



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:14 AM BST

PDB ID : 6W1R
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.23 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|---------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.13 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |

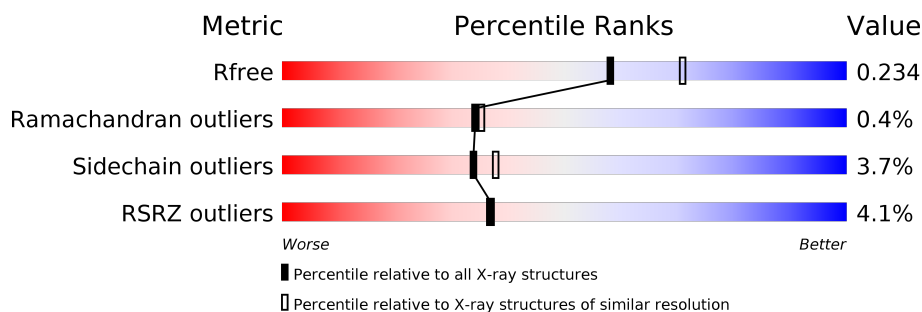
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2391 (2.26-2.22) |
| Ramachandran outliers | 138981 | 2489 (2.26-2.22) |
| Sidechain outliers | 138945 | 2490 (2.26-2.22) |
| RSRZ outliers | 127900 | 2353 (2.26-2.22) |

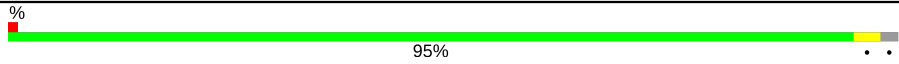
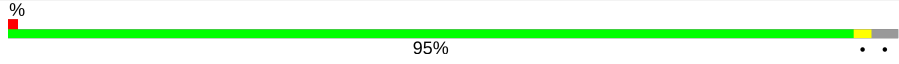
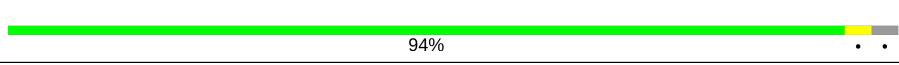
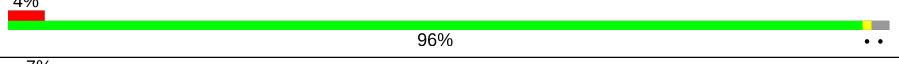
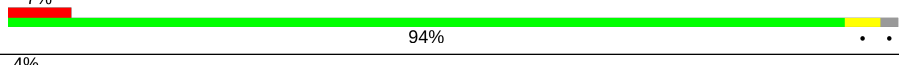
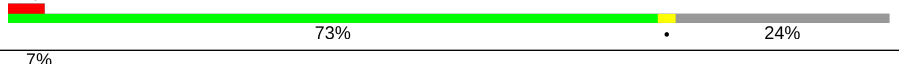
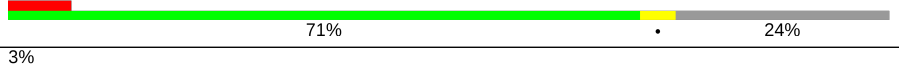
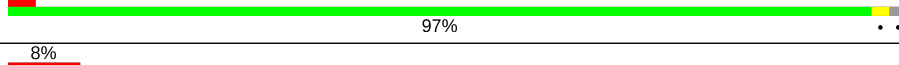
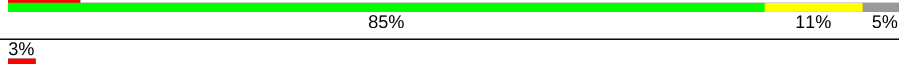
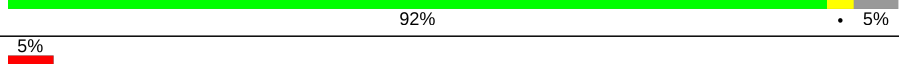
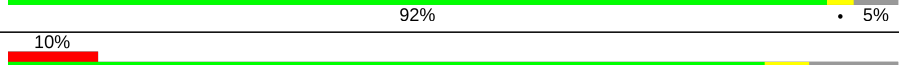
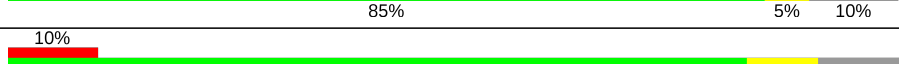

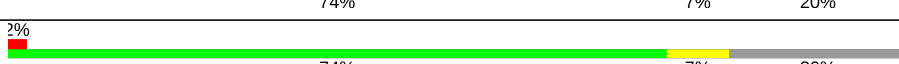
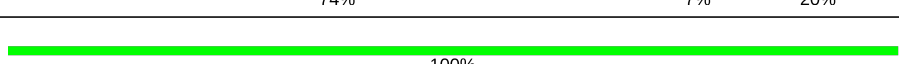
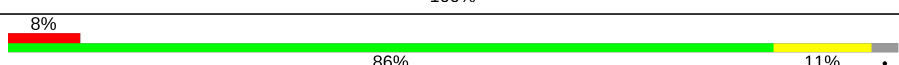
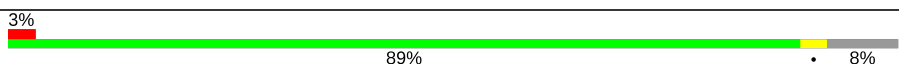
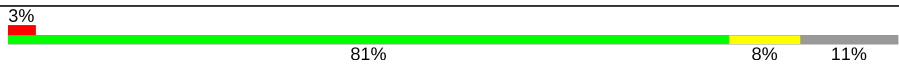
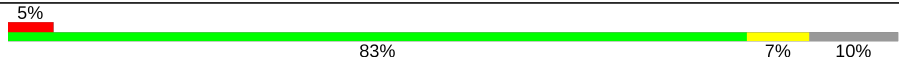

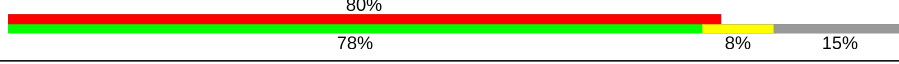
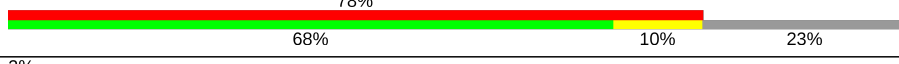
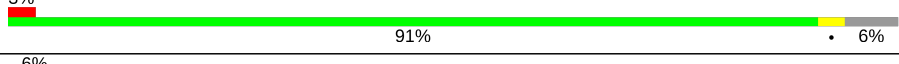
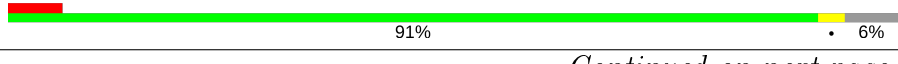

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 | <div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div> |
| 1 | a | 344 | <div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>..</div> </div> |
| 2 | B | 506 | <div> <div>%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div>.</div> </div> |
| 2 | b | 506 | <div> <div>4%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div>.</div> </div> |
| 3 | C | 461 | <div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div>..</div> </div> |

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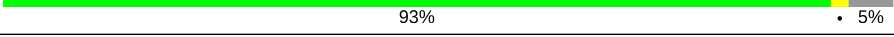


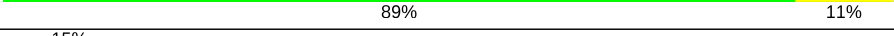

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 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 | 40 |  |
| 14 | r | 40 |  |
| 15 | T | 32 |  |
| 15 | t | 32 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 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 | 403 | X | - | - | - |
| 22 | CLA | A | 404 | X | - | - | - |
| 22 | CLA | A | 409 | X | - | - | - |
| 22 | CLA | B | 602 | 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 | - | - | - |

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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 | 508 | 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 | - | - | - |
| 22 | CLA | D | 405 | X | - | - | - |
| 22 | CLA | H | 101 | X | - | - | - |
| 22 | CLA | a | 402 | X | - | - | - |
| 22 | CLA | a | 403 | X | - | - | - |
| 22 | CLA | a | 405 | X | - | - | - |
| 22 | CLA | a | 411 | X | - | - | - |
| 22 | CLA | b | 601 | X | - | - | - |
| 22 | CLA | b | 602 | 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 | 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 | 508 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 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 | c | 514 | X | - | - | - |
| 22 | CLA | d | 402 | X | - | - | - |
| 22 | CLA | d | 403 | X | - | - | - |

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105311 atoms, of which 52566 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 | 60 | 0 |
| | | | 6031 | 2014 | 2942 | 509 | 547 | 19 | | | |
| 1 | a | 334 | Total | C | H | N | O | S | 0 | 60 | 0 |
| | | | 6019 | 2011 | 2933 | 509 | 547 | 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 |
| | | | 7864 | 2631 | 3859 | 666 | 695 | 13 | | | |
| 2 | b | 505 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 7800 | 2610 | 3822 | 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 | 10 | 0 |
| | | | 6876 | 2283 | 3397 | 580 | 602 | 14 | | | |
| 3 | c | 451 | Total | C | H | N | O | S | 0 | 10 | 0 |
| | | | 7021 | 2324 | 3468 | 596 | 619 | 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 | 1 | 0 |
| | | | 5350 | 1806 | 2624 | 445 | 463 | 12 | | | |
| 4 | d | 341 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 5362 | 1810 | 2630 | 445 | 465 | 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 | 0 | 1 | 0 |
| | | | 1316 | 436 | 650 | 107 | 123 | | | |
| 5 | e | 82 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1311 | 434 | 647 | 108 | 122 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 6 | F | 34 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 556 | 187 | 281 | 45 | 42 | | | |
| 6 | f | 34 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 556 | 187 | 281 | 45 | 42 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 7 | H | 65 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 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 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| I | 1 | FME | - | initiating methionine | UNP Q8DJZ6 |
| i | 1 | FME | - | initiating methionine | UNP Q8DJZ6 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 9 | J | 36 | Total | C | 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 | | | |
| 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 |
| | | | 3698 | 1168 | 1828 | 313 | 385 | | | |
| 13 | o | 244 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 3718 | 1170 | 1844 | 317 | 383 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 14 | R | 34 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 569 | 184 | 298 | 47 | 40 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|
| 14 | r | 31 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 493 | 162 | 253 | 42 | 36 | | | |

- 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 |
| | | | 519 | 181 | 261 | 36 | 39 | 2 | | |
| 15 | t | 30 | Total | C | H | N | O | S | 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 |
| | | | 1546 | 491 | 772 | 129 | 154 | | | |
| 16 | u | 97 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1546 | 491 | 772 | 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 |
| | | | 2132 | 675 | 1068 | 177 | 208 | 4 | | |
| 17 | v | 137 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2132 | 675 | 1068 | 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 | | | |

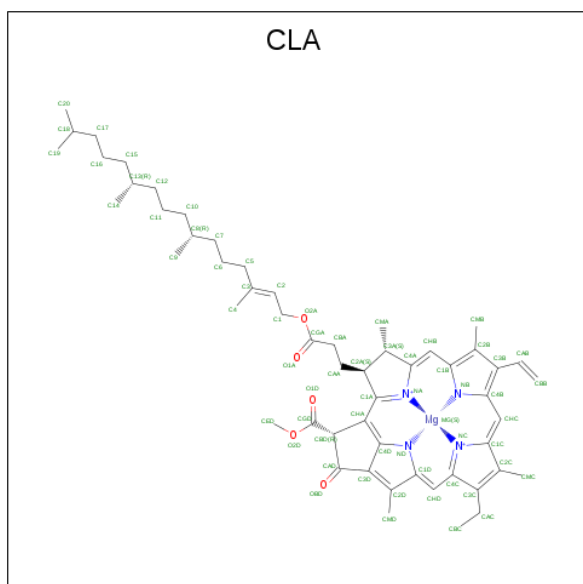
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

| 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 (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: 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 | | |

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

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|---------|--------|--------|---------|---------|
| 22 | C | 1 | Total 117 | C 49 | H 58 | 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 | 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 | H | 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 | 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 |

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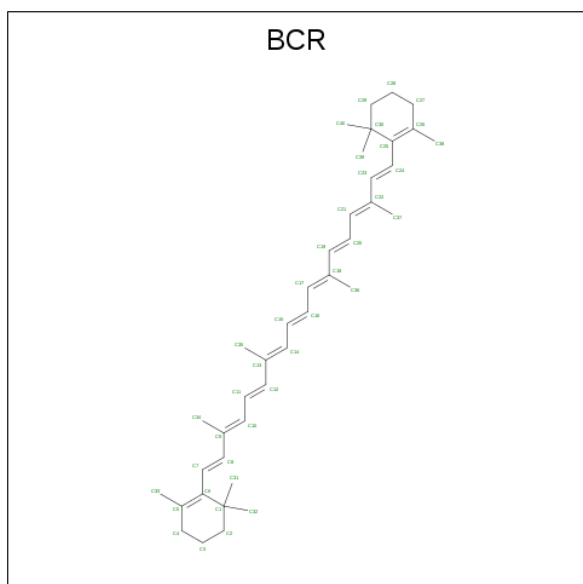
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | b | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 |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

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

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23 | A | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | B | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

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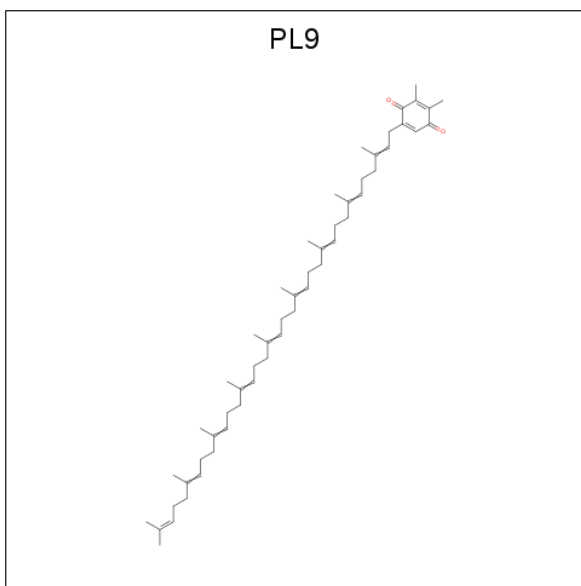
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23 | C | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | D | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | K | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | K | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | T | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | X | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | a | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | b | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | c | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | d | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | h | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | k | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | k | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |
| 23 | t | 1 | Total | C | H | 0 | 0 |
| | | | 96 | 40 | 56 | | |

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

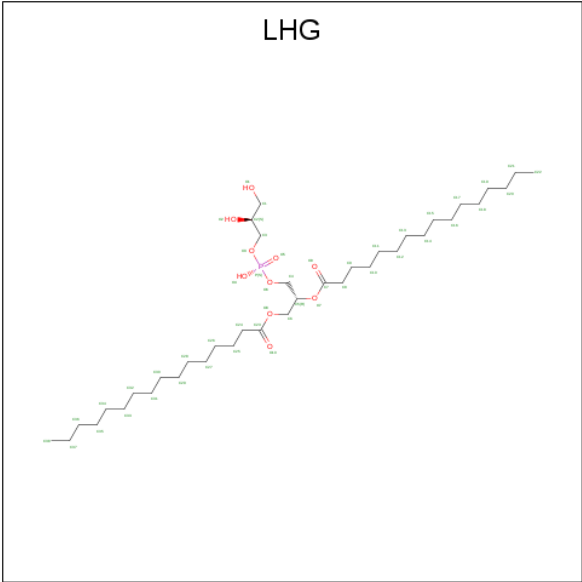
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 24 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 24 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by author).



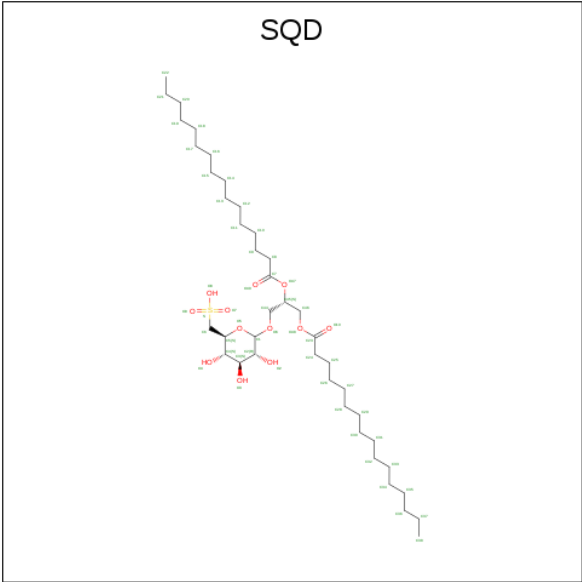
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 25 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 25 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 25 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



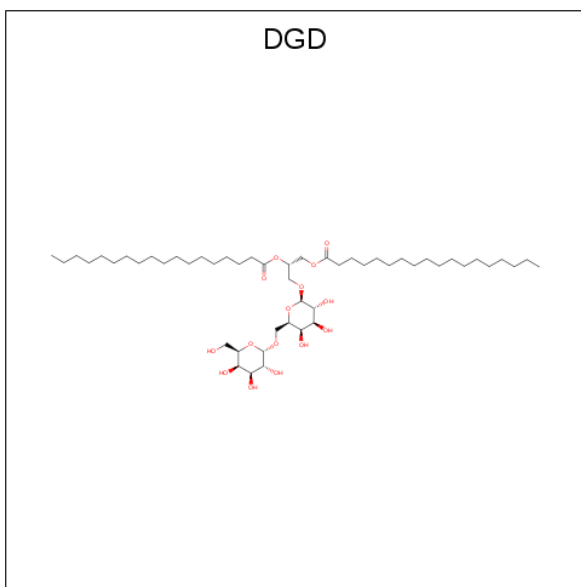
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 26 | A | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 112 | 36 | 65 | 10 | 1 | | |
| 26 | A | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 122 | 38 | 73 | 10 | 1 | | |
| 26 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 121 | 38 | 72 | 10 | 1 | | |
| 26 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 122 | 38 | 73 | 10 | 1 | | |
| 26 | L | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 122 | 38 | 73 | 10 | 1 | | |
| 26 | a | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 122 | 38 | 73 | 10 | 1 | | |
| 26 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 121 | 38 | 72 | 10 | 1 | | |
| 26 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 89 | 28 | 50 | 10 | 1 | | |
| 26 | e | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 97 | 31 | 55 | 10 | 1 | | |
| 26 | l | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 121 | 38 | 72 | 10 | 1 | | |

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



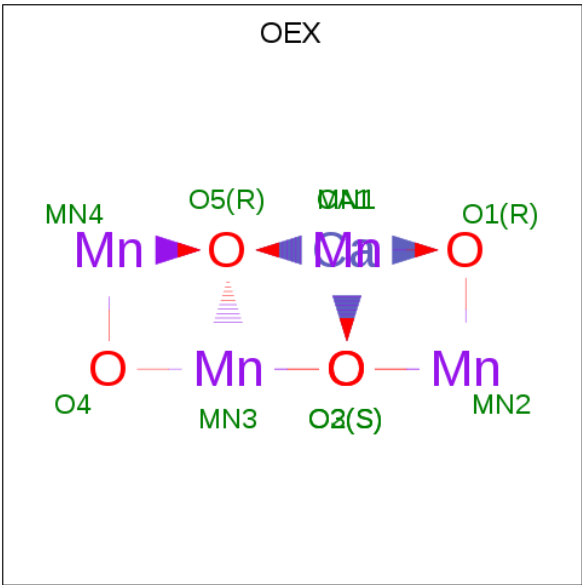
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 27 | A | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 122 | 39 | 70 | 12 | 1 | | |
| 27 | A | 1 | Total | C | H | O | | 0 | 0 |
| | | | 104 | 35 | 65 | 4 | | | |
| 27 | B | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 131 | 41 | 77 | 12 | 1 | | |
| 27 | F | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 81 | 25 | 45 | 10 | 1 | | |
| 27 | L | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 114 | 36 | 65 | 12 | 1 | | |
| 27 | a | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 130 | 41 | 76 | 12 | 1 | | |
| 27 | a | 1 | Total | C | H | O | | 0 | 0 |
| | | | 92 | 31 | 56 | 5 | | | |
| 27 | d | 1 | Total | C | H | O | S | 0 | 0 |
| | | | 89 | 28 | 48 | 12 | 1 | | |

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



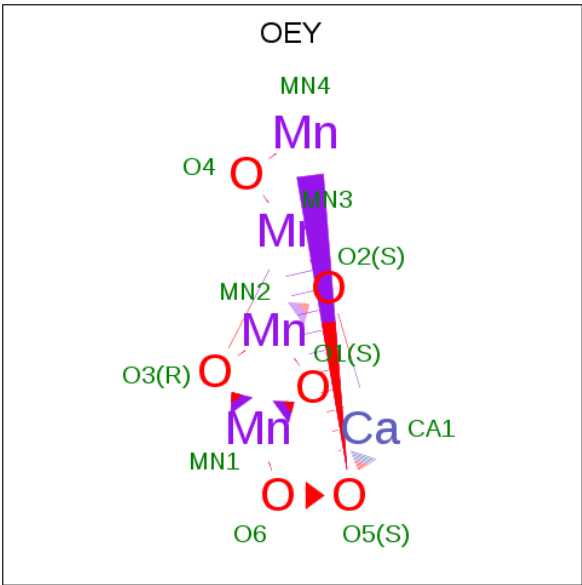
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 28 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 160 | 51 | 94 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 142 | 47 | 80 | 15 | | |
| 28 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |
| 28 | H | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |
| 28 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |
| 28 | h | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 47 | 79 | 15 | | |

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



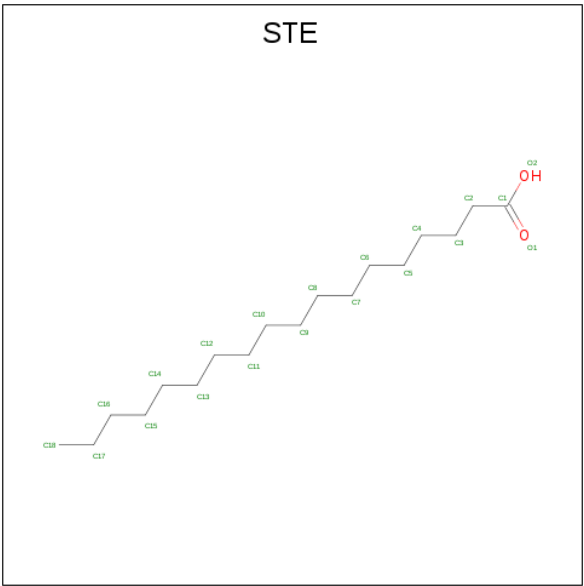
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 29 | A | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 10 | 1 | 4 | 5 | | |
| 29 | a | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 10 | 1 | 4 | 5 | | |

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



| 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 STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 43 | 15 | 26 | 2 | | |
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 46 | 16 | 28 | 2 | | |
| 31 | B | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 31 | B | 1 | Total | C | H | | 0 | 0 |
| | | | 41 | 15 | 26 | | | |
| 31 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | C | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 31 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | H | 1 | Total | C | H | | 0 | 0 |
| | | | 53 | 18 | 35 | | | |
| 31 | I | 1 | Total | C | H | | 0 | 0 |
| | | | 41 | 15 | 26 | | | |
| 31 | J | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |

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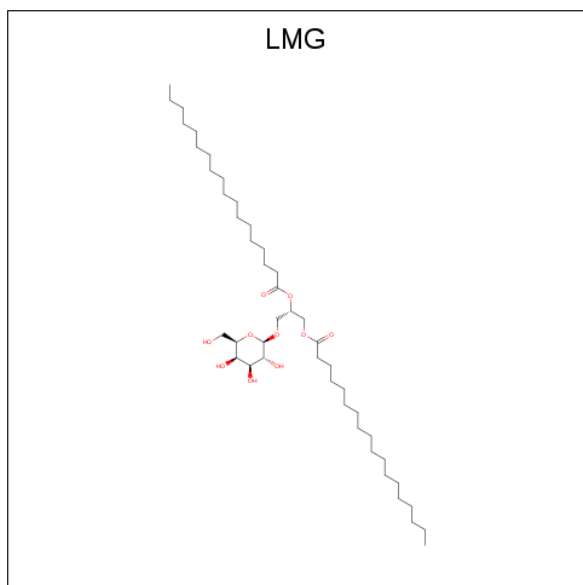
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | L | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | M | 1 | Total | C | H | O | 0 | 0 |
| | | | 37 | 13 | 22 | 2 | | |
| 31 | M | 1 | Total | C | H | | 0 | 0 |
| | | | 26 | 10 | 16 | | | |
| 31 | M | 1 | Total | C | H | | 0 | 0 |
| | | | 53 | 18 | 35 | | | |
| 31 | R | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | T | 1 | Total | C | H | | 0 | 0 |
| | | | 47 | 16 | 31 | | | |
| 31 | T | 1 | Total | C | H | | 0 | 0 |
| | | | 44 | 15 | 29 | | | |
| 31 | Z | 1 | Total | C | H | | 0 | 0 |
| | | | 20 | 8 | 12 | | | |
| 31 | a | 1 | Total | C | H | | 0 | 0 |
| | | | 26 | 10 | 16 | | | |
| 31 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | b | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | b | 1 | Total | C | H | O | 0 | 0 |
| | | | 40 | 14 | 24 | 2 | | |
| 31 | b | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | b | 1 | Total | C | H | | 0 | 0 |
| | | | 26 | 10 | 16 | | | |
| 31 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 43 | 15 | 26 | 2 | | |
| 31 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 55 | 18 | 35 | 2 | | |
| 31 | h | 1 | Total | C | H | | 0 | 0 |
| | | | 41 | 14 | 27 | | | |
| 31 | j | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | t | 1 | Total | C | H | O | 0 | 0 |
| | | | 34 | 12 | 20 | 2 | | |

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



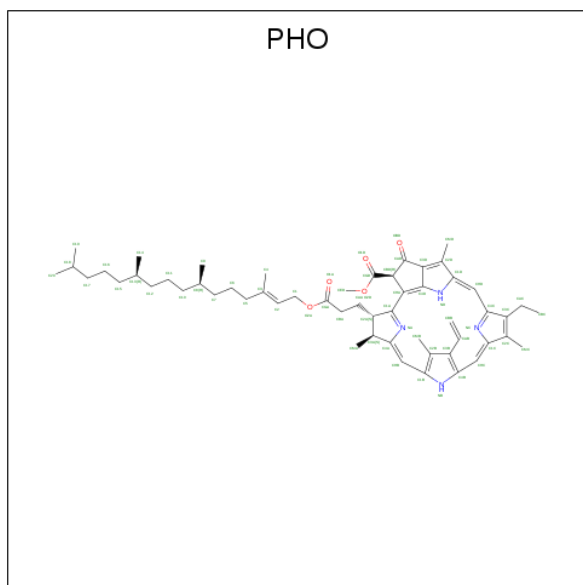
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 32 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 114 | 38 | 66 | 10 | | |
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 122 | 41 | 71 | 10 | | |
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 78 | 27 | 45 | 6 | | |
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 68 | 24 | 40 | 4 | | |
| 32 | M | 1 | Total | C | H | O | 0 | 0 |
| | | | 122 | 41 | 71 | 10 | | |
| 32 | Y | 1 | Total | C | H | O | 0 | 0 |
| | | | 113 | 38 | 65 | 10 | | |
| 32 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 140 | 45 | 85 | 10 | | |
| 32 | b | 1 | Total | C | H | O | 0 | 0 |
| | | | 141 | 45 | 86 | 10 | | |
| 32 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 80 | 27 | 43 | 10 | | |
| 32 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 117 | 38 | 69 | 10 | | |

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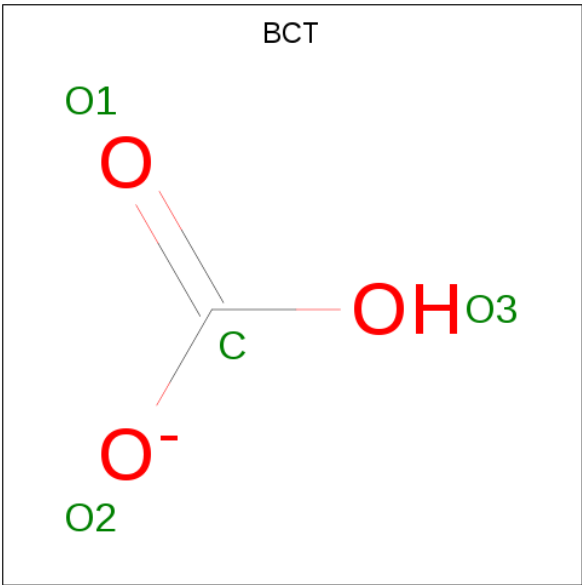
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 32 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 116 | 39 | 67 | 10 | | |
| 32 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 101 | 34 | 57 | 10 | | |
| 32 | m | 1 | Total | C | H | O | 0 | 0 |
| | | | 123 | 41 | 72 | 10 | | |

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



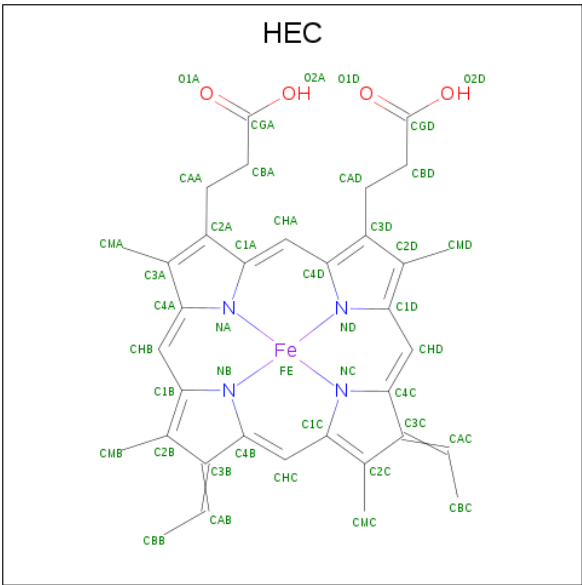
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 33 | D | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | |
| 33 | D | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | |
| 33 | a | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | |
| 33 | d | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 138 | 55 | 74 | 4 | 5 | | |

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 35 | F | 1 | Total | C | Fe | H | N | O | 0 | 0 |
| | | | 75 | 34 | 1 | 32 | 4 | 4 | | |
| 35 | V | 1 | Total | C | Fe | H | N | O | 0 | 0 |
| | | | 73 | 34 | 1 | 30 | 4 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 35 | f | 1 | Total | C | Fe | H | N | O | 0 | 0 |
| | | | 75 | 34 | 1 | 32 | 4 | 4 | | |
| 35 | v | 1 | Total | C | Fe | H | N | O | 0 | 0 |
| | | | 73 | 34 | 1 | 30 | 4 | 4 | | |

- Molecule 36 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 36 | A | 119 | Total | O | 0 | 8 |
| | | | 119 | 119 | | |
| 36 | B | 148 | Total | O | 0 | 0 |
| | | | 148 | 148 | | |
| 36 | C | 118 | Total | O | 0 | 0 |
| | | | 118 | 118 | | |
| 36 | D | 98 | Total | O | 0 | 0 |
| | | | 98 | 98 | | |
| 36 | E | 21 | Total | O | 0 | 0 |
| | | | 21 | 21 | | |
| 36 | F | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 36 | H | 26 | Total | O | 0 | 0 |
| | | | 26 | 26 | | |
| 36 | I | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 36 | J | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 36 | K | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 36 | L | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 36 | M | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 36 | O | 71 | Total | O | 0 | 0 |
| | | | 71 | 71 | | |
| 36 | R | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | T | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 36 | U | 31 | Total | O | 0 | 0 |
| | | | 31 | 31 | | |
| 36 | V | 51 | Total | O | 0 | 0 |
| | | | 51 | 51 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 36 | X | 9 | Total O 9 9 | 0 | 0 |
| 36 | Y | 4 | Total O 4 4 | 0 | 0 |
| 36 | Z | 2 | Total O 2 2 | 0 | 0 |
| 36 | a | 114 | Total O 114 114 | 0 | 8 |
| 36 | b | 126 | Total O 126 126 | 0 | 0 |
| 36 | c | 122 | Total O 122 122 | 0 | 0 |
| 36 | d | 94 | Total O 94 94 | 0 | 0 |
| 36 | e | 13 | Total O 13 13 | 0 | 0 |
| 36 | f | 2 | Total O 2 2 | 0 | 0 |
| 36 | h | 21 | Total O 21 21 | 0 | 0 |
| 36 | i | 8 | Total O 8 8 | 0 | 0 |
| 36 | j | 8 | Total O 8 8 | 0 | 0 |
| 36 | k | 6 | Total O 6 6 | 0 | 0 |
| 36 | l | 8 | Total O 8 8 | 0 | 0 |
| 36 | m | 7 | Total O 7 7 | 0 | 0 |
| 36 | o | 67 | Total O 67 67 | 0 | 0 |
| 36 | r | 1 | Total O 1 1 | 0 | 0 |
| 36 | t | 5 | Total O 5 5 | 0 | 0 |
| 36 | u | 41 | Total O 41 41 | 0 | 0 |
| 36 | v | 31 | Total O 31 31 | 0 | 0 |
| 36 | x | 9 | Total O 9 9 | 0 | 0 |

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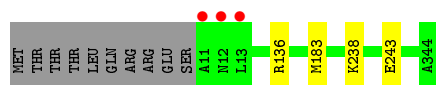
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 36 | y | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | z | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

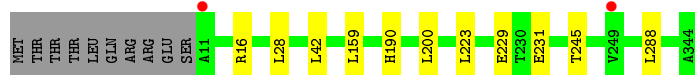
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

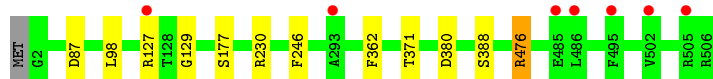
- Molecule 1: Photosystem II protein D1 1



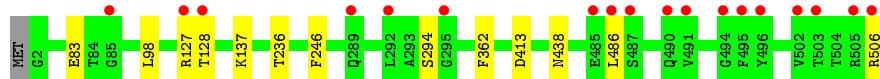
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

[illegible]

- Chain D:  95%

| Category | Count |
|----------|-------|
| MET | 1 |
| THR | 1 |
| ILE | 1 |
| ALA | 1 |
| ILE | 1 |
| GLY | 1 |
| ARG | 1 |
| ALA | 1 |
| PRO | 1 |
| ALA | 1 |
| GLU | 1 |
| R12 | 1 |
| V154 | 1 |
| R180 | 1 |
| E227 | 2 |
| G228 | 2 |
| A229 | 2 |
| K264 | 1 |
| R294 | 1 |
| M329 | 1 |
| L352 | 1 |

- Chain d:  94%

| | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | THR | IIE | ALA | IIE | GLY | ARG | ALA | PRO | ALA | GLU | R12 | L90 | R180 | F181 | L182 | R233 | L259 | L272 | L291 | M292 | L293 | E307 | L321 | M329 | L352 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|

- Chain E:  4% 96%

- Chain e:  94% 7%

Diagram illustrating the 12-mer sequence: MET, ALA, G3, T4, R8, R61, L65, Q74, F79, Q82, L83, K84. Red dots are placed above the T4, R61, Q74, F79, Q82, L83, and K84 segments.

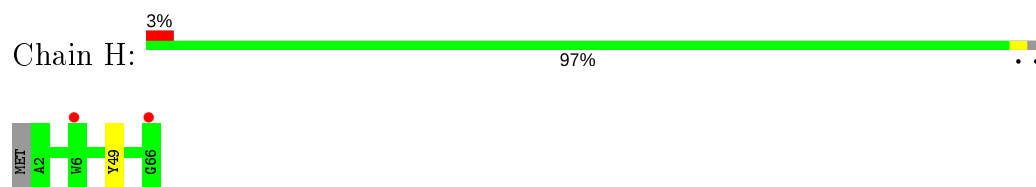
- Chain F:  4% 73% 24%

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 1. The x-axis lists amino acids: MET, THR, SER, ASN, THR, PRO, ASN, GLN, GLU, PRO, VAL, S12, Y13, T25, and R45. The bars for S12 and Y13 are green and reach approximately 0.8 bits. The bar for T25 is yellow and reaches approximately 0.4 bits. The bar for R45 is green and reaches approximately 0.3 bits. All other amino acids have bars that are very short, below 0.1 bits. There are two red dots above the S12 and Y13 bars.

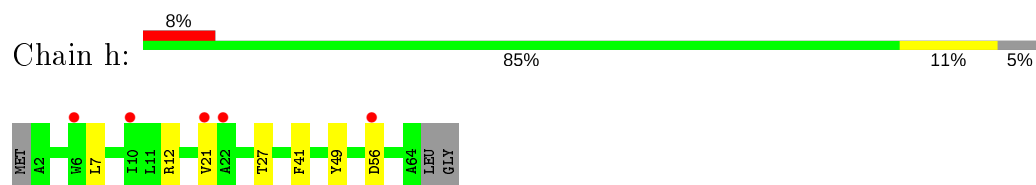
- Chain f:  7% 71% 24%

| Protein Family | Count |
|----------------|-------|
| MET | 12 |
| THR | 10 |
| SER | 7 |
| ASN | 9 |
| THR | 12 |
| PRO | 10 |
| ASN | 12 |
| GLN | 12 |
| GLU | 12 |
| PRO | 12 |
| VAL | 12 |
| S12 | 12 |
| V13 | 12 |
| P14 | 12 |
| I15 | 12 |
| V23 | 6 |
| V28 | 6 |
| R45 | 6 |

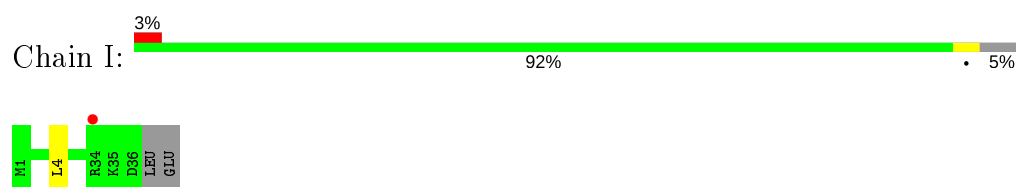
- Molecule 7: Photosystem II reaction center protein H



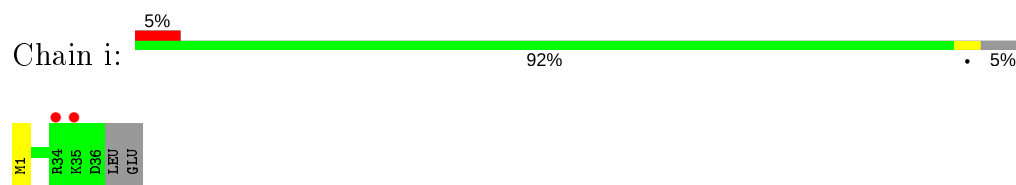
- Molecule 7: Photosystem II reaction center protein H



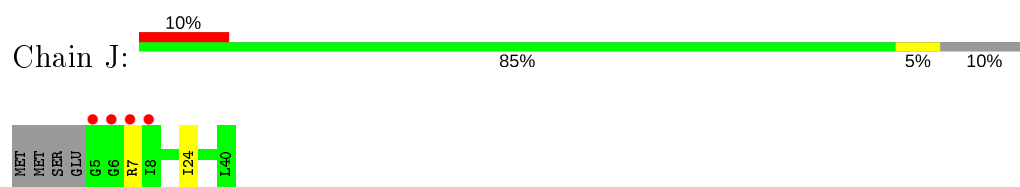
- Molecule 8: Photosystem II reaction center protein I



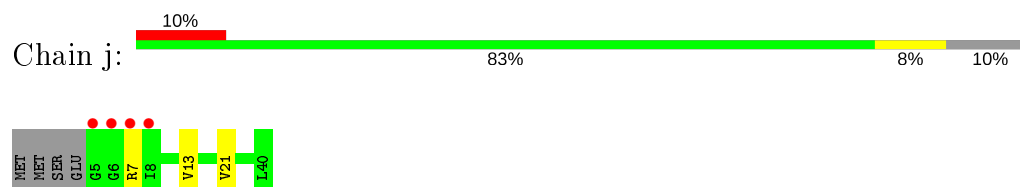
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

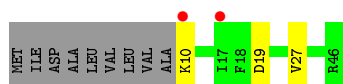


- Molecule 9: Photosystem II reaction center protein J

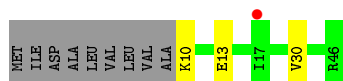
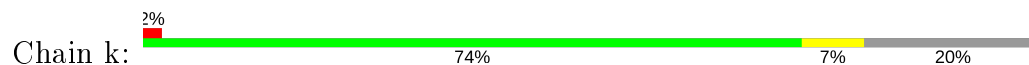


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

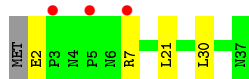
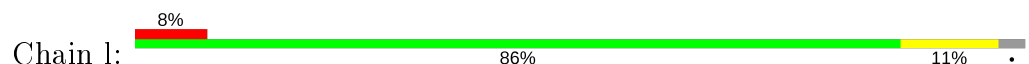


- Molecule 11: Photosystem II reaction center protein L

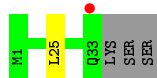
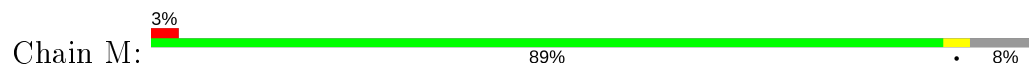


There are no outlier residues recorded for this chain.

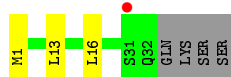
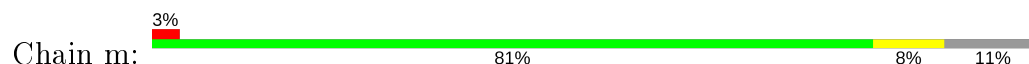
- Molecule 11: Photosystem II reaction center protein L



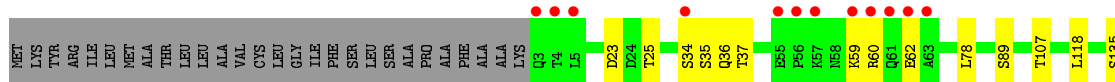
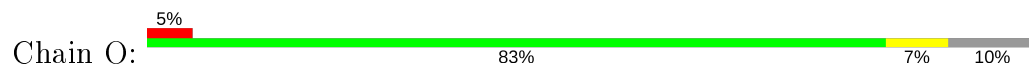
- Molecule 12: Photosystem II reaction center protein M



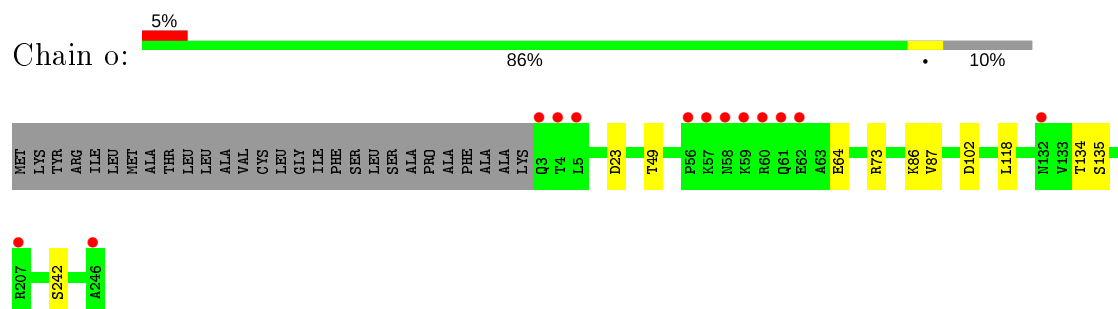
- Molecule 12: Photosystem II reaction center protein M



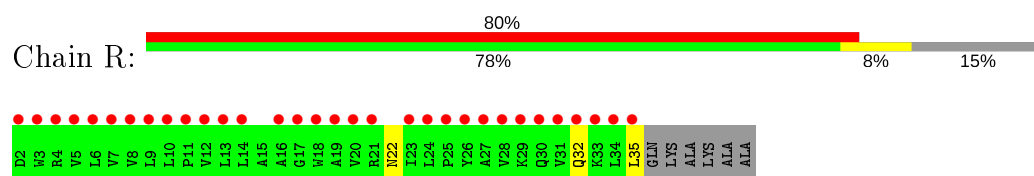
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



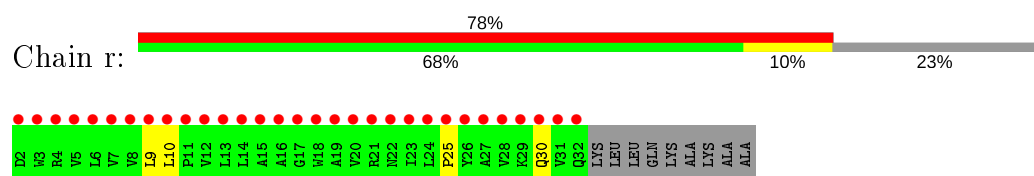
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



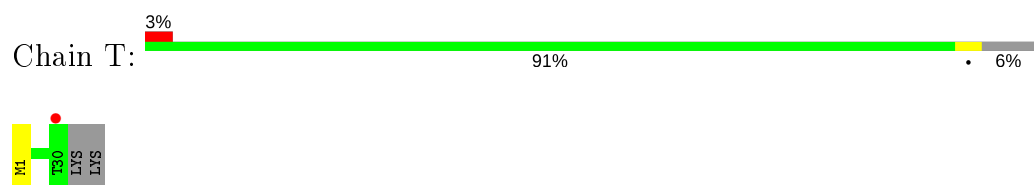
- Molecule 14: Photosystem II protein Y



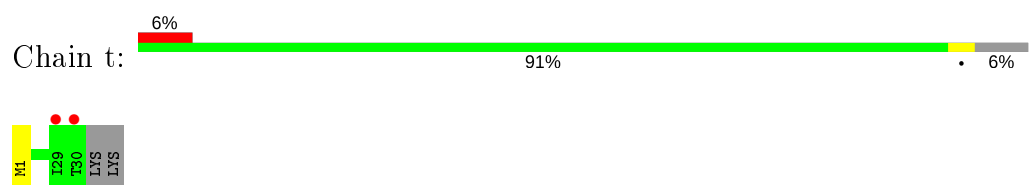
- Molecule 14: Photosystem II protein Y



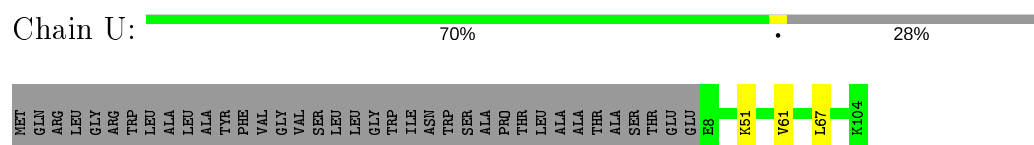
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

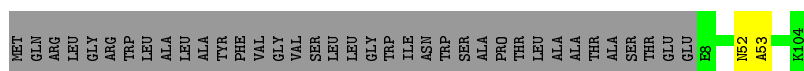


- Molecule 16: Photosystem II 12 kDa extrinsic protein



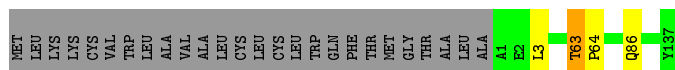
- Molecule 16: Photosystem II 12 kDa extrinsic protein





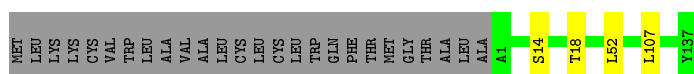
- Molecule 17: Cytochrome c-550

Chain V: 82% 16%



- Molecule 17: Cytochrome c-550

Chain v: 82% 16%



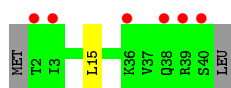
- Molecule 18: Photosystem II reaction center X protein

Chain X: 5% 88% 5% 7%



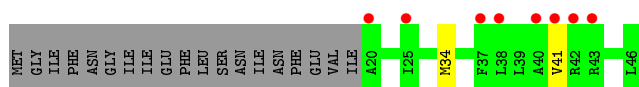
- Molecule 18: Photosystem II reaction center X protein

Chain x: 15% 93% 5%



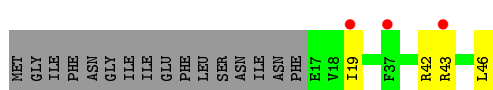
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 17% 54% 41%



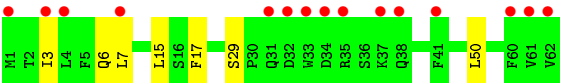
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 7% 57% 9% 35%

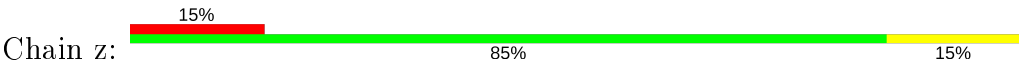


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 24% 89% 11%



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 33.70 – 2.23 33.70 – 2.23 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (33.70-2.23) 85.1 (33.70-2.23) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.61 (at 2.22Å) | Xtriage |
| Refinement program | PHENIX 1.17.1 _3660 | Depositor |
| R, R_{free} | 0.172 , 0.235 0.172 , 0.234 | Depositor DCC |
| R_{free} test set | 3445 reflections (0.89%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 29.6 | Xtriage |
| Anisotropy | 0.206 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 61.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 105311 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: LHG, STE, OEY, OEX, PHO, DGD, CL, SQD, CLA, PL9, FE2, HEC, BCT, FME, BCR, LMG

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 | 0.59 | 0/3187 | 0.69 | 4/4342 (0.1%) |
| 1 | a | 0.59 | 0/3184 | 0.73 | 6/4338 (0.1%) |
| 2 | B | 0.65 | 1/4161 (0.0%) | 0.70 | 3/5669 (0.1%) |
| 2 | b | 0.61 | 0/4118 | 0.69 | 0/5611 |
| 3 | C | 0.62 | 0/3621 | 0.69 | 2/4930 (0.0%) |
| 3 | c | 0.59 | 0/3693 | 0.66 | 0/5026 |
| 4 | D | 0.68 | 0/2820 | 0.69 | 1/3840 (0.0%) |
| 4 | d | 0.63 | 0/2829 | 0.70 | 0/3852 |
| 5 | E | 0.55 | 0/688 | 0.60 | 0/940 |
| 5 | e | 0.50 | 0/683 | 0.60 | 0/932 |
| 6 | F | 0.49 | 0/284 | 0.60 | 0/387 |
| 6 | f | 0.50 | 0/284 | 0.61 | 0/387 |
| 7 | H | 0.59 | 0/523 | 0.66 | 0/713 |
| 7 | h | 0.57 | 0/511 | 0.69 | 0/697 |
| 8 | I | 0.63 | 0/293 | 0.70 | 0/396 |
| 8 | i | 0.70 | 0/293 | 0.63 | 0/396 |
| 9 | J | 0.53 | 0/263 | 0.63 | 0/356 |
| 9 | j | 0.53 | 0/263 | 0.65 | 0/356 |
| 10 | K | 0.49 | 0/303 | 0.60 | 0/416 |
| 10 | k | 0.54 | 0/303 | 0.66 | 0/416 |
| 11 | L | 0.72 | 0/311 | 0.76 | 0/422 |
| 11 | l | 0.65 | 0/303 | 0.66 | 0/412 |
| 12 | M | 0.69 | 0/249 | 0.69 | 0/341 |
| 12 | m | 0.70 | 0/244 | 0.73 | 0/334 |
| 13 | O | 0.61 | 0/1904 | 0.75 | 1/2585 (0.0%) |
| 13 | o | 0.63 | 0/1905 | 0.75 | 1/2583 (0.0%) |
| 14 | R | 0.45 | 0/277 | 0.53 | 0/380 |
| 14 | r | 0.38 | 0/246 | 0.48 | 0/339 |
| 15 | T | 0.78 | 0/257 | 0.69 | 0/349 |
| 15 | t | 0.73 | 0/255 | 0.69 | 0/346 |
| 16 | U | 0.56 | 0/785 | 0.69 | 0/1064 |
| 16 | u | 0.62 | 0/785 | 0.72 | 0/1064 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | V | 0.61 | 0/1085 | 0.73 | 1/1473 (0.1%) |
| 17 | v | 0.53 | 0/1085 | 0.65 | 0/1473 |
| 18 | X | 0.51 | 0/284 | 0.63 | 0/384 |
| 18 | x | 0.43 | 0/289 | 0.56 | 0/391 |
| 19 | Y | 0.52 | 0/197 | 0.62 | 0/264 |
| 19 | y | 0.40 | 0/219 | 0.62 | 0/294 |
| 20 | Z | 0.47 | 0/490 | 0.54 | 0/669 |
| 20 | z | 0.44 | 0/488 | 0.55 | 0/666 |
| All | All | 0.61 | 1/43962 (0.0%) | 0.69 | 19/59833 (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 |
|-----|-------|---------------------|---------------------|
| 16 | u | 0 | 1 |
| 17 | V | 0 | 1 |
| All | All | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 129 | GLY | C-N | -5.76 | 1.20 | 1.34 |

The worst 5 of 19 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|--------|--------|-------------|----------|
| 1 | a | 190[A] | HIS | O-C-N | -10.10 | 106.55 | 122.70 |
| 1 | a | 190[B] | HIS | O-C-N | -10.10 | 106.55 | 122.70 |
| 1 | a | 190[A] | HIS | CA-C-N | 8.05 | 134.92 | 117.20 |
| 1 | a | 190[B] | HIS | CA-C-N | 8.05 | 134.92 | 117.20 |
| 1 | a | 190[A] | HIS | C-N-CA | 7.16 | 139.60 | 121.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 17 | V | 63 | THR | Peptide |
| 16 | u | 52 | ASN | 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 | 391/344 (114%) | 379 (97%) | 12 (3%) | 0 | 100 | 100 |
| 1 | a | 391/344 (114%) | 381 (97%) | 10 (3%) | 0 | 100 | 100 |
| 2 | B | 508/506 (100%) | 498 (98%) | 10 (2%) | 0 | 100 | 100 |
| 2 | b | 503/506 (99%) | 486 (97%) | 15 (3%) | 2 (0%) | 34 | 35 |
| 3 | C | 450/461 (98%) | 438 (97%) | 11 (2%) | 1 (0%) | 47 | 53 |
| 3 | c | 459/461 (100%) | 445 (97%) | 13 (3%) | 1 (0%) | 47 | 53 |
| 4 | D | 339/352 (96%) | 330 (97%) | 9 (3%) | 0 | 100 | 100 |
| 4 | d | 340/352 (97%) | 330 (97%) | 10 (3%) | 0 | 100 | 100 |
| 5 | E | 81/84 (96%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 80/84 (95%) | 75 (94%) | 4 (5%) | 1 (1%) | 12 | 7 |
| 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%) | 56 (89%) | 7 (11%) | 0 | 100 | 100 |
| 7 | h | 61/66 (92%) | 57 (93%) | 4 (7%) | 0 | 100 | 100 |
| 8 | I | 34/38 (90%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | i | 34/38 (90%) | 32 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | J | 34/40 (85%) | 31 (91%) | 2 (6%) | 1 (3%) | 4 | 1 |
| 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%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |

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| 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%) | 223 (92%) | 13 (5%) | 7 (3%) | 4 | 1 |
| 13 | o | 242/272 (89%) | 229 (95%) | 12 (5%) | 1 (0%) | 34 | 35 |
| 14 | R | 32/40 (80%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 14 | r | 29/40 (72%) | 23 (79%) | 4 (14%) | 2 (7%) | 1 | 0 |
| 15 | T | 28/32 (88%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 15 | t | 28/32 (88%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 16 | U | 95/134 (71%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 16 | u | 95/134 (71%) | 89 (94%) | 5 (5%) | 1 (1%) | 14 | 9 |
| 17 | V | 135/163 (83%) | 128 (95%) | 6 (4%) | 1 (1%) | 22 | 20 |
| 17 | v | 135/163 (83%) | 127 (94%) | 8 (6%) | 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%) | 24 (86%) | 2 (7%) | 2 (7%) | 1 | 0 |
| 20 | Z | 60/62 (97%) | 48 (80%) | 12 (20%) | 0 | 100 | 100 |
| 20 | z | 60/62 (97%) | 57 (95%) | 2 (3%) | 1 (2%) | 9 | 4 |
| All | All | 5374/5690 (94%) | 5161 (96%) | 192 (4%) | 21 (0%) | 34 | 35 |

5 of 21 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 36 | GLN |
| 13 | O | 59 | LYS |
| 13 | O | 60 | ARG |
| 13 | O | 62 | GLU |
| 17 | V | 64 | 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 | 320/280 (114%) | 318 (99%) | 2 (1%) | 86 | 90 |
| 1 | a | 319/280 (114%) | 309 (97%) | 10 (3%) | 40 | 46 |
| 2 | B | 408/404 (101%) | 399 (98%) | 9 (2%) | 52 | 59 |
| 2 | b | 402/404 (100%) | 391 (97%) | 11 (3%) | 44 | 51 |
| 3 | C | 353/362 (98%) | 343 (97%) | 10 (3%) | 43 | 49 |
| 3 | c | 361/362 (100%) | 345 (96%) | 16 (4%) | 28 | 30 |
| 4 | D | 277/283 (98%) | 272 (98%) | 5 (2%) | 59 | 66 |
| 4 | d | 278/283 (98%) | 267 (96%) | 11 (4%) | 31 | 34 |
| 5 | E | 72/73 (99%) | 70 (97%) | 2 (3%) | 43 | 49 |
| 5 | e | 71/73 (97%) | 69 (97%) | 2 (3%) | 43 | 49 |
| 6 | F | 28/39 (72%) | 27 (96%) | 1 (4%) | 35 | 39 |
| 6 | f | 28/39 (72%) | 26 (93%) | 2 (7%) | 14 | 11 |
| 7 | H | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 | 64 |
| 7 | h | 53/55 (96%) | 46 (87%) | 7 (13%) | 4 | 2 |
| 8 | I | 32/34 (94%) | 31 (97%) | 1 (3%) | 40 | 46 |
| 8 | i | 32/34 (94%) | 32 (100%) | 0 | 100 | 100 |
| 9 | J | 24/28 (86%) | 23 (96%) | 1 (4%) | 30 | 32 |
| 9 | j | 24/28 (86%) | 21 (88%) | 3 (12%) | 4 | 2 |
| 10 | K | 30/37 (81%) | 27 (90%) | 3 (10%) | 7 | 4 |
| 10 | k | 30/37 (81%) | 27 (90%) | 3 (10%) | 7 | 4 |
| 11 | L | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 11 | l | 34/35 (97%) | 30 (88%) | 4 (12%) | 5 | 2 |
| 12 | M | 28/32 (88%) | 27 (96%) | 1 (4%) | 35 | 39 |
| 12 | m | 28/32 (88%) | 26 (93%) | 2 (7%) | 14 | 11 |
| 13 | O | 206/228 (90%) | 195 (95%) | 11 (5%) | 22 | 21 |
| 13 | o | 207/228 (91%) | 198 (96%) | 9 (4%) | 29 | 31 |
| 14 | R | 28/32 (88%) | 25 (89%) | 3 (11%) | 6 | 3 |
| 14 | r | 23/32 (72%) | 21 (91%) | 2 (9%) | 10 | 6 |
| 15 | T | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 15 | t | 25/28 (89%) | 25 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 16 | U | 84/112 (75%) | 81 (96%) | 3 (4%) | 35 | 39 |
| 16 | u | 84/112 (75%) | 84 (100%) | 0 | 100 | 100 |
| 17 | V | 117/138 (85%) | 115 (98%) | 2 (2%) | 60 | 68 |
| 17 | v | 117/138 (85%) | 113 (97%) | 4 (3%) | 37 | 42 |
| 18 | X | 31/34 (91%) | 29 (94%) | 2 (6%) | 17 | 14 |
| 18 | x | 31/34 (91%) | 30 (97%) | 1 (3%) | 39 | 44 |
| 19 | Y | 19/37 (51%) | 17 (90%) | 2 (10%) | 7 | 3 |
| 19 | y | 22/37 (60%) | 20 (91%) | 2 (9%) | 9 | 6 |
| 20 | Z | 52/52 (100%) | 45 (86%) | 7 (14%) | 4 | 1 |
| 20 | z | 51/52 (98%) | 43 (84%) | 8 (16%) | 2 | 1 |
| All | All | 4444/4646 (96%) | 4281 (96%) | 163 (4%) | 34 | 38 |

5 of 163 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 231 | GLU |
| 3 | c | 99 | VAL |
| 17 | v | 52 | LEU |
| 1 | a | 288 | LEU |
| 2 | b | 362 | PHE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | X | 38 | GLN |
| 20 | Z | 38 | GLN |
| 4 | d | 61 | HIS |
| 17 | V | 86 | GLN |
| 2 | b | 490 | 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 |
| 15 | FME | T | 1 | 15 | 8,9,10 | 1.11 | 1 (12%) | 7,9,11 | 1.40 | 2 (28%) |
| 8 | FME | I | 1 | 8 | 8,9,10 | 1.00 | 0 | 7,9,11 | 0.97 | 0 |
| 12 | FME | M | 1 | 12 | 8,9,10 | 0.86 | 0 | 7,9,11 | 0.92 | 0 |
| 8 | FME | i | 1 | 8 | 8,9,10 | 1.15 | 1 (12%) | 7,9,11 | 0.52 | 0 |
| 15 | FME | t | 1 | 15 | 8,9,10 | 1.34 | 1 (12%) | 7,9,11 | 0.78 | 0 |
| 12 | FME | m | 1 | 12 | 8,9,10 | 1.02 | 1 (12%) | 7,9,11 | 1.21 | 1 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 15 | FME | T | 1 | 15 | - | 1/7/9/11 | - |
| 8 | FME | I | 1 | 8 | - | 2/7/9/11 | - |
| 12 | FME | M | 1 | 12 | - | 1/7/9/11 | - |
| 8 | FME | i | 1 | 8 | - | 2/7/9/11 | - |
| 15 | FME | t | 1 | 15 | - | 2/7/9/11 | - |
| 12 | FME | m | 1 | 12 | - | 0/7/9/11 | - |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15 | t | 1 | FME | CA-N | -3.00 | 1.42 | 1.46 |
| 12 | m | 1 | FME | CA-N | -2.24 | 1.43 | 1.46 |
| 8 | i | 1 | FME | CA-N | -2.09 | 1.43 | 1.46 |
| 15 | T | 1 | FME | CB-CA | 2.06 | 1.57 | 1.53 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 15 | T | 1 | FME | CA-N-CN | 2.91 | 127.29 | 122.82 |
| 12 | m | 1 | FME | CA-N-CN | -2.35 | 119.21 | 122.82 |
| 15 | T | 1 | FME | CG-CB-CA | 2.03 | 118.59 | 112.95 |

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 32 | LMG | b | 621 | - | 55,55,55 | 0.91 | 3 (5%) | 63,63,63 | 1.52 | 10 (15%) |
| 22 | CLA | c | 514 | - | 59,73,73 | 1.42 | 6 (10%) | 67,113,113 | 1.46 | 7 (10%) |
| 26 | LHG | D | 412 | - | 48,48,48 | 0.96 | 3 (6%) | 51,54,54 | 1.34 | 7 (13%) |
| 23 | BCR | b | 618 | - | 41,41,41 | 1.25 | 2 (4%) | 56,56,56 | 1.37 | 7 (12%) |
| 27 | SQD | F | 102 | - | 35,36,54 | 1.03 | 3 (8%) | 42,45,65 | 1.88 | 9 (21%) |
| 31 | STE | a | 415 | - | 9,9,19 | 0.53 | 0 | 8,8,19 | 0.54 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | DGD | H | 102 | - | 63,63,67 | 1.30 | 8 (12%) | 77,77,81 | 1.34 | 7 (9%) |
| 22 | CLA | B | 604 | - | 59,73,73 | 1.50 | 8 (13%) | 67,113,113 | 2.19 | 14 (20%) |
| 31 | STE | b | 620 | - | 16,19,19 | 0.45 | 0 | 15,19,19 | 0.83 | 0 |
| 33 | PHO | a | 404 | - | 67,69,69 | 1.08 | 7 (10%) | 85,99,99 | 1.13 | 6 (7%) |
| 22 | CLA | c | 513 | - | 59,73,73 | 1.52 | 6 (10%) | 67,113,113 | 1.66 | 14 (20%) |
| 22 | CLA | B | 616 | - | 54,68,73 | 1.79 | 10 (18%) | 61,107,113 | 1.75 | 10 (16%) |
| 31 | STE | C | 521 | - | 15,15,19 | 0.53 | 0 | 14,14,19 | 0.52 | 0 |
| 22 | CLA | c | 506 | - | 59,73,73 | 1.57 | 7 (11%) | 67,113,113 | 1.82 | 15 (22%) |
| 23 | BCR | t | 101 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.47 | 11 (19%) |
| 22 | CLA | A | 402 | - | 59,73,73 | 1.51 | 7 (11%) | 67,113,113 | 1.69 | 13 (19%) |
| 23 | BCR | X | 101 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.36 | 8 (14%) |
| 31 | STE | R | 101 | - | 8,11,19 | 0.49 | 0 | 7,11,19 | 0.70 | 0 |
| 26 | LHG | D | 409 | - | 48,48,48 | 1.30 | 5 (10%) | 51,54,54 | 1.25 | 7 (13%) |
| 23 | BCR | d | 404 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.14 | 6 (10%) |
| 32 | LMG | C | 516 | - | 48,48,55 | 1.19 | 3 (6%) | 56,56,63 | 1.53 | 9 (16%) |
| 31 | STE | T | 103 | - | 14,14,19 | 0.50 | 0 | 13,13,19 | 0.71 | 0 |
| 31 | STE | M | 104 | - | 17,17,19 | 0.36 | 0 | 16,16,19 | 0.88 | 0 |
| 22 | CLA | C | 506 | - | 59,73,73 | 1.64 | 7 (11%) | 67,113,113 | 1.66 | 12 (17%) |
| 23 | BCR | K | 102 | - | 41,41,41 | 1.06 | 2 (4%) | 56,56,56 | 1.37 | 9 (16%) |
| 22 | CLA | c | 508 | 36 | 59,73,73 | 1.41 | 6 (10%) | 67,113,113 | 1.68 | 14 (20%) |
| 25 | PL9 | A | 408 | - | 55,55,55 | 1.65 | 12 (21%) | 68,69,69 | 1.75 | 18 (26%) |
| 31 | STE | c | 501 | - | 8,11,19 | 0.45 | 0 | 7,11,19 | 0.60 | 0 |
| 31 | STE | T | 102 | - | 15,15,19 | 0.45 | 0 | 14,14,19 | 0.81 | 0 |
| 22 | CLA | c | 509 | - | 58,72,73 | 1.64 | 7 (12%) | 65,111,113 | 1.57 | 9 (13%) |
| 35 | HEC | F | 101 | 5,6 | 26,50,50 | 2.50 | 5 (19%) | 18,82,82 | 2.37 | 6 (33%) |
| 23 | BCR | c | 516 | - | 41,41,41 | 1.16 | 4 (9%) | 56,56,56 | 1.56 | 9 (16%) |
| 22 | CLA | C | 510 | - | 59,73,73 | 1.47 | 7 (11%) | 67,113,113 | 1.47 | 8 (11%) |
| 33 | PHO | d | 401 | - | 67,69,69 | 1.22 | 8 (11%) | 85,99,99 | 1.30 | 9 (10%) |
| 22 | CLA | c | 511 | - | 59,73,73 | 1.56 | 6 (10%) | 67,113,113 | 1.70 | 14 (20%) |
| 22 | CLA | C | 503 | - | 59,73,73 | 1.71 | 9 (15%) | 67,113,113 | 1.74 | 10 (14%) |
| 22 | CLA | C | 508 | - | 59,73,73 | 1.57 | 8 (13%) | 67,113,113 | 1.41 | 7 (10%) |
| 22 | CLA | b | 610 | 36 | 59,73,73 | 1.20 | 7 (11%) | 67,113,113 | 1.51 | 13 (19%) |
| 23 | BCR | B | 618 | - | 41,41,41 | 1.07 | 3 (7%) | 56,56,56 | 1.43 | 10 (17%) |
| 35 | HEC | v | 201 | 17 | 26,50,50 | 2.37 | 3 (11%) | 18,82,82 | 2.08 | 6 (33%) |
| 22 | CLA | b | 602 | - | 59,73,73 | 1.36 | 9 (15%) | 67,113,113 | 1.56 | 10 (14%) |
| 22 | CLA | c | 505 | 36 | 54,68,73 | 1.48 | 6 (11%) | 61,107,113 | 1.57 | 12 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 27 | SQD | a | 414 | - | 35,35,54 | 1.10 | 2 (5%) | 37,37,65 | 1.30 | 3 (8%) |
| 28 | DGD | h | 102 | - | 63,63,67 | 1.28 | 9 (14%) | 77,77,81 | 1.40 | 9 (11%) |
| 31 | STE | I | 101 | - | 14,14,19 | 0.62 | 0 | 13,13,19 | 0.43 | 0 |
| 29 | OEX | A | 415[A] | 1,3,36 | 0,15,15 | 0.00 | - | - | | |
| 22 | CLA | d | 402 | - | 59,73,73 | 1.21 | 7 (11%) | 67,113,113 | 1.27 | 11 (16%) |
| 32 | LMG | c | 523 | - | 49,49,55 | 1.06 | 5 (10%) | 57,57,63 | 1.30 | 4 (7%) |
| 25 | PL9 | a | 410 | - | 55,55,55 | 0.94 | 3 (5%) | 68,69,69 | 1.61 | 9 (13%) |
| 32 | LMG | d | 408 | - | 44,44,55 | 1.03 | 4 (9%) | 52,52,63 | 1.27 | 6 (11%) |
| 22 | CLA | b | 608 | - | 59,73,73 | 1.87 | 10 (16%) | 67,113,113 | 1.43 | 11 (16%) |
| 31 | STE | B | 625 | - | 14,14,19 | 0.46 | 0 | 13,13,19 | 0.79 | 0 |
| 22 | CLA | B | 606 | - | 59,73,73 | 1.73 | 8 (13%) | 67,113,113 | 1.51 | 10 (14%) |
| 22 | CLA | B | 614 | - | 59,73,73 | 1.53 | 6 (10%) | 67,113,113 | 1.34 | 11 (16%) |
| 31 | STE | C | 520 | - | 8,11,19 | 0.57 | 0 | 7,11,19 | 0.47 | 0 |
| 27 | SQD | d | 409 | - | 40,41,54 | 1.14 | 4 (10%) | 49,52,65 | 1.99 | 13 (26%) |
| 28 | DGD | C | 518 | - | 63,63,67 | 1.11 | 5 (7%) | 77,77,81 | 1.37 | 11 (14%) |
| 28 | DGD | C | 519 | - | 63,63,67 | 1.15 | 10 (15%) | 77,77,81 | 1.38 | 8 (10%) |
| 23 | BCR | b | 619 | - | 41,41,41 | 1.00 | 2 (4%) | 56,56,56 | 1.40 | 7 (12%) |
| 22 | CLA | C | 507 | 36 | 59,73,73 | 1.56 | 8 (13%) | 67,113,113 | 1.69 | 9 (13%) |
| 22 | CLA | b | 606 | - | 59,73,73 | 1.62 | 5 (8%) | 67,113,113 | 1.83 | 13 (19%) |
| 22 | CLA | b | 611 | - | 59,73,73 | 1.39 | 8 (13%) | 67,113,113 | 1.64 | 14 (20%) |
| 31 | STE | j | 101 | - | 8,11,19 | 0.52 | 0 | 7,11,19 | 0.48 | 0 |
| 22 | CLA | C | 513 | - | 59,73,73 | 1.48 | 7 (11%) | 67,113,113 | 1.74 | 13 (19%) |
| 22 | CLA | b | 616 | - | 54,68,73 | 1.53 | 8 (14%) | 61,107,113 | 1.63 | 12 (19%) |
| 35 | HEC | V | 201 | 17 | 26,50,50 | 2.29 | 3 (11%) | 18,82,82 | 2.01 | 9 (50%) |
| 31 | STE | M | 103 | - | 9,9,19 | 0.53 | 0 | 8,8,19 | 0.51 | 0 |
| 31 | STE | B | 620 | - | 13,16,19 | 0.48 | 0 | 12,16,19 | 0.68 | 0 |
| 23 | BCR | k | 101 | - | 41,41,41 | 1.08 | 2 (4%) | 56,56,56 | 1.08 | 4 (7%) |
| 22 | CLA | c | 503 | - | 59,73,73 | 1.37 | 6 (10%) | 67,113,113 | 1.63 | 14 (20%) |
| 22 | CLA | B | 610 | 36 | 59,73,73 | 1.51 | 8 (13%) | 67,113,113 | 1.44 | 12 (17%) |
| 31 | STE | b | 622 | - | 12,15,19 | 0.64 | 0 | 11,15,19 | 0.56 | 0 |
| 22 | CLA | a | 411 | 36 | 59,73,73 | 1.66 | 6 (10%) | 67,113,113 | 1.40 | 9 (13%) |
| 22 | CLA | C | 512 | - | 59,73,73 | 1.58 | 8 (13%) | 67,113,113 | 1.45 | 10 (14%) |
| 26 | LHG | d | 407 | - | 38,38,48 | 1.03 | 2 (5%) | 41,44,54 | 1.14 | 2 (4%) |
| 31 | STE | B | 624 | - | 15,15,19 | 0.56 | 0 | 14,14,19 | 0.51 | 0 |
| 26 | LHG | A | 412 | - | 48,48,48 | 0.84 | 2 (4%) | 51,54,54 | 1.17 | 5 (9%) |
| 22 | CLA | b | 615 | - | 59,73,73 | 1.52 | 7 (11%) | 67,113,113 | 1.46 | 12 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | BCR | b | 617 | - | 41,41,41 | 0.98 | 3 (7%) | 56,56,56 | 1.30 | 8 (14%) |
| 27 | SQD | A | 413 | - | 38,38,54 | 1.09 | 4 (10%) | 40,40,65 | 1.43 | 4 (10%) |
| 22 | CLA | B | 613 | - | 59,73,73 | 1.67 | 7 (11%) | 67,113,113 | 1.64 | 16 (23%) |
| 23 | BCR | h | 101 | - | 41,41,41 | 0.97 | 2 (4%) | 56,56,56 | 1.36 | 10 (17%) |
| 27 | SQD | a | 413 | - | 53,54,54 | 0.94 | 4 (7%) | 62,65,65 | 1.94 | 12 (19%) |
| 26 | LHG | L | 102 | - | 48,48,48 | 0.75 | 2 (4%) | 51,54,54 | 1.15 | 2 (3%) |
| 35 | HEC | f | 101 | 5,6 | 26,50,50 | 2.33 | 3 (11%) | 18,82,82 | 2.54 | 4 (22%) |
| 32 | LMG | Y | 101 | - | 48,48,55 | 1.20 | 5 (10%) | 56,56,63 | 1.21 | 5 (8%) |
| 31 | STE | D | 413 | - | 16,19,19 | 0.38 | 0 | 15,19,19 | 0.94 | 0 |
| 27 | SQD | L | 101 | - | 48,49,54 | 0.95 | 2 (4%) | 57,60,65 | 2.50 | 18 (31%) |
| 22 | CLA | B | 605 | - | 59,73,73 | 1.31 | 6 (10%) | 67,113,113 | 1.43 | 13 (19%) |
| 22 | CLA | D | 405 | - | 59,73,73 | 1.20 | 5 (8%) | 67,113,113 | 1.50 | 11 (16%) |
| 22 | CLA | b | 607 | 36 | 59,73,73 | 1.48 | 4 (6%) | 67,113,113 | 1.64 | 12 (17%) |
| 32 | LMG | a | 417 | - | 55,55,55 | 1.57 | 10 (18%) | 63,63,63 | 1.50 | 12 (19%) |
| 22 | CLA | b | 612 | - | 59,73,73 | 1.33 | 5 (8%) | 67,113,113 | 1.86 | 13 (19%) |
| 22 | CLA | C | 504 | 36 | 53,67,73 | 1.63 | 6 (11%) | 59,105,113 | 1.44 | 9 (15%) |
| 32 | LMG | m | 101 | - | 51,51,55 | 1.14 | 4 (7%) | 59,59,63 | 1.59 | 9 (15%) |
| 22 | CLA | b | 613 | - | 59,73,73 | 1.57 | 7 (11%) | 67,113,113 | 1.43 | 10 (14%) |
| 31 | STE | c | 521 | - | 16,19,19 | 0.52 | 0 | 15,19,19 | 0.51 | 0 |
| 23 | BCR | c | 515 | - | 41,41,41 | 1.00 | 3 (7%) | 56,56,56 | 1.28 | 9 (16%) |
| 22 | CLA | B | 603 | - | 59,73,73 | 1.27 | 7 (11%) | 67,113,113 | 1.57 | 13 (19%) |
| 22 | CLA | C | 511 | 3 | 59,73,73 | 1.71 | 9 (15%) | 67,113,113 | 1.36 | 7 (10%) |
| 31 | STE | H | 103 | - | 17,17,19 | 0.47 | 0 | 16,16,19 | 0.69 | 0 |
| 23 | BCR | T | 101 | - | 41,41,41 | 1.05 | 3 (7%) | 56,56,56 | 1.22 | 3 (5%) |
| 22 | CLA | a | 402 | - | 59,73,73 | 1.61 | 5 (8%) | 67,113,113 | 1.35 | 13 (19%) |
| 22 | CLA | C | 505 | - | 59,73,73 | 1.66 | 7 (11%) | 67,113,113 | 1.56 | 11 (16%) |
| 22 | CLA | b | 605 | - | 59,73,73 | 1.35 | 6 (10%) | 67,113,113 | 1.74 | 11 (16%) |
| 31 | STE | Z | 101 | - | 7,7,19 | 0.50 | 0 | 6,6,19 | 0.33 | 0 |
| 26 | LHG | a | 412 | - | 48,48,48 | 1.07 | 5 (10%) | 51,54,54 | 1.42 | 9 (17%) |
| 22 | CLA | B | 615 | - | 59,73,73 | 1.69 | 7 (11%) | 67,113,113 | 1.69 | 8 (11%) |
| 28 | DGD | c | 518 | - | 63,63,67 | 1.08 | 3 (4%) | 77,77,81 | 1.23 | 5 (6%) |
| 23 | BCR | B | 617 | - | 41,41,41 | 1.05 | 2 (4%) | 56,56,56 | 1.55 | 11 (19%) |
| 31 | STE | a | 416 | - | 8,11,19 | 0.45 | 0 | 7,11,19 | 0.74 | 0 |
| 28 | DGD | c | 519 | - | 63,63,67 | 1.10 | 4 (6%) | 77,77,81 | 1.38 | 13 (16%) |
| 28 | DGD | C | 517 | - | 63,63,67 | 1.39 | 9 (14%) | 77,77,81 | 1.39 | 12 (15%) |
| 22 | CLA | d | 403 | - | 59,73,73 | 1.64 | 9 (15%) | 67,113,113 | 1.22 | 4 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | LHG | A | 410 | - | 46,46,48 | 1.19 | 5 (10%) | 49,52,54 | 1.16 | 4 (8%) |
| 31 | STE | L | 103 | - | 8,11,19 | 0.51 | 0 | 7,11,19 | 0.73 | 0 |
| 30 | OEY | a | 419[B] | 1,3,36 | 0,16,16 | 0.00 | - | - | | |
| 34 | BCT | a | 409 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 33 | PHO | D | 401 | - | 67,69,69 | 1.20 | 11 (16%) | 85,99,99 | 1.13 | 8 (9%) |
| 32 | LMG | c | 522 | - | 48,48,55 | 1.19 | 4 (8%) | 56,56,63 | 1.25 | 6 (10%) |
| 22 | CLA | A | 403 | 36 | 59,73,73 | 1.56 | 7 (11%) | 67,113,113 | 1.48 | 10 (14%) |
| 22 | CLA | A | 409 | 36 | 59,73,73 | 1.30 | 5 (8%) | 67,113,113 | 1.47 | 10 (14%) |
| 22 | CLA | a | 405 | - | 59,73,73 | 1.44 | 8 (13%) | 67,113,113 | 1.34 | 10 (14%) |
| 31 | STE | B | 623 | - | 14,17,19 | 0.47 | 0 | 13,17,19 | 0.77 | 0 |
| 32 | LMG | D | 408 | - | 51,51,55 | 0.99 | 3 (5%) | 59,59,63 | 1.47 | 7 (11%) |
| 22 | CLA | B | 607 | 36 | 59,73,73 | 1.45 | 8 (13%) | 67,113,113 | 1.65 | 11 (16%) |
| 22 | CLA | B | 608 | - | 59,73,73 | 1.52 | 11 (18%) | 67,113,113 | 1.73 | 12 (17%) |
| 26 | LHG | e | 101 | - | 41,41,48 | 1.11 | 4 (9%) | 44,47,54 | 1.24 | 3 (6%) |
| 23 | BCR | k | 102 | - | 41,41,41 | 1.02 | 3 (7%) | 56,56,56 | 1.17 | 6 (10%) |
| 22 | CLA | C | 502 | - | 59,73,73 | 1.42 | 6 (10%) | 67,113,113 | 1.44 | 10 (14%) |
| 31 | STE | M | 102 | - | 11,14,19 | 0.54 | 0 | 10,14,19 | 0.57 | 0 |
| 27 | SQD | A | 411 | - | 51,52,54 | 1.09 | 5 (9%) | 60,63,65 | 2.18 | 15 (25%) |
| 33 | PHO | D | 402 | - | 67,69,69 | 1.25 | 9 (13%) | 85,99,99 | 1.14 | 8 (9%) |
| 22 | CLA | D | 404 | - | 59,73,73 | 1.49 | 7 (11%) | 67,113,113 | 1.57 | 11 (16%) |
| 22 | CLA | A | 404 | - | 48,62,73 | 1.41 | 10 (20%) | 53,99,113 | 1.57 | 7 (13%) |
| 34 | BCT | D | 403 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 31 | STE | d | 412 | - | 16,19,19 | 0.43 | 0 | 15,19,19 | 0.62 | 0 |
| 23 | BCR | B | 619 | - | 41,41,41 | 1.08 | 3 (7%) | 56,56,56 | 1.55 | 13 (23%) |
| 31 | STE | d | 411 | - | 16,19,19 | 0.44 | 0 | 15,19,19 | 0.67 | 0 |
| 22 | CLA | c | 507 | - | 59,73,73 | 1.33 | 7 (11%) | 67,113,113 | 1.50 | 11 (16%) |
| 32 | LMG | D | 411 | - | 20,26,55 | 0.83 | 0 | 18,26,63 | 1.05 | 0 |
| 26 | LHG | l | 101 | - | 48,48,48 | 0.79 | 1 (2%) | 51,54,54 | 1.25 | 6 (11%) |
| 23 | BCR | C | 514 | - | 41,41,41 | 1.25 | 4 (9%) | 56,56,56 | 1.30 | 5 (8%) |
| 22 | CLA | B | 611 | - | 59,73,73 | 1.41 | 8 (13%) | 67,113,113 | 1.44 | 10 (14%) |
| 22 | CLA | b | 601 | 36 | 59,73,73 | 1.64 | 7 (11%) | 67,113,113 | 1.70 | 9 (13%) |
| 31 | STE | J | 101 | - | 8,11,19 | 0.33 | 0 | 7,11,19 | 0.77 | 0 |
| 31 | STE | B | 601 | - | 8,11,19 | 0.38 | 0 | 7,11,19 | 0.70 | 0 |
| 30 | OEY | A | 416[B] | 1,3,36 | 0,16,16 | 0.00 | - | - | | |
| 32 | LMG | M | 101 | - | 51,51,55 | 0.86 | 1 (1%) | 59,59,63 | 1.37 | 11 (18%) |
| 23 | BCR | C | 515 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.36 | 8 (14%) |
| 23 | BCR | K | 101 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.31 | 9 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | b | 603 | - | 59,73,73 | 1.62 | 10 (16%) | 67,113,113 | 1.58 | 11 (16%) |
| 31 | STE | h | 103 | - | 13,13,19 | 0.43 | 0 | 12,12,19 | 0.61 | 0 |
| 31 | STE | B | 622 | - | 8,11,19 | 0.49 | 0 | 7,11,19 | 0.78 | 0 |
| 22 | CLA | b | 614 | - | 59,73,73 | 1.40 | 10 (16%) | 67,113,113 | 1.39 | 7 (10%) |
| 22 | CLA | c | 512 | 3 | 59,73,73 | 1.65 | 6 (10%) | 67,113,113 | 1.51 | 6 (8%) |
| 23 | BCR | a | 406 | - | 41,41,41 | 1.03 | 3 (7%) | 56,56,56 | 1.35 | 5 (8%) |
| 22 | CLA | C | 501 | - | 59,73,73 | 1.66 | 8 (13%) | 67,113,113 | 1.35 | 9 (13%) |
| 22 | CLA | b | 604 | - | 59,73,73 | 1.50 | 5 (8%) | 67,113,113 | 2.19 | 17 (25%) |
| 23 | BCR | A | 405 | - | 41,41,41 | 1.16 | 1 (2%) | 56,56,56 | 1.42 | 10 (17%) |
| 22 | CLA | a | 403 | 36 | 59,73,73 | 1.43 | 9 (15%) | 67,113,113 | 1.69 | 11 (16%) |
| 22 | CLA | c | 510 | - | 59,73,73 | 1.42 | 6 (10%) | 67,113,113 | 1.77 | 11 (16%) |
| 27 | SQD | B | 621 | - | 53,54,54 | 0.94 | 2 (3%) | 62,65,65 | 2.19 | 16 (25%) |
| 22 | CLA | c | 502 | - | 59,73,73 | 1.33 | 7 (11%) | 67,113,113 | 1.51 | 13 (19%) |
| 29 | OEX | a | 418[A] | 1,3,36 | 0,15,15 | 0.00 | - | - | - | - |
| 25 | PL9 | d | 405 | - | 55,55,55 | 1.47 | 7 (12%) | 68,69,69 | 1.62 | 11 (16%) |
| 22 | CLA | B | 602 | - | 59,73,73 | 1.51 | 6 (10%) | 67,113,113 | 1.70 | 13 (19%) |
| 28 | DGD | A | 414 | - | 67,67,67 | 1.41 | 9 (13%) | 81,81,81 | 1.41 | 13 (16%) |
| 31 | STE | C | 522 | - | 8,11,19 | 0.49 | 0 | 7,11,19 | 0.87 | 0 |
| 22 | CLA | B | 612 | - | 59,73,73 | 1.43 | 7 (11%) | 67,113,113 | 1.54 | 7 (10%) |
| 22 | CLA | c | 504 | - | 59,73,73 | 1.44 | 8 (13%) | 67,113,113 | 1.35 | 4 (5%) |
| 22 | CLA | B | 609 | - | 59,73,73 | 1.50 | 7 (11%) | 67,113,113 | 1.87 | 9 (13%) |
| 25 | PL9 | D | 407 | - | 55,55,55 | 1.18 | 3 (5%) | 68,69,69 | 1.88 | 18 (26%) |
| 32 | LMG | D | 410 | - | 31,31,55 | 1.23 | 4 (12%) | 33,33,63 | 1.14 | 3 (9%) |
| 23 | BCR | D | 406 | - | 41,41,41 | 1.14 | 2 (4%) | 56,56,56 | 1.28 | 8 (14%) |
| 22 | CLA | H | 101 | 36 | 59,73,73 | 1.68 | 8 (13%) | 67,113,113 | 1.42 | 8 (11%) |
| 26 | LHG | d | 406 | - | 48,48,48 | 0.79 | 2 (4%) | 51,54,54 | 1.16 | 1 (1%) |
| 31 | STE | b | 623 | - | 16,19,19 | 0.60 | 0 | 15,19,19 | 0.58 | 0 |
| 31 | STE | d | 410 | - | 13,16,19 | 0.34 | 0 | 12,16,19 | 1.00 | 0 |
| 32 | LMG | c | 520 | - | 37,37,55 | 1.13 | 4 (10%) | 45,45,63 | 1.36 | 7 (15%) |
| 31 | STE | t | 102 | - | 10,13,19 | 0.53 | 0 | 9,13,19 | 0.69 | 0 |
| 31 | STE | b | 624 | - | 9,9,19 | 0.46 | 0 | 8,8,19 | 0.48 | 0 |
| 22 | CLA | C | 509 | - | 59,73,73 | 1.46 | 8 (13%) | 67,113,113 | 1.53 | 10 (14%) |
| 22 | CLA | b | 609 | - | 59,73,73 | 1.80 | 8 (13%) | 67,113,113 | 1.66 | 14 (20%) |
| 28 | DGD | c | 517 | - | 63,63,67 | 1.35 | 8 (12%) | 77,77,81 | 1.42 | 13 (16%) |

