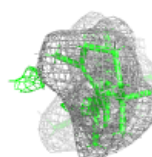
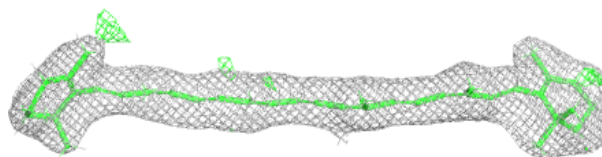
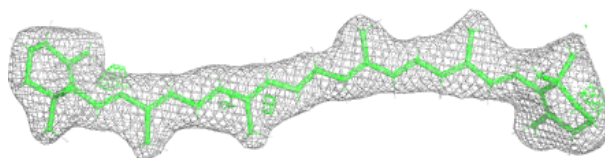


Electron density around BCR Y 101:

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

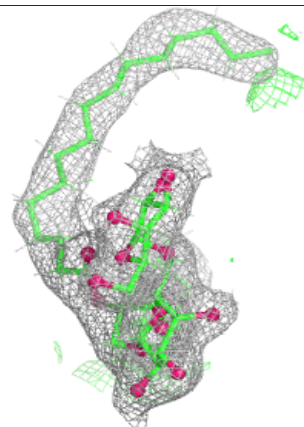
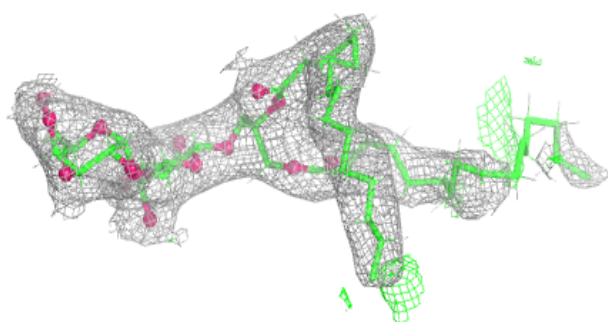
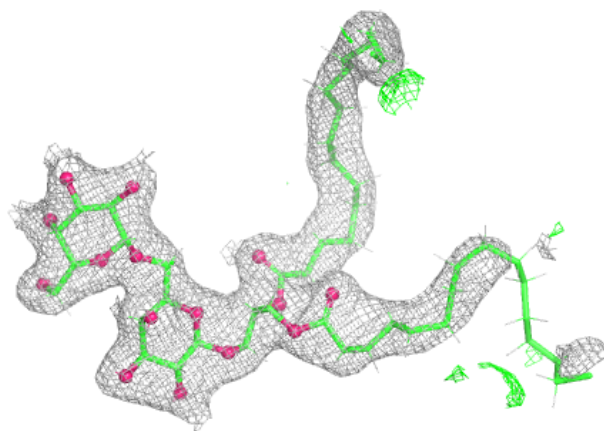
**Electron density around BCR b 618:**

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

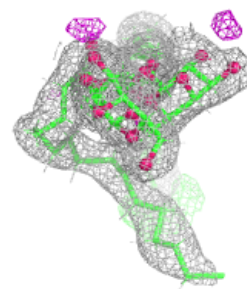
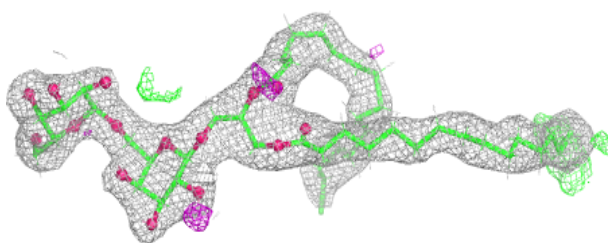
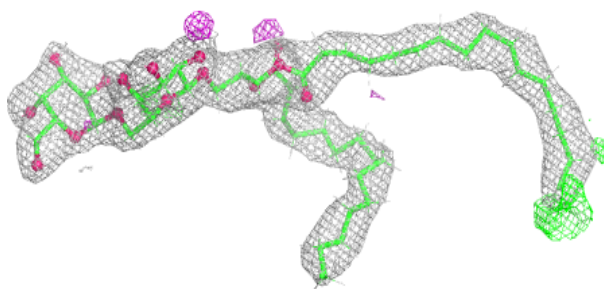


Electron density around DGD C 517:

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

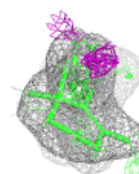
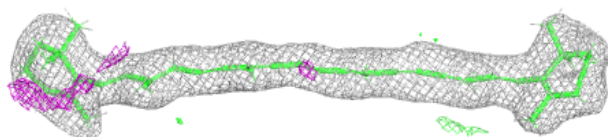
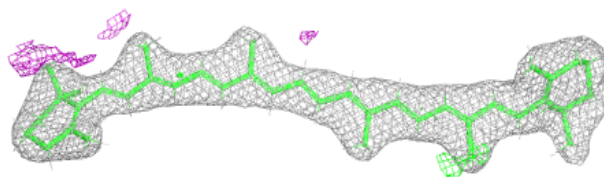
**Electron density around DGD H 102:**

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

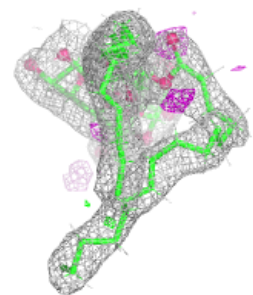
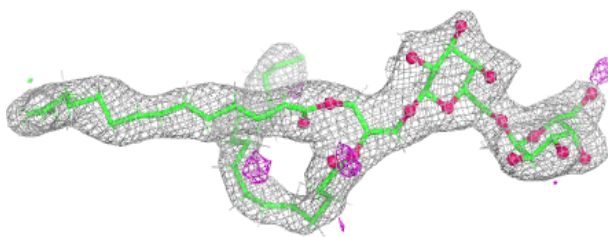
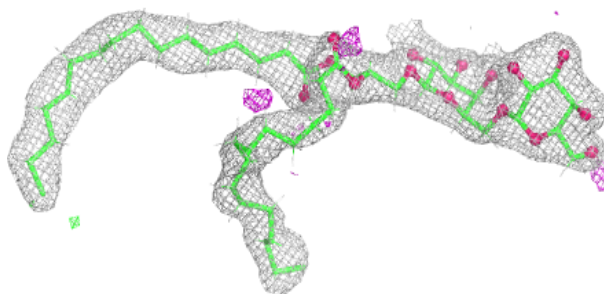


Electron density around BCR B 618:

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

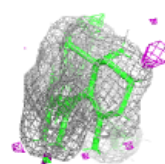
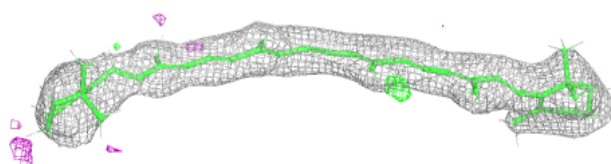
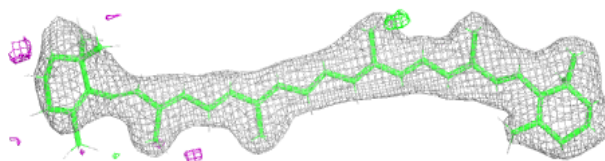
**Electron density around DGD h 102:**

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

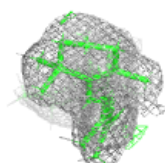
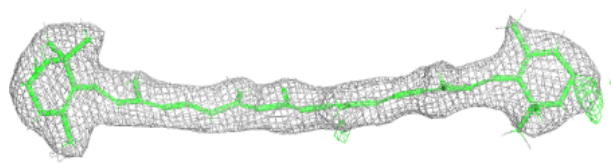
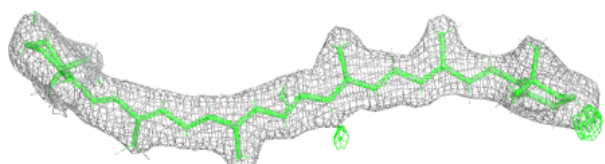


Electron density around BCR D 405:

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

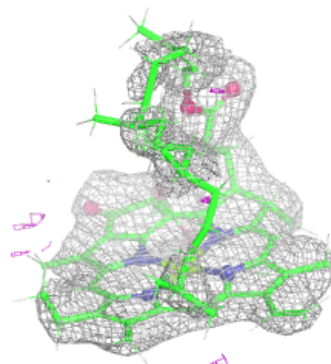
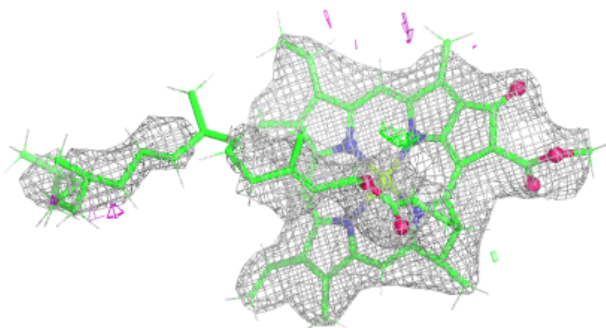
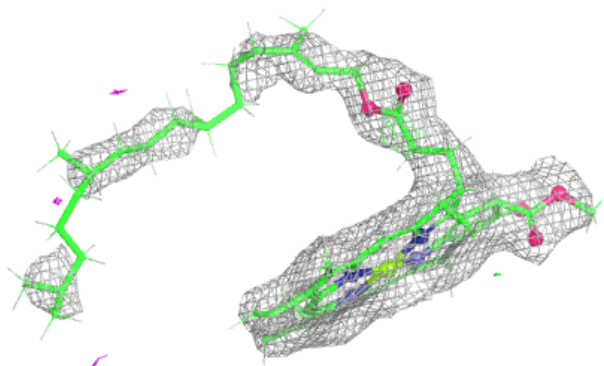
**Electron density around BCR H 101:**

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

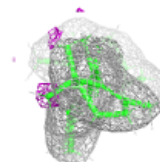
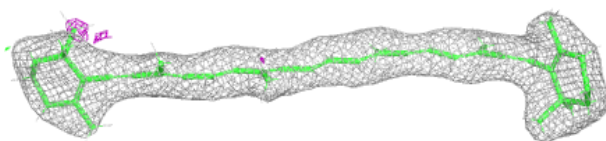
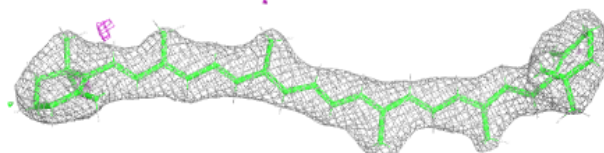


Electron density around CLA c 513:

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

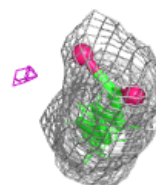
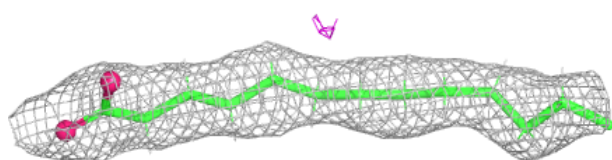
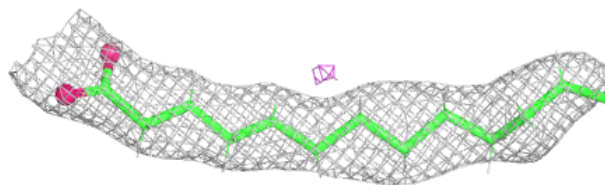
**Electron density around BCR c 515:**

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

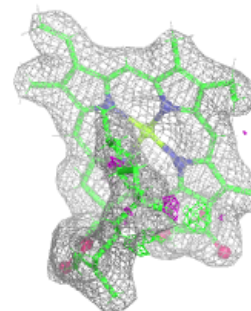
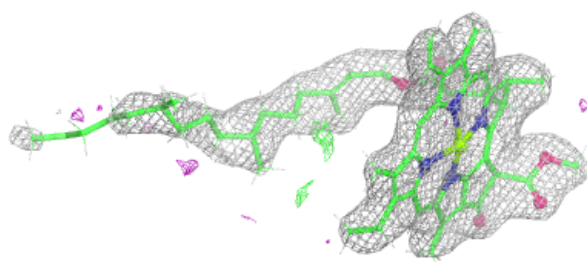
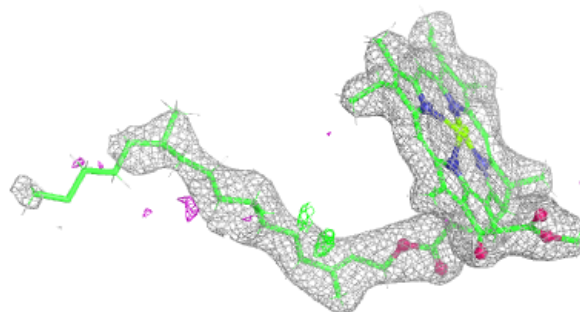


Electron density around STE M 102:

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

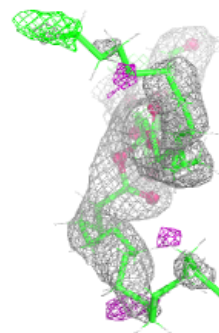
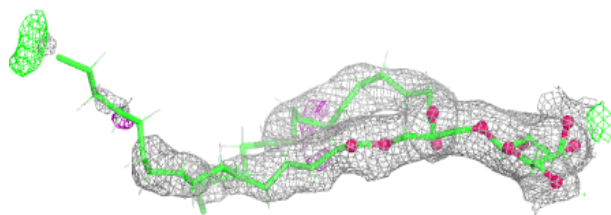
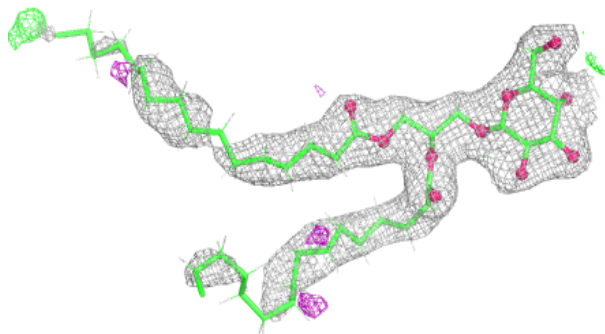
**Electron density around CLA c 508:**

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



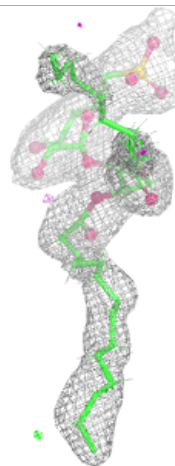
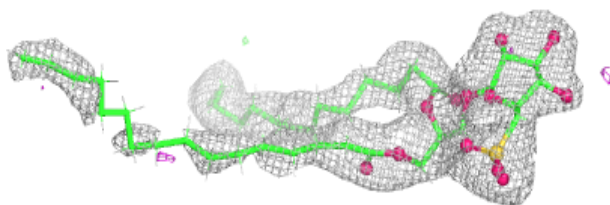
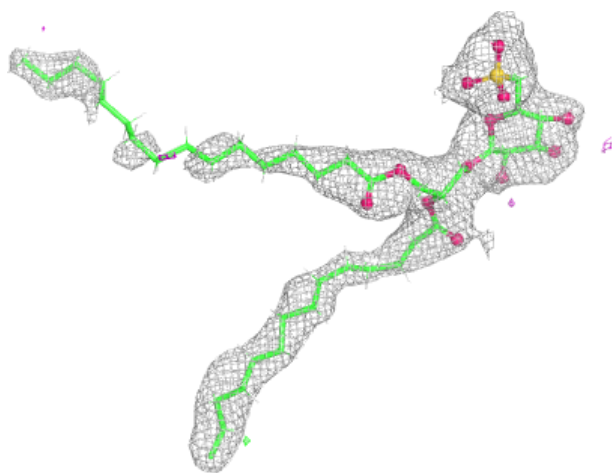
Electron density around LMG D 407:

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



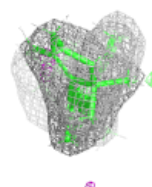
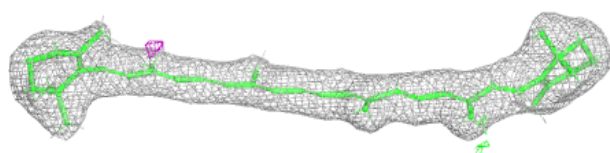
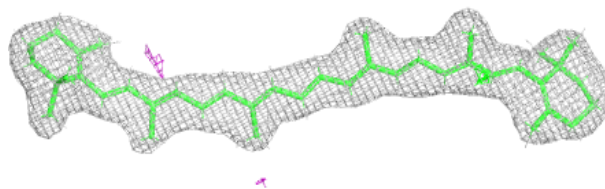
Electron density around SQD A 412:

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

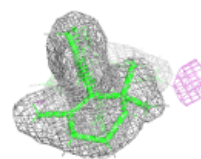
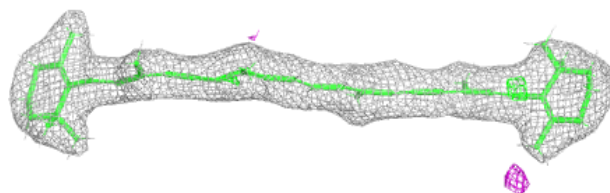
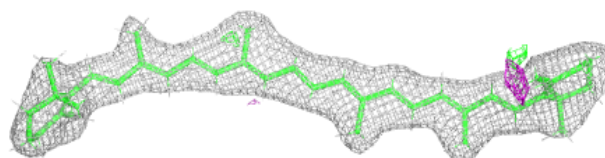


Electron density around BCR B 619:

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

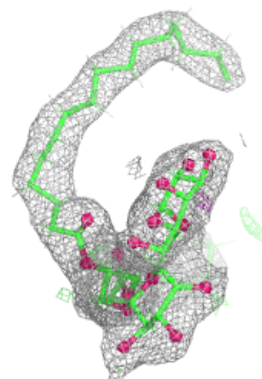
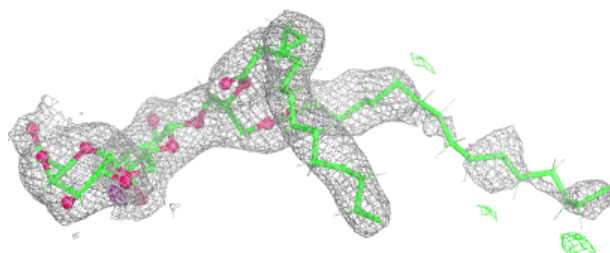
**Electron density around BCR C 514:**

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

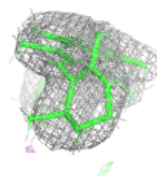
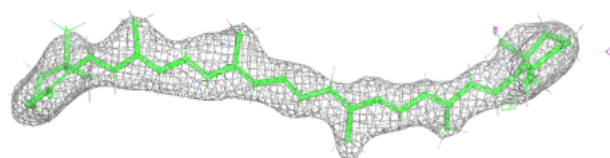
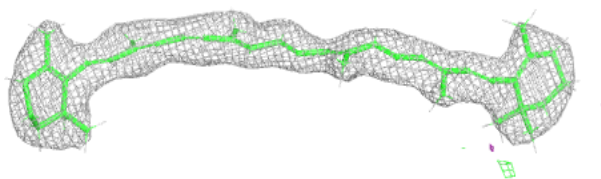


Electron density around DGD c 518:

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

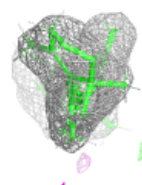
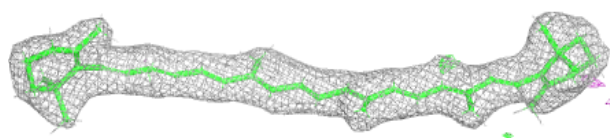
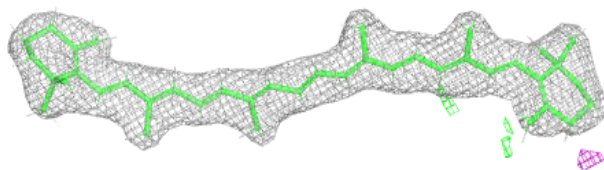
**Electron density around BCR C 515:**

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

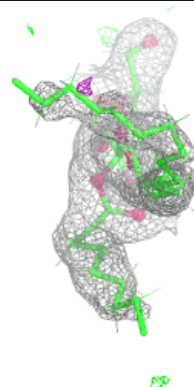
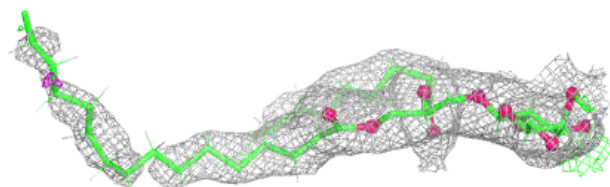
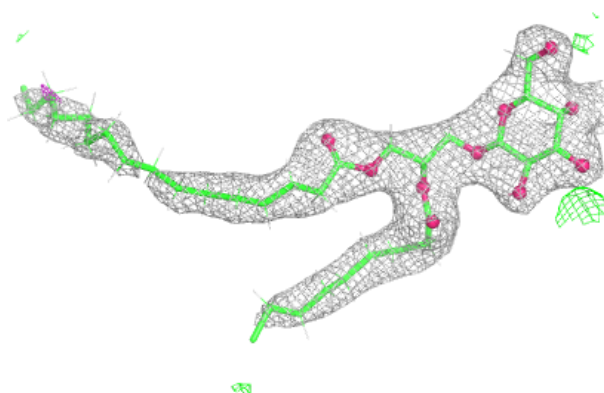


Electron density around BCR b 619:

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

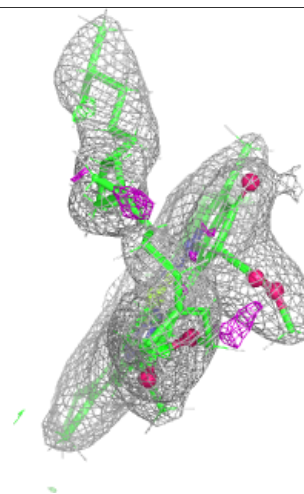
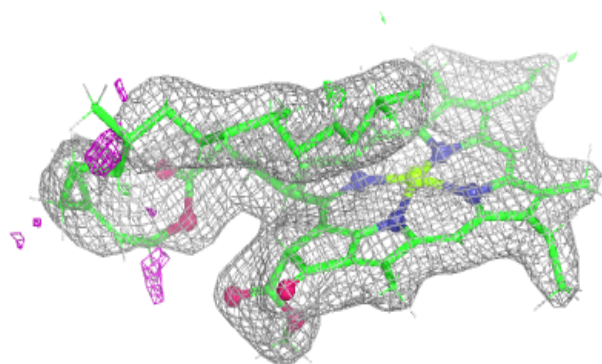
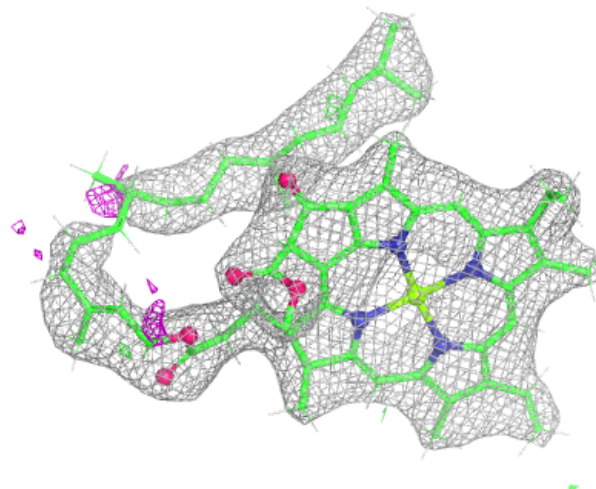
**Electron density around LMG d 412:**