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 |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | LMG | b | 621 | - | - | 25/50/70/70 | 0/1/1/1 |
| 22 | CLA | c | 514 | - | 3/3/25/25 | 9/37/135/135 | - |
| 26 | LHG | D | 412 | - | - | 15/53/53/53 | - |
| 23 | BCR | b | 618 | - | - | 4/29/63/63 | 0/2/2/2 |
| 27 | SQD | F | 102 | - | - | 15/28/48/69 | 0/1/1/1 |
| 31 | STE | a | 415 | - | - | 3/7/7/17 | - |
| 28 | DGD | H | 102 | - | - | 17/51/91/95 | 0/2/2/2 |
| 22 | CLA | B | 604 | - | 3/3/25/25 | 10/37/135/135 | - |
| 31 | STE | b | 620 | - | - | 8/15/17/17 | - |
| 33 | PHO | a | 404 | - | - | 8/53/103/103 | 0/5/6/6 |
| 22 | CLA | c | 513 | - | 3/3/25/25 | 18/37/135/135 | - |
| 22 | CLA | B | 616 | - | 3/3/24/25 | 8/31/129/135 | - |
| 31 | STE | C | 521 | - | - | 6/13/13/17 | - |
| 22 | CLA | c | 506 | - | 2/2/25/25 | 12/37/135/135 | - |
| 23 | BCR | t | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 402 | - | 3/3/25/25 | 8/37/135/135 | - |
| 23 | BCR | X | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 31 | STE | R | 101 | - | - | 3/7/9/17 | - |
| 23 | BCR | c | 516 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | BCR | d | 404 | - | - | 5/29/63/63 | 0/2/2/2 |
| 32 | LMG | C | 516 | - | - | 16/43/63/70 | 0/1/1/1 |
| 31 | STE | T | 103 | - | - | 8/12/12/17 | - |
| 31 | STE | M | 104 | - | - | 7/15/15/17 | - |
| 22 | CLA | C | 506 | - | 3/3/25/25 | 13/37/135/135 | - |
| 23 | BCR | K | 102 | - | - | 11/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 508 | 36 | 3/3/25/25 | 12/37/135/135 | - |
| 25 | PL9 | A | 408 | - | - | 21/53/73/73 | 0/1/1/1 |
| 31 | STE | c | 501 | - | - | 5/7/9/17 | - |
| 31 | STE | T | 102 | - | - | 10/13/13/17 | - |
| 22 | CLA | c | 509 | - | 3/3/24/25 | 5/36/134/135 | - |
| 35 | HEC | F | 101 | 5,6 | - | 0/6/54/54 | - |
| 26 | LHG | D | 409 | - | - | 22/53/53/53 | - |
| 22 | CLA | C | 510 | - | 3/3/25/25 | 6/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 33 | PHO | d | 401 | - | - | 9/53/103/103 | 0/5/6/6 |
| 22 | CLA | c | 511 | - | 3/3/25/25 | 11/37/135/135 | - |
| 22 | CLA | C | 503 | - | 3/3/25/25 | 3/37/135/135 | - |
| 22 | CLA | C | 508 | - | 2/2/25/25 | 8/37/135/135 | - |
| 22 | CLA | b | 610 | 36 | 3/3/25/25 | 5/37/135/135 | - |
| 23 | BCR | B | 618 | - | - | 4/29/63/63 | 0/2/2/2 |
| 35 | HEC | v | 201 | 17 | - | 0/6/54/54 | - |
| 22 | CLA | b | 602 | - | 1/1/25/25 | 6/37/135/135 | - |
| 22 | CLA | c | 505 | 36 | 3/3/24/25 | 5/31/129/135 | - |
| 27 | SQD | a | 414 | - | - | 16/37/37/69 | - |
| 28 | DGD | h | 102 | - | - | 15/51/91/95 | 0/2/2/2 |
| 31 | STE | I | 101 | - | - | 4/12/12/17 | - |
| 31 | STE | B | 620 | - | - | 9/12/14/17 | - |
| 31 | STE | M | 102 | - | - | 8/10/12/17 | - |
| 32 | LMG | c | 523 | - | - | 22/44/64/70 | 0/1/1/1 |
| 27 | SQD | a | 413 | - | - | 25/49/69/69 | 0/1/1/1 |
| 32 | LMG | d | 408 | - | - | 11/39/59/70 | 0/1/1/1 |
| 22 | CLA | b | 608 | - | 2/2/25/25 | 7/37/135/135 | - |
| 31 | STE | B | 625 | - | - | 7/12/12/17 | - |
| 22 | CLA | B | 606 | - | 3/3/25/25 | 10/37/135/135 | - |
| 22 | CLA | B | 614 | - | 3/3/25/25 | 14/37/135/135 | - |
| 31 | STE | C | 520 | - | - | 3/7/9/17 | - |
| 27 | SQD | d | 409 | - | - | 13/36/56/69 | 0/1/1/1 |
| 28 | DGD | C | 518 | - | - | 22/51/91/95 | 0/2/2/2 |
| 28 | DGD | C | 519 | - | - | 18/51/91/95 | 0/2/2/2 |
| 23 | BCR | b | 619 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 507 | 36 | 3/3/25/25 | 5/37/135/135 | - |
| 22 | CLA | b | 606 | - | 3/3/25/25 | 4/37/135/135 | - |
| 22 | CLA | b | 611 | - | 3/3/25/25 | 8/37/135/135 | - |
| 31 | STE | j | 101 | - | - | 4/7/9/17 | - |
| 22 | CLA | C | 513 | - | 3/3/25/25 | 10/37/135/135 | - |
| 22 | CLA | b | 616 | - | 3/3/24/25 | 5/31/129/135 | - |
| 35 | HEC | V | 201 | 17 | - | 0/6/54/54 | - |
| 31 | STE | M | 103 | - | - | 2/7/7/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | BCR | k | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 503 | - | 2/2/25/25 | 8/37/135/135 | - |
| 22 | CLA | B | 610 | 36 | 3/3/25/25 | 5/37/135/135 | - |
| 31 | STE | b | 622 | - | - | 4/11/13/17 | - |
| 22 | CLA | a | 411 | 36 | 2/2/25/25 | 5/37/135/135 | - |
| 22 | CLA | C | 512 | - | 3/3/25/25 | 10/37/135/135 | - |
| 26 | LHG | d | 407 | - | - | 15/43/43/53 | - |
| 31 | STE | B | 624 | - | - | 10/13/13/17 | - |
| 26 | LHG | A | 412 | - | - | 28/53/53/53 | - |
| 22 | CLA | b | 615 | - | 3/3/25/25 | 3/37/135/135 | - |
| 23 | BCR | b | 617 | - | - | 6/29/63/63 | 0/2/2/2 |
| 27 | SQD | A | 413 | - | - | 18/39/39/69 | - |
| 22 | CLA | B | 613 | - | 3/3/25/25 | 12/37/135/135 | - |
| 23 | BCR | h | 101 | - | - | 8/29/63/63 | 0/2/2/2 |
| 25 | PL9 | a | 410 | - | - | 19/53/73/73 | 0/1/1/1 |
| 26 | LHG | L | 102 | - | - | 17/53/53/53 | - |
| 32 | LMG | Y | 101 | - | - | 22/43/63/70 | 0/1/1/1 |
| 31 | STE | D | 413 | - | - | 12/15/17/17 | - |
| 27 | SQD | L | 101 | - | - | 18/44/64/69 | 0/1/1/1 |
| 22 | CLA | B | 605 | - | 2/2/25/25 | 14/37/135/135 | - |
| 22 | CLA | D | 405 | - | 3/3/25/25 | 13/37/135/135 | - |
| 23 | BCR | B | 619 | - | - | 7/29/63/63 | 0/2/2/2 |
| 32 | LMG | a | 417 | - | - | 30/50/70/70 | 0/1/1/1 |
| 22 | CLA | b | 612 | - | 3/3/25/25 | 4/37/135/135 | - |
| 22 | CLA | C | 504 | 36 | 3/3/23/25 | 7/30/128/135 | - |
| 32 | LMG | m | 101 | - | - | 20/46/66/70 | 0/1/1/1 |
| 22 | CLA | b | 613 | - | 3/3/25/25 | 8/37/135/135 | - |
| 31 | STE | c | 521 | - | - | 8/15/17/17 | - |
| 23 | BCR | c | 515 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 603 | - | 3/3/25/25 | 12/37/135/135 | - |
| 22 | CLA | C | 511 | 3 | 3/3/25/25 | 8/37/135/135 | - |
| 31 | STE | H | 103 | - | - | 8/15/15/17 | - |
| 23 | BCR | T | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 22 | CLA | a | 402 | - | 3/3/25/25 | 5/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | C | 505 | - | 1/1/25/25 | 8/37/135/135 | - |
| 22 | CLA | b | 605 | - | 3/3/25/25 | 7/37/135/135 | - |
| 31 | STE | Z | 101 | - | - | 2/5/5/17 | - |
| 26 | LHG | a | 412 | - | - | 20/53/53/53 | - |
| 22 | CLA | B | 615 | - | 3/3/25/25 | 7/37/135/135 | - |
| 28 | DGD | c | 518 | - | - | 18/51/91/95 | 0/2/2/2 |
| 23 | BCR | B | 617 | - | - | 9/29/63/63 | 0/2/2/2 |
| 31 | STE | a | 416 | - | - | 4/7/9/17 | - |
| 28 | DGD | c | 519 | - | - | 18/51/91/95 | 0/2/2/2 |
| 28 | DGD | C | 517 | - | - | 18/51/91/95 | 0/2/2/2 |
| 22 | CLA | d | 403 | - | 2/2/25/25 | 6/37/135/135 | - |
| 26 | LHG | A | 410 | - | - | 23/51/51/53 | - |
| 31 | STE | L | 103 | - | - | 4/7/9/17 | - |
| 33 | PHO | D | 401 | - | - | 5/53/103/103 | 0/5/6/6 |
| 32 | LMG | c | 522 | - | - | 25/43/63/70 | 0/1/1/1 |
| 22 | CLA | A | 403 | 36 | 3/3/25/25 | 11/37/135/135 | - |
| 22 | CLA | A | 409 | 36 | 3/3/25/25 | 7/37/135/135 | - |
| 22 | CLA | a | 405 | - | 3/3/25/25 | 12/37/135/135 | - |
| 31 | STE | B | 623 | - | - | 8/13/15/17 | - |
| 32 | LMG | D | 408 | - | - | 15/46/66/70 | 0/1/1/1 |
| 22 | CLA | B | 607 | 36 | 3/3/25/25 | 14/37/135/135 | - |
| 22 | CLA | B | 608 | - | 3/3/25/25 | 3/37/135/135 | - |
| 26 | LHG | e | 101 | - | - | 24/46/46/53 | - |
| 23 | BCR | k | 102 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 502 | - | 3/3/25/25 | 8/37/135/135 | - |
| 22 | CLA | d | 402 | - | 1/1/25/25 | 6/37/135/135 | - |
| 27 | SQD | A | 411 | - | - | 24/47/67/69 | 0/1/1/1 |
| 33 | PHO | D | 402 | - | - | 4/53/103/103 | 0/5/6/6 |
| 22 | CLA | D | 404 | - | 1/1/25/25 | 8/37/135/135 | - |
| 22 | CLA | A | 404 | - | 3/3/22/25 | 1/24/122/135 | - |
| 35 | HEC | f | 101 | 5,6 | - | 0/6/54/54 | - |
| 31 | STE | d | 412 | - | - | 9/15/17/17 | - |
| 22 | CLA | b | 607 | 36 | 3/3/25/25 | 12/37/135/135 | - |
| 31 | STE | d | 411 | - | - | 9/15/17/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | c | 507 | - | 3/3/25/25 | 14/37/135/135 | - |
| 32 | LMG | D | 411 | - | - | 8/18/22/70 | - |
| 26 | LHG | l | 101 | - | - | 15/53/53/53 | - |
| 23 | BCR | C | 514 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 611 | - | 3/3/25/25 | 4/37/135/135 | - |
| 22 | CLA | b | 601 | 36 | 2/2/25/25 | 21/37/135/135 | - |
| 31 | STE | J | 101 | - | - | 2/7/9/17 | - |
| 31 | STE | B | 601 | - | - | 5/7/9/17 | - |
| 32 | LMG | M | 101 | - | - | 25/46/66/70 | 0/1/1/1 |
| 23 | BCR | C | 515 | - | - | 11/29/63/63 | 0/2/2/2 |
| 23 | BCR | K | 101 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | b | 603 | - | 3/3/25/25 | 4/37/135/135 | - |
| 31 | STE | h | 103 | - | - | 6/11/11/17 | - |
| 31 | STE | B | 622 | - | - | 5/7/9/17 | - |
| 22 | CLA | b | 614 | - | 3/3/25/25 | 17/37/135/135 | - |
| 22 | CLA | c | 512 | 3 | 3/3/25/25 | 3/37/135/135 | - |
| 23 | BCR | a | 406 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 501 | - | 3/3/25/25 | 2/37/135/135 | - |
| 22 | CLA | b | 604 | - | 3/3/25/25 | 10/37/135/135 | - |
| 23 | BCR | A | 405 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | a | 403 | 36 | 2/2/25/25 | 10/37/135/135 | - |
| 22 | CLA | c | 510 | - | 3/3/25/25 | 11/37/135/135 | - |
| 27 | SQD | B | 621 | - | - | 24/49/69/69 | 0/1/1/1 |
| 22 | CLA | c | 502 | - | 3/3/25/25 | 5/37/135/135 | - |
| 25 | PL9 | d | 405 | - | - | 17/53/73/73 | 0/1/1/1 |
| 22 | CLA | B | 602 | - | 3/3/25/25 | 9/37/135/135 | - |
| 28 | DGD | A | 414 | - | - | 27/55/95/95 | 0/2/2/2 |
| 31 | STE | C | 522 | - | - | 1/7/9/17 | - |
| 22 | CLA | B | 612 | - | 3/3/25/25 | 8/37/135/135 | - |
| 22 | CLA | c | 504 | - | 3/3/25/25 | 7/37/135/135 | - |
| 22 | CLA | B | 609 | - | 1/1/25/25 | 2/37/135/135 | - |
| 25 | PL9 | D | 407 | - | - | 12/53/73/73 | 0/1/1/1 |
| 32 | LMG | D | 410 | - | - | 13/33/33/70 | - |
| 23 | BCR | D | 406 | - | - | 4/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | H | 101 | 36 | 3/3/25/25 | 18/37/135/135 | - |
| 26 | LHG | d | 406 | - | - | 23/53/53/53 | - |
| 31 | STE | b | 623 | - | - | 9/15/17/17 | - |
| 31 | STE | d | 410 | - | - | 9/12/14/17 | - |
| 32 | LMG | c | 520 | - | - | 7/31/51/70 | 0/1/1/1 |
| 31 | STE | t | 102 | - | - | 4/9/11/17 | - |
| 31 | STE | b | 624 | - | - | 2/7/7/17 | - |
| 22 | CLA | C | 509 | - | 3/3/25/25 | 11/37/135/135 | - |
| 22 | CLA | b | 609 | - | 1/1/25/25 | 8/37/135/135 | - |
| 28 | DGD | c | 517 | - | - | 28/51/91/95 | 0/2/2/2 |

The worst 5 of 804 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 22 | H | 101 | CLA | C4B-NB | 8.96 | 1.43 | 1.35 |
| 22 | B | 613 | CLA | C4B-NB | 8.96 | 1.43 | 1.35 |
| 22 | C | 503 | CLA | C4B-NB | 8.41 | 1.42 | 1.35 |
| 22 | A | 403 | CLA | C4B-NB | 8.23 | 1.42 | 1.35 |
| 22 | b | 604 | CLA | C4B-NB | 8.15 | 1.42 | 1.35 |

The worst 5 of 1359 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22 | B | 604 | CLA | C4A-NA-C1A | 11.79 | 112.01 | 106.71 |
| 27 | L | 101 | SQD | O6-C1-C2 | 11.45 | 126.19 | 108.30 |
| 22 | b | 604 | CLA | C4A-NA-C1A | 10.51 | 111.43 | 106.71 |
| 22 | B | 615 | CLA | C4A-NA-C1A | 9.02 | 110.76 | 106.71 |
| 22 | B | 607 | CLA | C4A-NA-C1A | 8.90 | 110.71 | 106.71 |

5 of 189 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | c | 514 | CLA | NC |
| 22 | c | 514 | CLA | ND |
| 22 | c | 514 | CLA | NA |
| 22 | B | 604 | CLA | NC |
| 22 | B | 604 | CLA | ND |

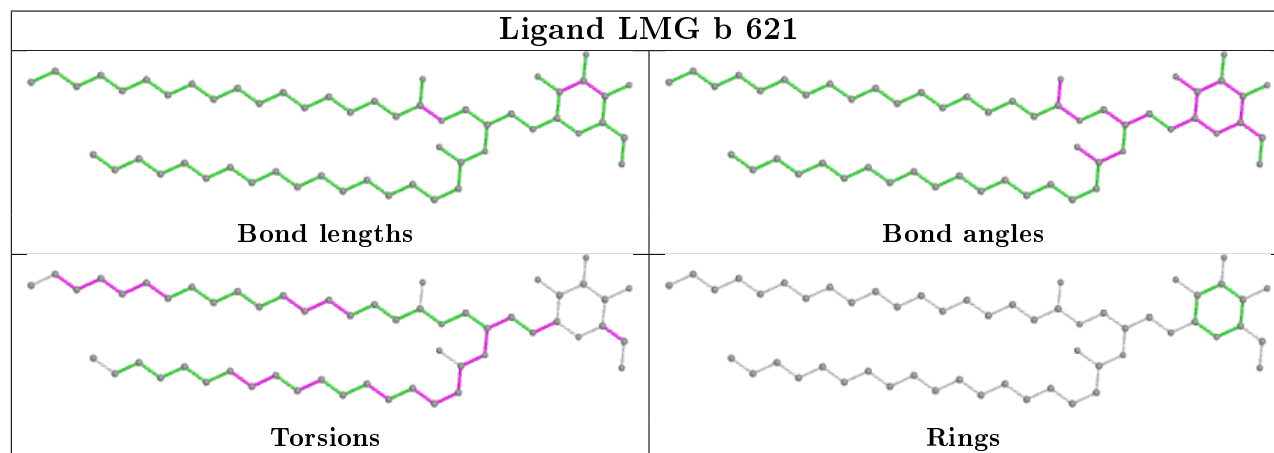
5 of 1829 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 32 | b | 621 | LMG | C2-C1-O1-C7 |
| 32 | b | 621 | LMG | O6-C1-O1-C7 |
| 26 | D | 412 | LHG | C1-C2-C3-O3 |
| 26 | D | 412 | LHG | C3-O3-P-O4 |
| 26 | D | 412 | LHG | C3-O3-P-O5 |

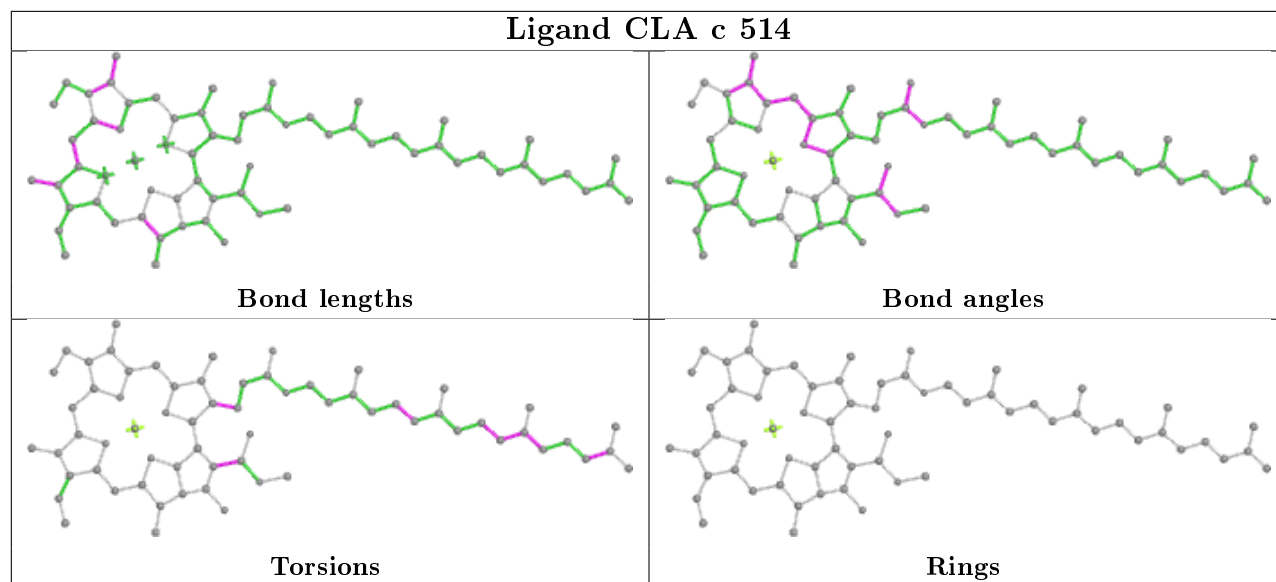
There are no ring outliers.

No monomer is involved in short contacts.

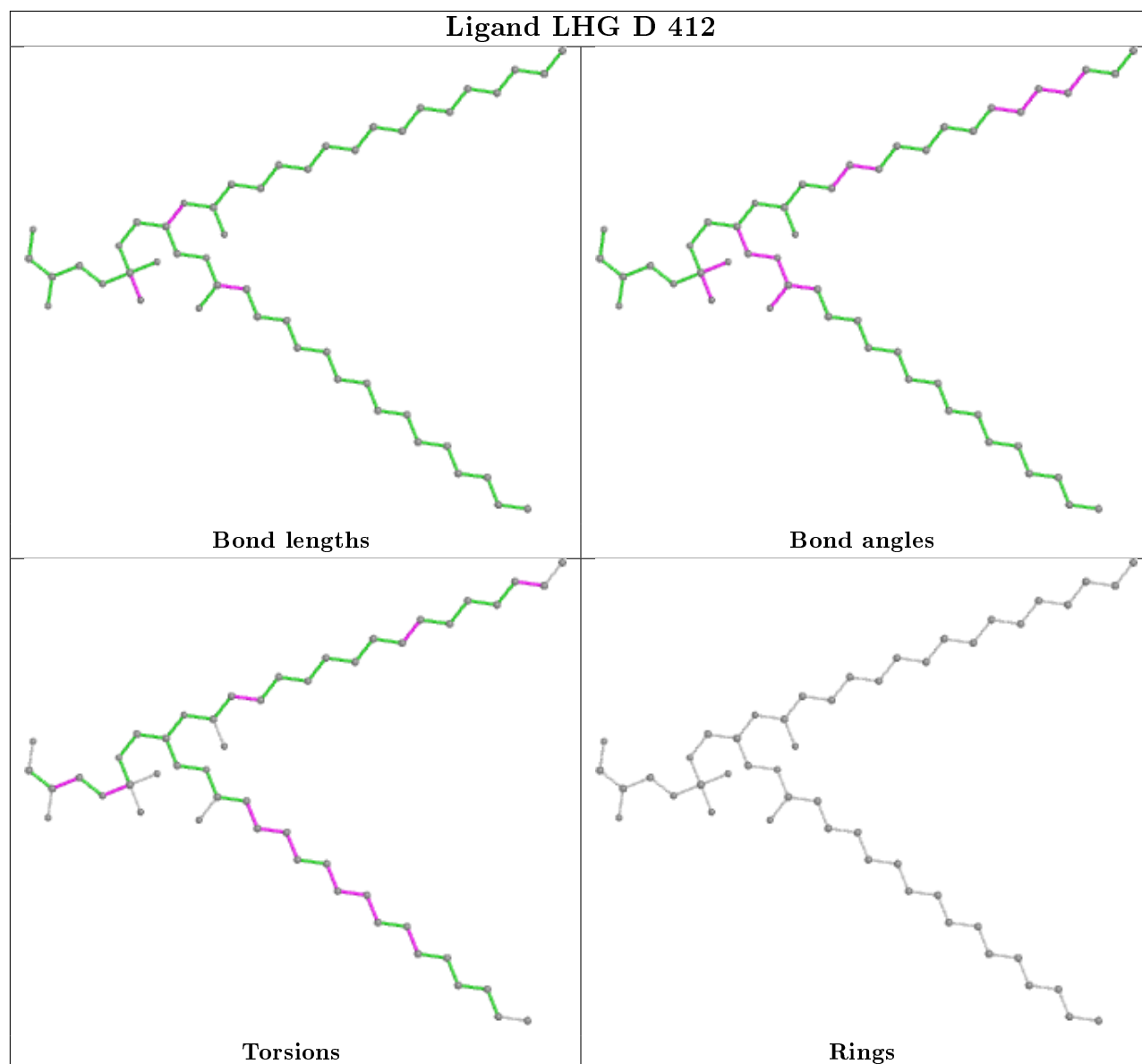
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

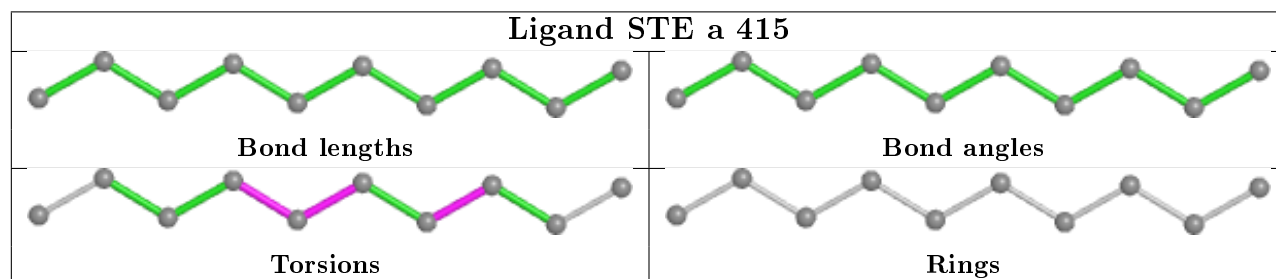
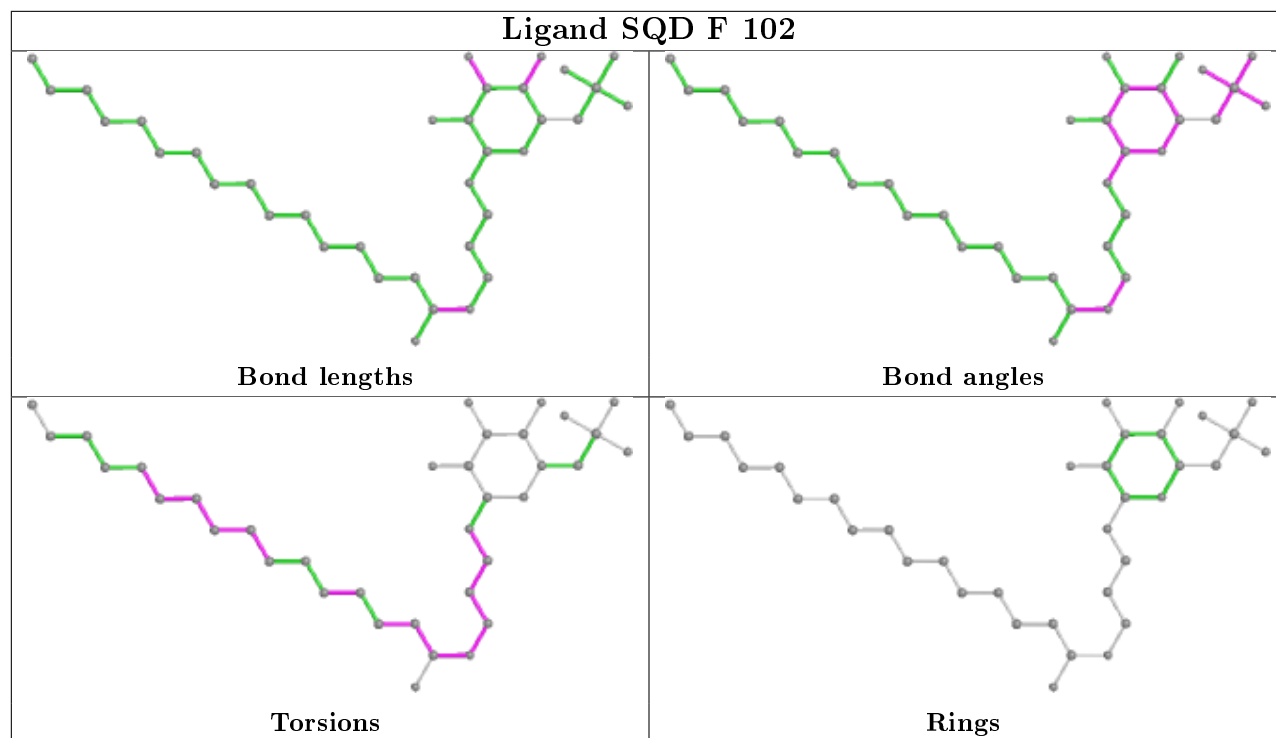
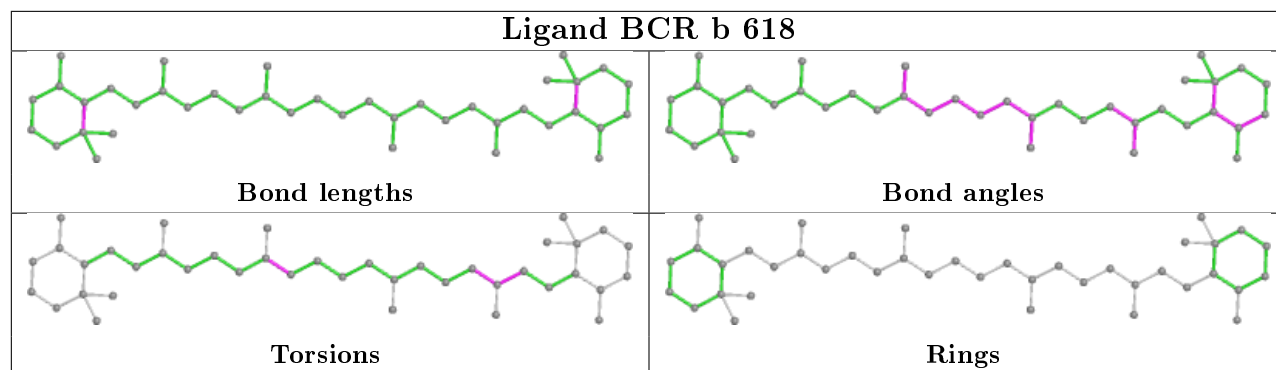


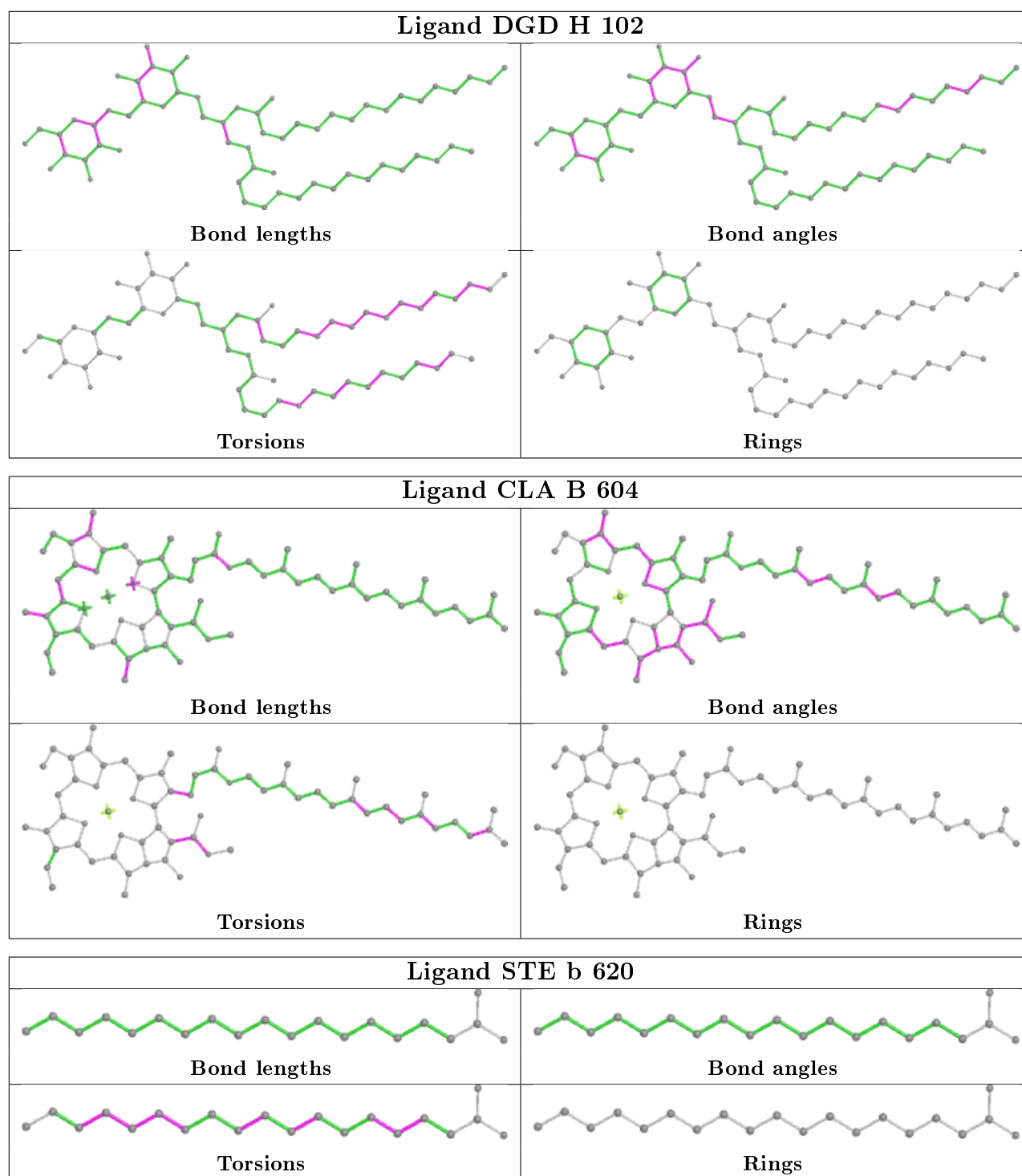
Ligand CLA c 514

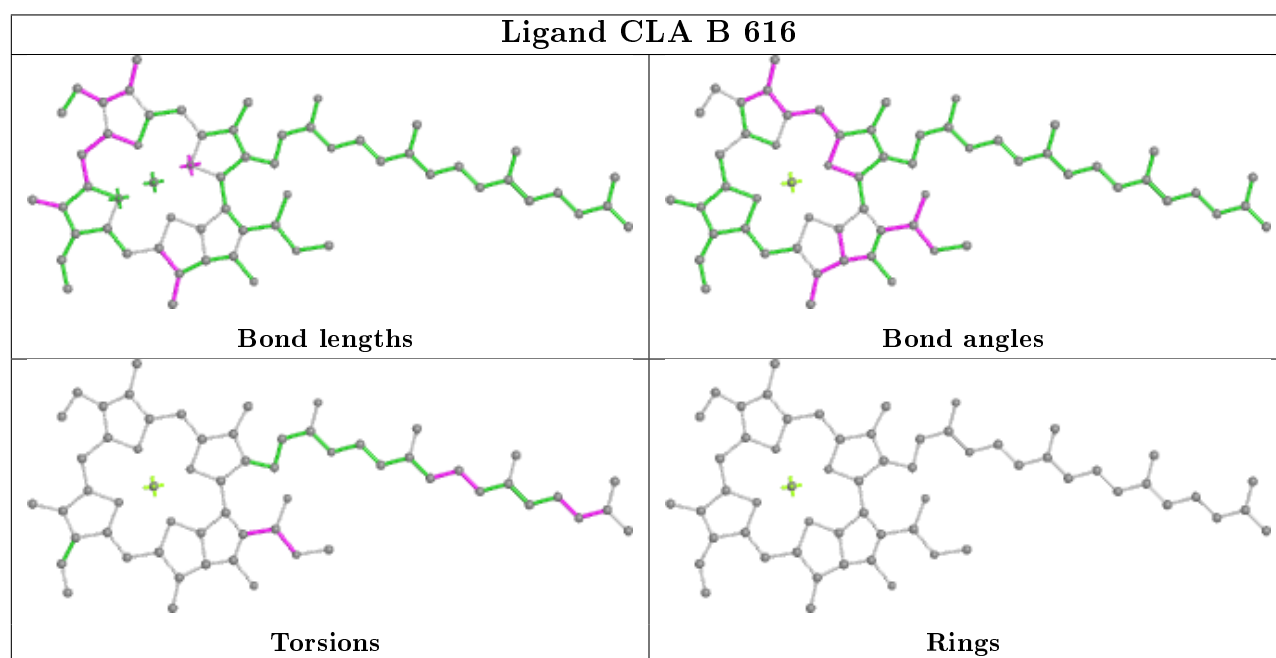
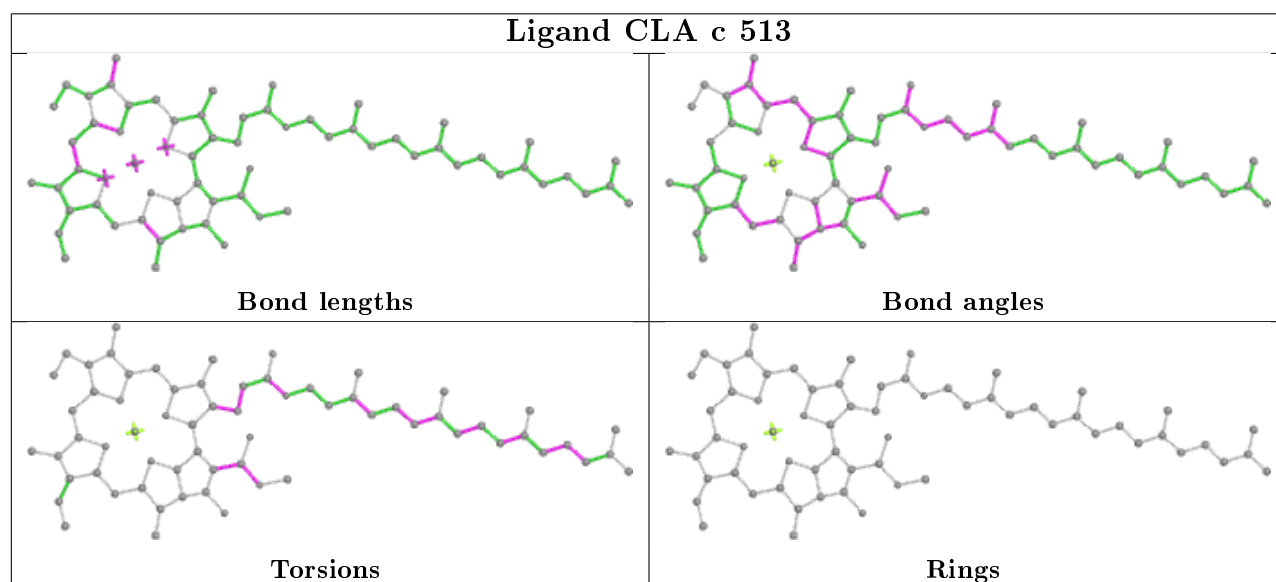
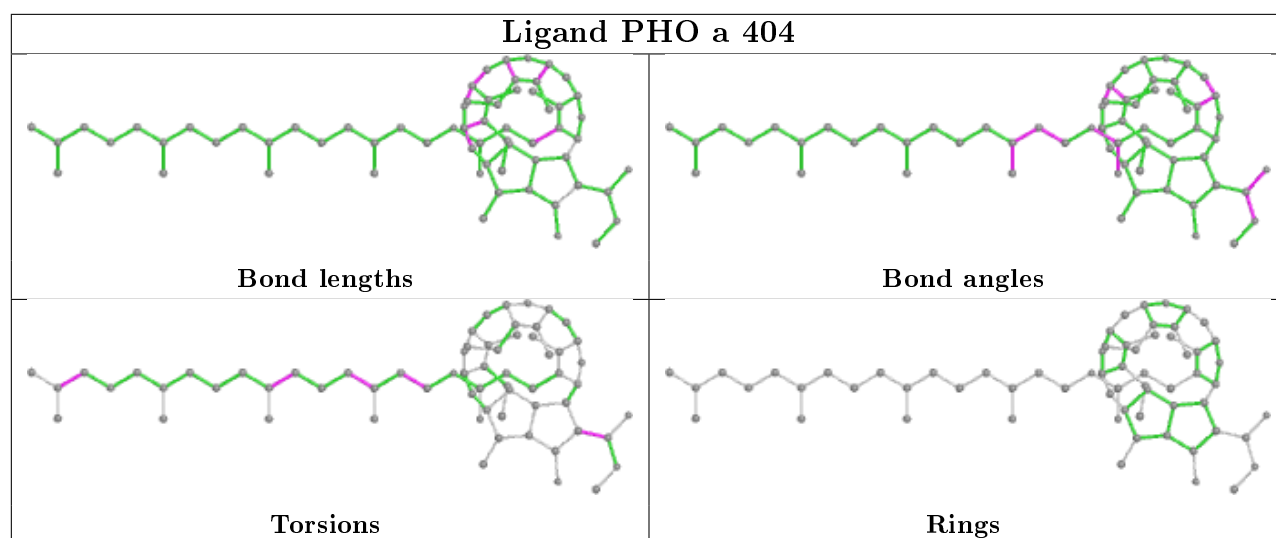


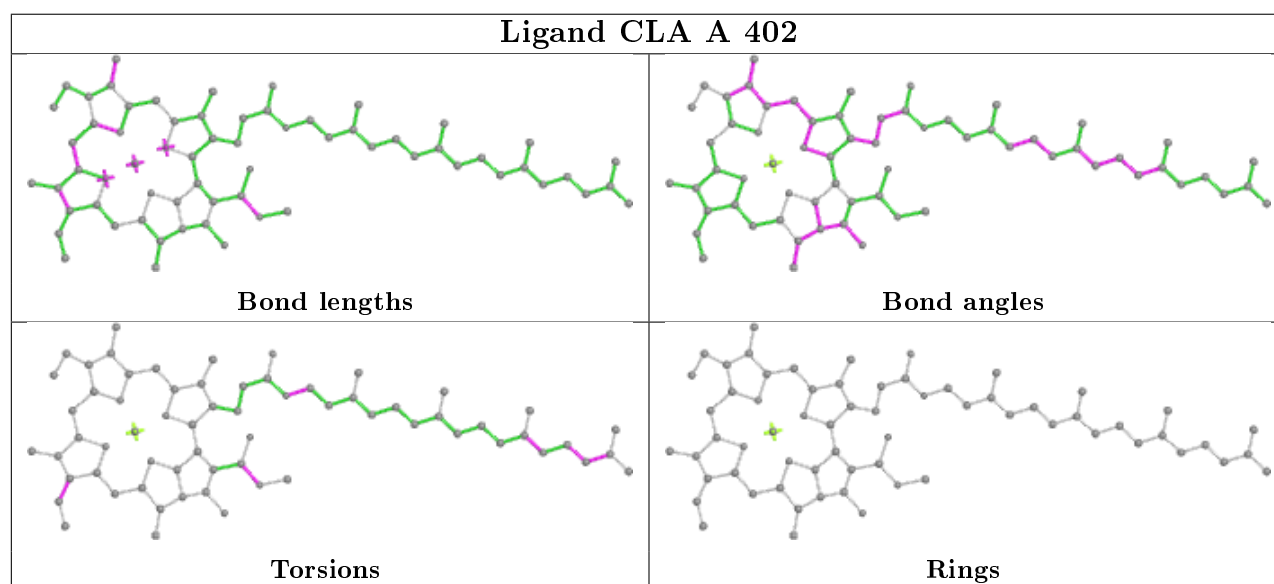
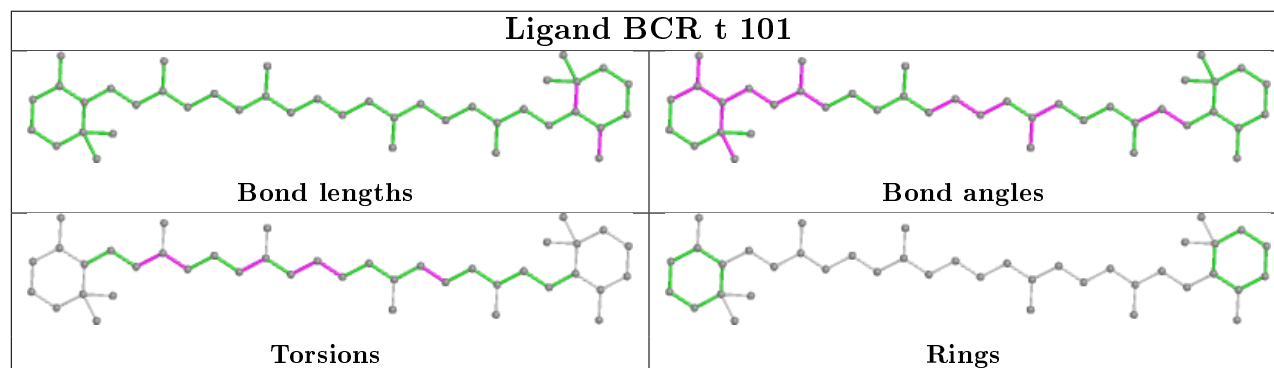
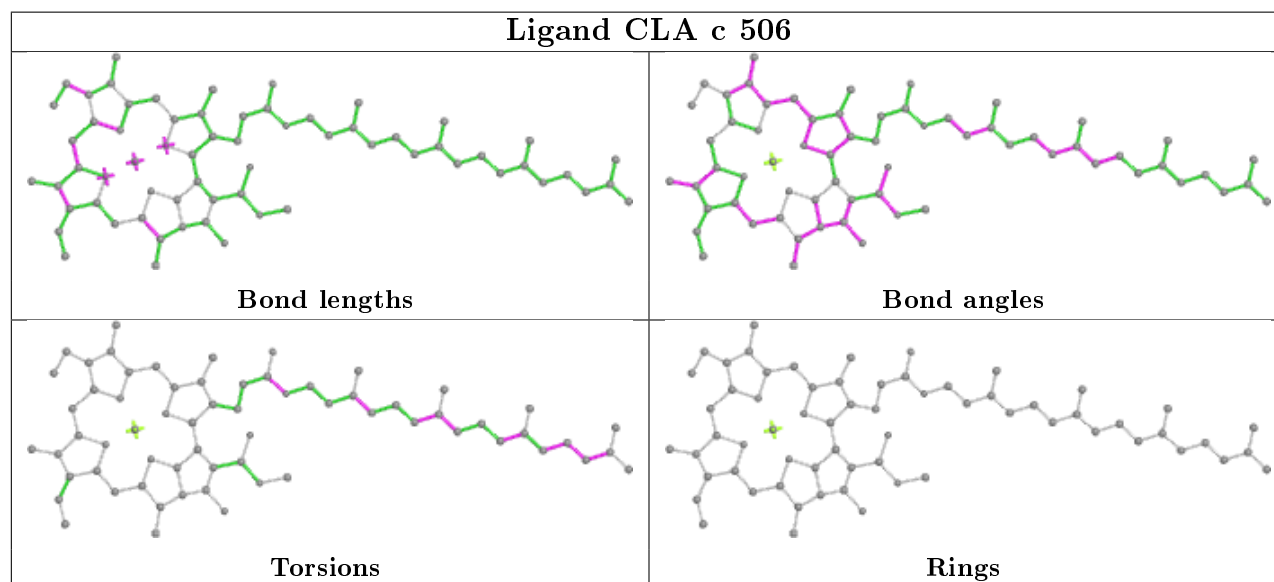
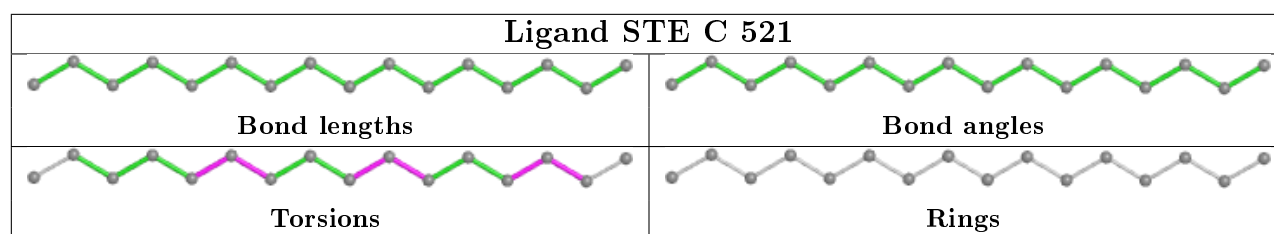
Ligand LHG D 412

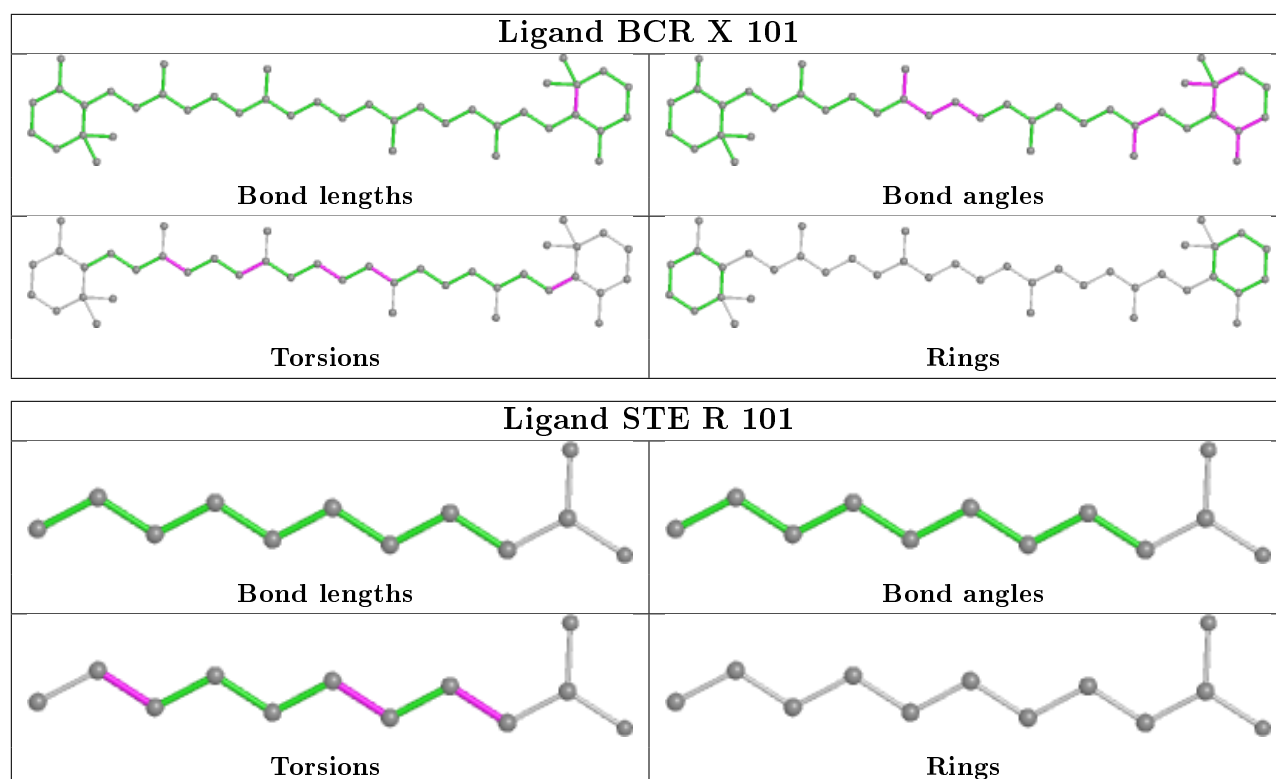


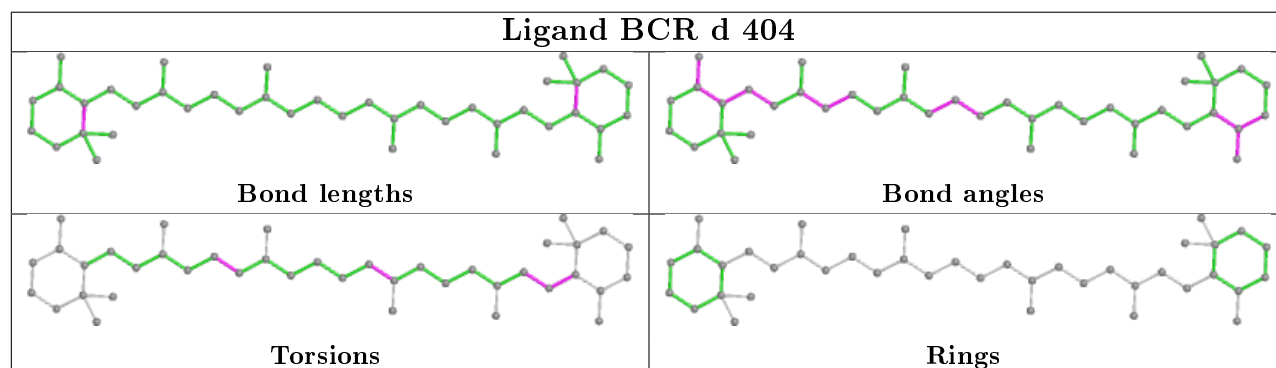
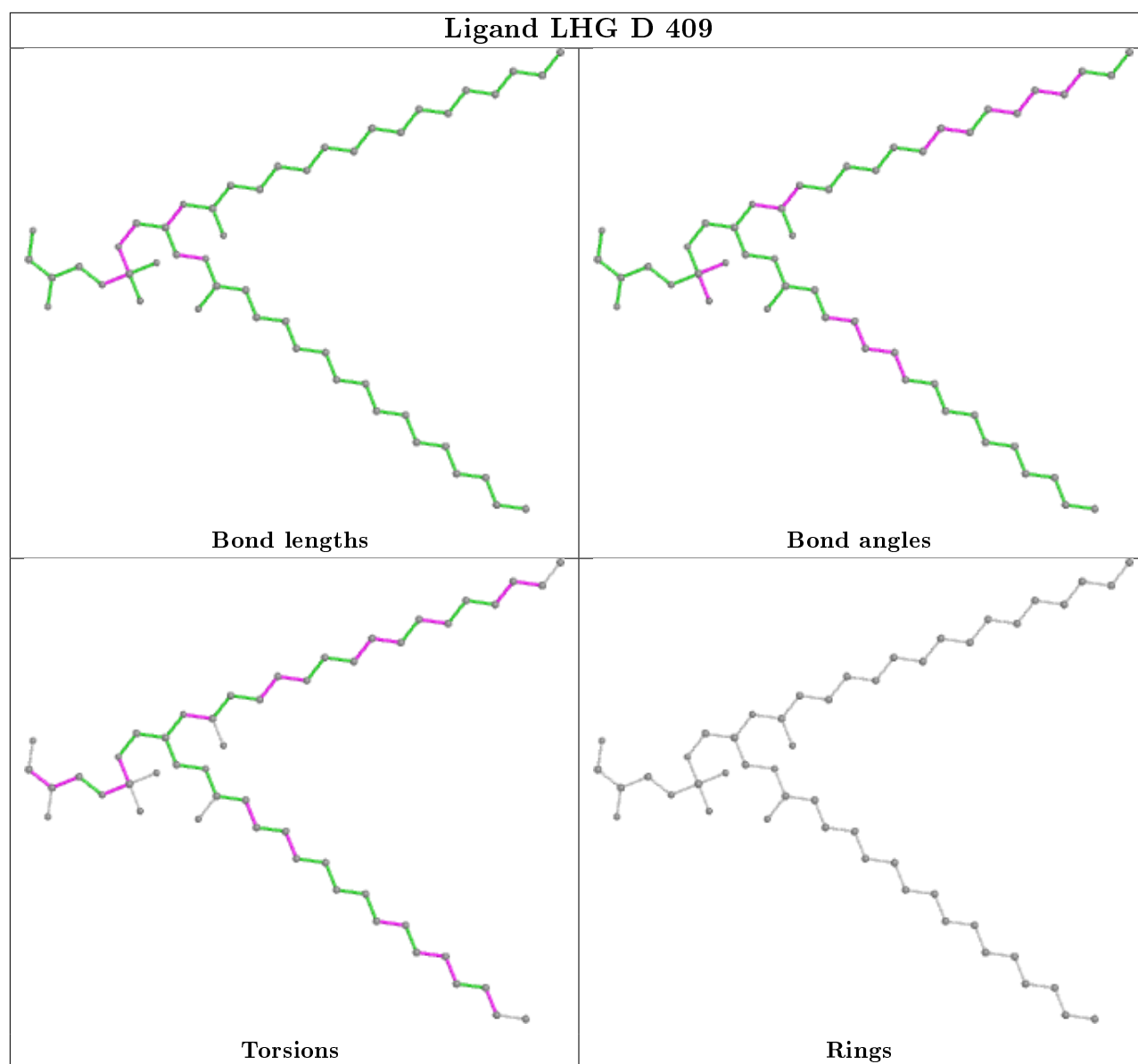


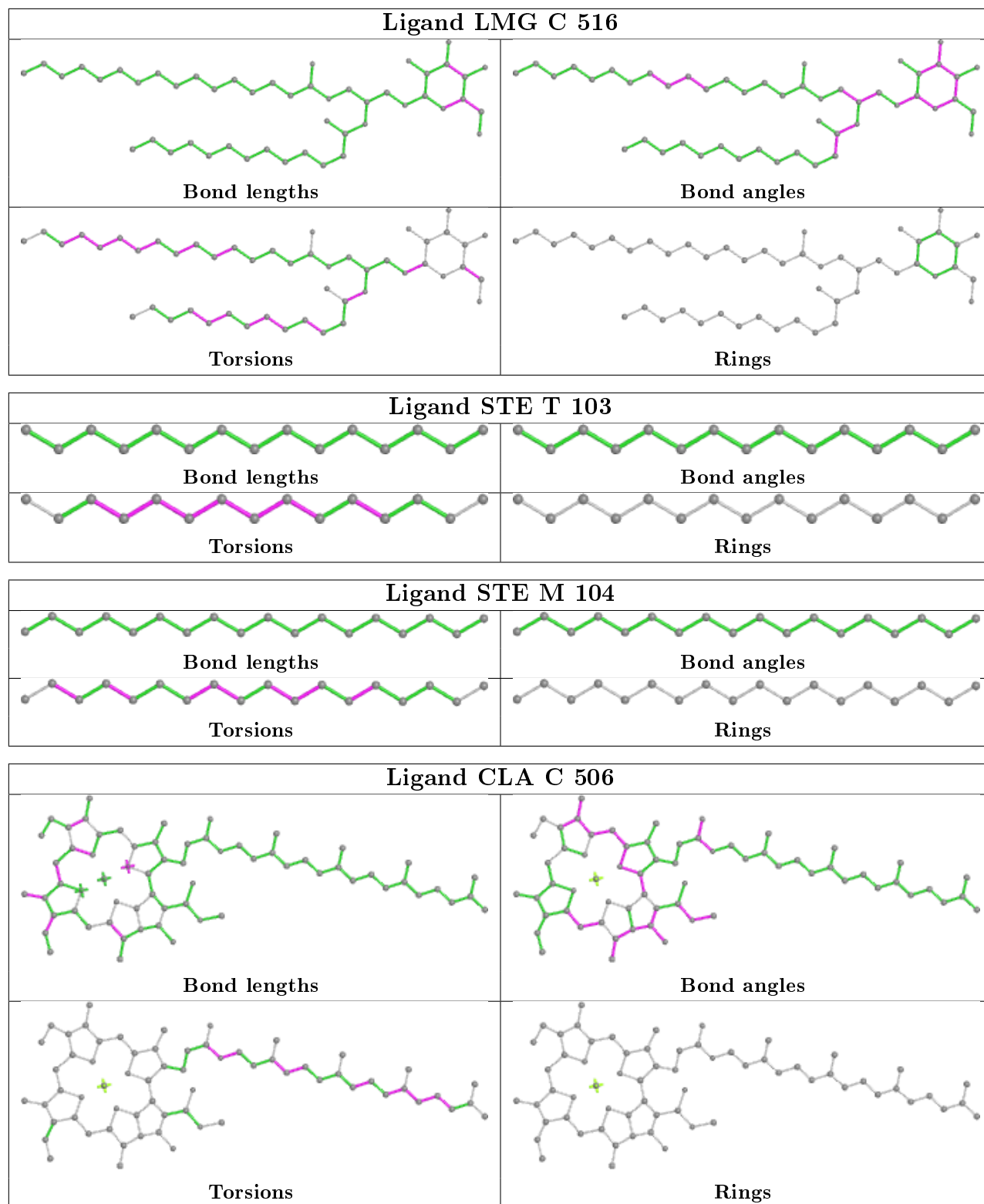


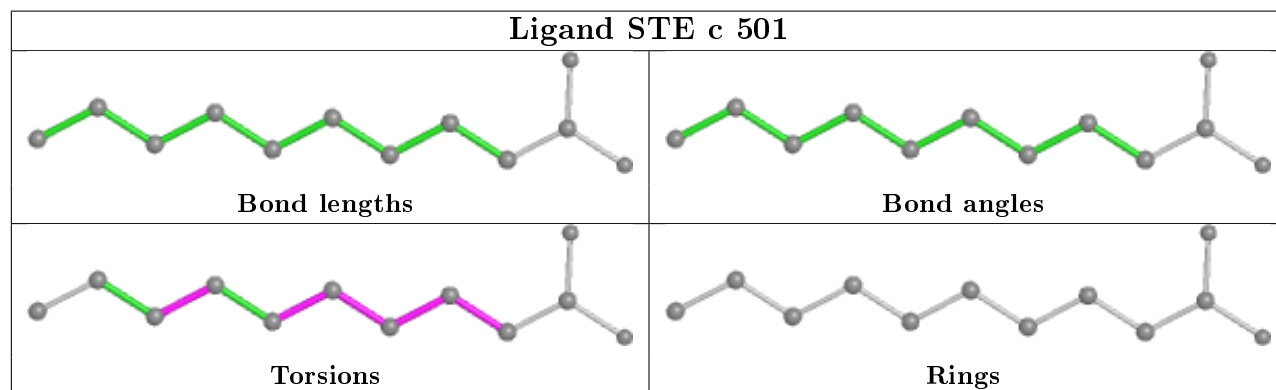
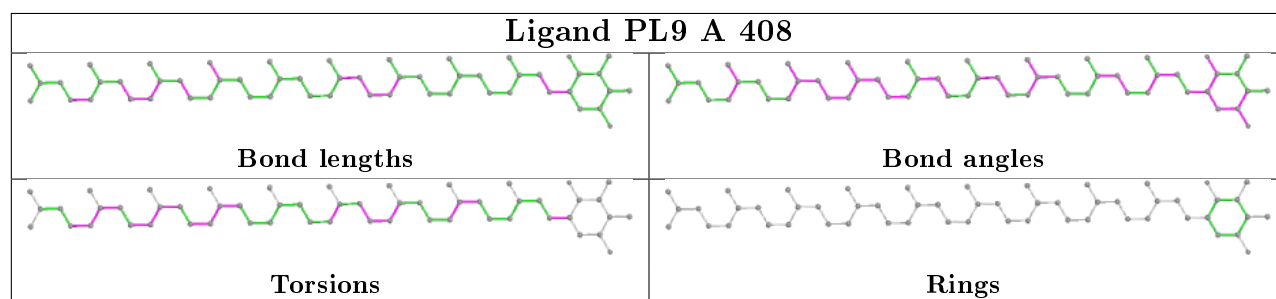
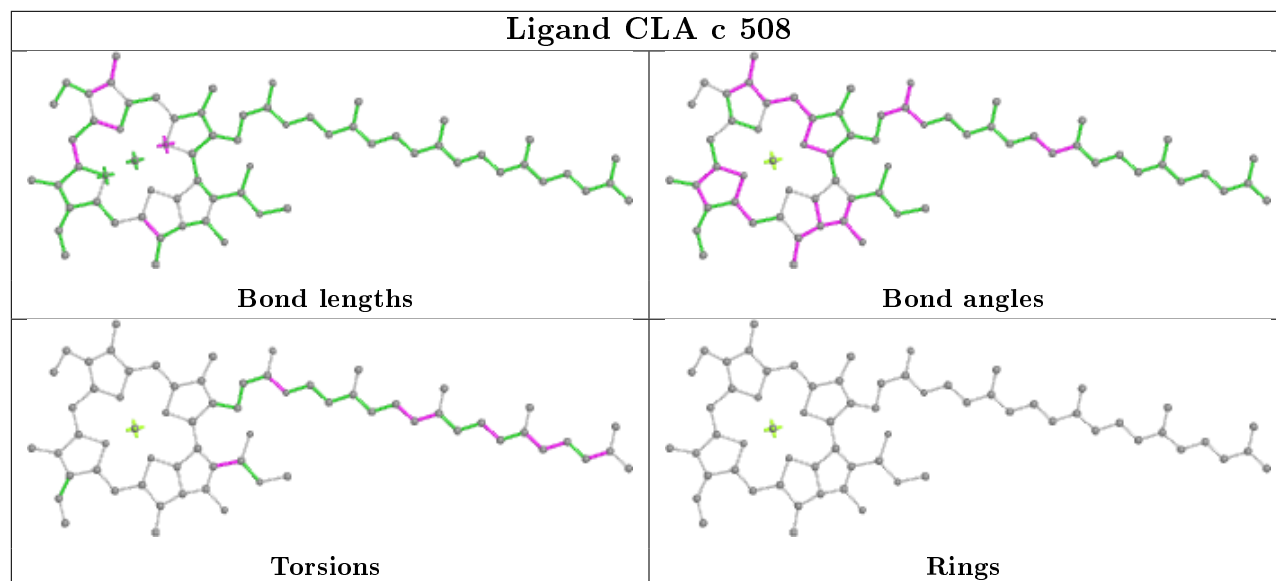
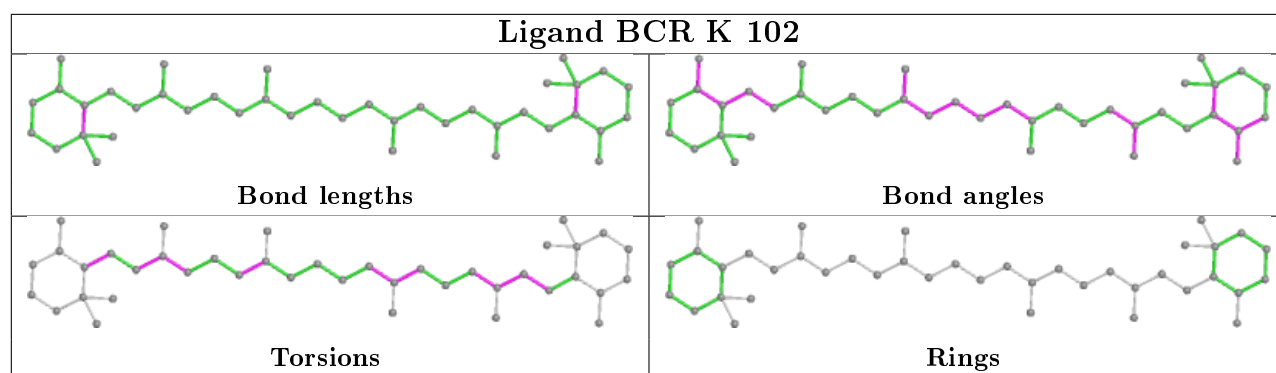


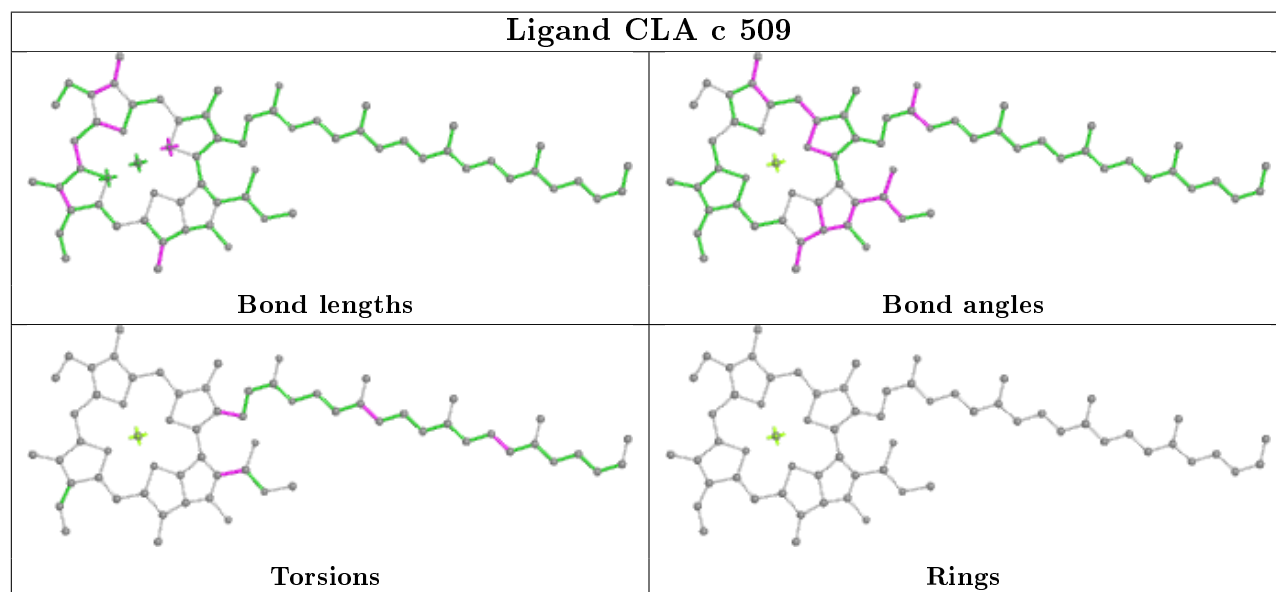
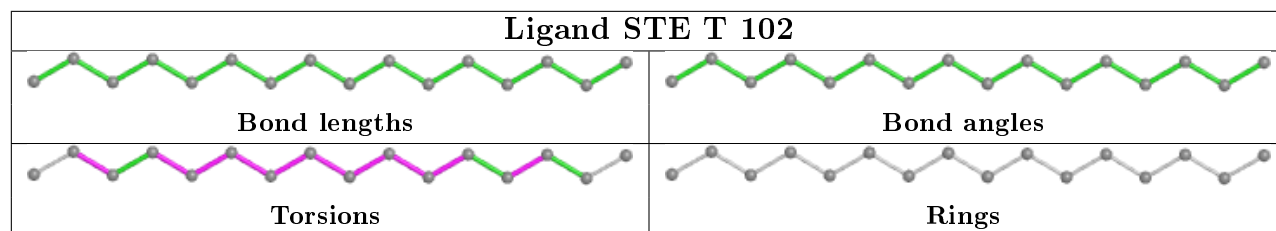




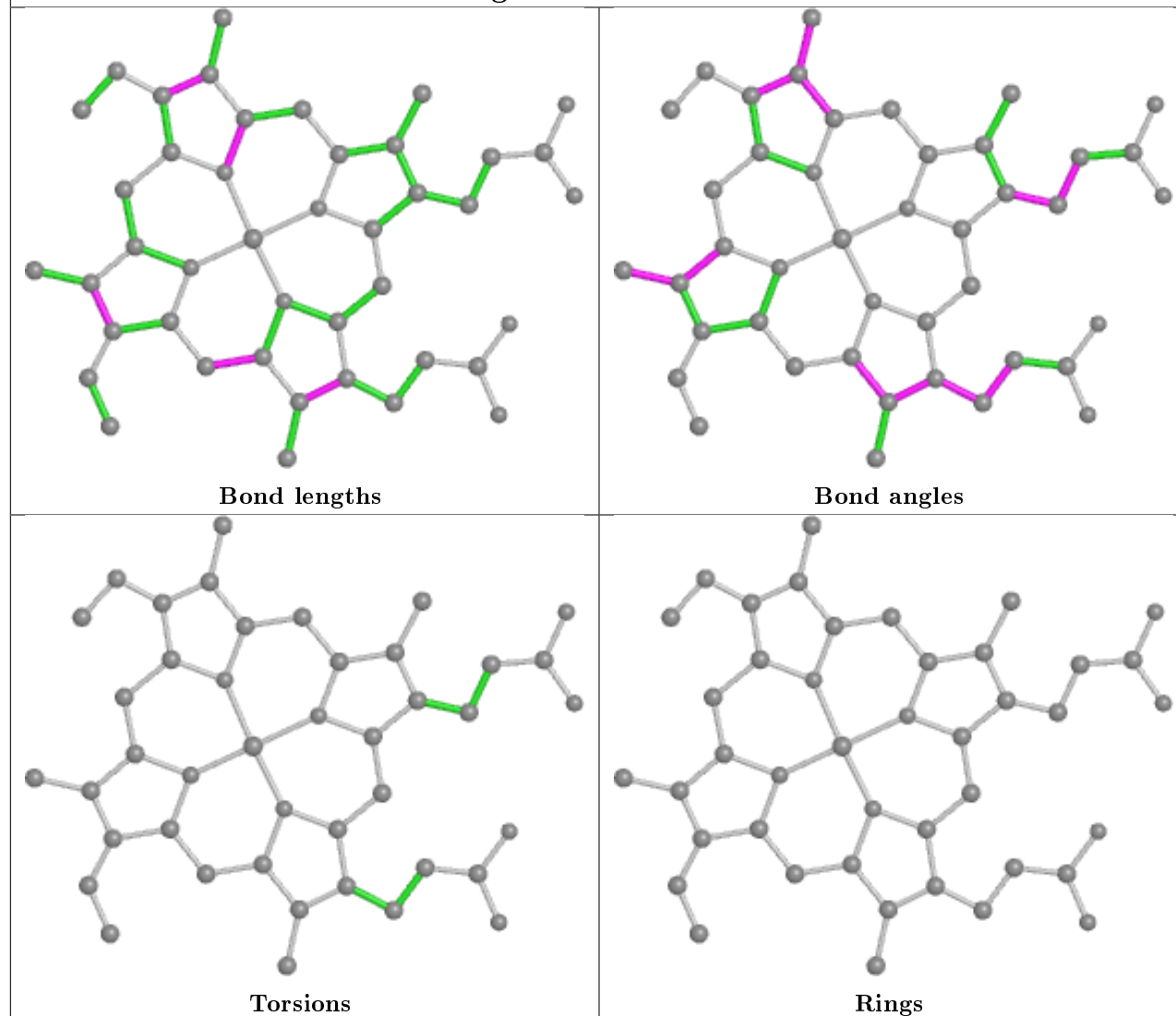




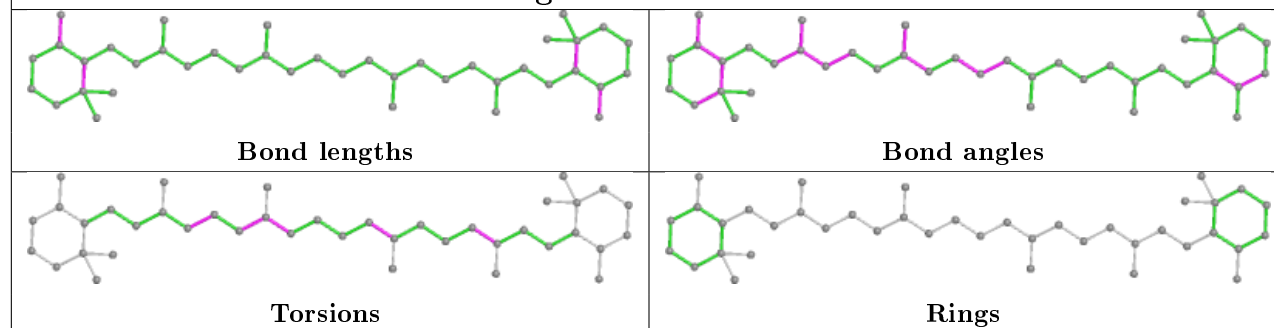




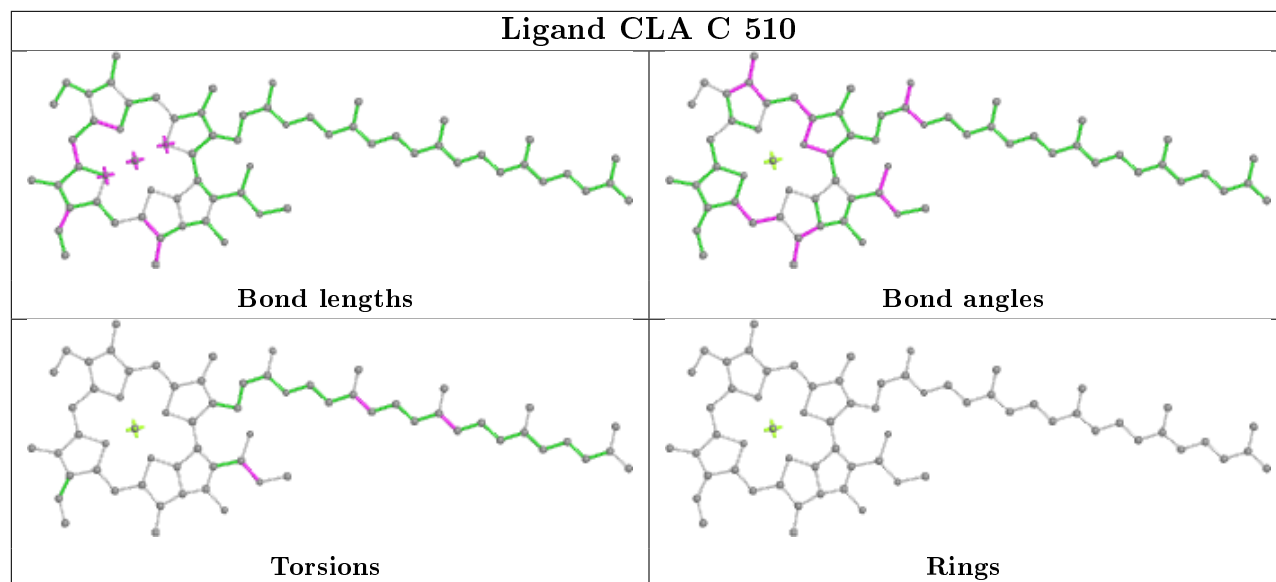
Ligand HEC F 101



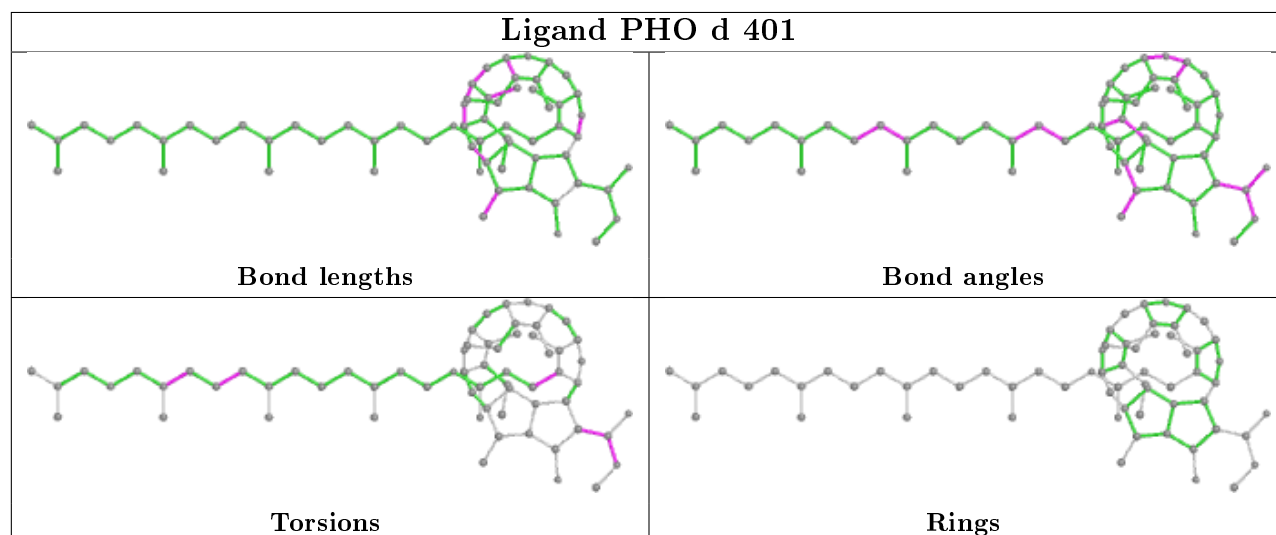
Ligand BCR c 516



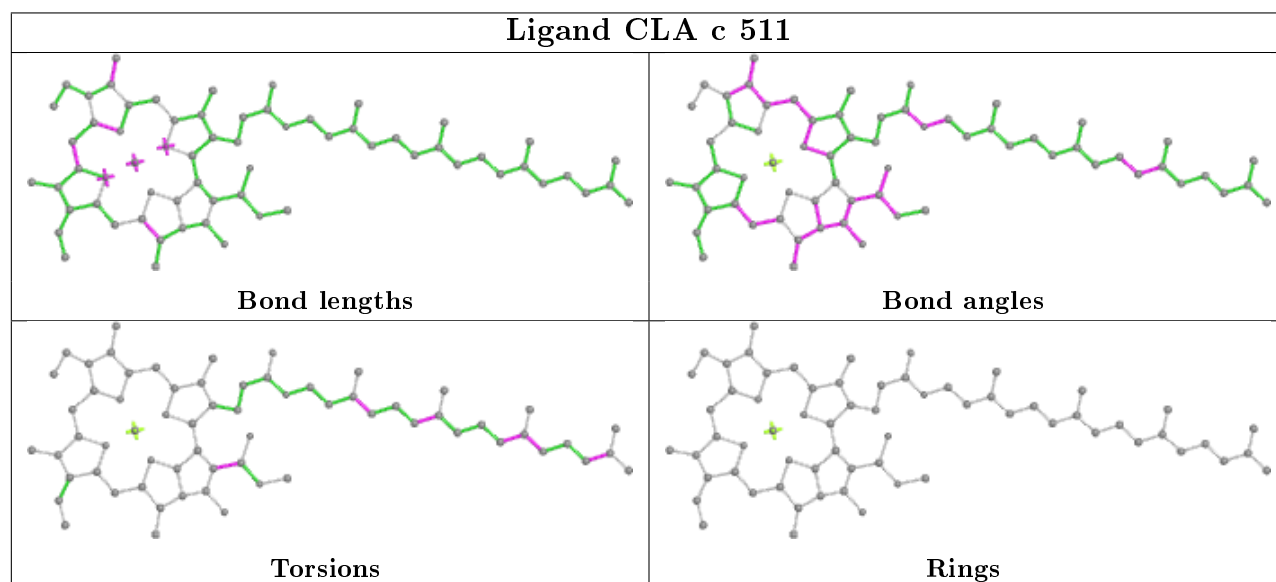
Ligand CLA C 510

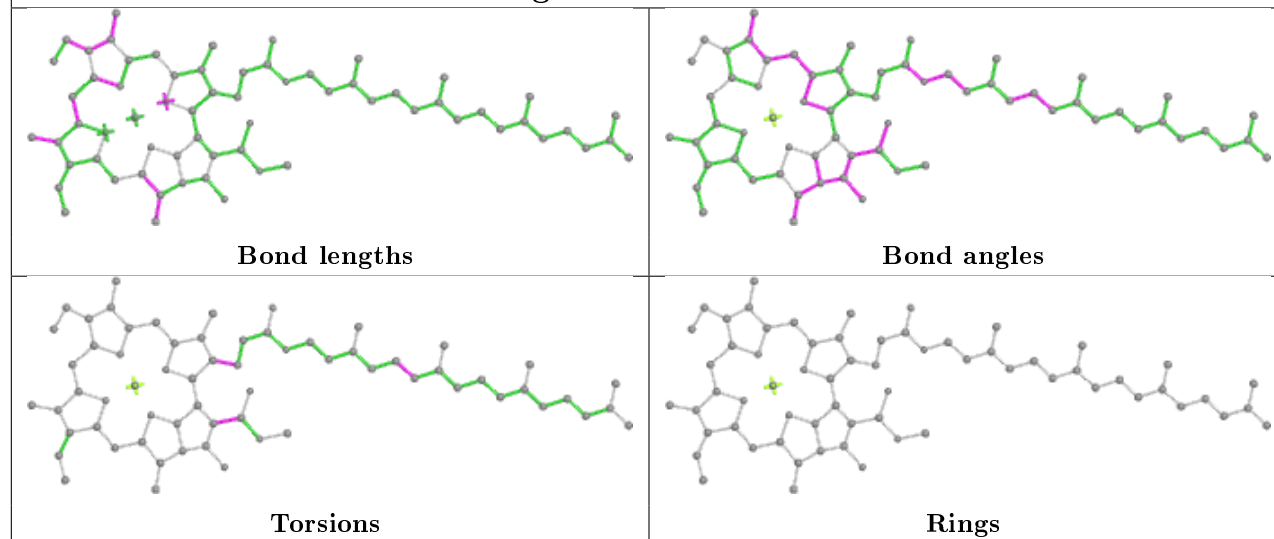
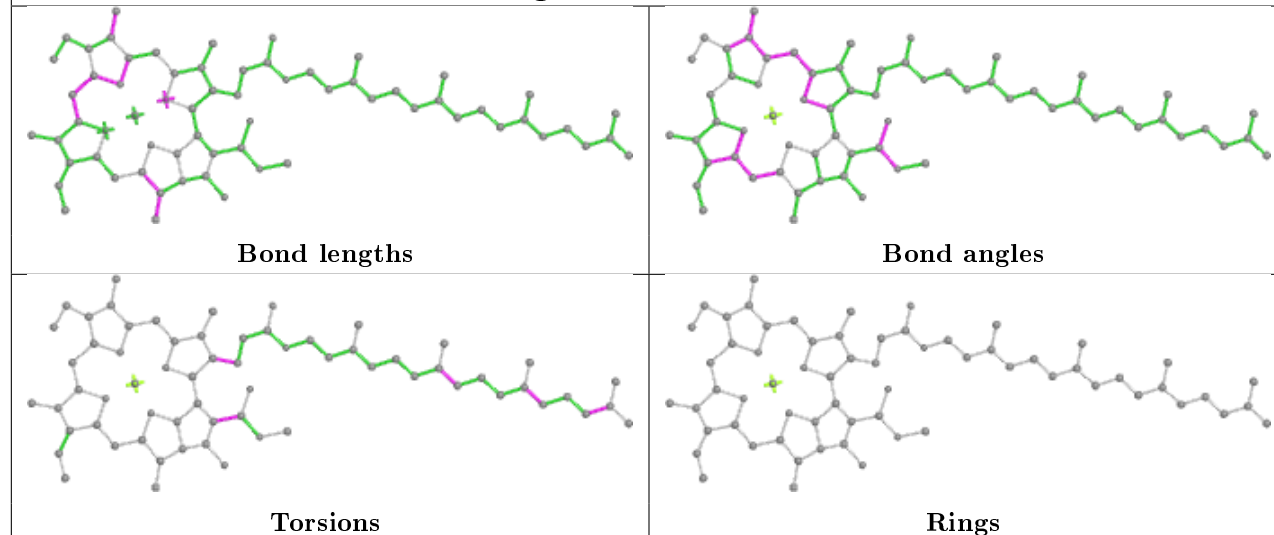
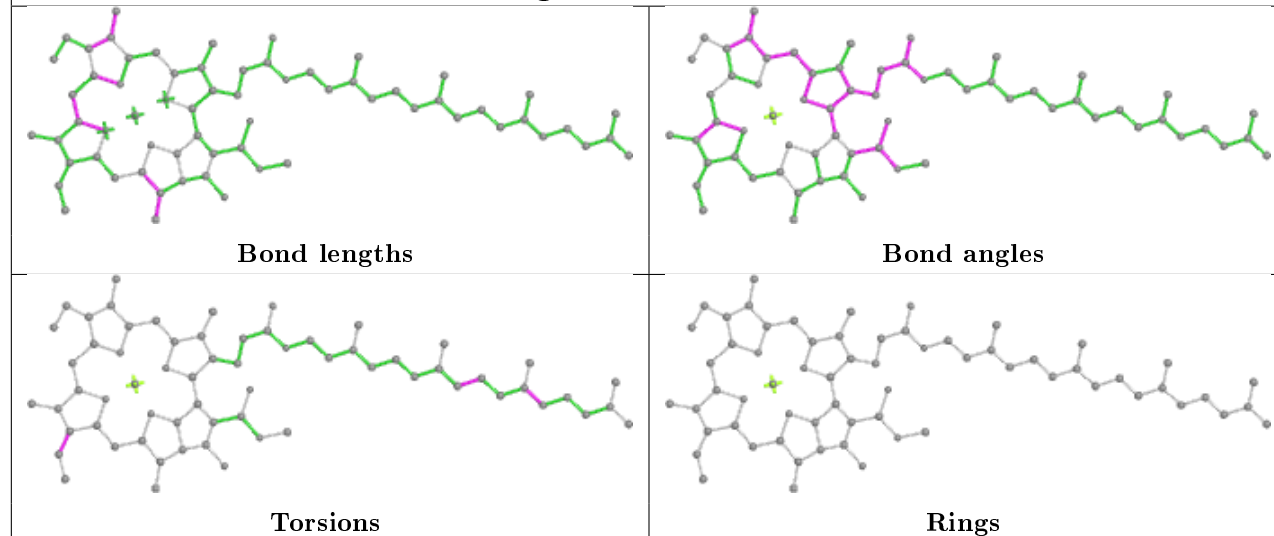


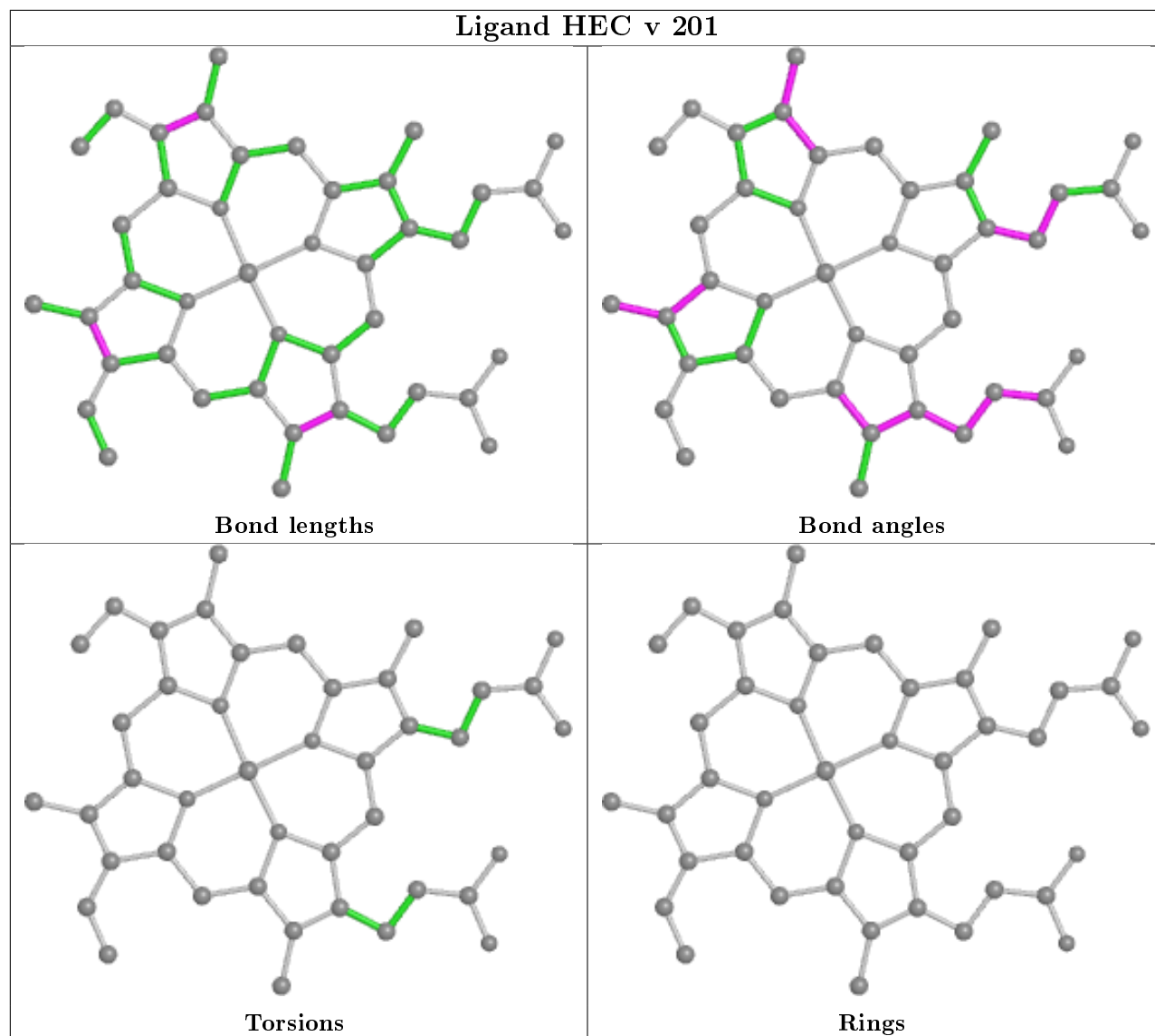
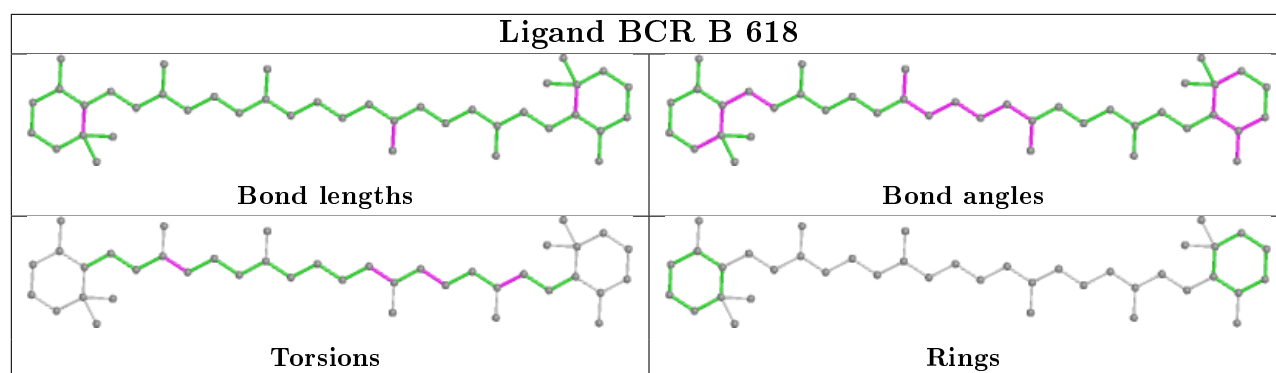
Ligand PHO d 401



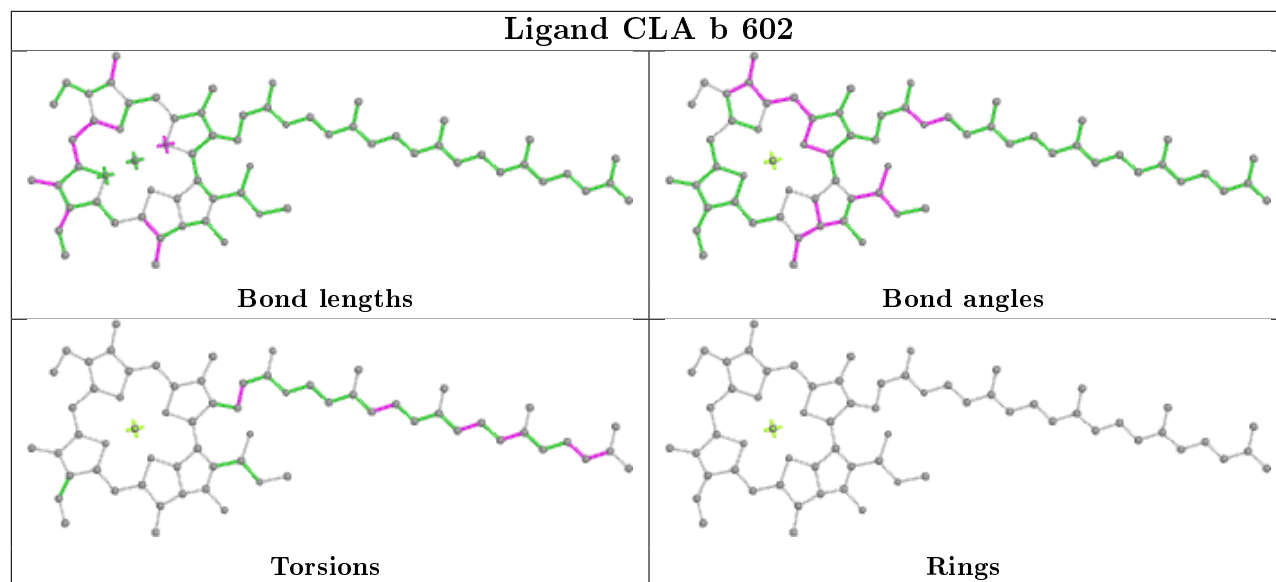
Ligand CLA c 511



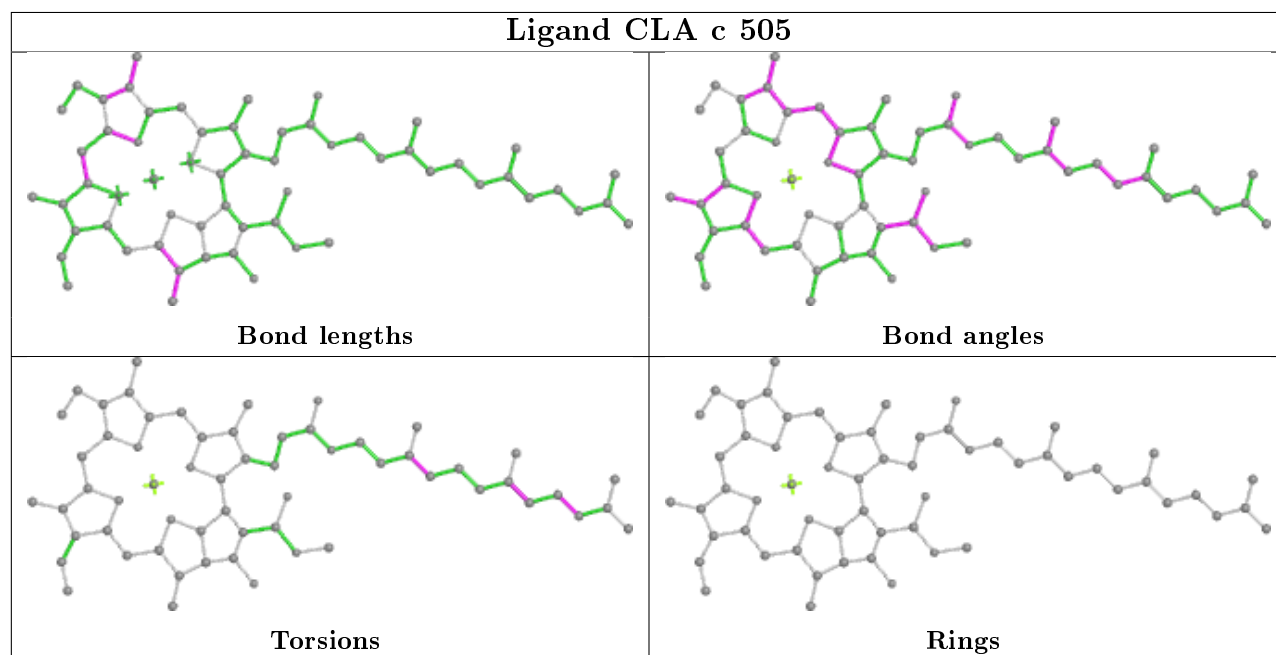
Ligand CLA C 503**Ligand CLA C 508****Ligand CLA b 610**



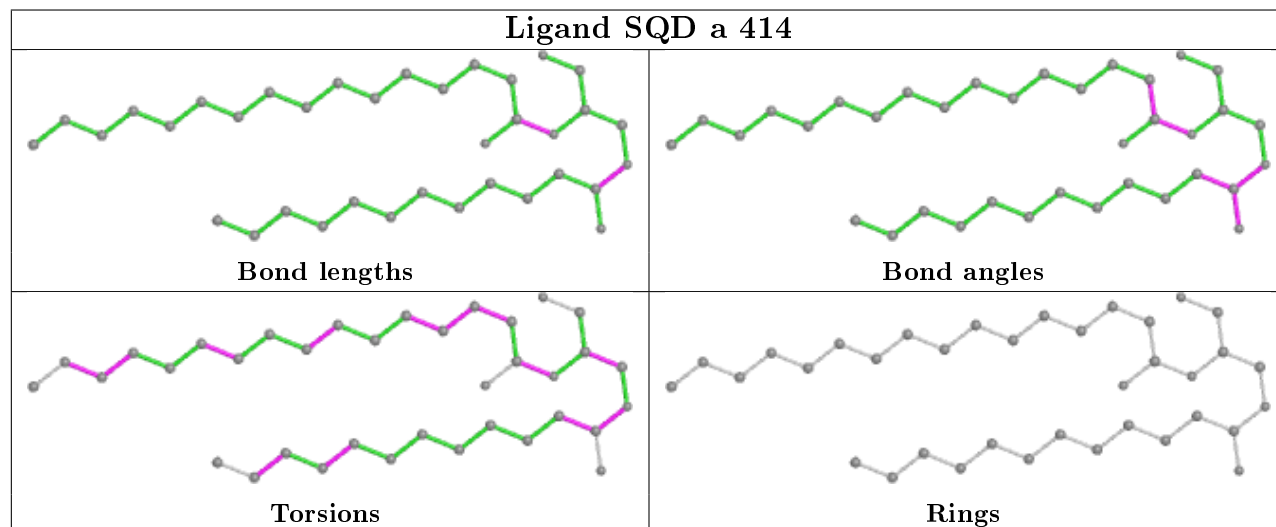
Ligand CLA b 602

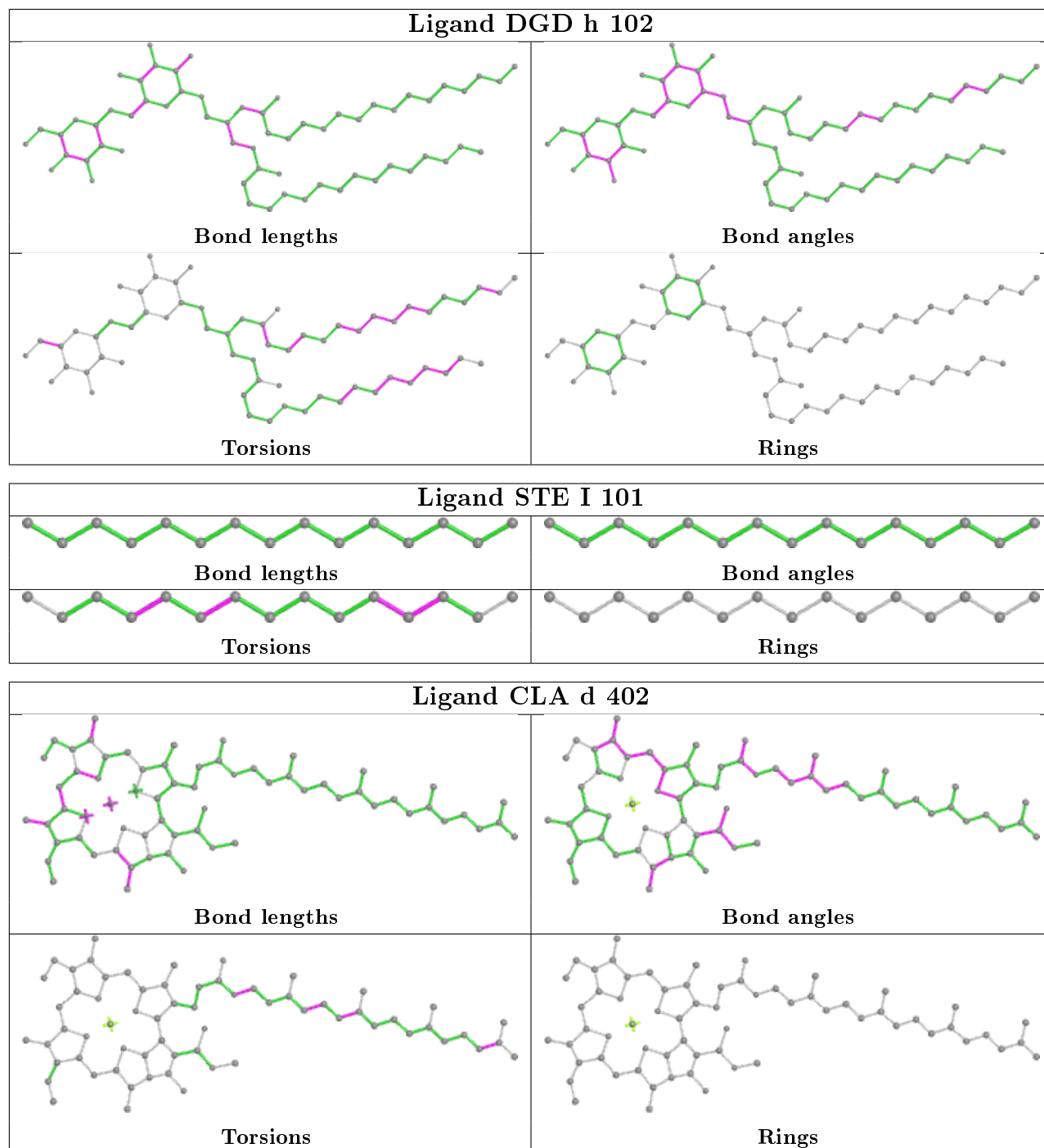


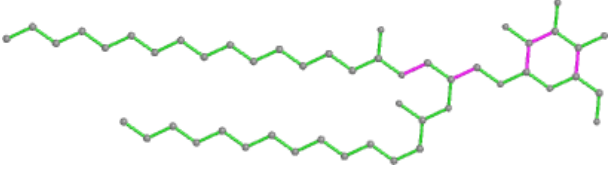
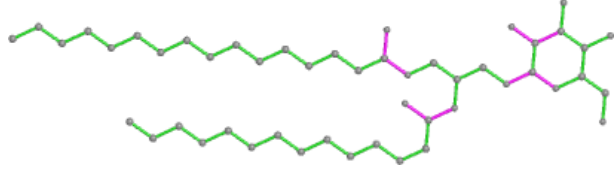
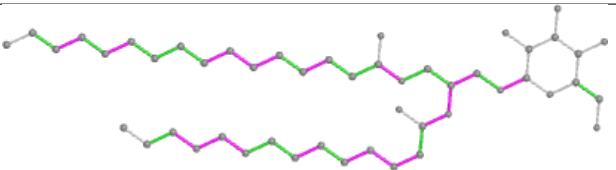
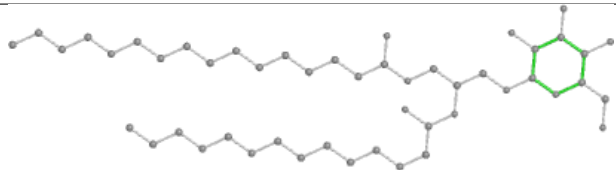
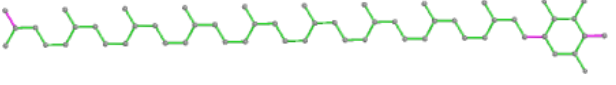
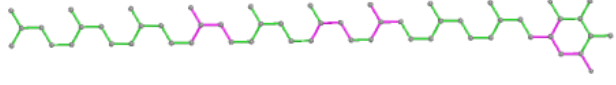
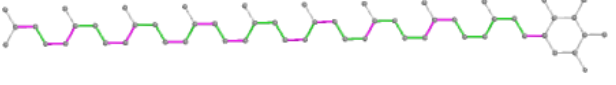
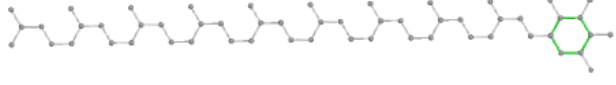
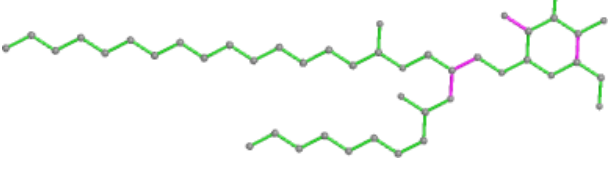
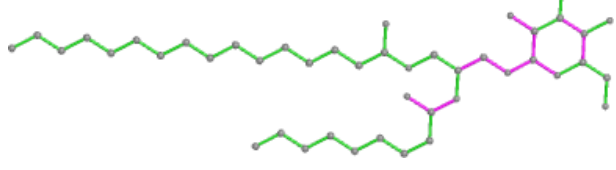
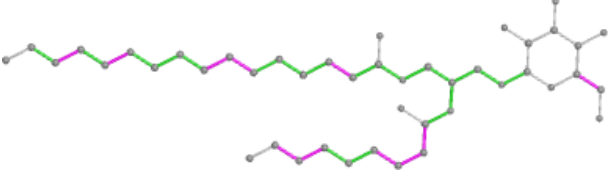
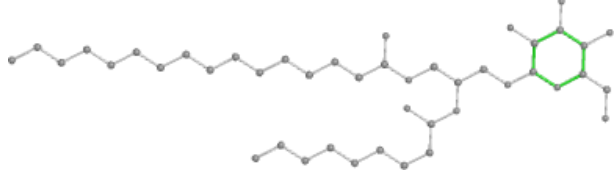
Ligand CLA c 505

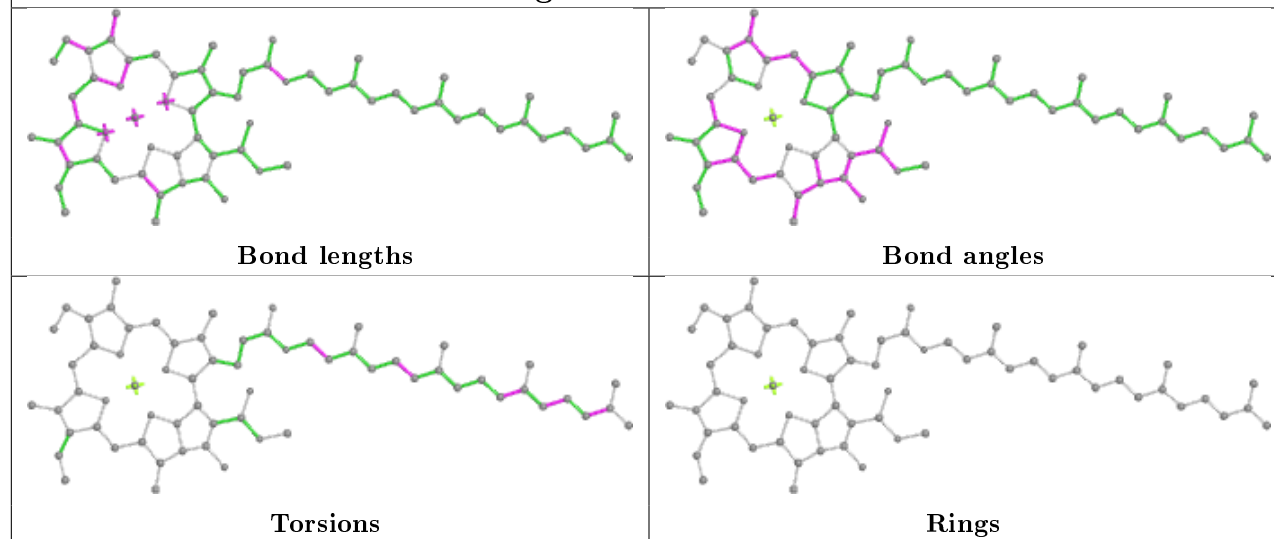
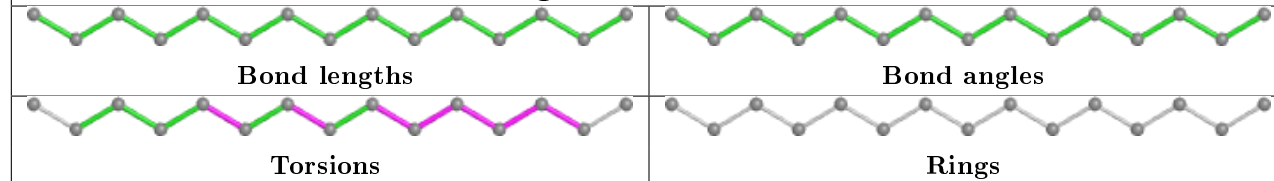
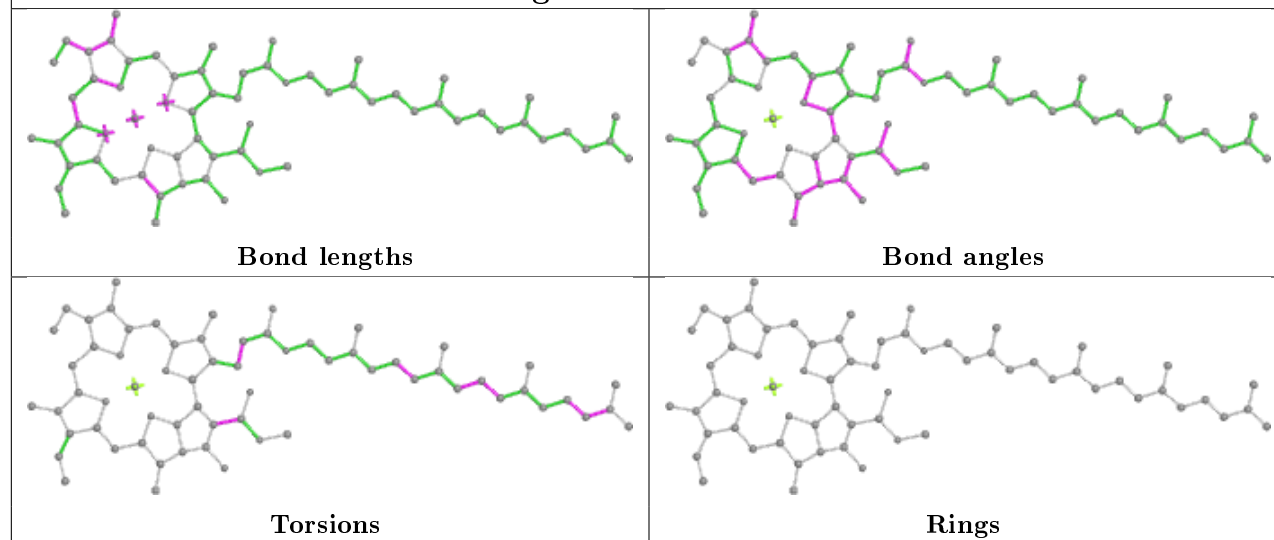


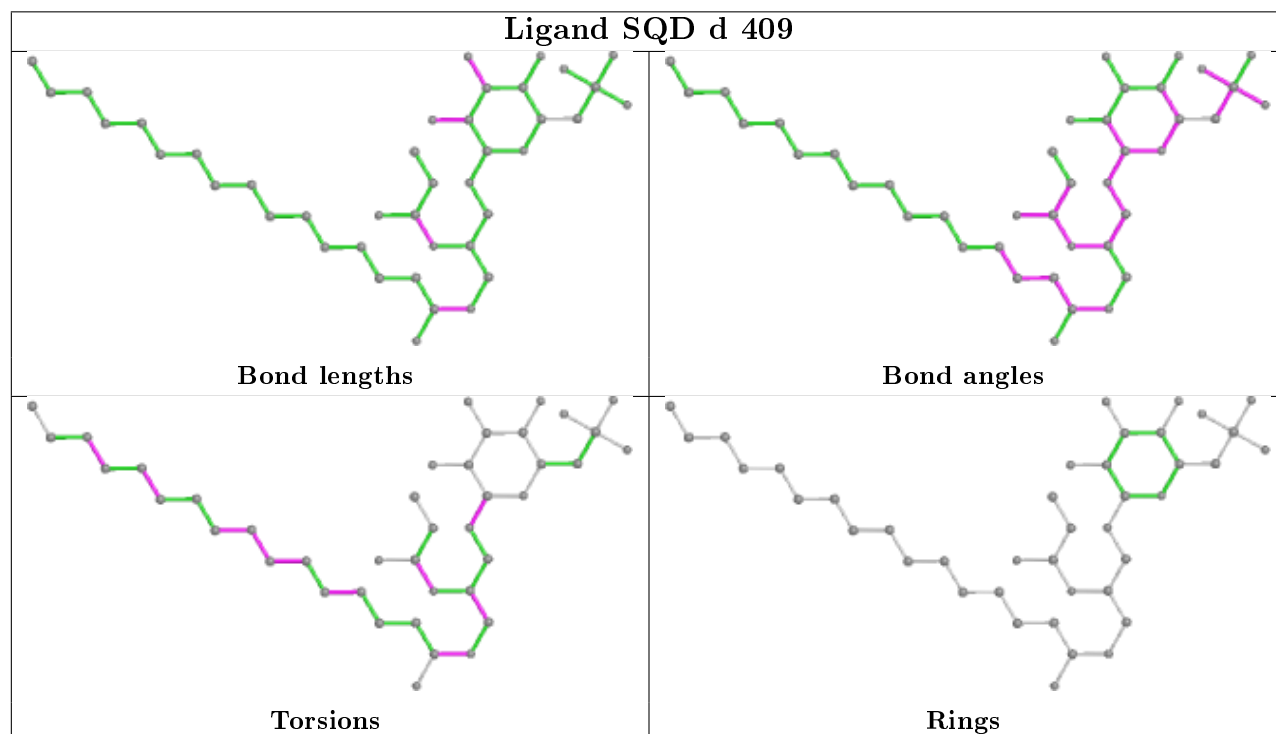
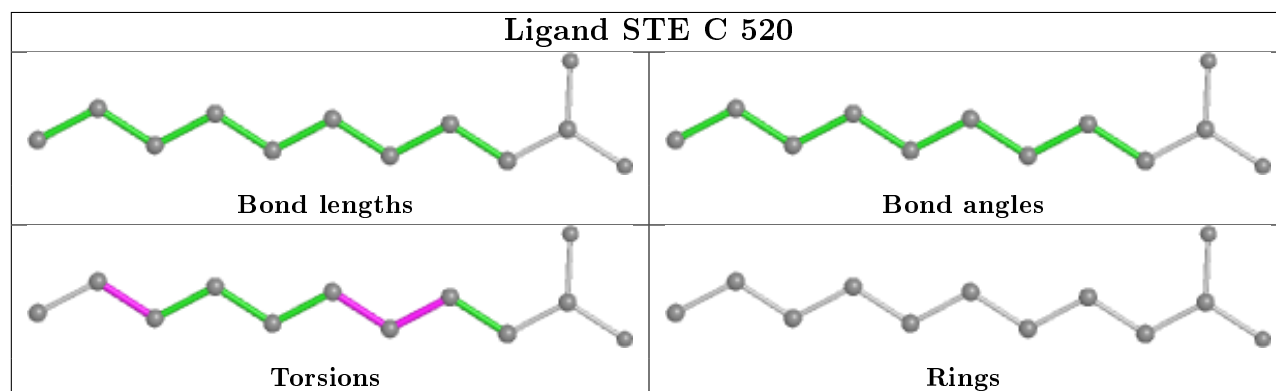
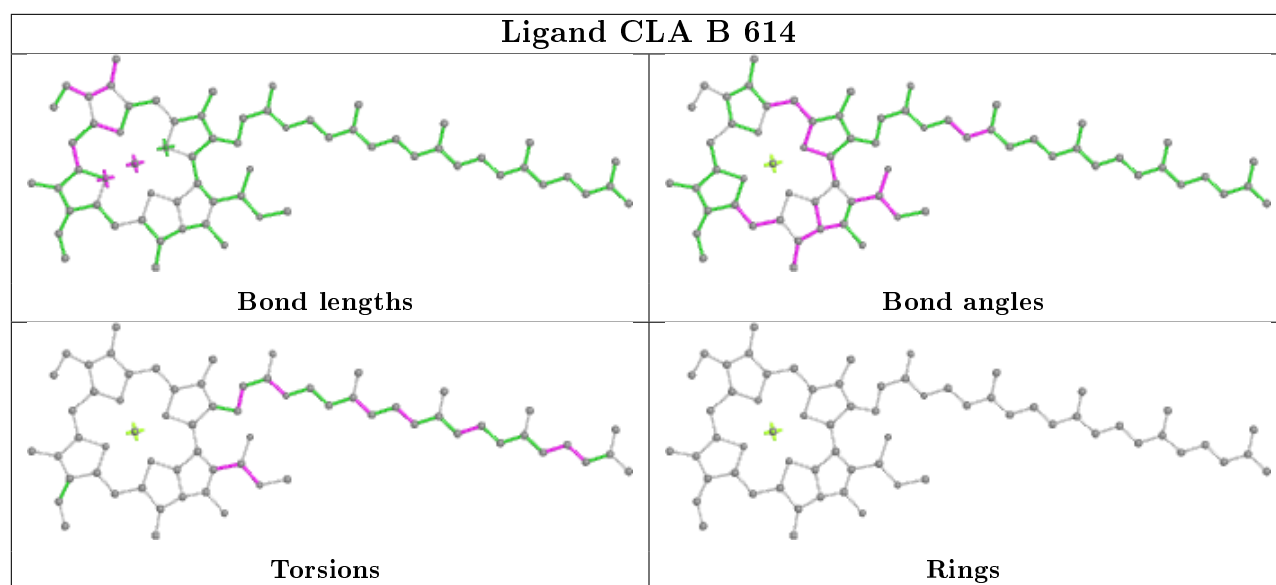
Ligand SQD a 414

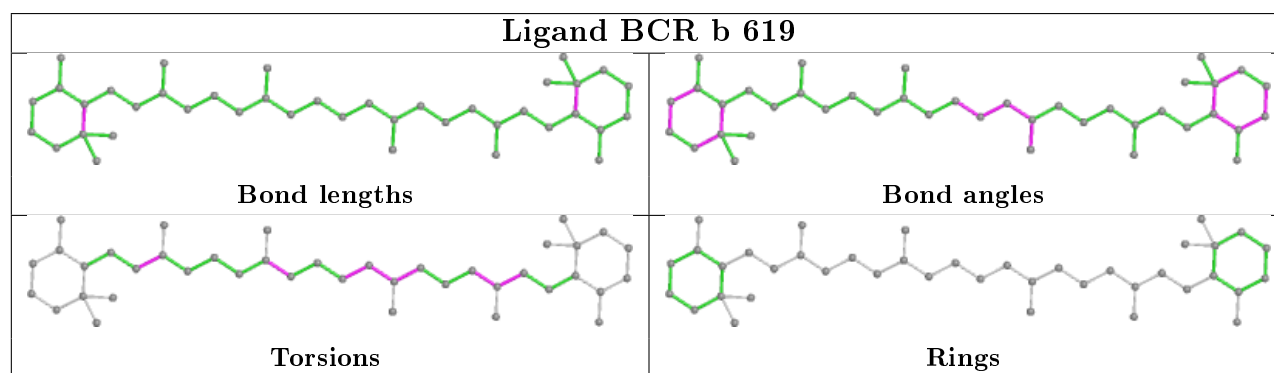
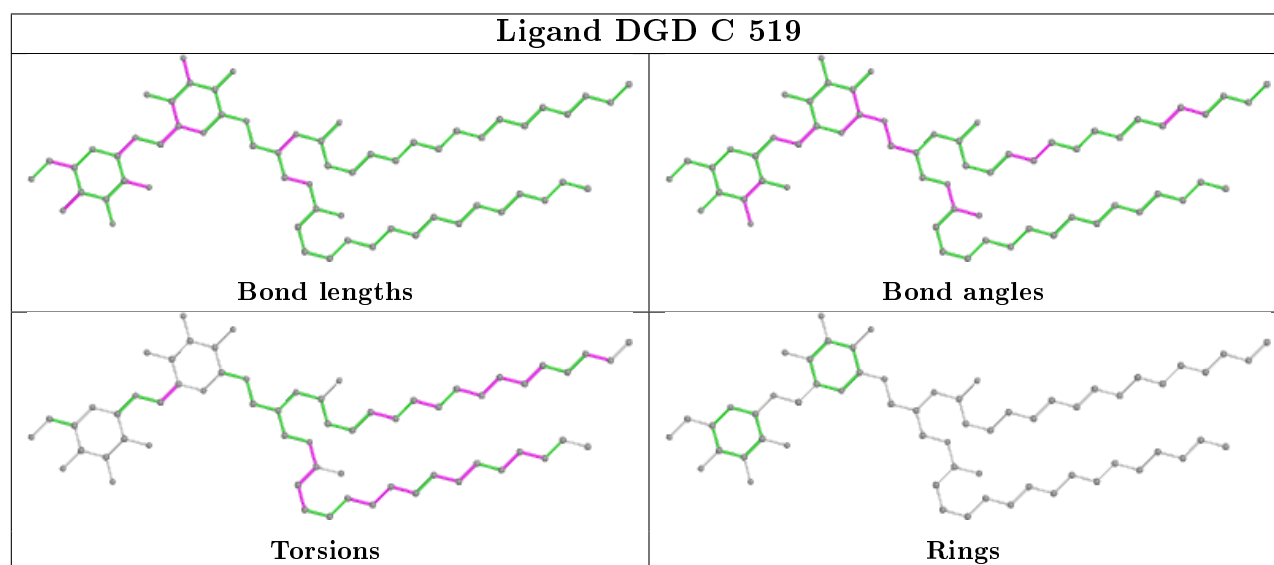
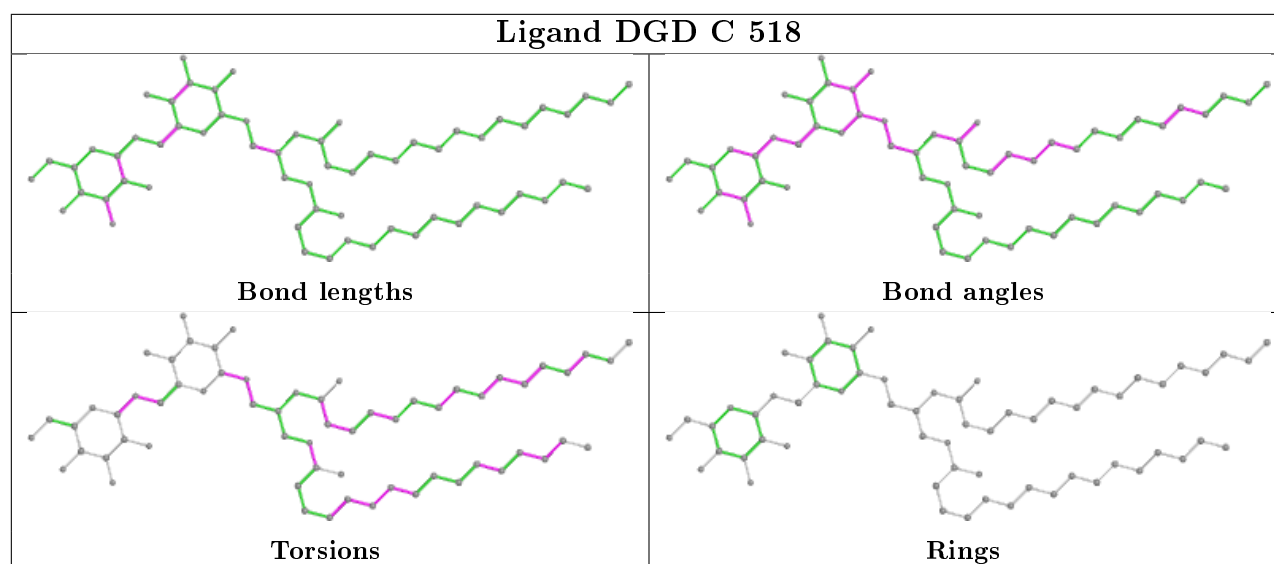


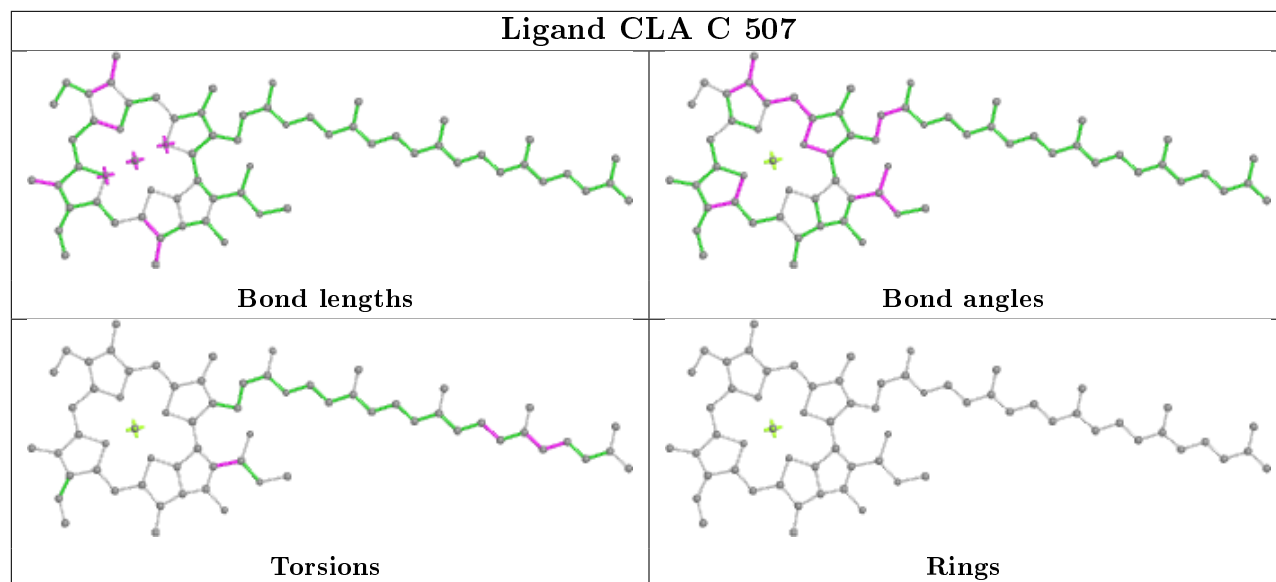
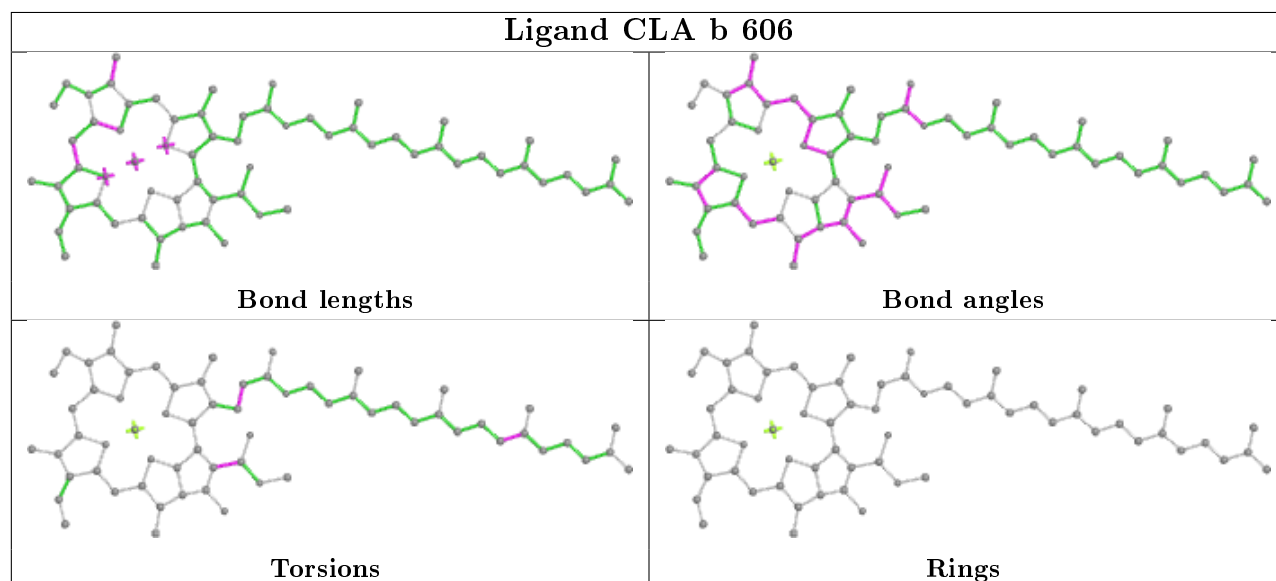
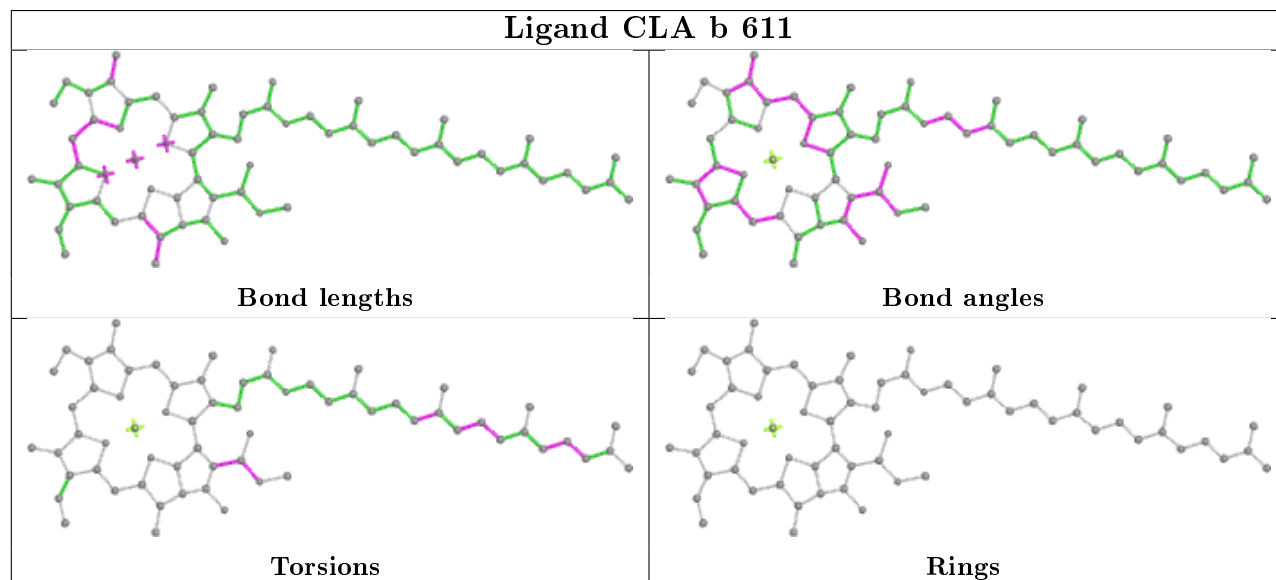


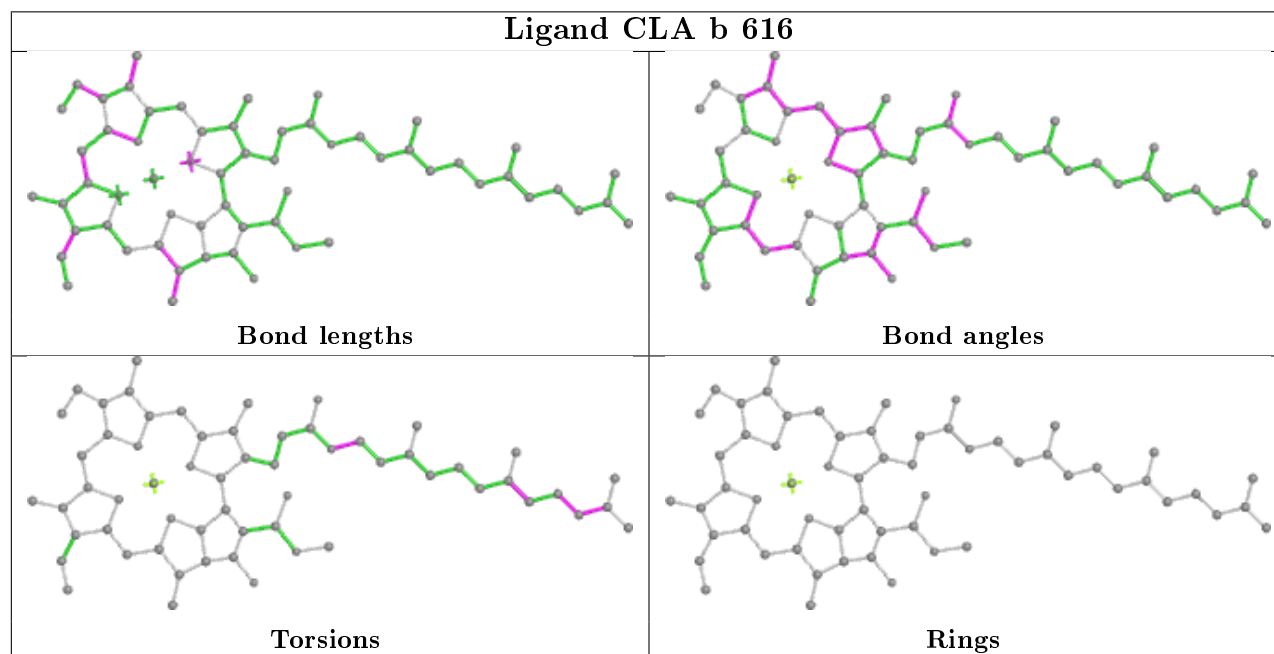
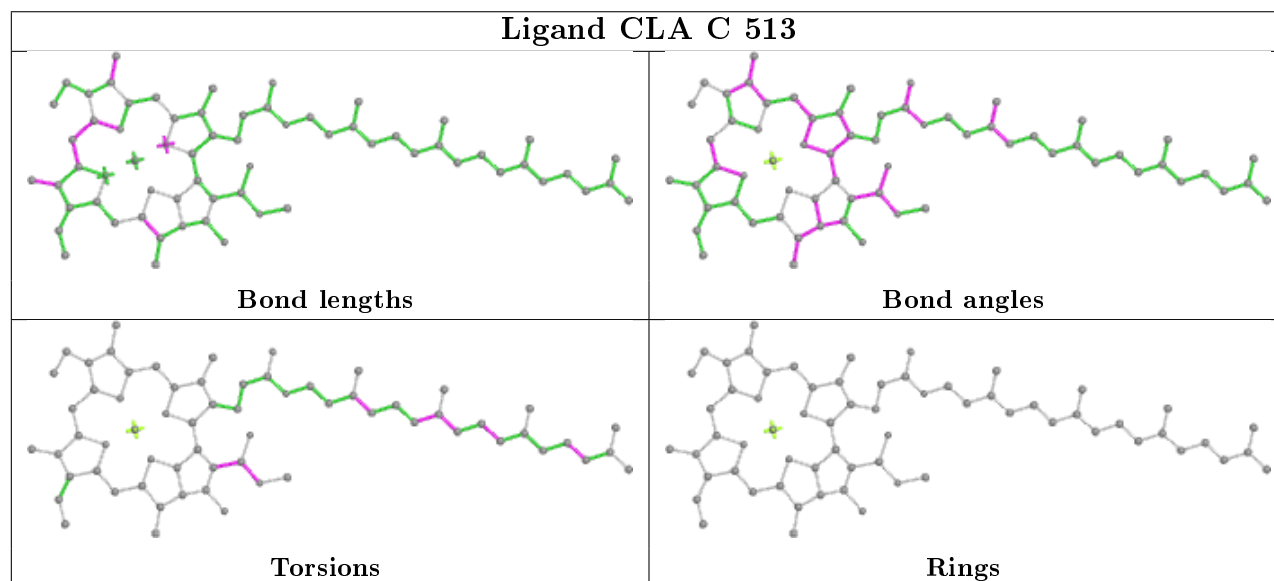
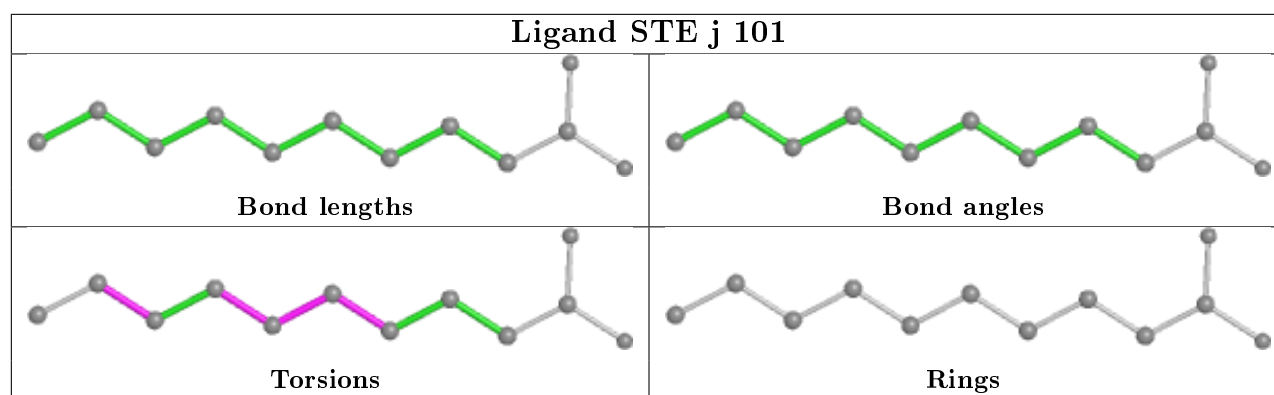
| Ligand LMG c 523 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand PL9 a 410 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand LMG d 408 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |

Ligand CLA b 608**Ligand STE B 625****Ligand CLA B 606**

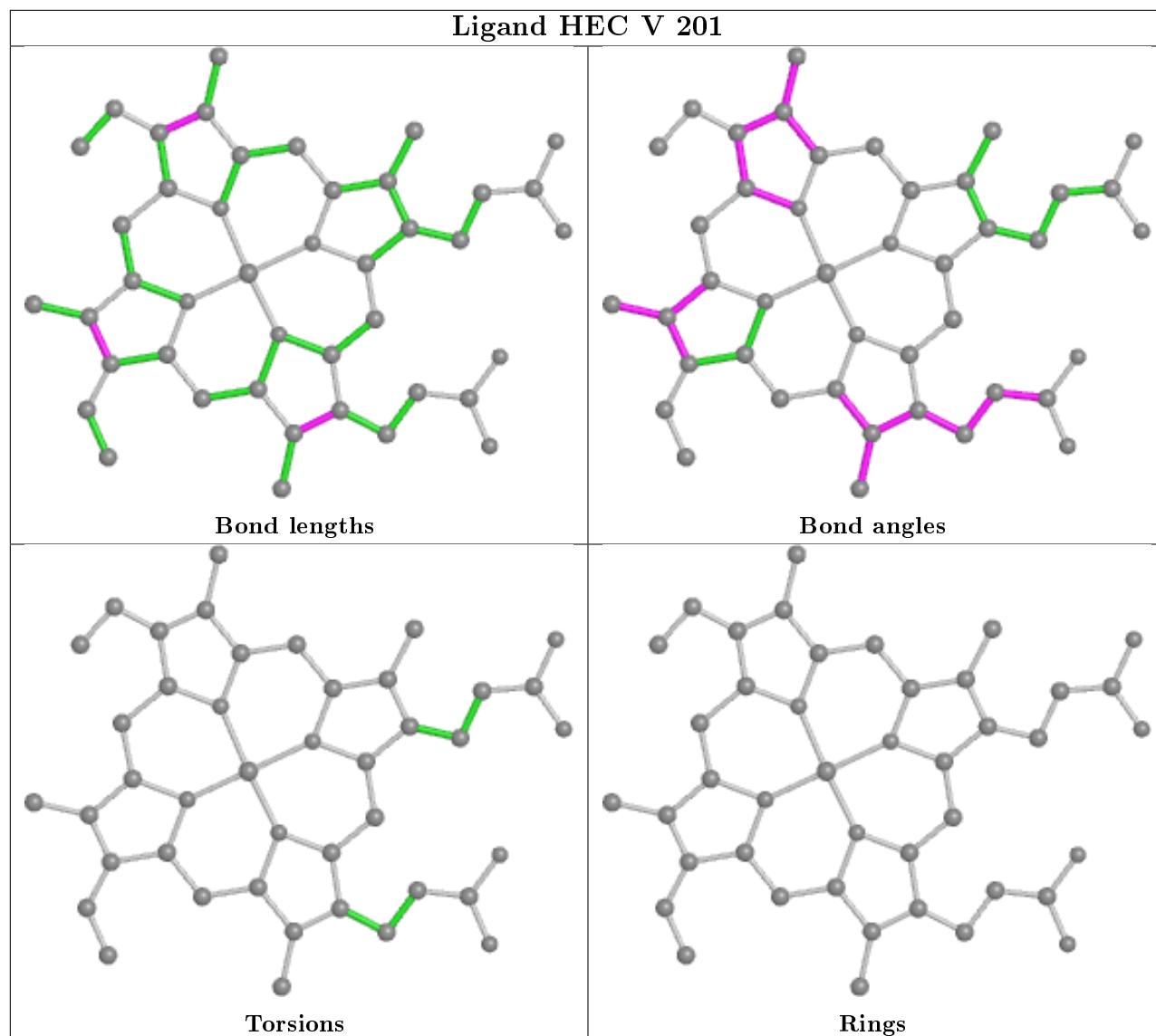




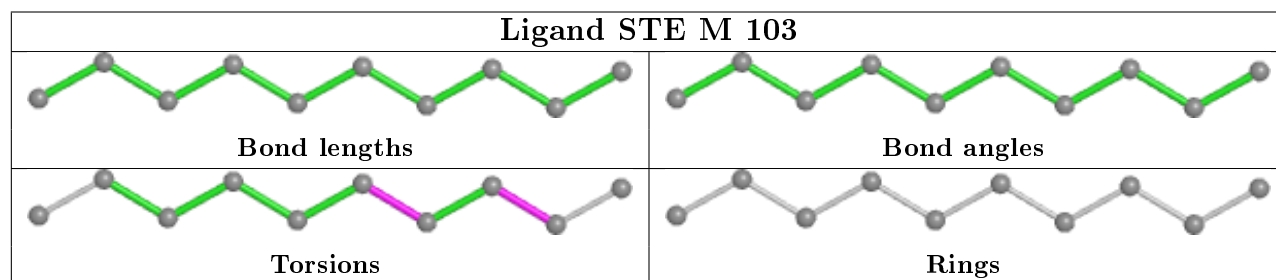
Ligand CLA C 507**Ligand CLA b 606****Ligand CLA b 611**



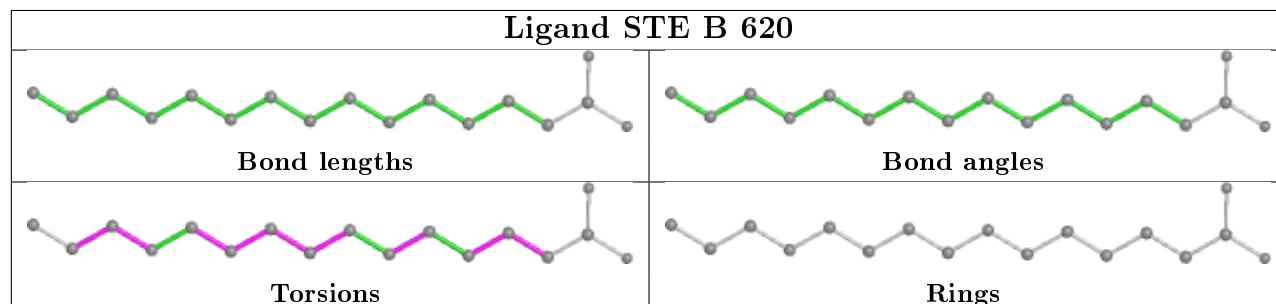
Ligand HEC V 201

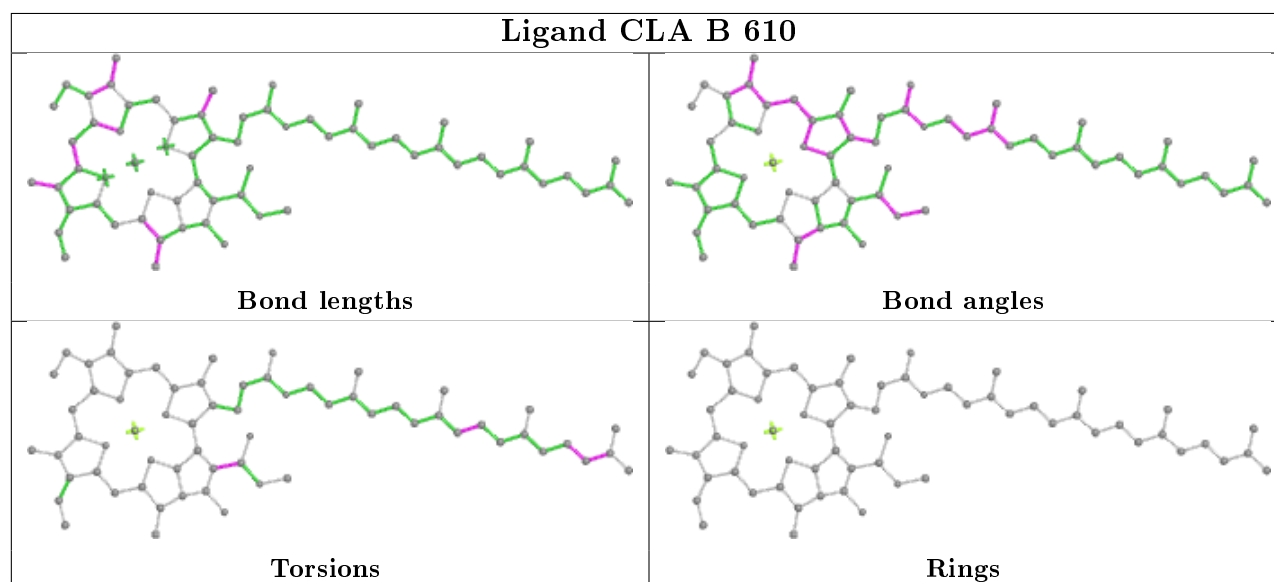
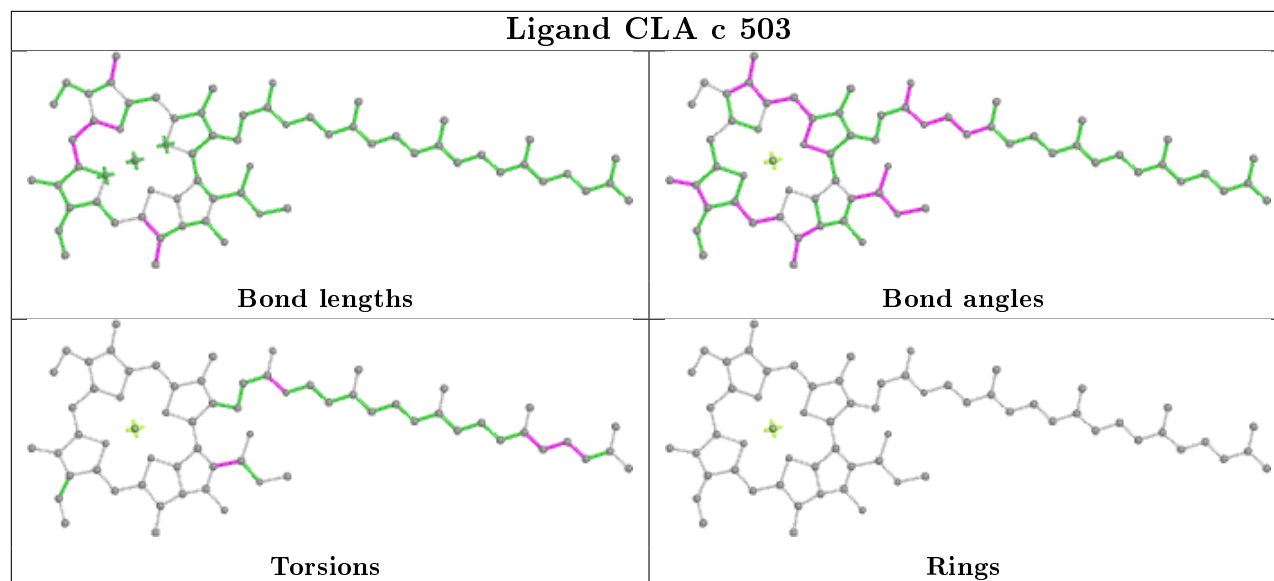
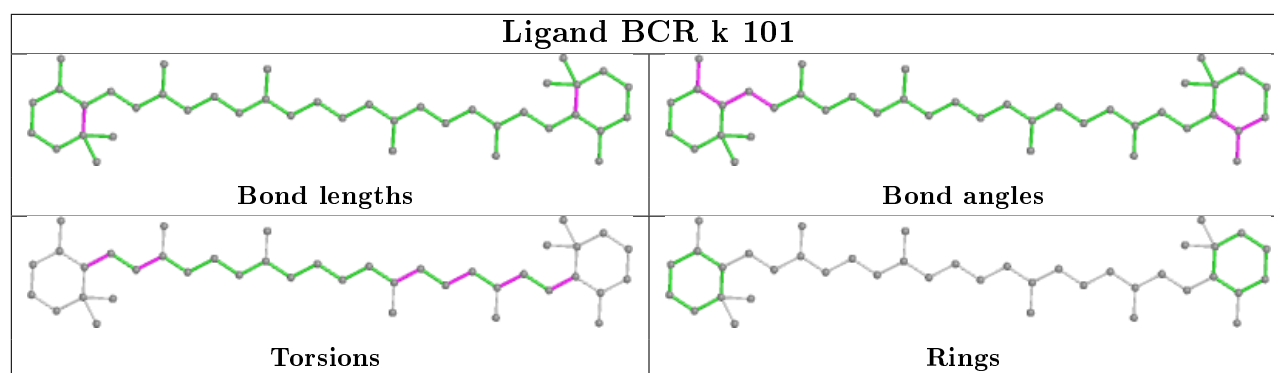


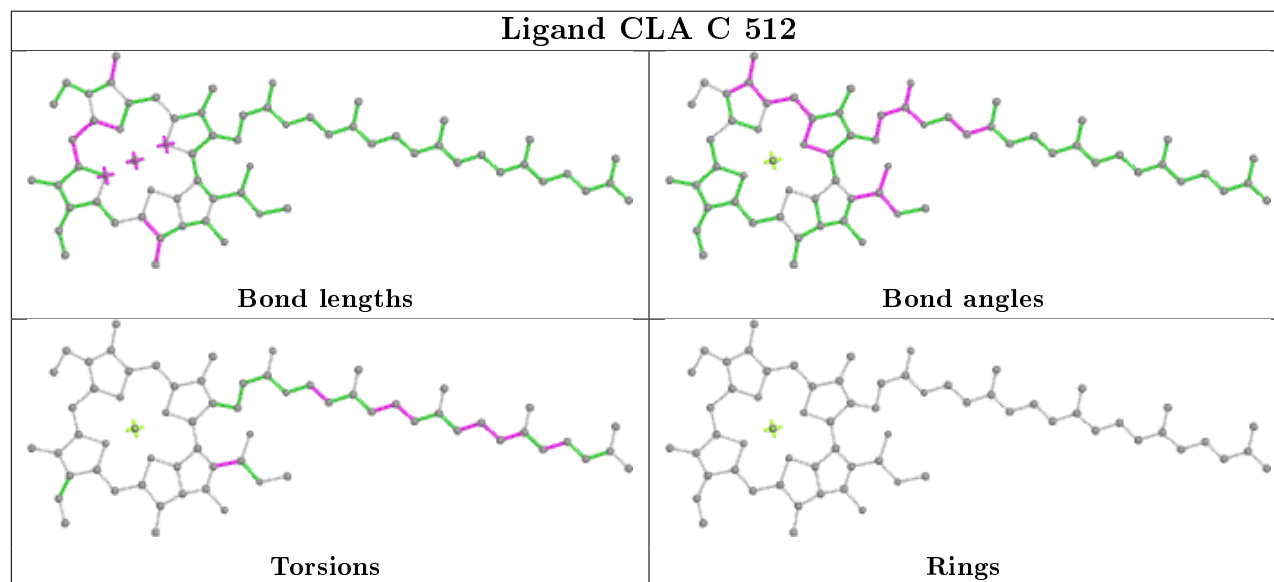
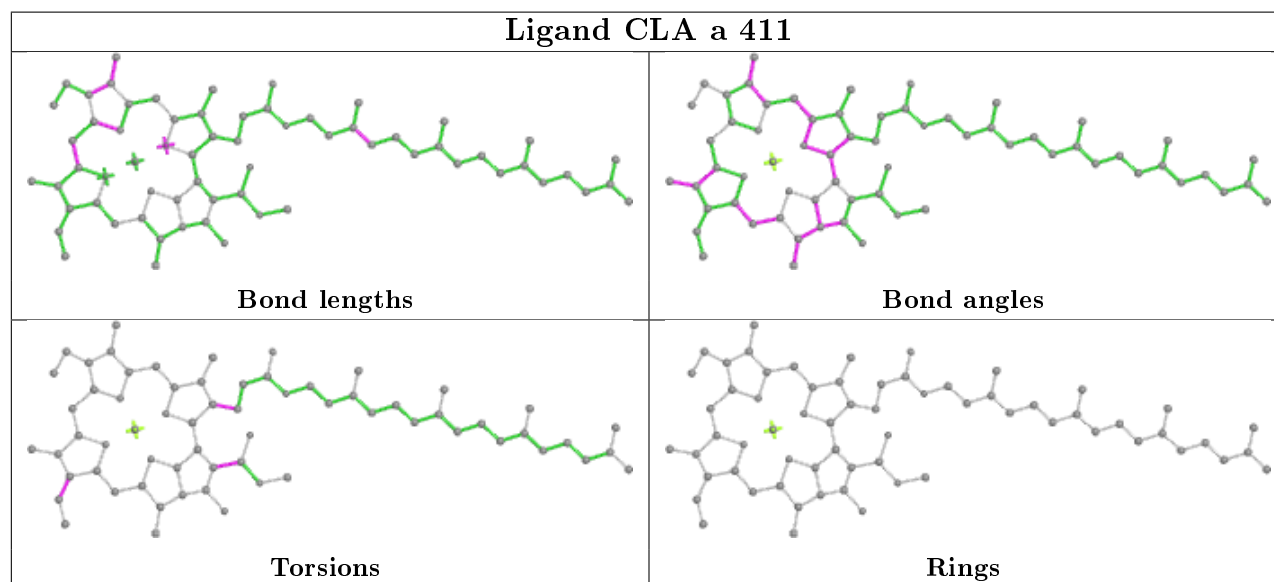
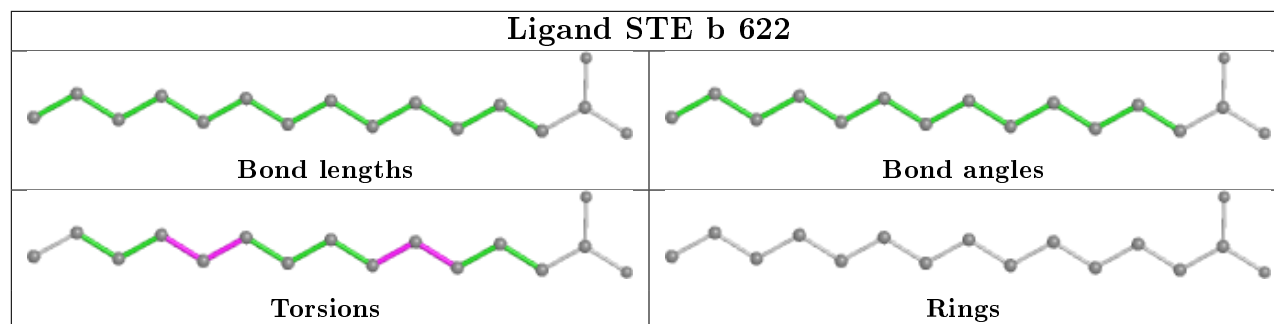
Ligand STE M 103

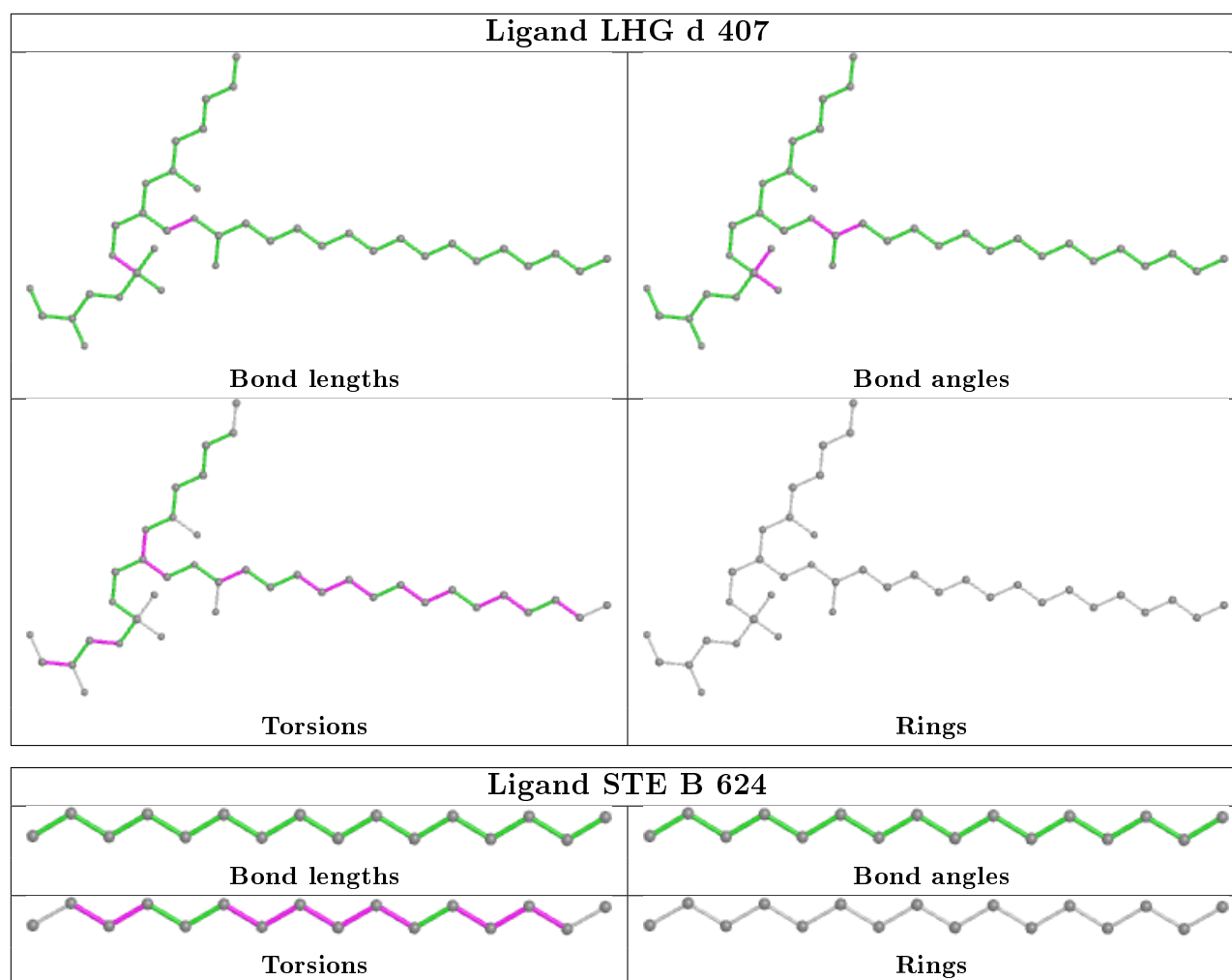


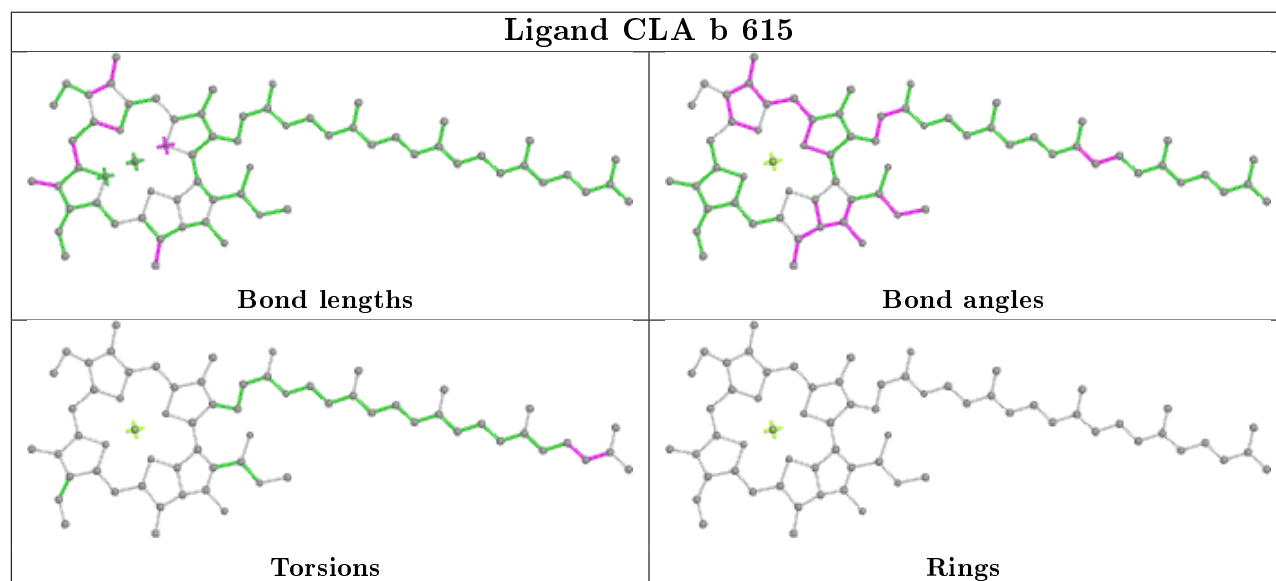
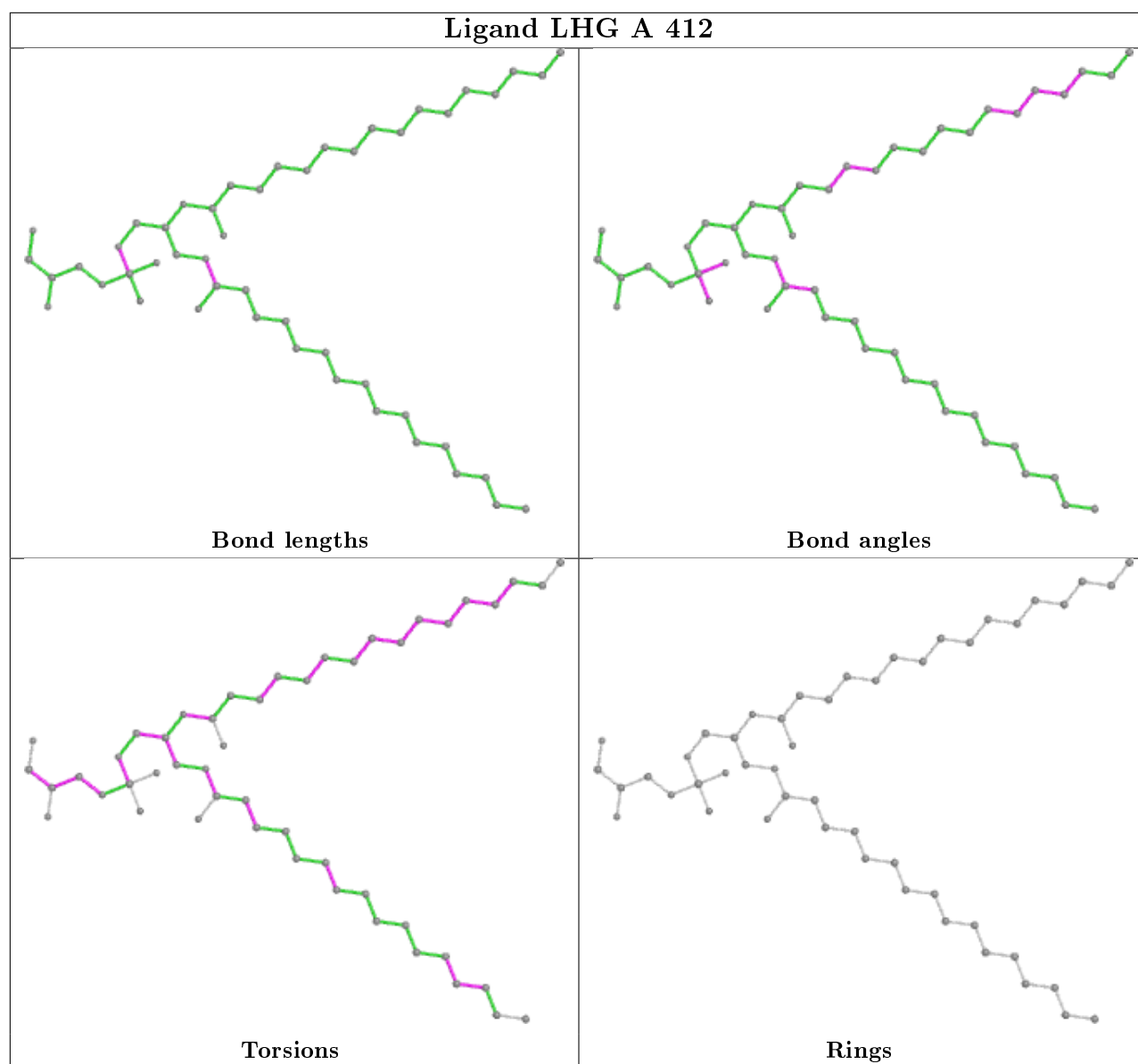
Ligand STE B 620

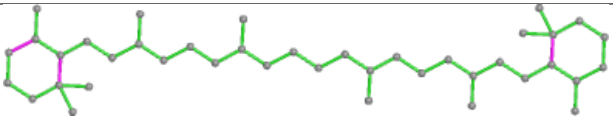
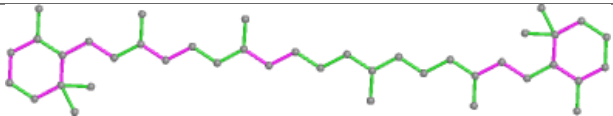
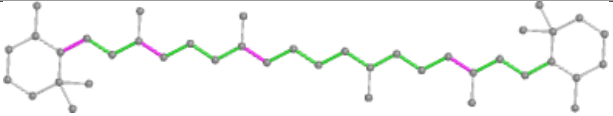
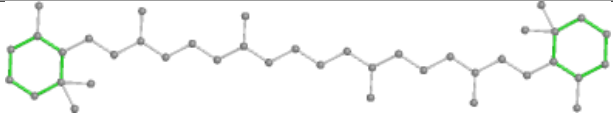