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



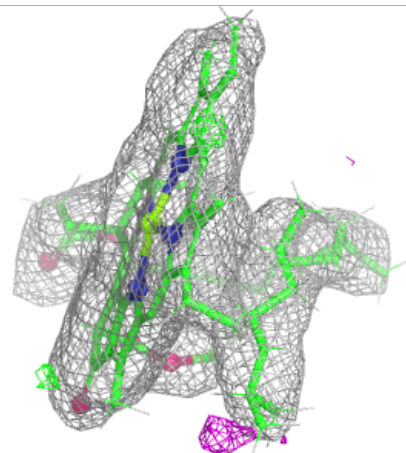
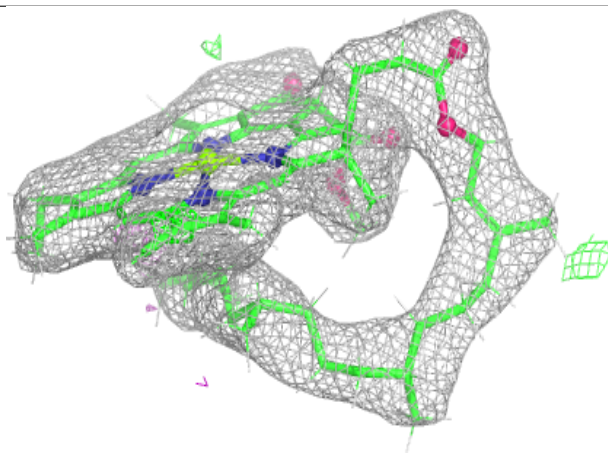
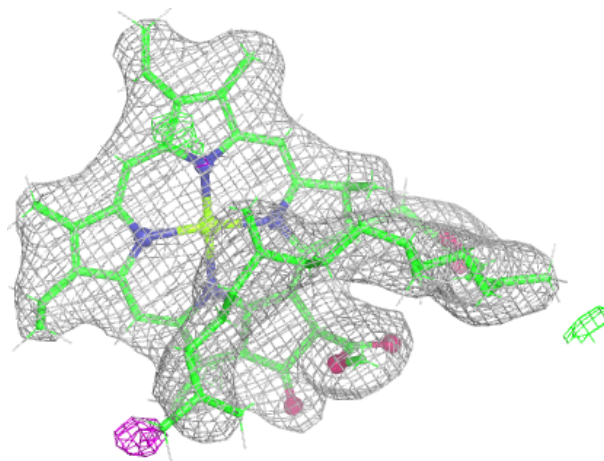
Electron density around CLA c 509:

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



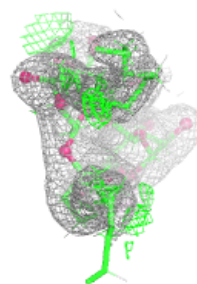
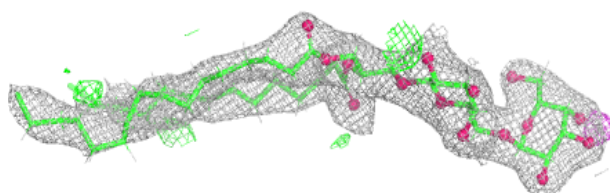
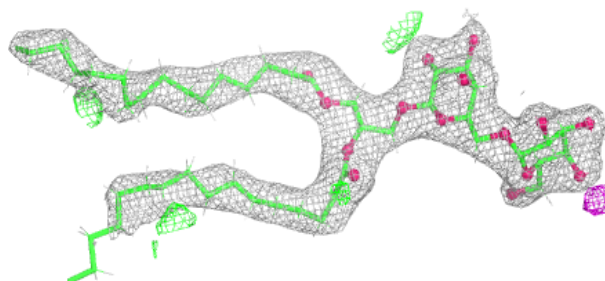
Electron density around CLA c 510:

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

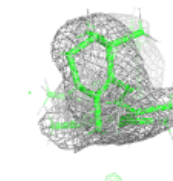
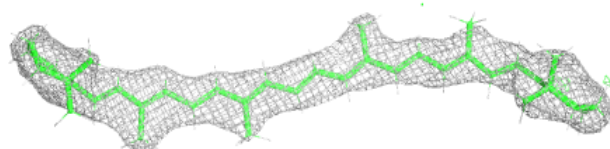
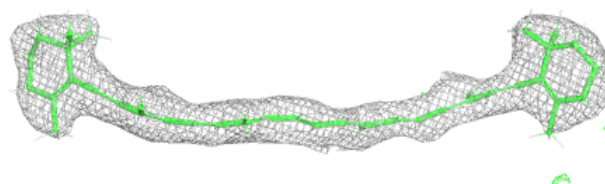


Electron density around DGD c 519:

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

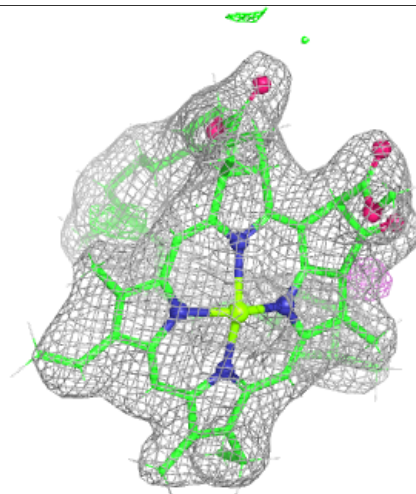
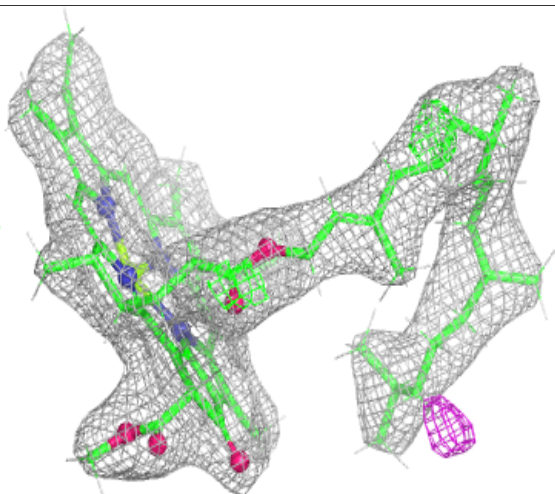
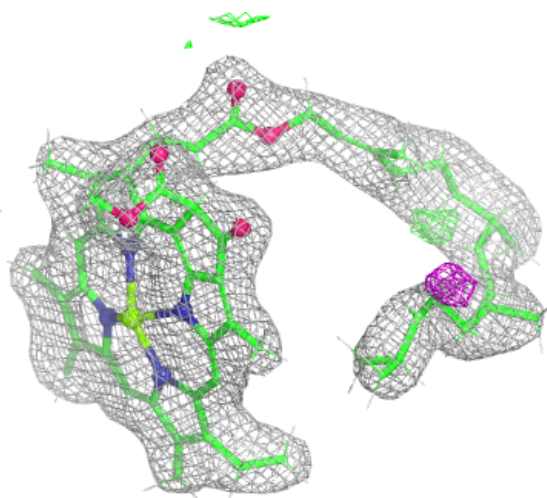
**Electron density around BCR c 516:**

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



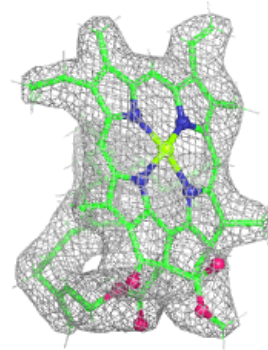
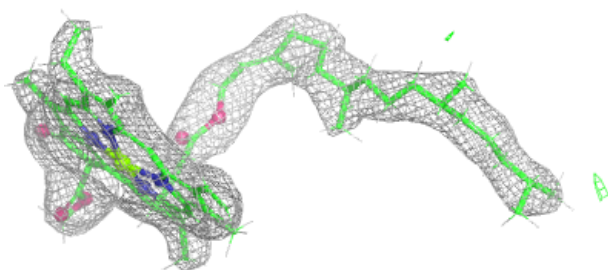
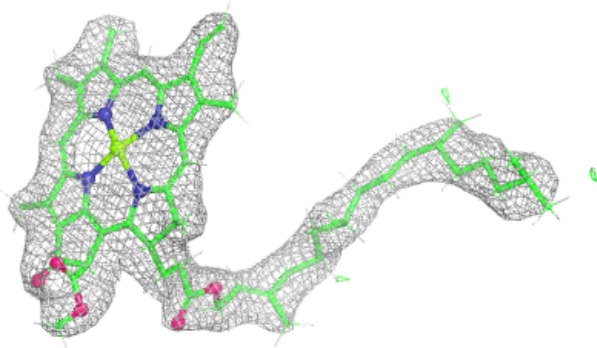
Electron density around CLA C 503:

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

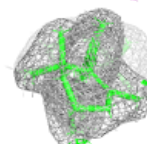
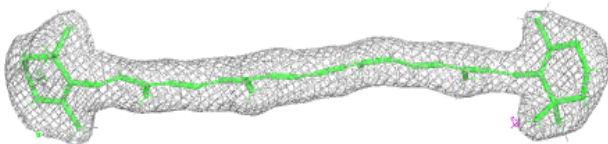
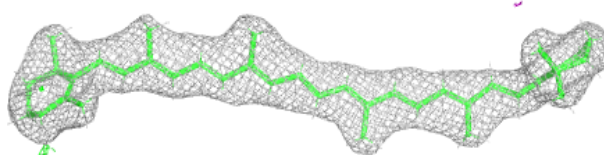


Electron density around CLA C 511:

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

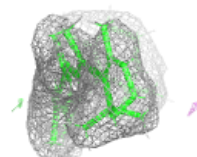
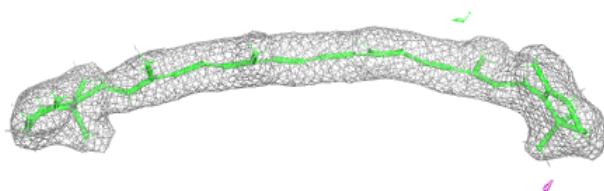
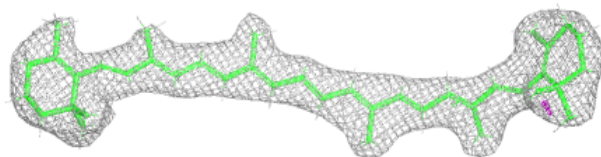
**Electron density around BCR A 406:**

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

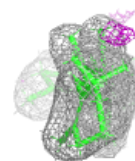
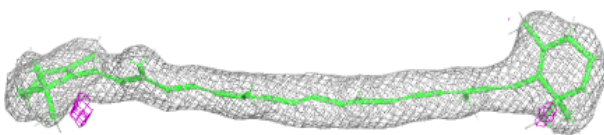
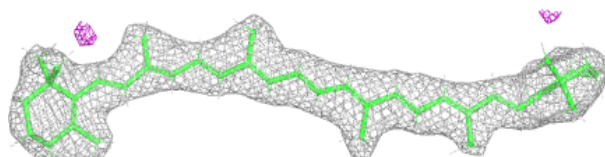


Electron density around BCR T 101:

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

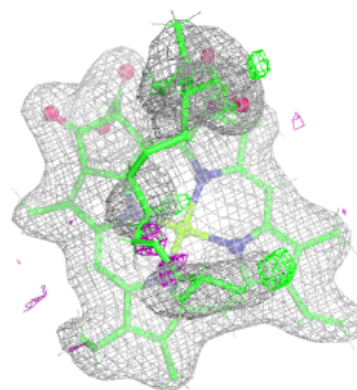
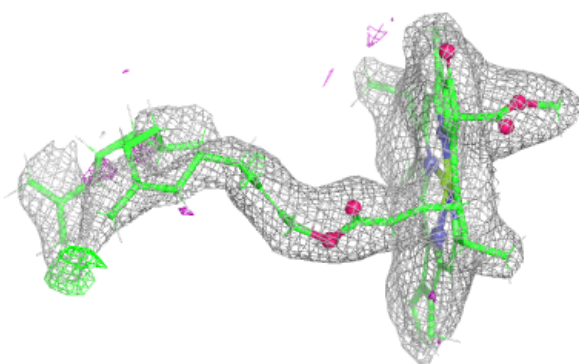
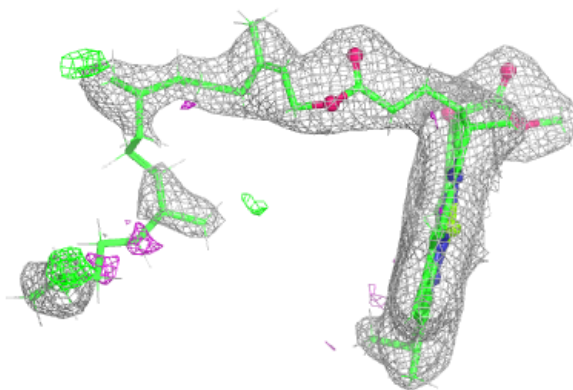
**Electron density around BCR B 617:**

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

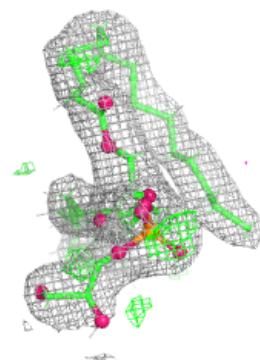
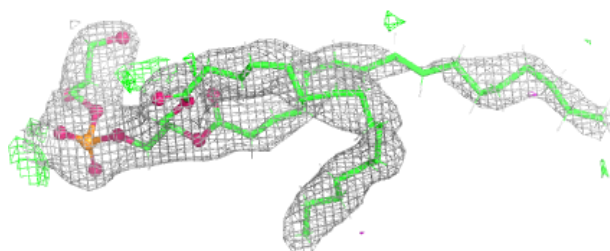
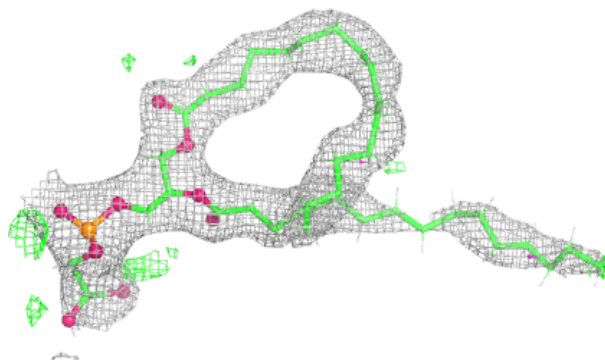


Electron density around CLA c 506:

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

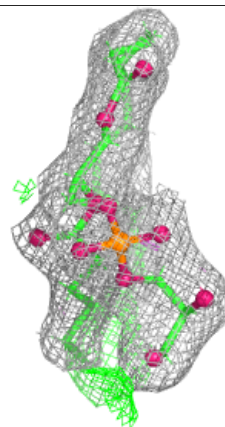
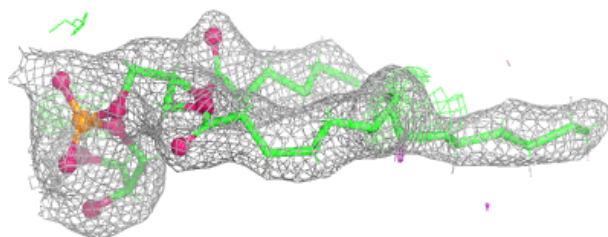
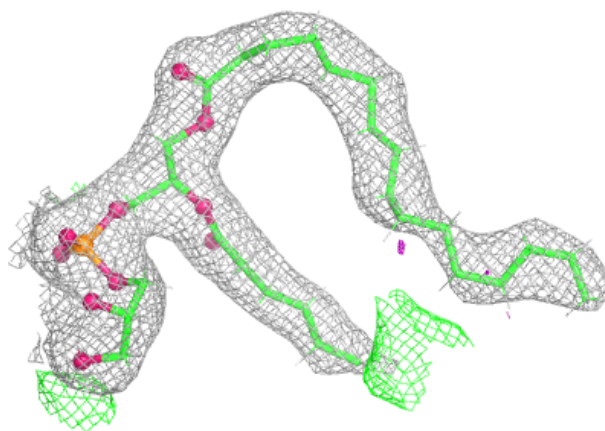
**Electron density around LHG d 408:**

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

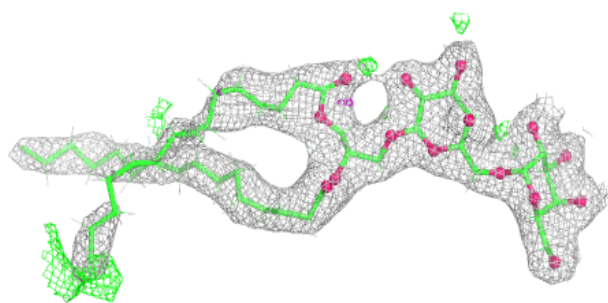
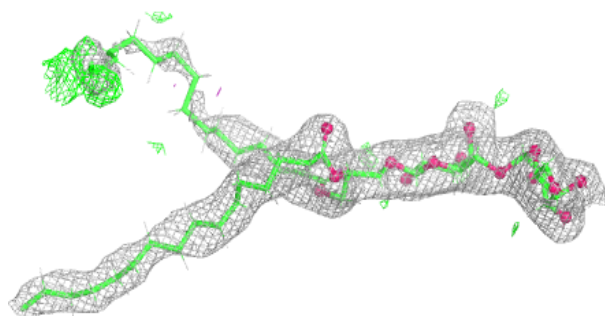


Electron density around LHG d 410:

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

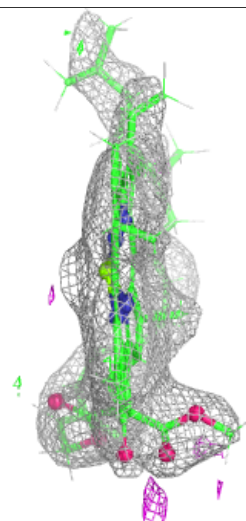
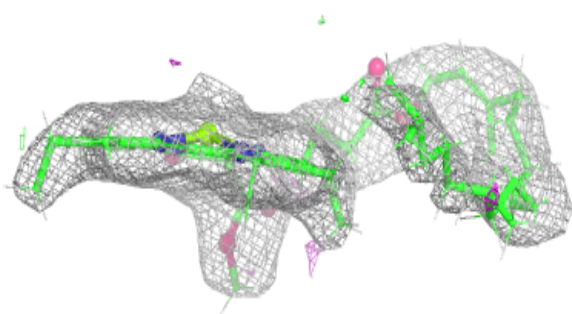
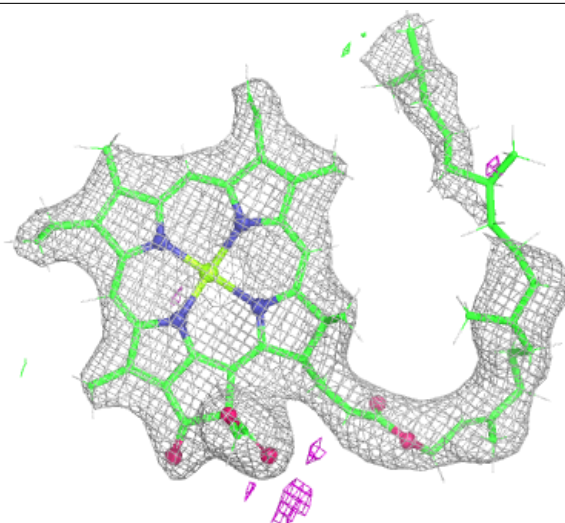
**Electron density around DGD C 516:**

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



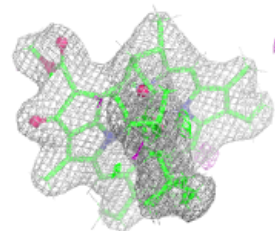
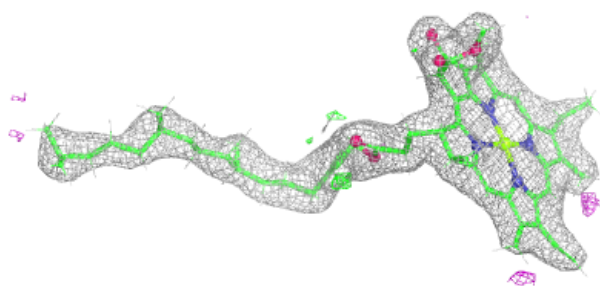
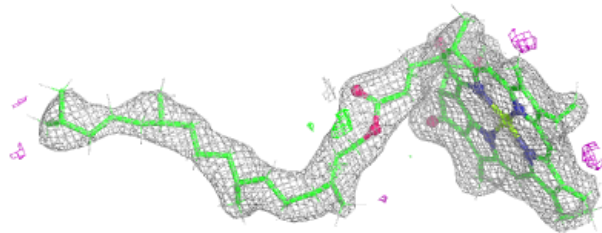
Electron density around CLA C 512:

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



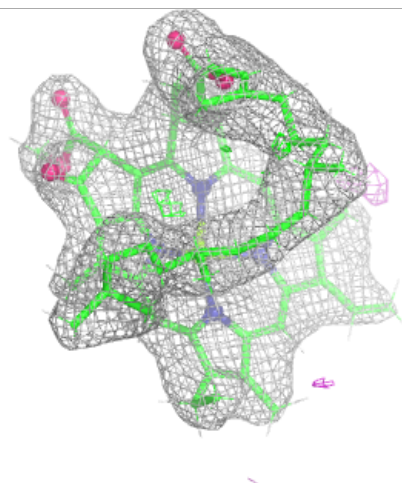
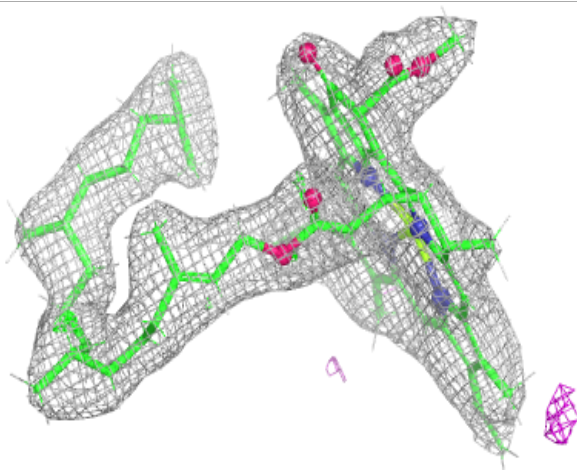
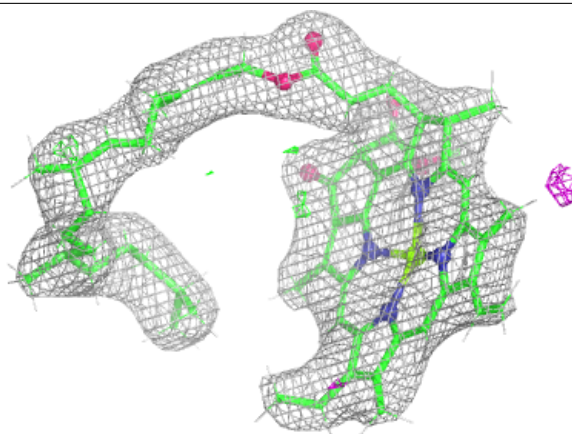
Electron density around CLA c 502:

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



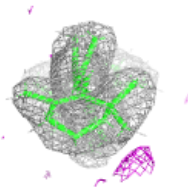
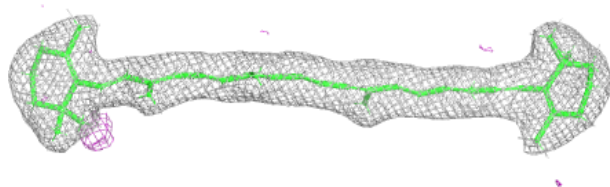
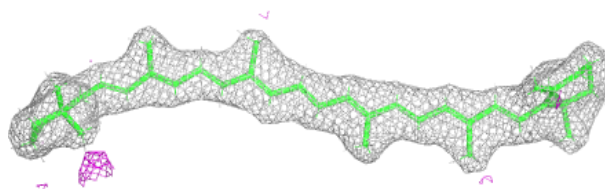
Electron density around CLA c 503:

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

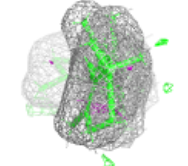
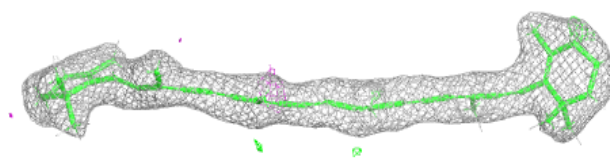
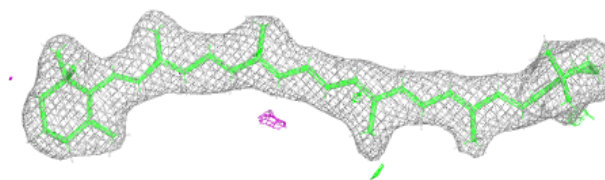


Electron density around BCR a 405:

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

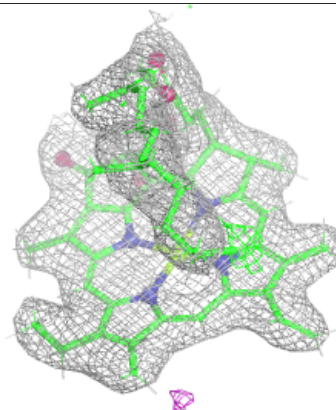
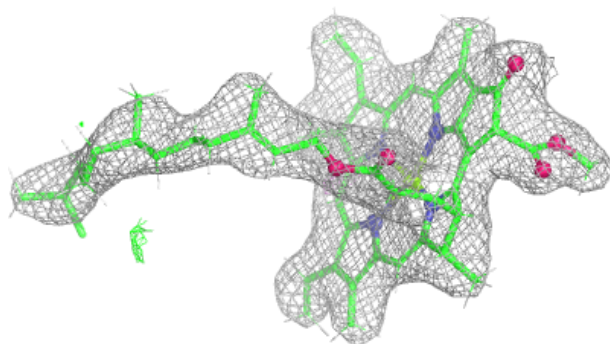
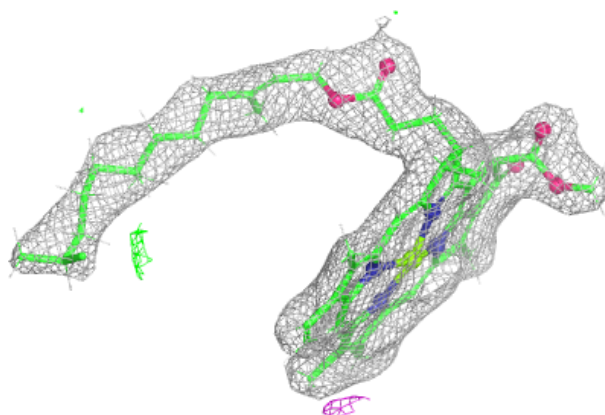
**Electron density around BCR b 617:**

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

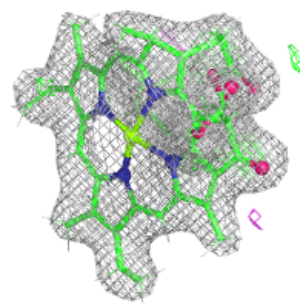
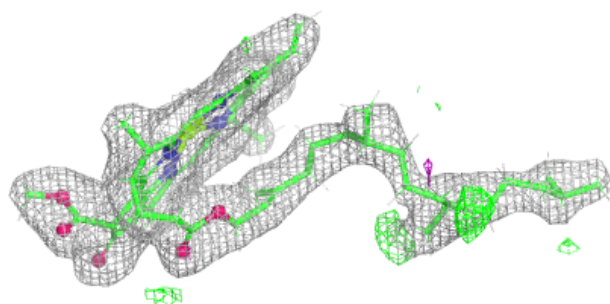
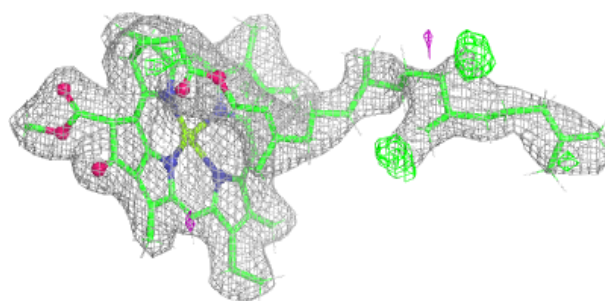


Electron density around CLA c 504:

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

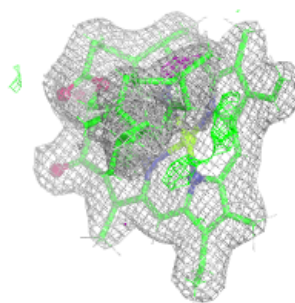
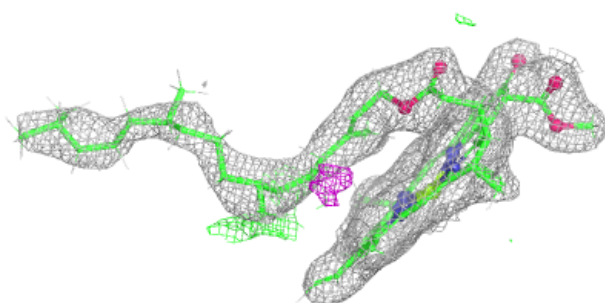
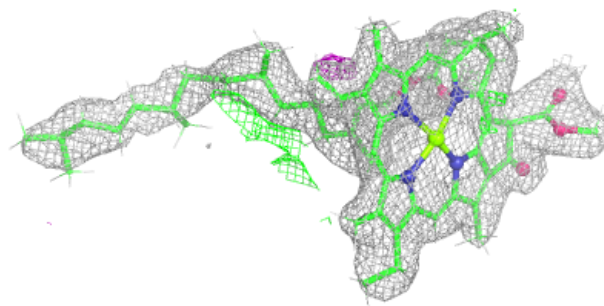
**Electron density around CLA c 505:**

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



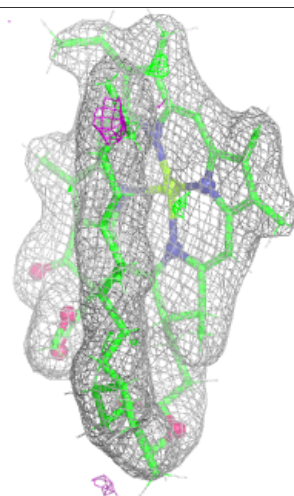
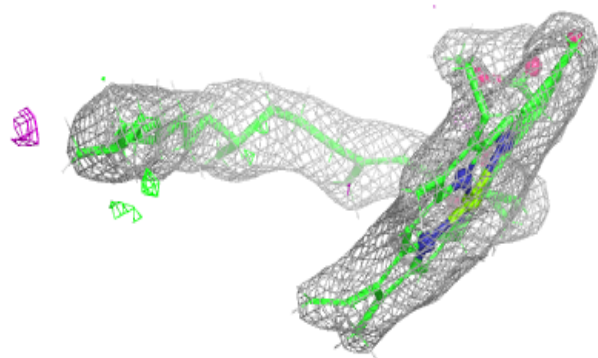
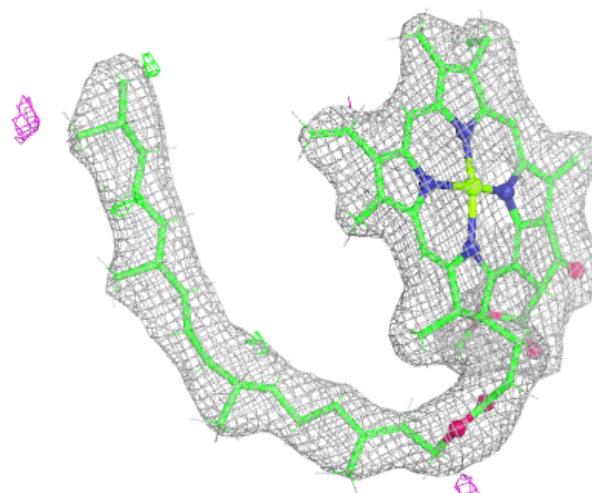
Electron density around CLA C 505:

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



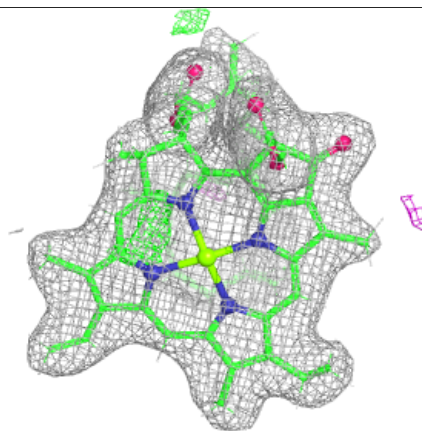
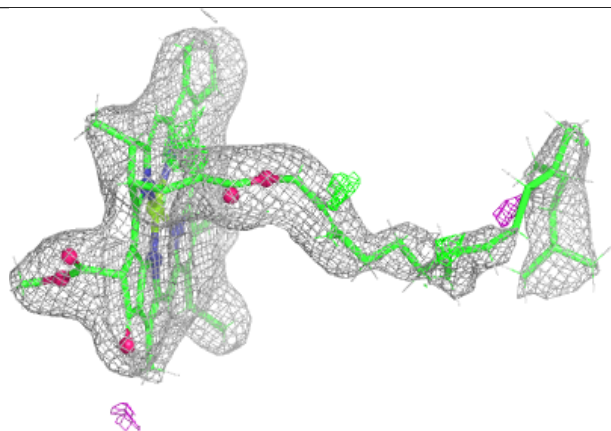
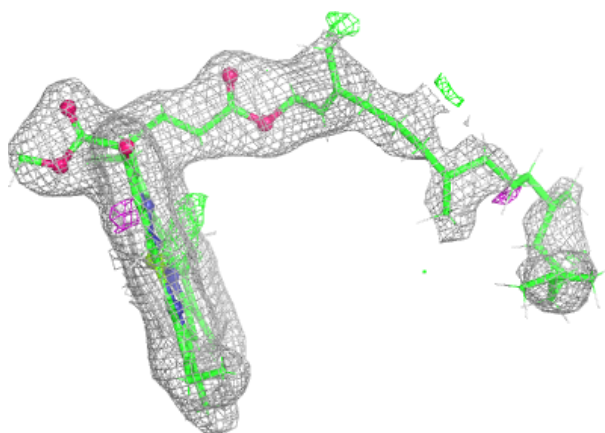
Electron density around CLA c 507:

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

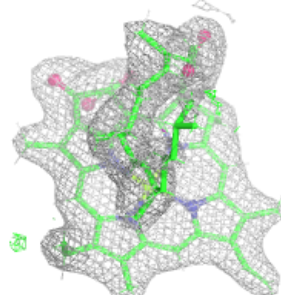
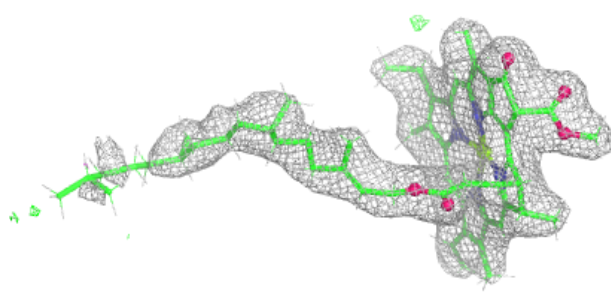
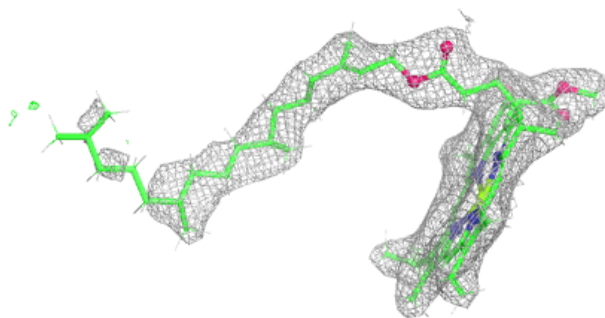


Electron density around CLA C 506:

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

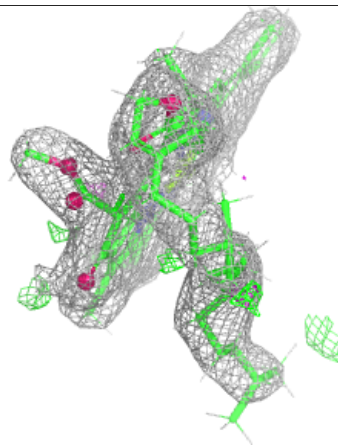
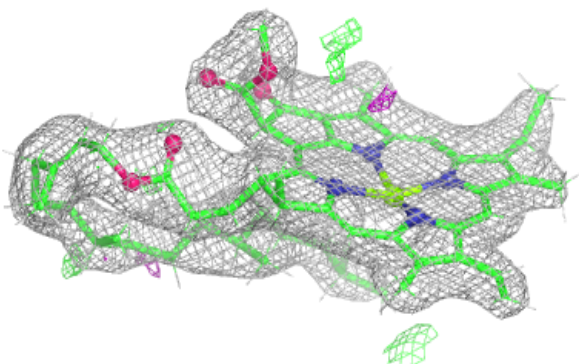
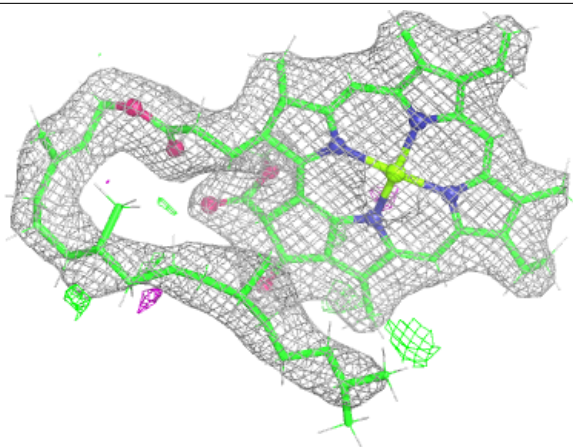
**Electron density around CLA C 508:**

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



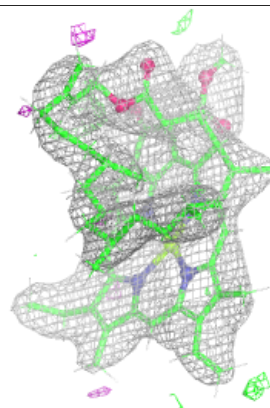
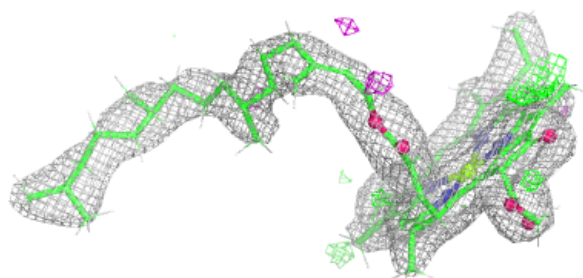
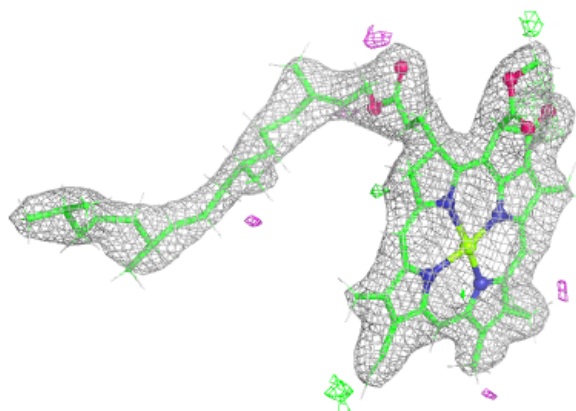
Electron density around CLA C 509:

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

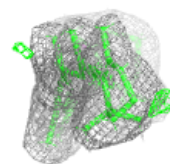
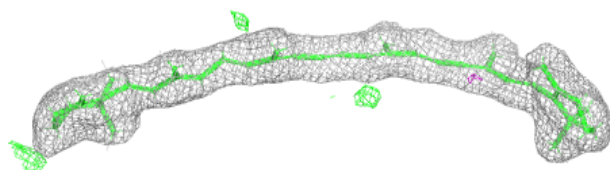
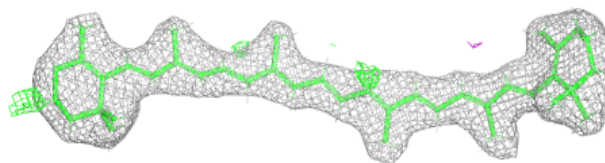


Electron density around CLA c 511:

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

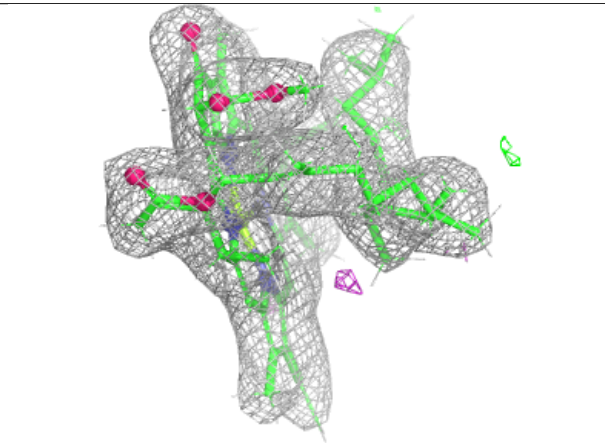
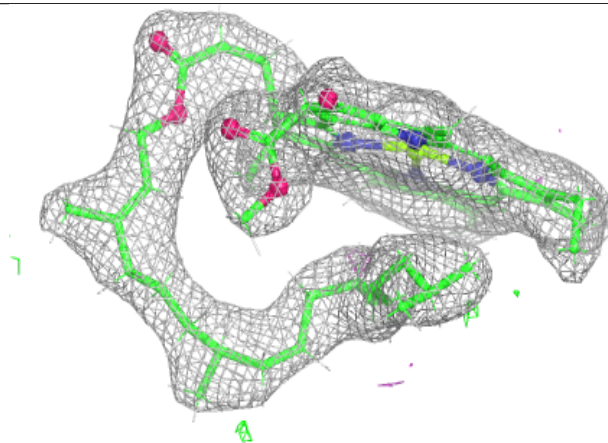
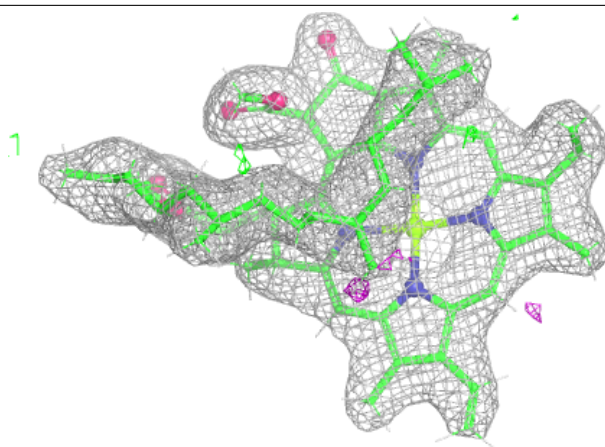
**Electron density around BCR t 101:**

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

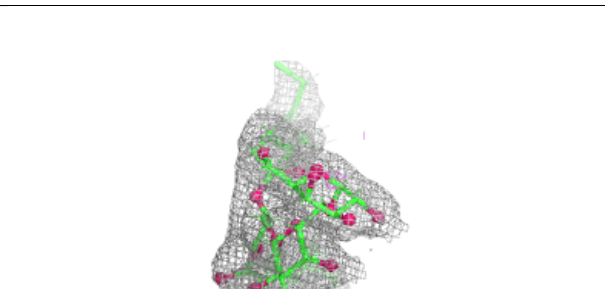
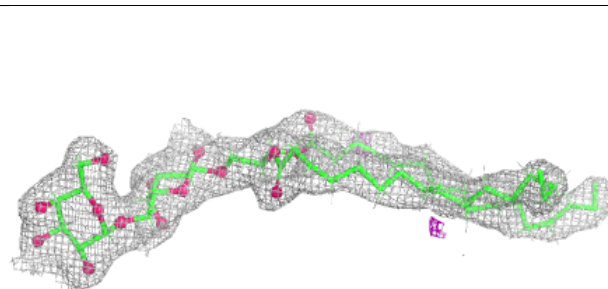
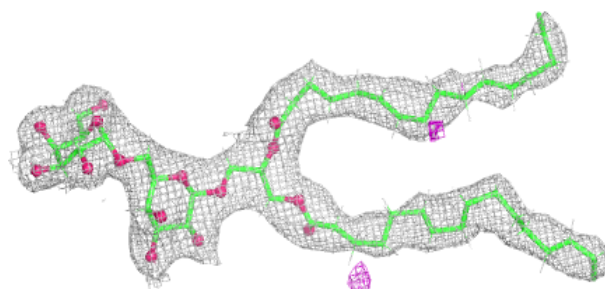


Electron density around CLA C 510:

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

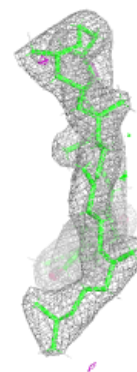
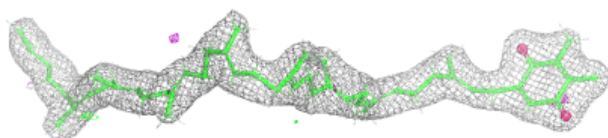
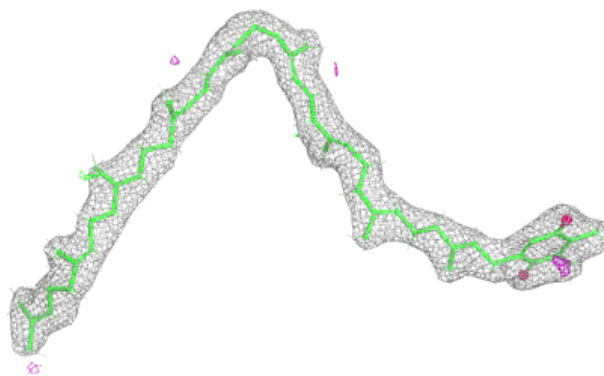
**Electron density around DGD C 518:**

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

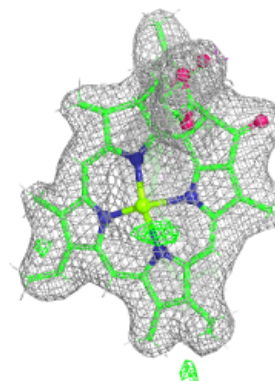
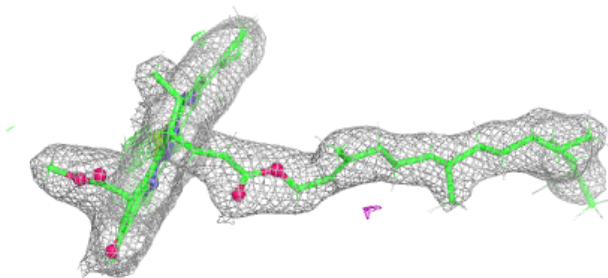
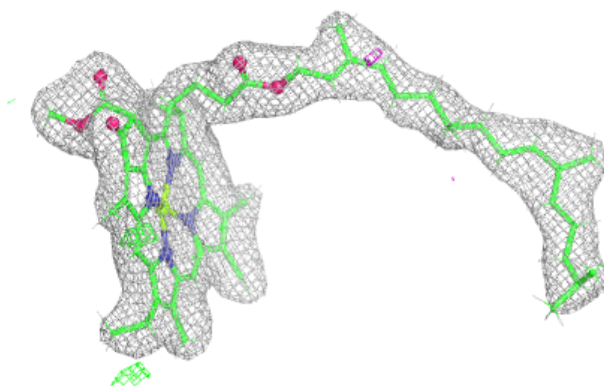


Electron density around PL9 D 406:

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

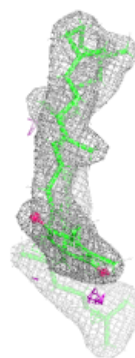
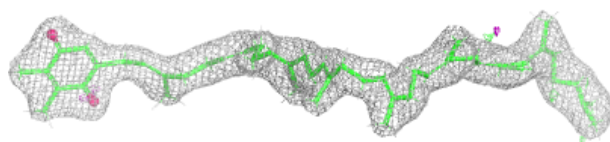
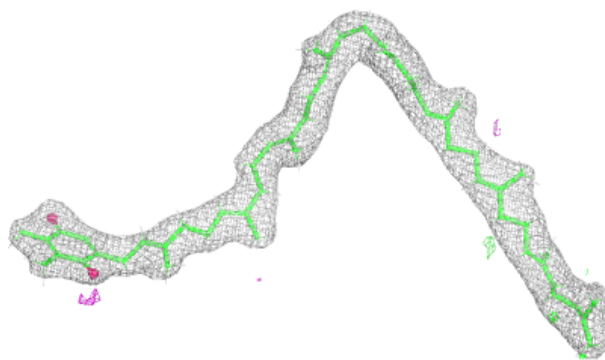
**Electron density around CLA B 609:**

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

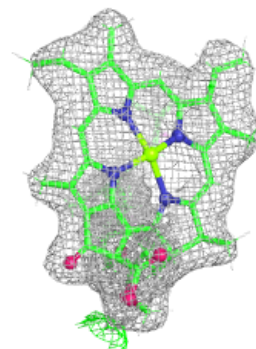
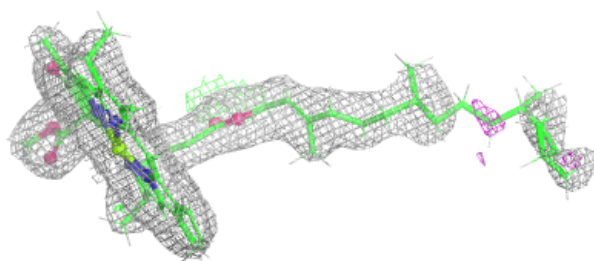
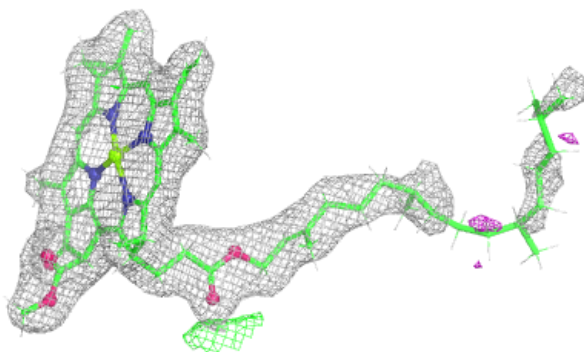


Electron density around PL9 d 407:

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

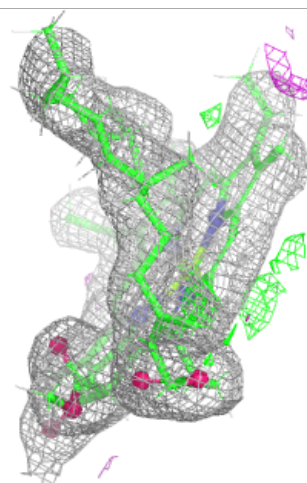
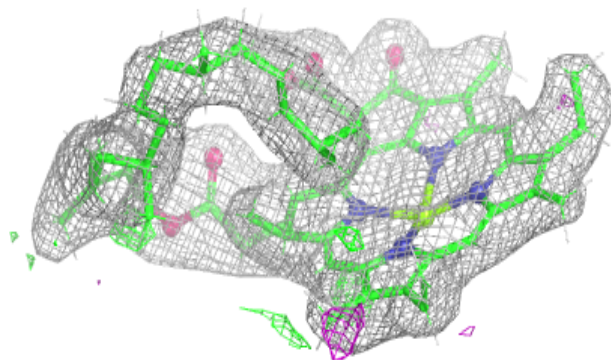
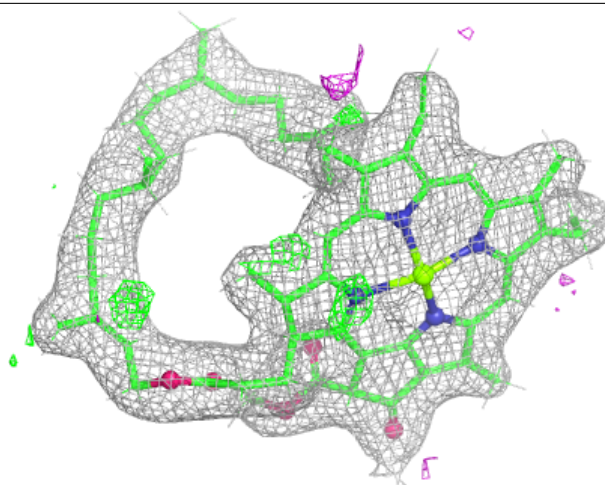
**Electron density around CLA d 405:**

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



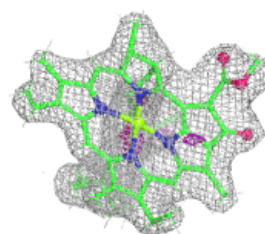
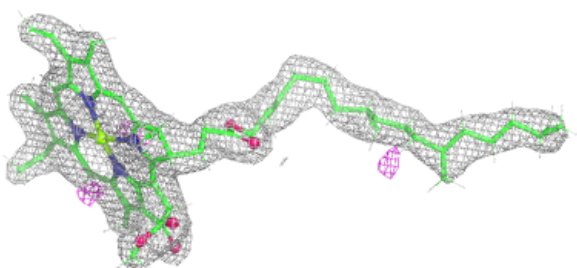
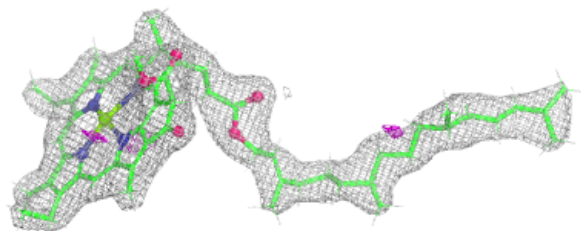
Electron density around CLA B 615:

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

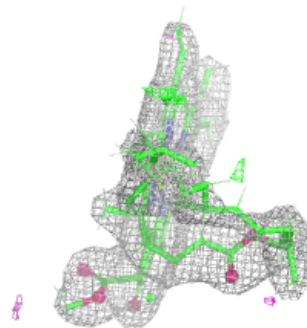
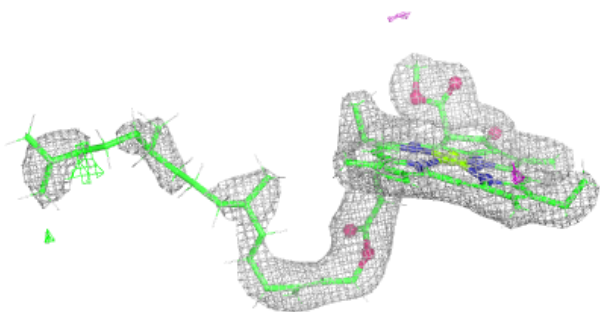
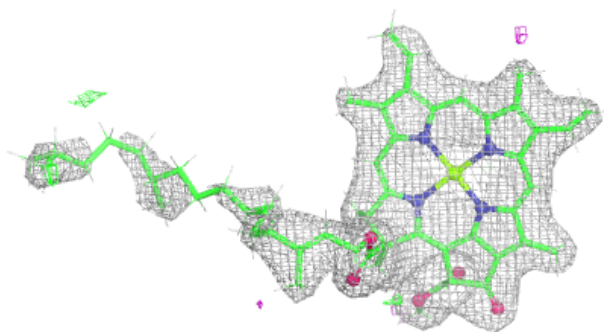


Electron density around CLA C 502:

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

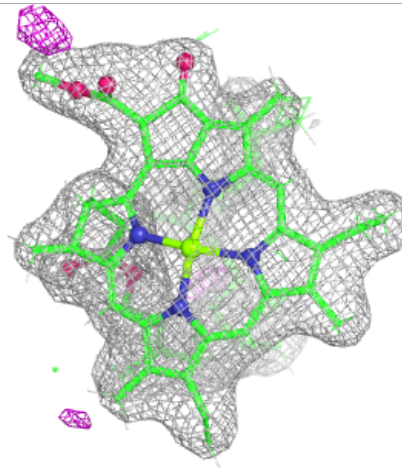
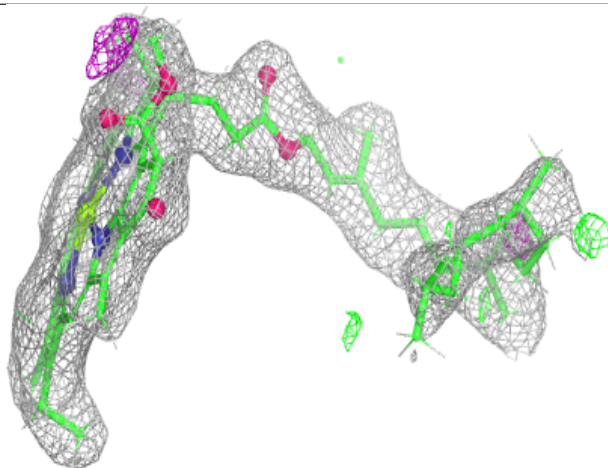
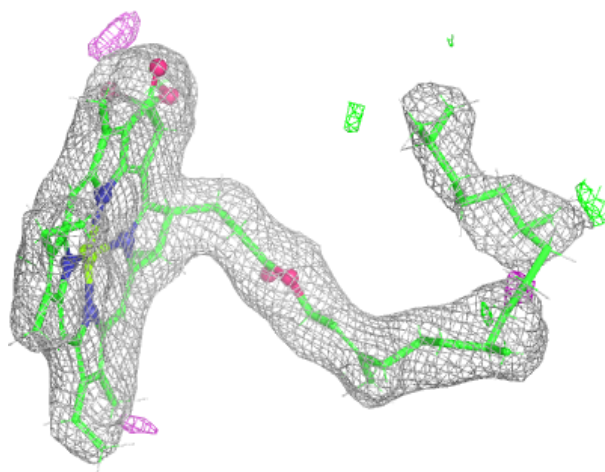
**Electron density around CLA a 403:**

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



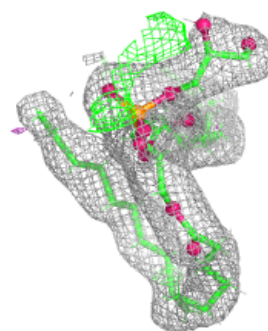
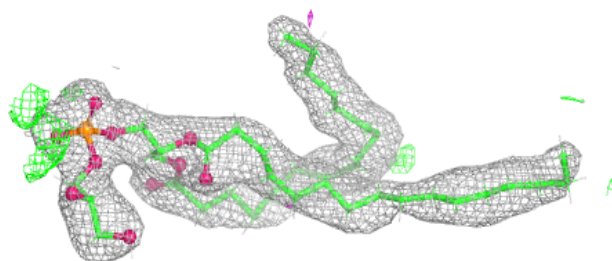
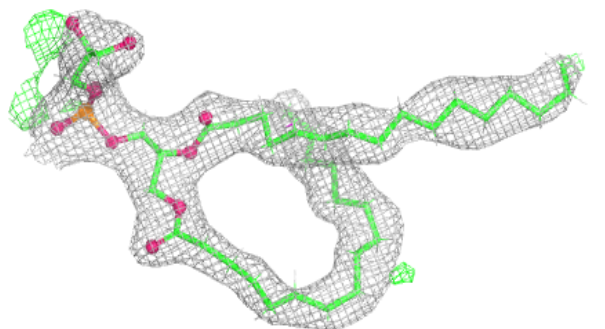
Electron density around CLA B 606:

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

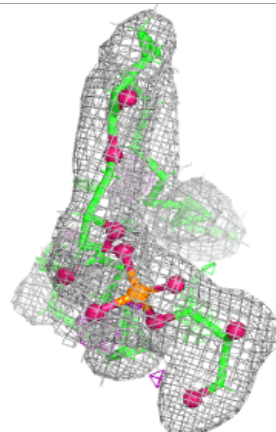
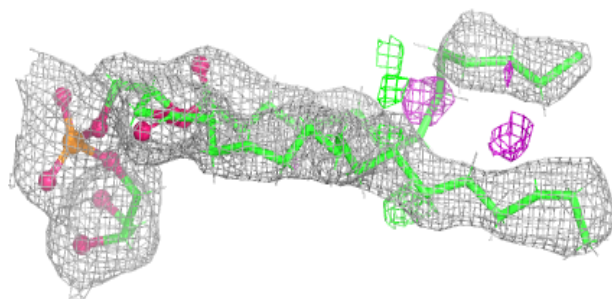
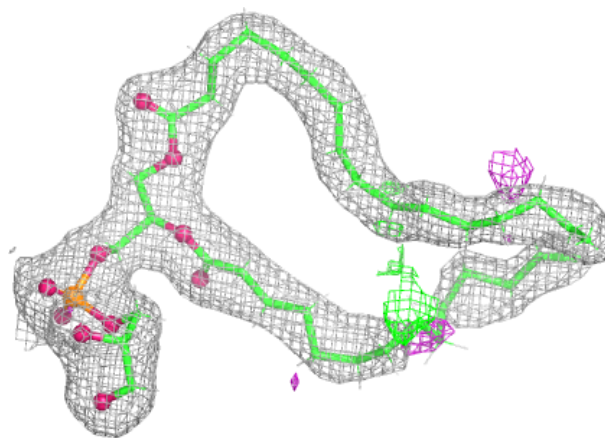


Electron density around LHG B 622:

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

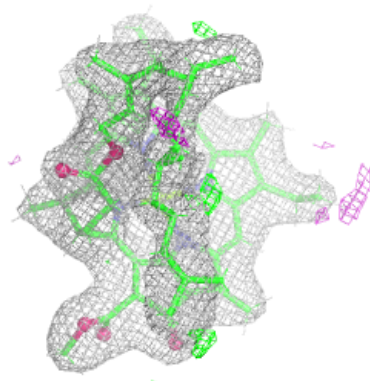
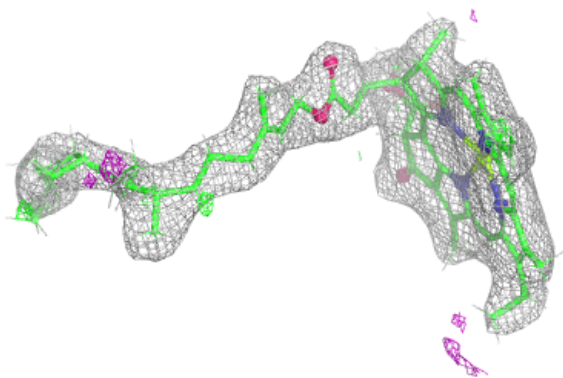
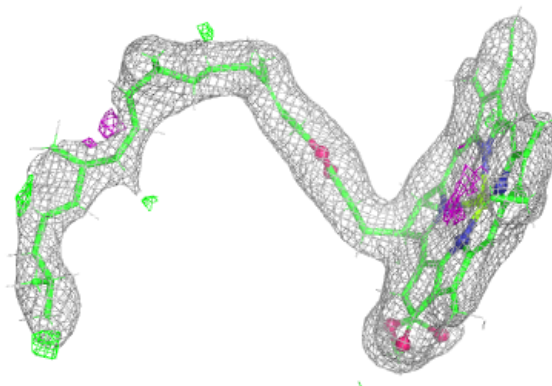
**Electron density around LHG D 409:**

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



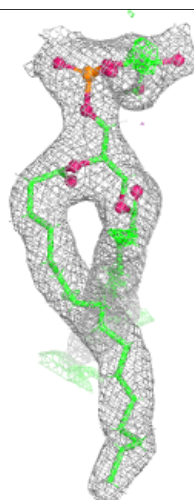
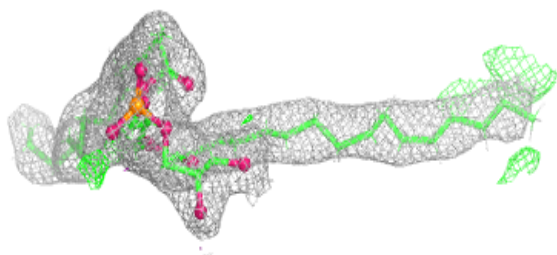
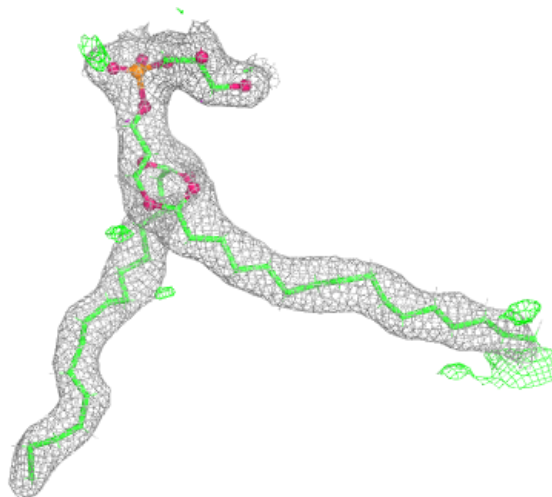
Electron density around CLA b 606:

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



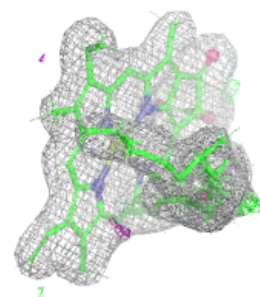
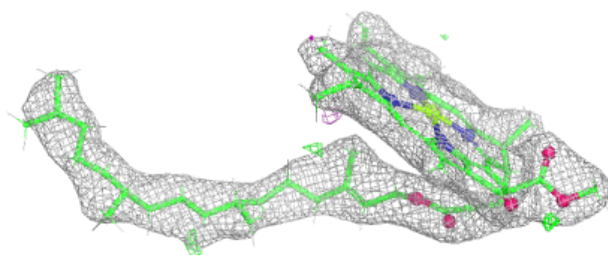
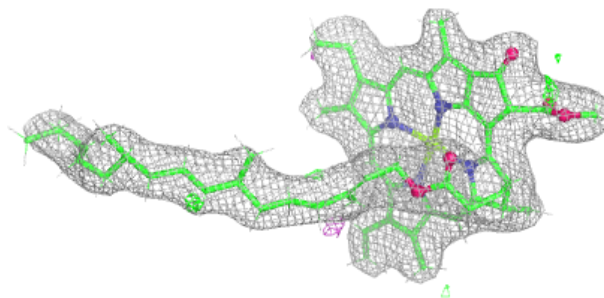
Electron density around LHG L 102:

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

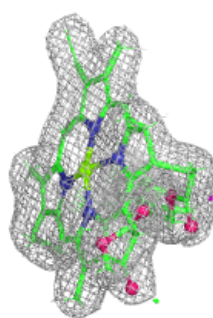
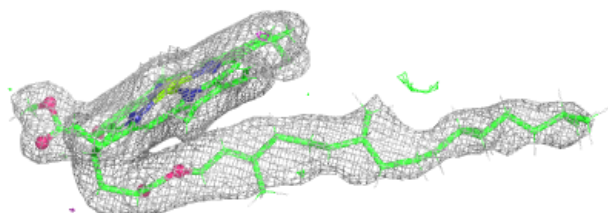
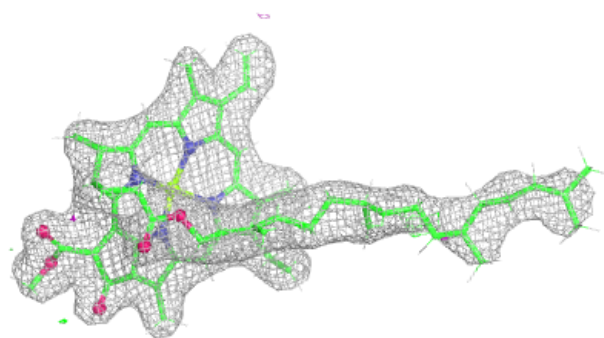


Electron density around CLA b 608:

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

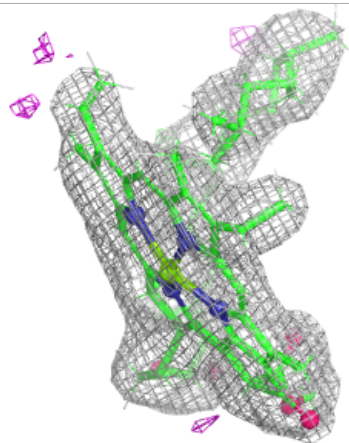
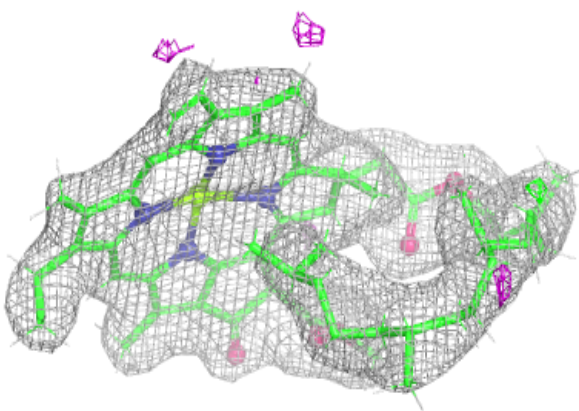
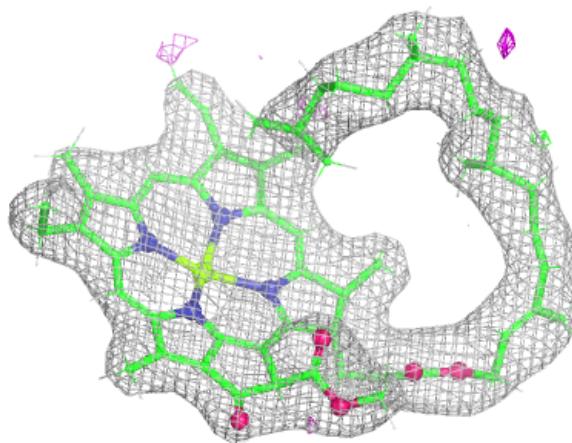
**Electron density around CLA b 614:**

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



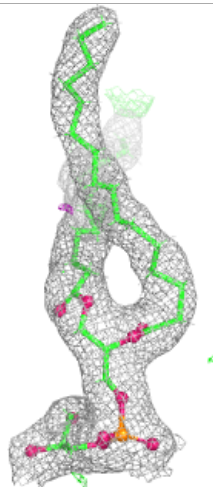
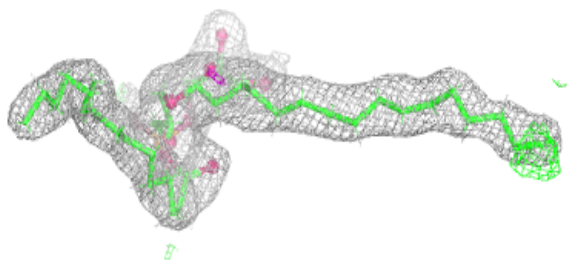
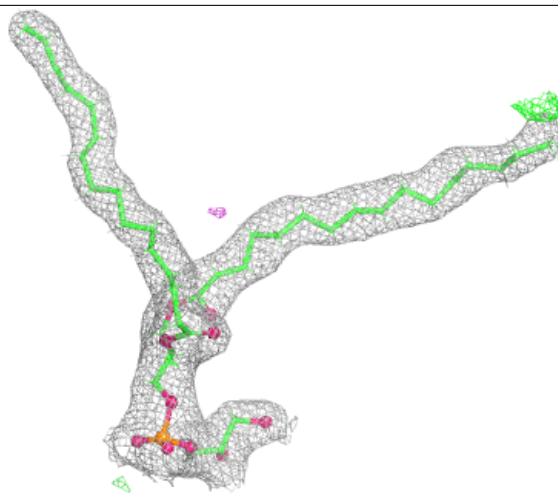
Electron density around CLA b 615:

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



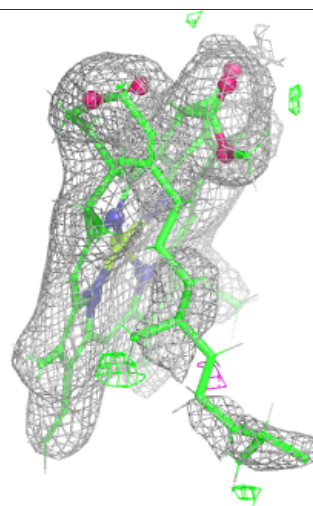
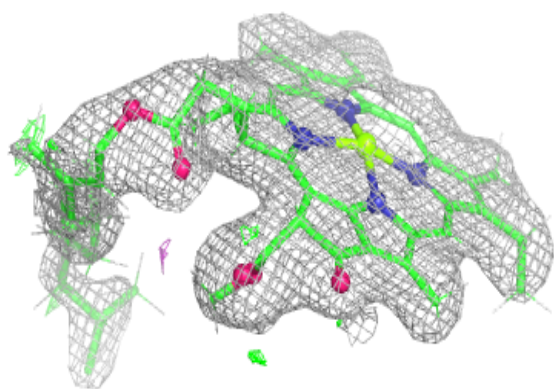
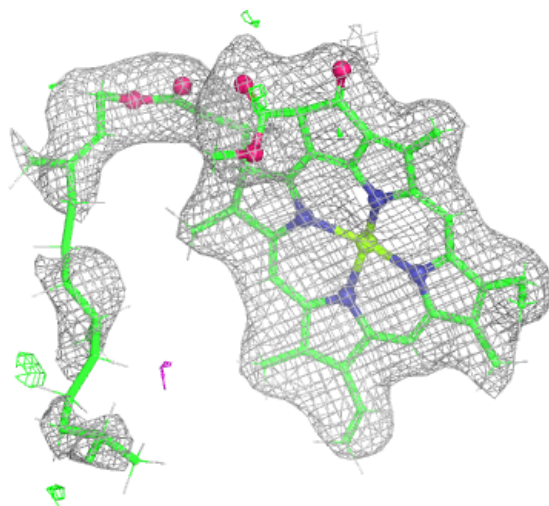
Electron density around LHG 1 101:

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



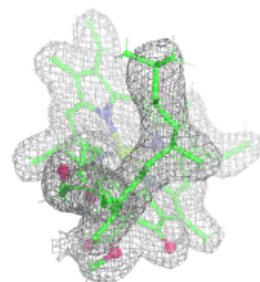
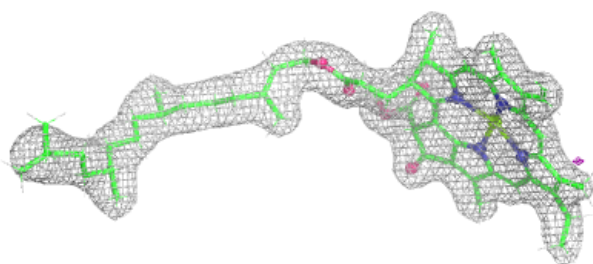
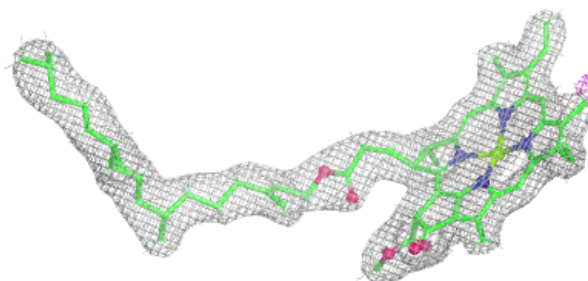
Electron density around CLA b 616:

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

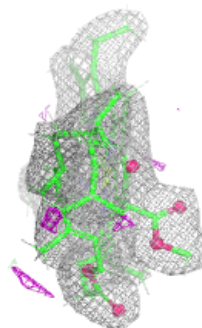
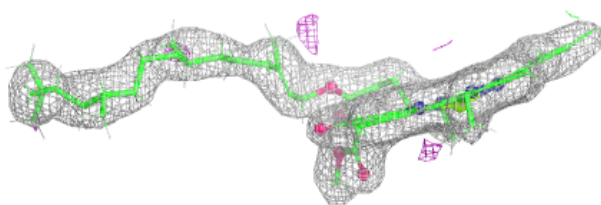
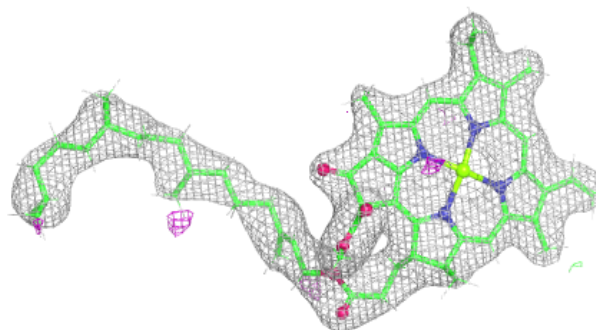


Electron density around CLA a 402:

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

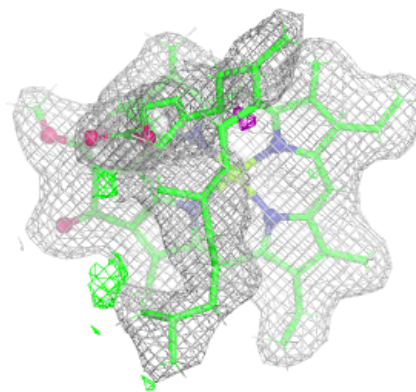
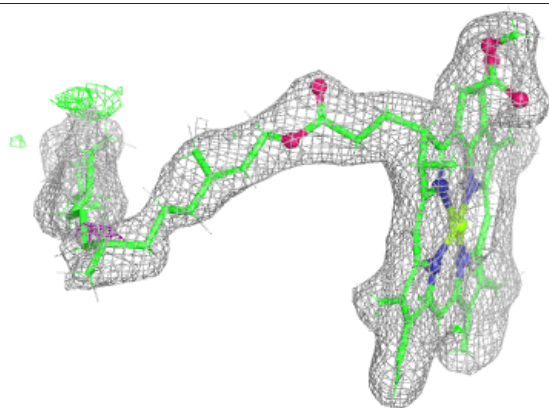
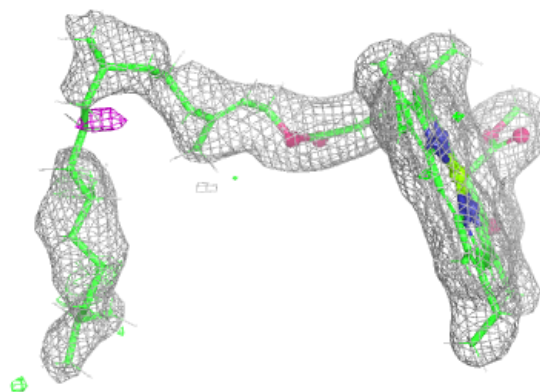
**Electron density around CLA B 602:**

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

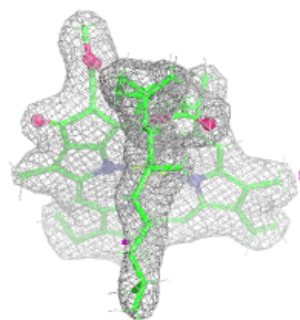
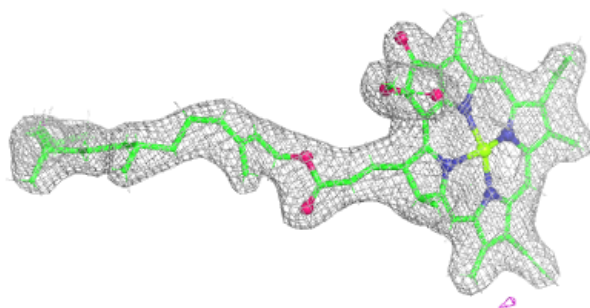
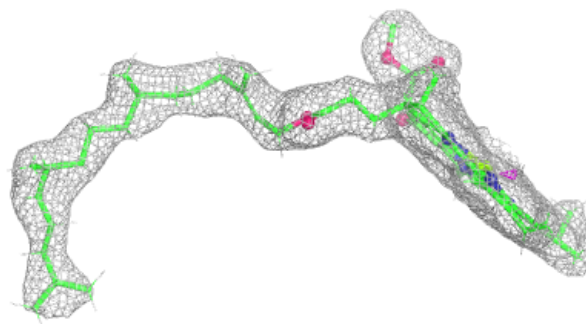


Electron density around CLA a 404:

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

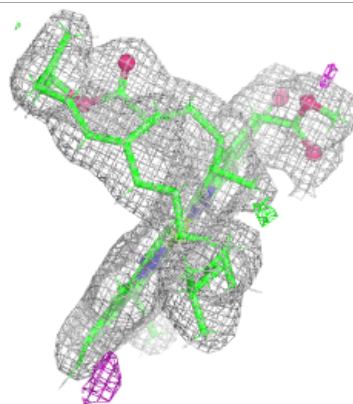
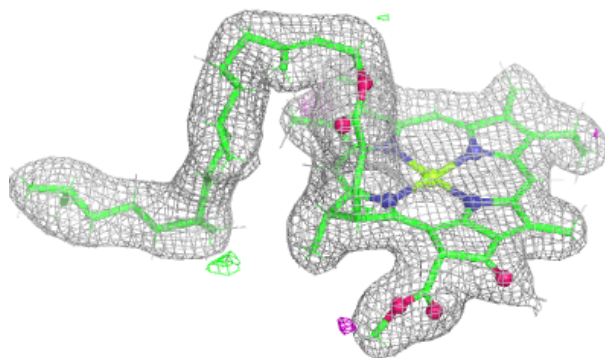
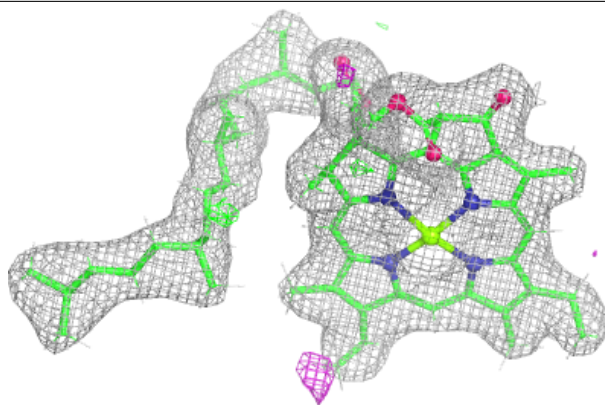
**Electron density around CLA d 403:**

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



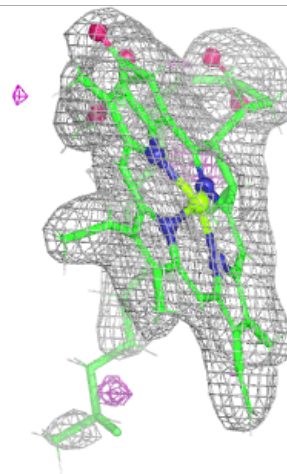
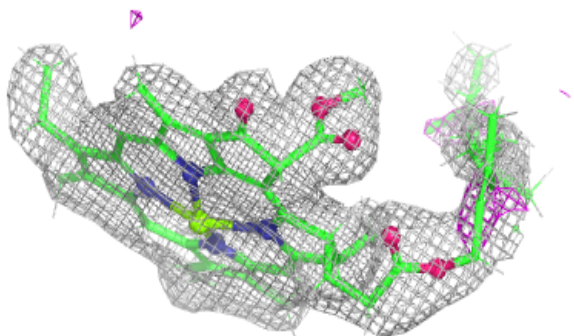
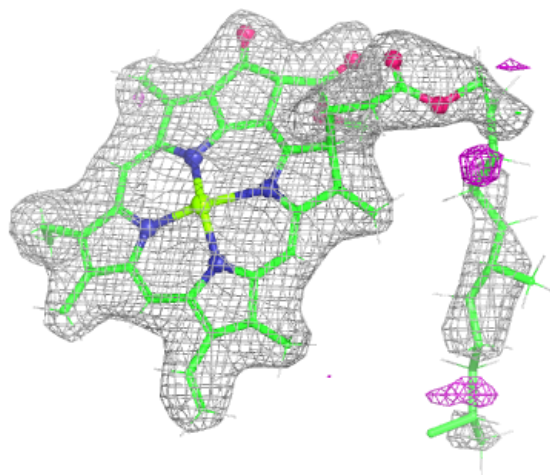
Electron density around CLA d 404:

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



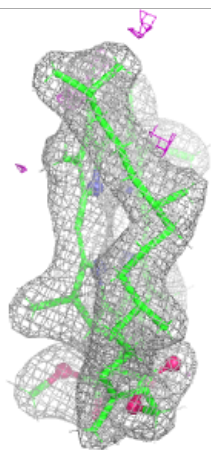
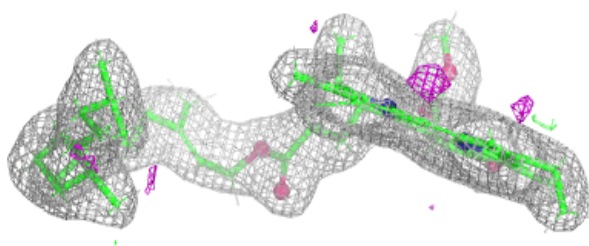
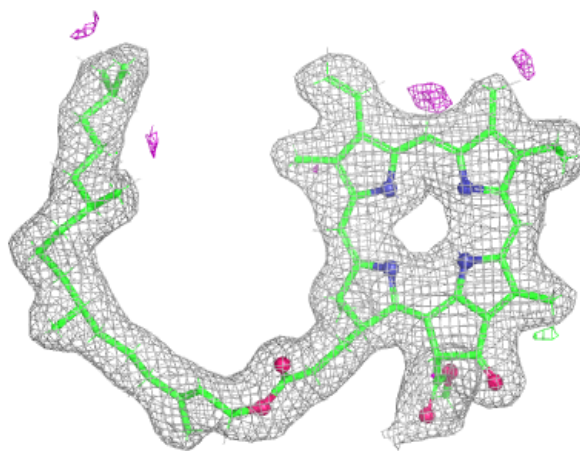
Electron density around CLA B 616:

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



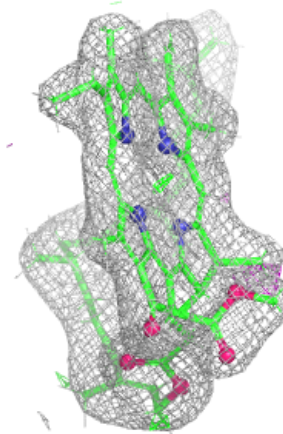
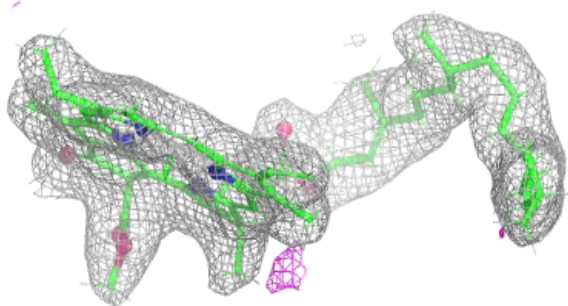
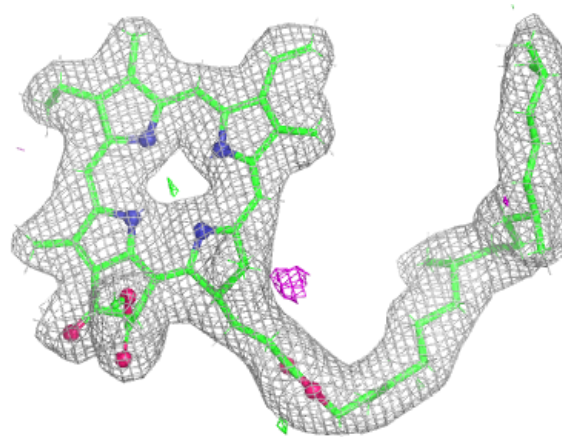
Electron density around PHO A 404:

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



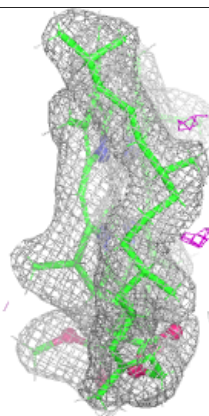
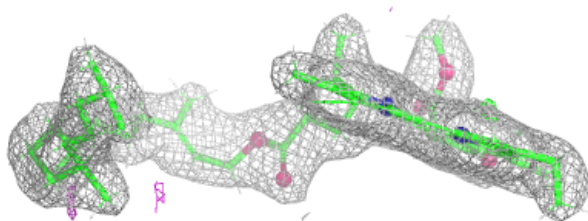
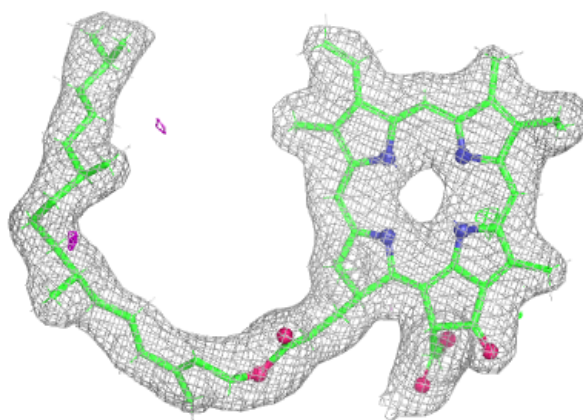
Electron density around PHO D 401:

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



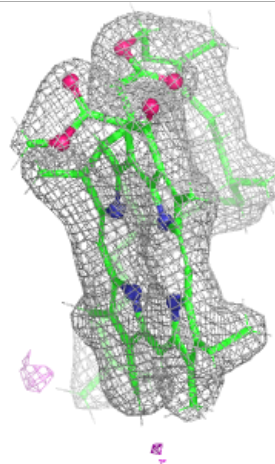
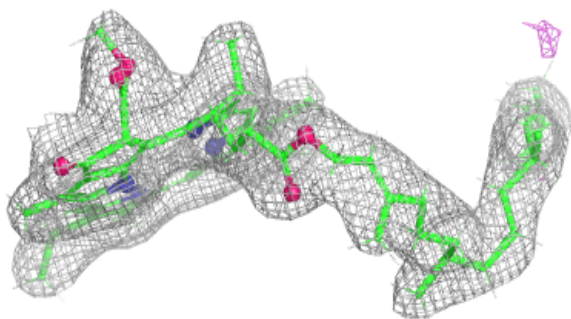
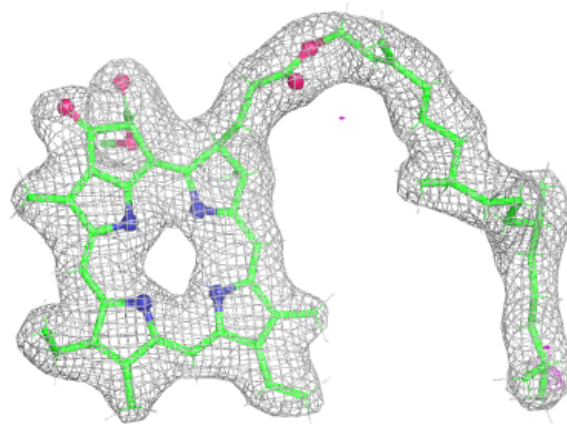
Electron density around PHO d 401:

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



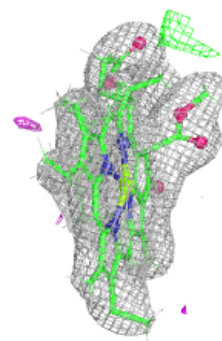
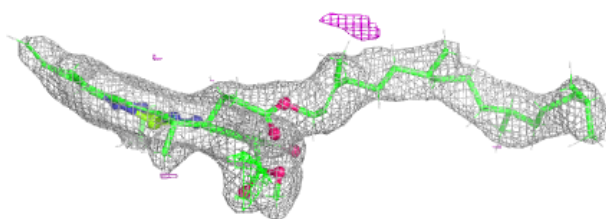
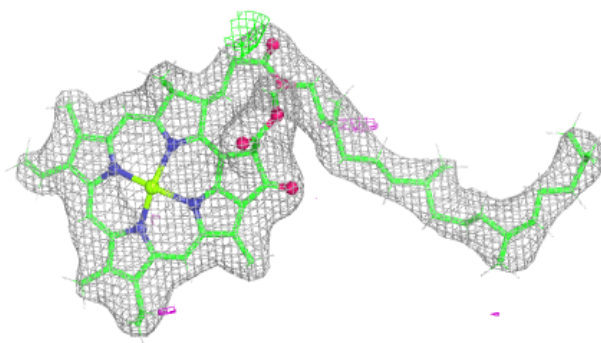
Electron density around PHO d 402:

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

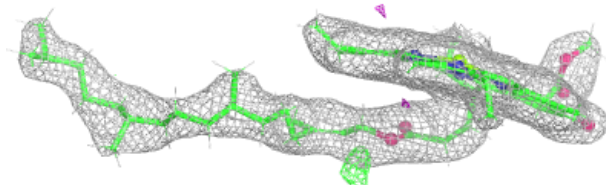
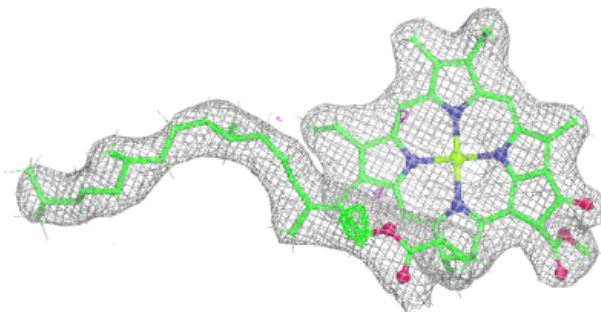


Electron density around CLA b 602:

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

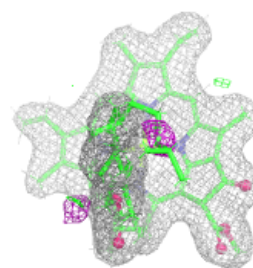
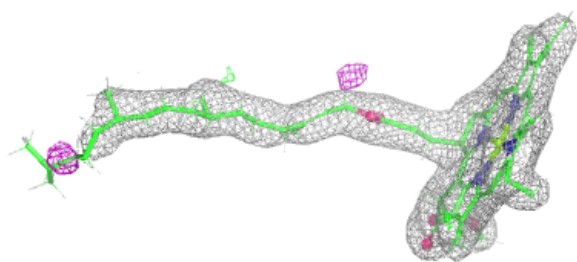
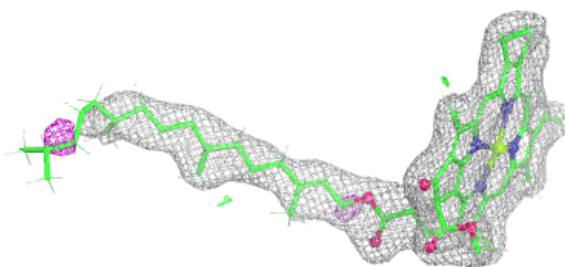
**Electron density around CLA b 603:**