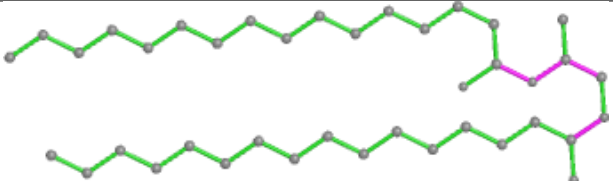
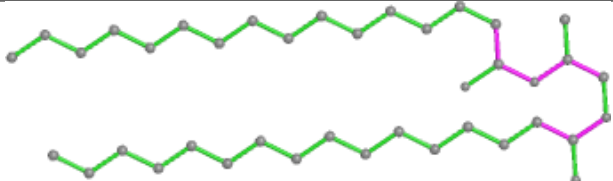
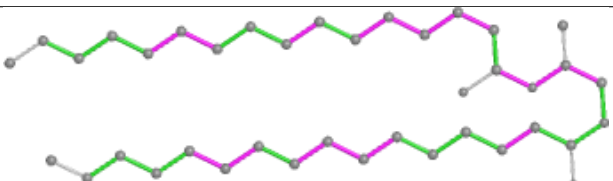
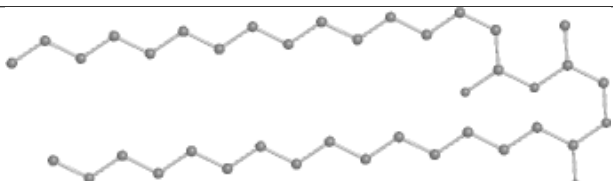


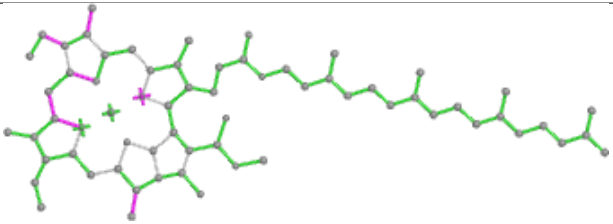
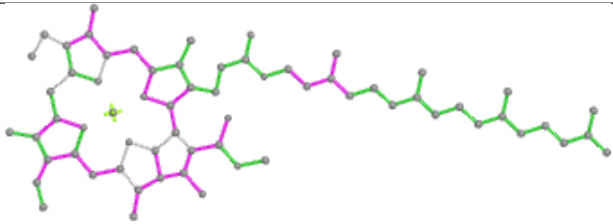
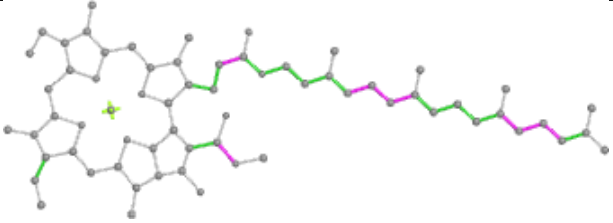
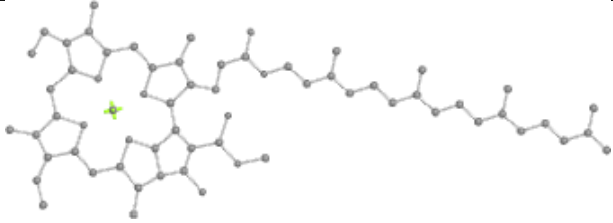


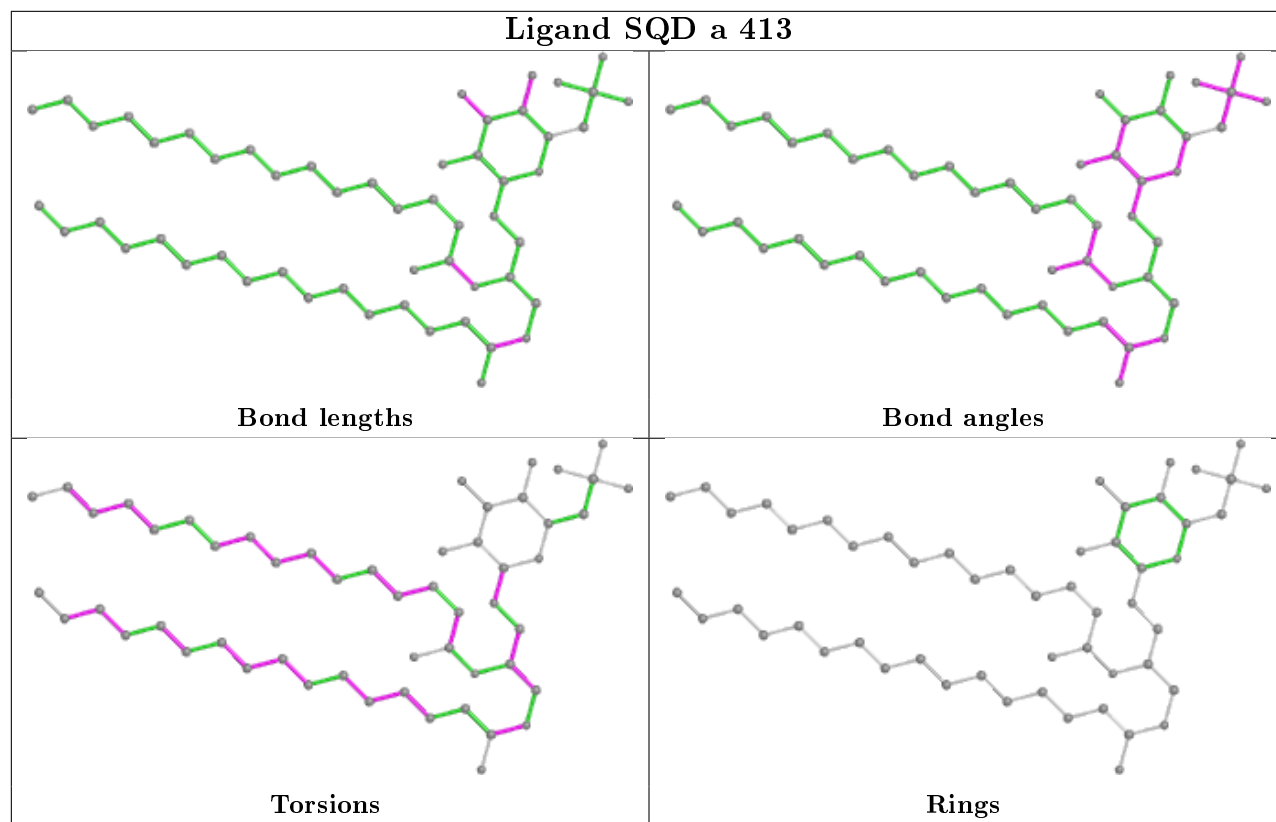
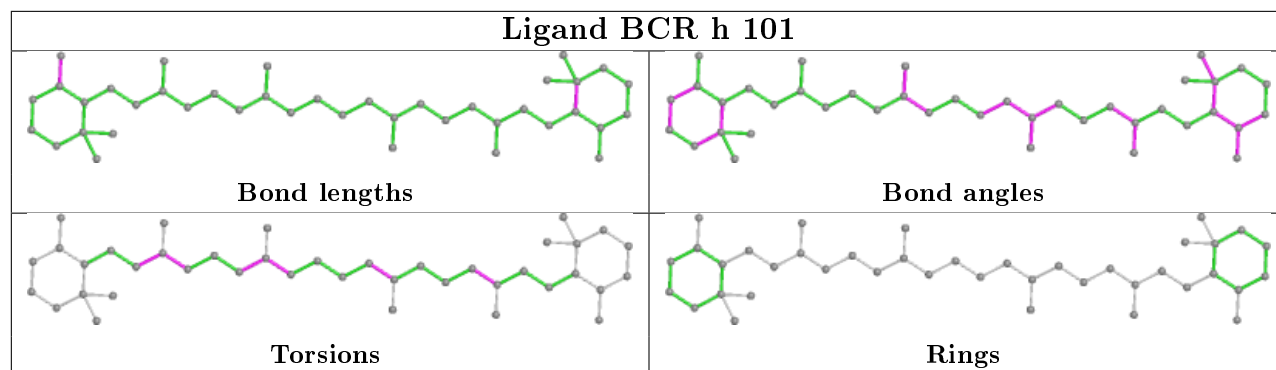


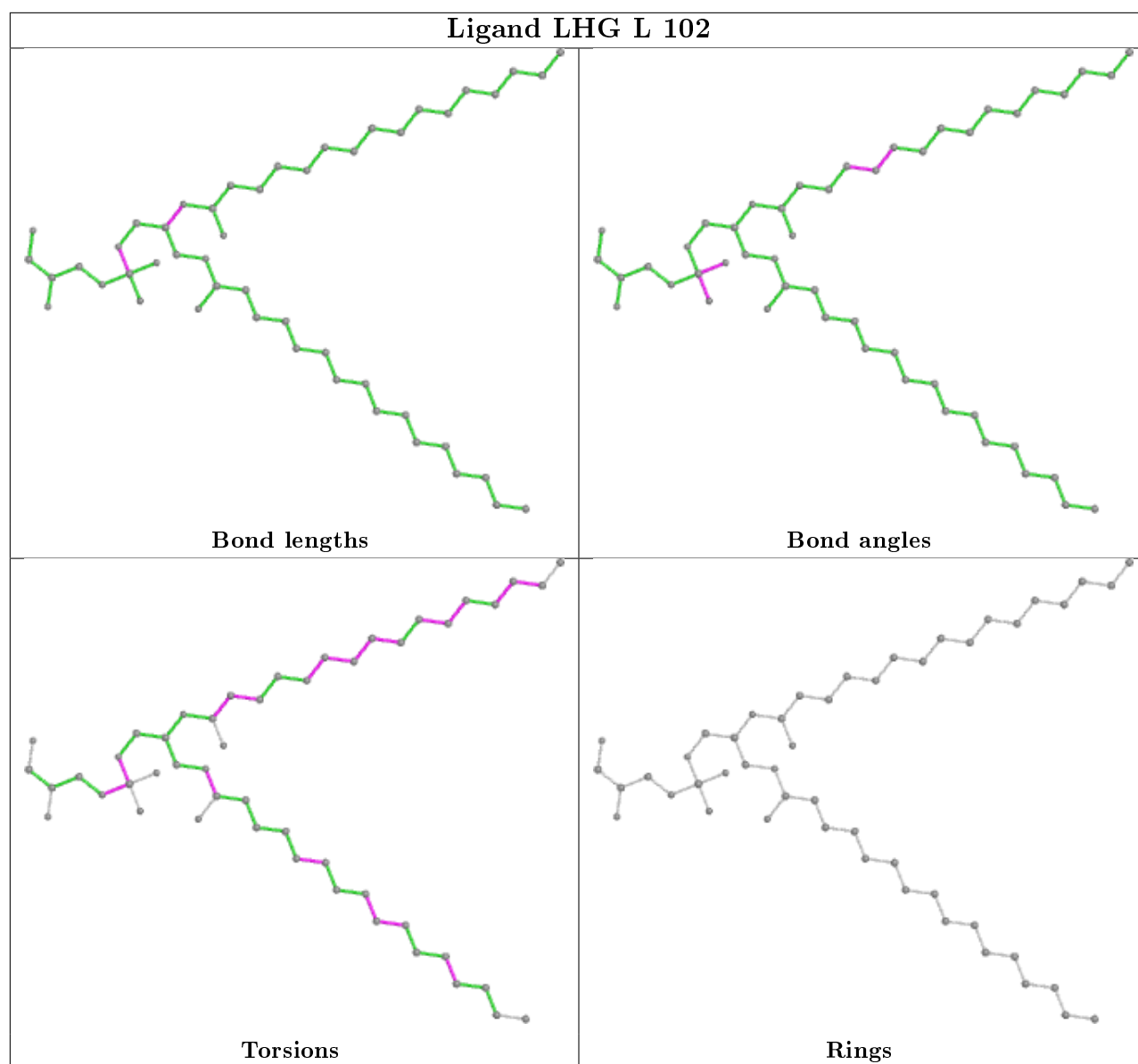


| Ligand BCR b 617 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

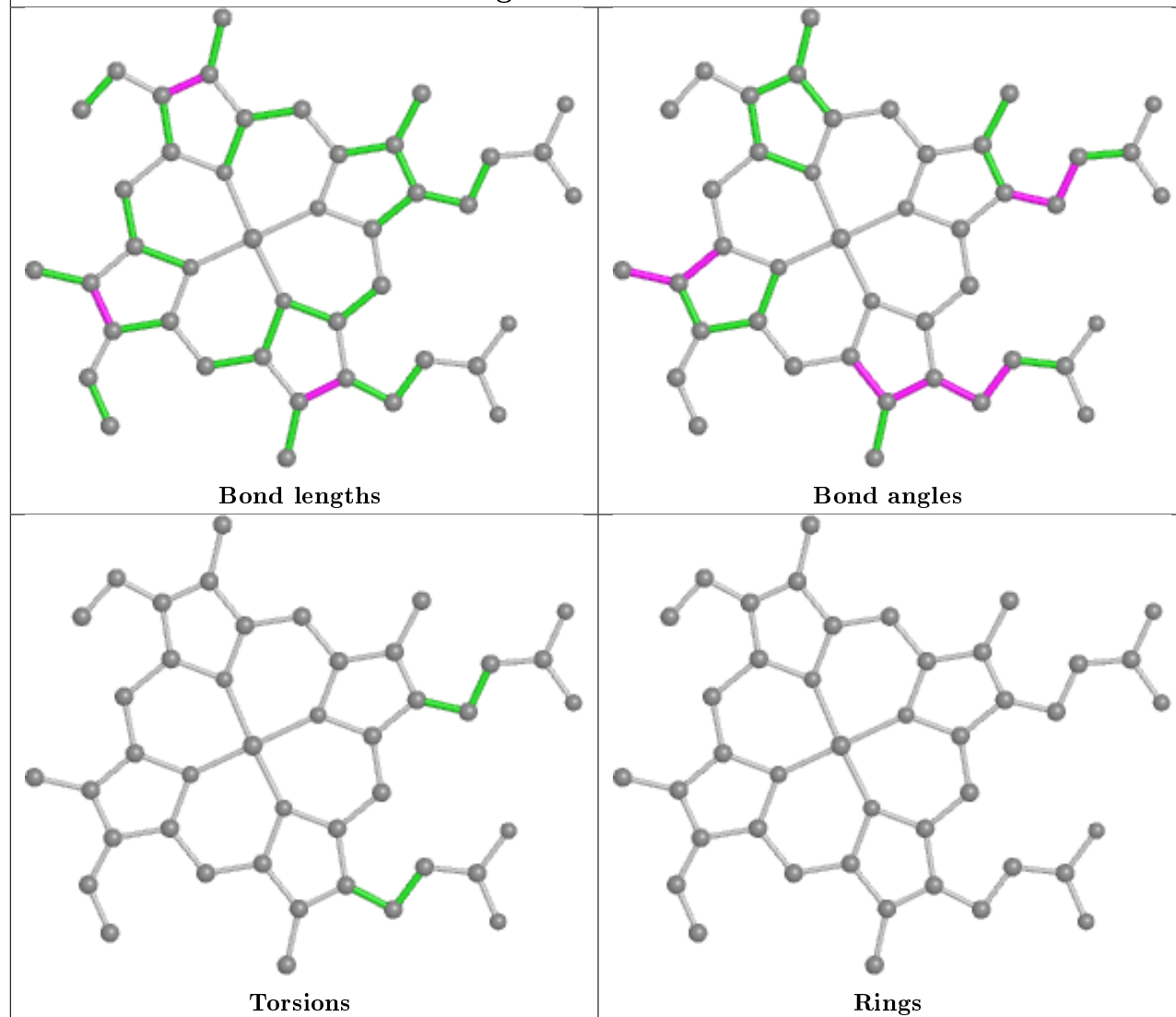
| Ligand SQD A 413 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA B 613 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

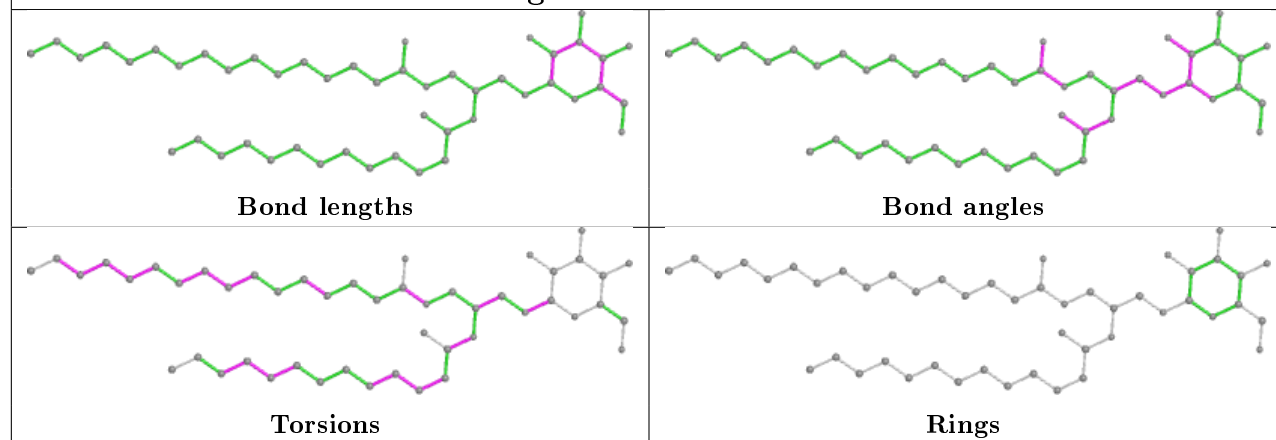


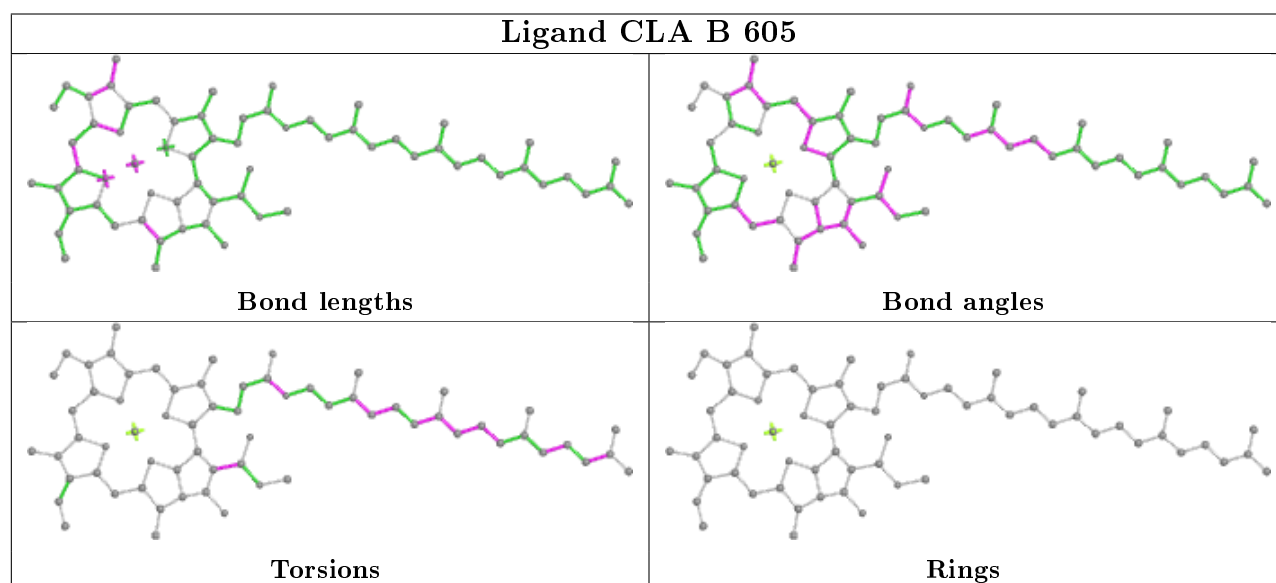
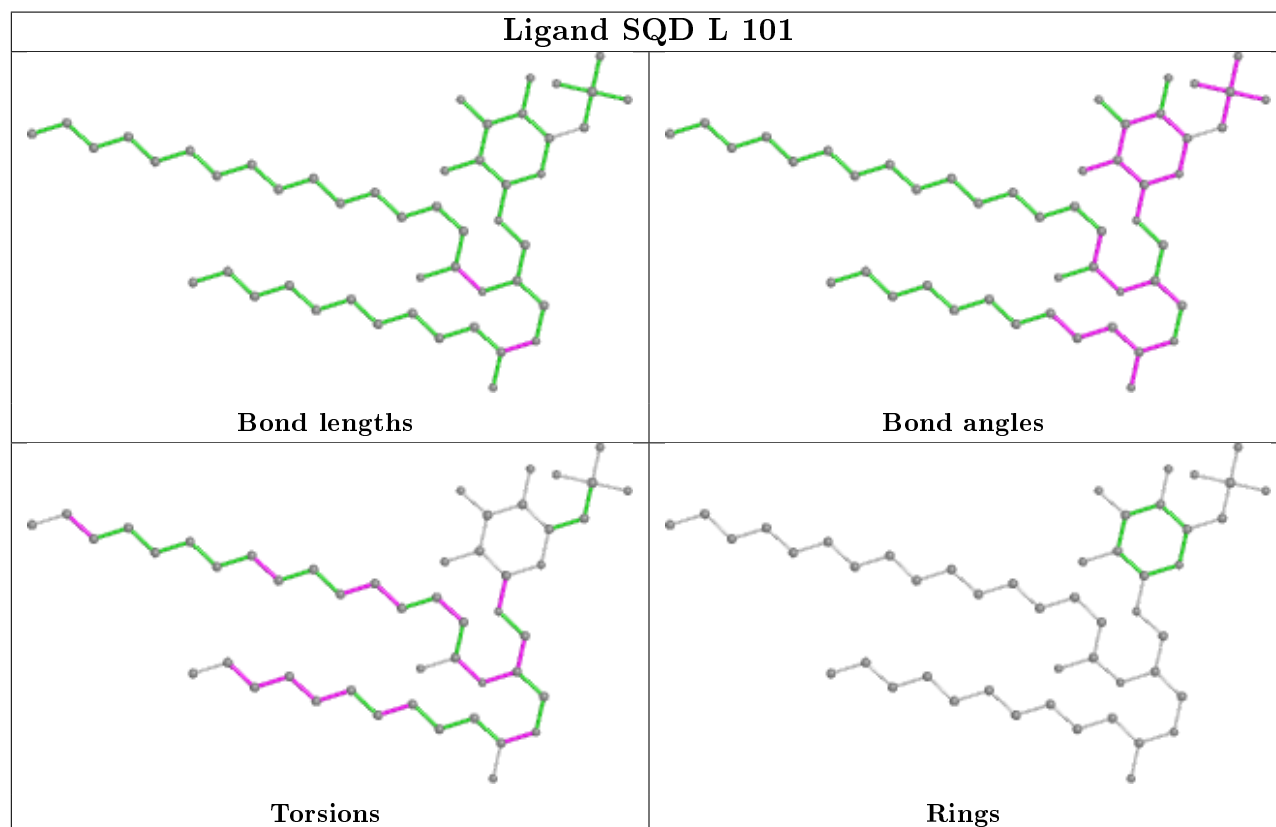
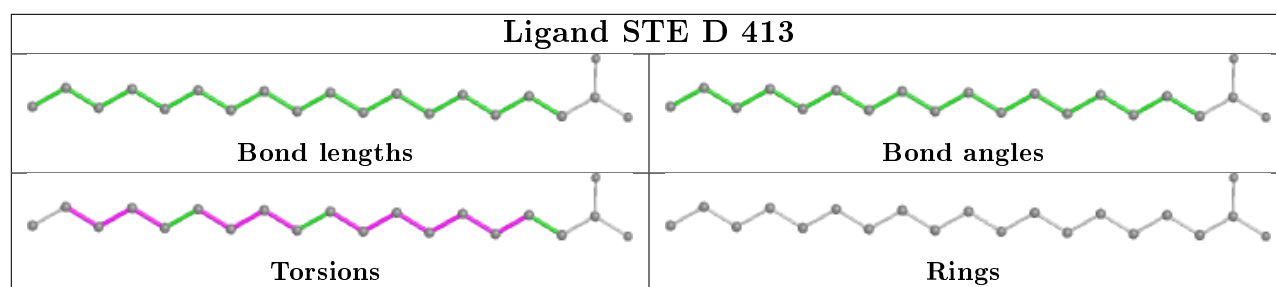


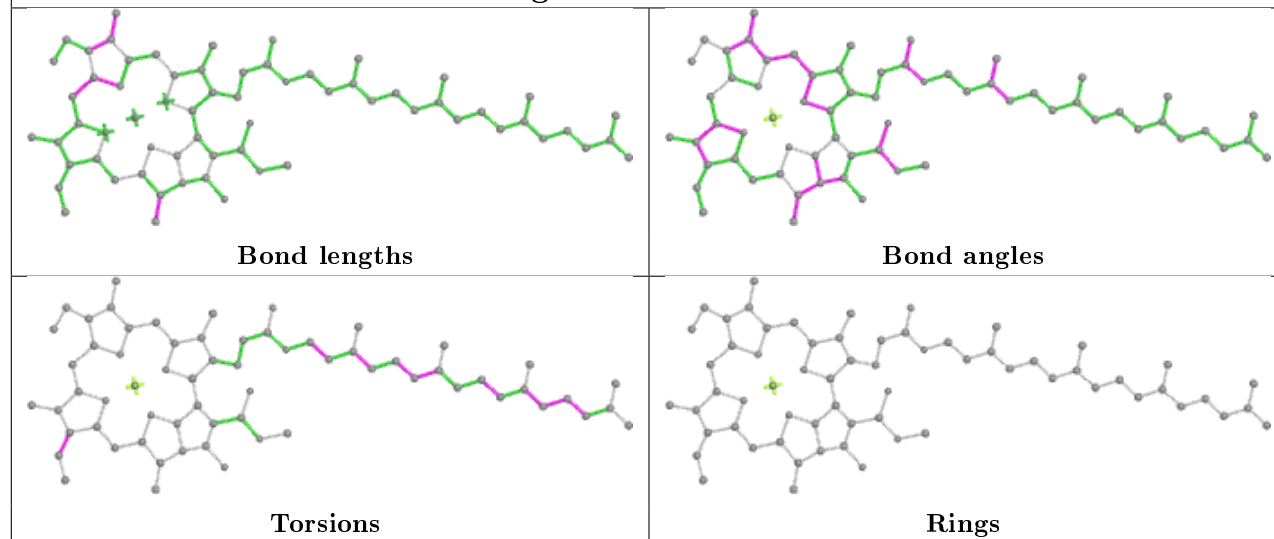
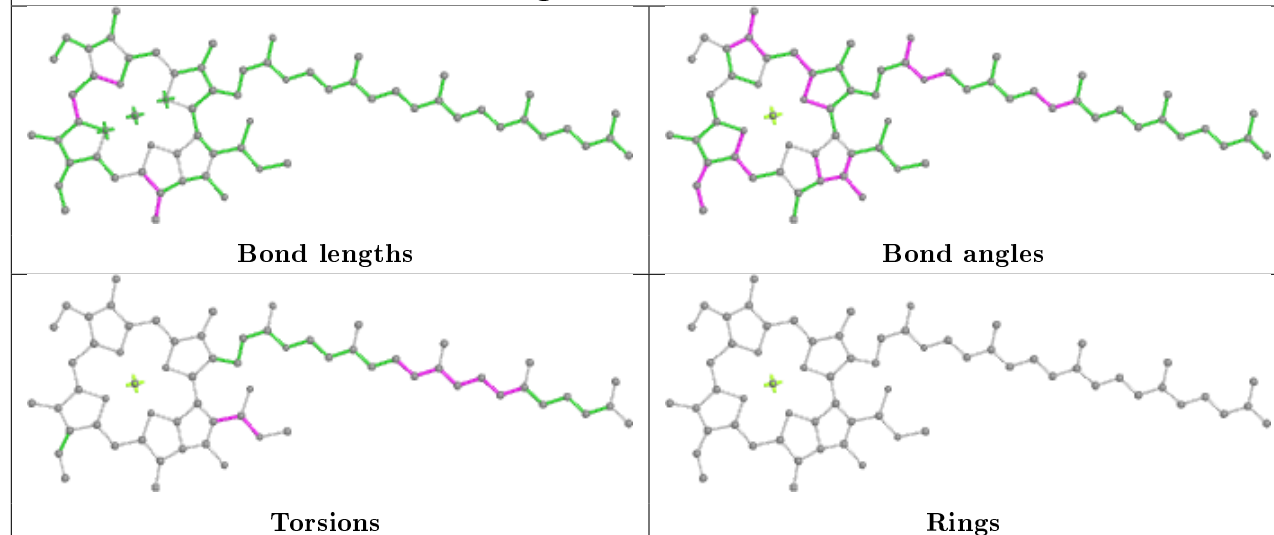
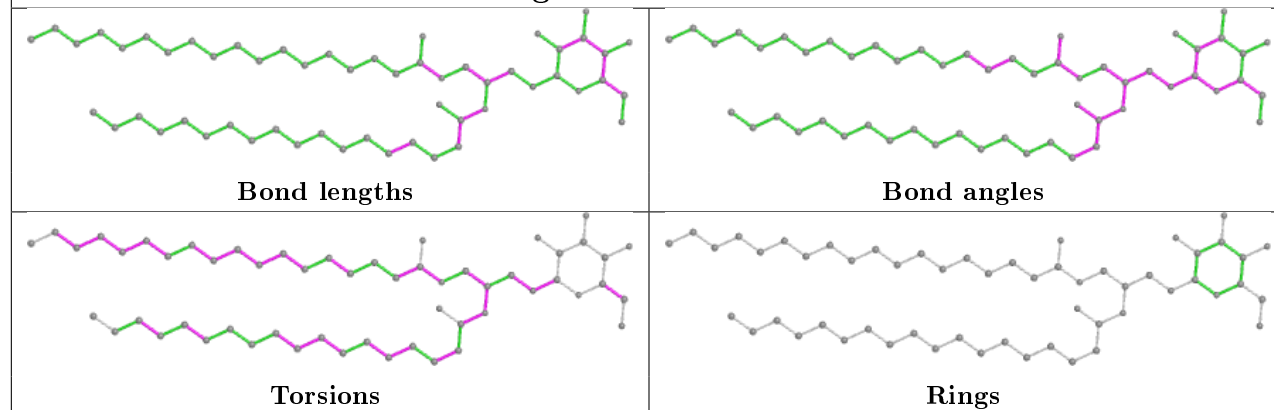
Ligand HEC f 101



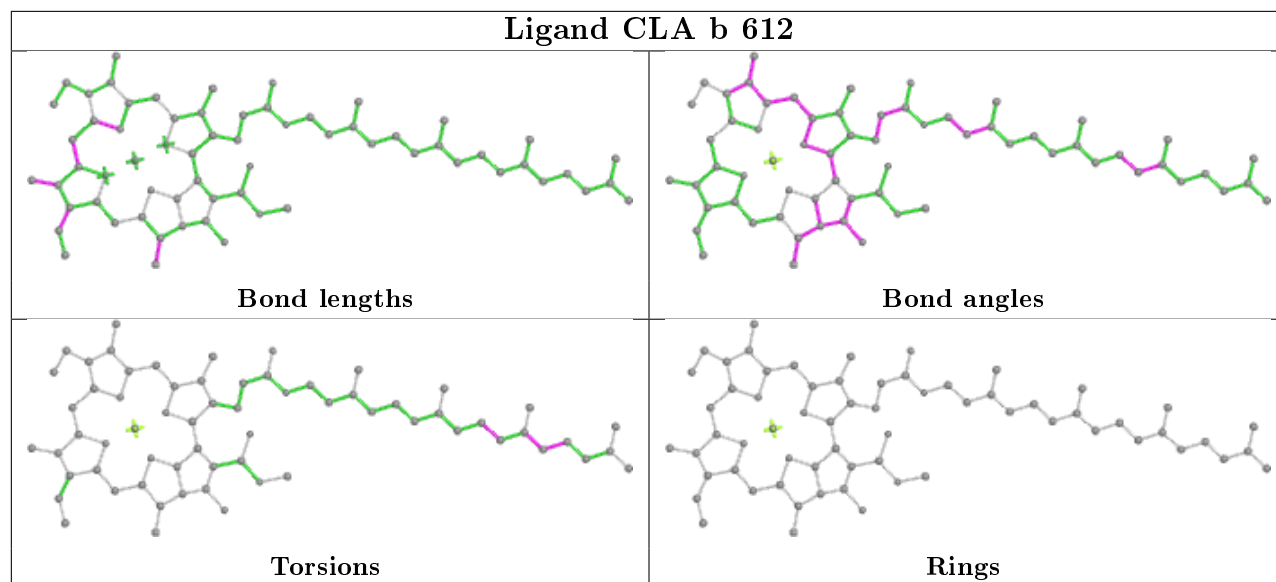
Ligand LMG Y 101



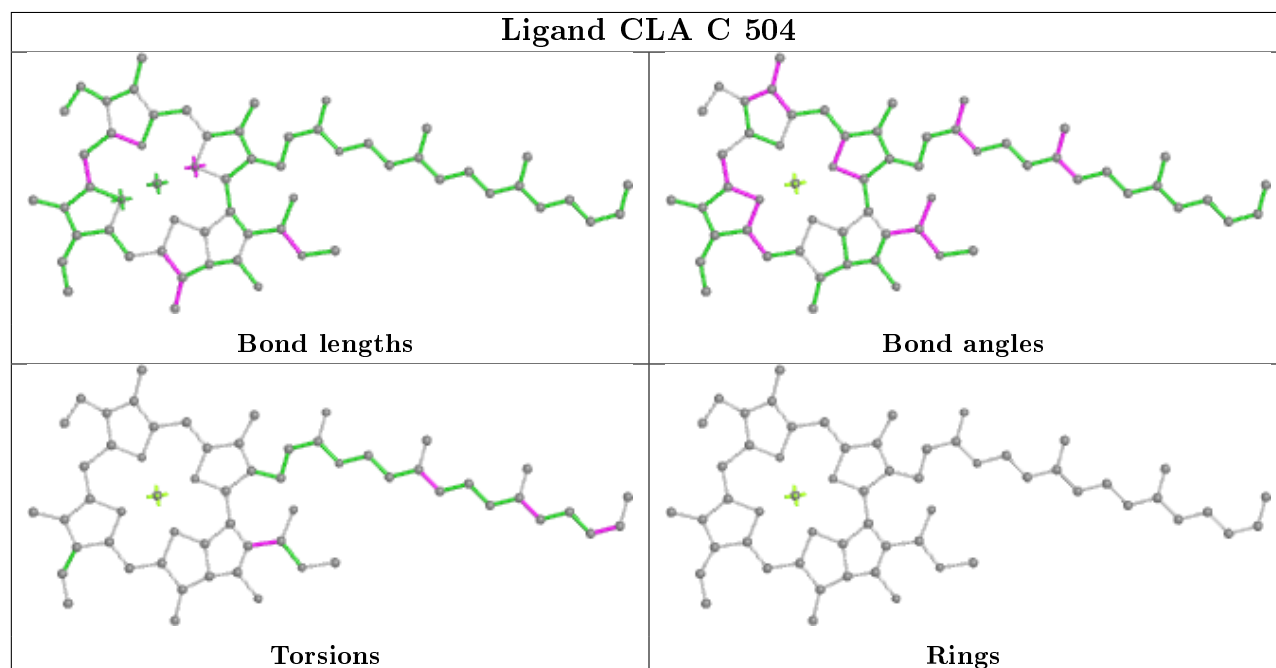


Ligand CLA D 405**Ligand CLA b 607****Ligand LMG a 417**

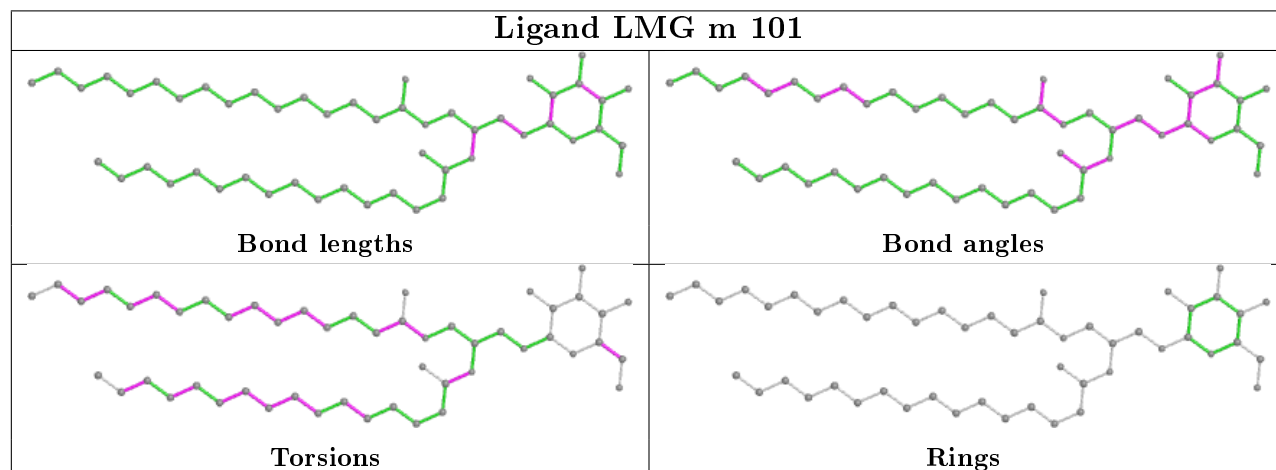
Ligand CLA b 612

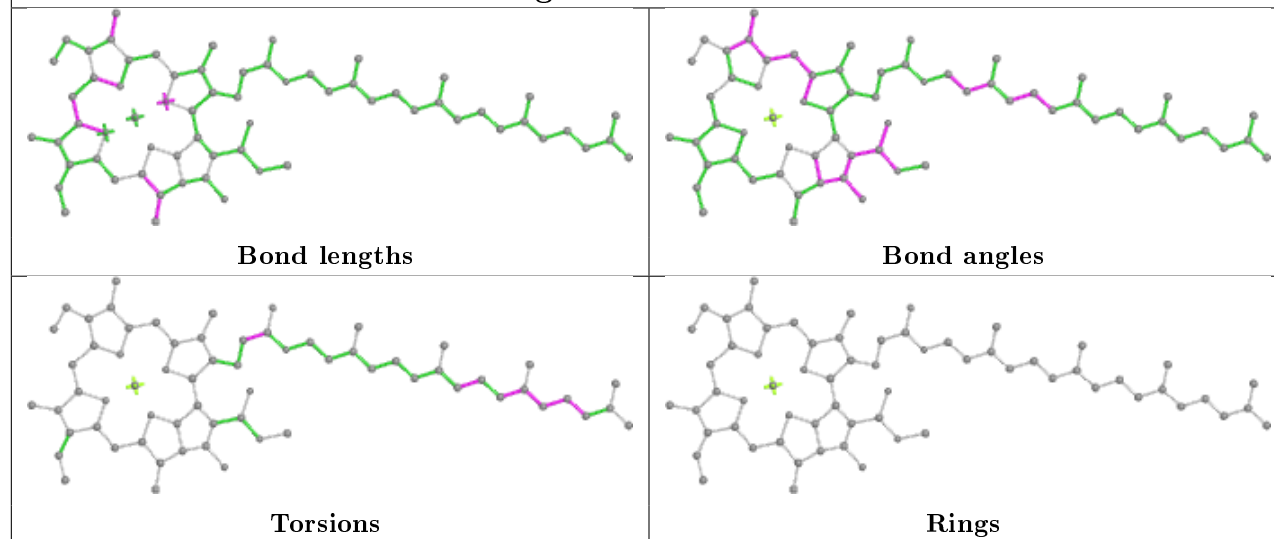
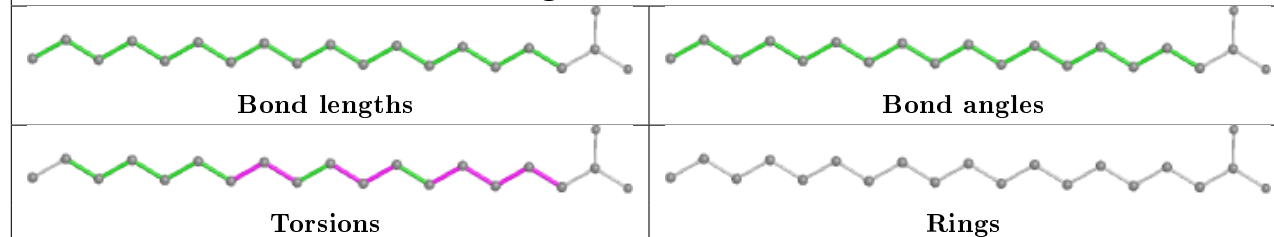
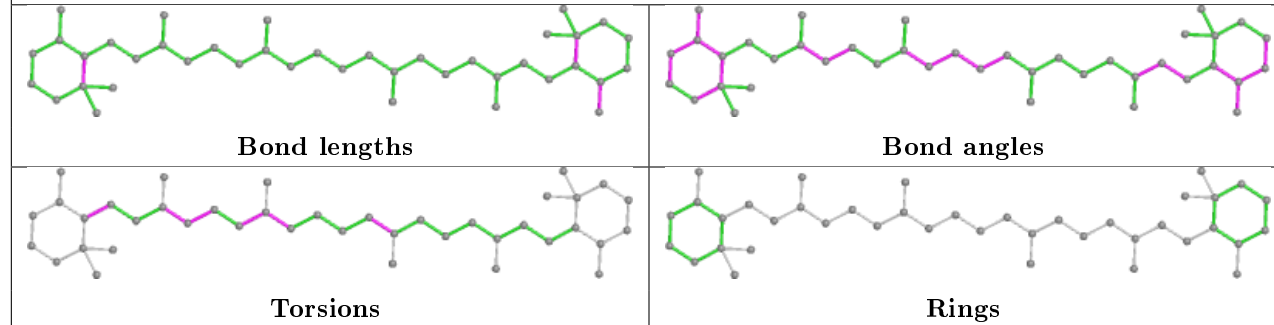


Ligand CLA C 504

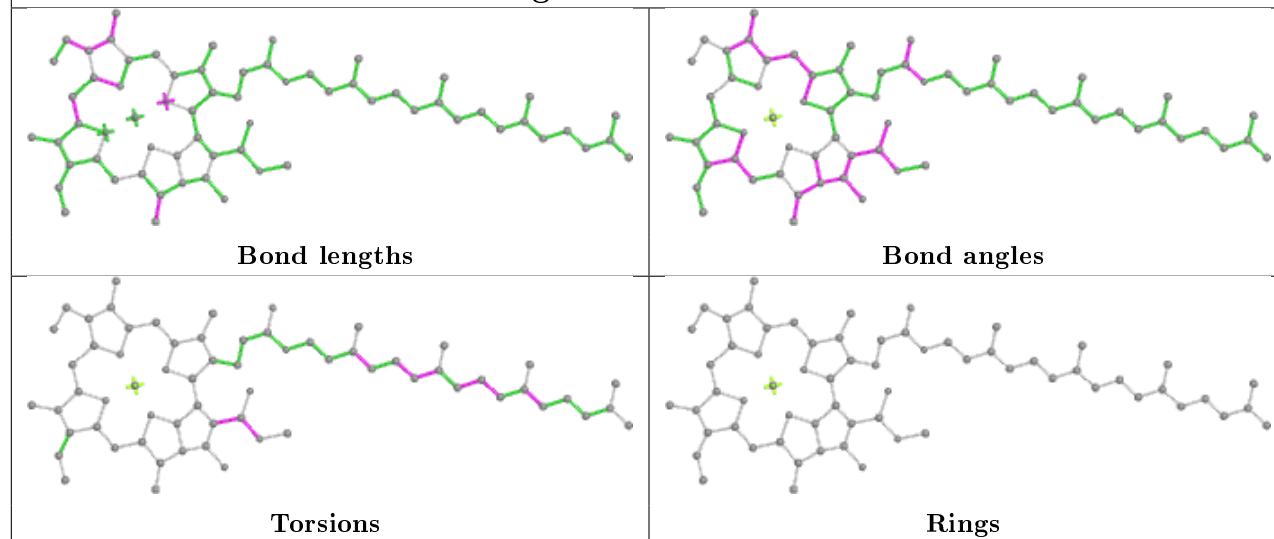


Ligand LMG m 101

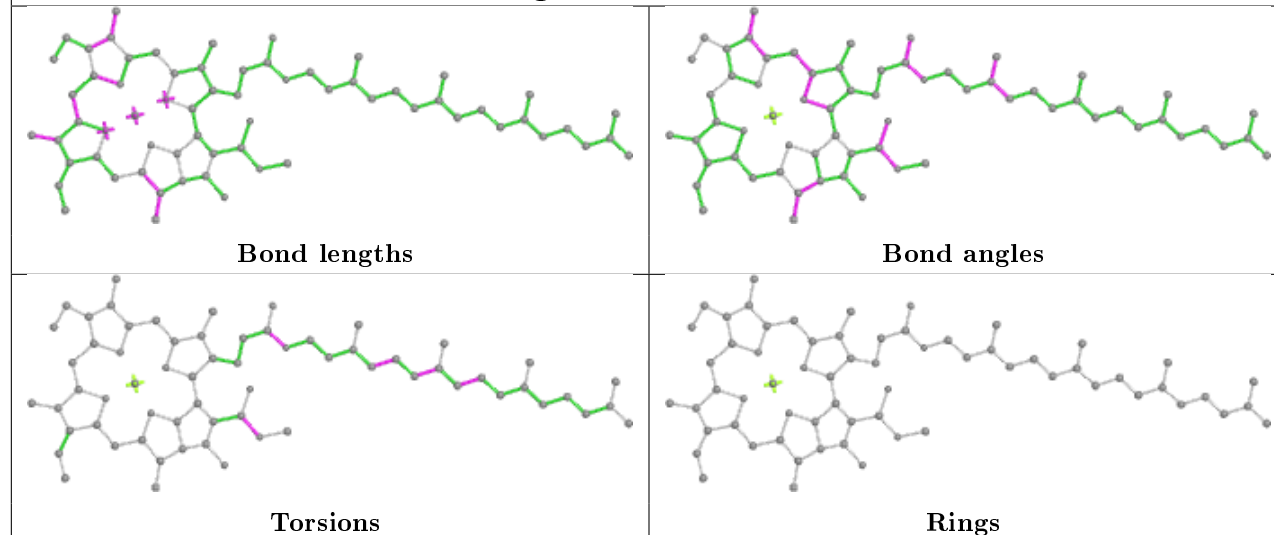


Ligand CLA b 613**Ligand STE c 521****Ligand BCR c 515**

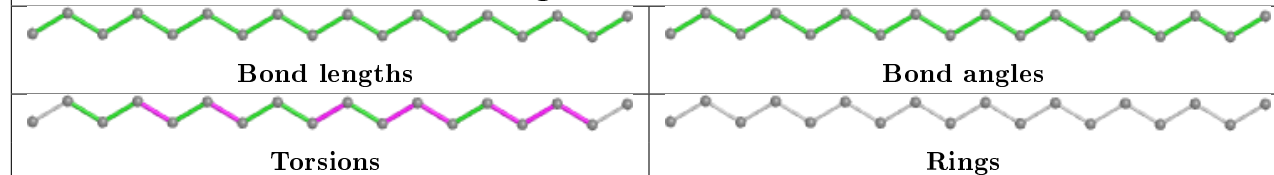
Ligand CLA B 603



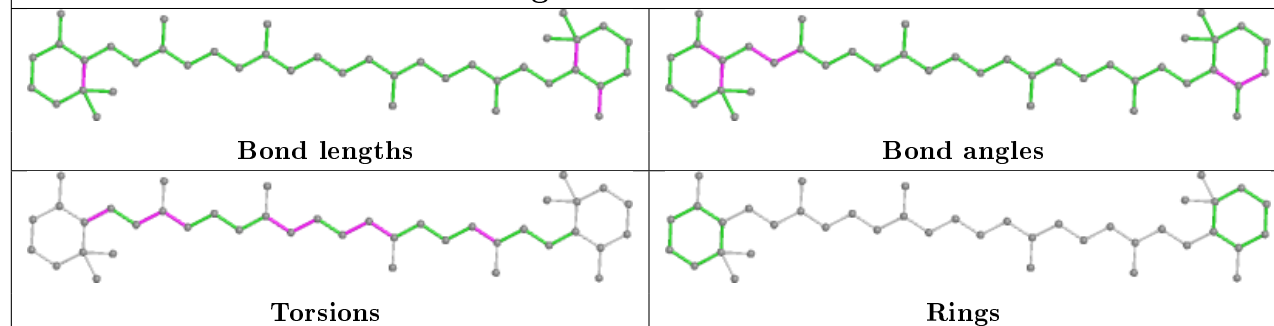
Ligand CLA C 511

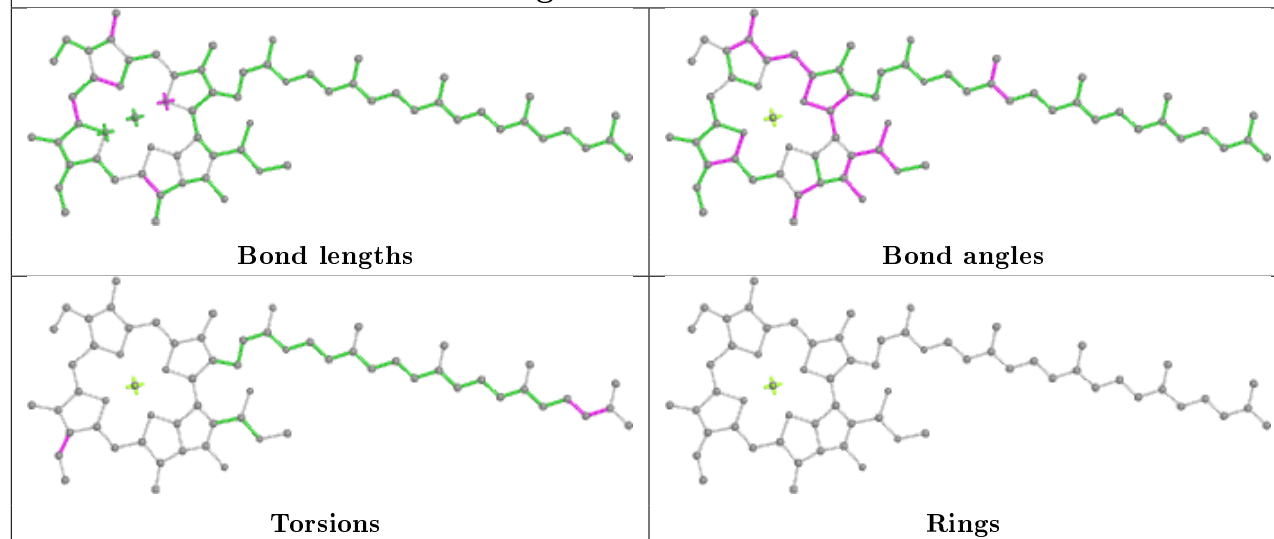
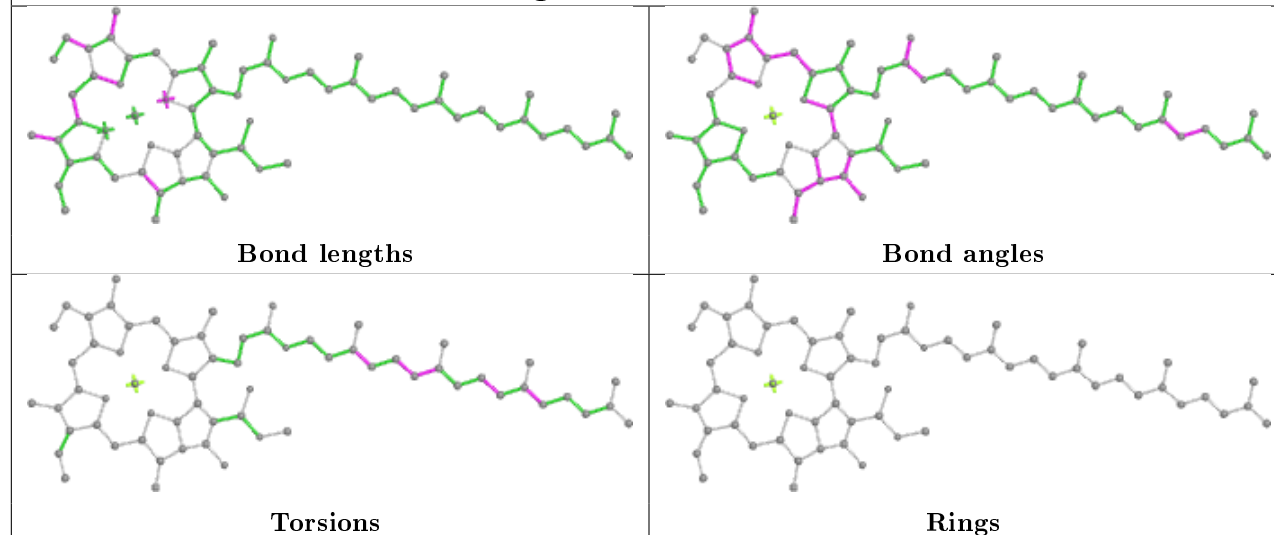
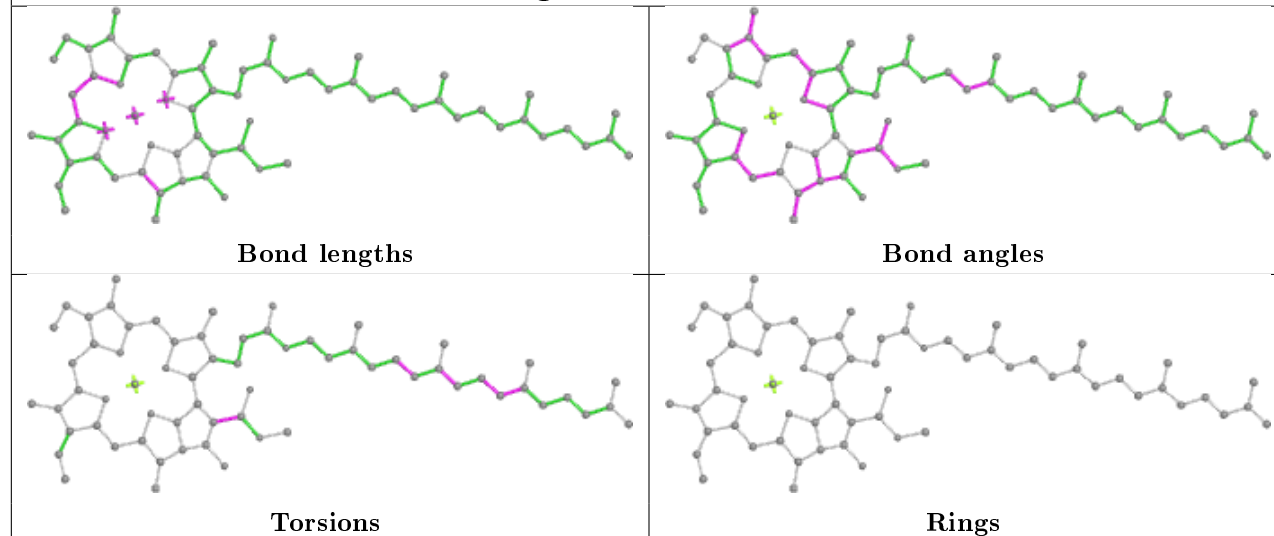


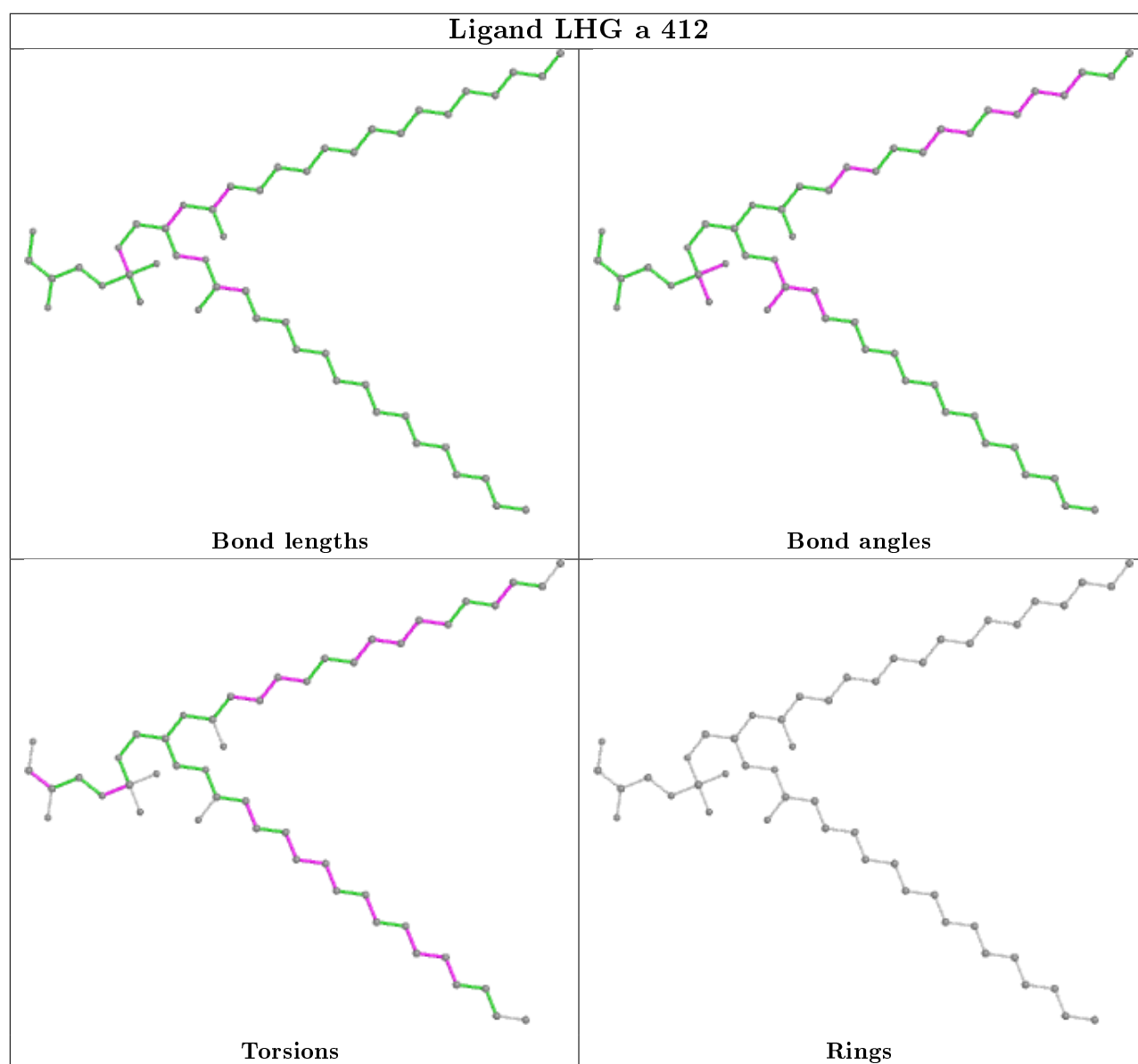
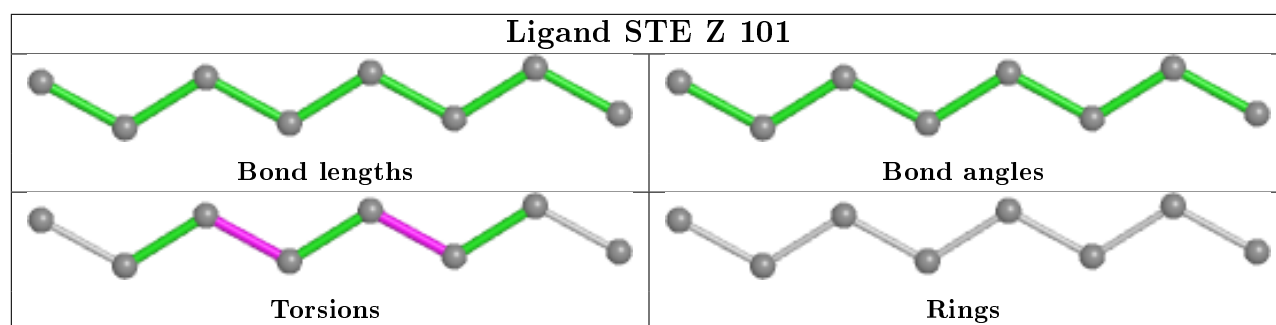
Ligand STE H 103

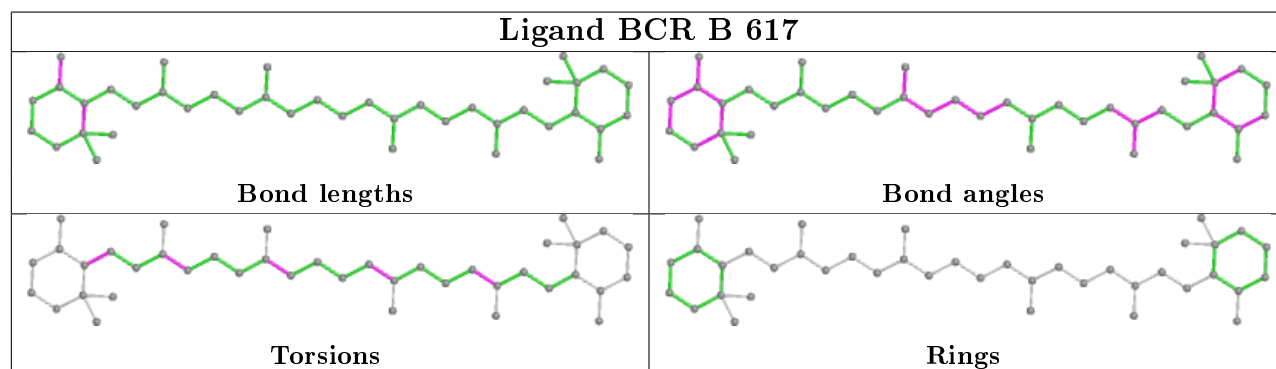
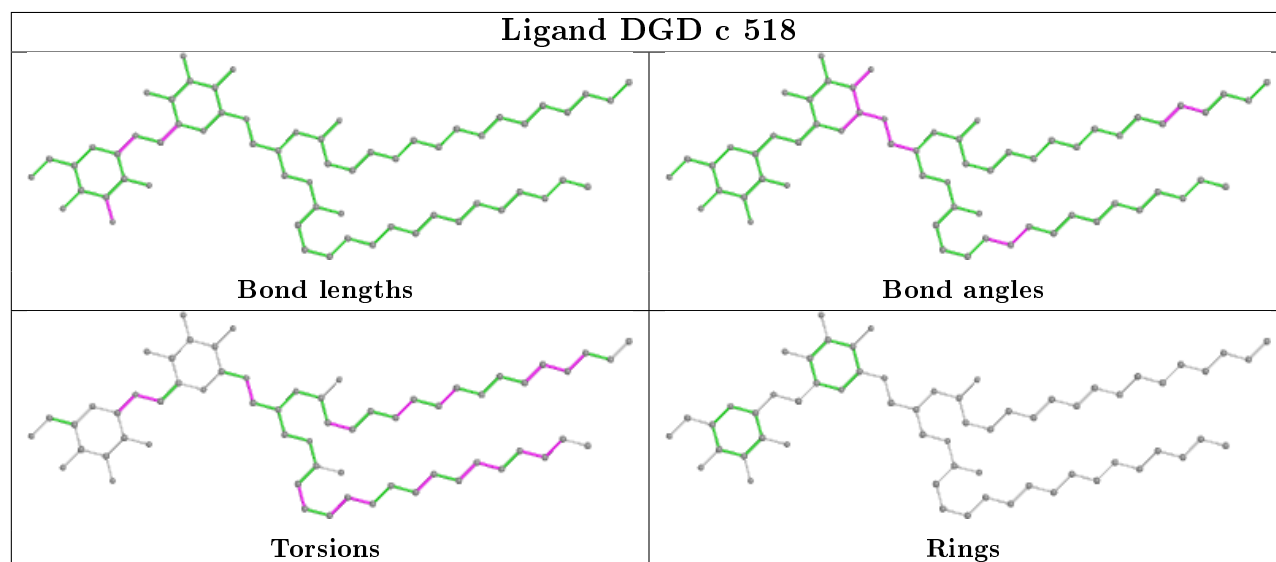
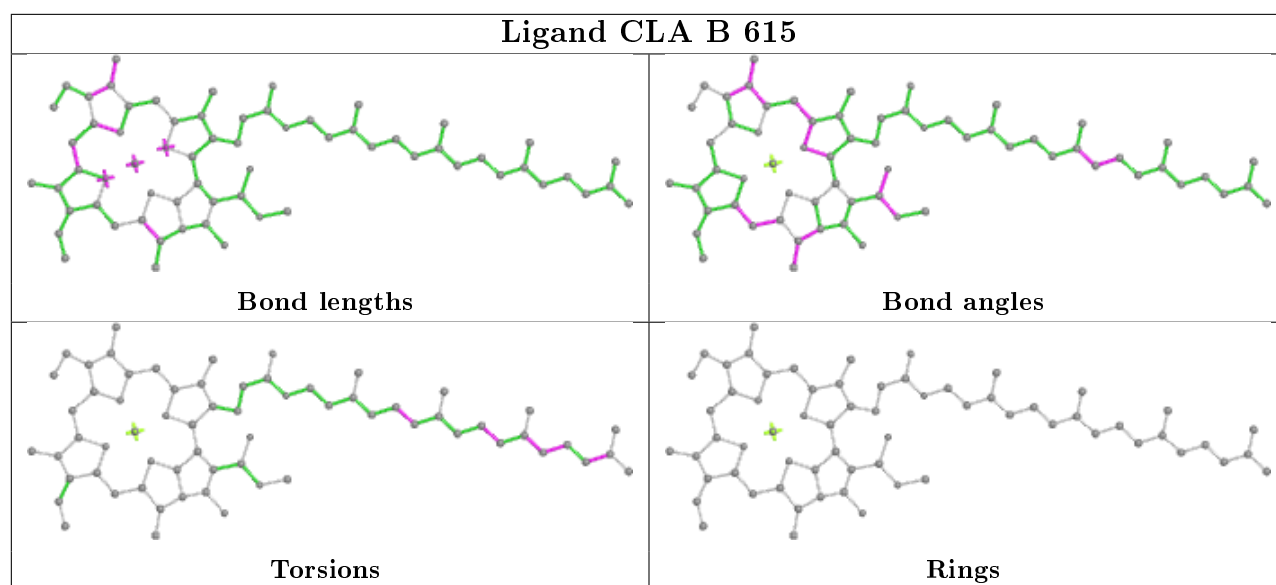


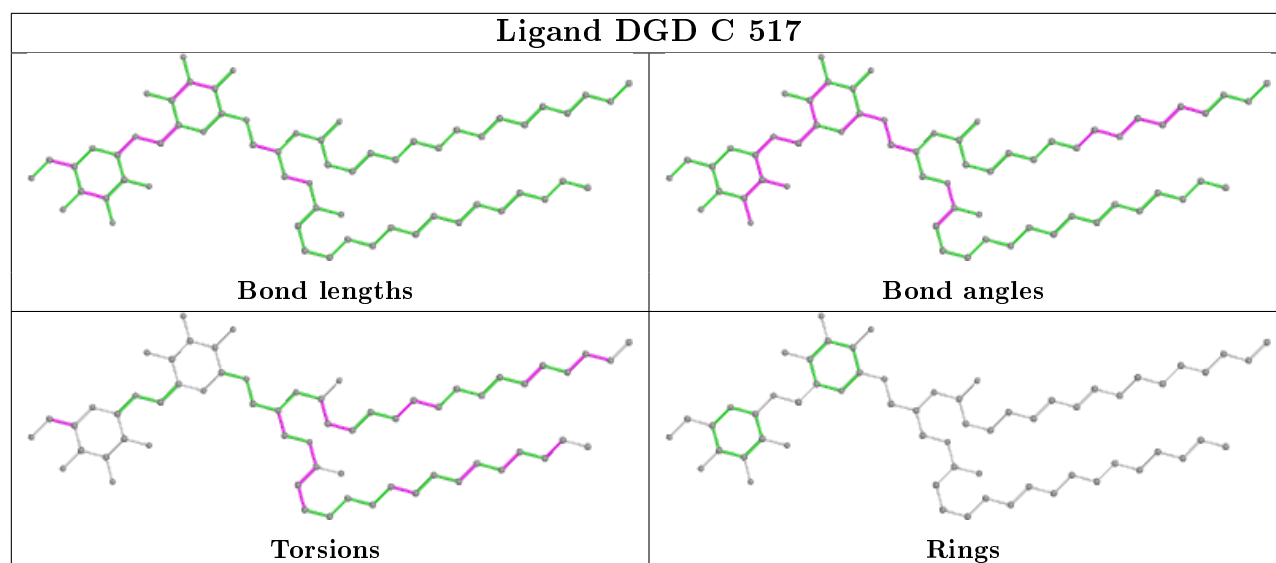
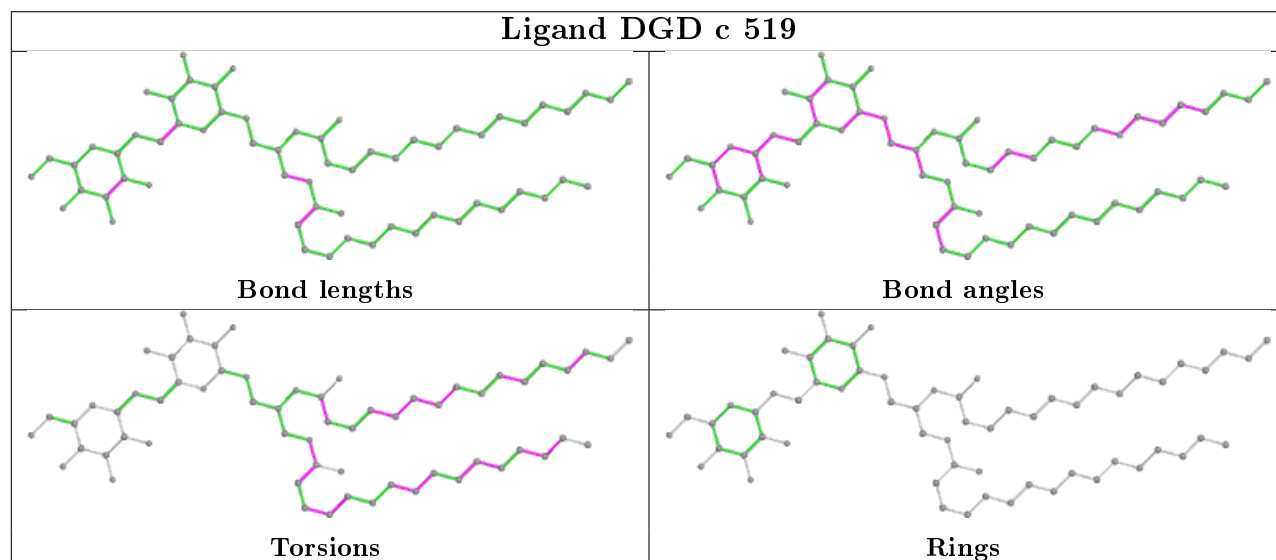
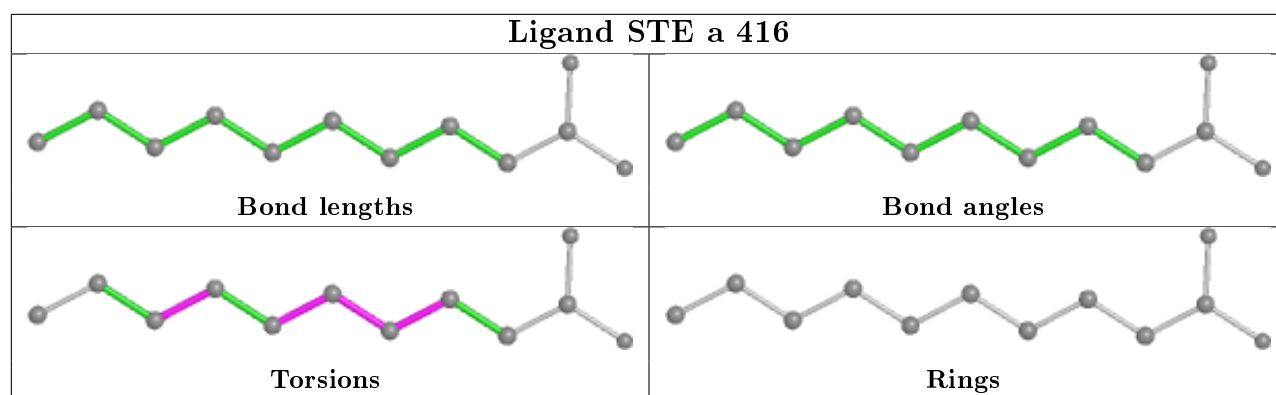
Ligand BCR T 101



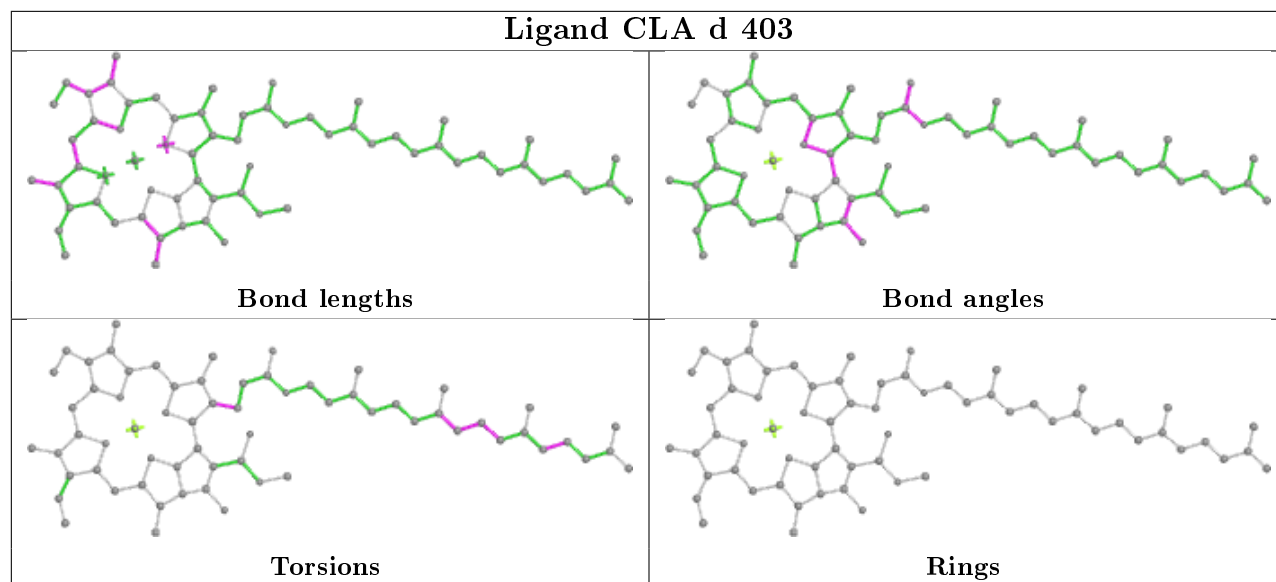
Ligand CLA a 402**Ligand CLA C 505****Ligand CLA b 605**



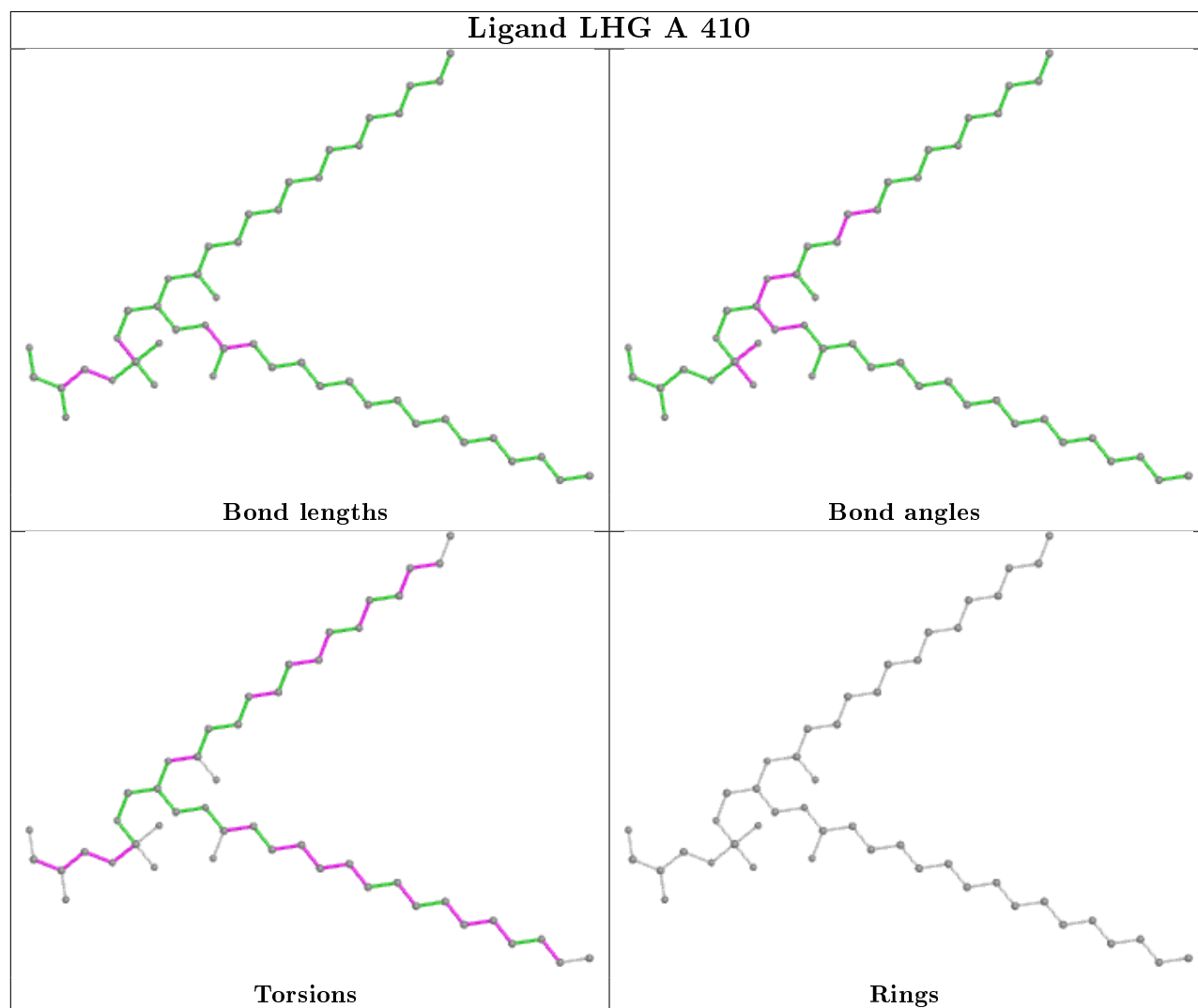


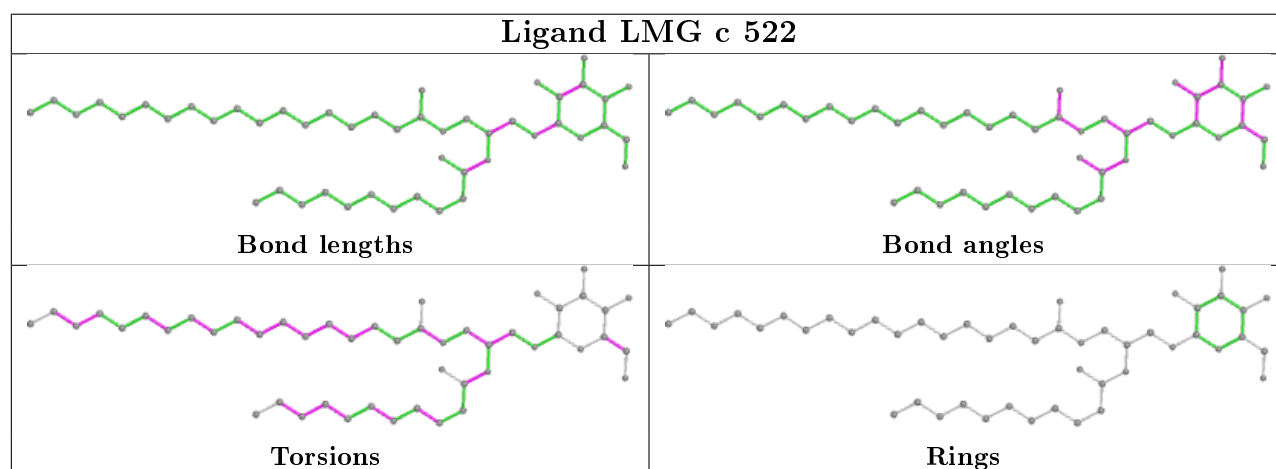
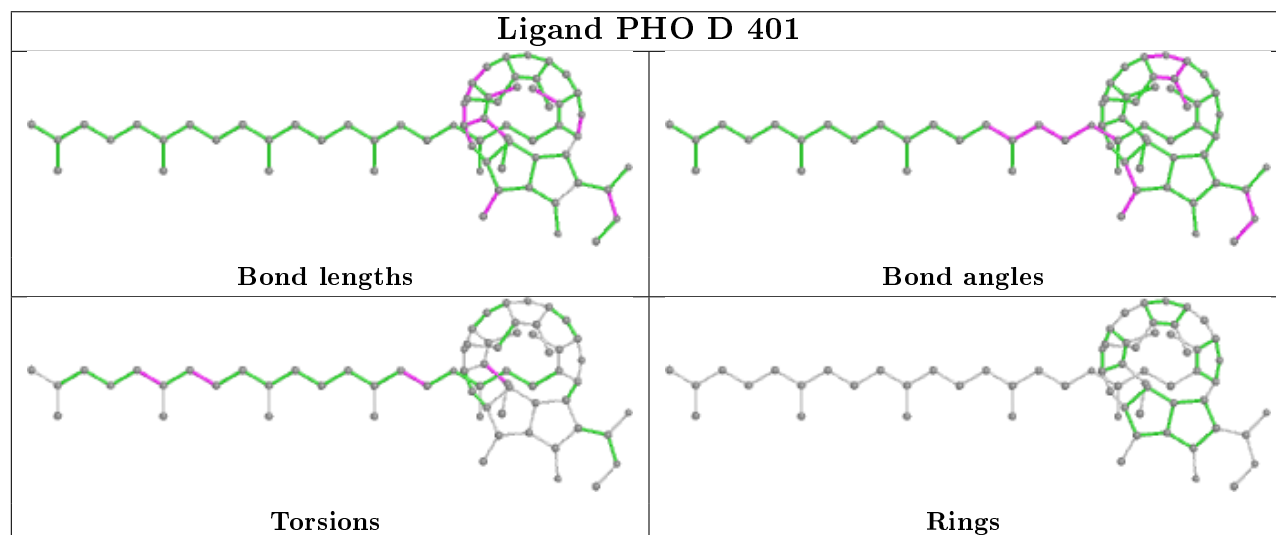
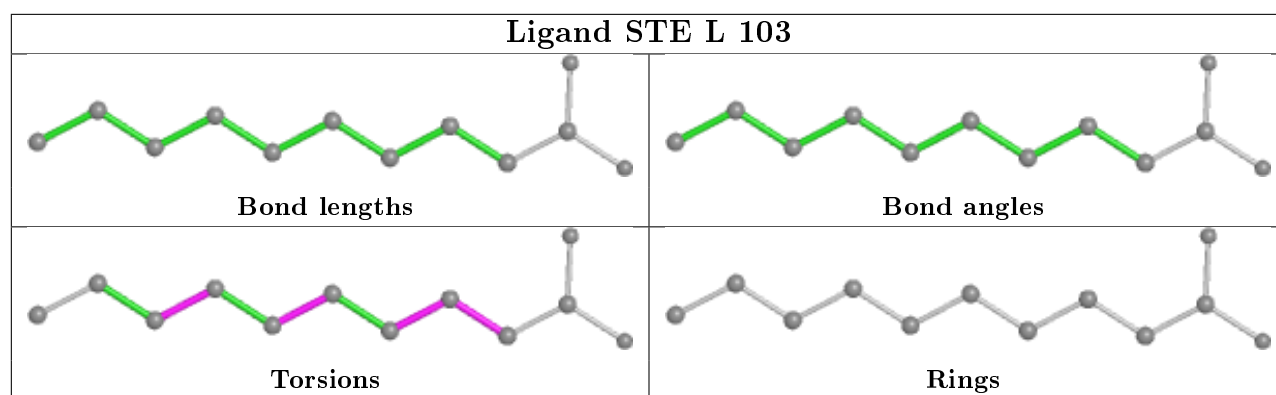