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

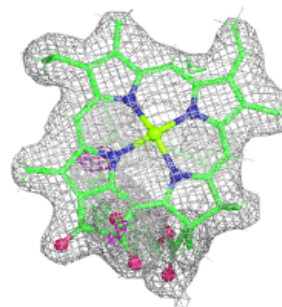
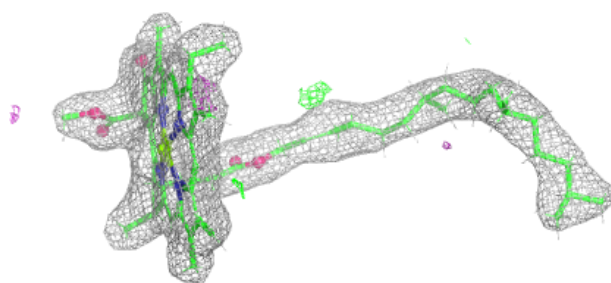
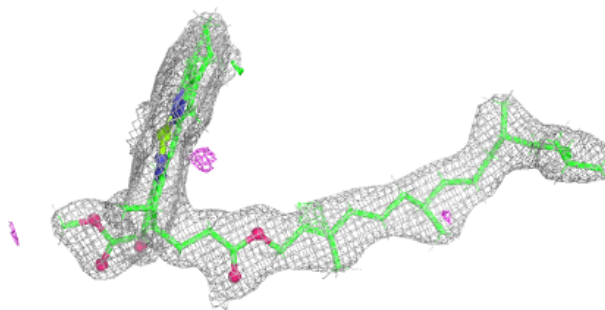


Electron density around CLA b 604:

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

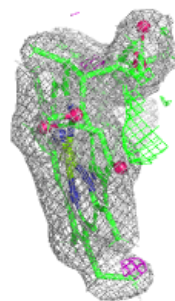
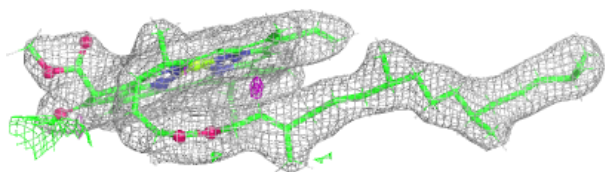
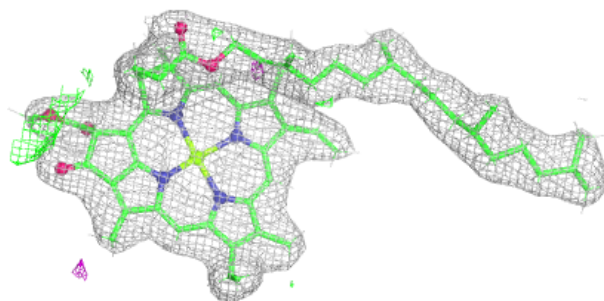
**Electron density around CLA b 605:**

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

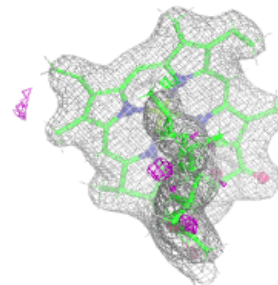
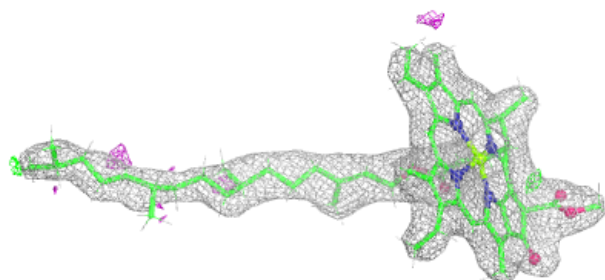
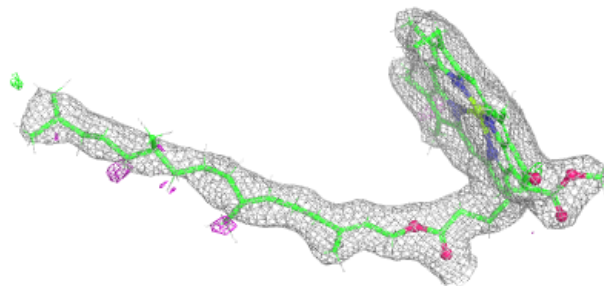


Electron density around CLA C 501:

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

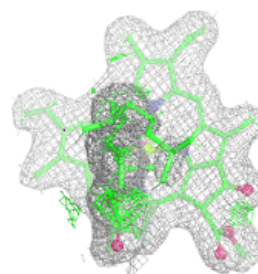
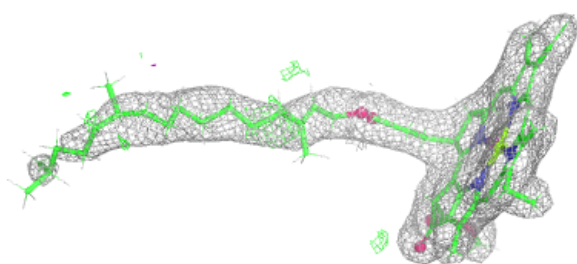
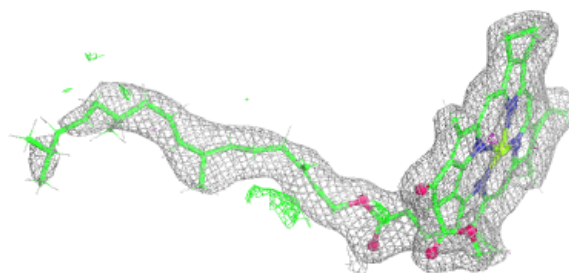
**Electron density around CLA b 607:**

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

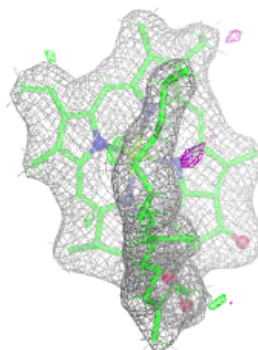
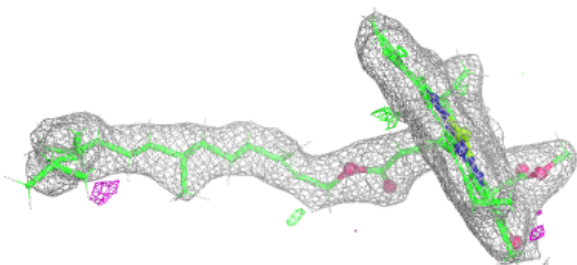
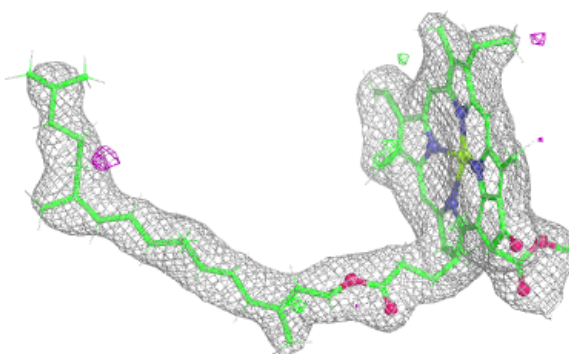


Electron density around CLA B 604:

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

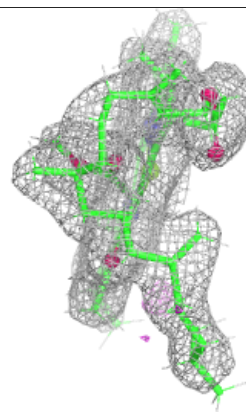
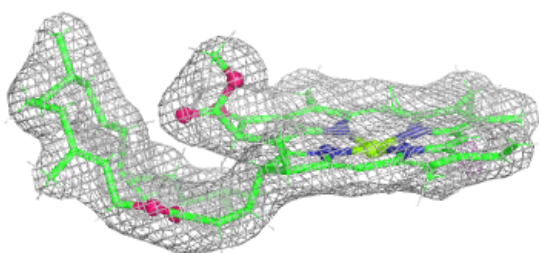
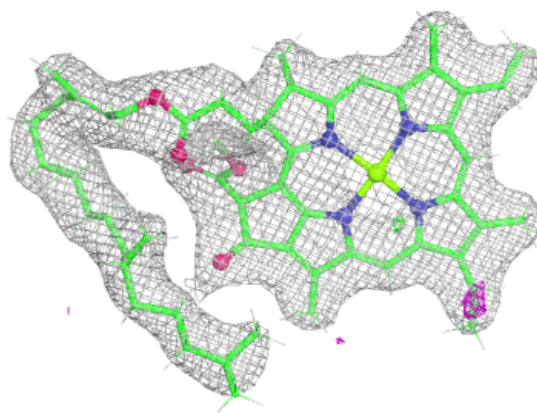
**Electron density around CLA b 609:**

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



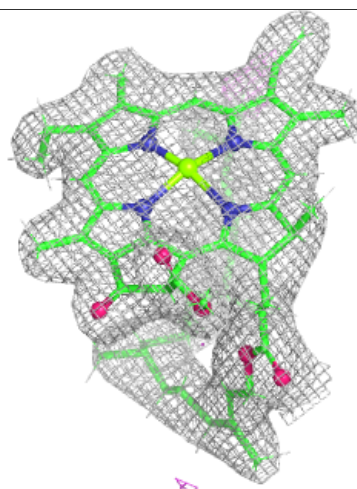
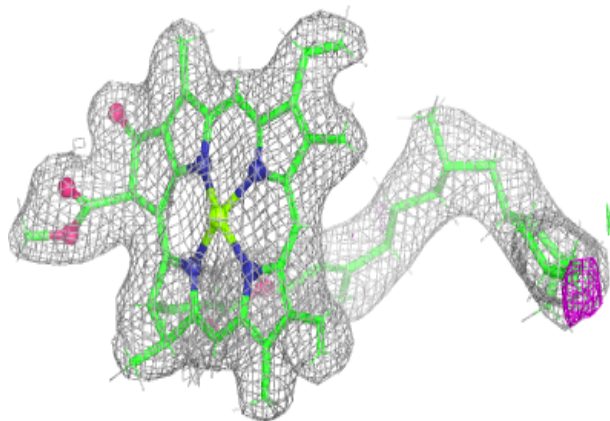
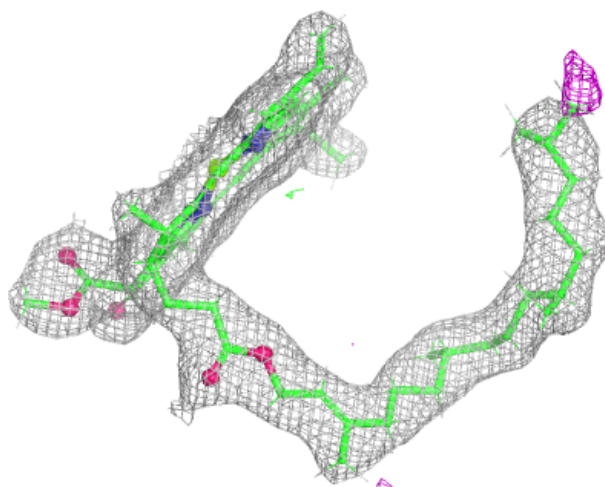
Electron density around CLA b 610:

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



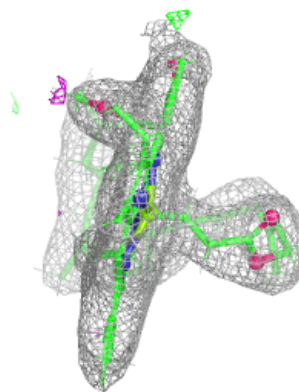
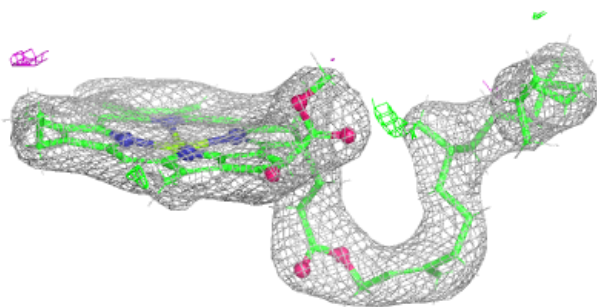
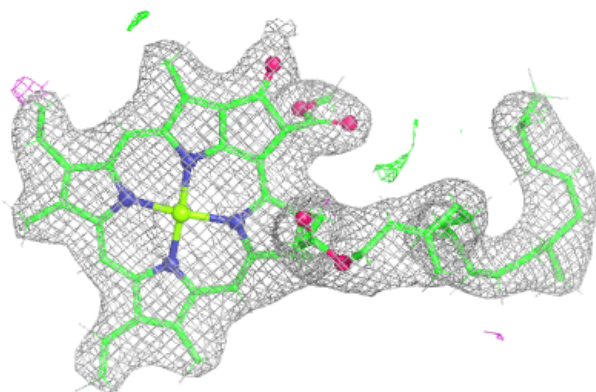
Electron density around CLA b 611:

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



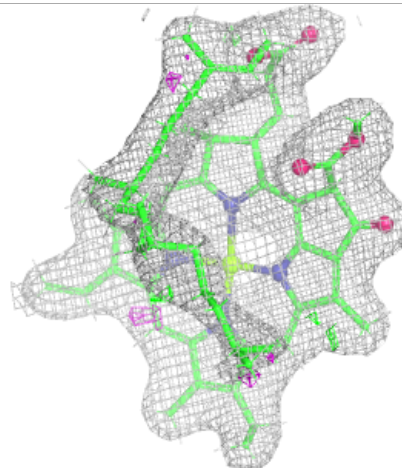
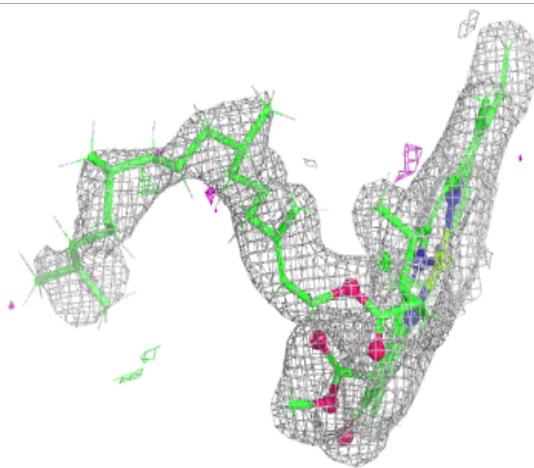
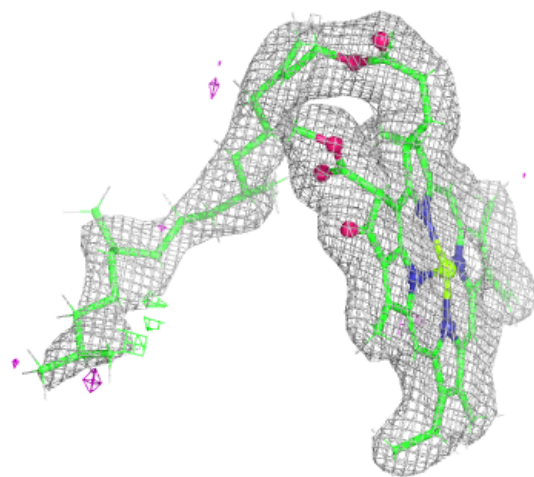
Electron density around CLA b 612:

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



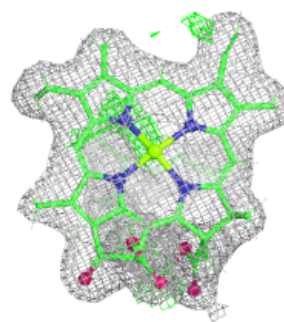
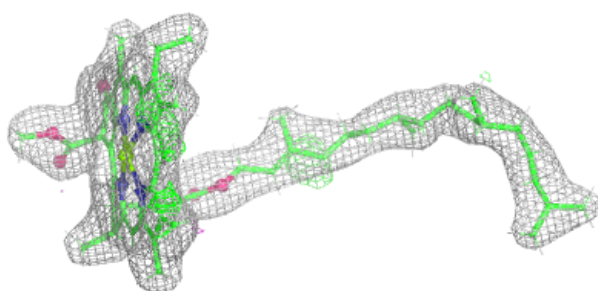
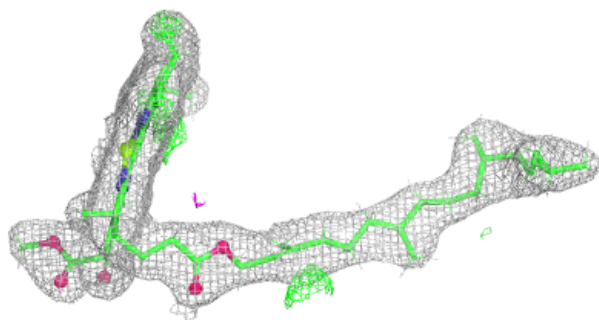
Electron density around CLA b 613:

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

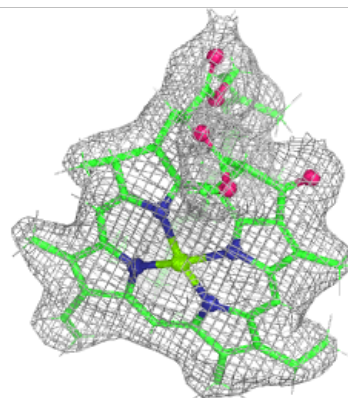
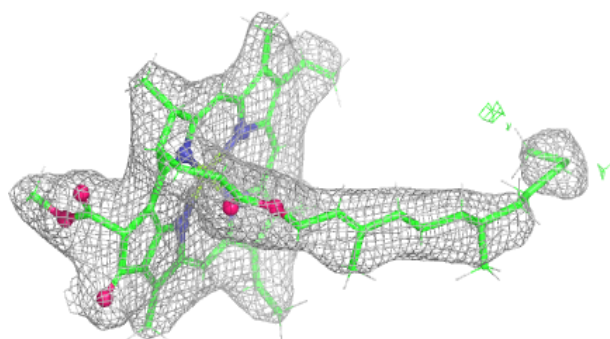
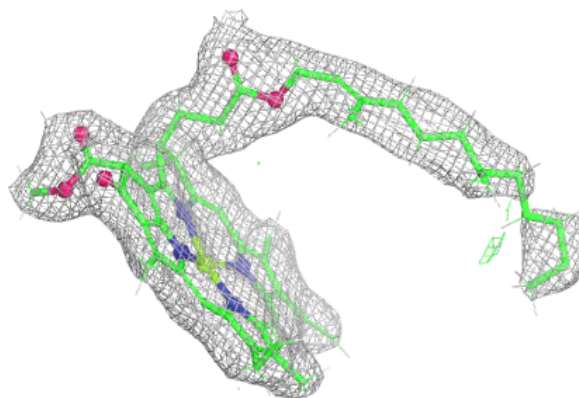


Electron density around CLA B 605:

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

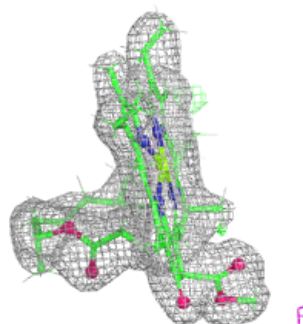
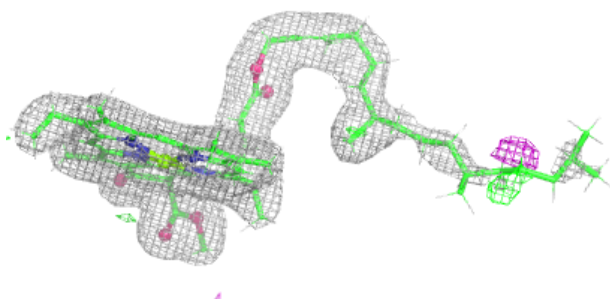
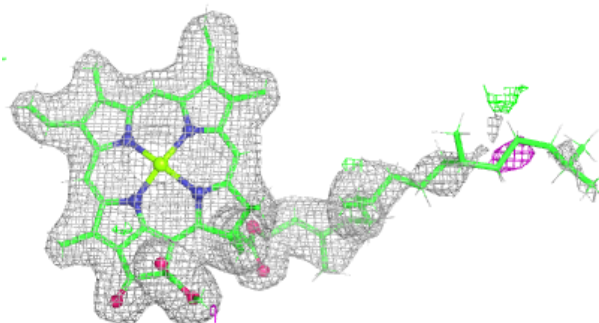
**Electron density around CLA C 504:**

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

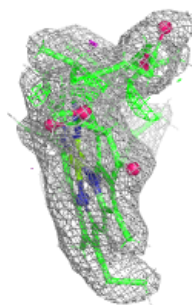
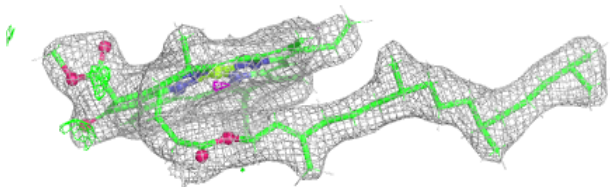
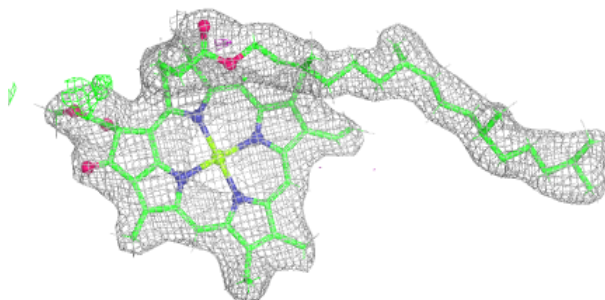


Electron density around CLA A 403:

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

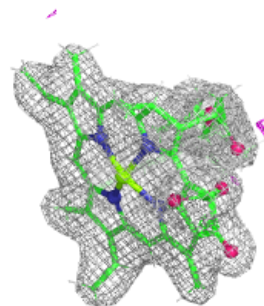
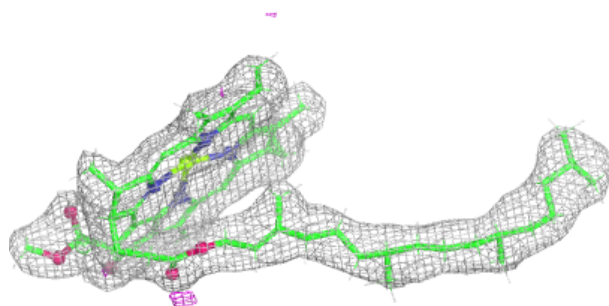
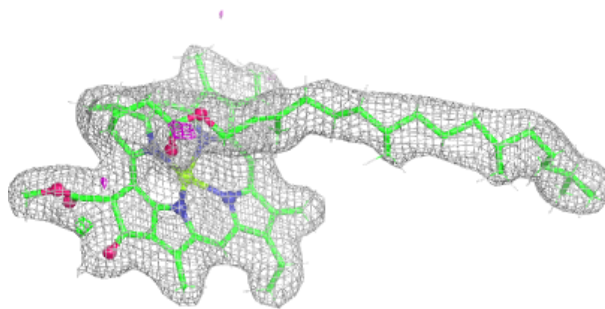
**Electron density around CLA c 501:**

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



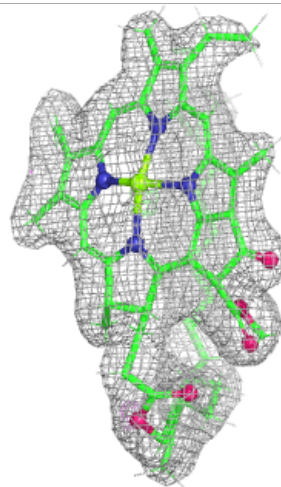
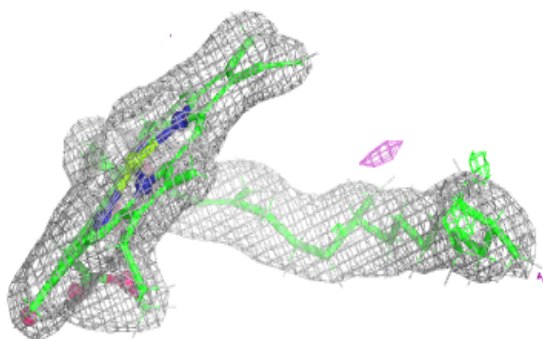
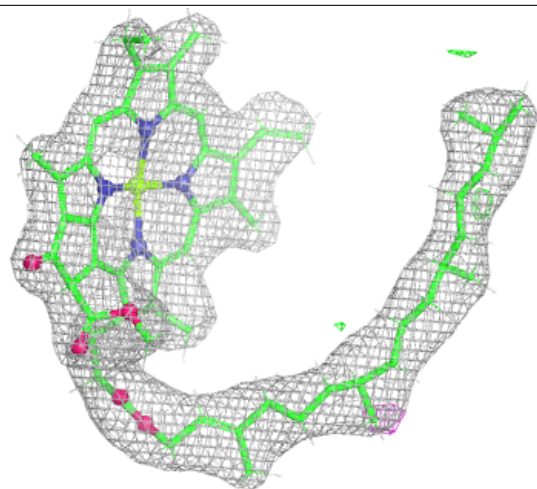
Electron density around CLA B 608:

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



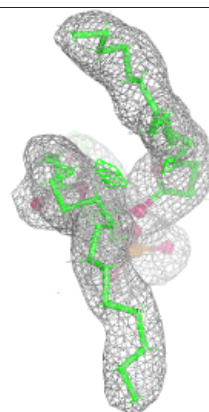
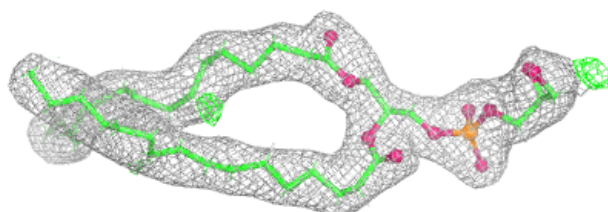
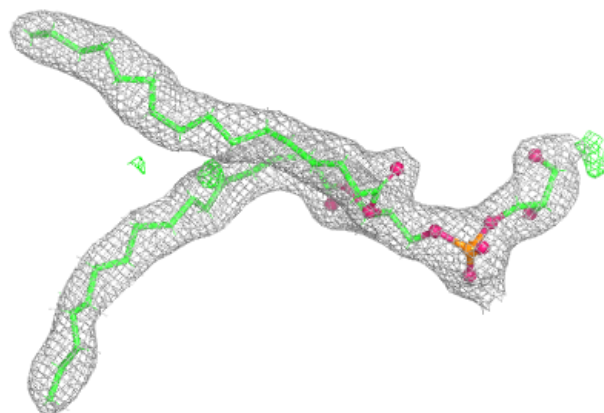
Electron density around CLA C 507:

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

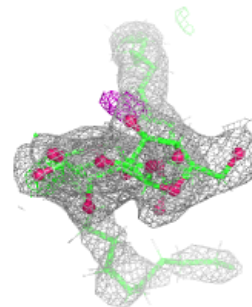
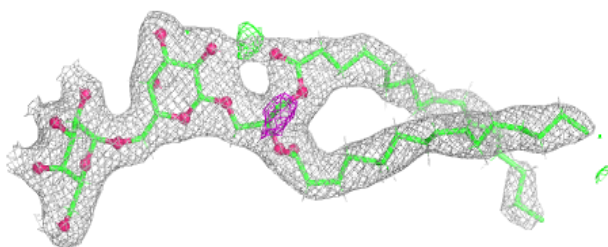
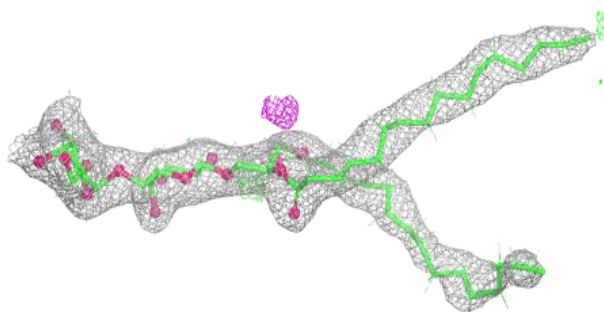


Electron density around LHG D 408:

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

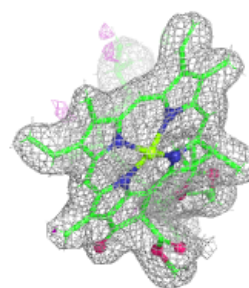
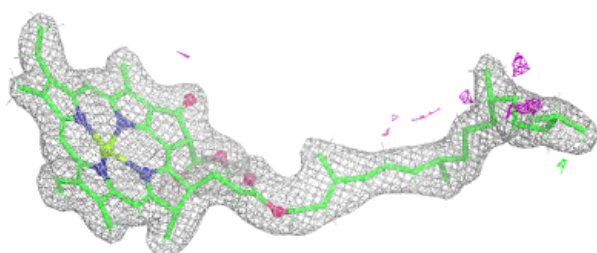
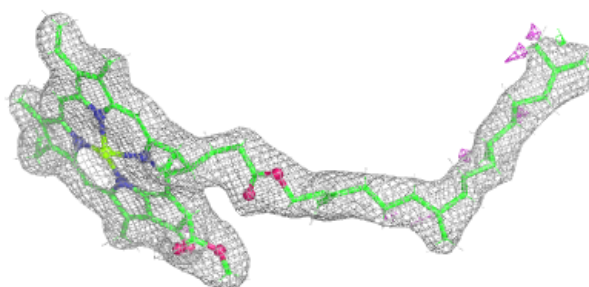
**Electron density around DGD c 517:**

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



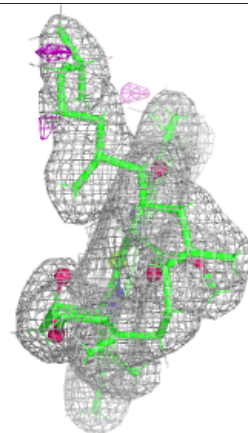
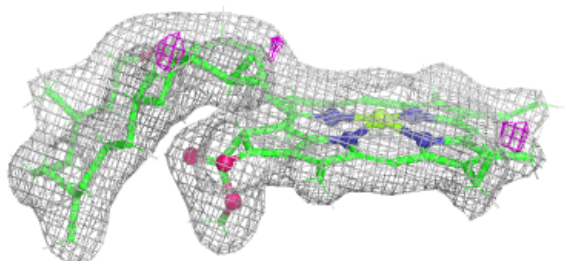
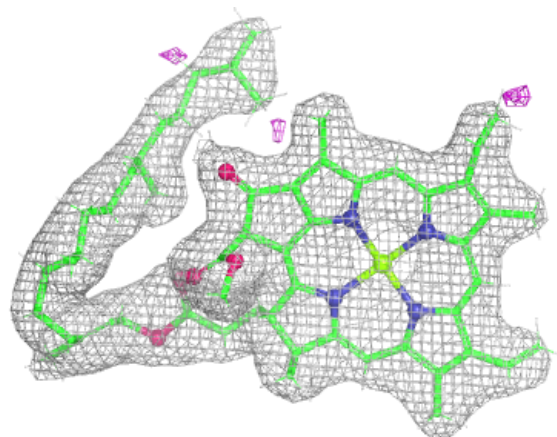
Electron density around CLA A 402:

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



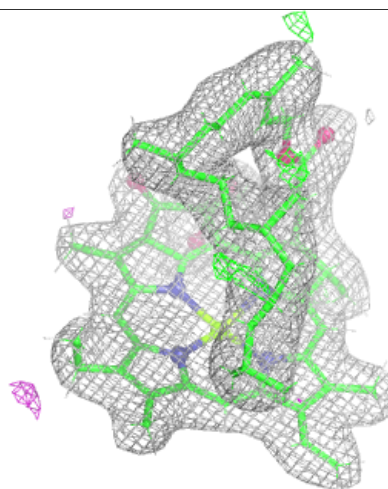
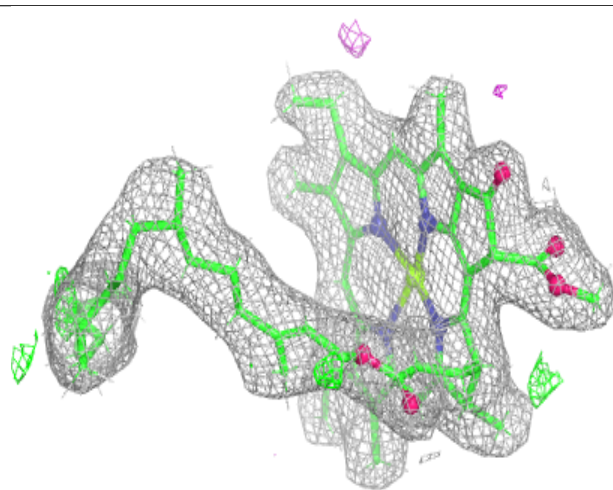
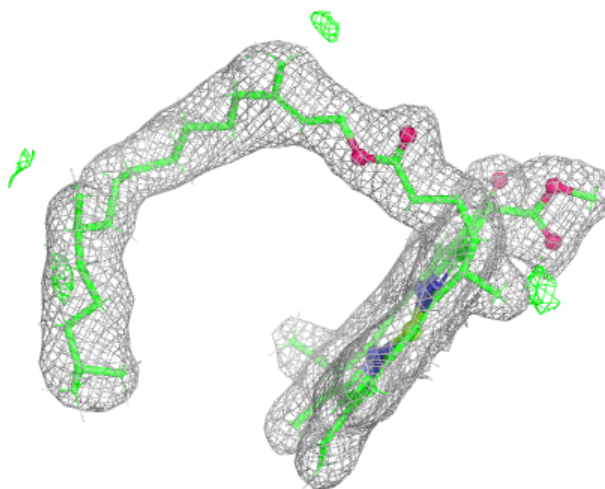
Electron density around CLA B 610:

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



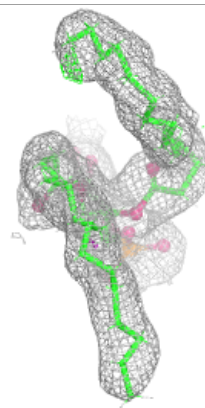
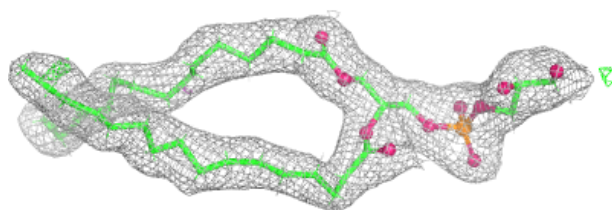
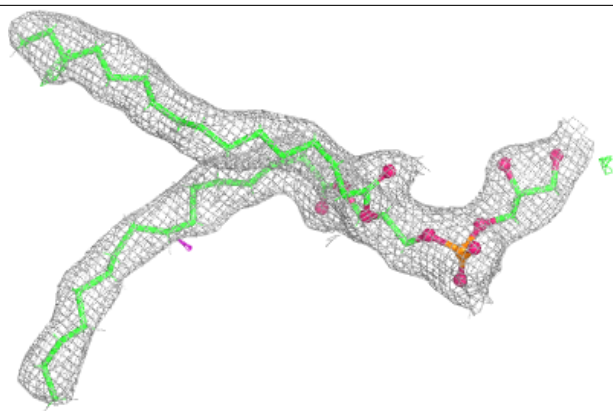
Electron density around CLA B 611:

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

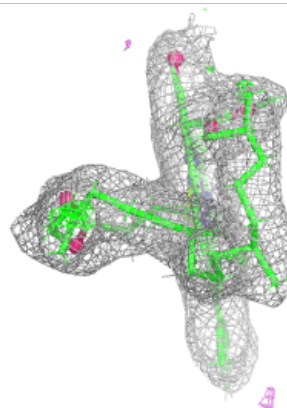
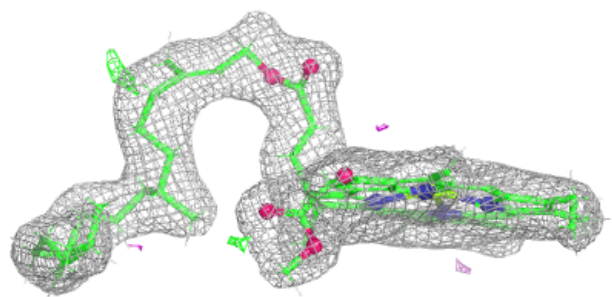
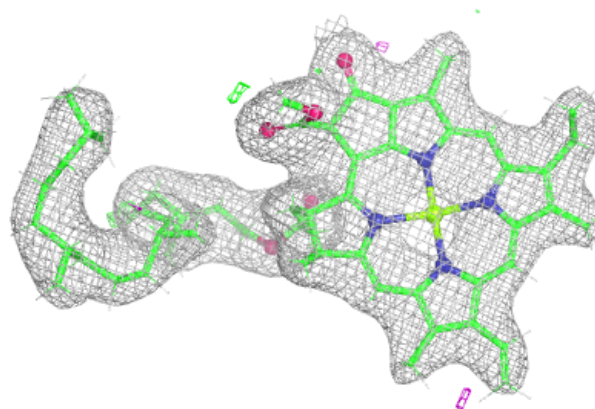


Electron density around LHG d 409:

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

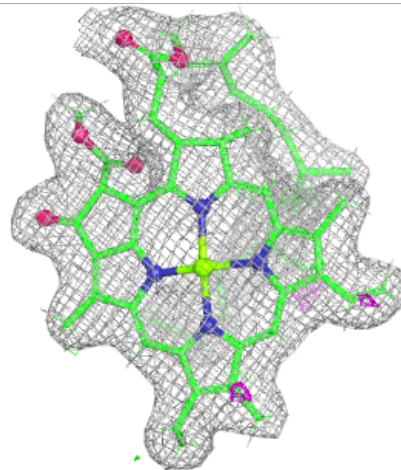
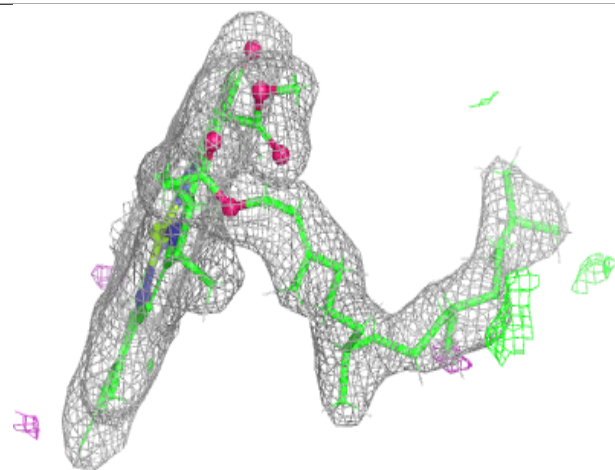
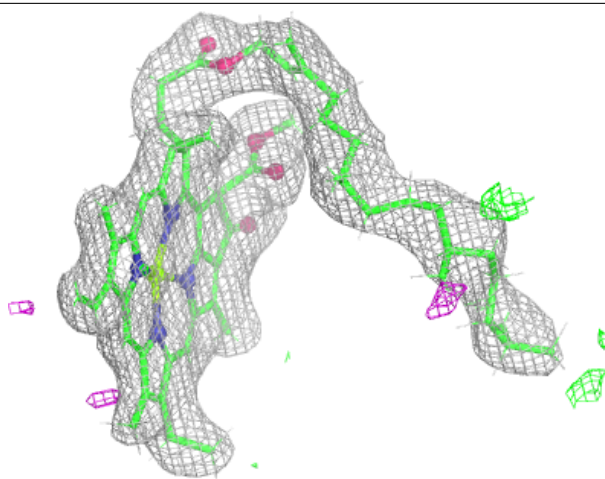
**Electron density around CLA B 612:**

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



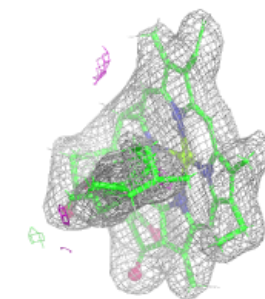
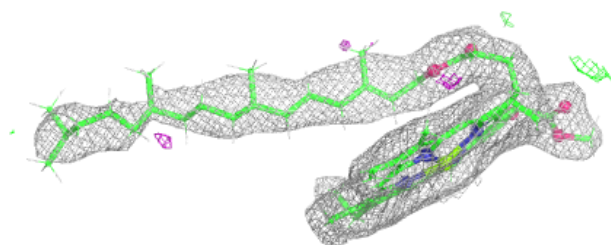
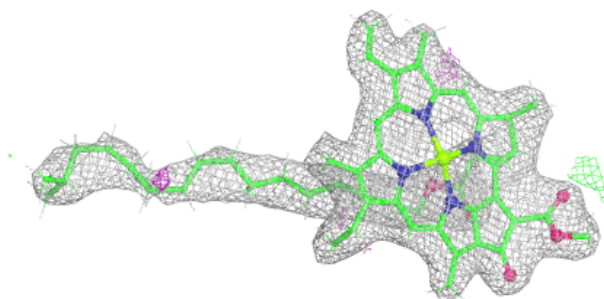
Electron density around CLA B 613:

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

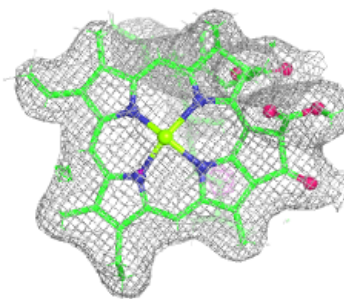
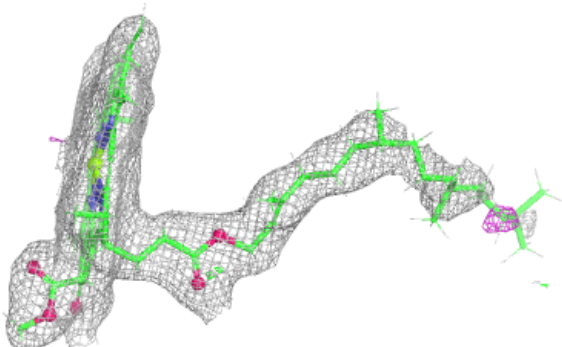
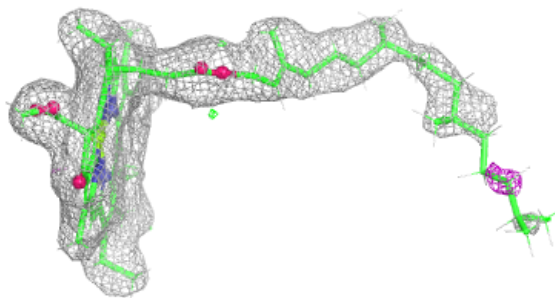


Electron density around CLA B 614:

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

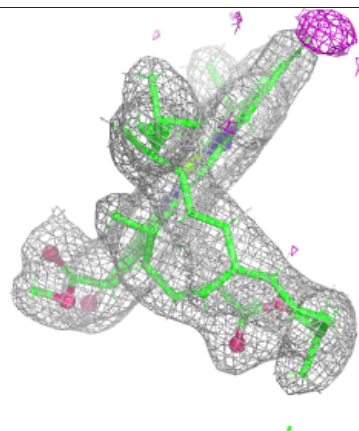
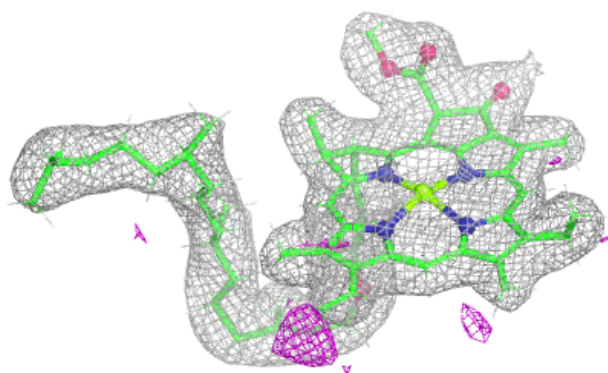
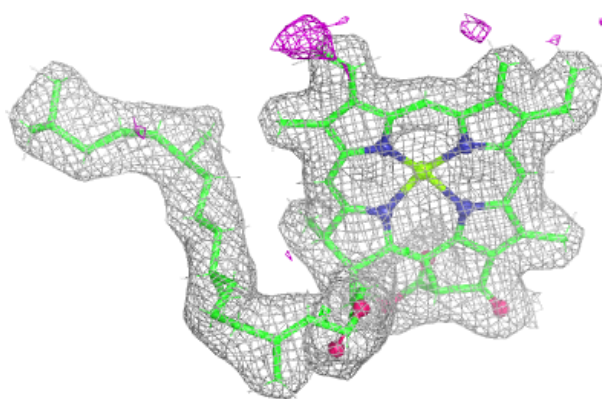
**Electron density around CLA D 404:**

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

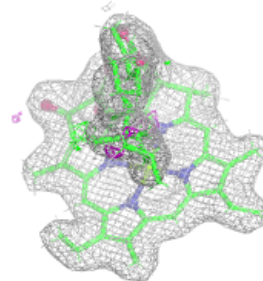
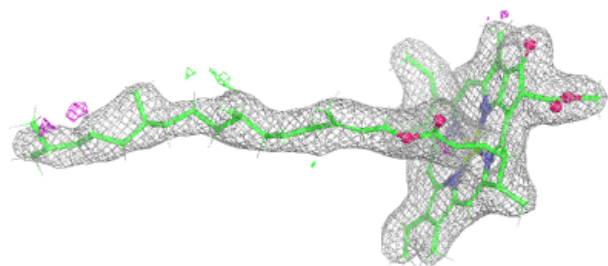
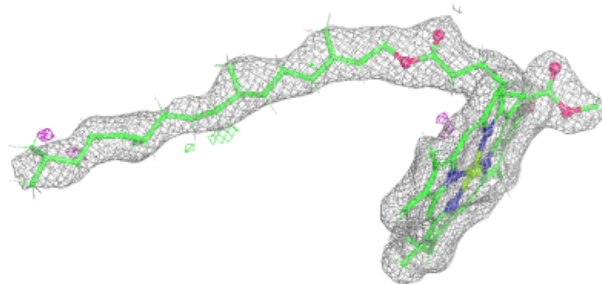


Electron density around CLA A 410:

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

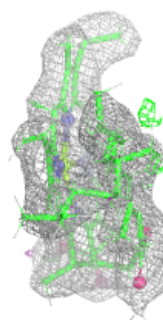
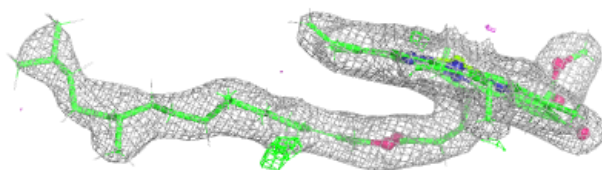
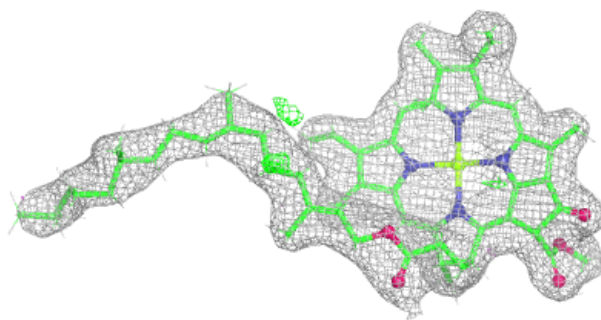
**Electron density around CLA B 607:**

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

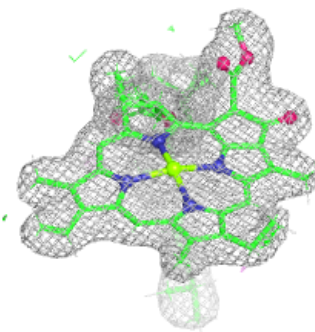
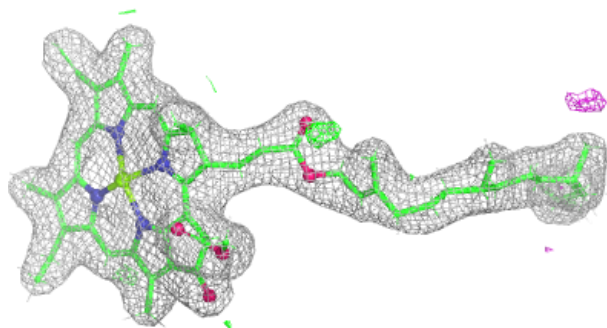
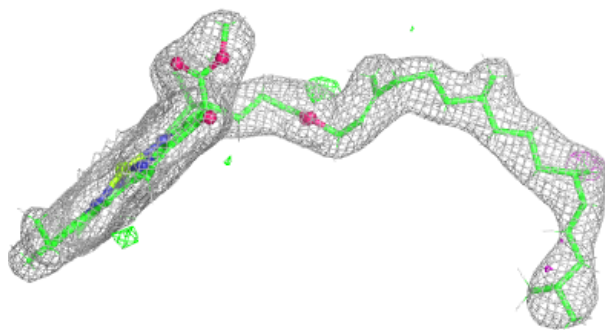


Electron density around CLA B 603:

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

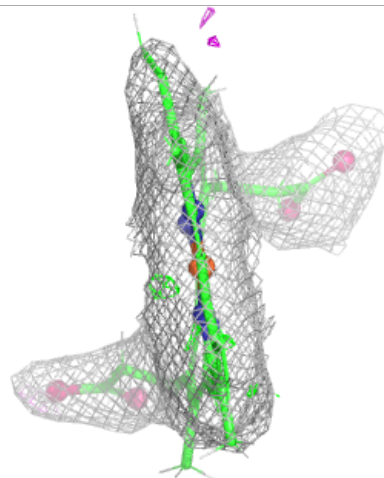
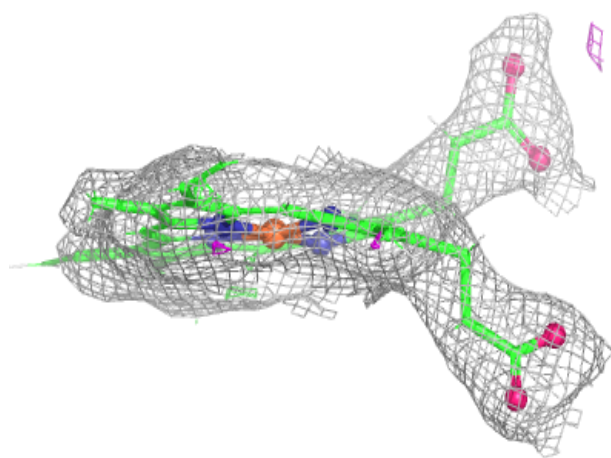
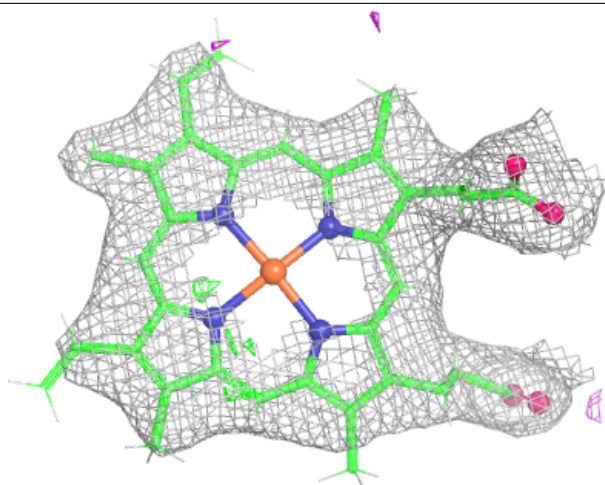
**Electron density around CLA D 403:**

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



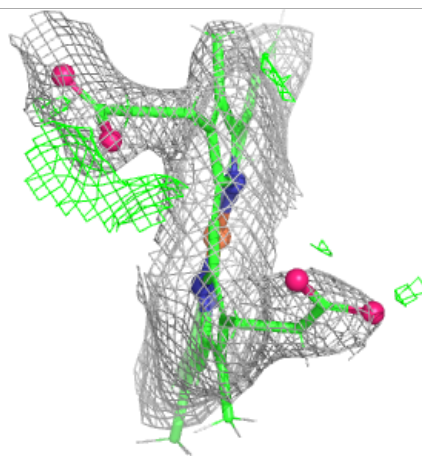
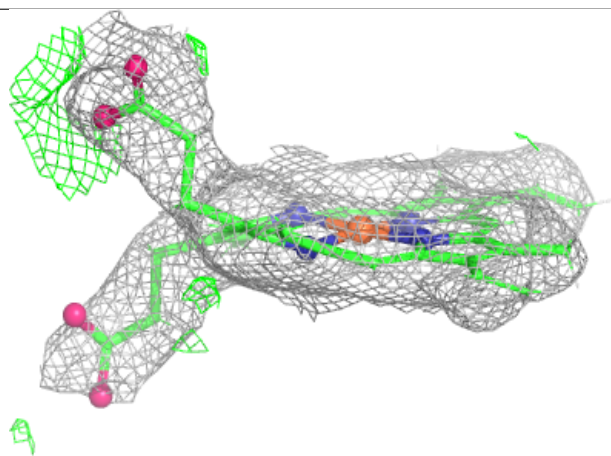
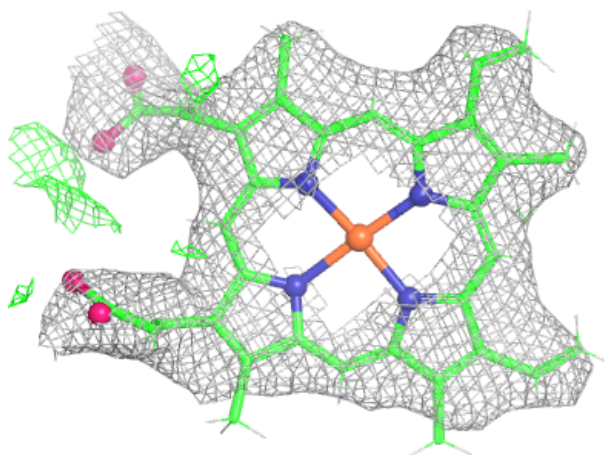
Electron density around HEM E 101:

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



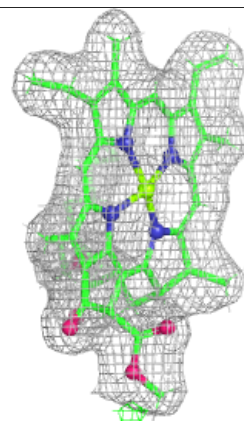
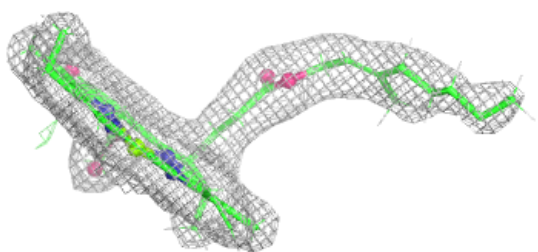
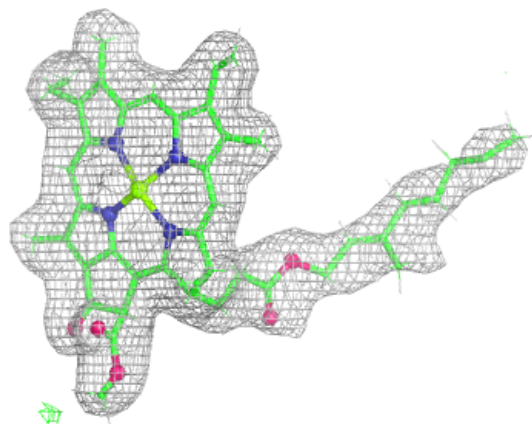
Electron density around HEM f 101:

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



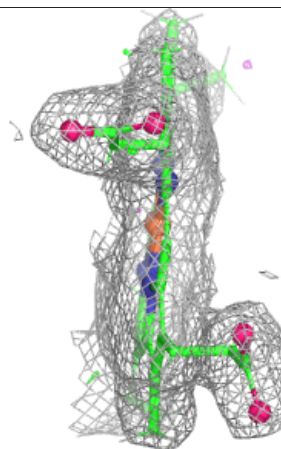
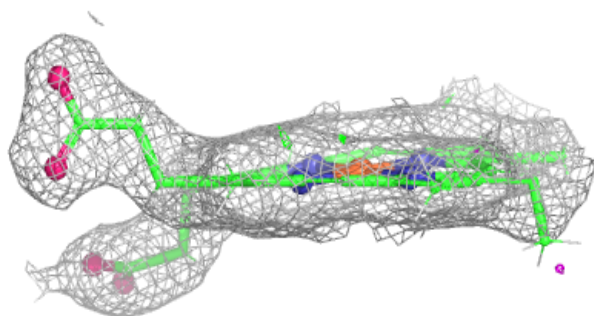
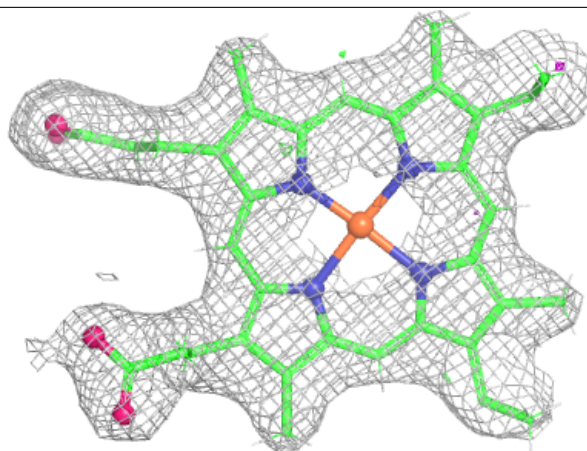
Electron density around CLA A 405:

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



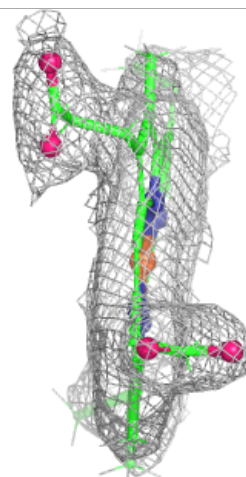
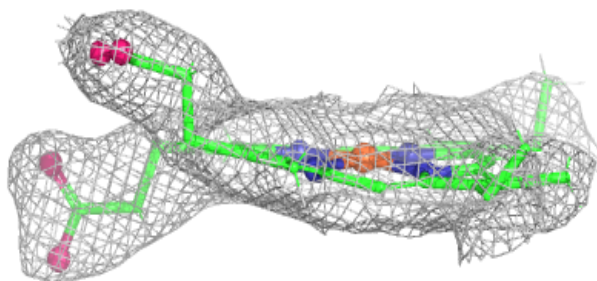
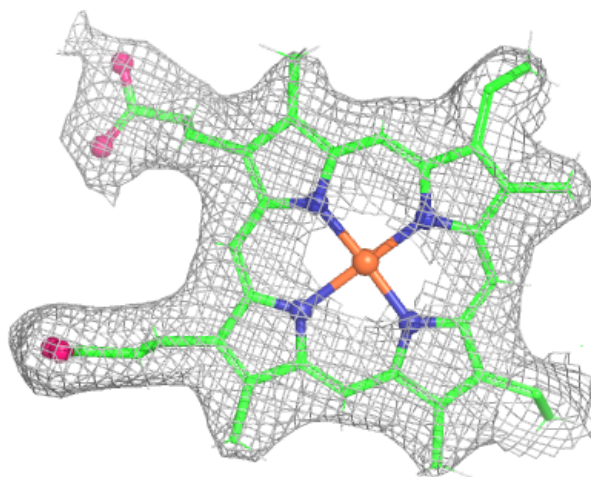
Electron density around HEC V 201:

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



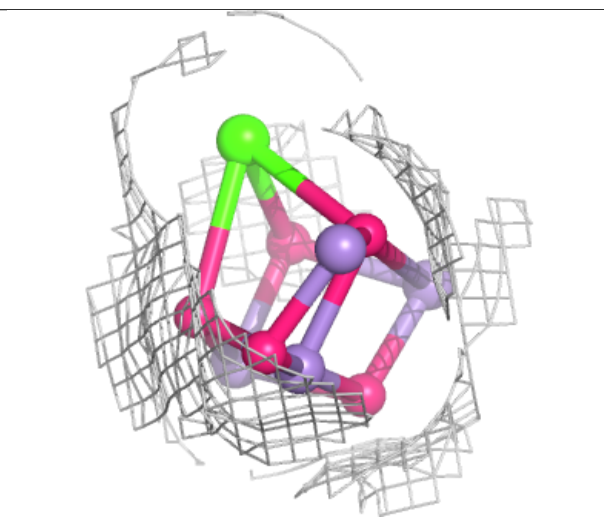
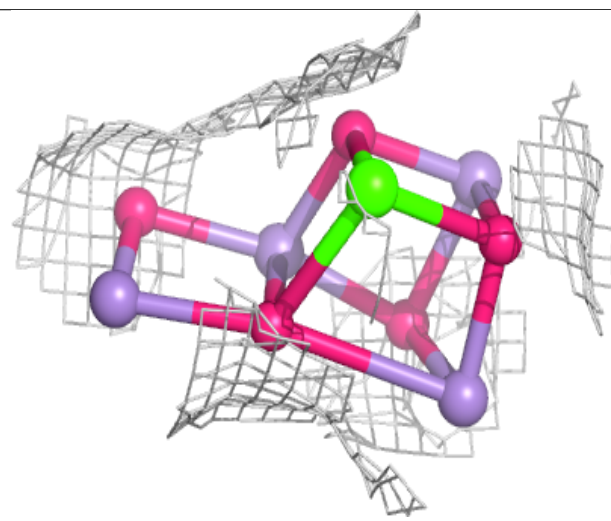
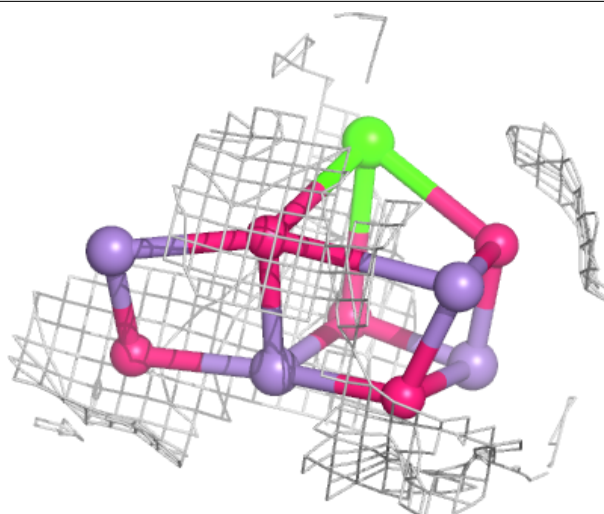
Electron density around HEC v 201:

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



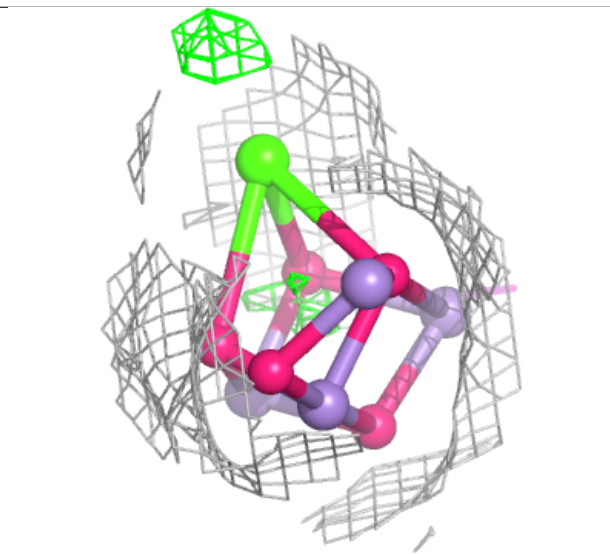
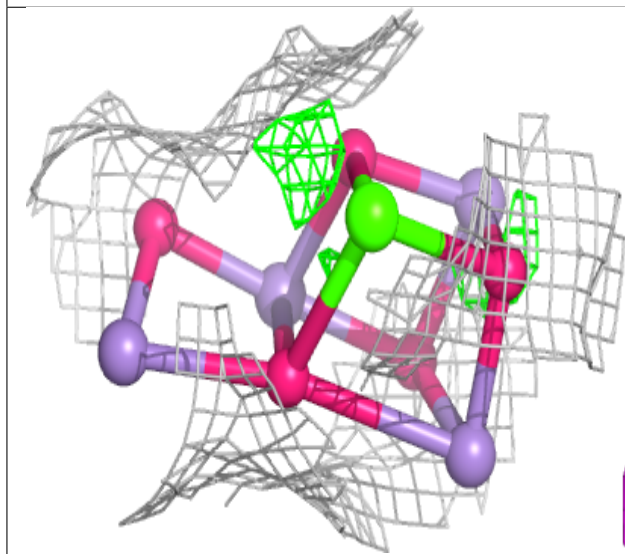
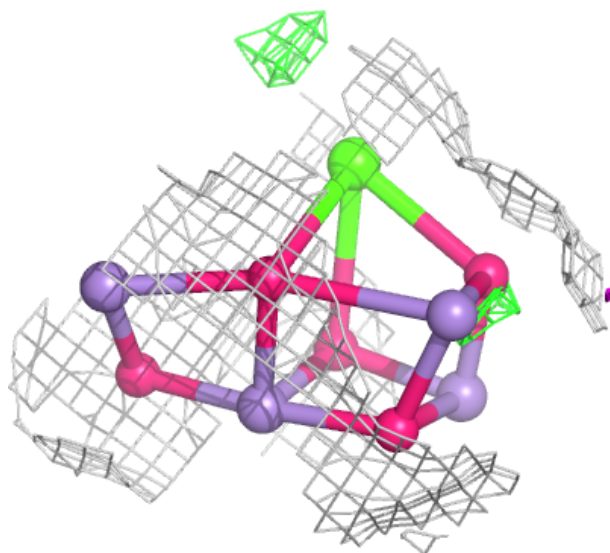
Electron density around OEX a 416 (A):

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



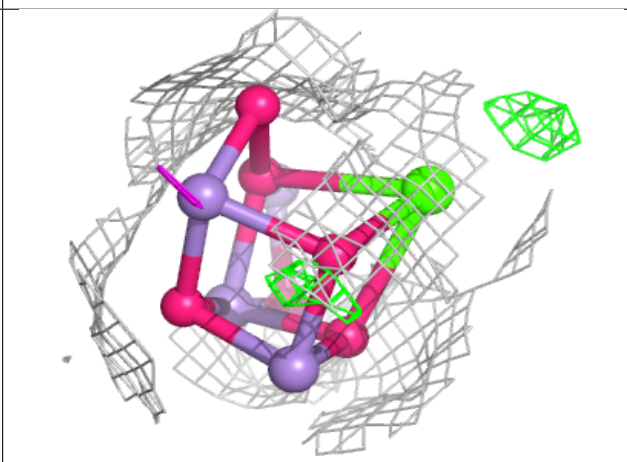
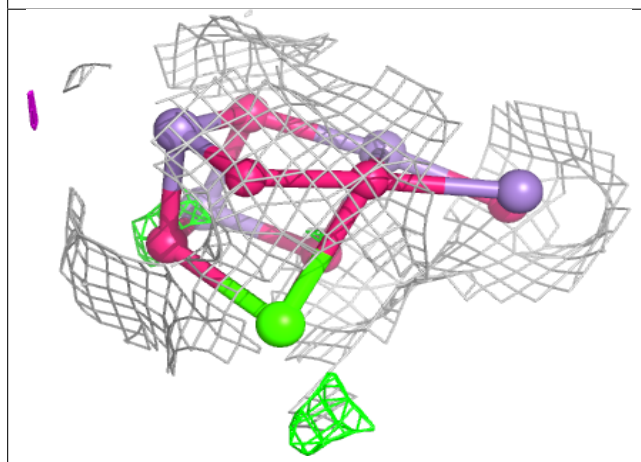
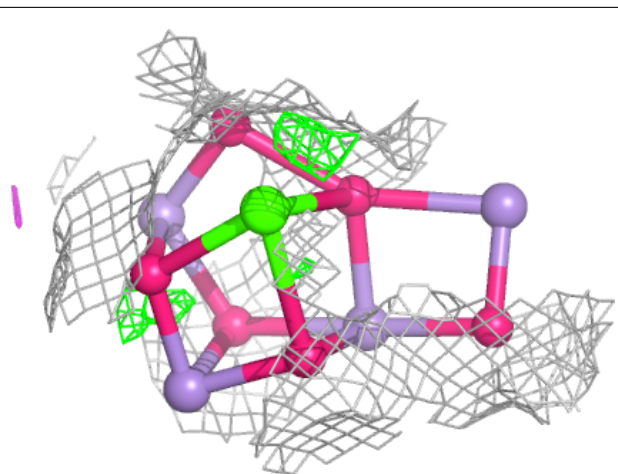
Electron density around OEX A 416 (A):

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



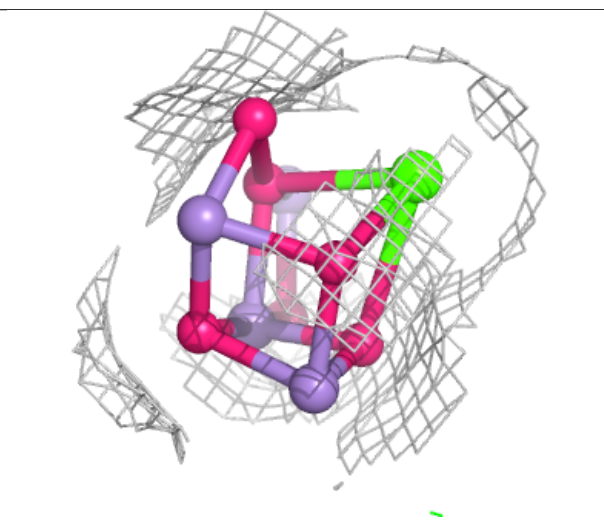
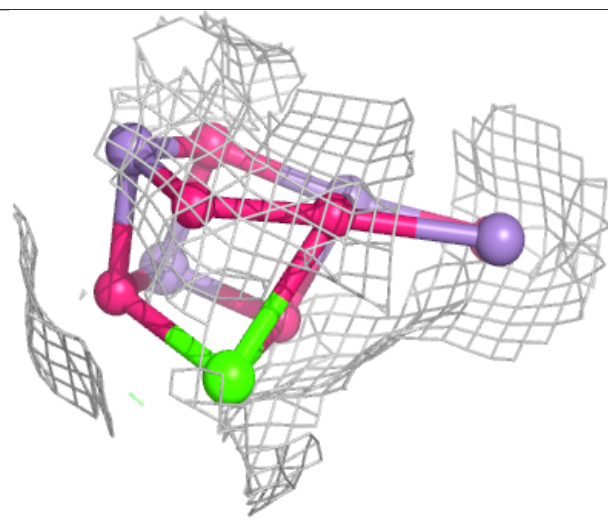
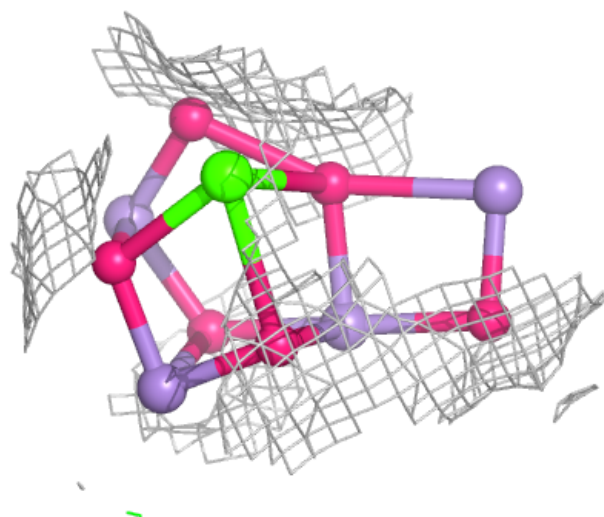
Electron density around OEY A 415 (B):

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



Electron density around OEY a 415 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.