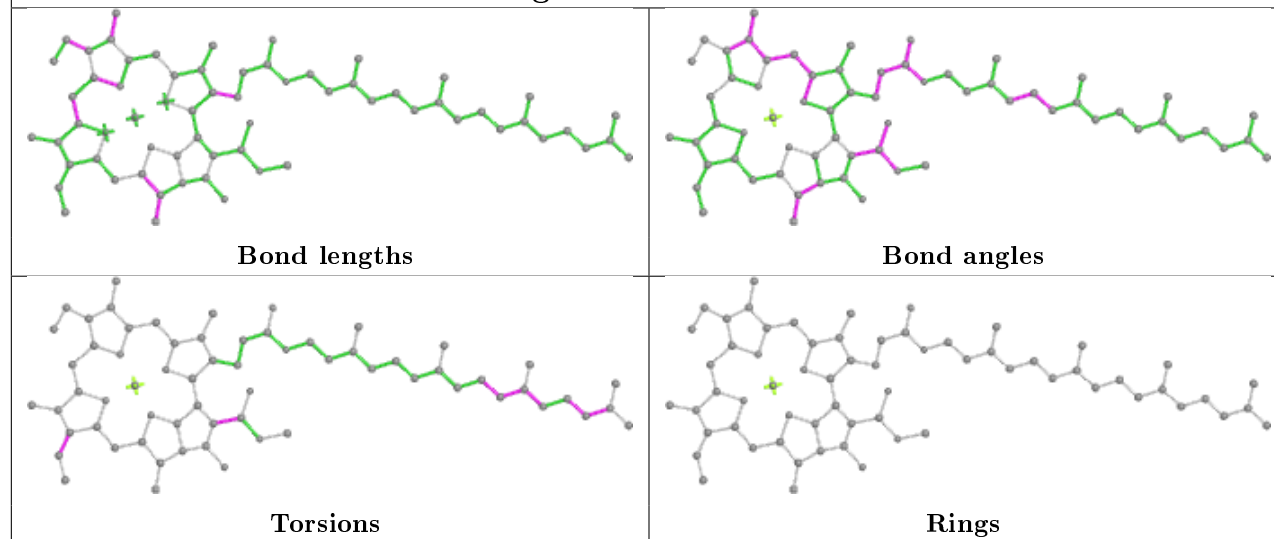
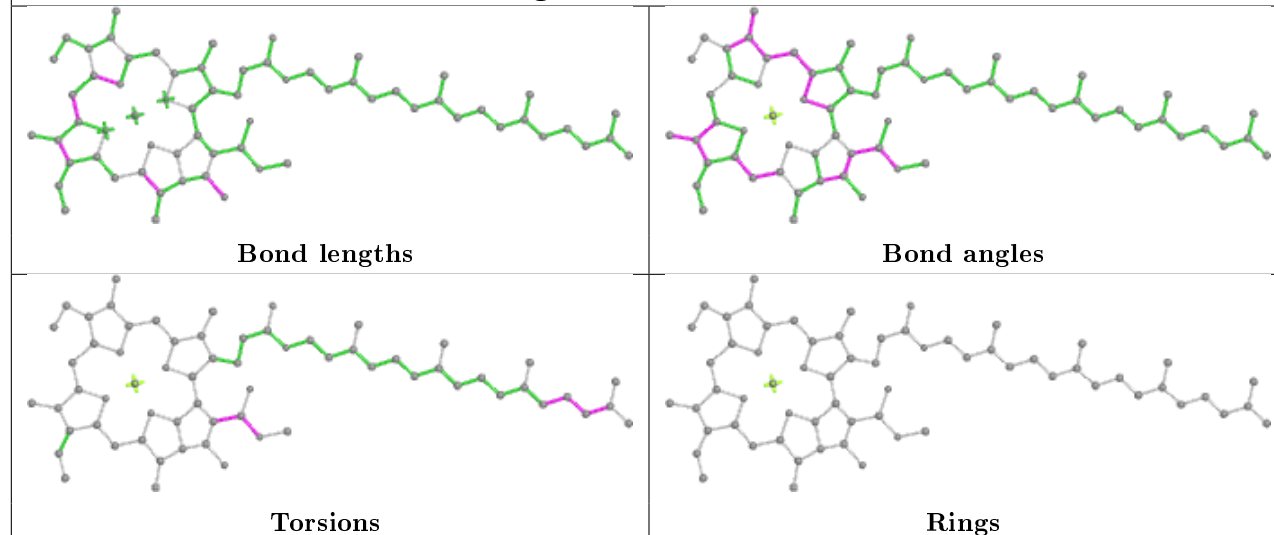
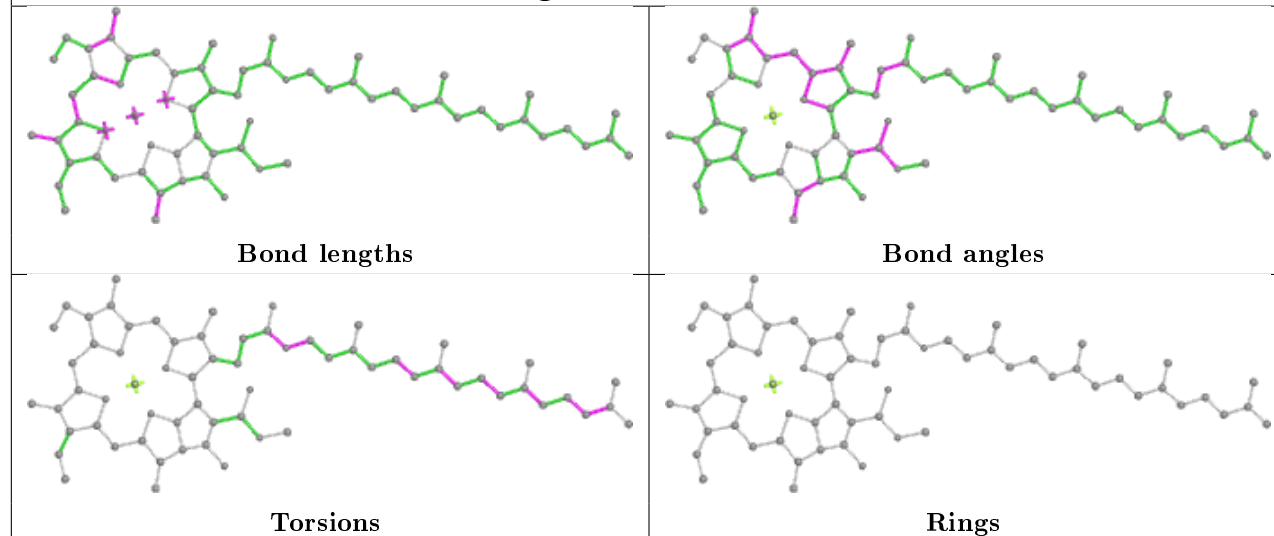
Ligand CLA d 403

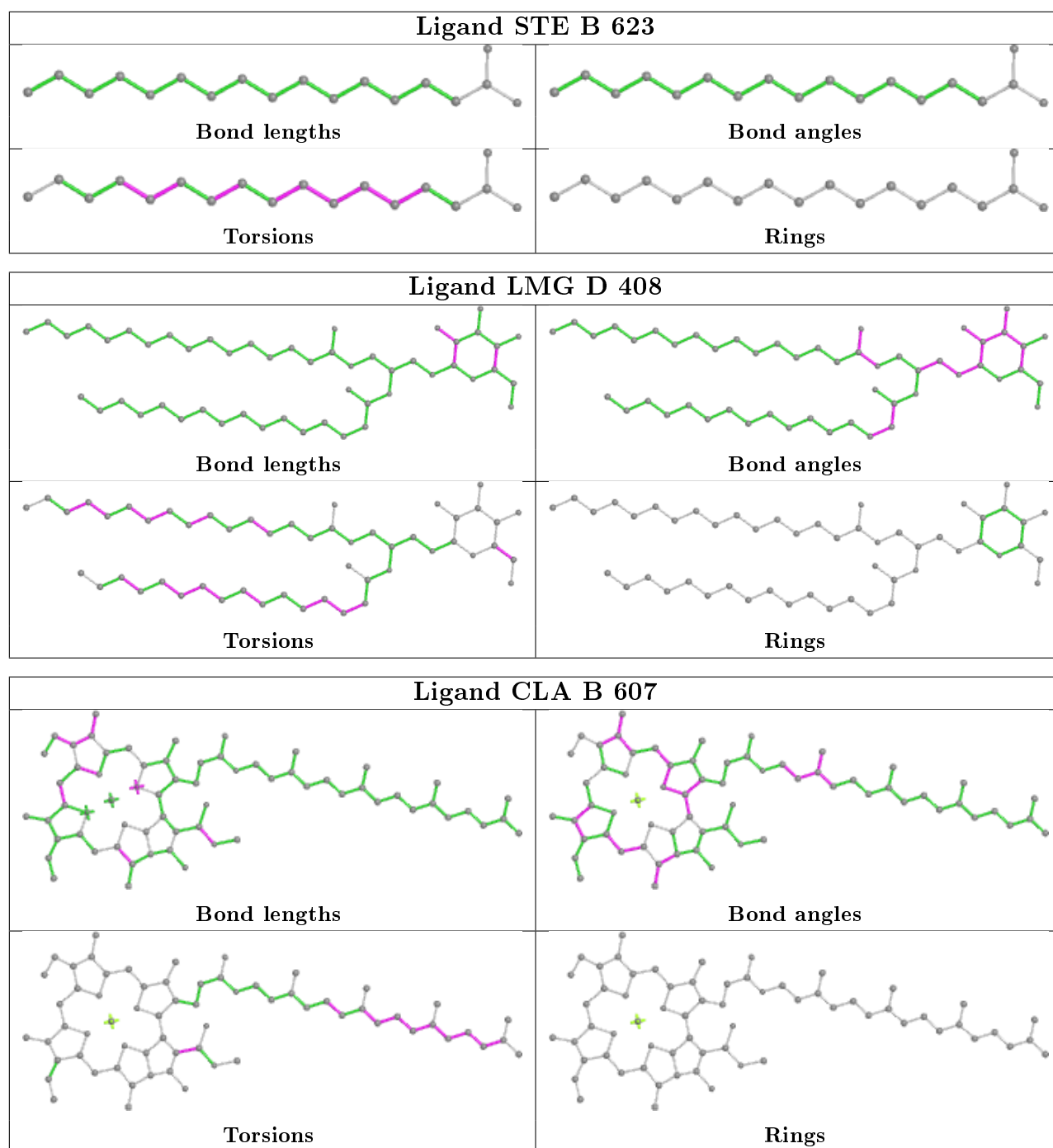


Ligand LHG A 410

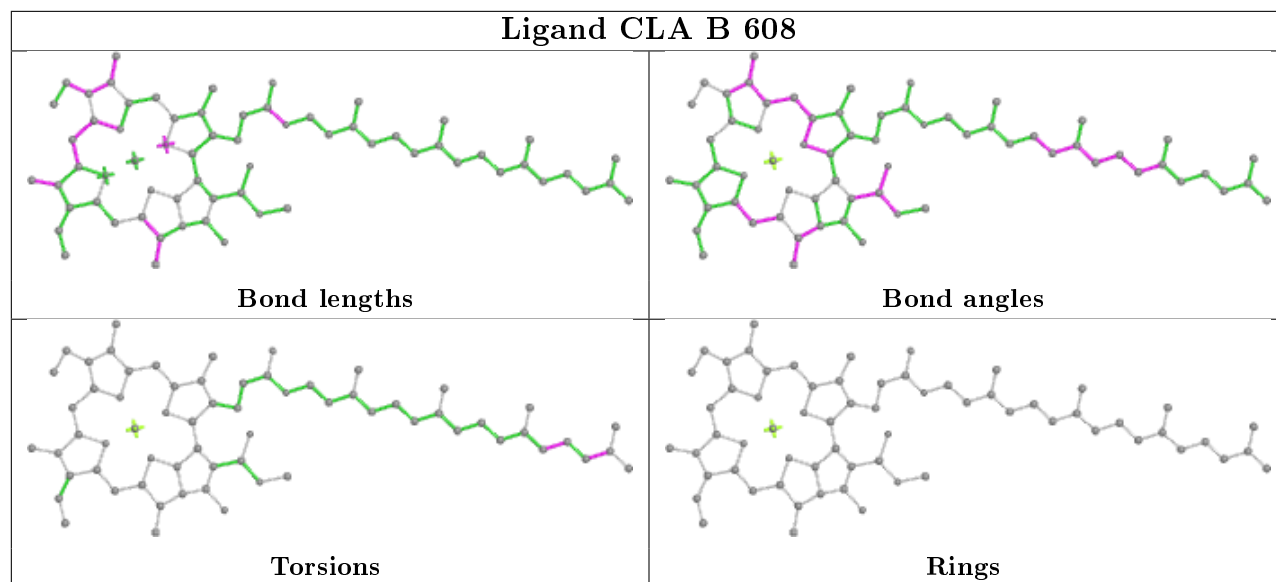




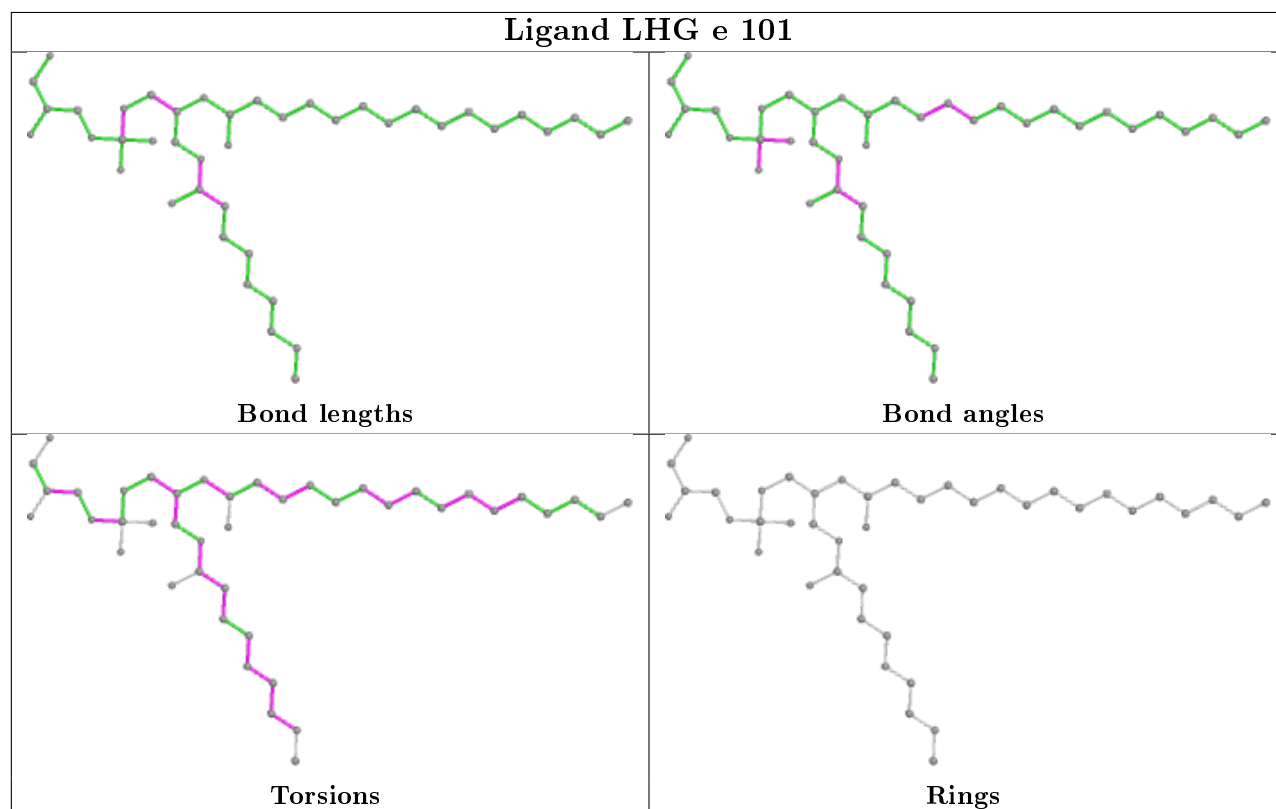
Ligand CLA A 403**Ligand CLA A 409****Ligand CLA a 405**



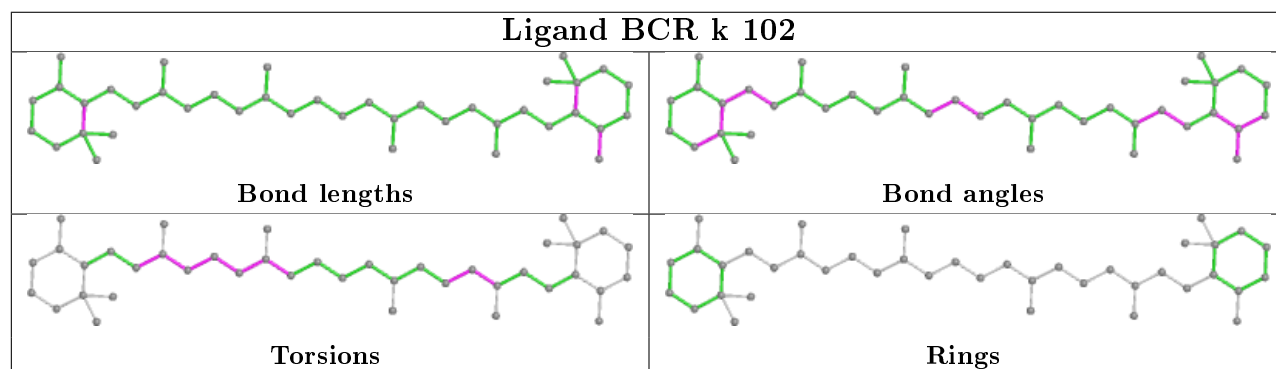
Ligand CLA B 608

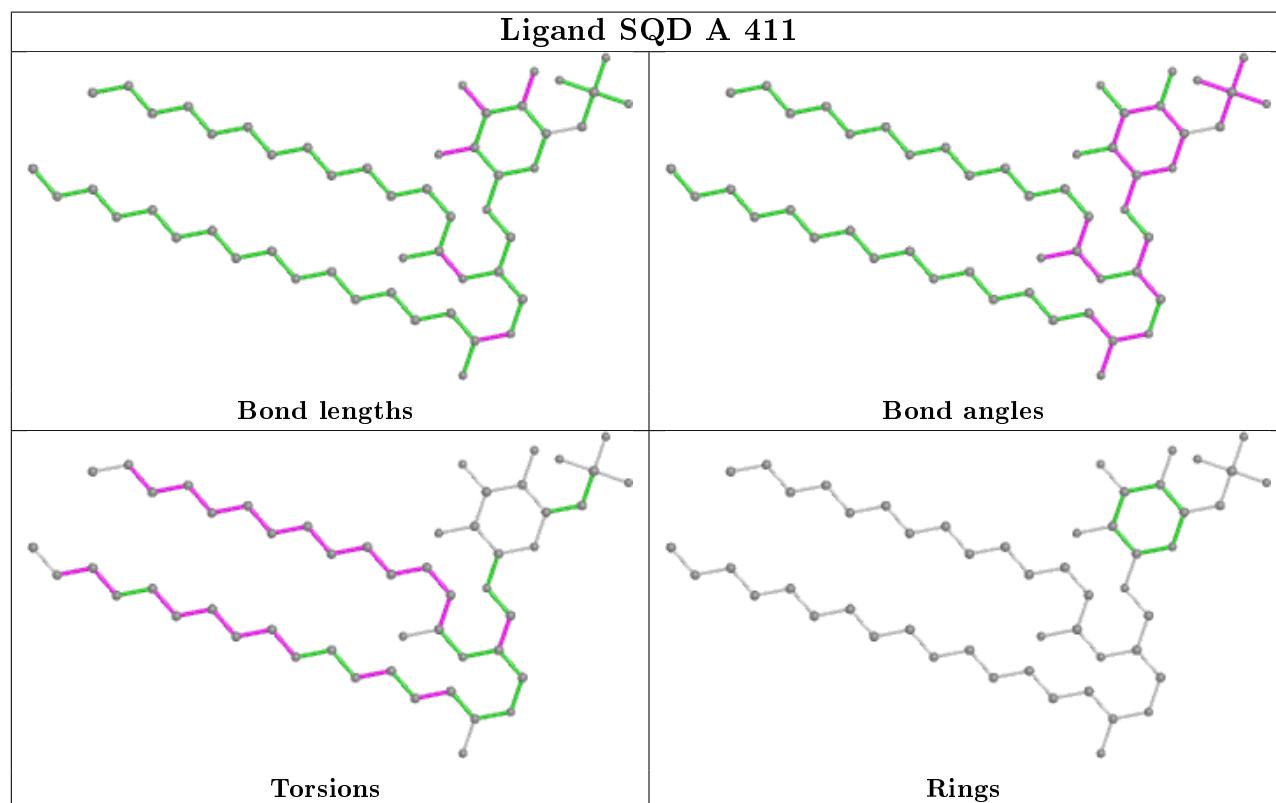
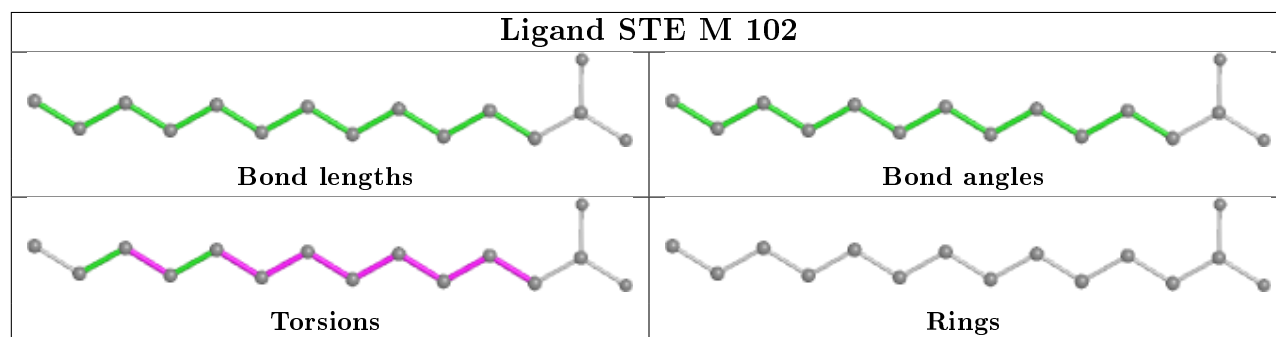
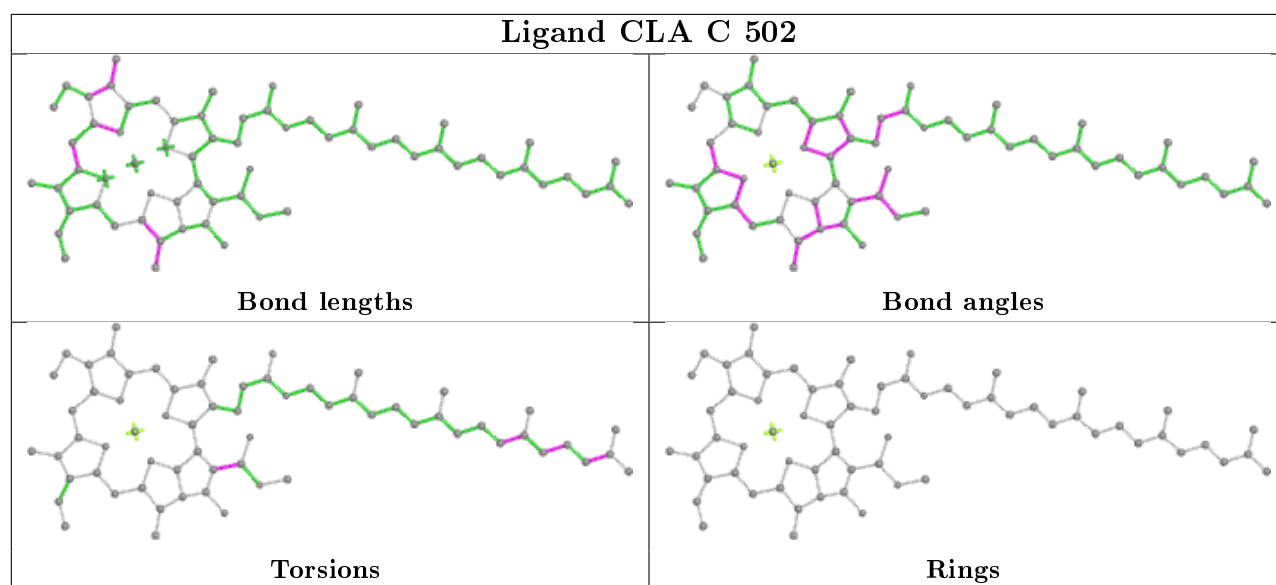


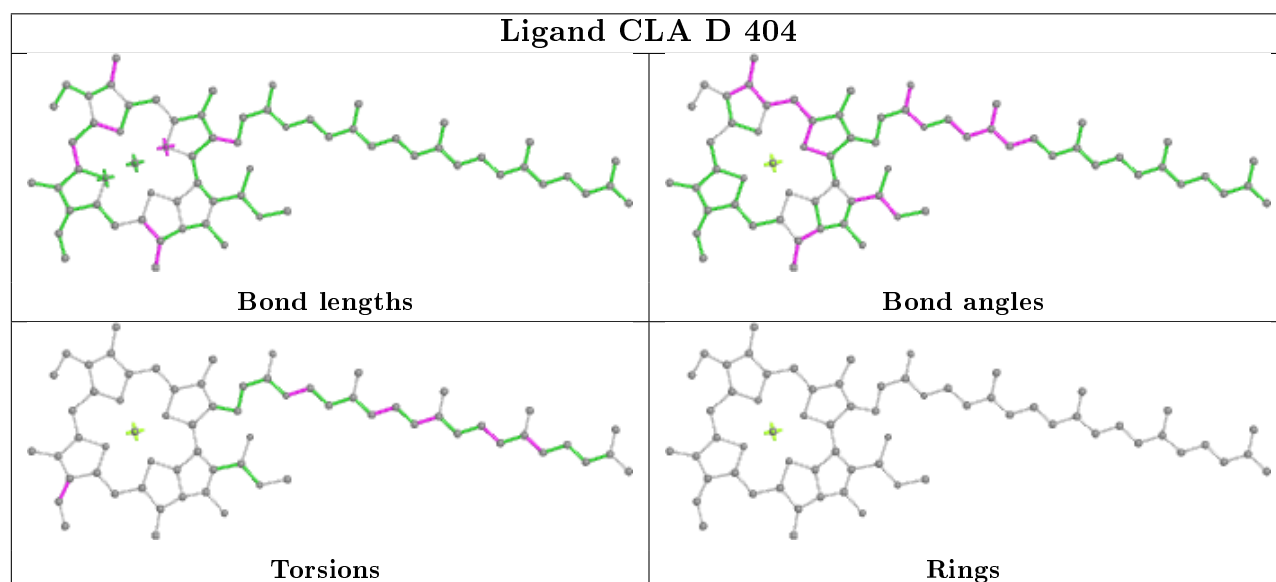
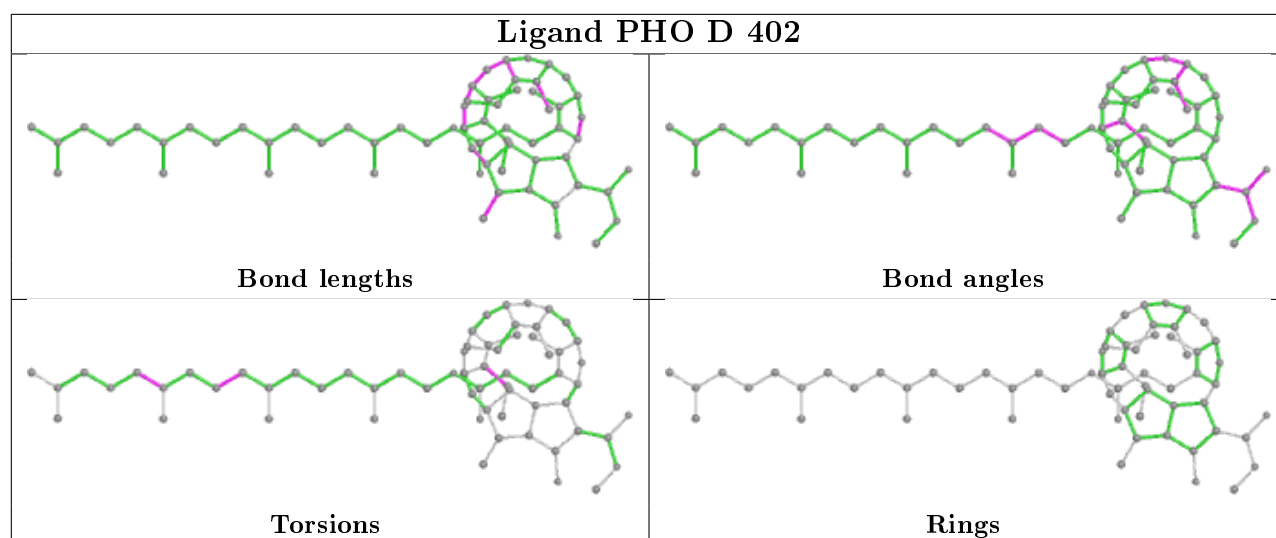
Ligand LHG e 101

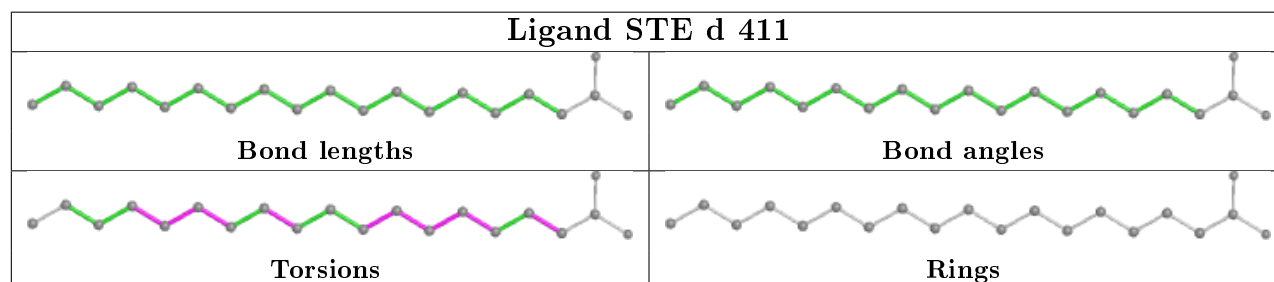
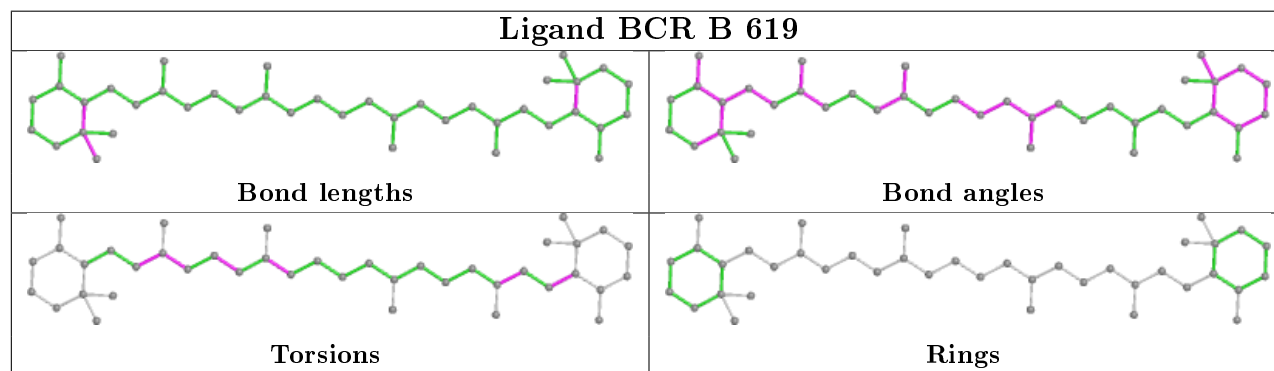
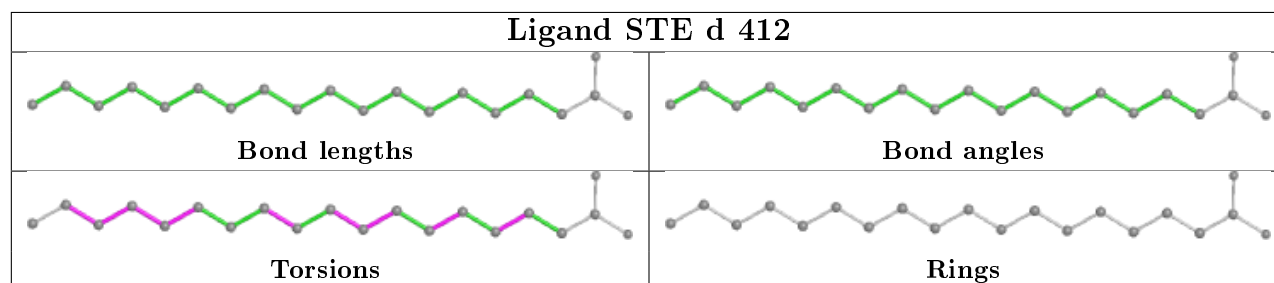
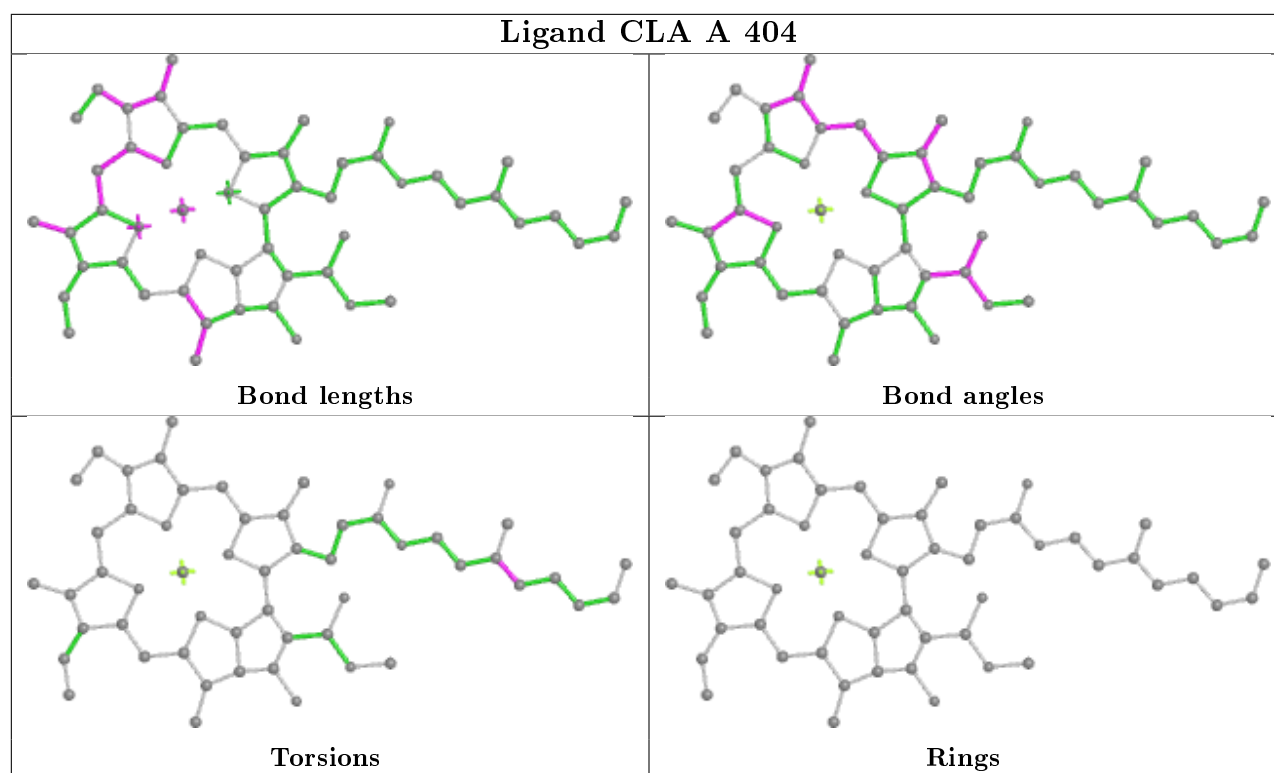


Ligand BCR k 102

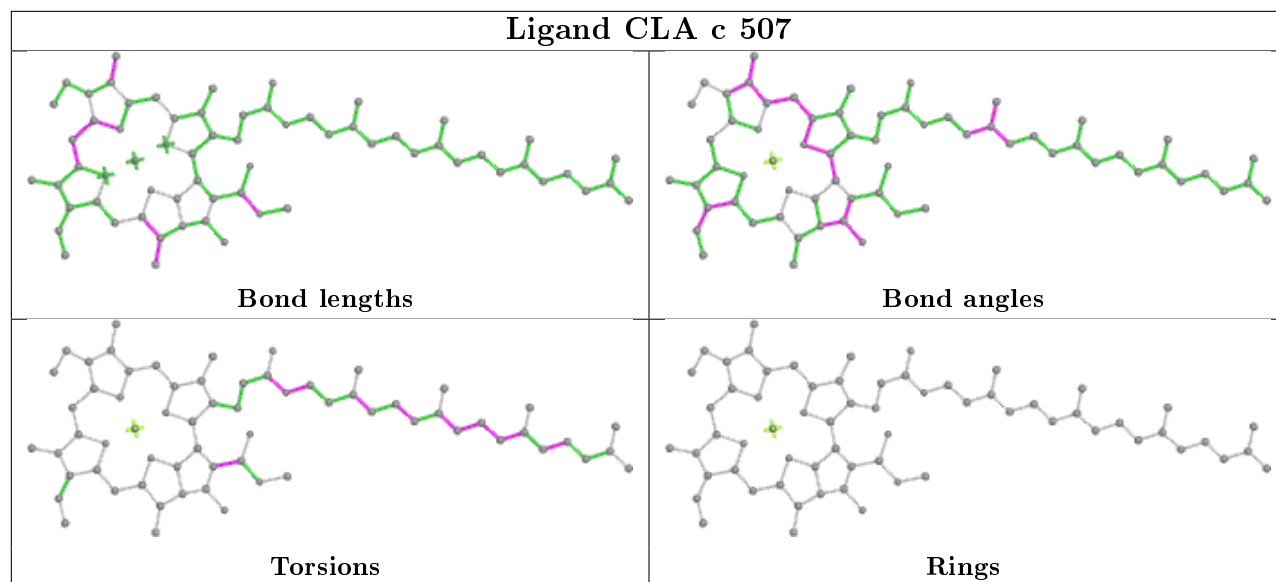




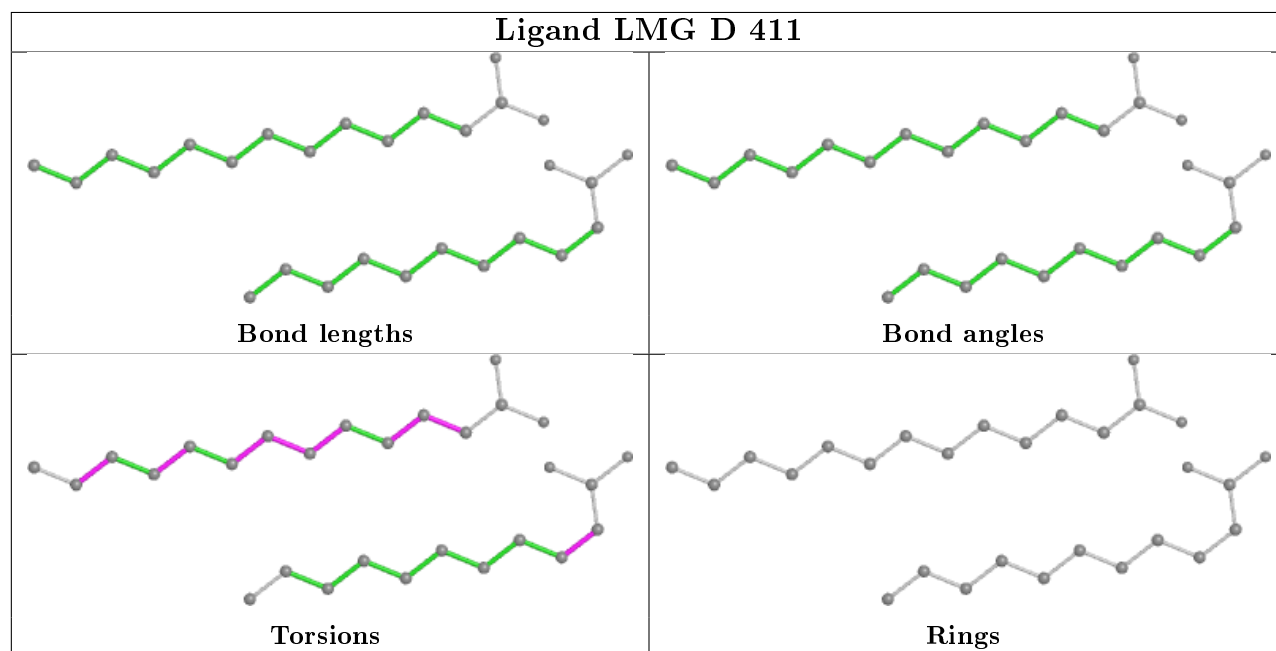




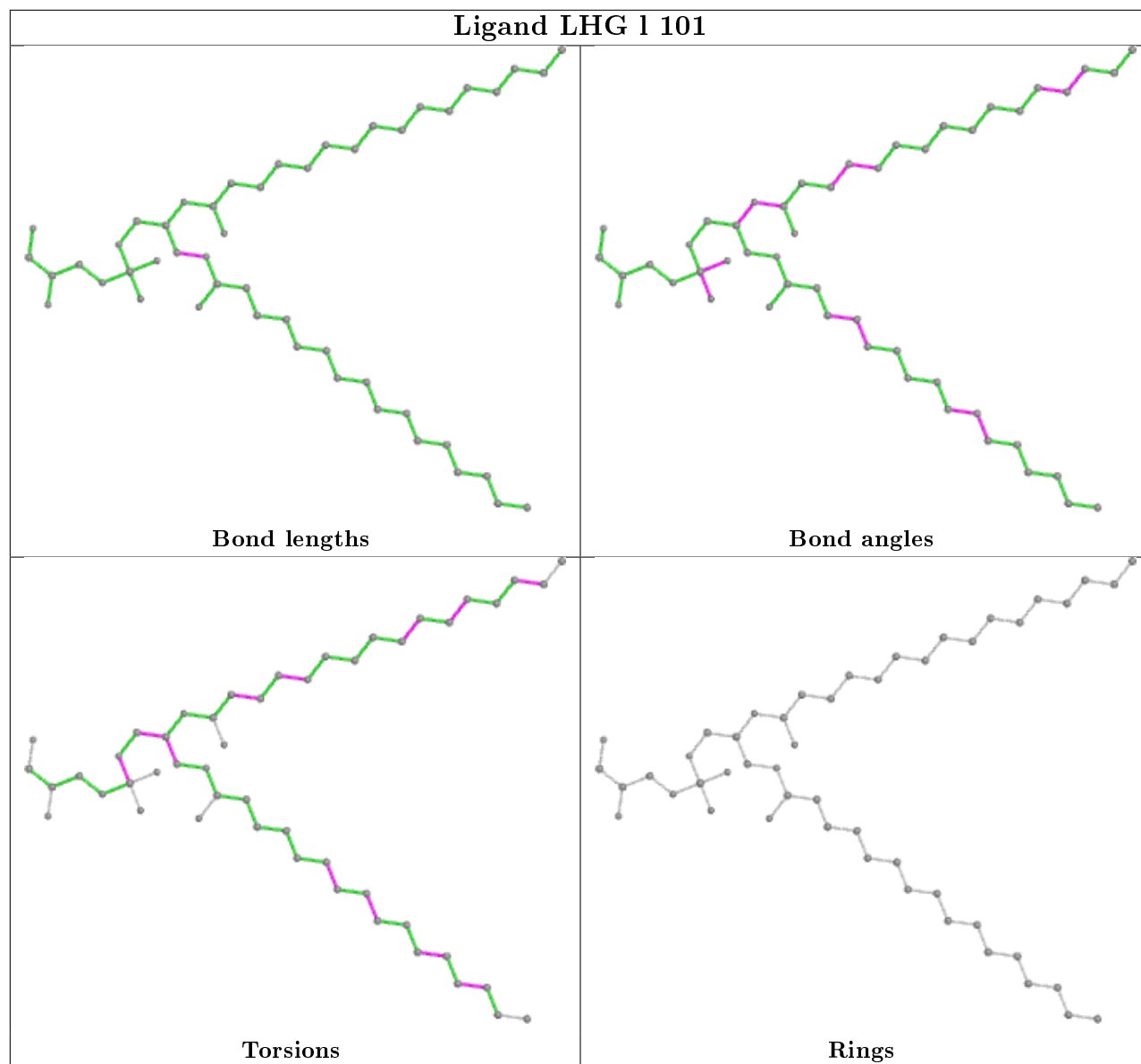
Ligand CLA c 507



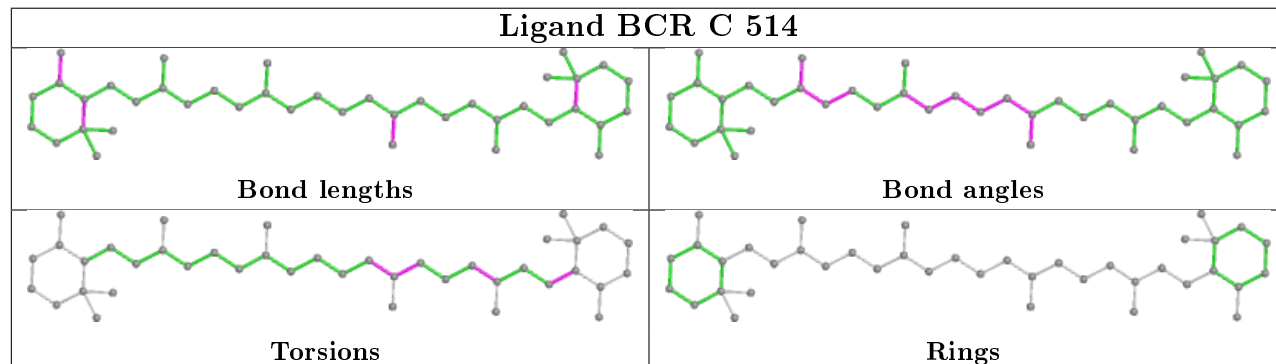
Ligand LMG D 411



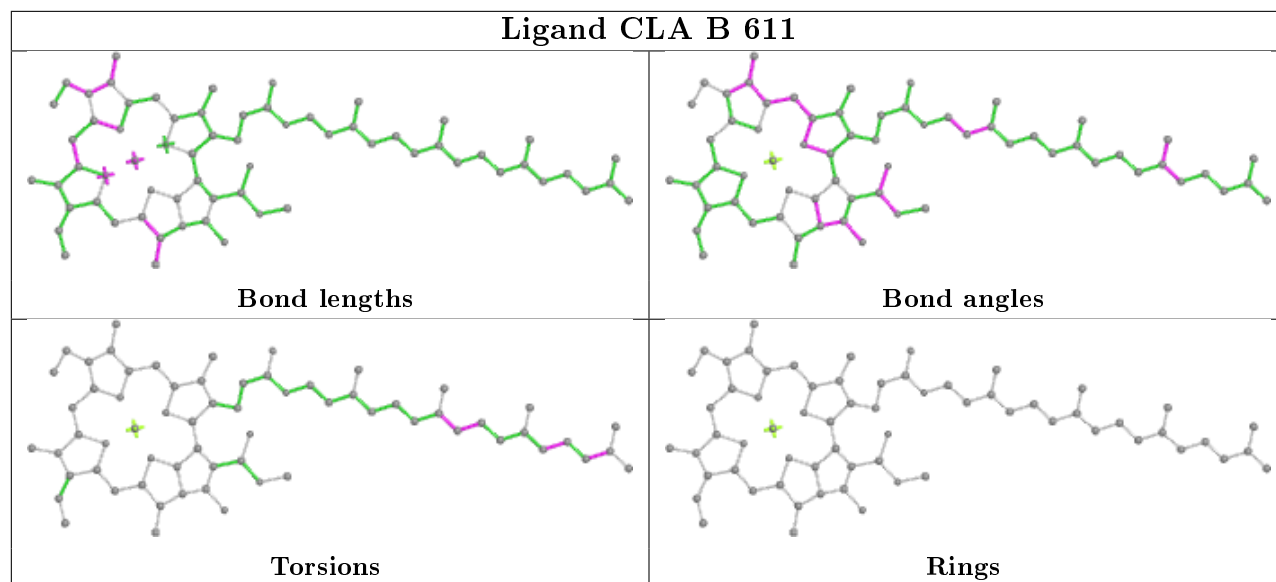
Ligand LHG 1 101



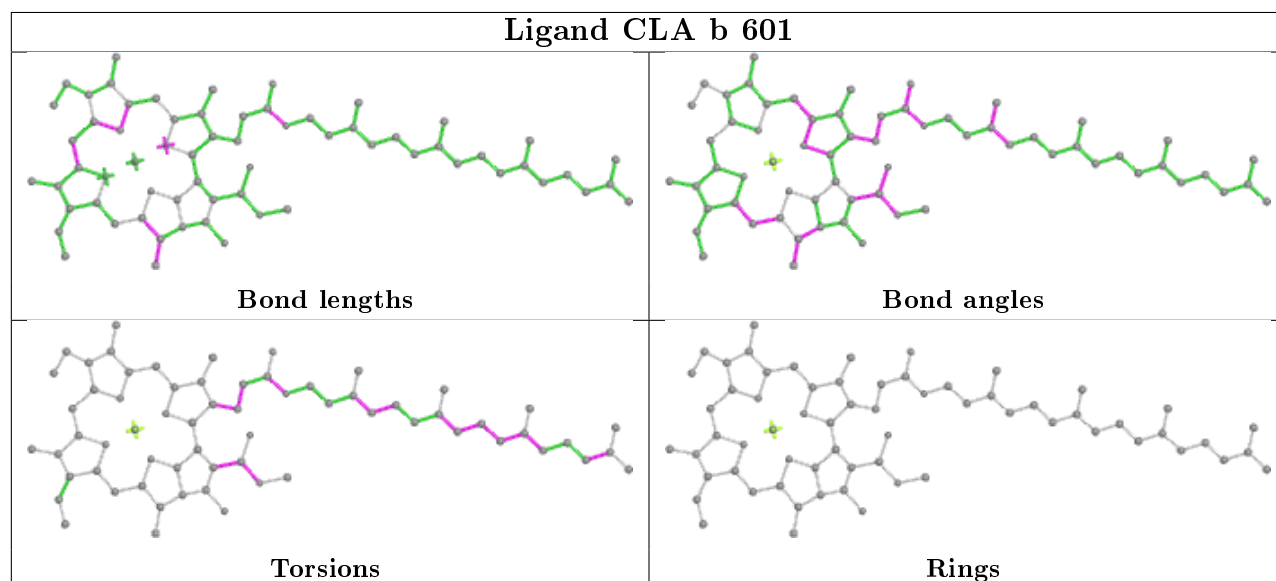
Ligand BCR C 514



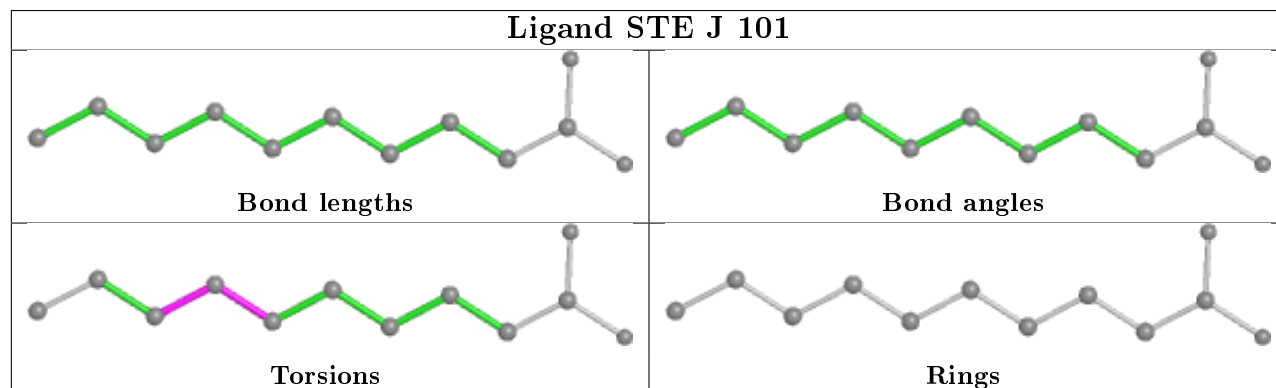
Ligand CLA B 611

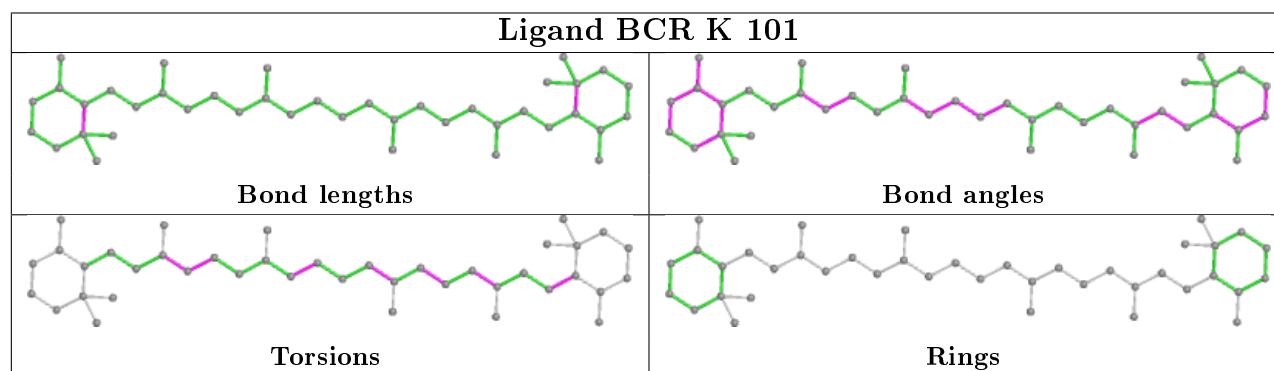
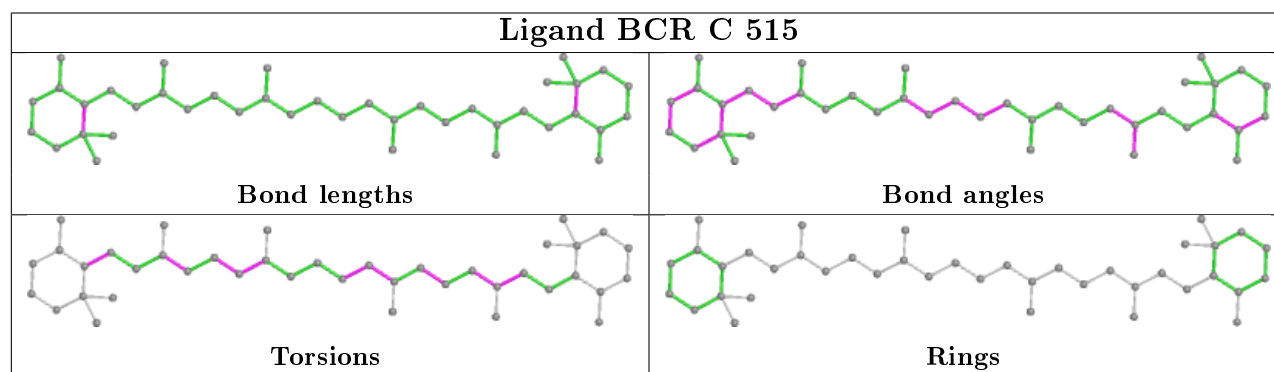
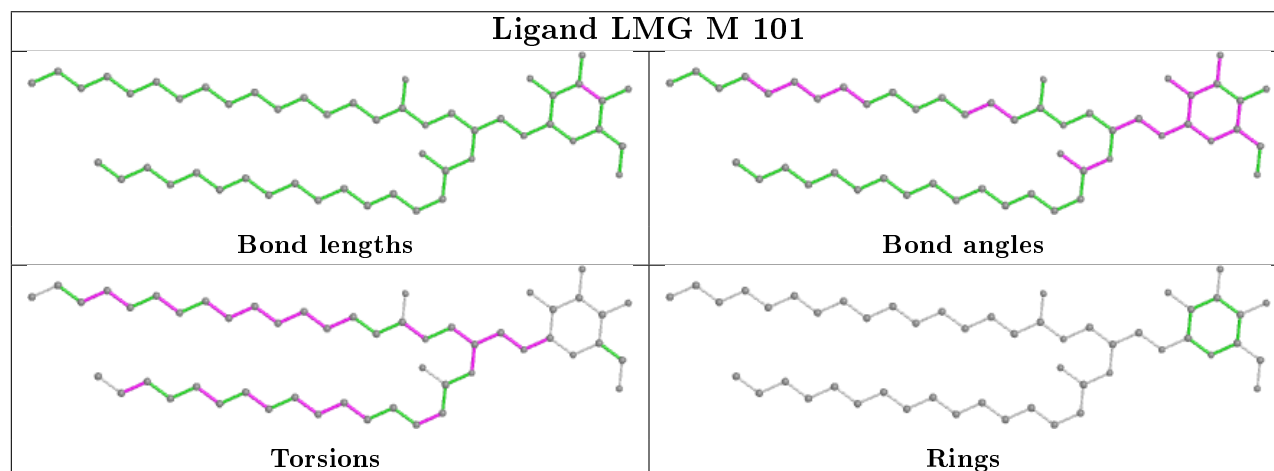
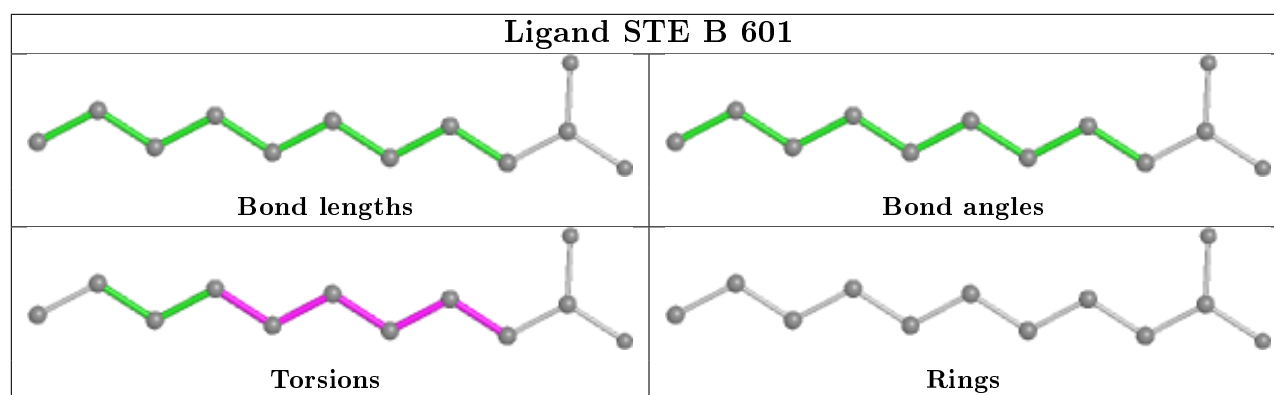


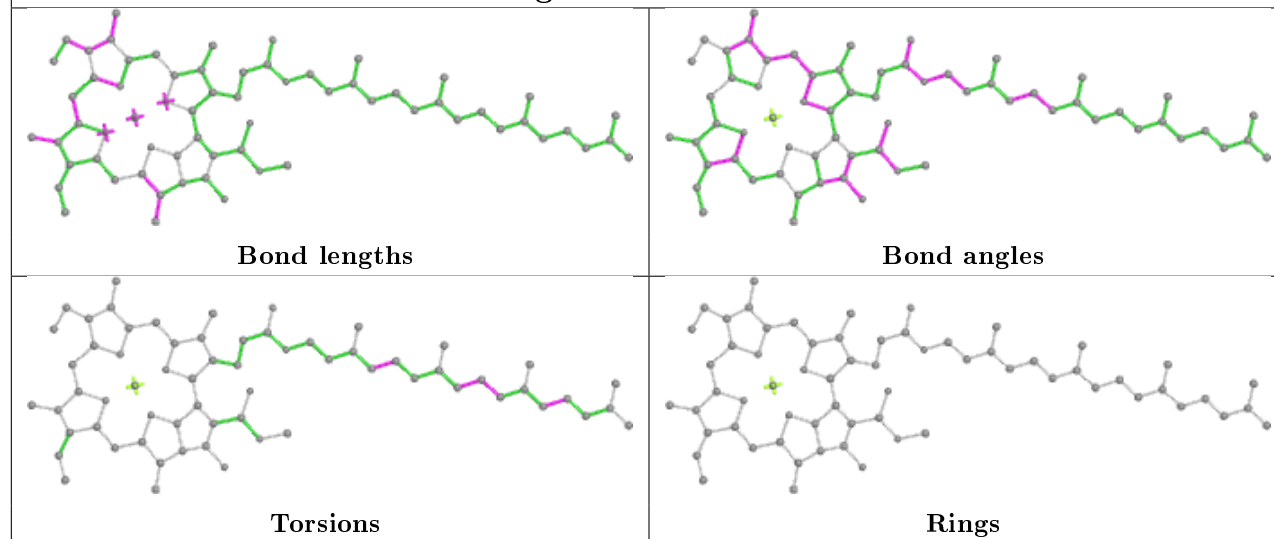
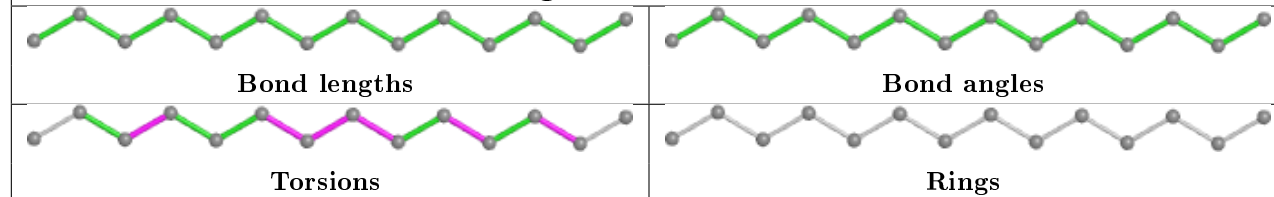
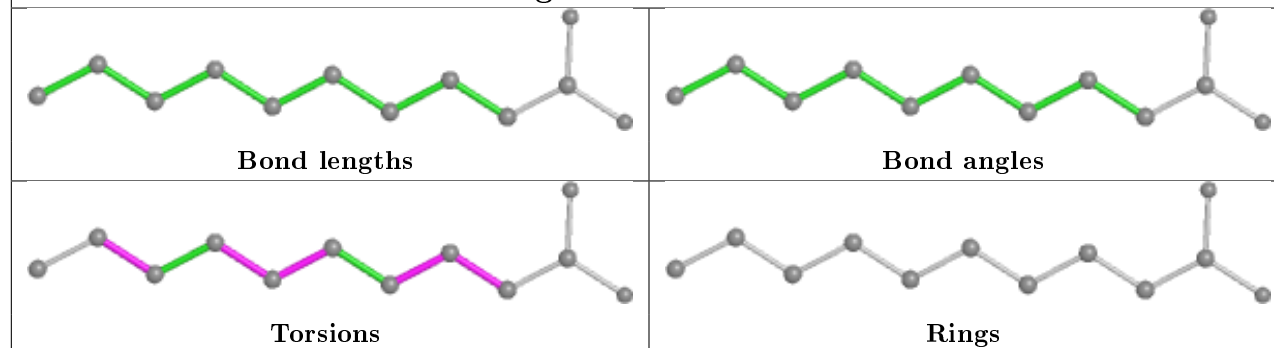
Ligand CLA b 601

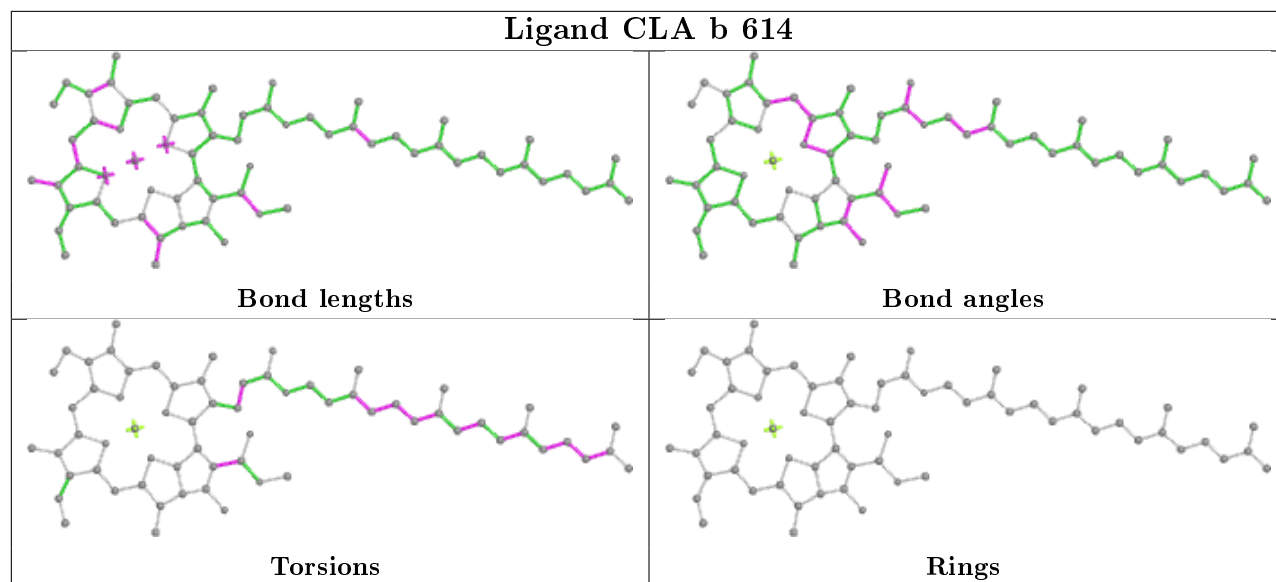
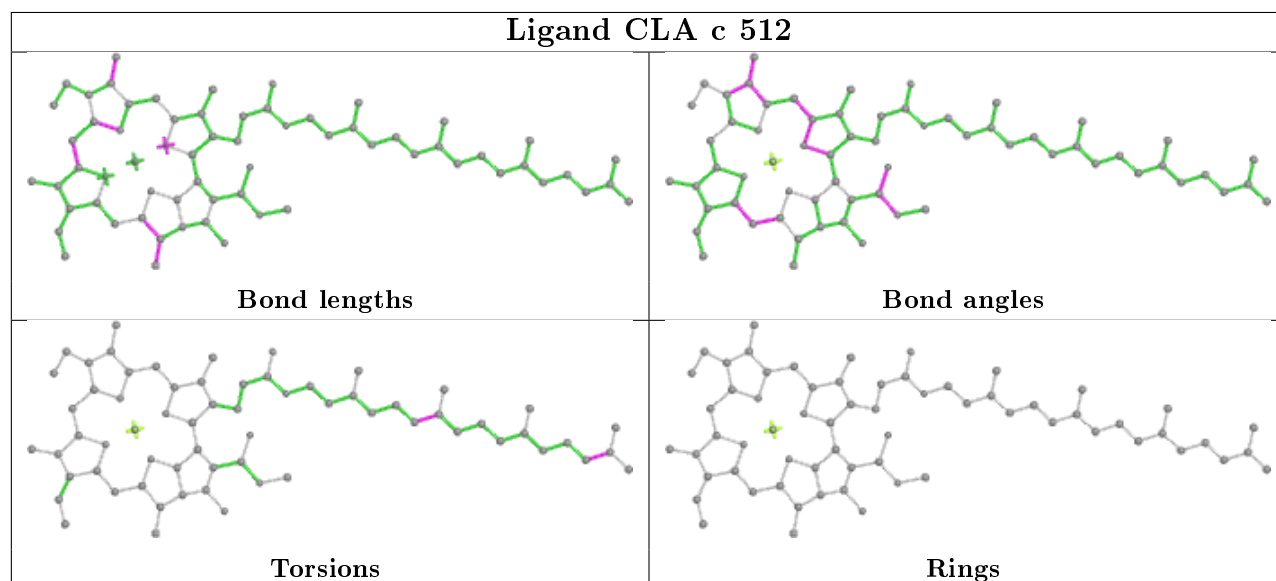
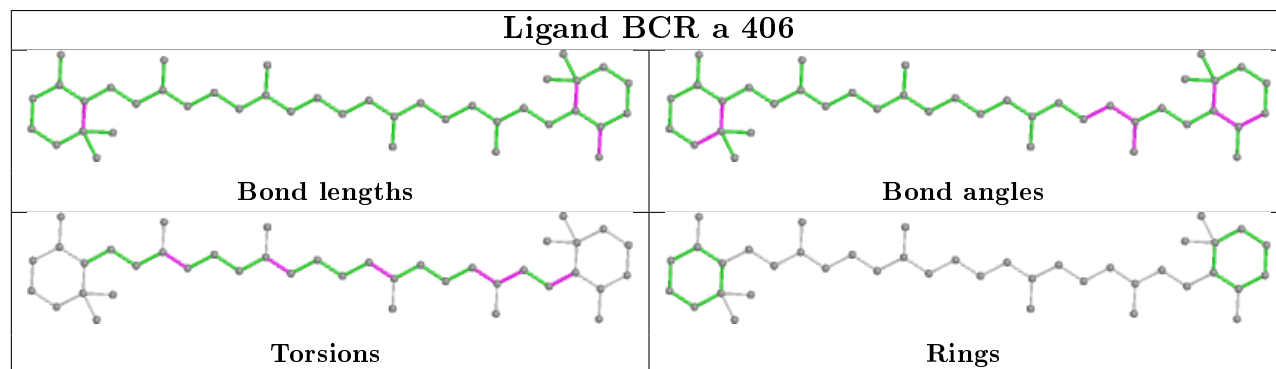


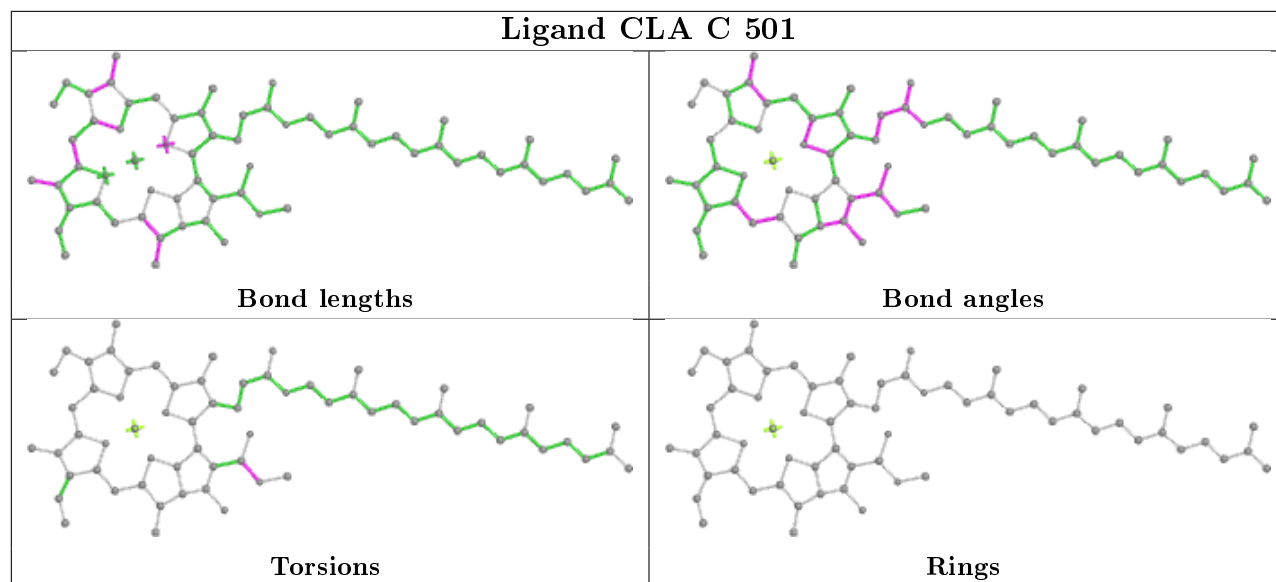
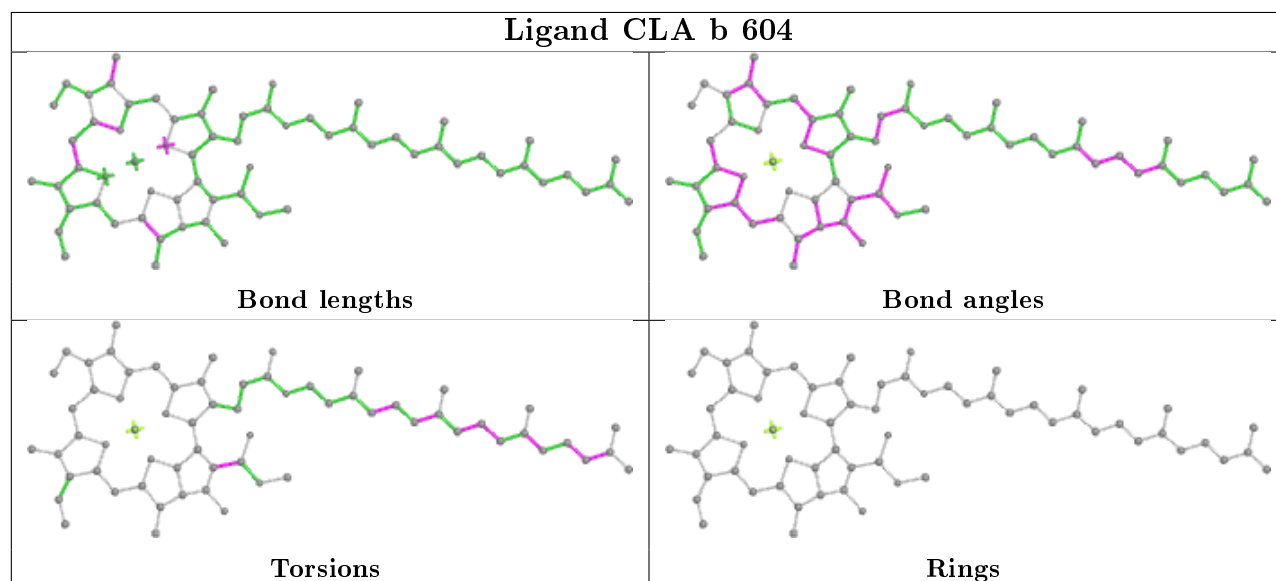
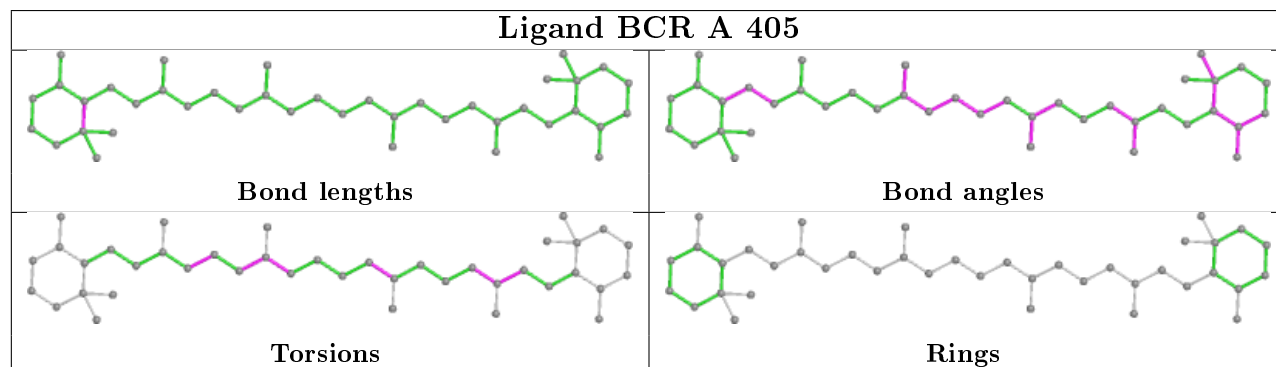
Ligand STE J 101

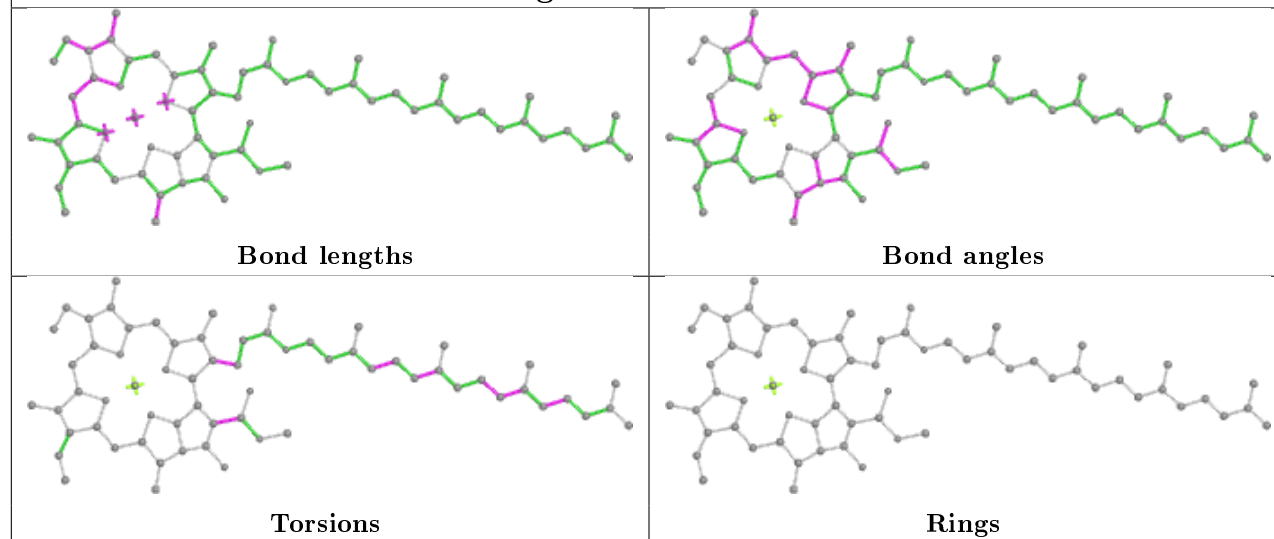
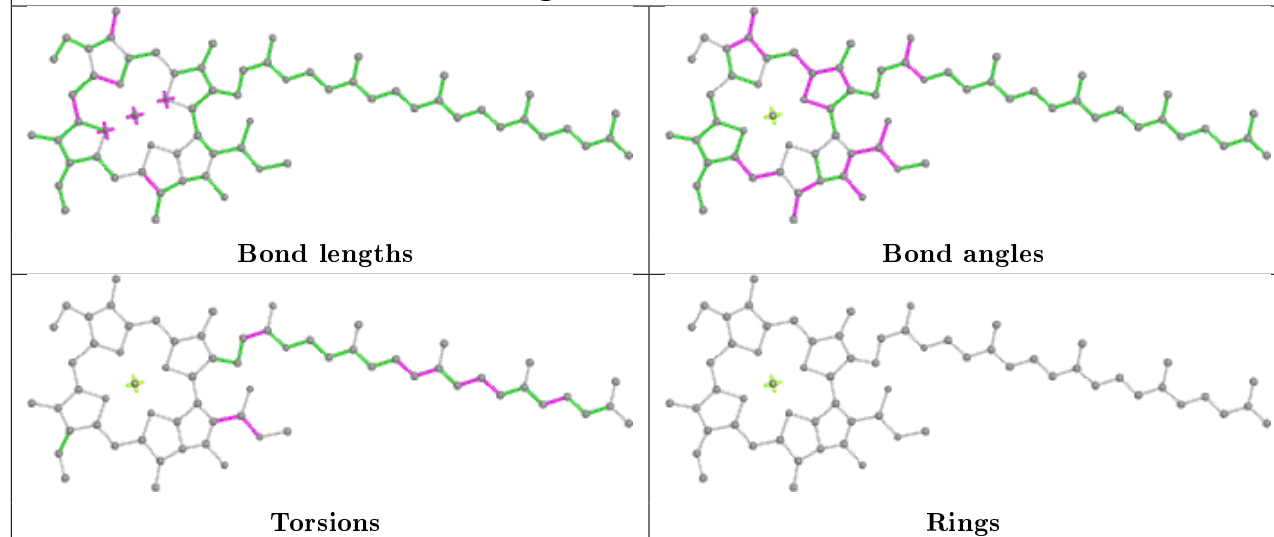


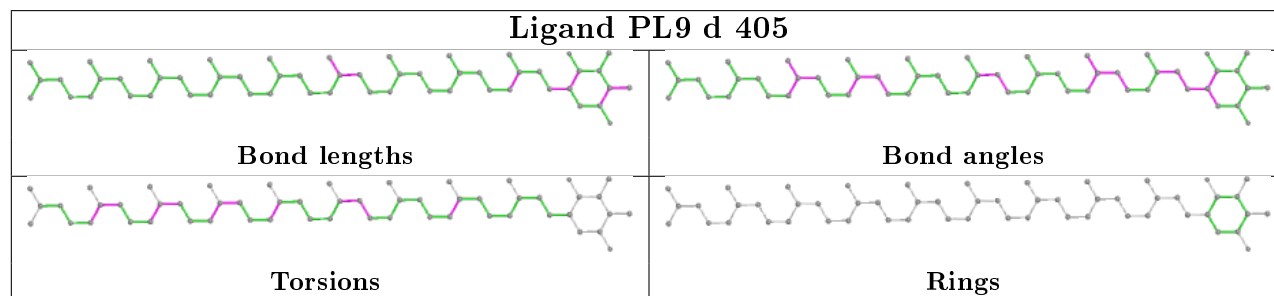
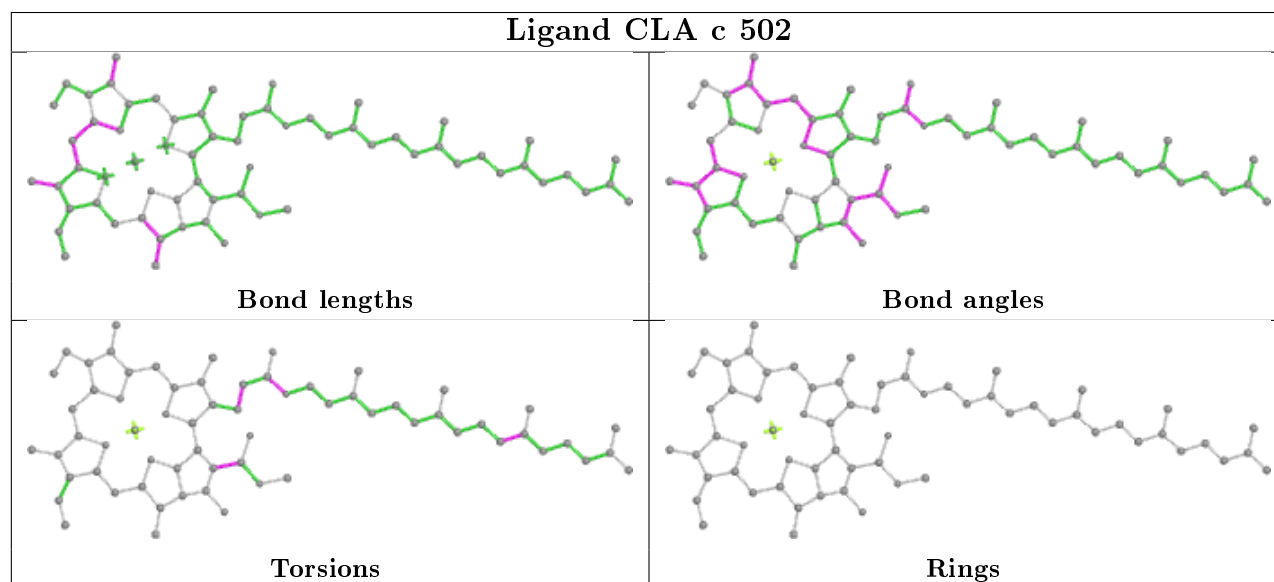
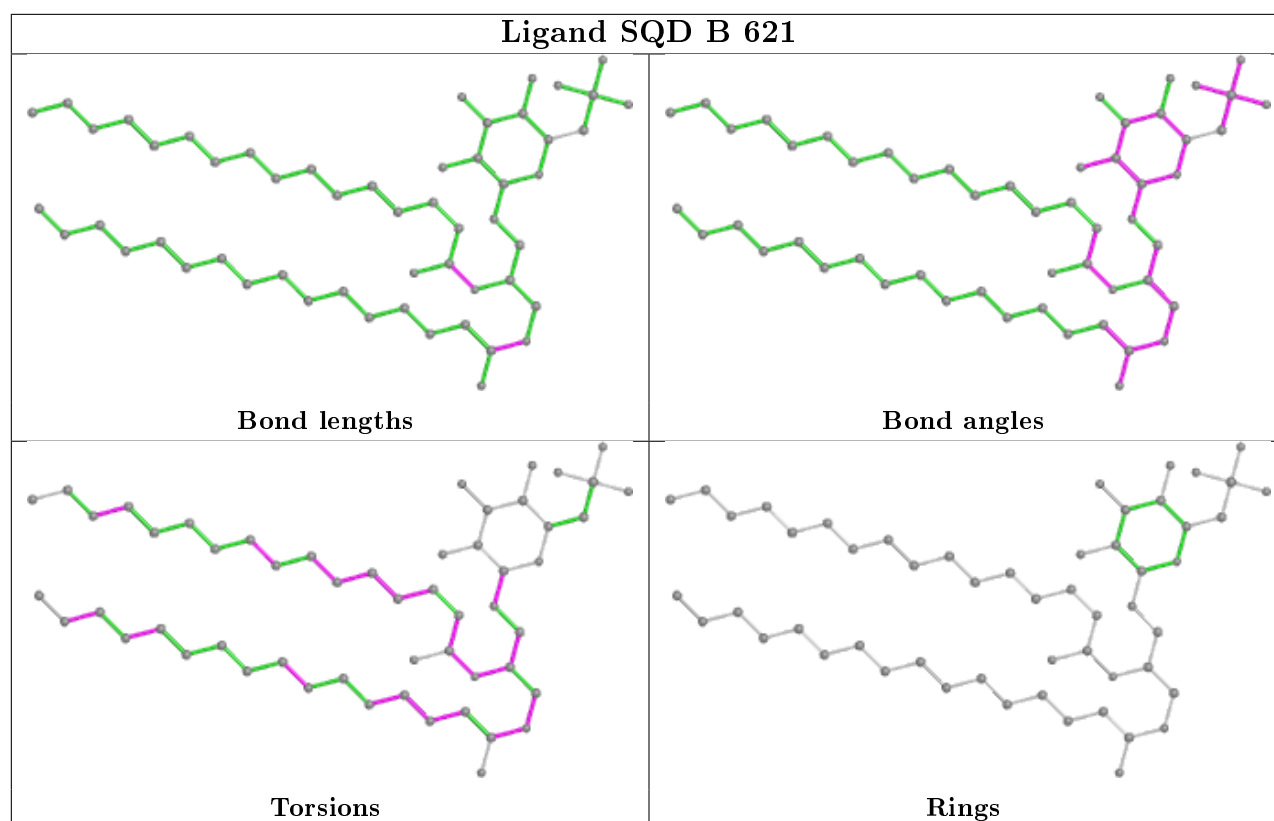


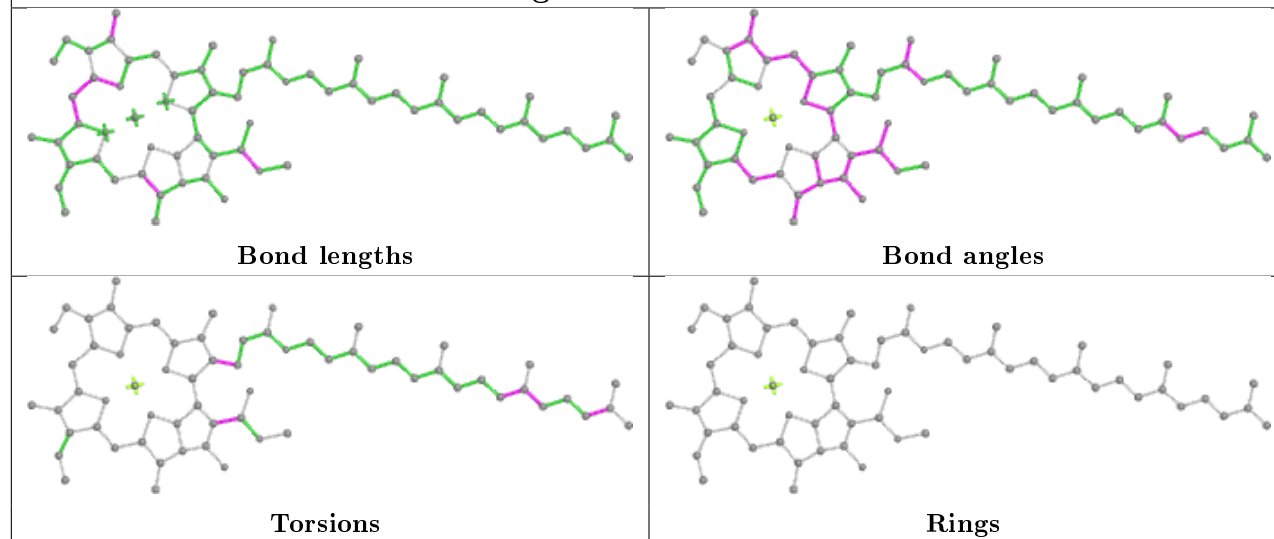
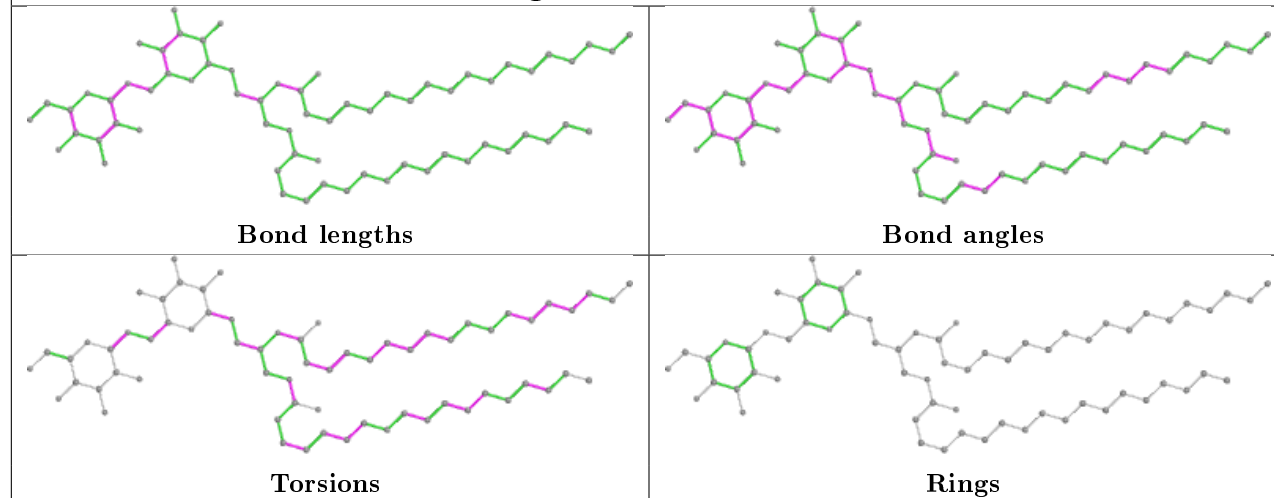
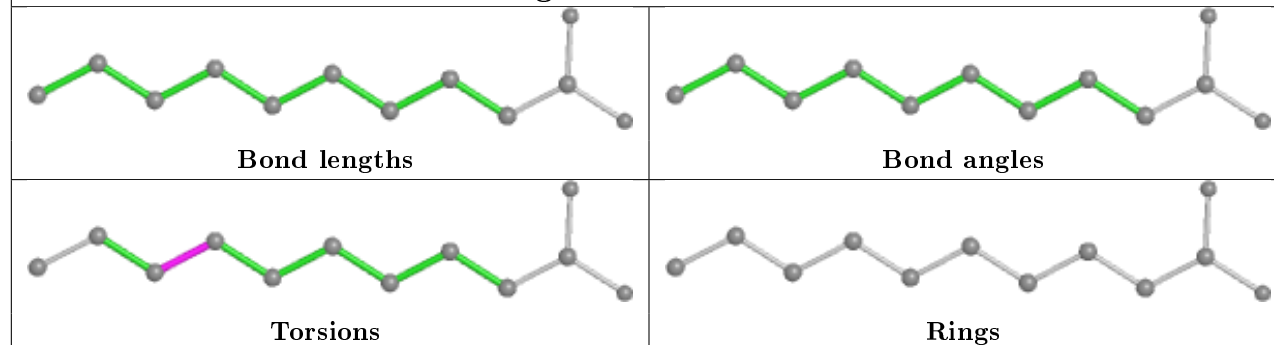
Ligand CLA b 603**Ligand STE h 103****Ligand STE B 622**

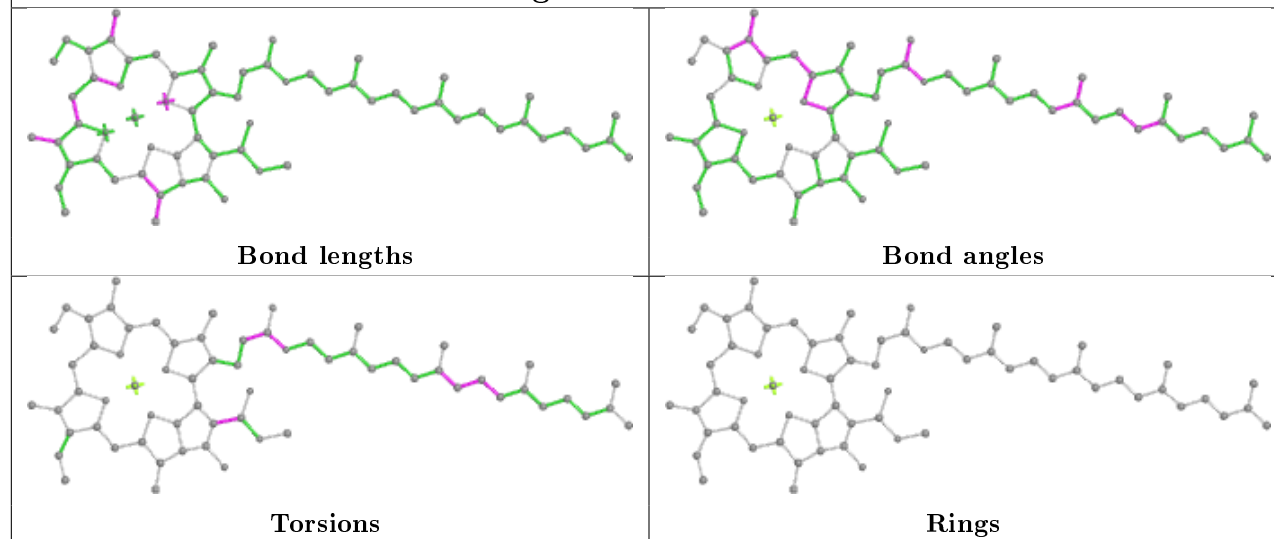
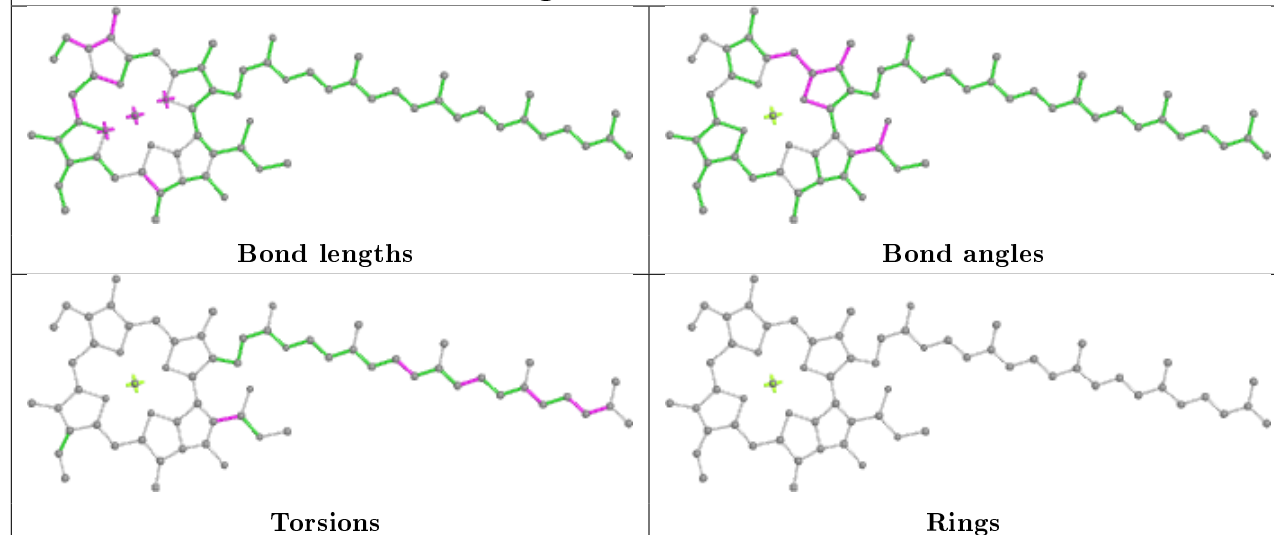
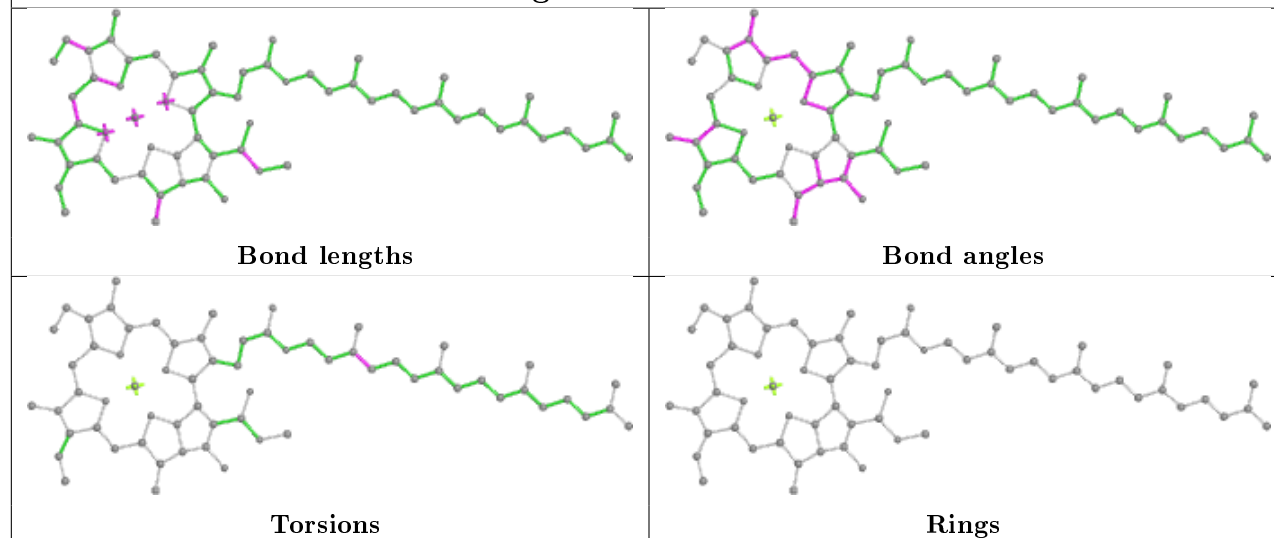
Ligand CLA b 614**Ligand CLA c 512****Ligand BCR a 406**

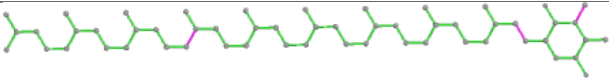
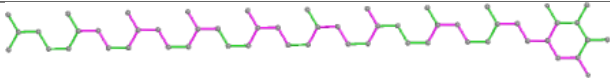
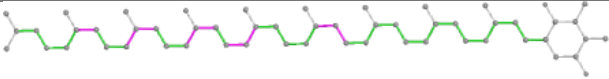
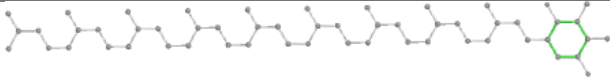
Ligand CLA C 501**Ligand CLA b 604****Ligand BCR A 405**

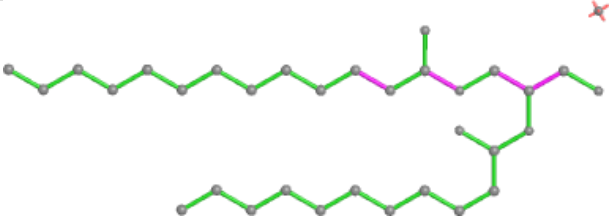
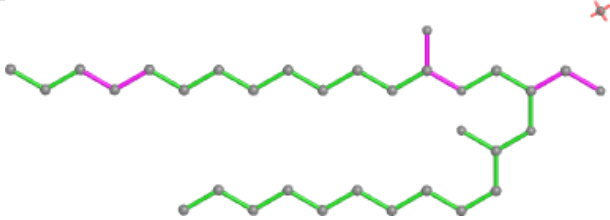
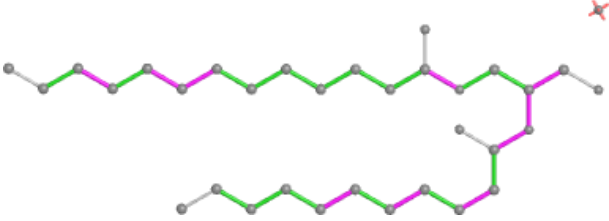
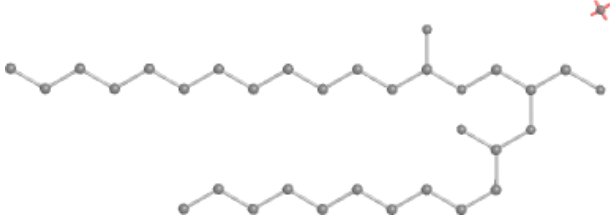
Ligand CLA a 403**Ligand CLA c 510**

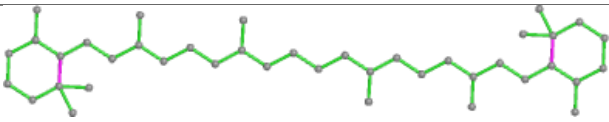
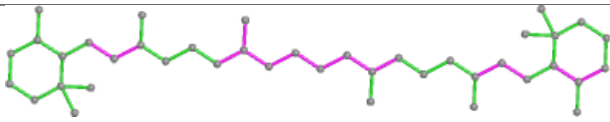
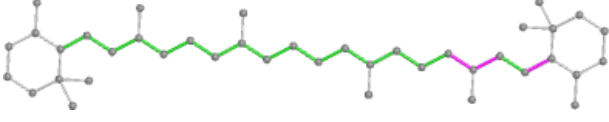
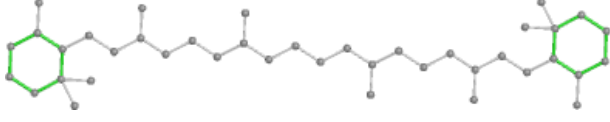


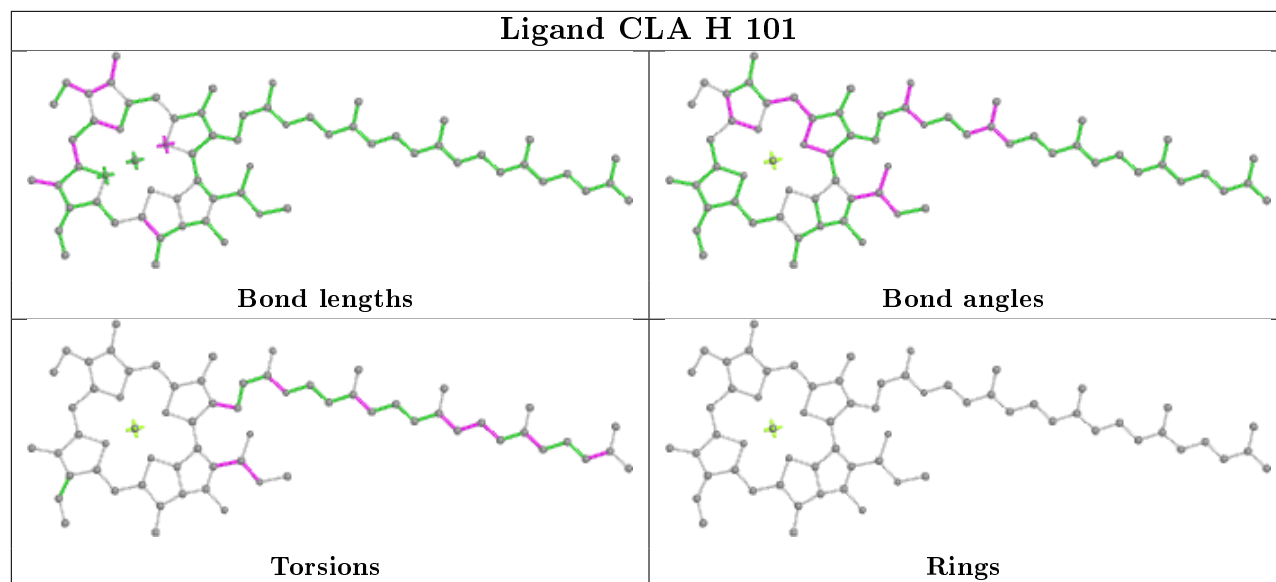
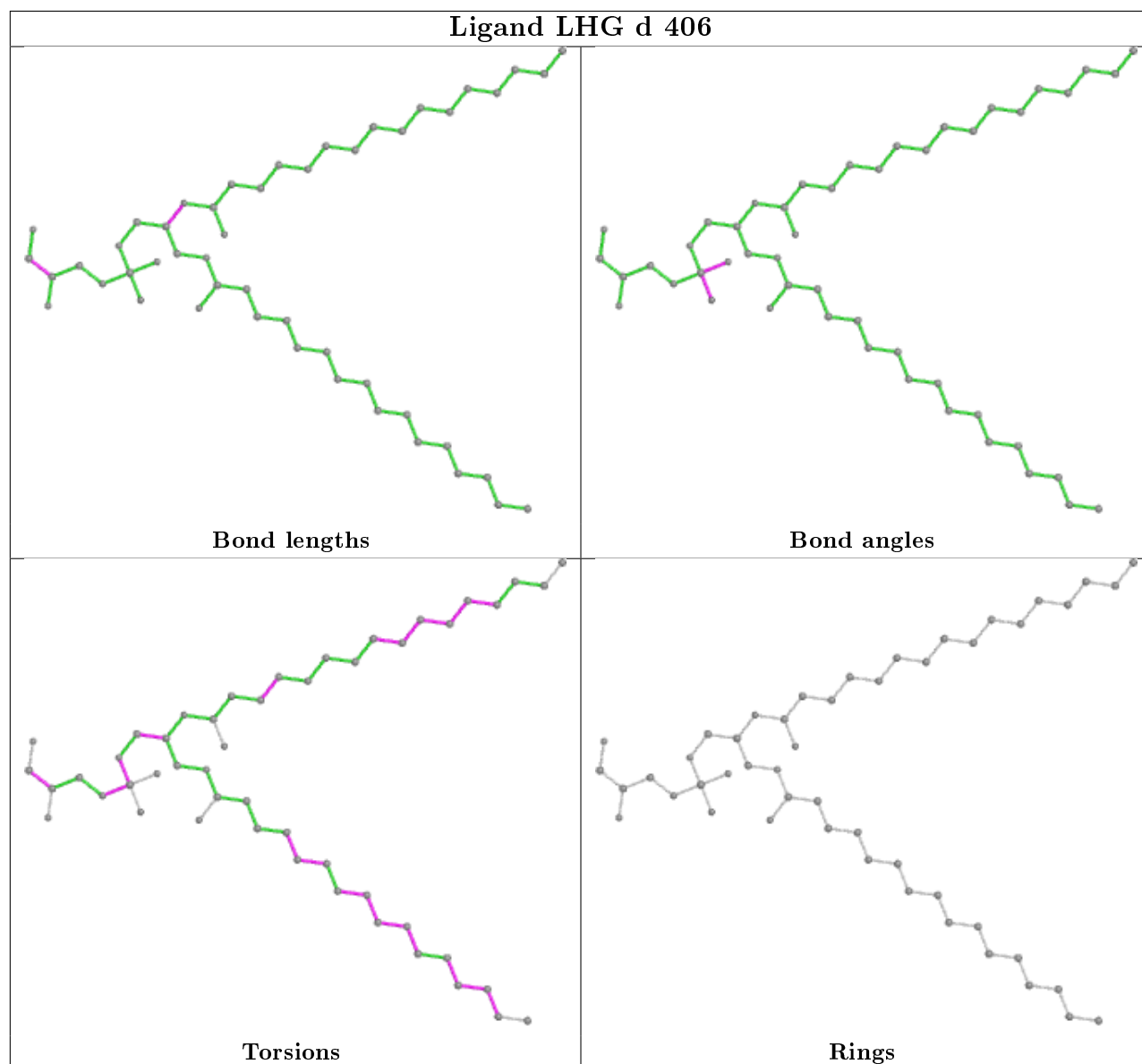
Ligand CLA B 602**Ligand DGD A 414****Ligand STE C 522**

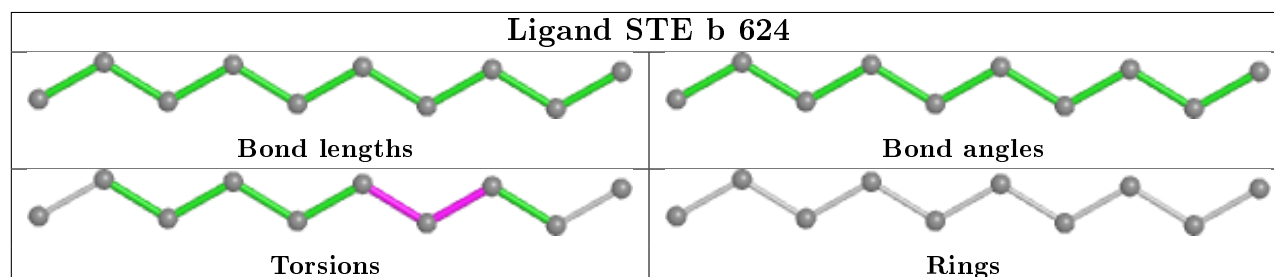
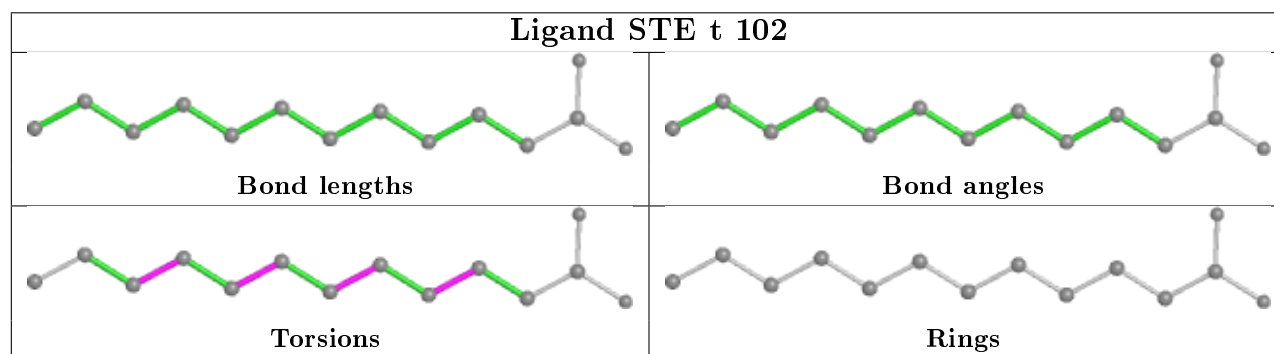
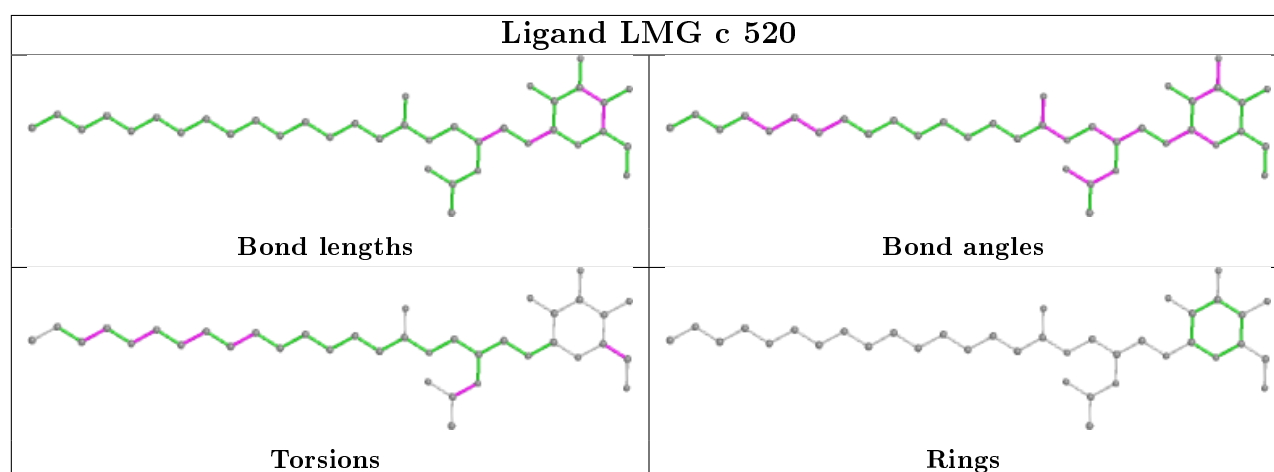
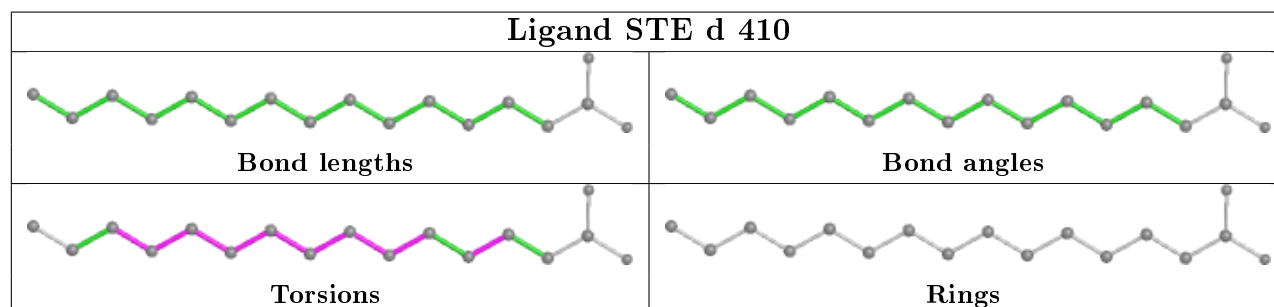
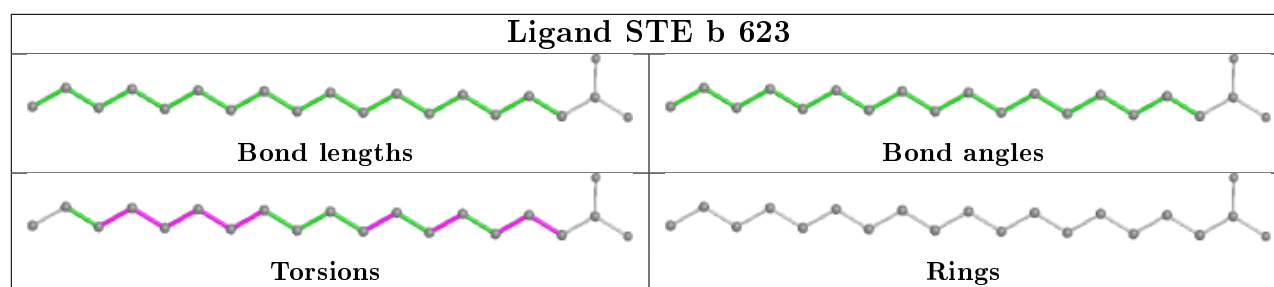
Ligand CLA B 612**Ligand CLA c 504****Ligand CLA B 609**

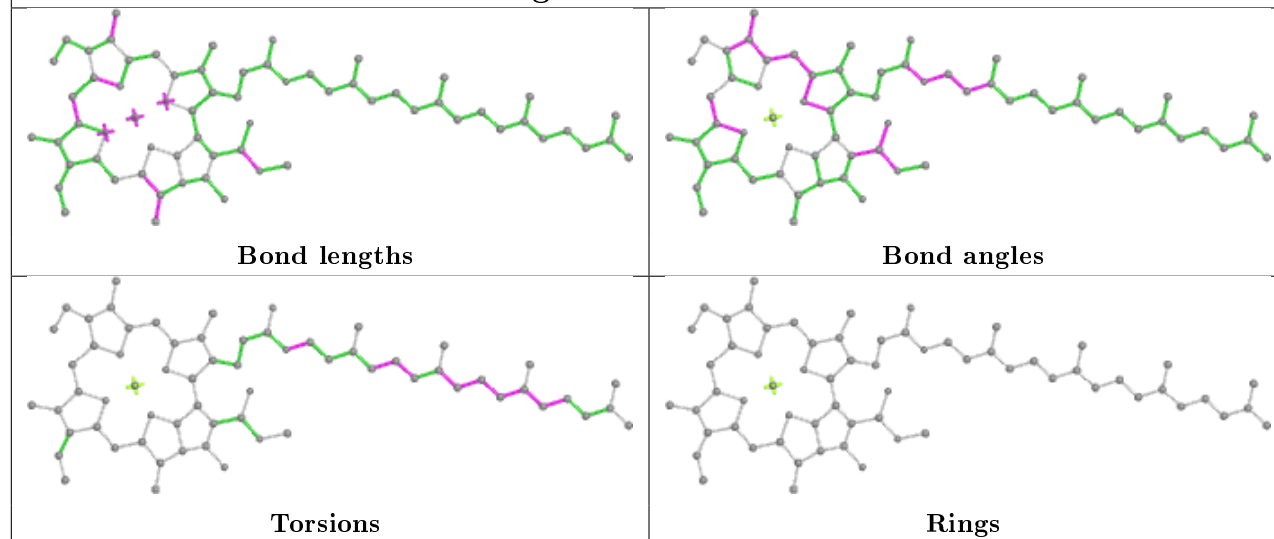
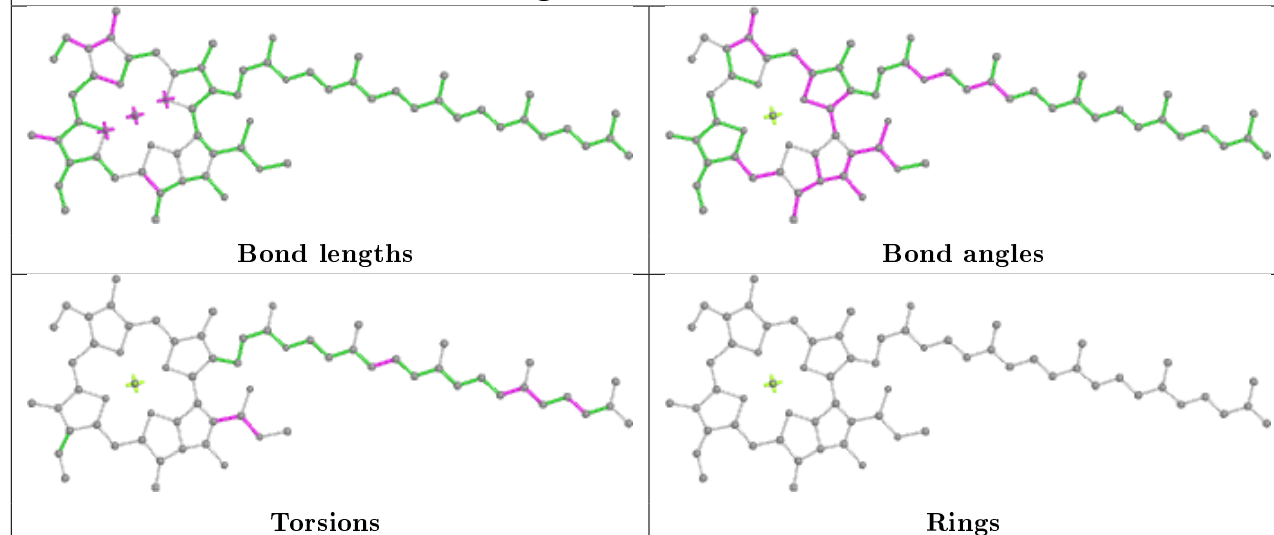
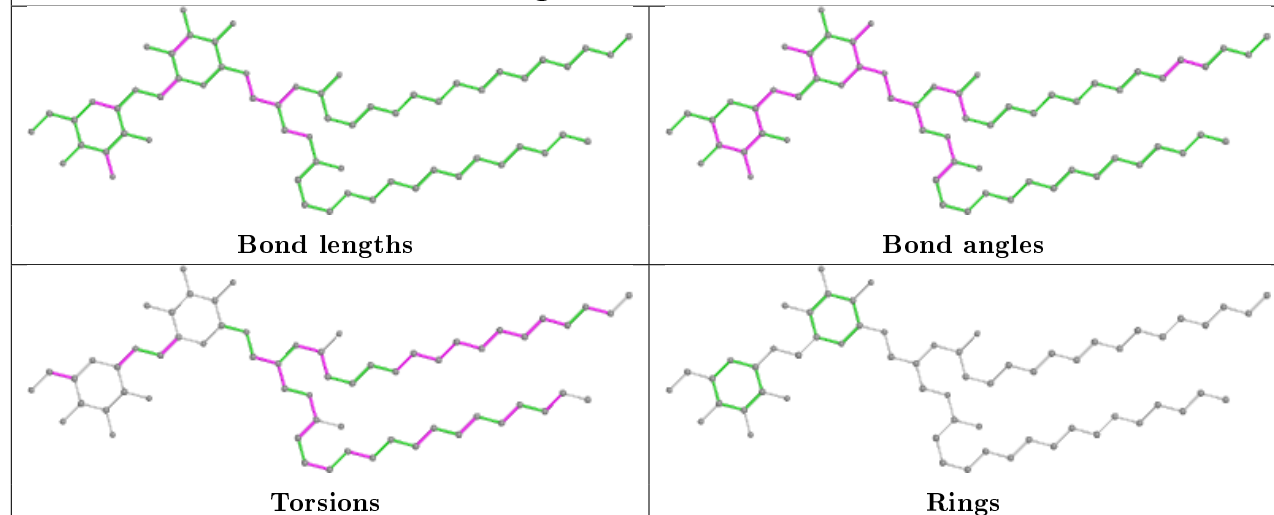
| Ligand PL9 D 407 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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

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

Ligand CLA H 101**Ligand LHG d 406**



Ligand CLA C 509**Ligand CLA b 609****Ligand DGD c 517**

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%) | -0.40 | 3 (0%) 84 84 | 26, 34, 55, 81 | 0 |
| 1 | a | 334/344 (97%) | -0.38 | 2 (0%) 89 89 | 24, 36, 62, 82 | 0 |
| 2 | B | 505/506 (99%) | -0.42 | 7 (1%) 75 76 | 26, 37, 68, 99 | 0 |
| 2 | b | 505/506 (99%) | -0.26 | 18 (3%) 42 42 | 28, 40, 77, 107 | 0 |
| 3 | C | 442/461 (95%) | -0.32 | 7 (1%) 72 73 | 29, 41, 58, 78 | 0 |
| 3 | c | 451/461 (97%) | -0.28 | 6 (1%) 77 78 | 29, 43, 66, 101 | 0 |
| 4 | D | 341/352 (96%) | -0.43 | 2 (0%) 89 89 | 25, 34, 55, 86 | 0 |
| 4 | d | 341/352 (96%) | -0.34 | 0 100 100 | 27, 38, 63, 82 | 0 |
| 5 | E | 82/84 (97%) | -0.05 | 3 (3%) 41 41 | 37, 58, 77, 85 | 0 |
| 5 | e | 82/84 (97%) | 0.18 | 6 (7%) 15 14 | 41, 65, 83, 99 | 0 |
| 6 | F | 34/45 (75%) | -0.39 | 2 (5%) 22 21 | 40, 48, 72, 95 | 0 |
| 6 | f | 34/45 (75%) | -0.23 | 3 (8%) 10 9 | 45, 53, 92, 104 | 0 |
| 7 | H | 65/66 (98%) | -0.12 | 2 (3%) 49 49 | 38, 46, 63, 76 | 0 |
| 7 | h | 63/66 (95%) | 0.21 | 5 (7%) 12 12 | 46, 55, 66, 75 | 0 |
| 8 | I | 35/38 (92%) | -0.33 | 1 (2%) 51 52 | 35, 42, 73, 88 | 0 |
| 8 | i | 35/38 (92%) | -0.20 | 2 (5%) 23 23 | 36, 44, 80, 82 | 0 |
| 9 | J | 36/40 (90%) | 0.03 | 4 (11%) 5 4 | 38, 52, 79, 96 | 0 |
| 9 | j | 36/40 (90%) | 0.10 | 4 (11%) 5 4 | 43, 56, 89, 104 | 0 |
| 10 | K | 37/46 (80%) | 0.13 | 2 (5%) 25 25 | 48, 58, 76, 86 | 0 |
| 10 | k | 37/46 (80%) | -0.12 | 1 (2%) 54 55 | 53, 60, 79, 83 | 0 |
| 11 | L | 37/37 (100%) | -0.55 | 0 100 100 | 29, 33, 65, 77 | 0 |
| 11 | l | 36/37 (97%) | -0.31 | 3 (8%) 11 11 | 27, 34, 72, 86 | 0 |
| 12 | M | 32/36 (88%) | -0.26 | 1 (3%) 49 49 | 30, 37, 66, 78 | 0 |
| 12 | m | 31/36 (86%) | -0.31 | 1 (3%) 47 47 | 30, 37, 59, 71 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | O | 244/272 (89%) | -0.15 | 13 (5%) 26 26 | 28, 45, 86, 126 | 0 |
| 13 | o | 244/272 (89%) | -0.22 | 13 (5%) 26 26 | 28, 44, 83, 124 | 0 |
| 14 | R | 34/40 (85%) | 3.40 | 32 (94%) 0 0 | 80, 93, 105, 110 | 0 |
| 14 | r | 31/40 (77%) | 5.55 | 31 (100%) 0 0 | 87, 118, 131, 136 | 0 |
| 15 | T | 29/32 (90%) | -0.42 | 1 (3%) 45 45 | 30, 35, 65, 81 | 0 |
| 15 | t | 29/32 (90%) | -0.30 | 2 (6%) 16 16 | 31, 37, 80, 81 | 0 |
| 16 | U | 97/134 (72%) | -0.40 | 0 100 100 | 36, 46, 68, 94 | 0 |
| 16 | u | 97/134 (72%) | -0.54 | 0 100 100 | 34, 44, 61, 85 | 0 |
| 17 | V | 137/163 (84%) | -0.65 | 0 100 100 | 31, 44, 59, 77 | 0 |
| 17 | v | 137/163 (84%) | -0.30 | 0 100 100 | 37, 50, 70, 80 | 0 |
| 18 | X | 38/41 (92%) | 0.13 | 2 (5%) 26 26 | 46, 58, 80, 85 | 0 |
| 18 | x | 39/41 (95%) | 0.41 | 6 (15%) 2 1 | 52, 65, 94, 106 | 0 |
| 19 | Y | 27/46 (58%) | 1.20 | 8 (29%) 0 0 | 58, 78, 89, 100 | 0 |
| 19 | y | 30/46 (65%) | 0.56 | 3 (10%) 7 6 | 63, 75, 92, 95 | 0 |
| 20 | Z | 62/62 (100%) | 0.73 | 15 (24%) 0 0 | 55, 73, 112, 128 | 0 |
| 20 | z | 62/62 (100%) | 0.75 | 9 (14%) 2 2 | 61, 73, 107, 119 | 0 |
| All | All | 5302/5690 (93%) | -0.20 | 220 (4%) 37 37 | 24, 42, 79, 136 | 0 |

The worst 5 of 220 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 14 | r | 14 | LEU | 12.2 |
| 14 | r | 9 | LEU | 9.0 |
| 14 | r | 10 | LEU | 8.5 |
| 14 | r | 28 | VAL | 8.2 |
| 2 | b | 495 | PHE | 7.8 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 15 | FME | T | 1 | 10/11 | 0.94 | 0.10 | 36,48,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 15 | FME | t | 1 | 10/11 | 0.95 | 0.09 | 34,48,77,77 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.96 | 0.10 | 47,57,75,77 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.96 | 0.15 | 48,61,80,82 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.97 | 0.15 | 46,59,70,75 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.97 | 0.13 | 40,57,76,89 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 31 | STE | R | 101 | 12/20 | 0.67 | 0.32 | 68,87,105,110 | 0 |
| 31 | STE | H | 103 | 18/20 | 0.69 | 0.32 | 56,85,97,102 | 0 |
| 26 | LHG | A | 412 | 49/49 | 0.79 | 0.26 | 46,87,119,124 | 0 |
| 23 | BCR | X | 101 | 40/40 | 0.79 | 0.17 | 34,54,70,73 | 0 |
| 32 | LMG | c | 522 | 48/55 | 0.79 | 0.24 | 42,81,110,115 | 0 |
| 31 | STE | a | 416 | 12/20 | 0.81 | 0.27 | 35,72,80,82 | 0 |
| 25 | PL9 | A | 408 | 55/55 | 0.81 | 0.27 | 42,71,90,93 | 0 |
| 26 | LHG | e | 101 | 42/49 | 0.81 | 0.28 | 60,94,114,125 | 0 |
| 31 | STE | T | 103 | 15/20 | 0.82 | 0.18 | 40,62,91,93 | 0 |
| 31 | STE | c | 521 | 20/20 | 0.82 | 0.22 | 45,65,94,110 | 0 |
| 31 | STE | B | 624 | 16/20 | 0.82 | 0.24 | 40,64,83,86 | 0 |
| 31 | STE | h | 103 | 14/20 | 0.82 | 0.26 | 57,74,88,95 | 0 |
| 32 | LMG | D | 410 | 33/55 | 0.82 | 0.19 | 42,60,95,106 | 0 |
| 22 | CLA | C | 512 | 65/65 | 0.83 | 0.20 | 41,62,105,110 | 0 |
| 31 | STE | b | 622 | 16/20 | 0.83 | 0.17 | 44,66,87,93 | 0 |
| 31 | STE | b | 623 | 20/20 | 0.83 | 0.21 | 44,66,96,98 | 0 |
| 31 | STE | B | 623 | 18/20 | 0.84 | 0.16 | 45,65,90,95 | 0 |
| 32 | LMG | c | 523 | 49/55 | 0.84 | 0.18 | 37,62,105,119 | 0 |
| 31 | STE | d | 412 | 20/20 | 0.84 | 0.19 | 53,75,97,103 | 0 |
| 25 | PL9 | a | 410 | 55/55 | 0.84 | 0.21 | 43,76,96,103 | 0 |
| 31 | STE | C | 522 | 12/20 | 0.84 | 0.14 | 40,56,65,69 | 0 |
| 22 | CLA | c | 513 | 65/65 | 0.84 | 0.16 | 47,65,103,110 | 0 |
| 23 | BCR | h | 101 | 40/40 | 0.84 | 0.17 | 41,63,87,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 31 | STE | I | 101 | 15/20 | 0.85 | 0.15 | 43,64,86,87 | 0 |
| 31 | STE | d | 411 | 20/20 | 0.85 | 0.25 | 49,67,82,86 | 0 |
| 22 | CLA | b | 601 | 65/65 | 0.85 | 0.19 | 52,76,101,103 | 0 |
| 31 | STE | b | 620 | 20/20 | 0.85 | 0.24 | 44,61,82,88 | 0 |
| 32 | LMG | b | 621 | 55/55 | 0.85 | 0.29 | 50,79,102,113 | 0 |
| 31 | STE | B | 625 | 15/20 | 0.85 | 0.19 | 43,66,83,92 | 0 |
| 31 | STE | a | 415 | 10/20 | 0.85 | 0.20 | 33,67,81,83 | 0 |
| 32 | LMG | a | 417 | 55/55 | 0.86 | 0.15 | 39,61,90,107 | 0 |
| 31 | STE | M | 103 | 10/20 | 0.86 | 0.18 | 40,54,63,72 | 0 |
| 28 | DGD | A | 414 | 66/66 | 0.86 | 0.17 | 43,67,92,99 | 0 |
| 31 | STE | c | 501 | 12/20 | 0.86 | 0.17 | 44,72,81,86 | 0 |
| 31 | STE | Z | 101 | 8/20 | 0.86 | 0.18 | 42,63,77,77 | 0 |
| 22 | CLA | C | 513 | 65/65 | 0.86 | 0.21 | 51,69,108,113 | 0 |
| 31 | STE | B | 620 | 17/20 | 0.87 | 0.14 | 39,56,72,81 | 0 |
| 31 | STE | B | 601 | 12/20 | 0.87 | 0.41 | 56,74,93,94 | 0 |
| 31 | STE | M | 102 | 15/20 | 0.87 | 0.15 | 43,60,73,74 | 0 |
| 23 | BCR | K | 102 | 40/40 | 0.87 | 0.13 | 42,61,76,76 | 0 |
| 22 | CLA | H | 101 | 65/65 | 0.87 | 0.16 | 43,68,99,105 | 0 |
| 31 | STE | B | 622 | 12/20 | 0.87 | 0.13 | 35,58,68,76 | 0 |
| 27 | SQD | B | 621 | 54/54 | 0.88 | 0.15 | 41,64,93,101 | 0 |
| 22 | CLA | c | 514 | 65/65 | 0.88 | 0.20 | 47,72,110,119 | 0 |
| 27 | SQD | d | 409 | 41/54 | 0.88 | 0.20 | 59,95,120,123 | 0 |
| 32 | LMG | Y | 101 | 48/55 | 0.88 | 0.18 | 50,77,102,109 | 0 |
| 27 | SQD | L | 101 | 49/54 | 0.88 | 0.13 | 42,64,97,117 | 0 |
| 31 | STE | C | 521 | 16/20 | 0.88 | 0.15 | 46,61,71,77 | 0 |
| 27 | SQD | a | 414 | 36/54 | 0.88 | 0.17 | 24,66,100,107 | 0 |
| 31 | STE | b | 624 | 10/20 | 0.88 | 0.28 | 41,58,71,73 | 0 |
| 31 | STE | D | 413 | 20/20 | 0.89 | 0.17 | 38,56,85,86 | 0 |
| 31 | STE | M | 104 | 18/20 | 0.89 | 0.15 | 37,51,85,94 | 0 |
| 32 | LMG | C | 516 | 48/55 | 0.89 | 0.15 | 37,60,85,102 | 0 |
| 31 | STE | C | 520 | 12/20 | 0.89 | 0.13 | 45,63,73,76 | 0 |
| 27 | SQD | A | 413 | 39/54 | 0.89 | 0.17 | 45,70,99,104 | 0 |
| 32 | LMG | D | 411 | 28/55 | 0.89 | 0.15 | 35,54,68,74 | 0 |
| 23 | BCR | k | 101 | 40/40 | 0.89 | 0.14 | 40,67,80,83 | 0 |
| 31 | STE | T | 102 | 16/20 | 0.89 | 0.15 | 40,55,78,91 | 0 |
| 31 | STE | L | 103 | 12/20 | 0.89 | 0.19 | 55,70,86,96 | 0 |
| 23 | BCR | k | 102 | 40/40 | 0.90 | 0.18 | 40,58,70,72 | 0 |
| 22 | CLA | C | 502 | 65/65 | 0.90 | 0.16 | 32,48,65,66 | 0 |
| 31 | STE | t | 102 | 14/20 | 0.90 | 0.12 | 39,51,63,69 | 0 |
| 23 | BCR | D | 406 | 40/40 | 0.90 | 0.14 | 33,49,89,93 | 0 |
| 22 | CLA | a | 405 | 65/65 | 0.91 | 0.14 | 22,40,94,108 | 0 |
| 23 | BCR | d | 404 | 40/40 | 0.91 | 0.13 | 36,56,96,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22 | CLA | c | 503 | 65/65 | 0.91 | 0.16 | 35,47,65,71 | 0 |
| 32 | LMG | M | 101 | 51/55 | 0.91 | 0.13 | 34,54,82,89 | 0 |
| 28 | DGD | C | 518 | 62/66 | 0.91 | 0.14 | 38,59,101,119 | 0 |
| 22 | CLA | D | 405 | 65/65 | 0.91 | 0.14 | 24,45,110,127 | 0 |
| 31 | STE | j | 101 | 12/20 | 0.91 | 0.17 | 47,65,78,79 | 0 |
| 32 | LMG | m | 101 | 51/55 | 0.91 | 0.14 | 31,58,83,98 | 0 |
| 22 | CLA | C | 507 | 65/65 | 0.92 | 0.15 | 30,48,65,71 | 0 |
| 27 | SQD | F | 102 | 36/54 | 0.92 | 0.18 | 53,78,93,101 | 0 |
| 22 | CLA | c | 509 | 64/65 | 0.92 | 0.15 | 36,53,103,122 | 0 |
| 23 | BCR | K | 101 | 40/40 | 0.92 | 0.15 | 45,63,78,89 | 0 |
| 22 | CLA | b | 616 | 60/65 | 0.92 | 0.15 | 33,50,91,95 | 0 |
| 23 | BCR | c | 515 | 40/40 | 0.92 | 0.18 | 46,65,82,84 | 0 |
| 22 | CLA | b | 615 | 65/65 | 0.92 | 0.14 | 30,46,67,79 | 0 |
| 23 | BCR | C | 514 | 40/40 | 0.92 | 0.12 | 30,47,59,73 | 0 |
| 32 | LMG | D | 408 | 51/55 | 0.93 | 0.18 | 33,65,95,99 | 0 |
| 28 | DGD | c | 519 | 62/66 | 0.93 | 0.14 | 31,59,86,90 | 0 |
| 22 | CLA | c | 504 | 65/65 | 0.93 | 0.15 | 35,50,61,64 | 0 |
| 22 | CLA | d | 403 | 65/65 | 0.93 | 0.14 | 32,55,102,112 | 0 |
| 23 | BCR | b | 619 | 40/40 | 0.93 | 0.10 | 34,53,64,73 | 0 |
| 23 | BCR | C | 515 | 40/40 | 0.93 | 0.16 | 45,60,79,83 | 0 |
| 22 | CLA | B | 616 | 60/65 | 0.93 | 0.14 | 27,46,107,121 | 0 |
| 22 | CLA | B | 615 | 65/65 | 0.93 | 0.13 | 26,43,65,70 | 0 |
| 32 | LMG | c | 520 | 37/55 | 0.93 | 0.15 | 49,70,89,90 | 0 |
| 22 | CLA | c | 507 | 65/65 | 0.93 | 0.13 | 33,54,91,108 | 0 |
| 32 | LMG | d | 408 | 44/55 | 0.93 | 0.15 | 36,61,95,103 | 0 |
| 22 | CLA | C | 503 | 65/65 | 0.94 | 0.15 | 35,51,62,64 | 0 |
| 22 | CLA | C | 505 | 65/65 | 0.94 | 0.15 | 27,47,70,73 | 0 |
| 22 | CLA | C | 508 | 65/65 | 0.94 | 0.14 | 30,51,113,130 | 0 |
| 23 | BCR | B | 618 | 40/40 | 0.94 | 0.10 | 30,43,56,61 | 0 |
| 28 | DGD | c | 518 | 62/66 | 0.94 | 0.12 | 37,57,94,108 | 0 |
| 23 | BCR | B | 617 | 40/40 | 0.94 | 0.13 | 29,46,63,67 | 0 |
| 23 | BCR | b | 617 | 40/40 | 0.94 | 0.12 | 31,49,60,63 | 0 |
| 22 | CLA | b | 602 | 65/65 | 0.94 | 0.15 | 29,47,70,76 | 0 |
| 23 | BCR | b | 618 | 40/40 | 0.94 | 0.11 | 26,46,60,67 | 0 |
| 22 | CLA | a | 403 | 65/65 | 0.94 | 0.14 | 29,45,101,111 | 0 |
| 22 | CLA | c | 510 | 65/65 | 0.94 | 0.19 | 32,54,72,73 | 0 |
| 27 | SQD | a | 413 | 54/54 | 0.94 | 0.15 | 47,66,94,98 | 0 |
| 22 | CLA | B | 602 | 65/65 | 0.94 | 0.17 | 27,41,68,77 | 0 |
| 28 | DGD | h | 102 | 62/66 | 0.94 | 0.12 | 37,53,67,76 | 0 |
| 22 | CLA | c | 508 | 65/65 | 0.94 | 0.14 | 33,48,64,75 | 0 |
| 22 | CLA | c | 506 | 65/65 | 0.94 | 0.17 | 30,49,70,81 | 0 |
| 25 | PL9 | D | 407 | 55/55 | 0.94 | 0.12 | 25,39,51,66 | 0 |

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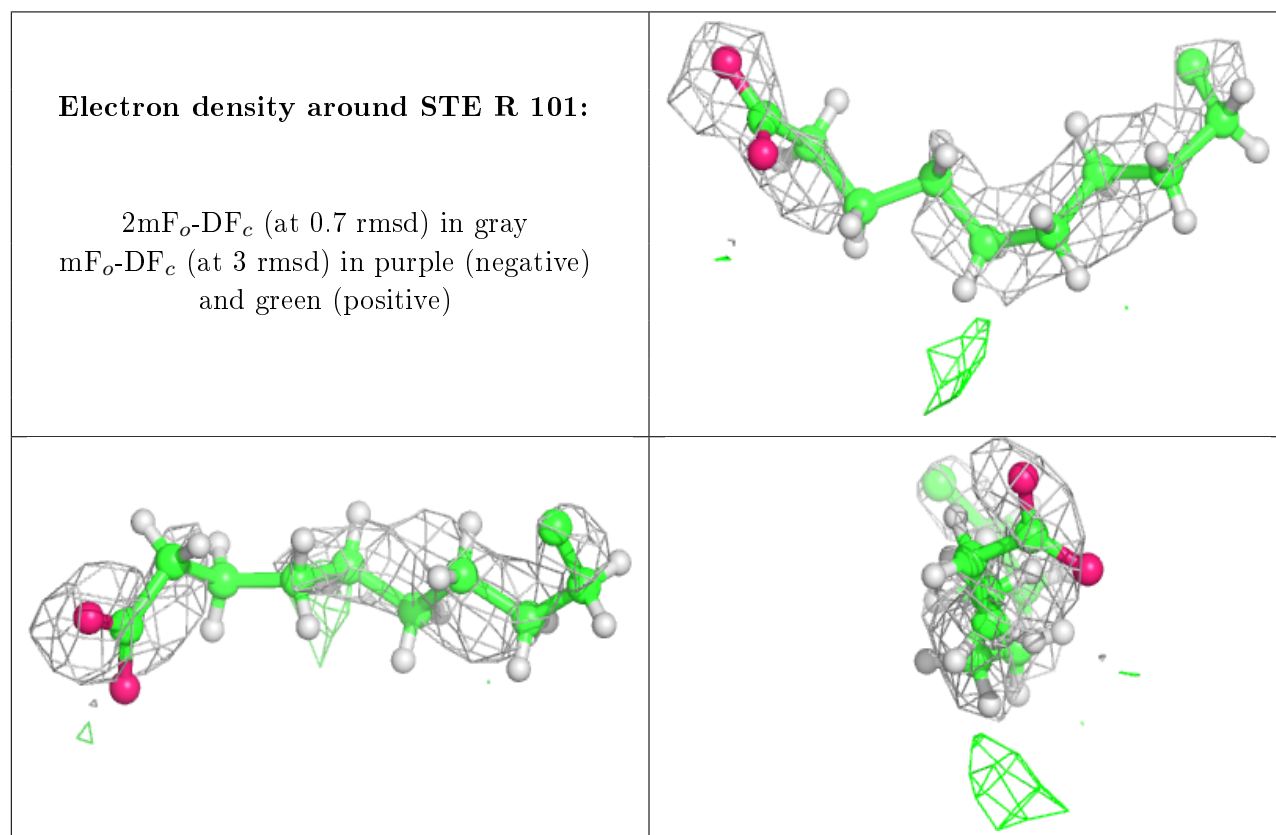
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28 | DGD | H | 102 | 62/66 | 0.94 | 0.11 | 31,51,65,77 | 0 |
| 22 | CLA | B | 604 | 65/65 | 0.94 | 0.13 | 22,37,79,93 | 0 |
| 22 | CLA | C | 504 | 59/65 | 0.94 | 0.12 | 33,47,84,103 | 0 |
| 22 | CLA | C | 506 | 65/65 | 0.94 | 0.12 | 28,48,91,99 | 0 |
| 22 | CLA | B | 606 | 65/65 | 0.94 | 0.11 | 20,41,72,78 | 0 |
| 31 | STE | d | 410 | 17/20 | 0.94 | 0.12 | 44,60,69,76 | 0 |
| 23 | BCR | B | 619 | 40/40 | 0.94 | 0.10 | 28,47,61,74 | 0 |
| 22 | CLA | C | 510 | 65/65 | 0.94 | 0.15 | 31,52,70,74 | 0 |
| 22 | CLA | C | 511 | 65/65 | 0.94 | 0.11 | 38,56,75,80 | 0 |
| 22 | CLA | C | 509 | 65/65 | 0.94 | 0.19 | 29,50,70,77 | 0 |
| 22 | CLA | b | 609 | 65/65 | 0.94 | 0.14 | 32,51,76,78 | 0 |
| 22 | CLA | b | 614 | 65/65 | 0.95 | 0.12 | 29,43,84,94 | 0 |
| 22 | CLA | c | 512 | 65/65 | 0.95 | 0.12 | 40,61,79,85 | 0 |
| 22 | CLA | C | 501 | 65/65 | 0.95 | 0.12 | 28,42,53,62 | 0 |
| 22 | CLA | b | 604 | 65/65 | 0.95 | 0.14 | 28,41,91,114 | 0 |
| 23 | BCR | A | 405 | 40/40 | 0.95 | 0.09 | 26,40,48,51 | 0 |
| 22 | CLA | b | 608 | 65/65 | 0.95 | 0.15 | 29,48,70,87 | 0 |
| 22 | CLA | b | 613 | 65/65 | 0.95 | 0.14 | 22,41,82,90 | 0 |
| 27 | SQD | A | 411 | 52/54 | 0.95 | 0.16 | 41,66,102,108 | 0 |
| 22 | CLA | A | 404 | 54/65 | 0.95 | 0.11 | 21,36,64,77 | 0 |
| 23 | BCR | c | 516 | 40/40 | 0.95 | 0.11 | 31,50,77,78 | 0 |
| 22 | CLA | b | 606 | 65/65 | 0.95 | 0.12 | 30,45,78,87 | 0 |
| 22 | CLA | B | 603 | 65/65 | 0.95 | 0.17 | 23,38,66,74 | 0 |
| 22 | CLA | B | 609 | 65/65 | 0.95 | 0.13 | 28,46,66,74 | 0 |
| 28 | DGD | C | 517 | 62/66 | 0.95 | 0.13 | 27,42,78,88 | 0 |
| 22 | CLA | b | 611 | 65/65 | 0.95 | 0.13 | 20,39,63,71 | 0 |
| 26 | LHG | l | 101 | 49/49 | 0.95 | 0.11 | 34,51,60,72 | 0 |
| 26 | LHG | A | 410 | 47/49 | 0.95 | 0.13 | 34,53,93,105 | 0 |
| 22 | CLA | c | 511 | 65/65 | 0.95 | 0.15 | 35,54,72,75 | 0 |
| 31 | STE | J | 101 | 12/20 | 0.95 | 0.12 | 48,64,78,79 | 0 |
| 23 | BCR | T | 101 | 40/40 | 0.95 | 0.09 | 27,46,64,66 | 0 |
| 22 | CLA | A | 403 | 65/65 | 0.95 | 0.14 | 24,40,103,110 | 0 |
| 28 | DGD | C | 519 | 62/66 | 0.95 | 0.12 | 29,55,84,94 | 0 |
| 22 | CLA | b | 605 | 65/65 | 0.95 | 0.15 | 29,41,60,66 | 0 |
| 22 | CLA | a | 411 | 65/65 | 0.95 | 0.13 | 21,37,47,52 | 0 |
| 26 | LHG | a | 412 | 49/49 | 0.95 | 0.13 | 33,53,75,84 | 0 |
| 28 | DGD | c | 517 | 62/66 | 0.95 | 0.12 | 28,46,79,95 | 0 |
| 23 | BCR | a | 406 | 40/40 | 0.96 | 0.08 | 24,37,48,58 | 0 |
| 33 | PHO | d | 401 | 64/64 | 0.96 | 0.09 | 27,44,54,62 | 0 |
| 22 | CLA | d | 402 | 65/65 | 0.96 | 0.12 | 25,40,65,80 | 0 |
| 22 | CLA | b | 612 | 65/65 | 0.96 | 0.17 | 22,39,54,60 | 0 |
| 33 | PHO | D | 402 | 64/64 | 0.96 | 0.14 | 26,37,46,47 | 0 |

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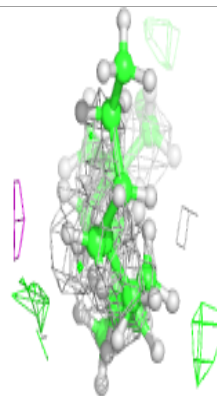
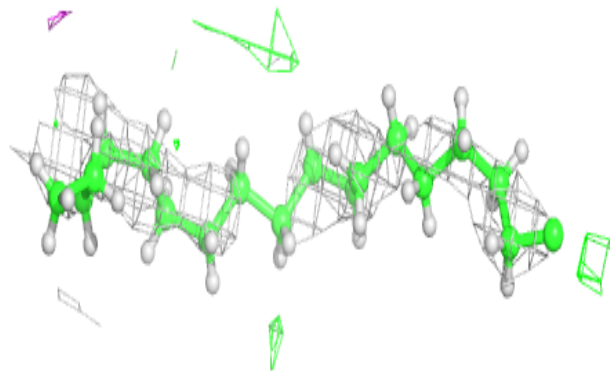
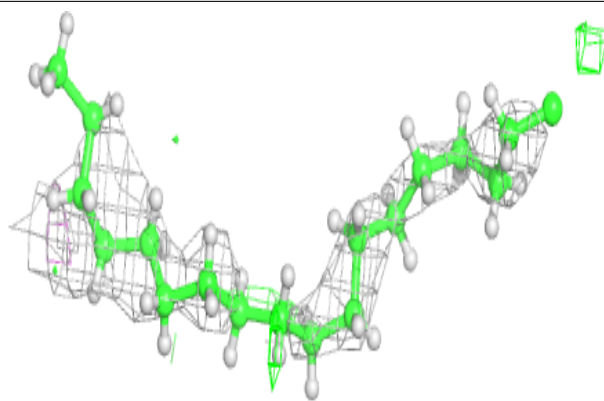
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 22 | CLA | D | 404 | 65/65 | 0.96 | 0.12 | 19,33,58,67 | 0 |
| 22 | CLA | c | 505 | 60/65 | 0.96 | 0.11 | 37,54,82,90 | 0 |
| 22 | CLA | c | 502 | 65/65 | 0.96 | 0.13 | 29,44,56,62 | 0 |
| 25 | PL9 | d | 405 | 55/55 | 0.96 | 0.11 | 26,40,51,54 | 0 |
| 22 | CLA | A | 402 | 65/65 | 0.96 | 0.10 | 18,33,51,69 | 0 |
| 26 | LHG | D | 412 | 49/49 | 0.96 | 0.12 | 34,48,69,76 | 0 |
| 22 | CLA | B | 613 | 65/65 | 0.96 | 0.14 | 21,38,77,88 | 0 |
| 22 | CLA | B | 612 | 65/65 | 0.96 | 0.15 | 24,37,51,56 | 0 |
| 22 | CLA | B | 610 | 65/65 | 0.96 | 0.14 | 22,36,47,54 | 0 |
| 22 | CLA | B | 614 | 65/65 | 0.96 | 0.15 | 24,41,87,101 | 0 |
| 35 | HEC | f | 101 | 43/43 | 0.96 | 0.12 | 48,65,89,92 | 0 |
| 33 | PHO | D | 401 | 64/64 | 0.96 | 0.10 | 21,34,45,48 | 0 |
| 33 | PHO | a | 404 | 64/64 | 0.96 | 0.13 | 24,34,44,44 | 0 |
| 22 | CLA | b | 610 | 65/65 | 0.96 | 0.17 | 27,43,56,64 | 0 |
| 22 | CLA | A | 409 | 65/65 | 0.96 | 0.10 | 23,34,56,61 | 0 |
| 22 | CLA | a | 402 | 65/65 | 0.96 | 0.11 | 22,34,48,60 | 0 |
| 26 | LHG | d | 407 | 39/49 | 0.96 | 0.10 | 35,53,78,84 | 0 |
| 22 | CLA | B | 605 | 65/65 | 0.96 | 0.15 | 25,37,51,53 | 0 |
| 22 | CLA | b | 603 | 65/65 | 0.96 | 0.15 | 25,43,77,92 | 0 |
| 22 | CLA | B | 607 | 65/65 | 0.96 | 0.11 | 22,35,71,80 | 0 |
| 22 | CLA | B | 608 | 65/65 | 0.96 | 0.12 | 23,39,63,69 | 0 |
| 23 | BCR | t | 101 | 40/40 | 0.96 | 0.09 | 25,43,56,57 | 0 |
| 22 | CLA | b | 607 | 65/65 | 0.96 | 0.11 | 22,43,71,75 | 0 |
| 35 | HEC | v | 201 | 43/43 | 0.97 | 0.12 | 30,41,55,57 | 0 |
| 26 | LHG | L | 102 | 49/49 | 0.97 | 0.13 | 30,47,62,69 | 0 |
| 35 | HEC | V | 201 | 43/43 | 0.97 | 0.12 | 28,37,45,54 | 0 |
| 22 | CLA | B | 611 | 65/65 | 0.97 | 0.15 | 23,34,51,51 | 0 |
| 26 | LHG | D | 409 | 49/49 | 0.97 | 0.10 | 26,43,55,62 | 0 |
| 26 | LHG | d | 406 | 49/49 | 0.97 | 0.10 | 30,46,60,68 | 0 |
| 35 | HEC | F | 101 | 43/43 | 0.97 | 0.11 | 40,57,70,79 | 0 |
| 34 | BCT | a | 409 | 4/4 | 0.98 | 0.21 | 32,35,48,57 | 0 |
| 34 | BCT | D | 403 | 4/4 | 0.98 | 0.17 | 33,37,44,45 | 0 |
| 24 | CL | A | 407 | 1/1 | 0.99 | 0.04 | 36,36,36,36 | 0 |
| 24 | CL | A | 406 | 1/1 | 0.99 | 0.09 | 34,34,34,34 | 0 |
| 29 | OEX | a | 418[A] | 10/10 | 0.99 | 0.11 | 33,39,42,43 | 10 |
| 24 | CL | a | 407 | 1/1 | 0.99 | 0.03 | 32,32,32,32 | 0 |
| 29 | OEX | A | 415[A] | 10/10 | 0.99 | 0.14 | 36,38,42,43 | 10 |
| 24 | CL | a | 408 | 1/1 | 0.99 | 0.03 | 34,34,34,34 | 0 |
| 30 | OEY | a | 419[B] | 11/11 | 0.99 | 0.12 | 18,23,28,29 | 11 |
| 30 | OEY | A | 416[B] | 11/11 | 0.99 | 0.14 | 18,23,28,28 | 11 |
| 21 | FE2 | a | 401 | 1/1 | 1.00 | 0.11 | 38,38,38,38 | 0 |
| 21 | FE2 | A | 401 | 1/1 | 1.00 | 0.14 | 37,37,37,37 | 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.



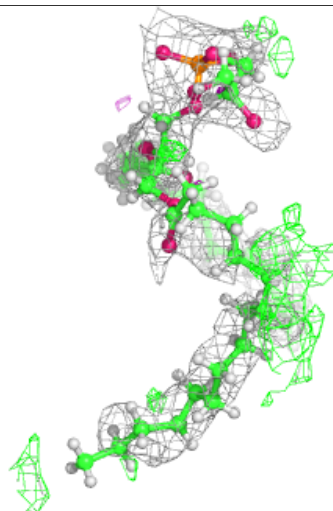
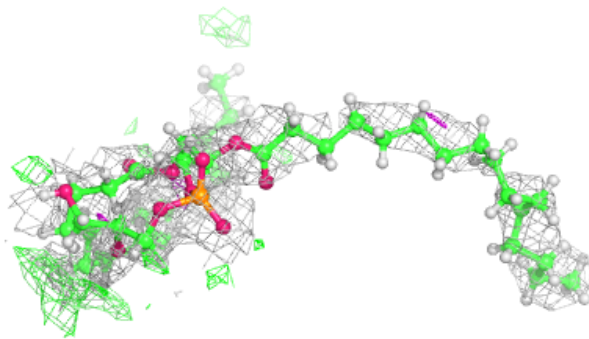
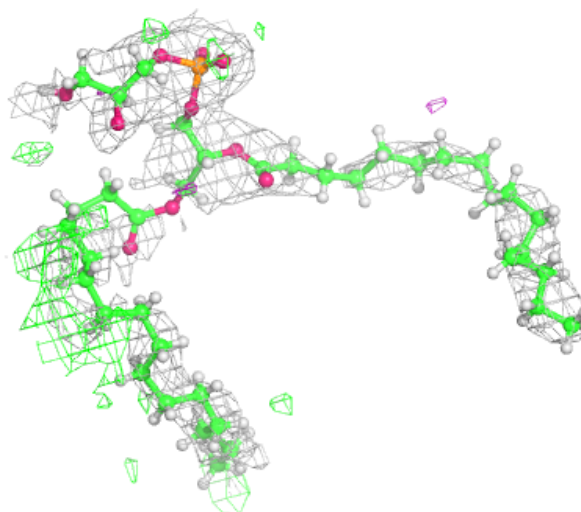
Electron density around STE H 103:

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



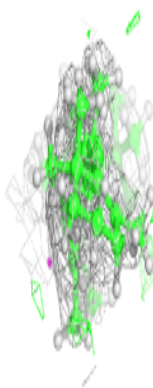
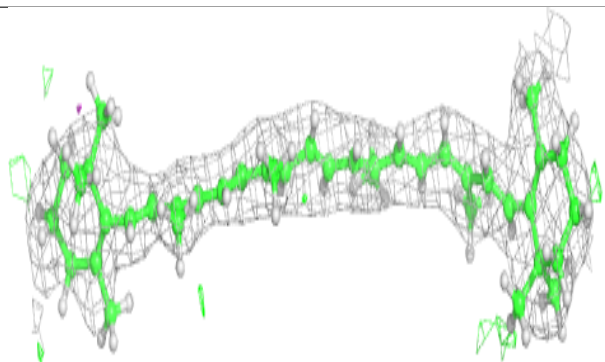
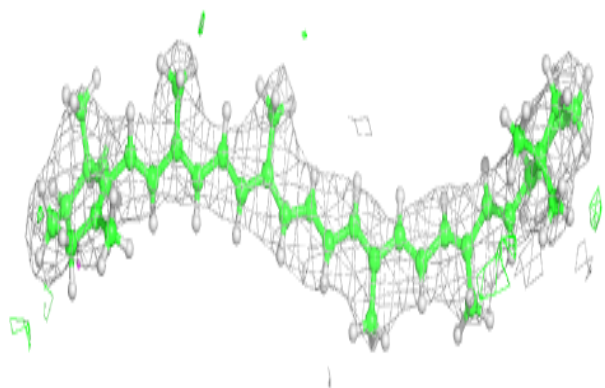
Electron density around LHG A 412:

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

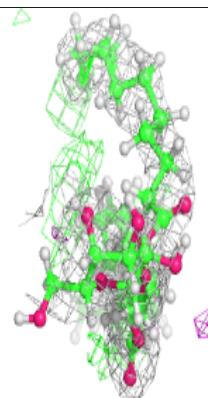
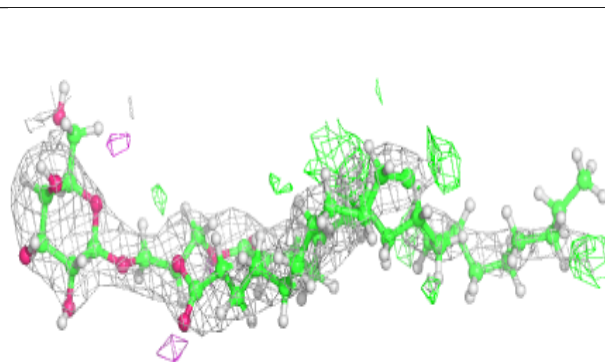
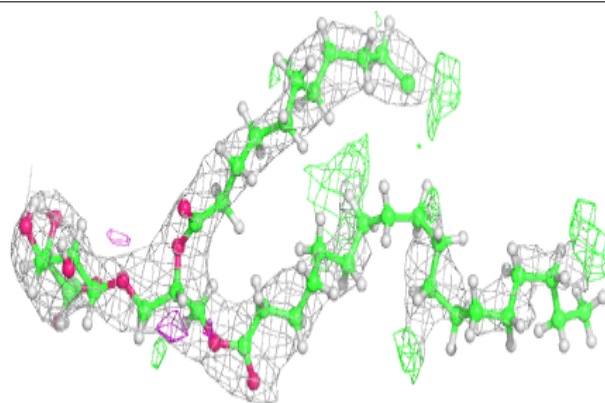


Electron density around BCR X 101:

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

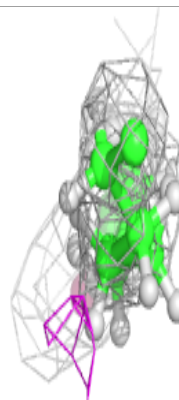
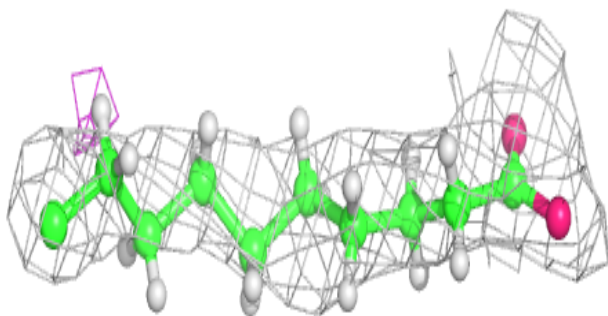
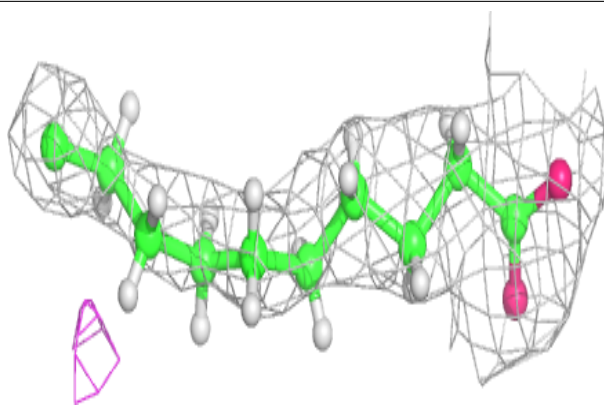
**Electron density around LMG c 522:**

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

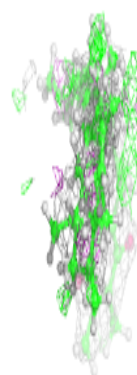
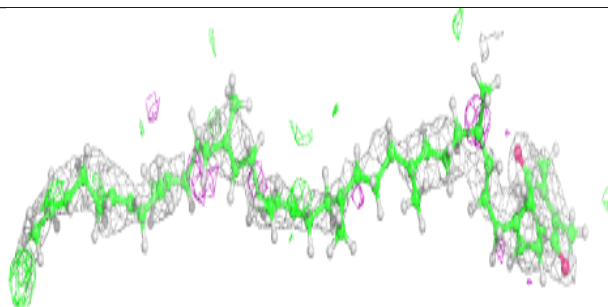
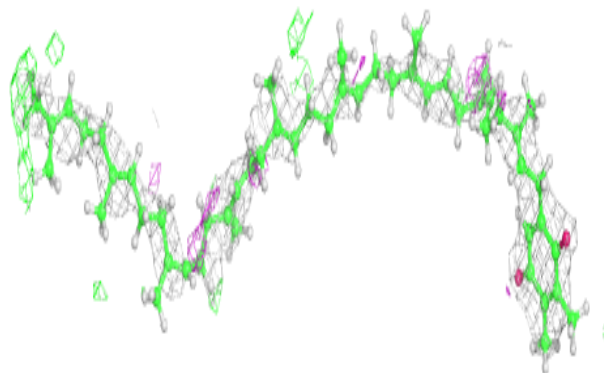


Electron density around STE a 416:

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

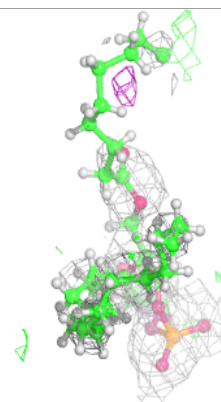
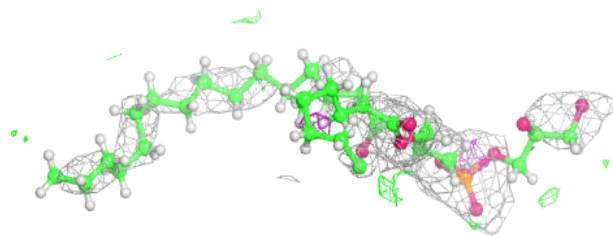
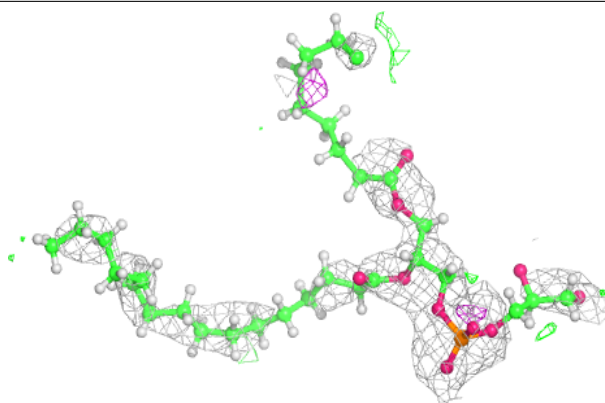
**Electron density around PL9 A 408:**

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

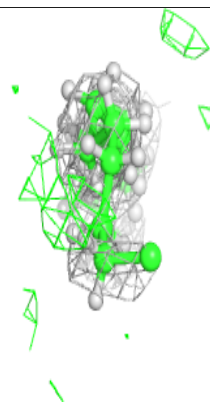
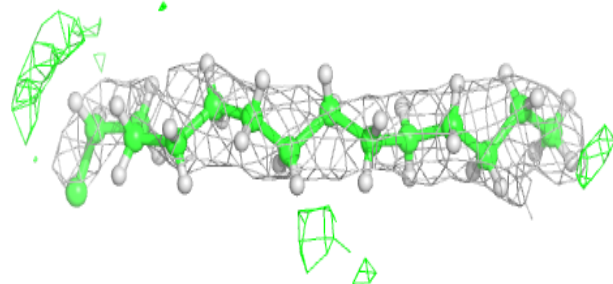
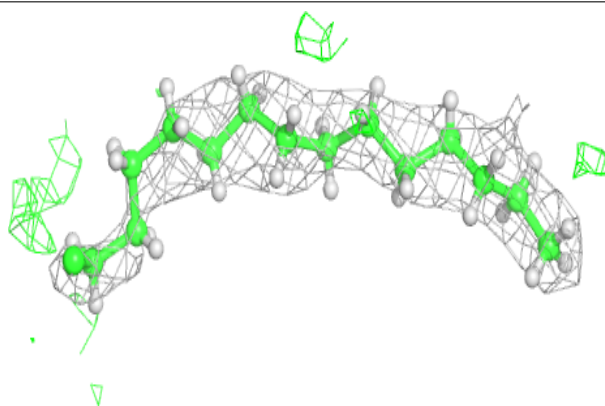


Electron density around LHG e 101:

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

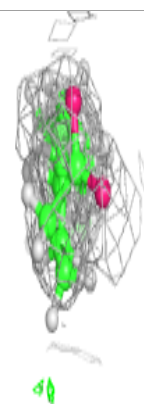
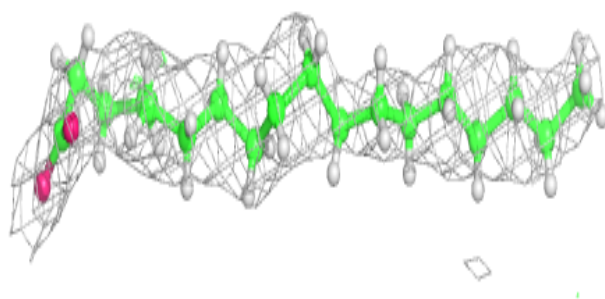
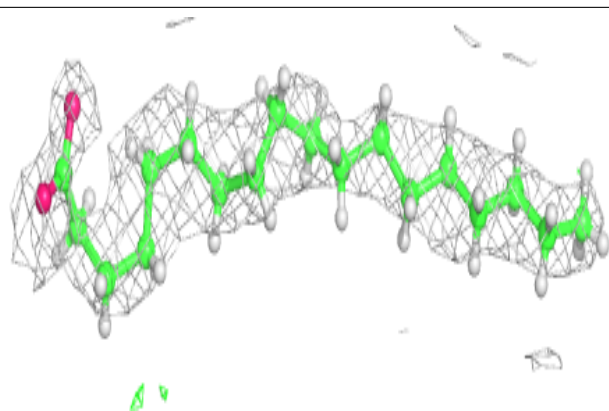
**Electron density around STE T 103:**

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

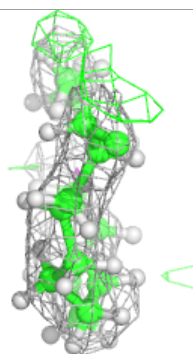
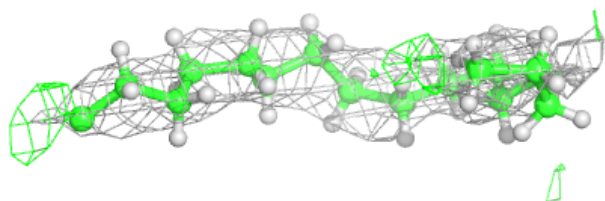
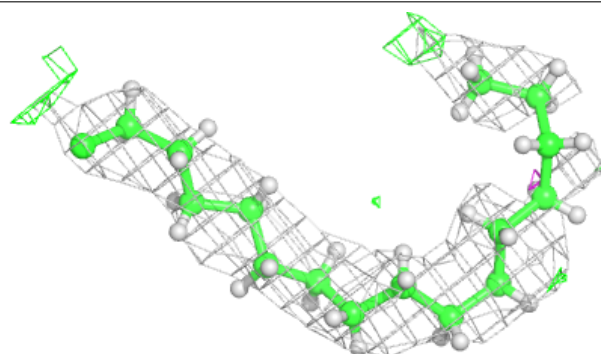


Electron density around STE c 521:

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

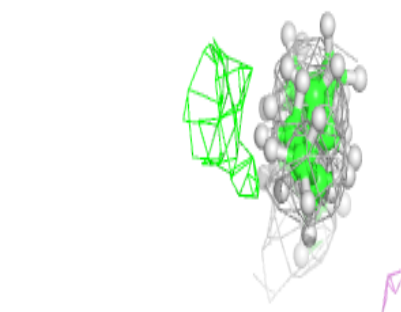
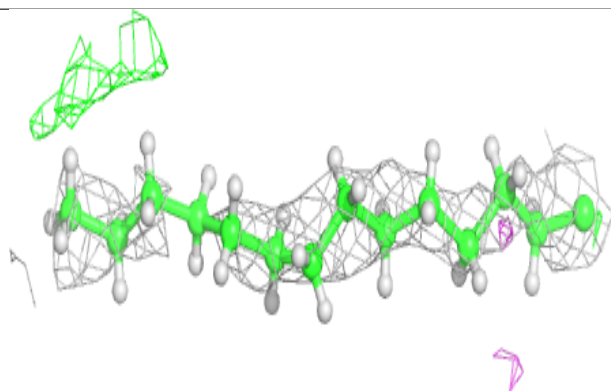
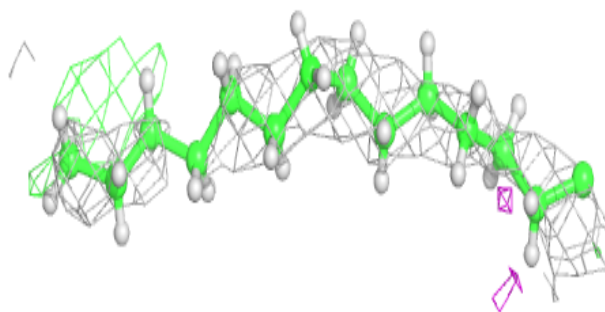
**Electron density around STE B 624:**

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

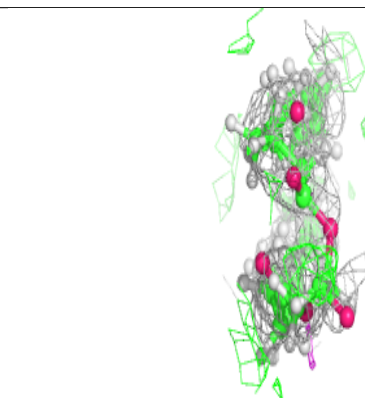
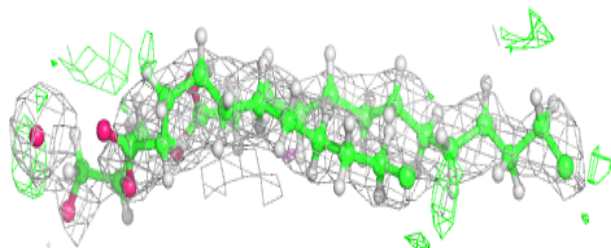
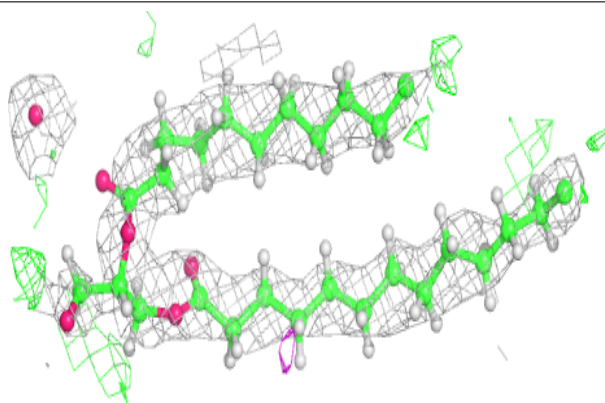


Electron density around STE h 103:

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

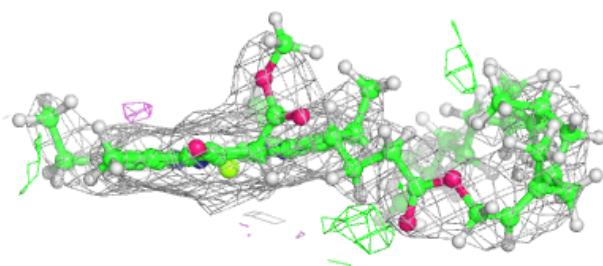
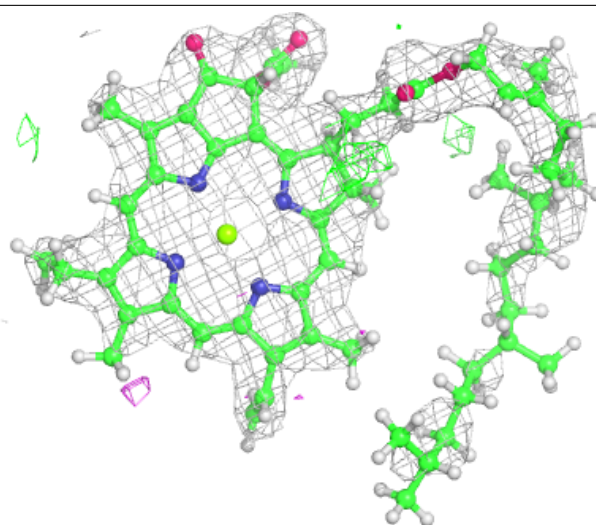
**Electron density around LMG D 410:**

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



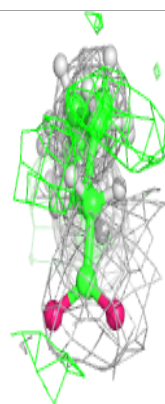
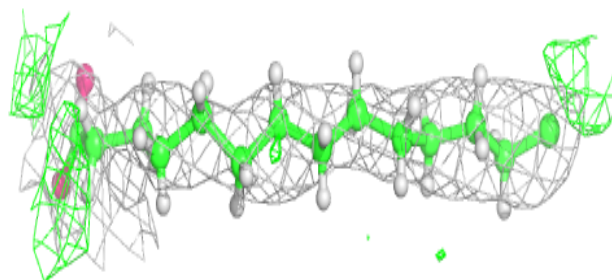
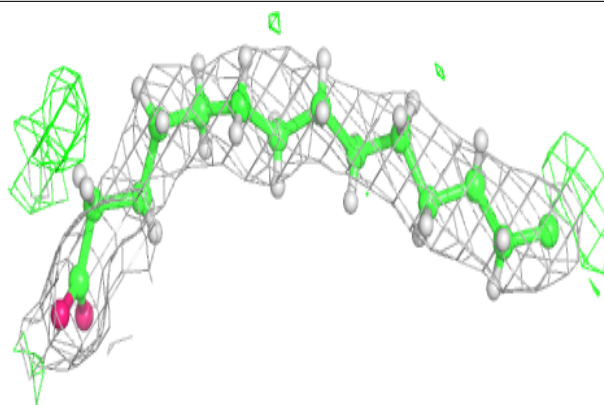
Electron density around CLA C 512:

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

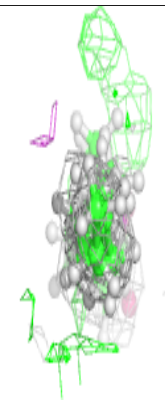
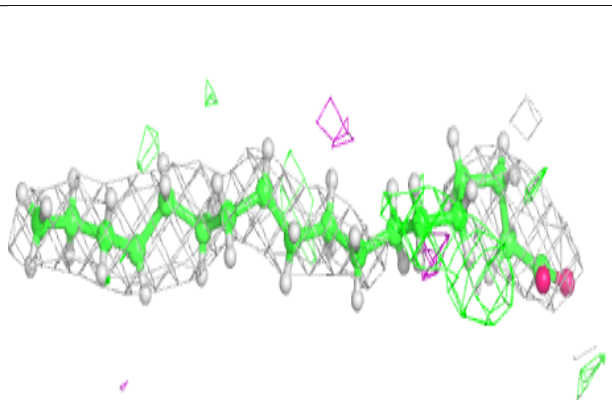
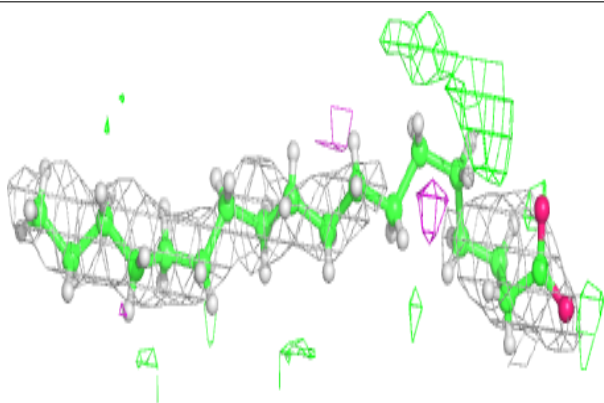


Electron density around STE b 622:

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

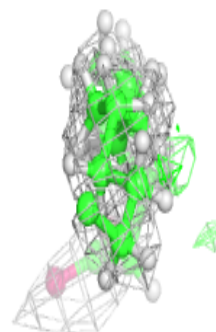
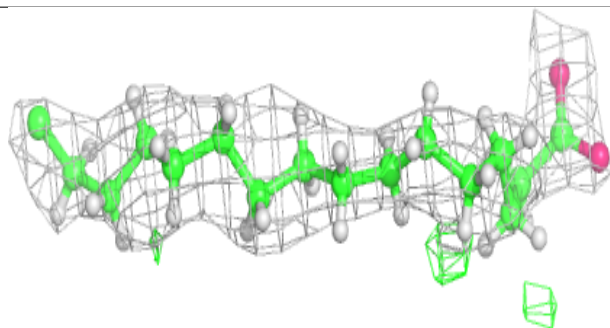
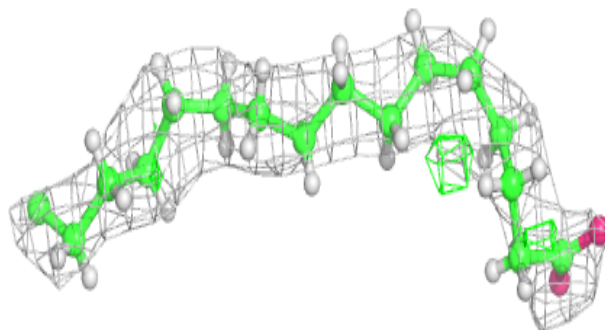
**Electron density around STE b 623:**

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

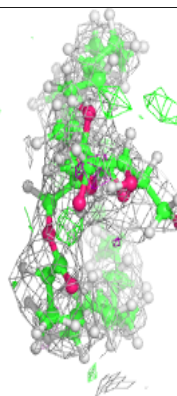
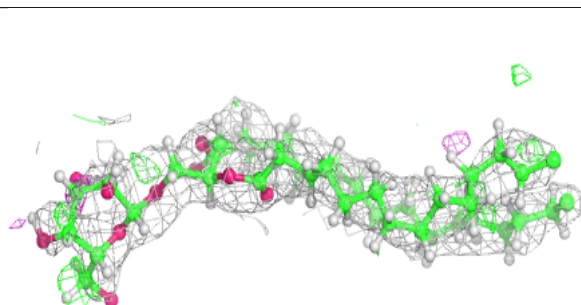
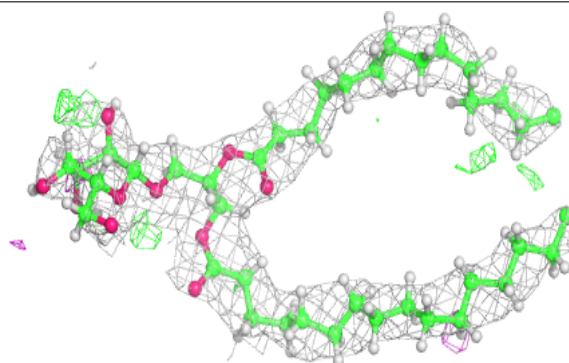


Electron density around STE B 623:

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

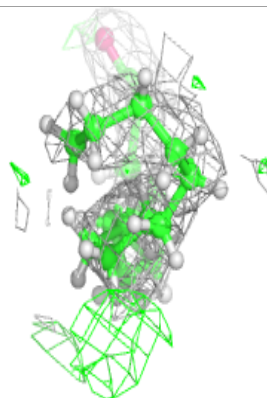
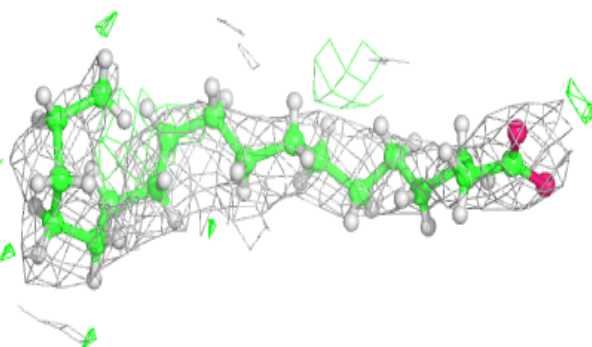
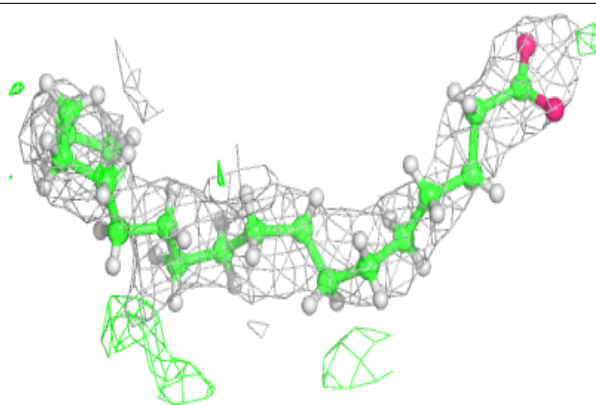
**Electron density around LMG c 523:**

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

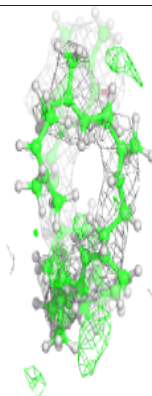
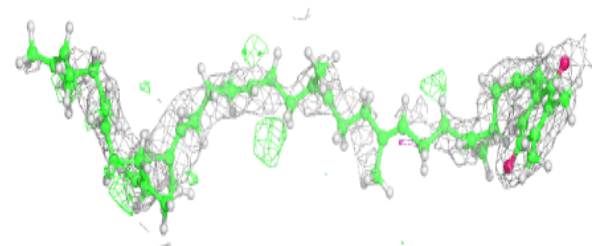
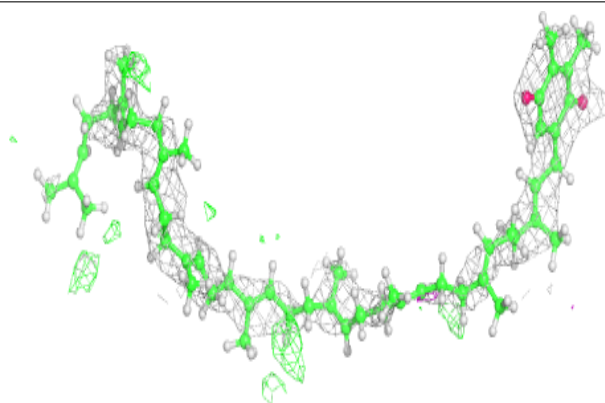


Electron density around STE d 412:

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

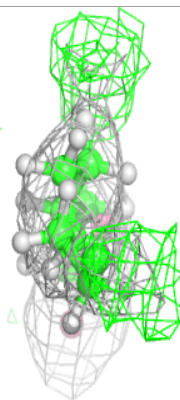
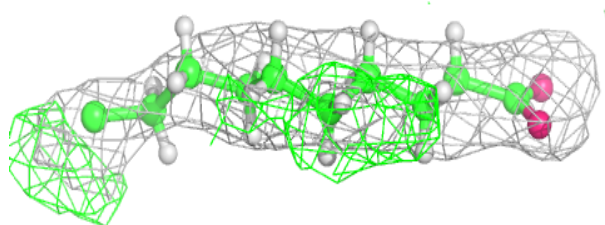
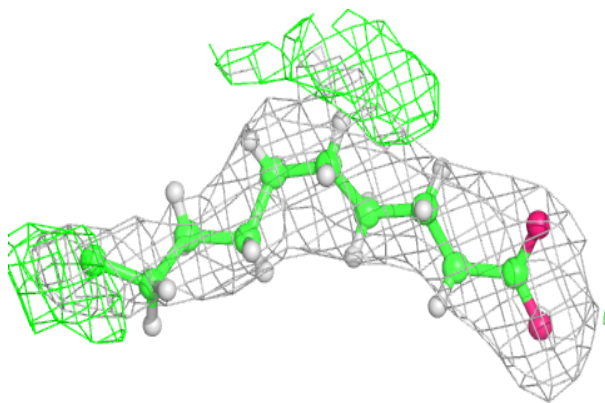
**Electron density around PL9 a 410:**

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



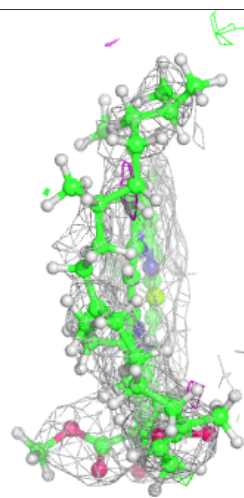
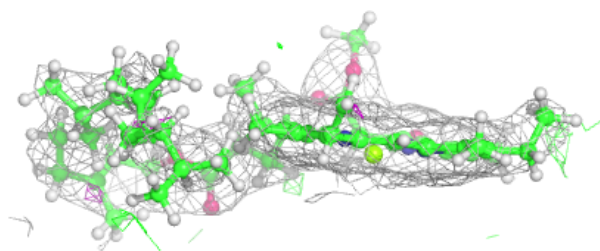
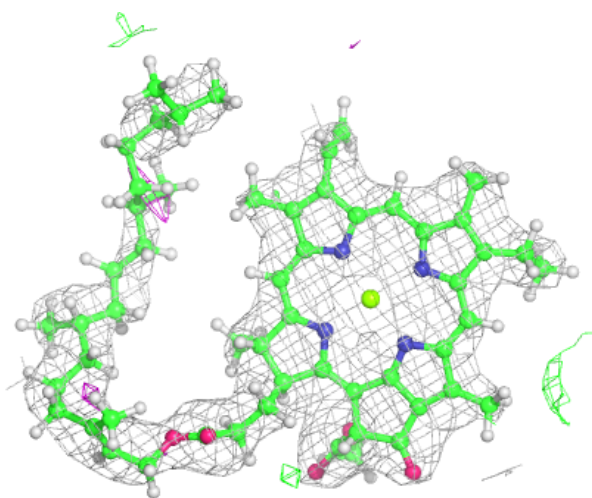
Electron density around STE C 522:

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



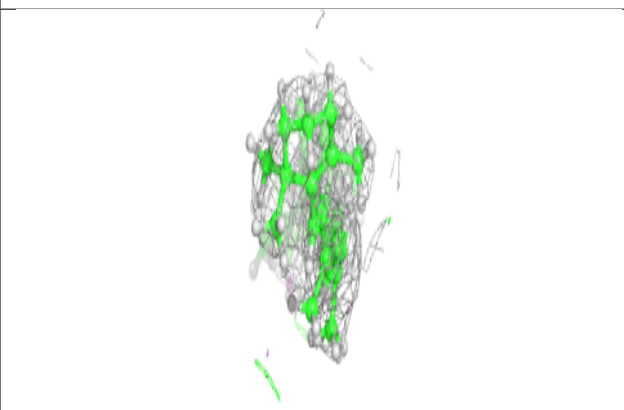
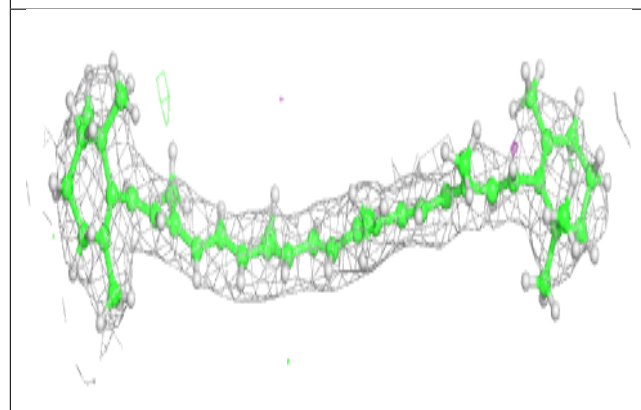
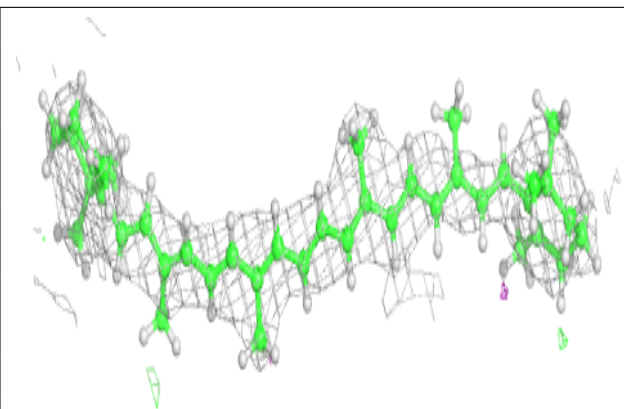
Electron density around CLA c 513:

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

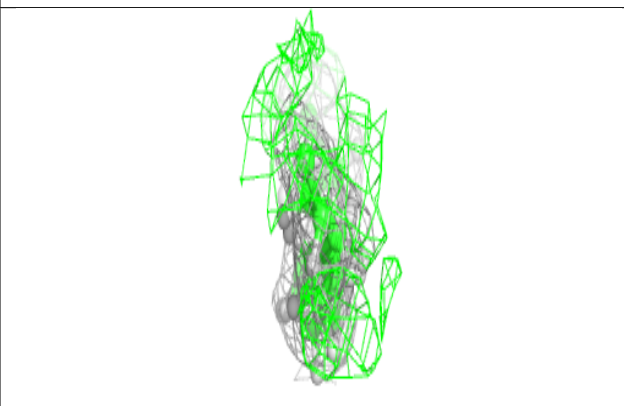
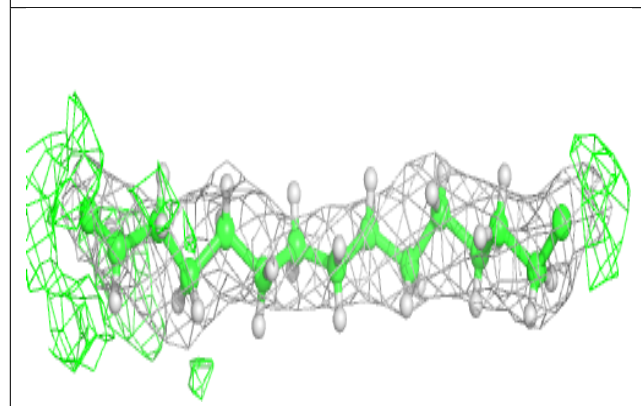
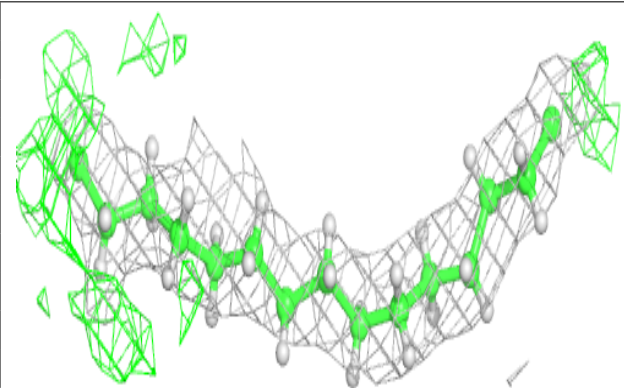


Electron density around BCR h 101:

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

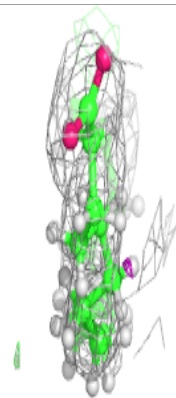
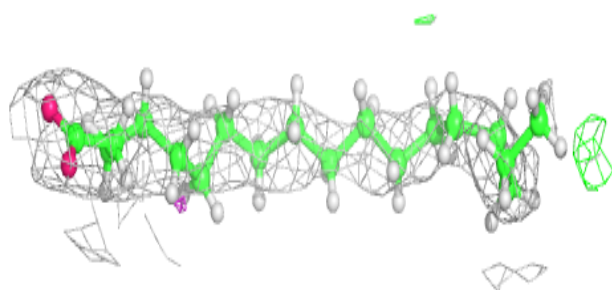
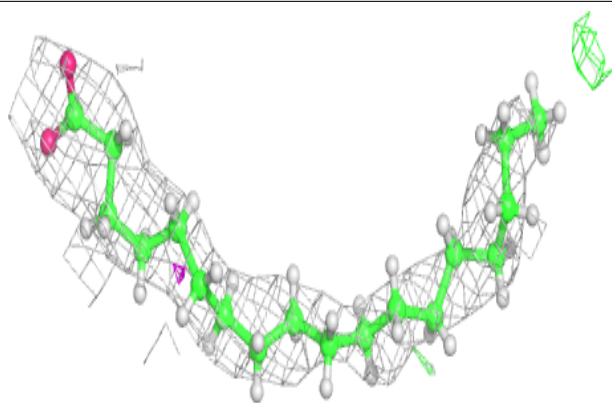
**Electron density around STE I 101:**

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

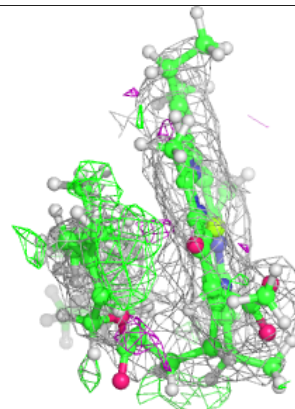
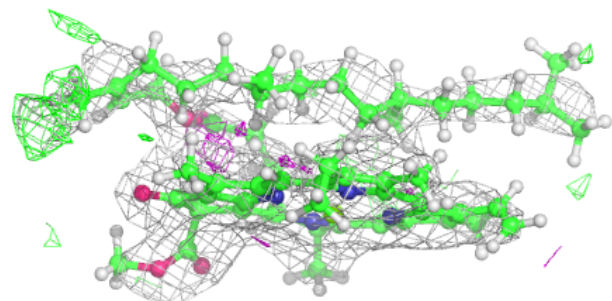
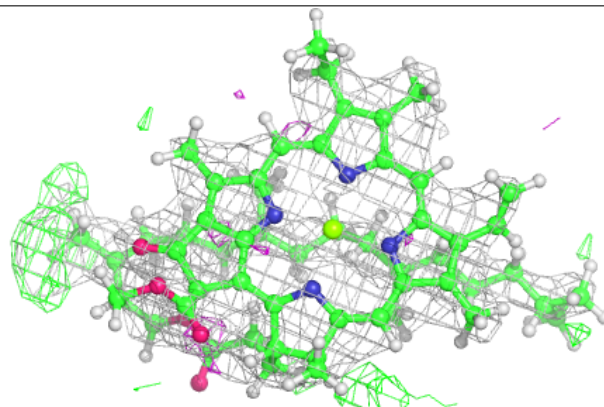


Electron density around STE d 411:

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

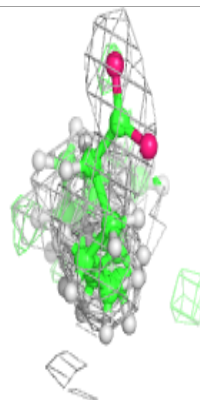
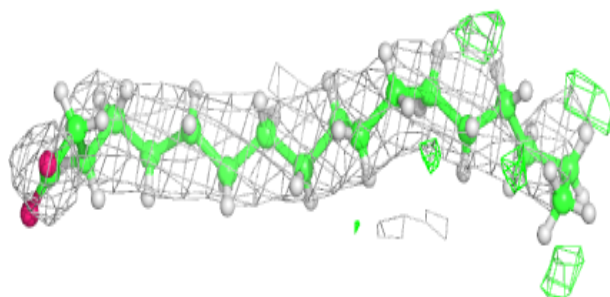
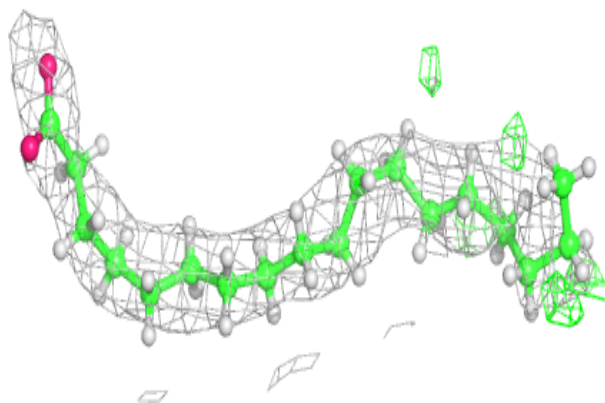
**Electron density around CLA b 601:**

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

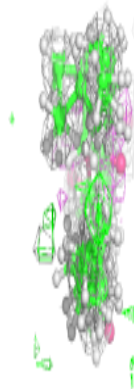
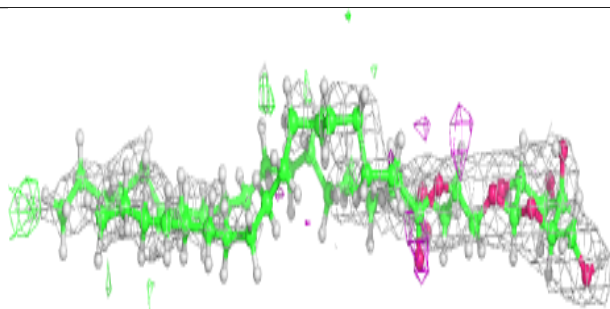
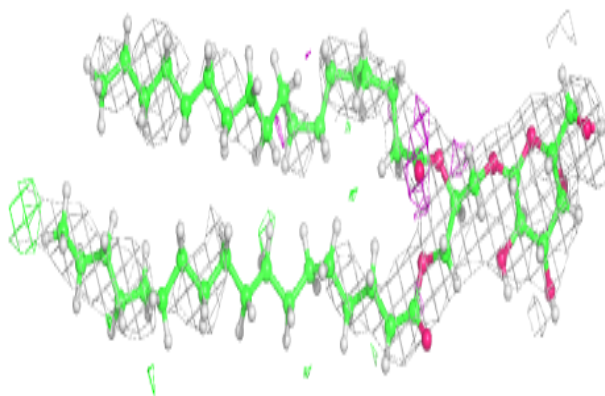


Electron density around STE b 620:

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

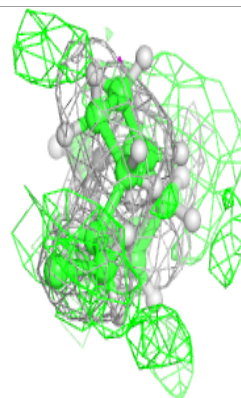
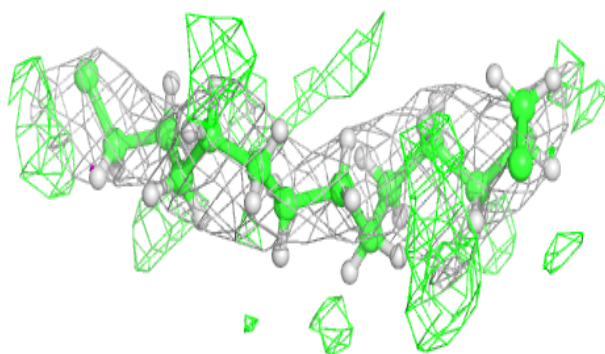
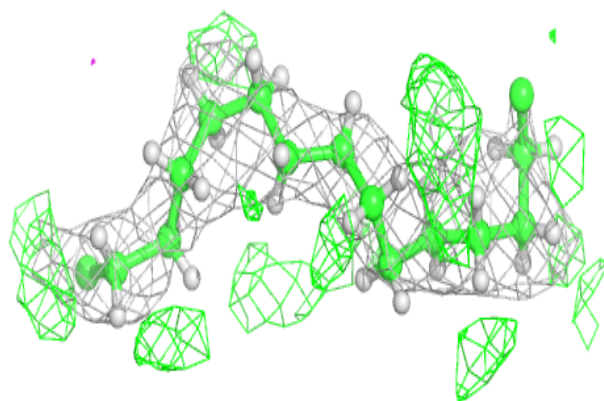
**Electron density around LMG b 621:**

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

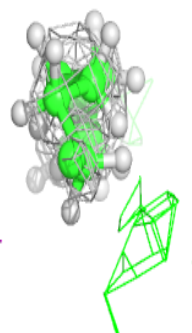
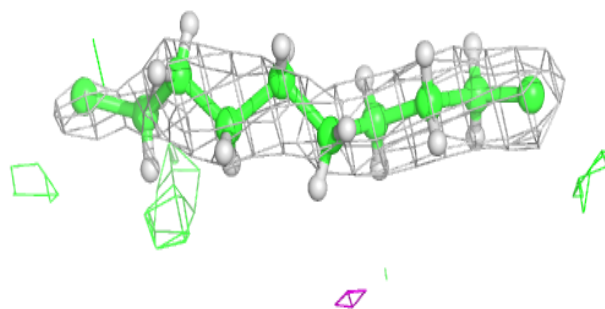
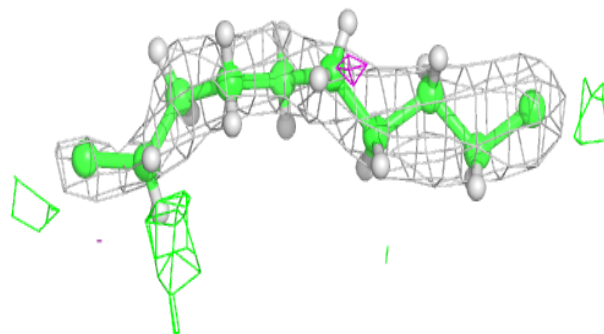


Electron density around STE B 625:

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

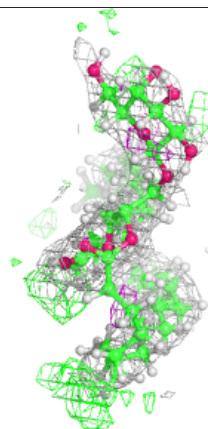
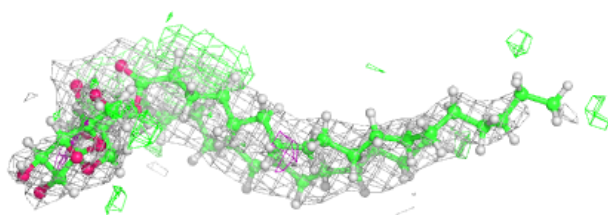
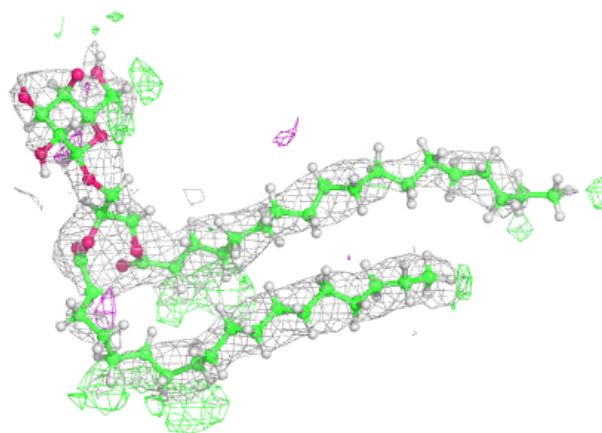
**Electron density around STE a 415:**

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

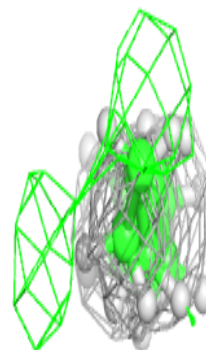
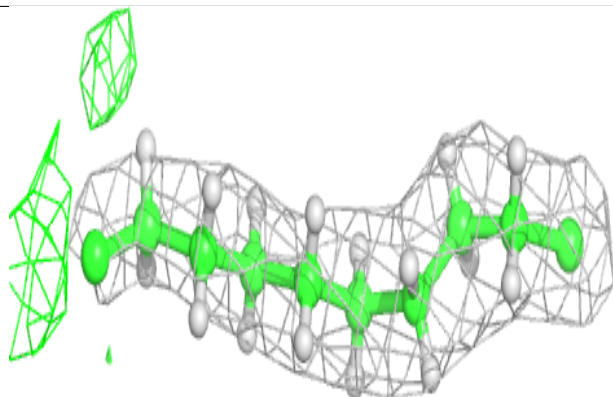
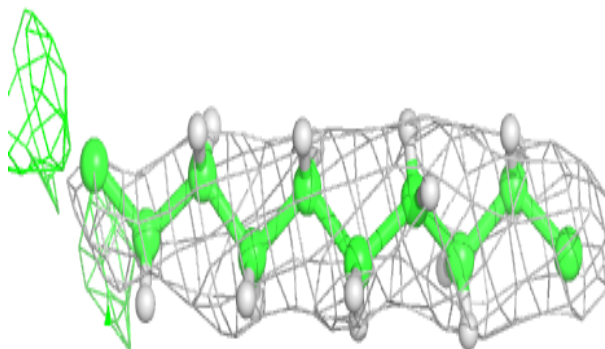


Electron density around LMG a 417:

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

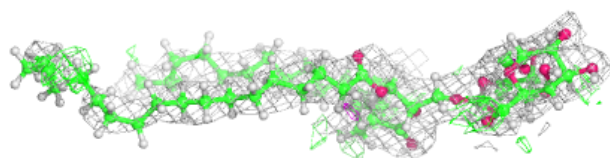
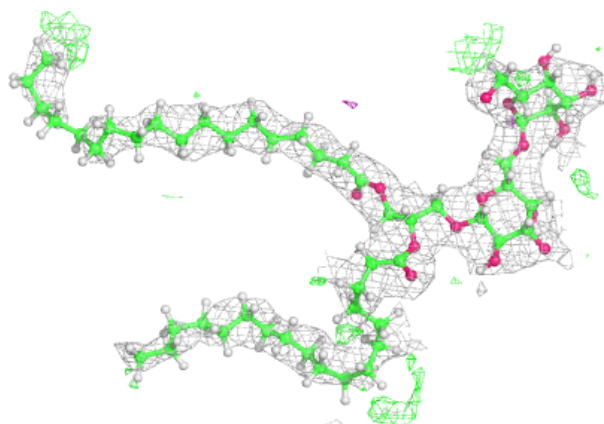
**Electron density around STE M 103:**

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

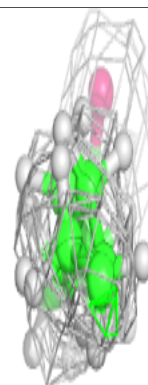
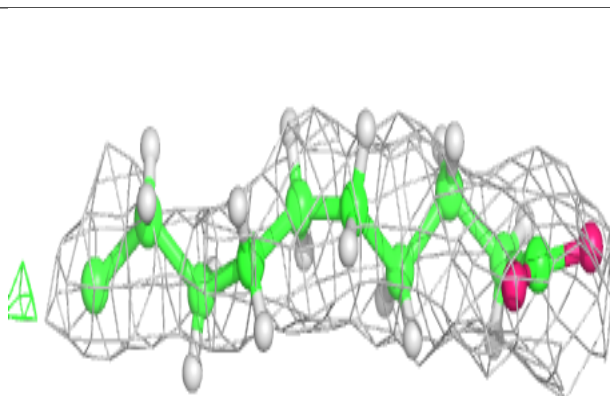
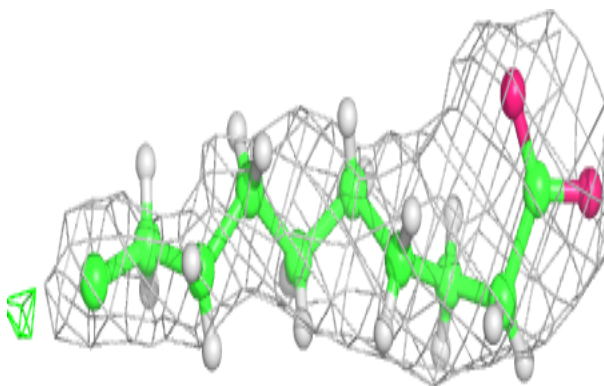


Electron density around DGD A 414:

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

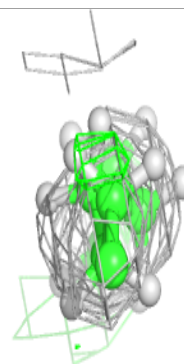
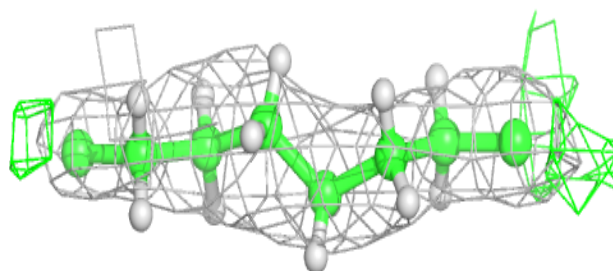
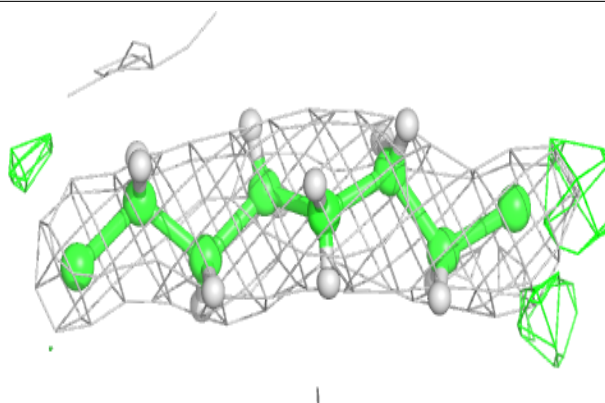
**Electron density around STE c 501:**

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

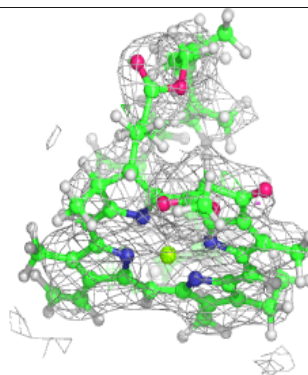
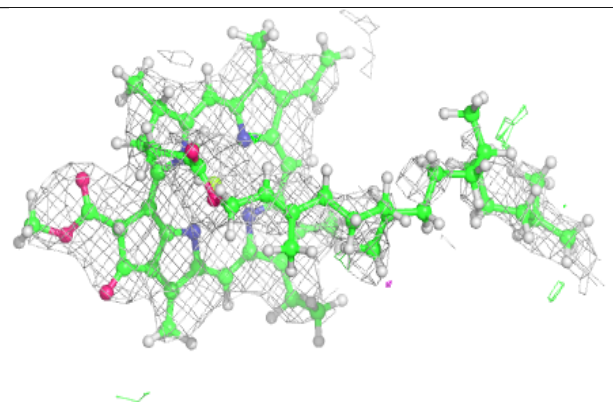
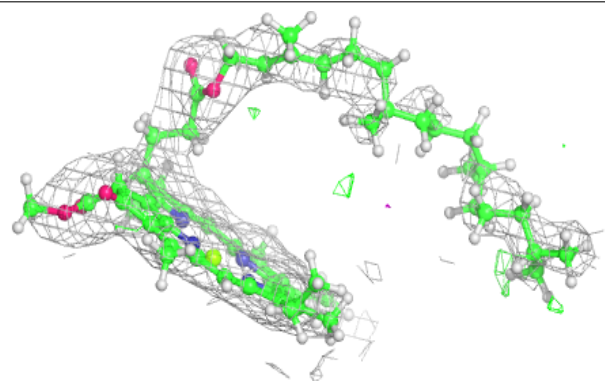


Electron density around STE Z 101:

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

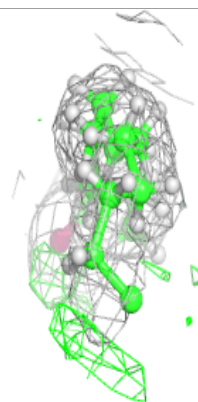
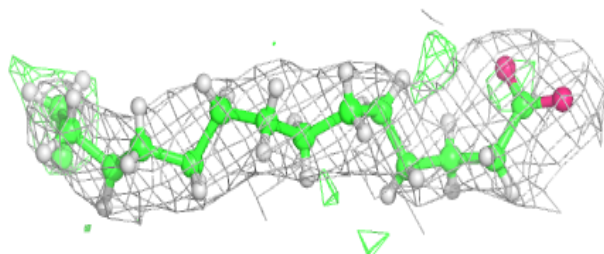
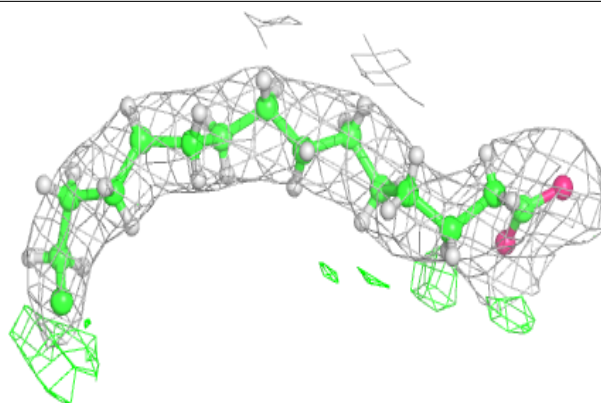
**Electron density around CLA C 513:**

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

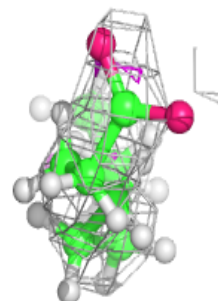
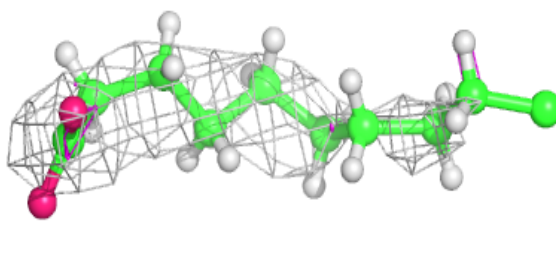
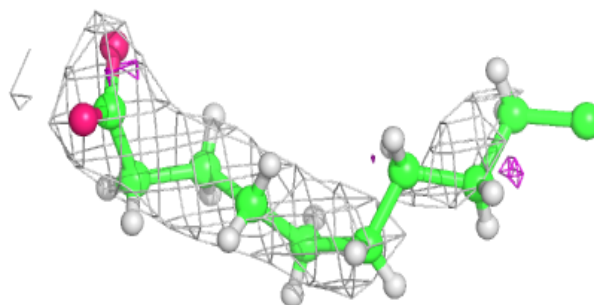


Electron density around STE B 620:

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

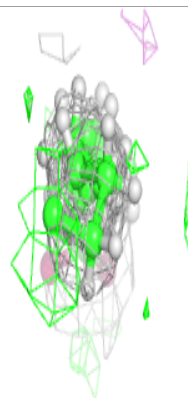
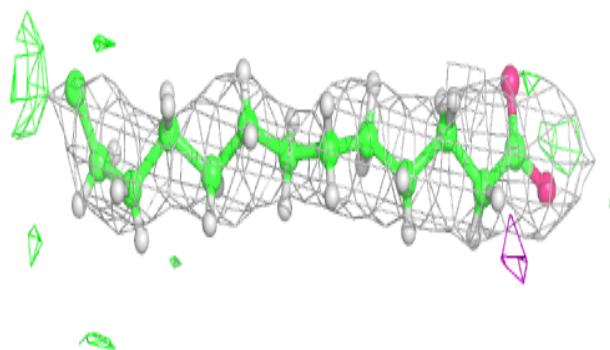
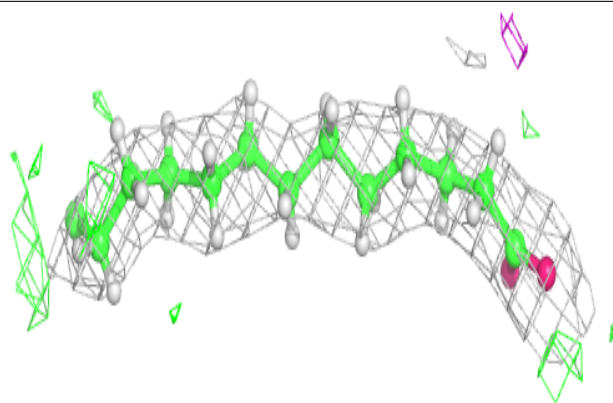
**Electron density around STE B 601:**

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

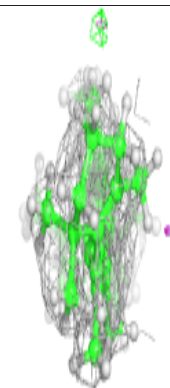
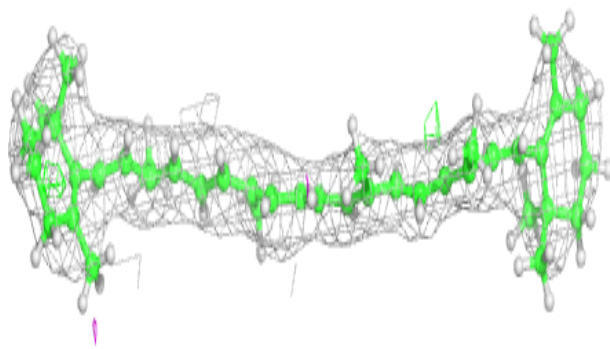
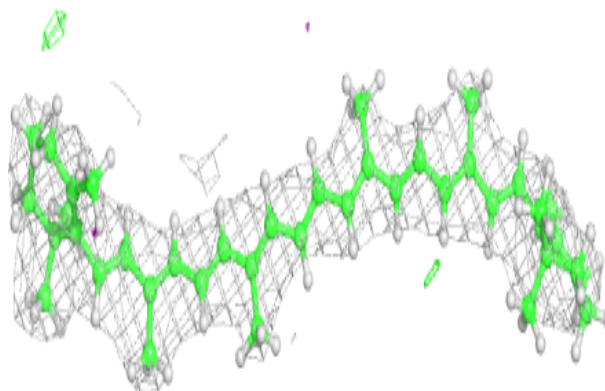


Electron density around STE M 102:

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

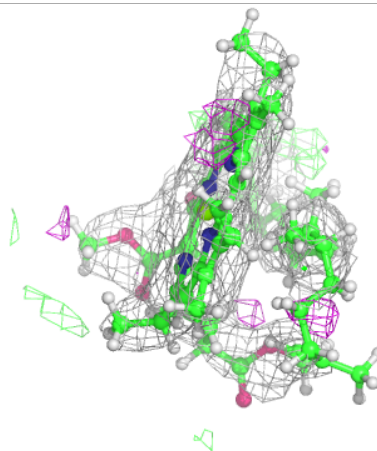
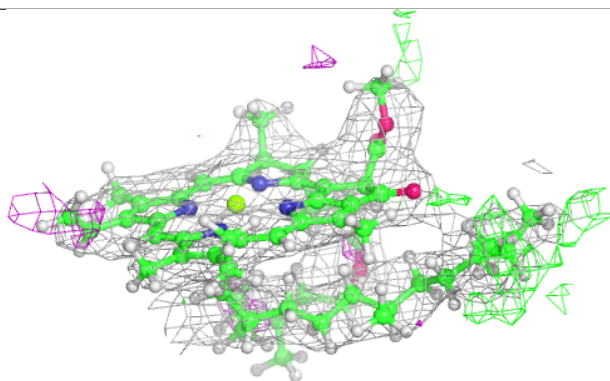
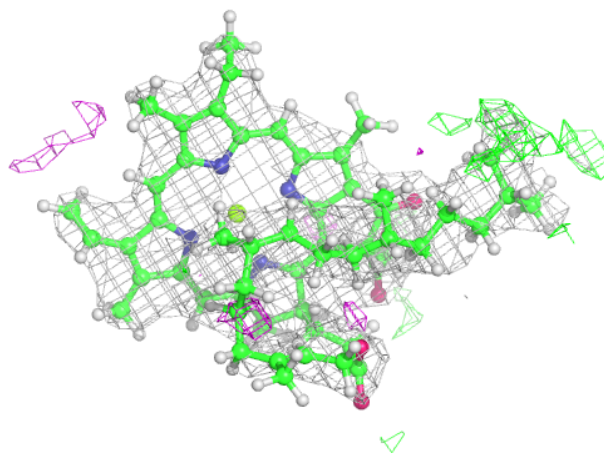
**Electron density around BCR K 102:**

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



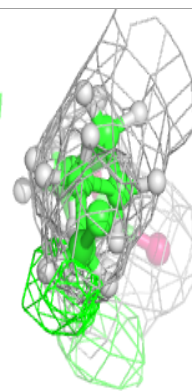
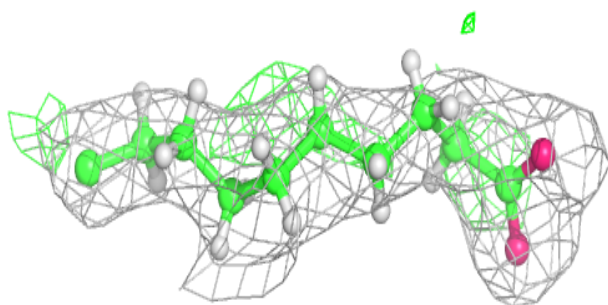
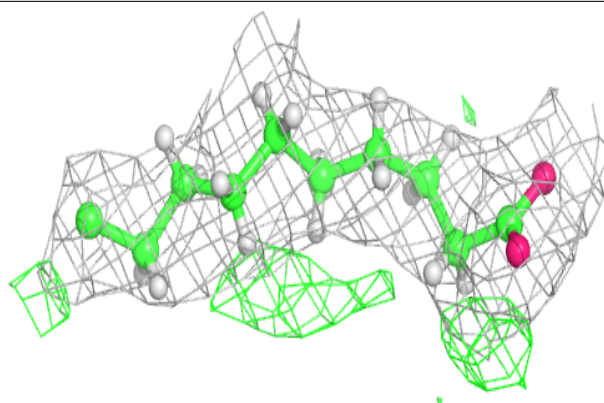
Electron density around CLA H 101:

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

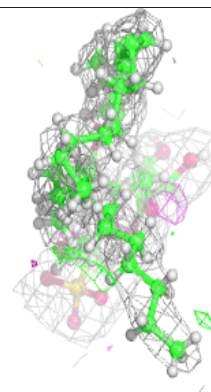
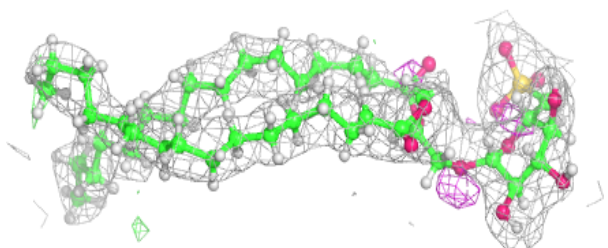
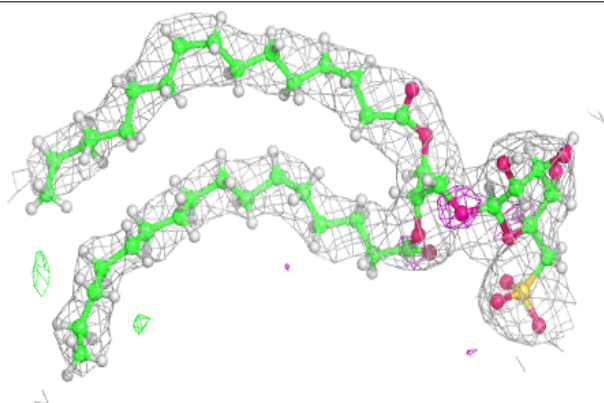


Electron density around STE B 622:

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

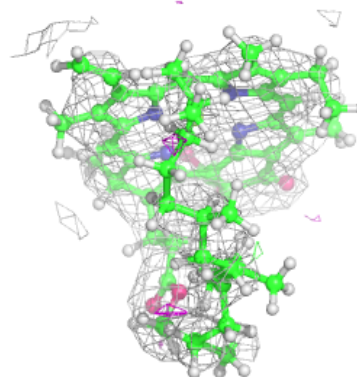
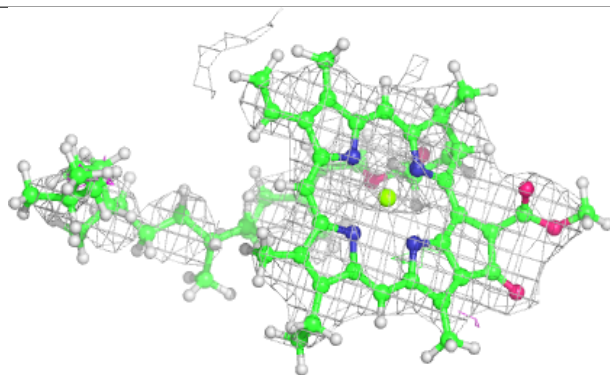
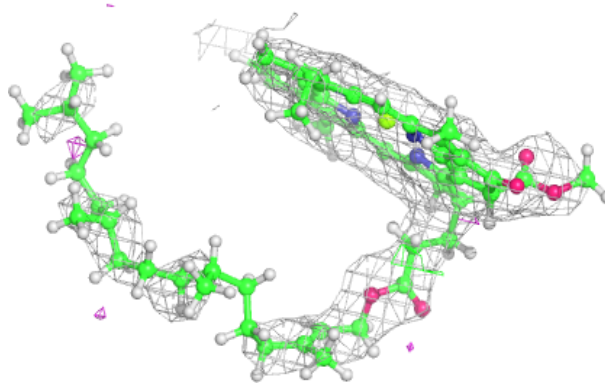
**Electron density around SQD B 621:**

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

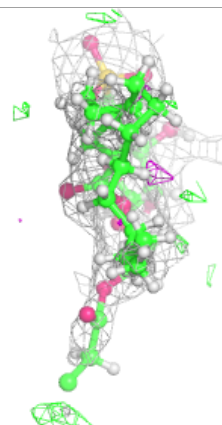
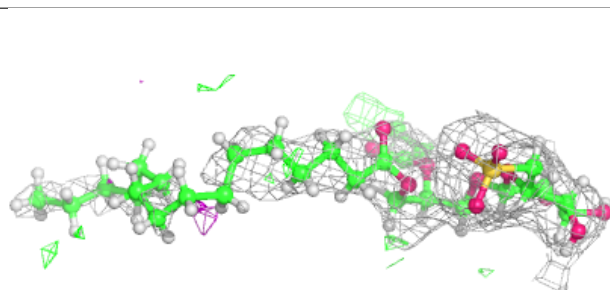
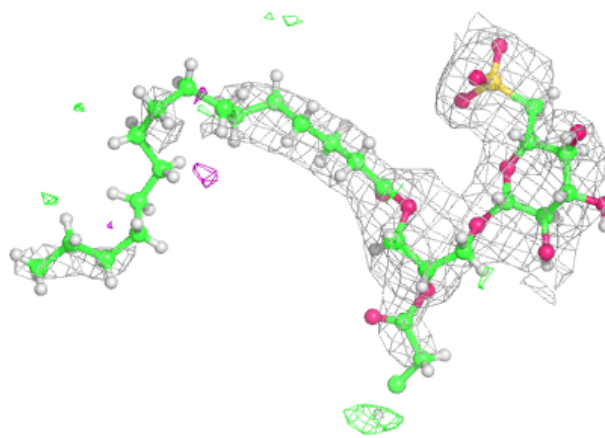


Electron density around CLA c 514:

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

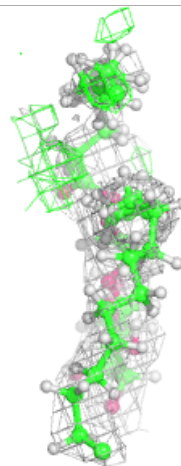
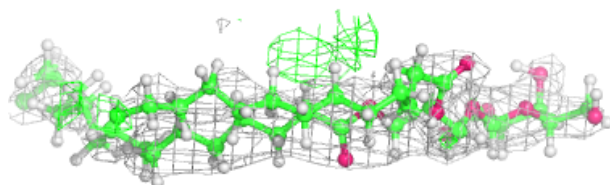
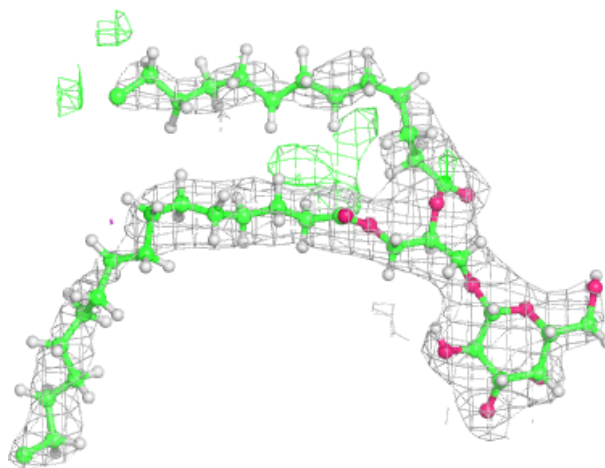
**Electron density around SQD d 409:**

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



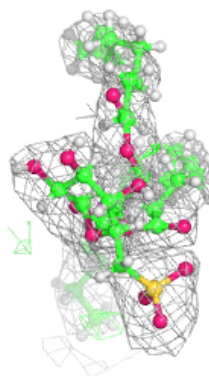
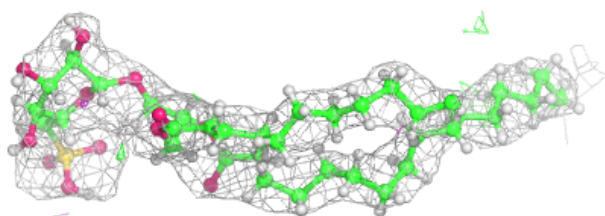
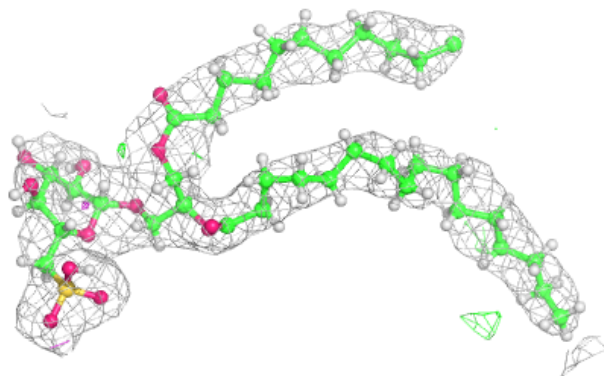
Electron density around LMG Y 101:

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

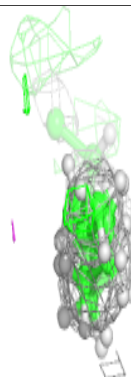
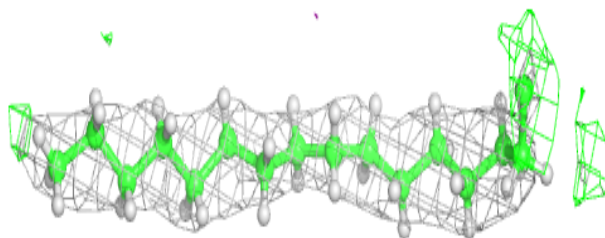
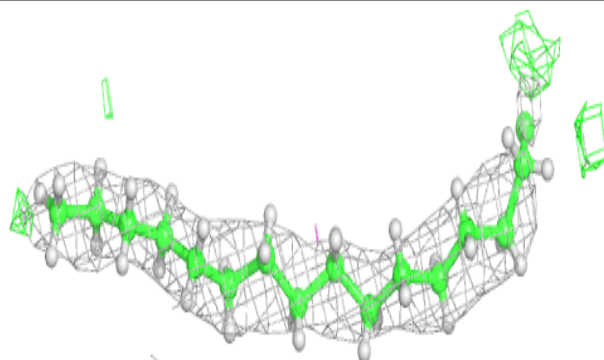


Electron density around SQD L 101:

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

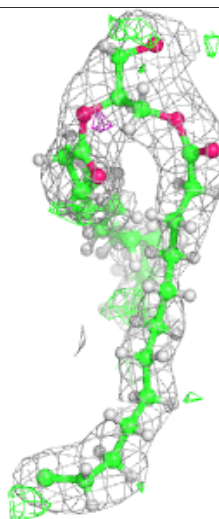
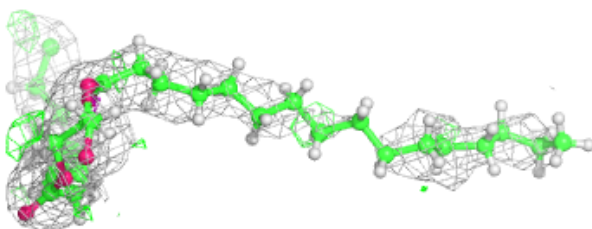
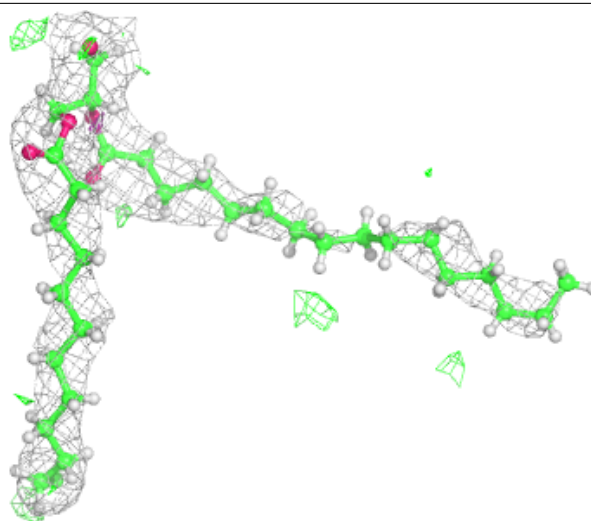
**Electron density around STE C 521:**

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



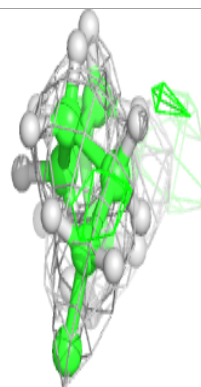
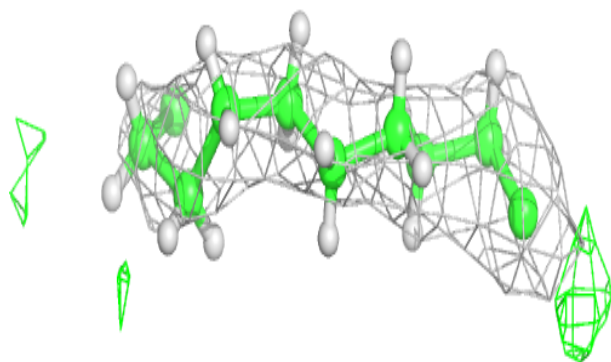
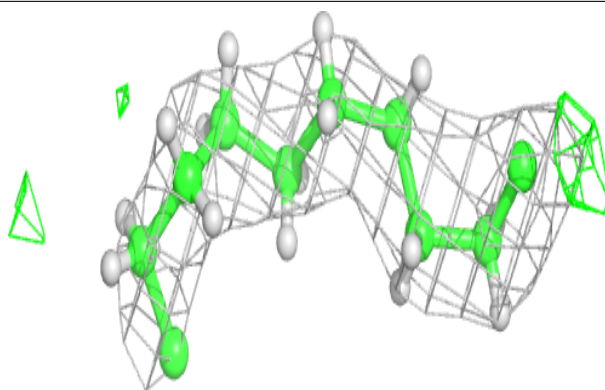
Electron density around SQD a 414:

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

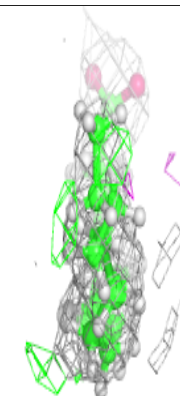
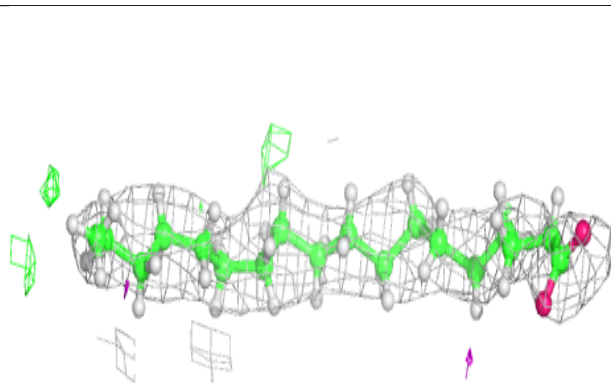
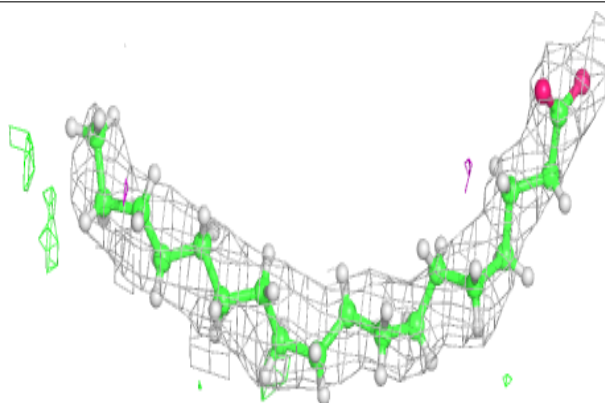


Electron density around STE b 624:

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

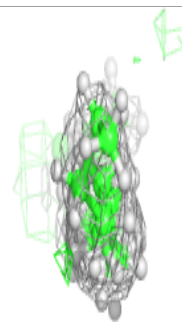
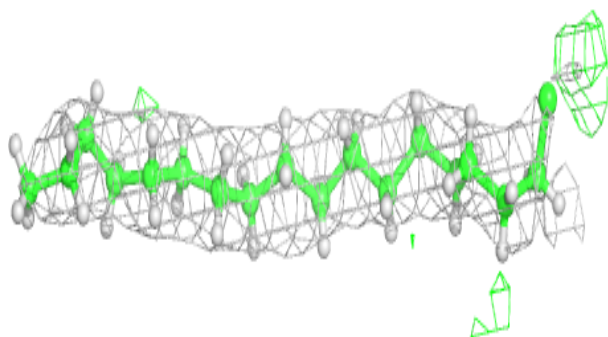
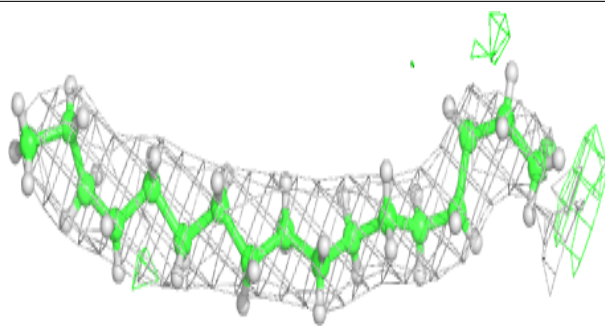
**Electron density around STE D 413:**

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

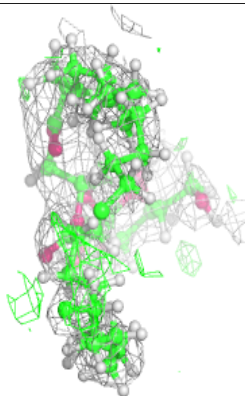
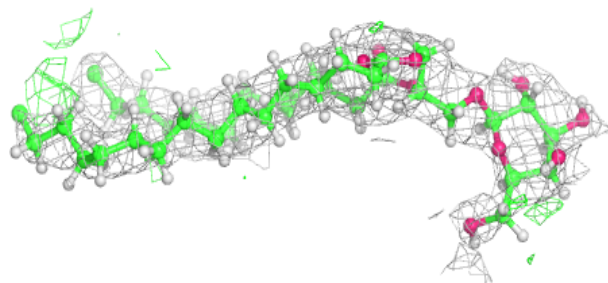
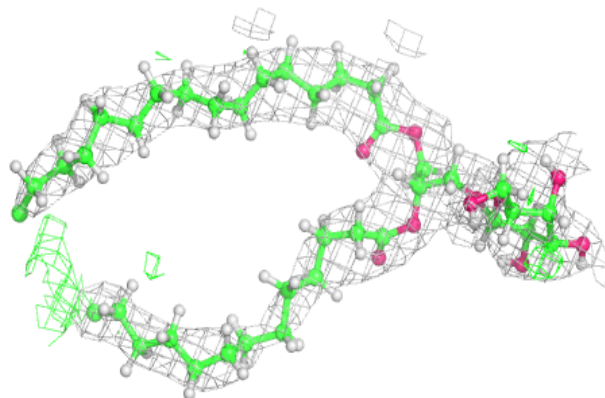


Electron density around STE M 104:

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

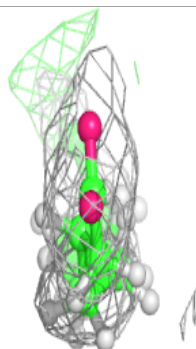
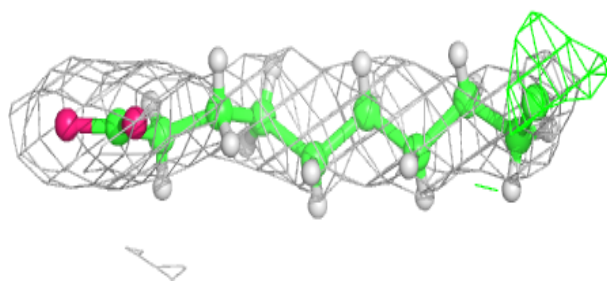
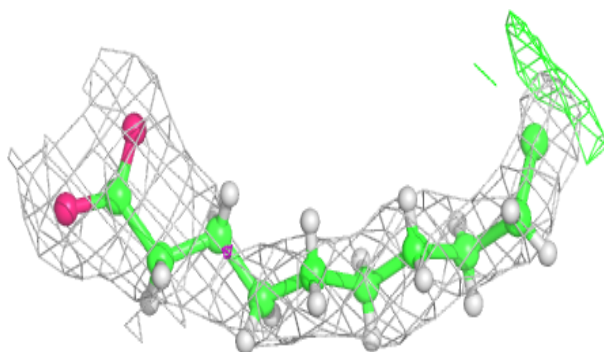
**Electron density around LMG C 516:**

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



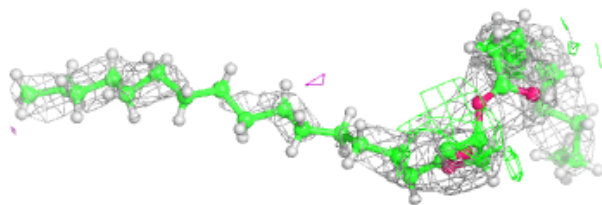
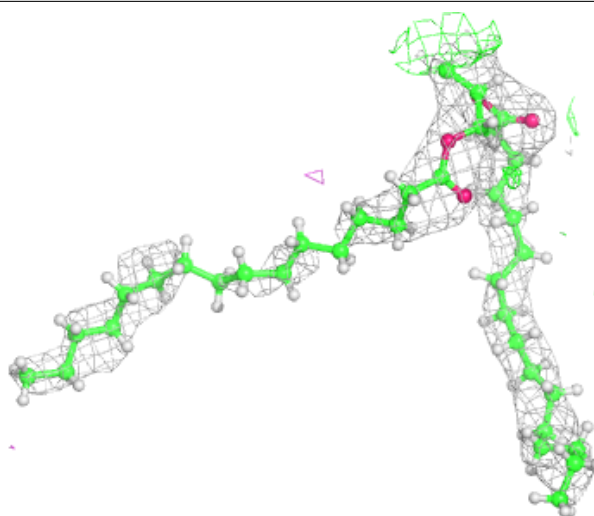
Electron density around STE C 520:

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



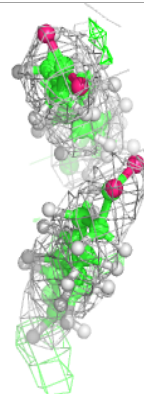
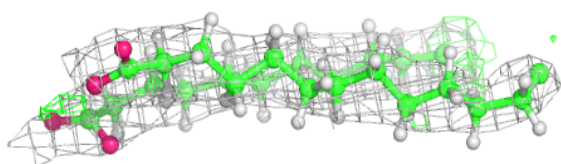
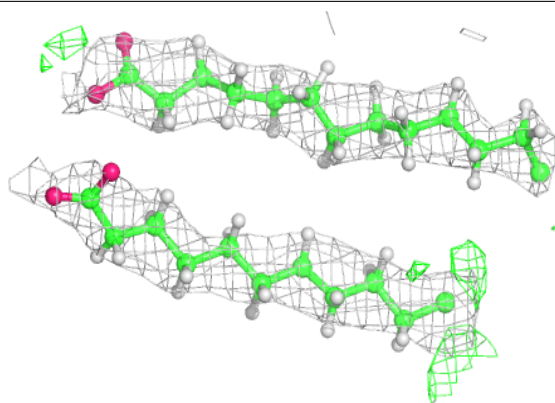
Electron density around SQD A 413:

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

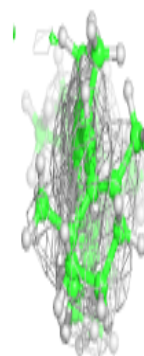
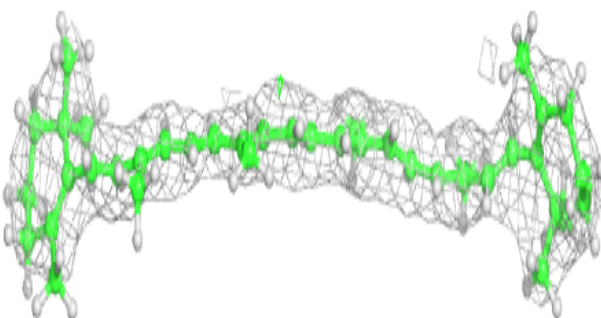
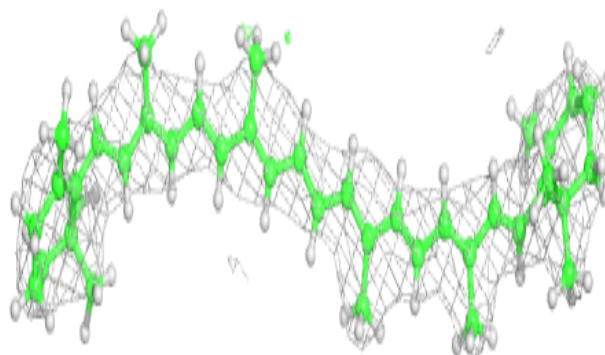


Electron density around LMG D 411:

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

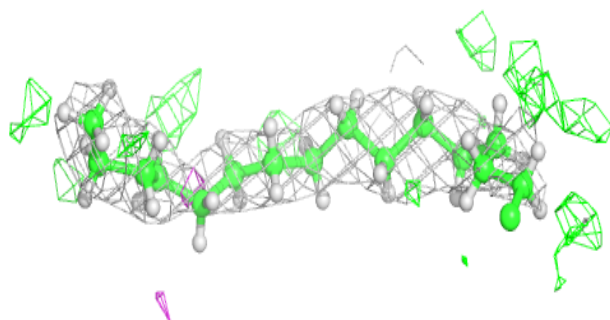
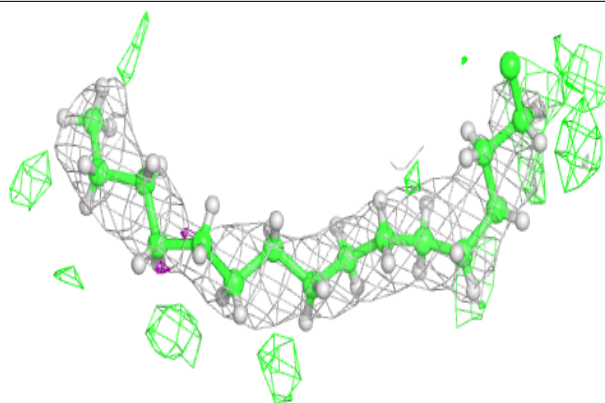
**Electron density around BCR k 101:**

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

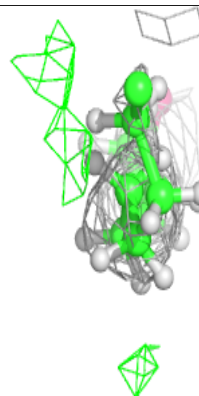
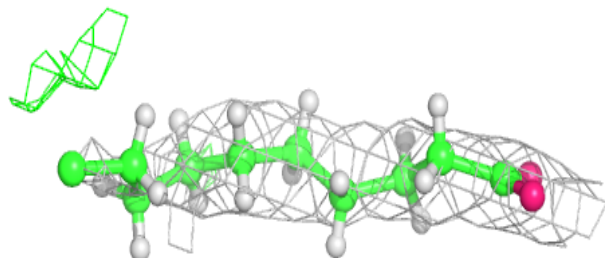
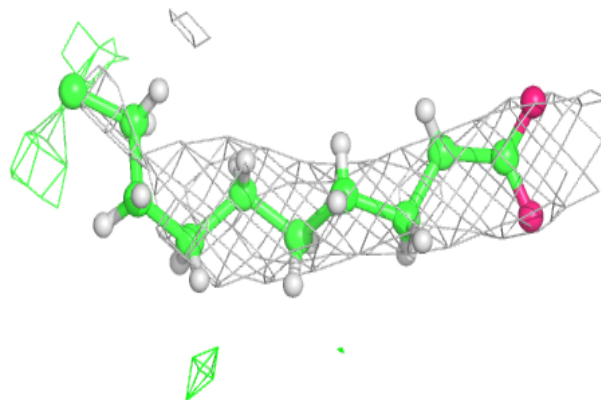


Electron density around STE T 102:

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

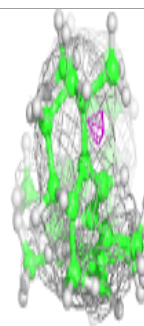
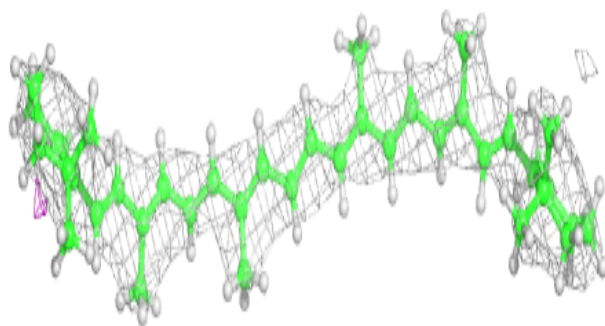
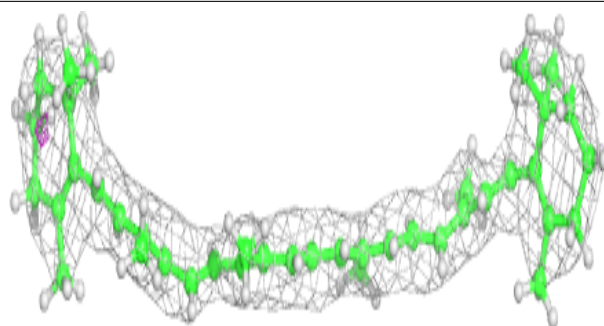
**Electron density around STE L 103:**

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

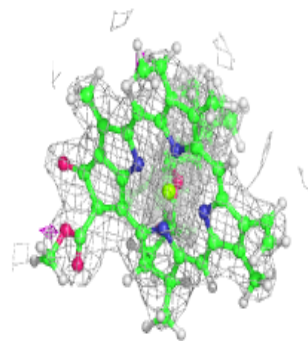
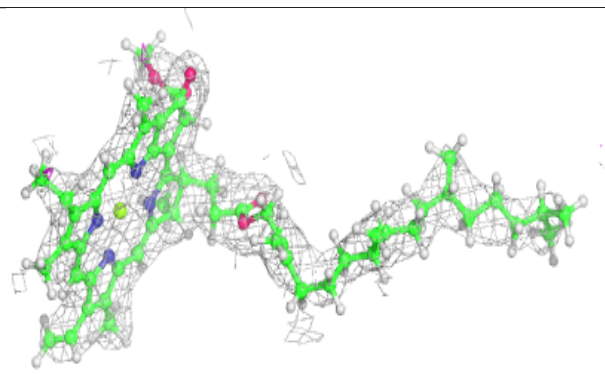
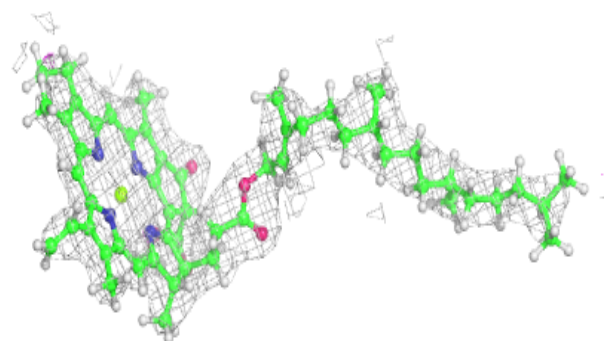


Electron density around BCR k 102:

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

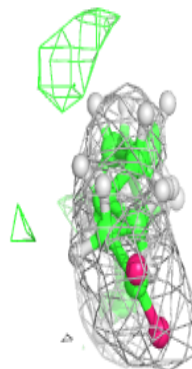
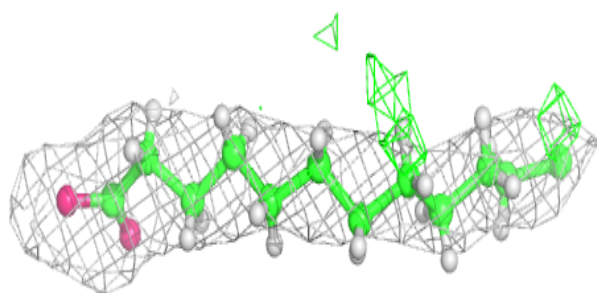
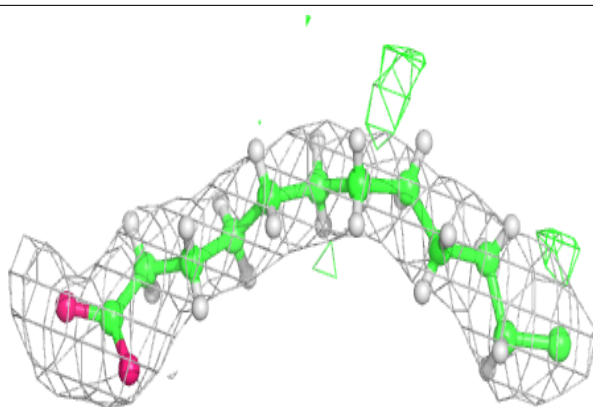
**Electron density around CLA C 502:**

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

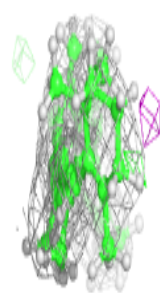
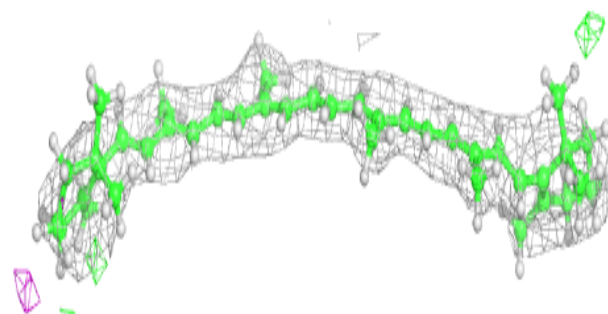
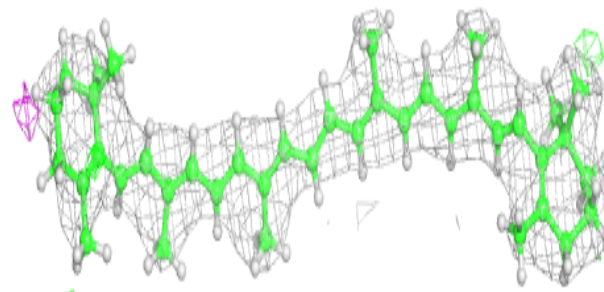


Electron density around STE t 102:

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

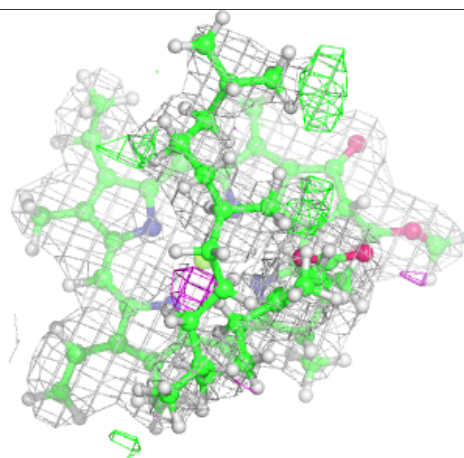
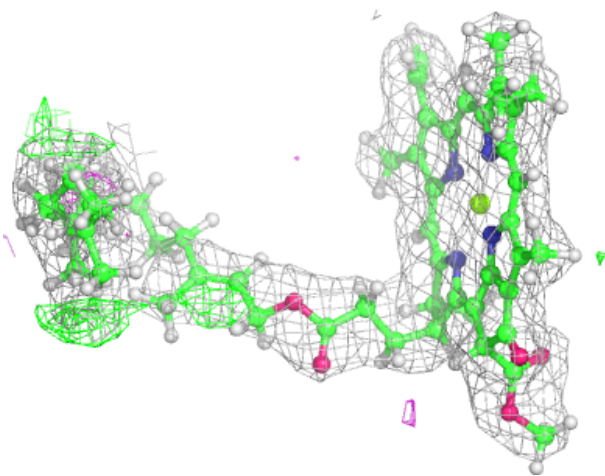
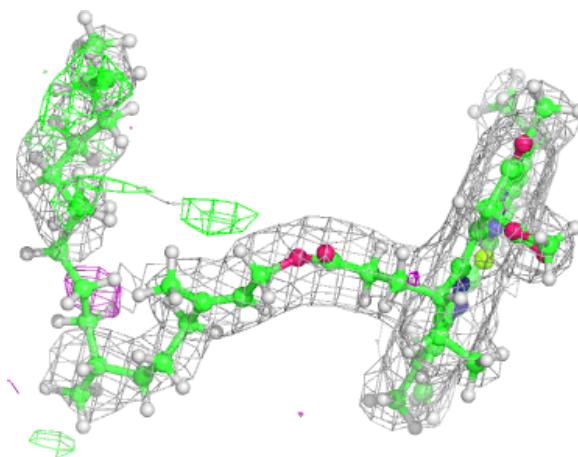
**Electron density around BCR D 406:**

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



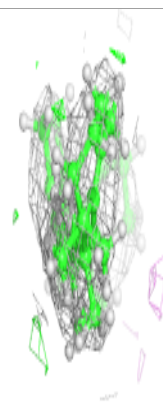
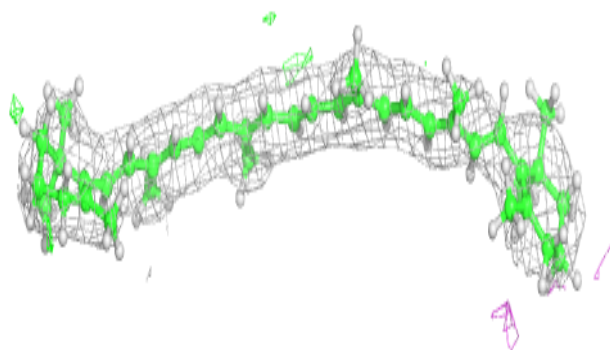
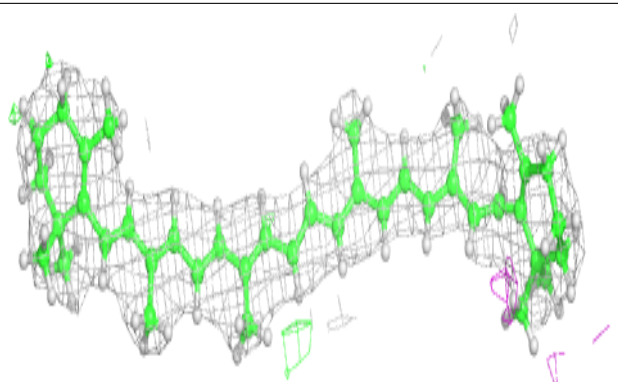
Electron density around CLA a 405:

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

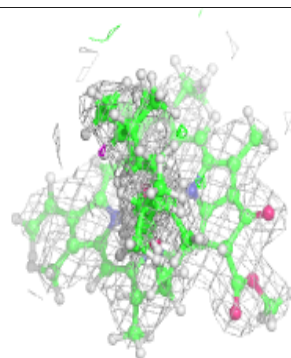
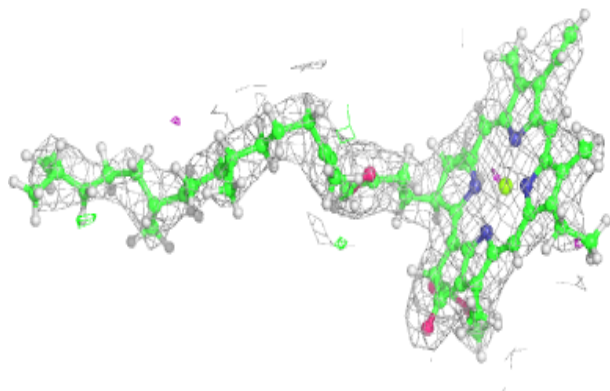
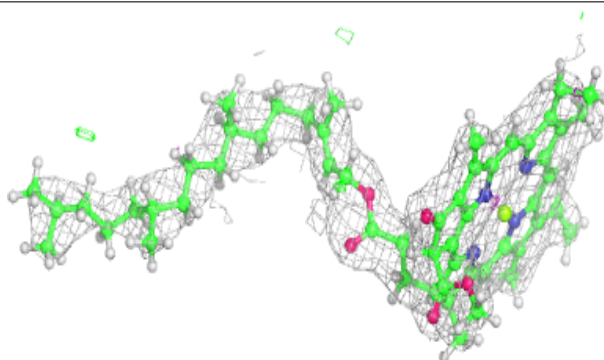


Electron density around BCR d 404:

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

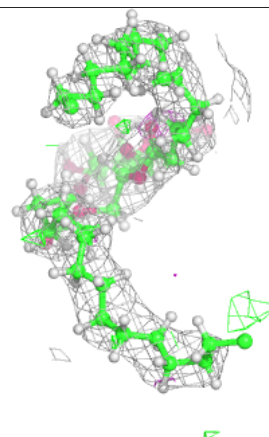
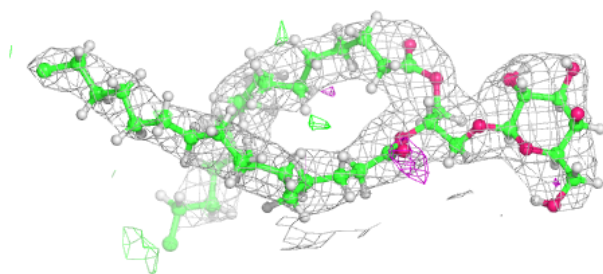
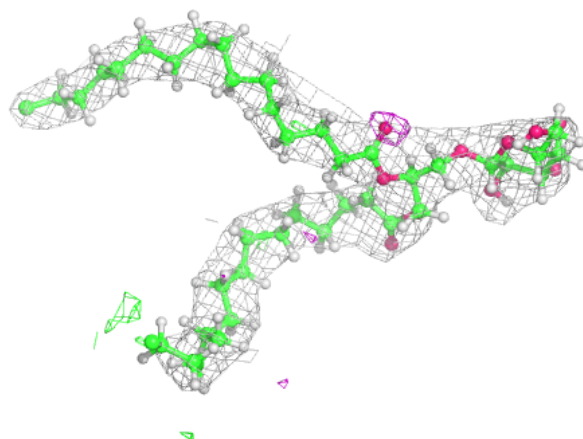
**Electron density around CLA c 503:**

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



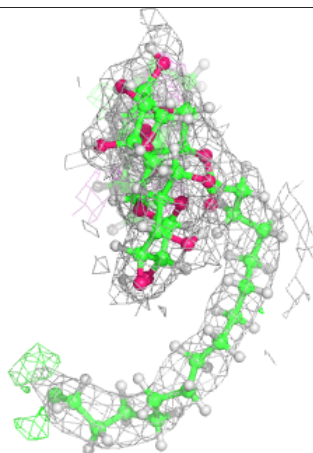
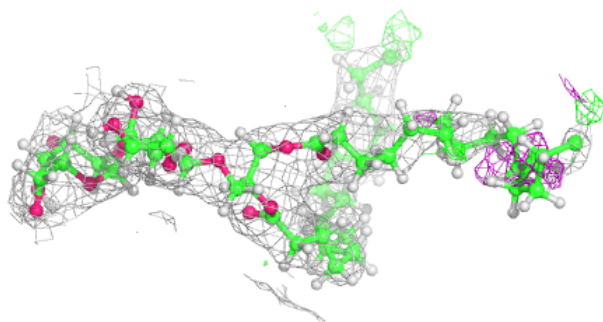
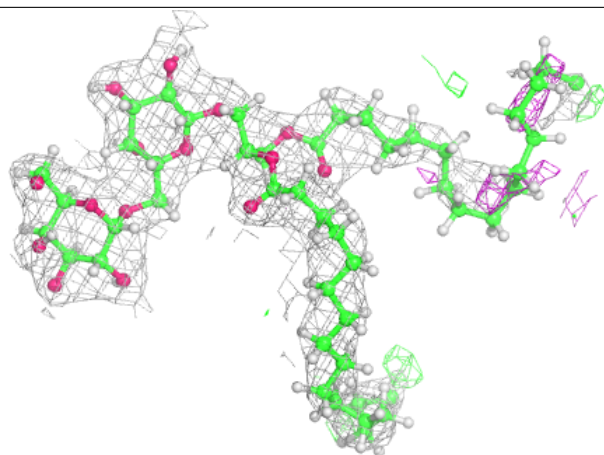
Electron density around LMG M 101:

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



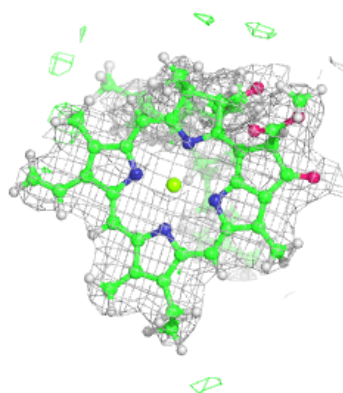
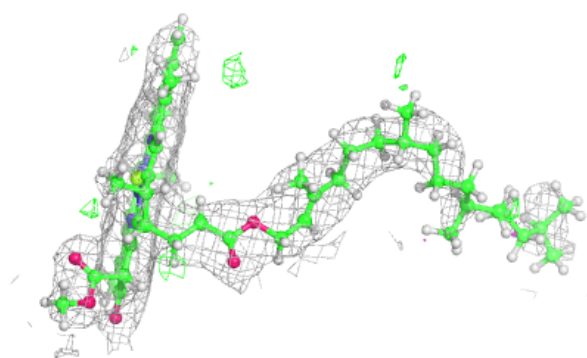
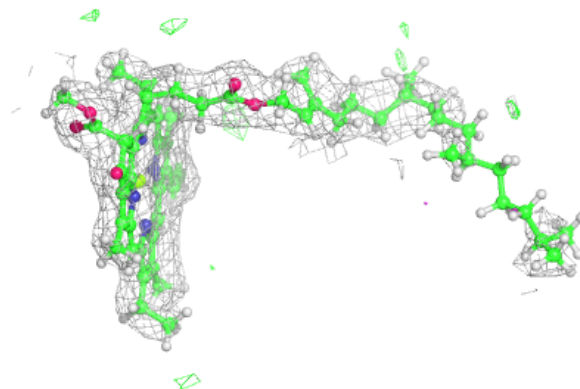
Electron density around DGD C 518:

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

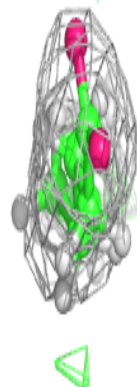
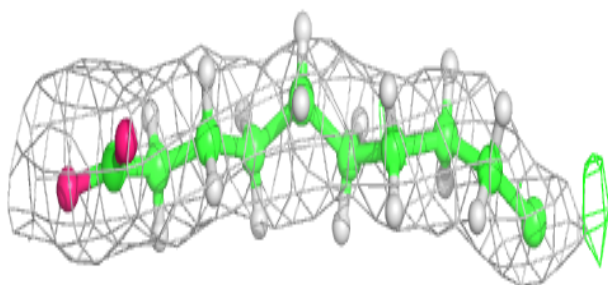
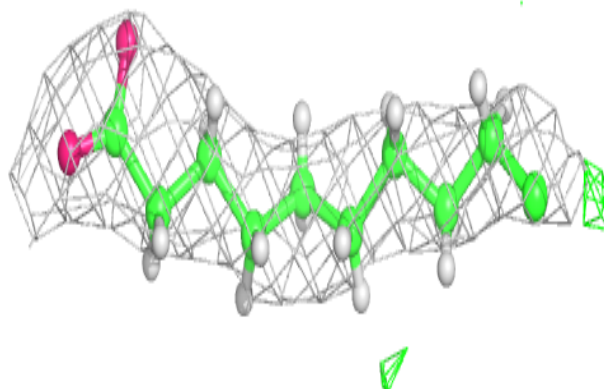


Electron density around CLA D 405:

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

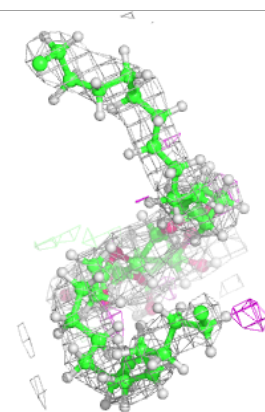
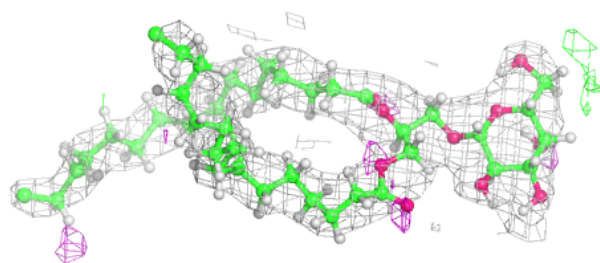
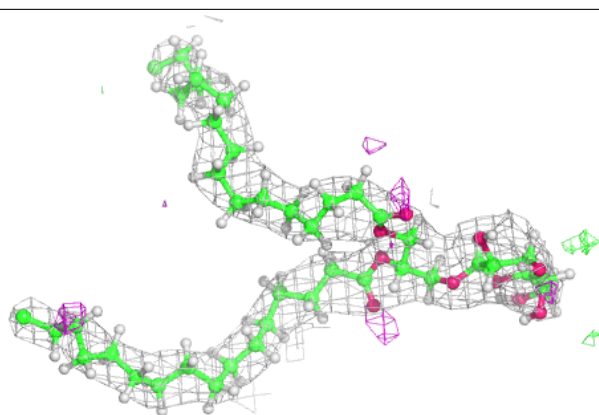
**Electron density around STE j 101:**

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



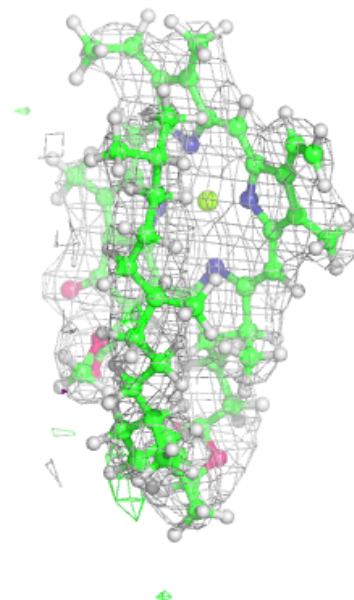
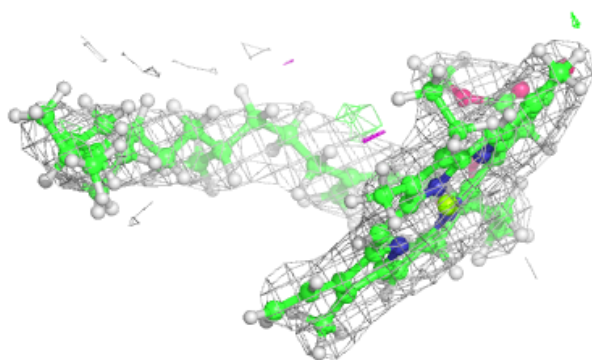
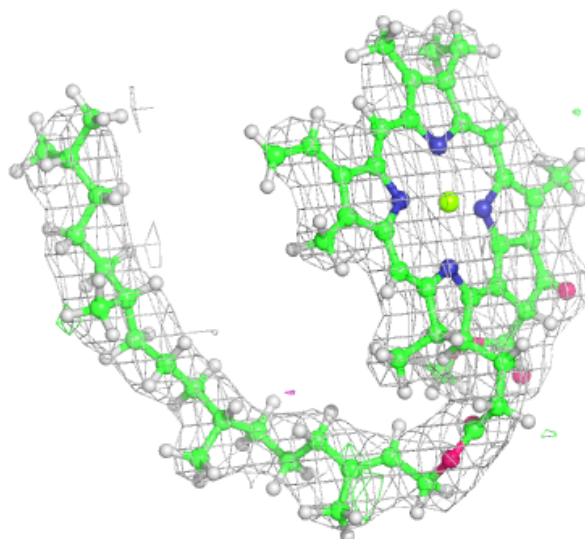
Electron density around LMG m 101:

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



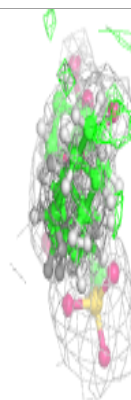
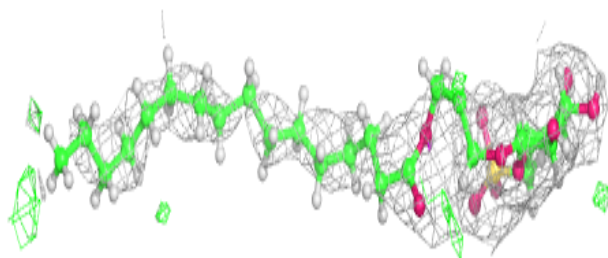
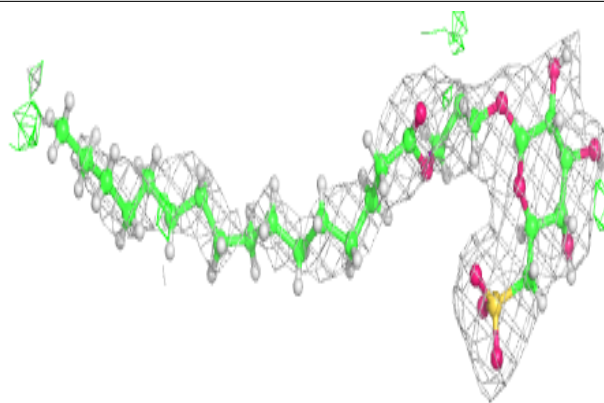
Electron density around CLA C 507:

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

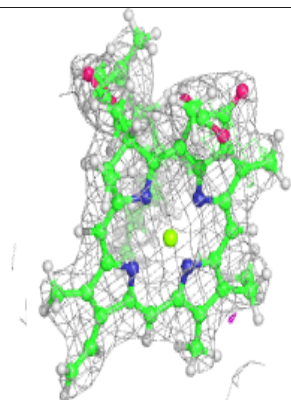
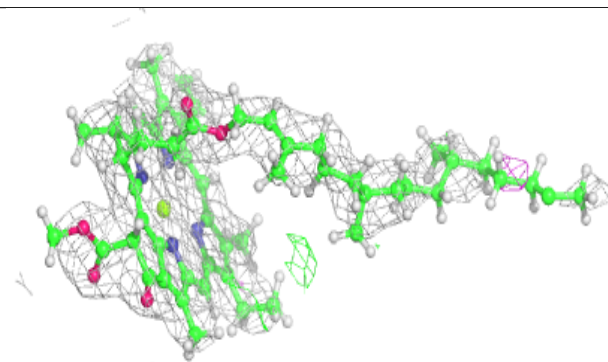
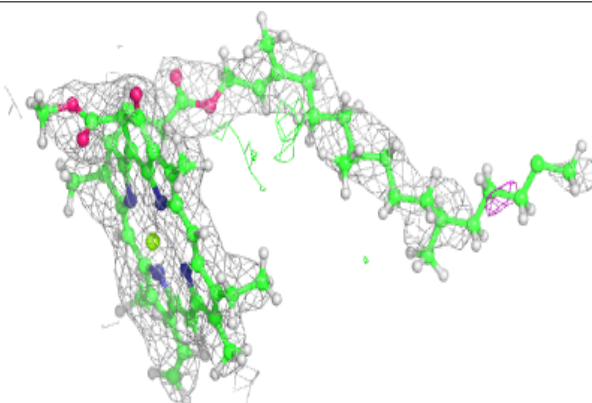


Electron density around SQD F 102:

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

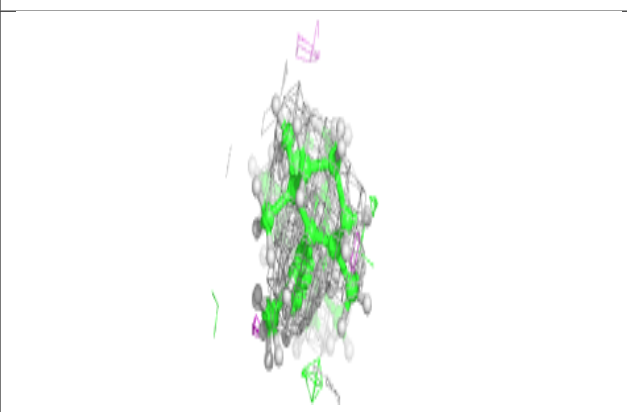
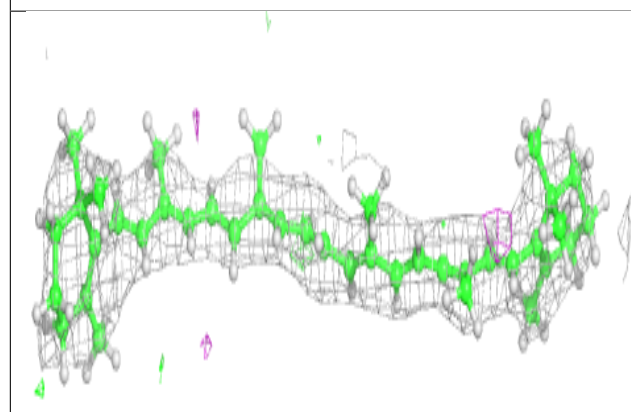
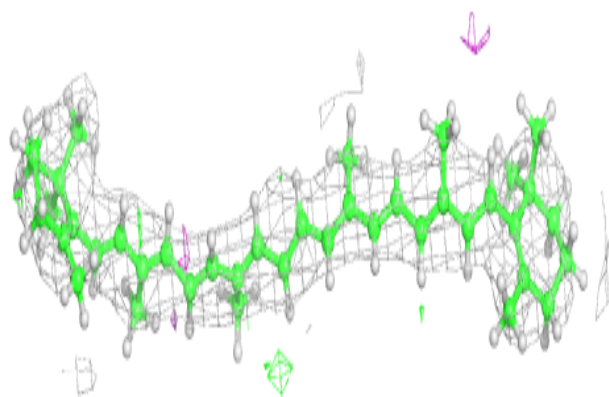
**Electron density around CLA c 509:**

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



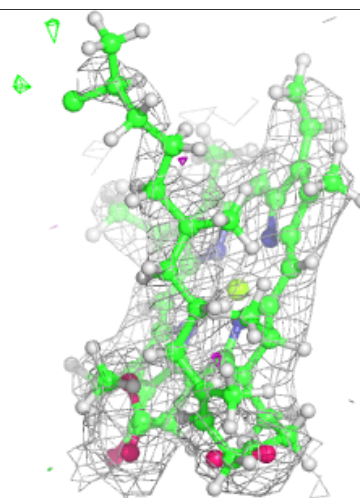
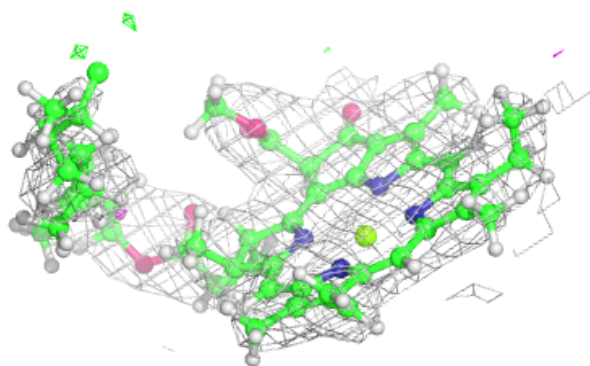
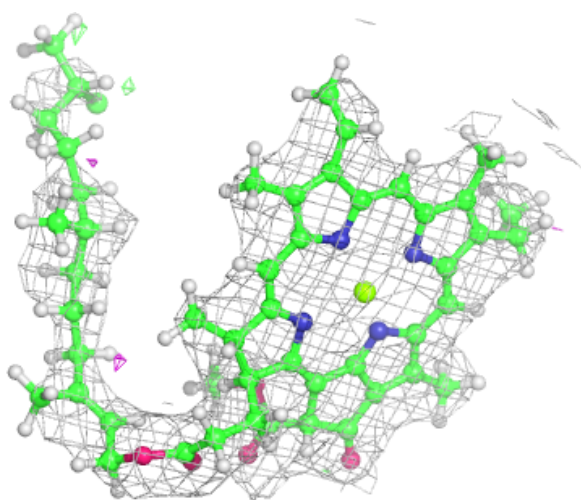
Electron density around BCR K 101:

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



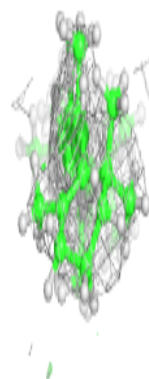
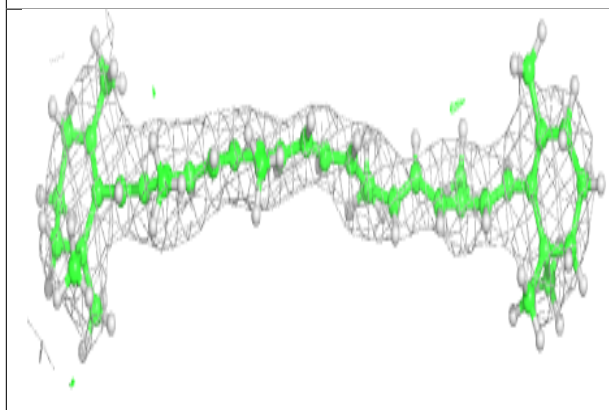
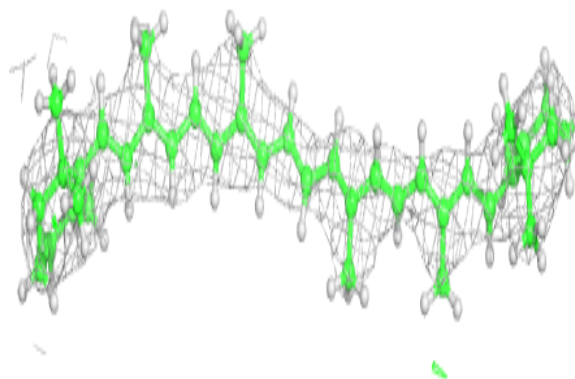
Electron density around CLA b 616:

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



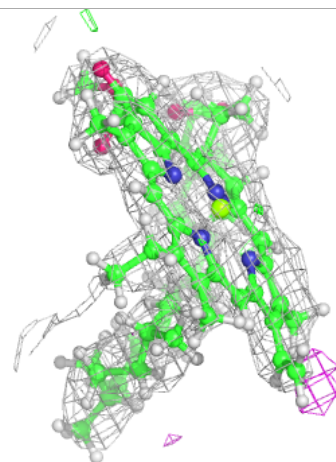
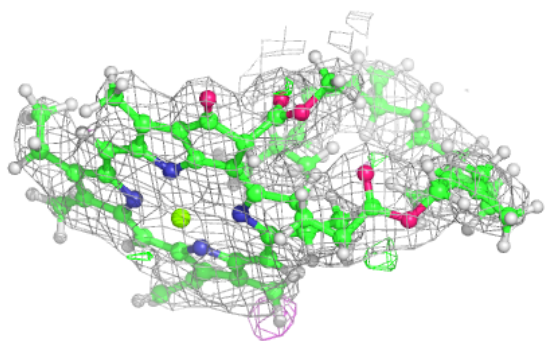
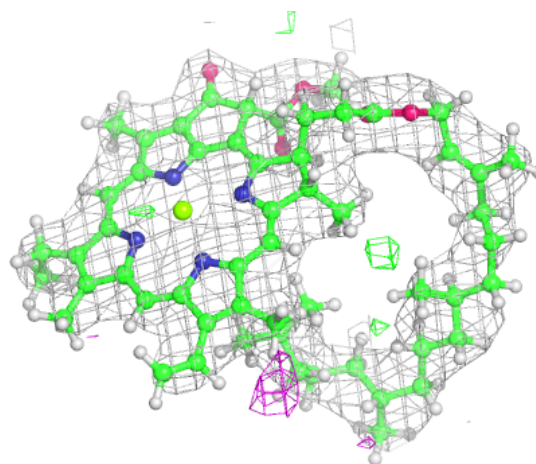
Electron density around BCR c 515:

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



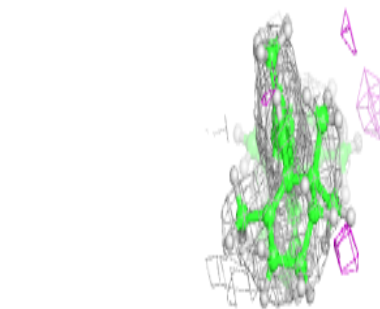
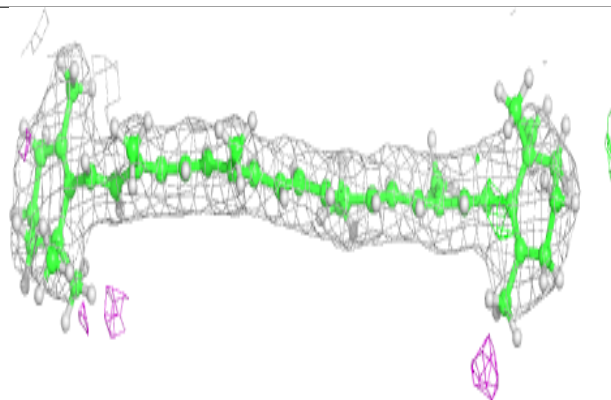
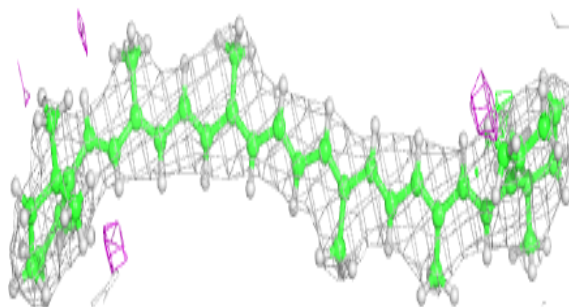
Electron density around CLA b 615:

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

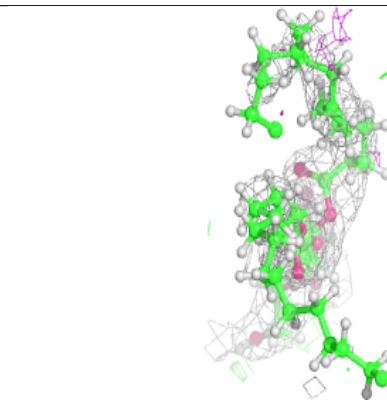
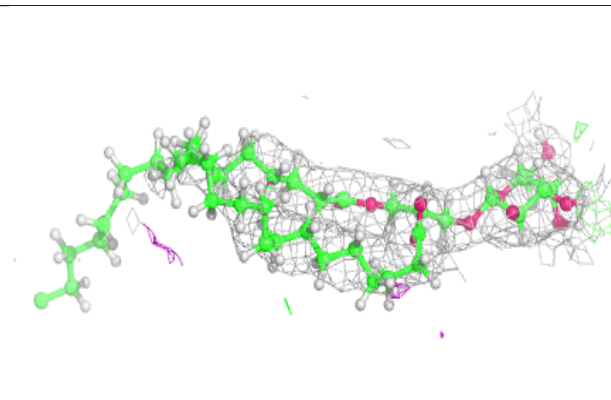
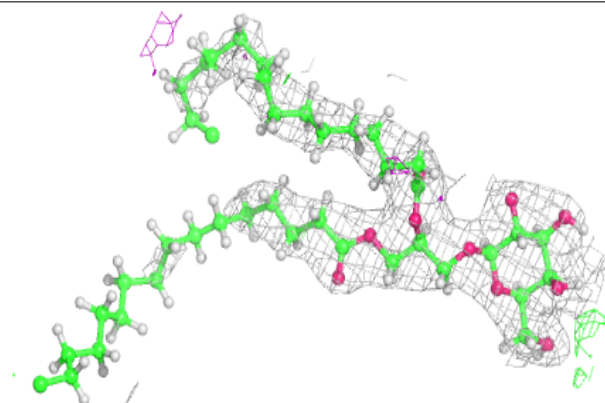


Electron density around BCR C 514:

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

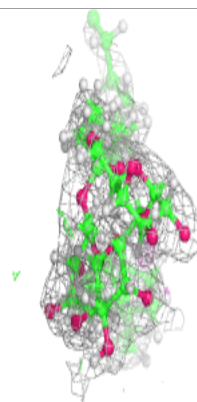
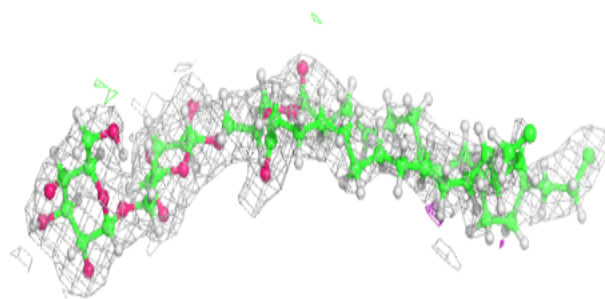
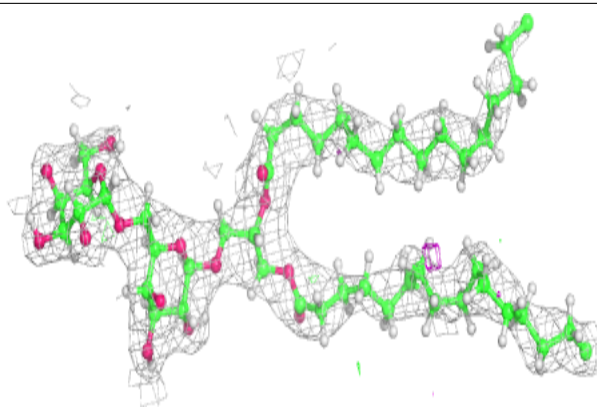
**Electron density around LMG D 408:**

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



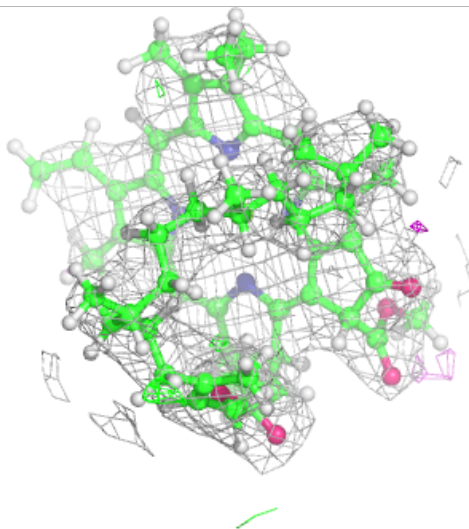
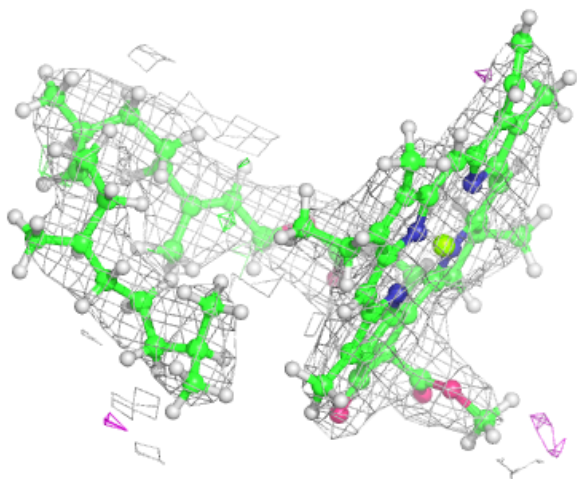
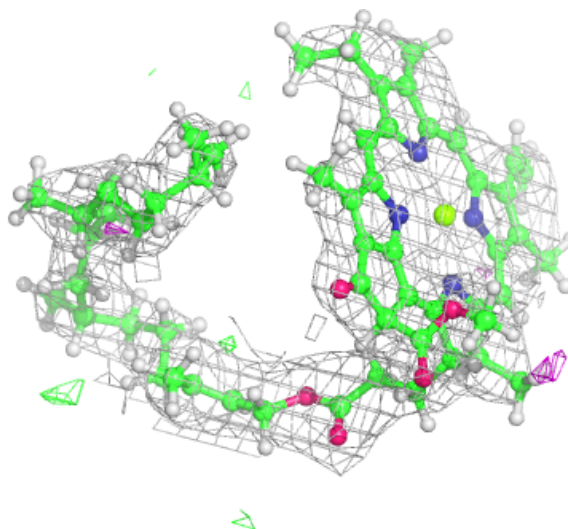
Electron density around DGD c 519:

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



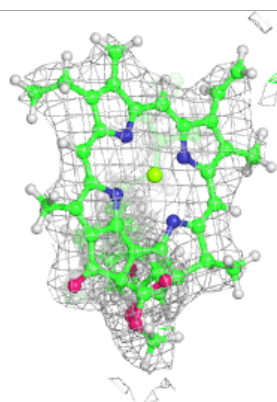
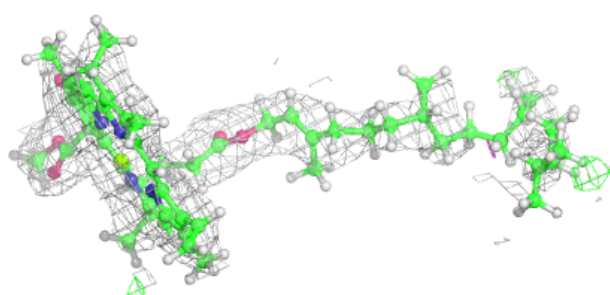
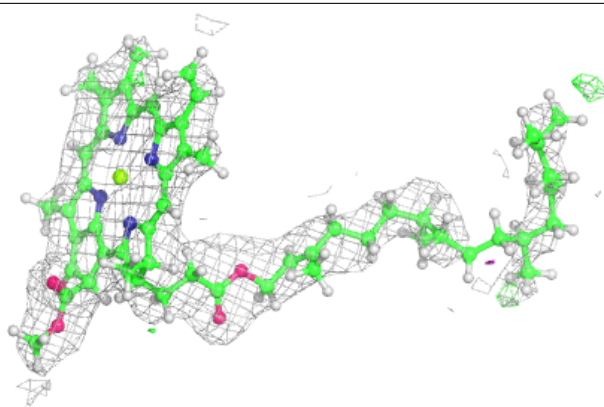
Electron density around CLA c 504:

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

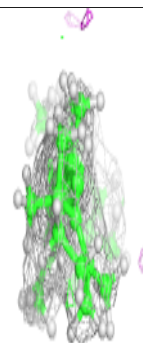
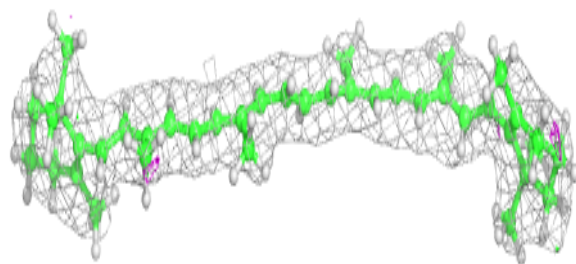
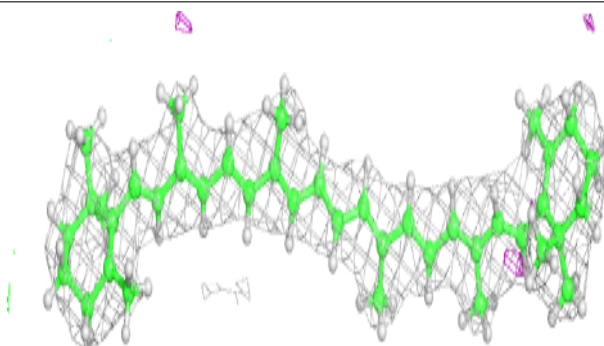


Electron density around CLA d 403:

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

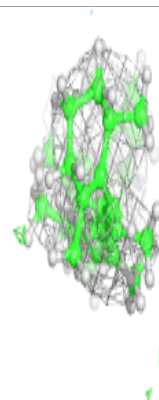
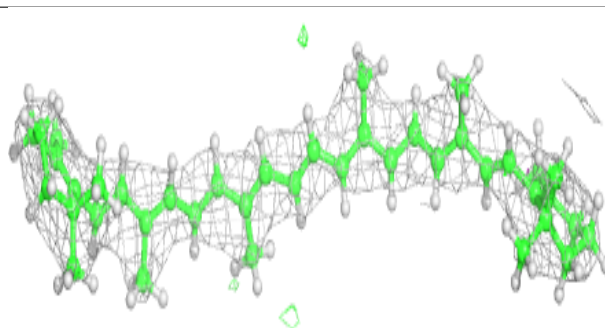
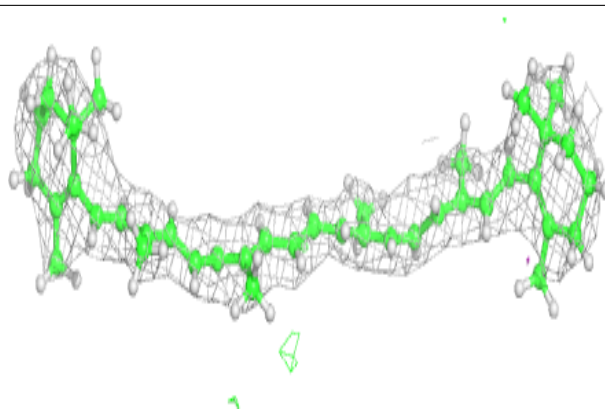
**Electron density around BCR b 619:**

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



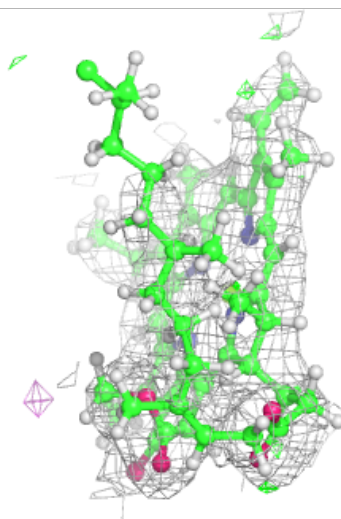
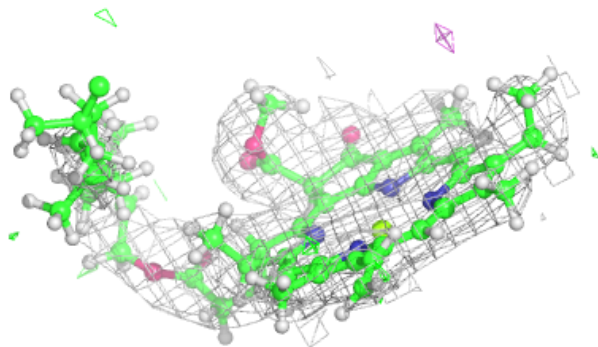
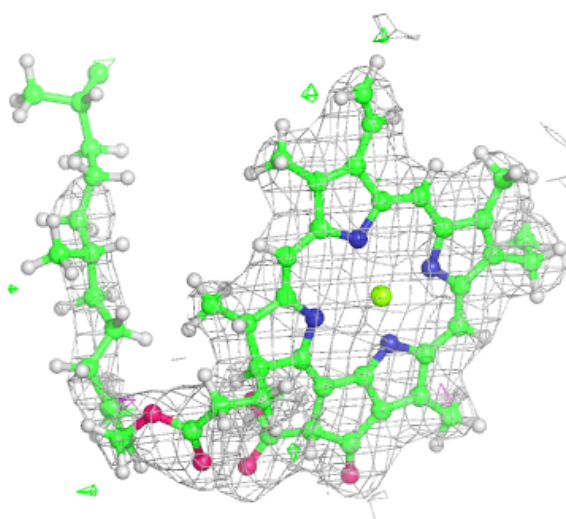
Electron density around BCR C 515:

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



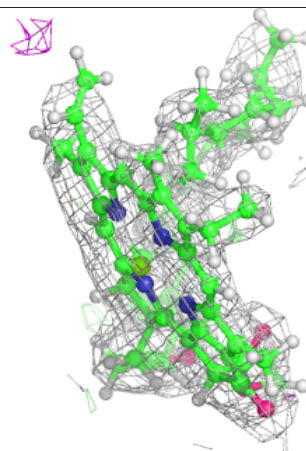
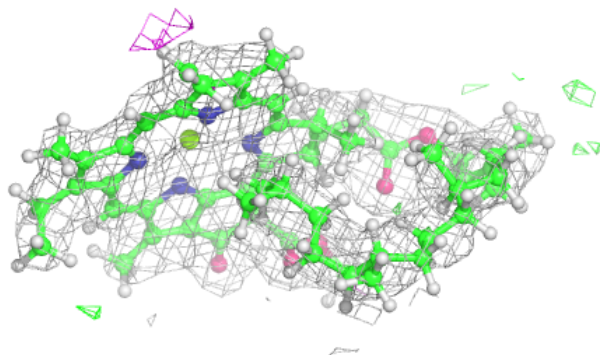
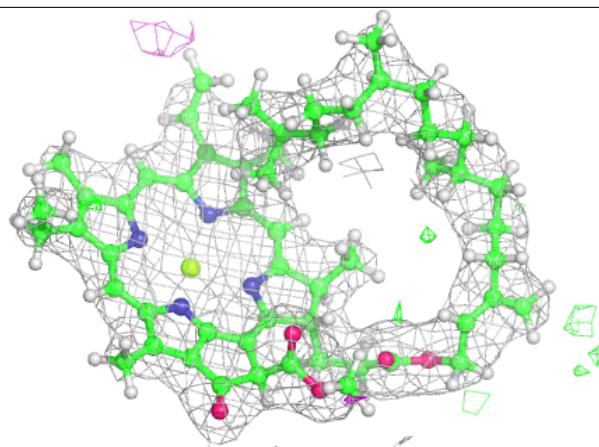
Electron density around CLA B 616:

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

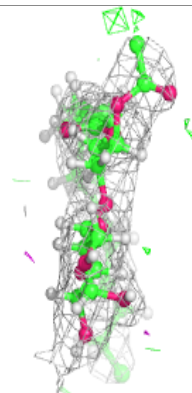
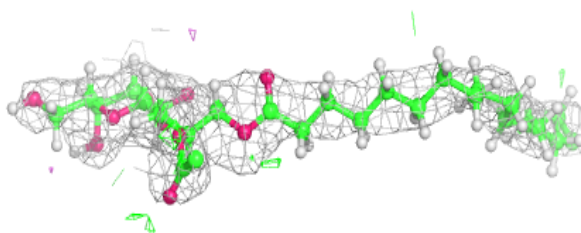
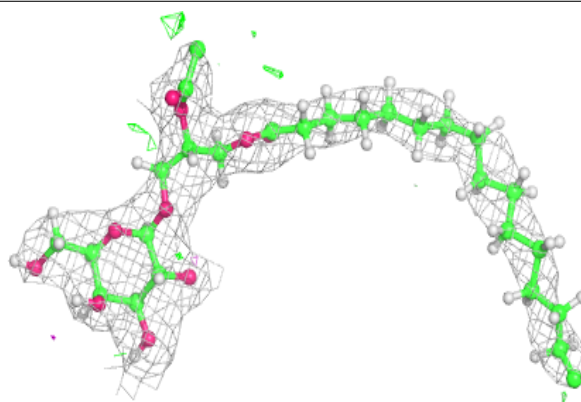


Electron density around CLA B 615:

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

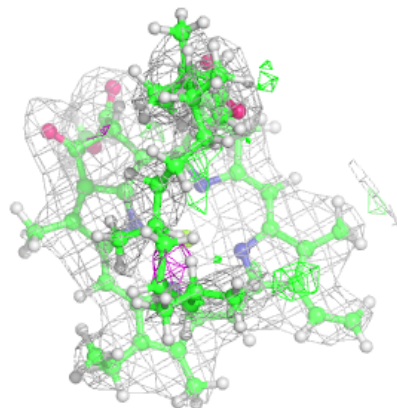
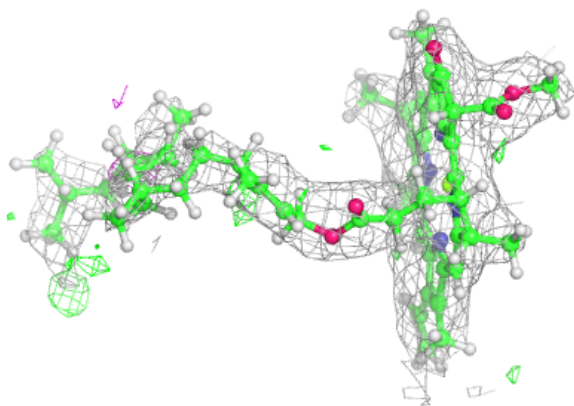
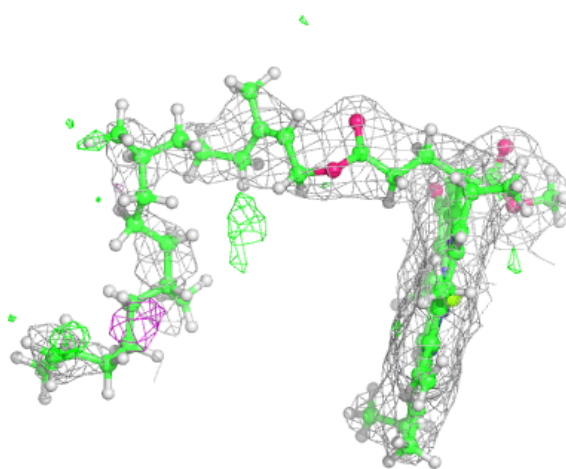
**Electron density around LMG c 520:**

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



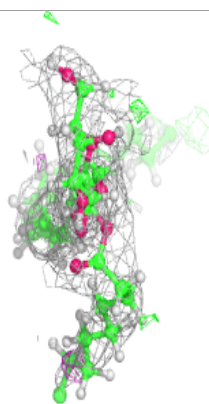
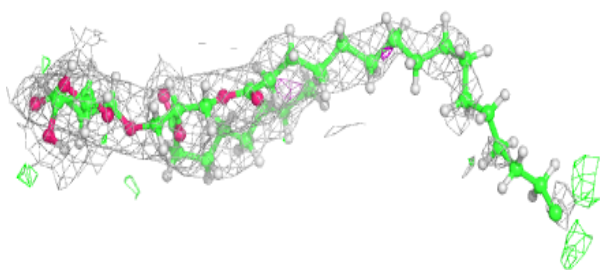
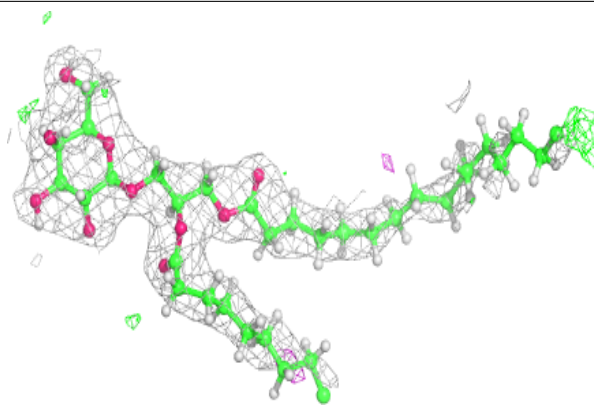
Electron density around CLA c 507:

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



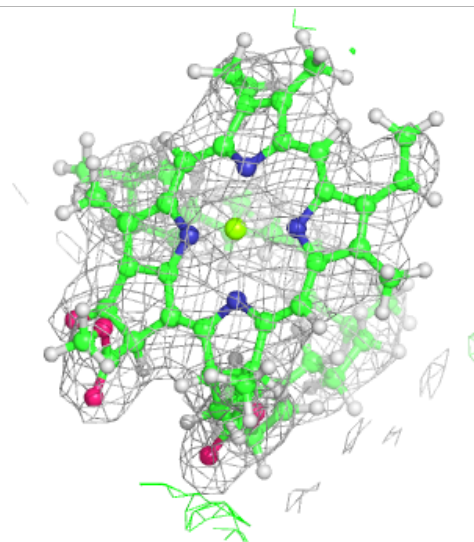
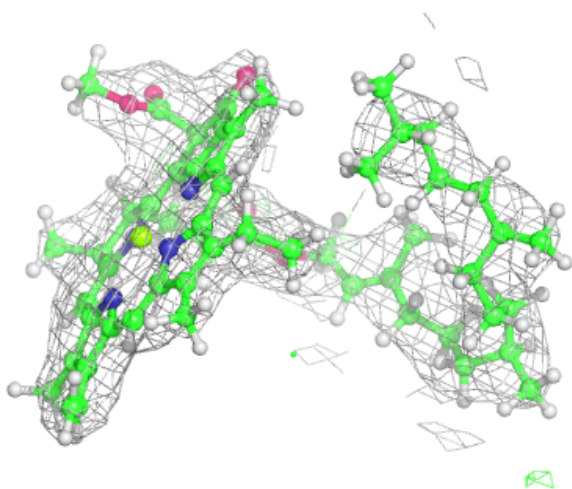
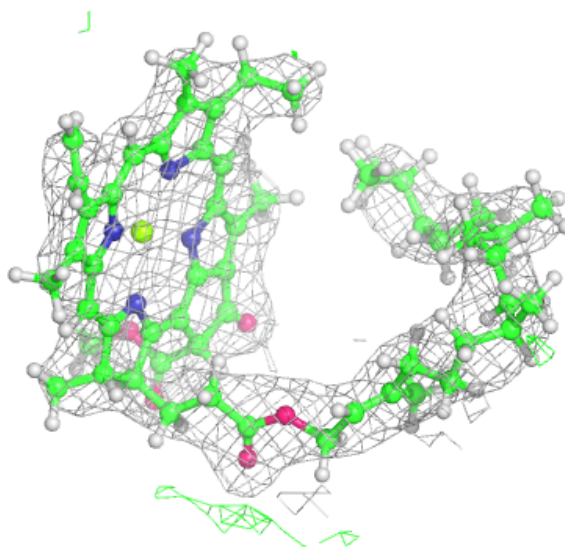
Electron density around LMG d 408:

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



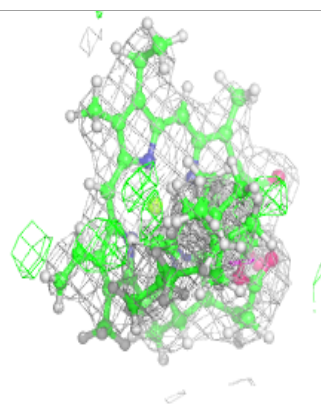
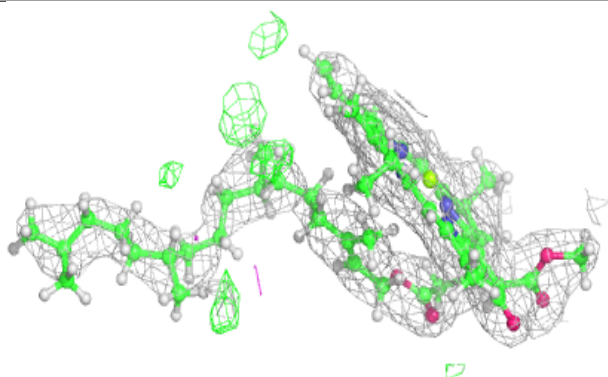
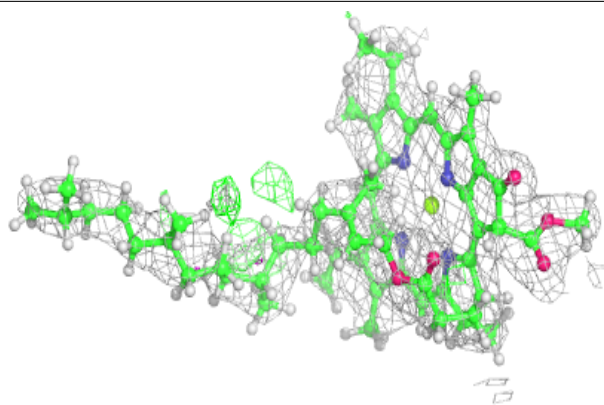
Electron density around CLA C 503:

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

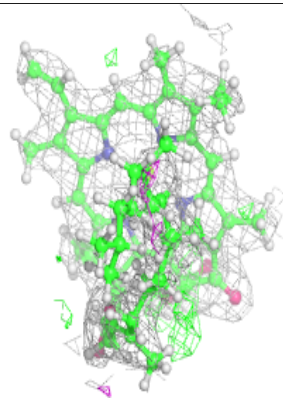
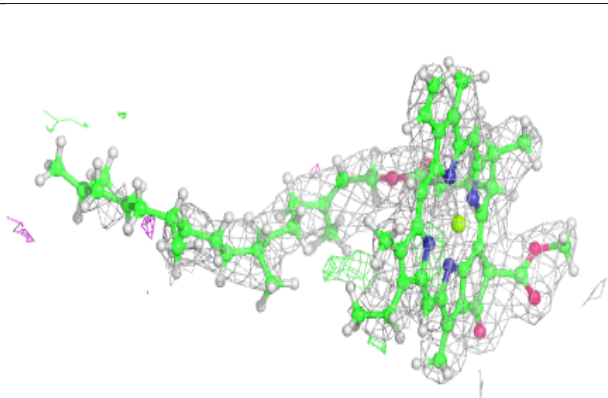
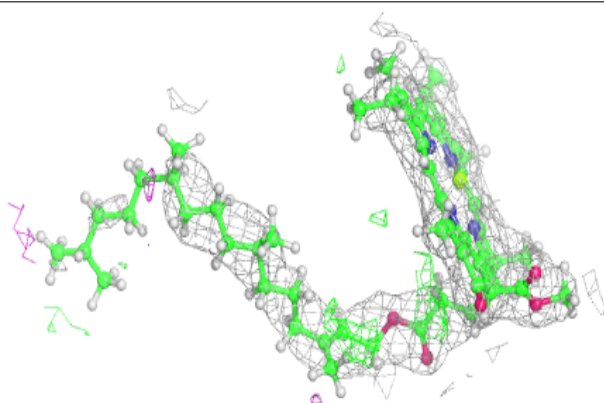


Electron density around CLA C 505:

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

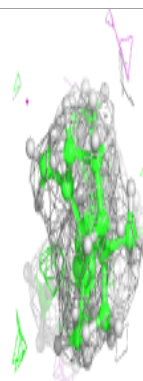
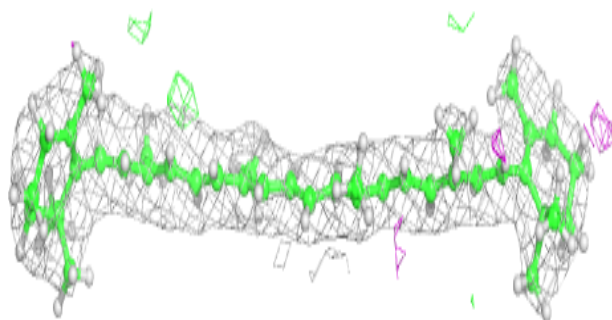
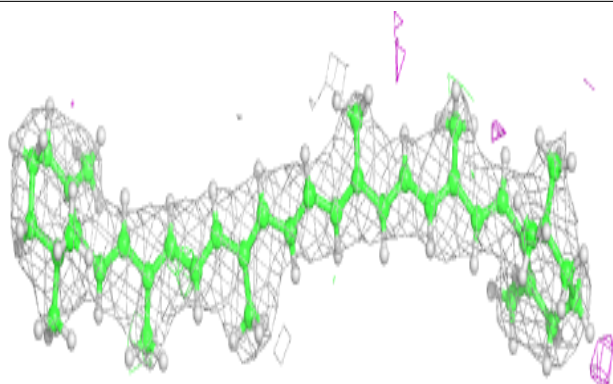
**Electron density around CLA C 508:**

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

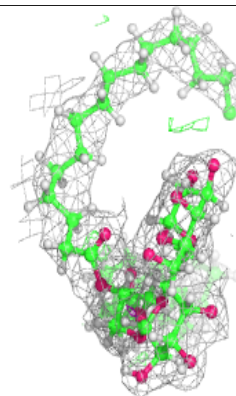
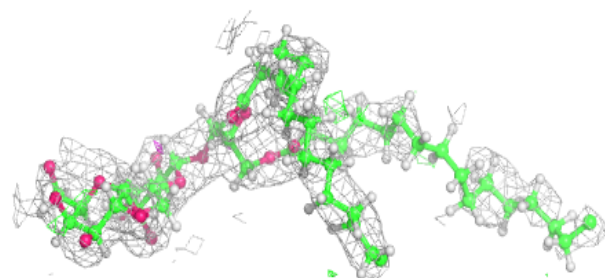
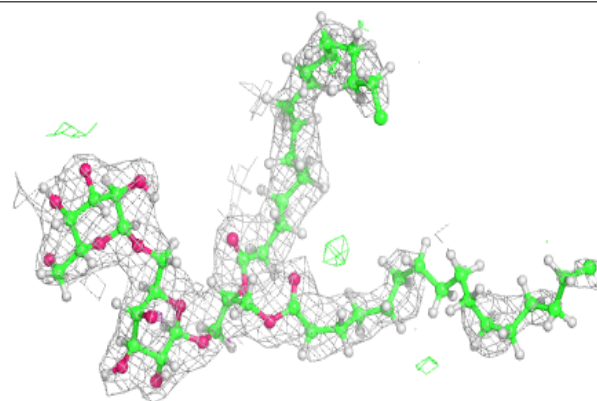


Electron density around BCR B 618:

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

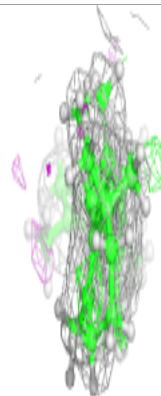
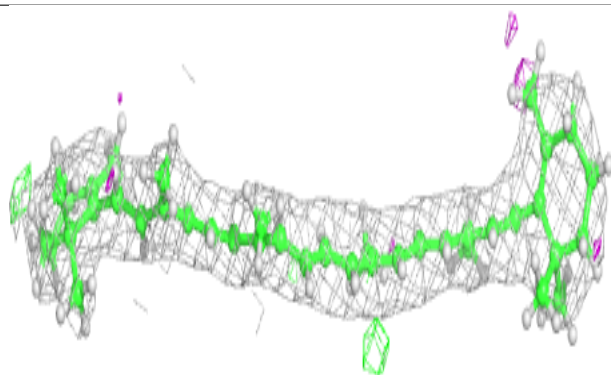
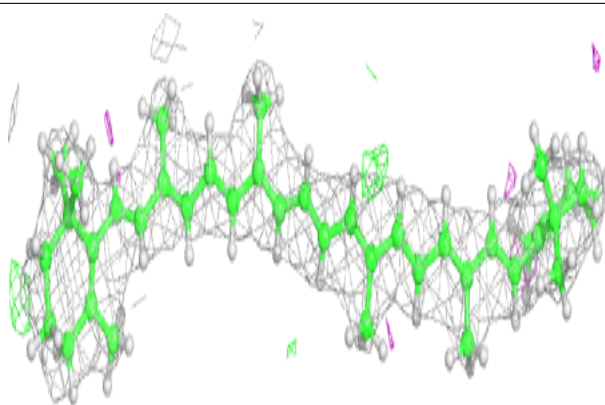
**Electron density around DGD c 518:**

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

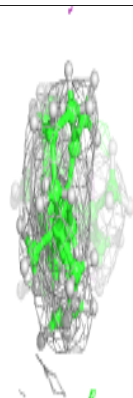
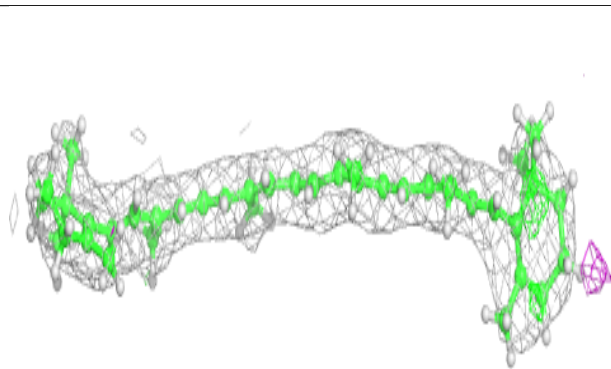
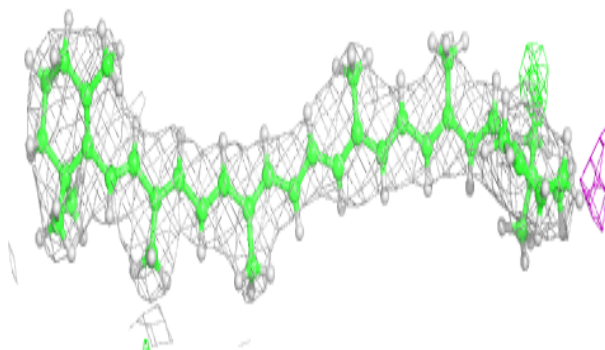


Electron density around BCR B 617:

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

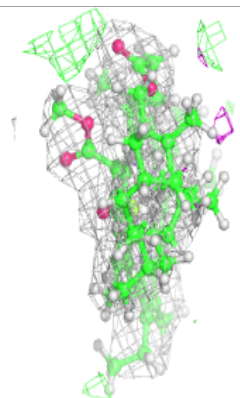
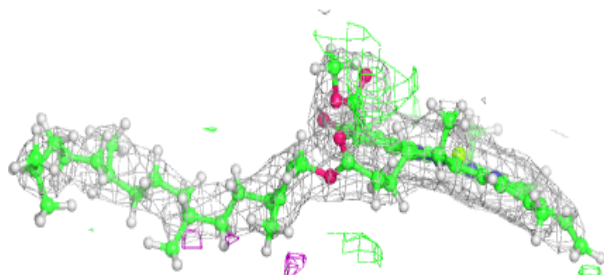
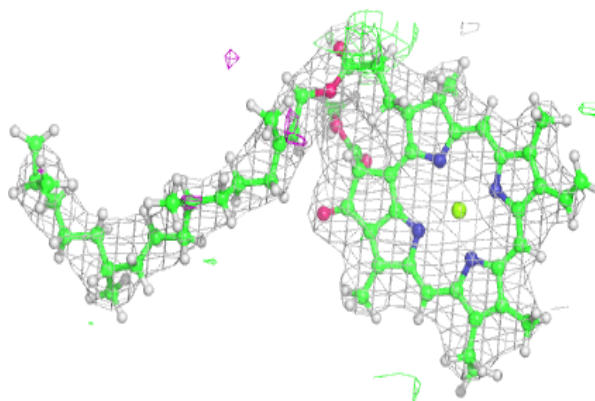
**Electron density around BCR b 617:**

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

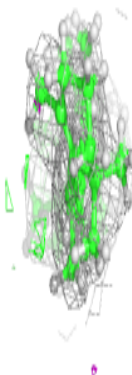
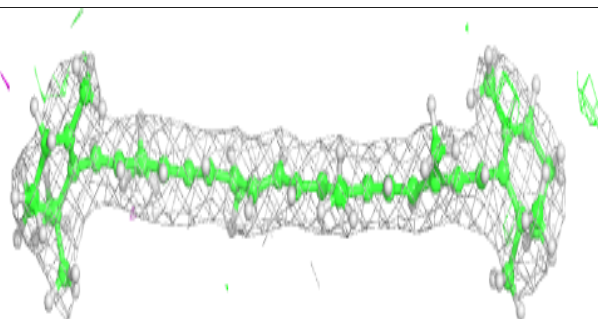
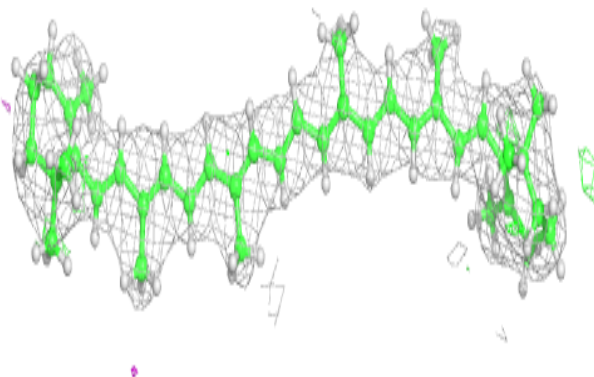


Electron density around CLA b 602:

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

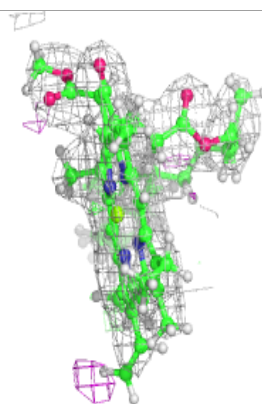
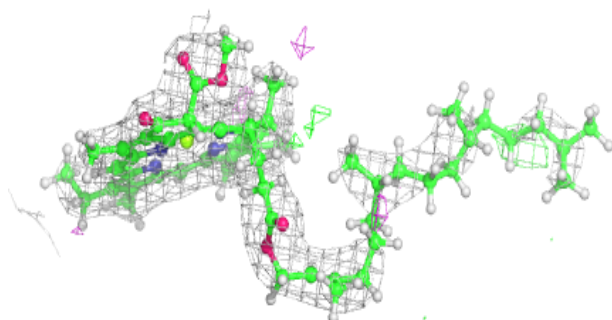
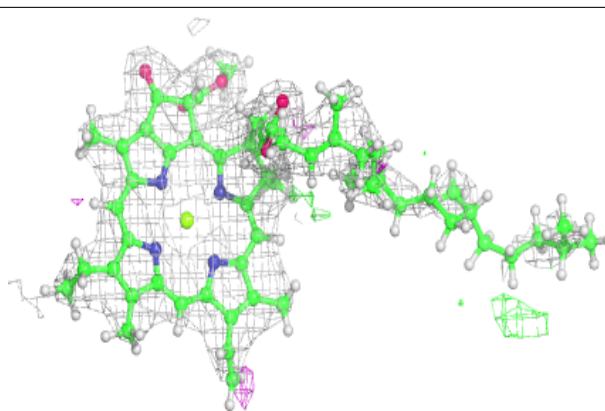
**Electron density around BCR b 618:**

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



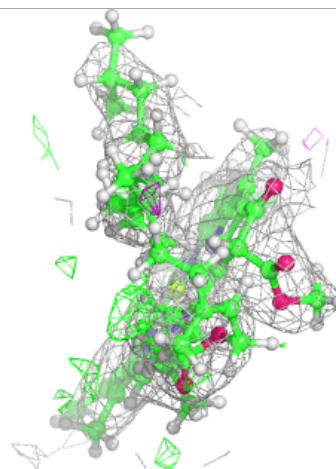
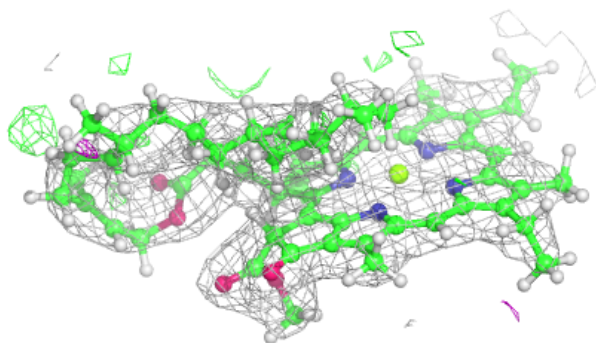
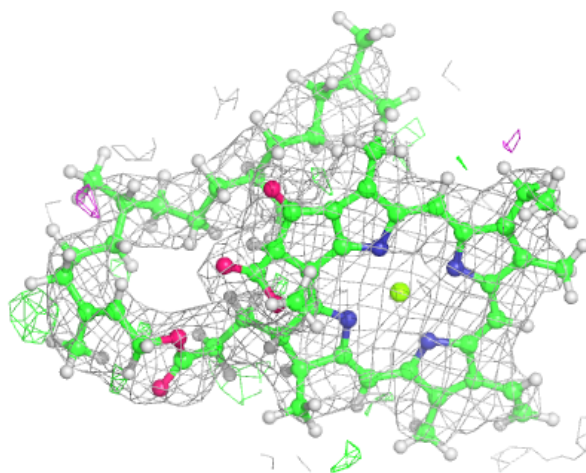
Electron density around CLA a 403:

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



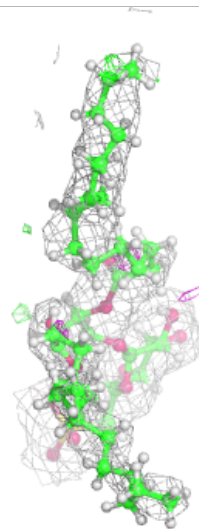
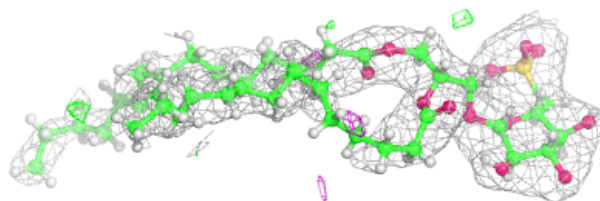
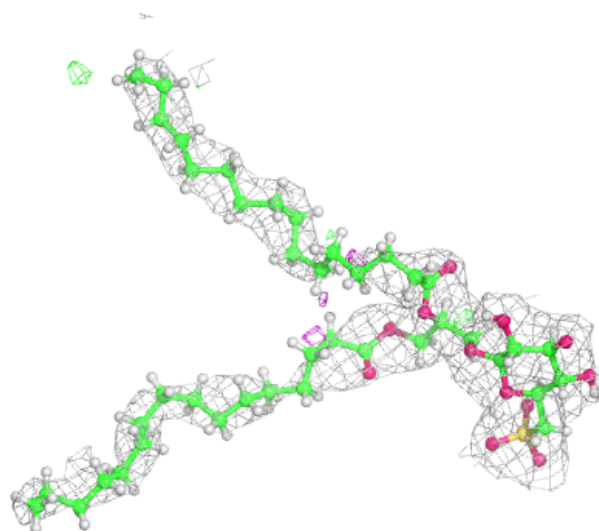
Electron density around CLA c 510:

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



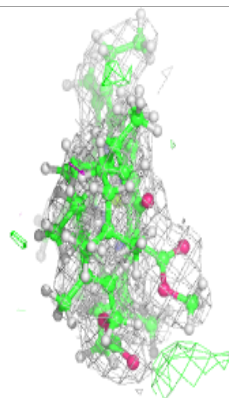
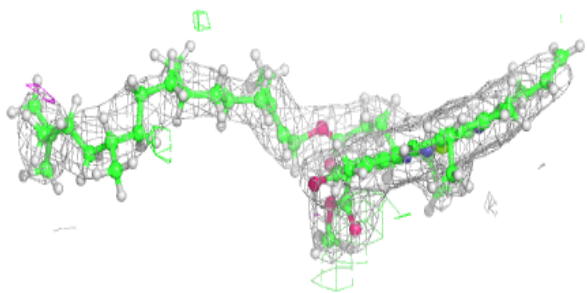
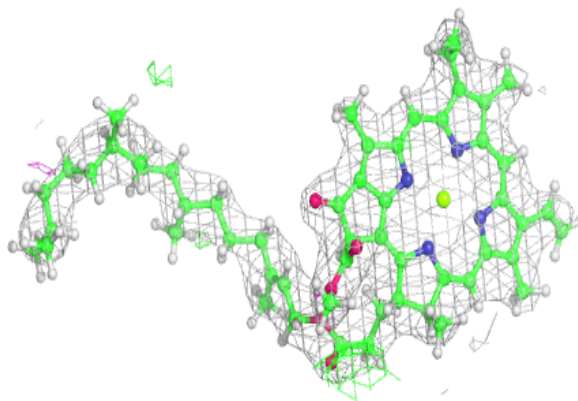
Electron density around SQD a 413:

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

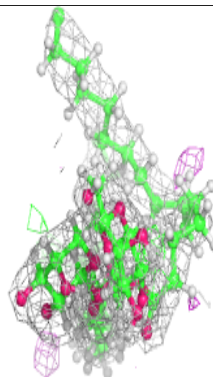
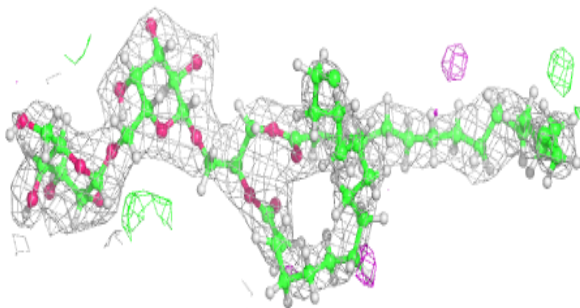
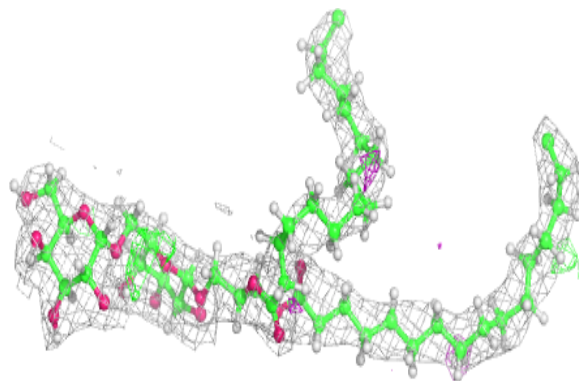


Electron density around CLA B 602:

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

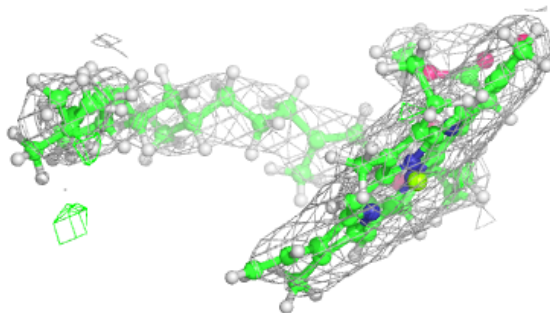
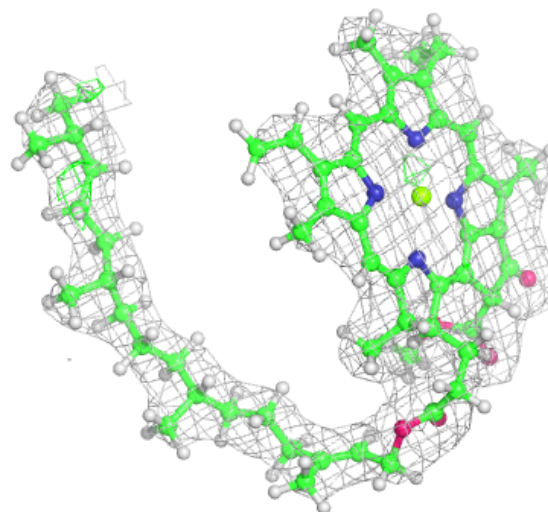
**Electron density around DGD h 102:**

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



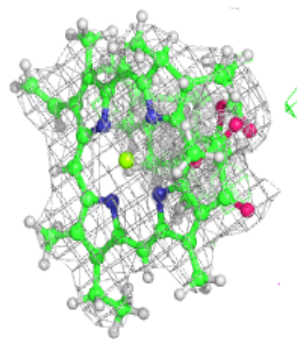
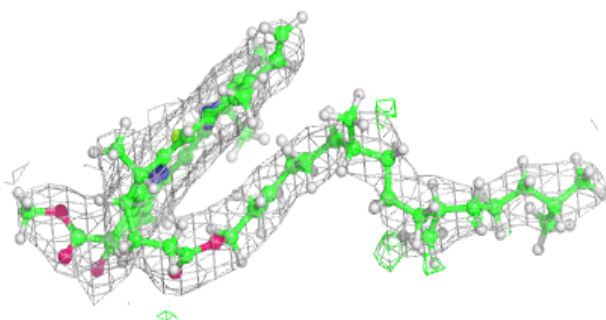
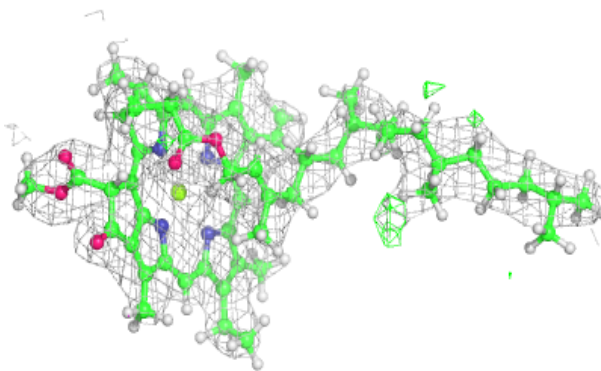
Electron density around CLA c 508:

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

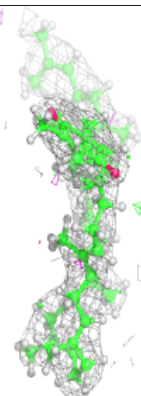
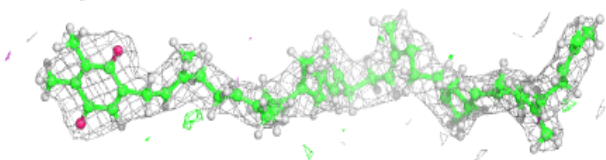
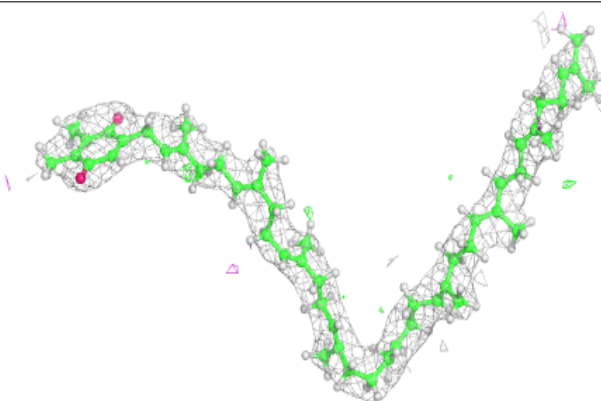


Electron density around CLA c 506:

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

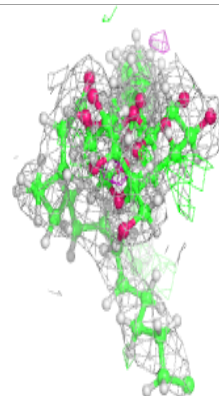
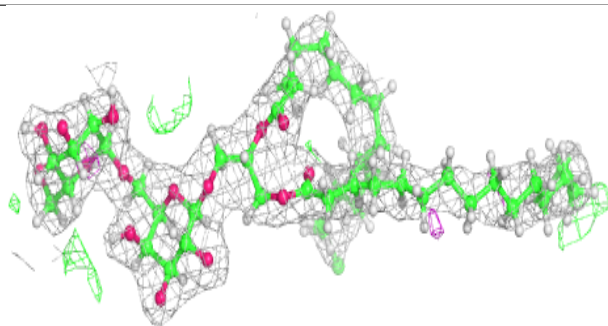
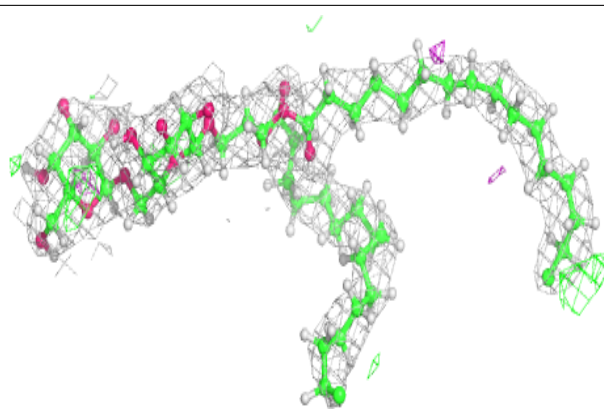
**Electron density around PL9 D 407:**

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

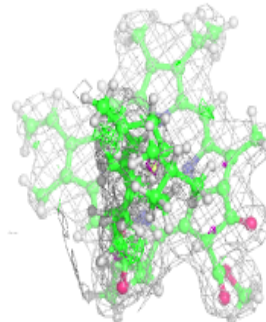
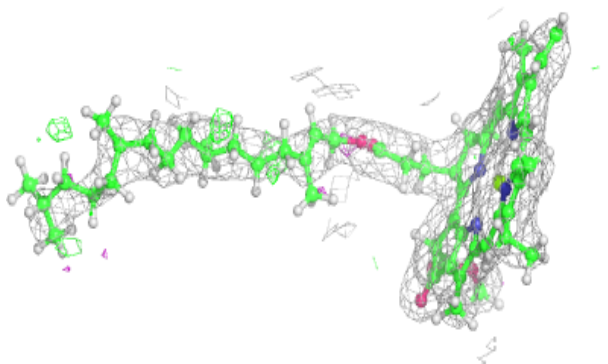
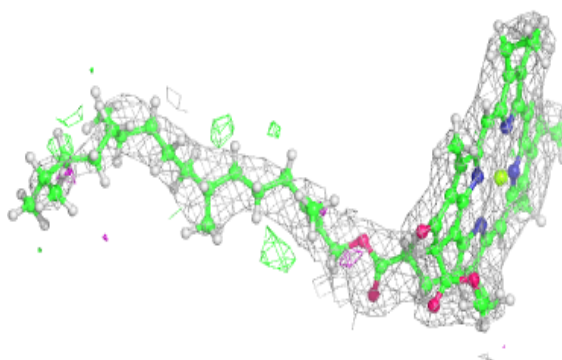


Electron density around DGD H 102:

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

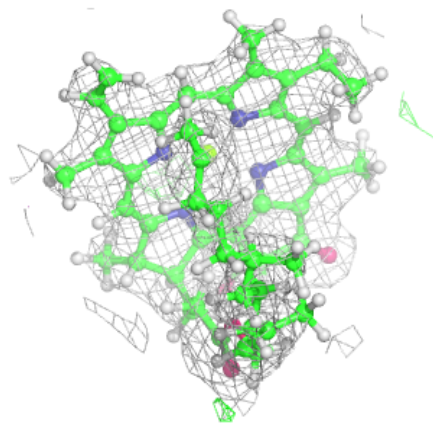
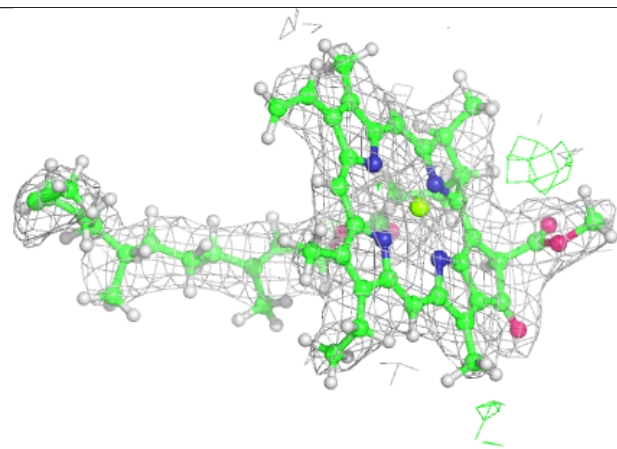
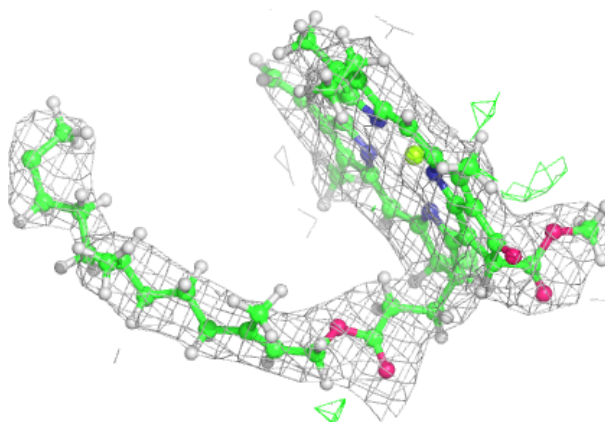
**Electron density around CLA B 604:**

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



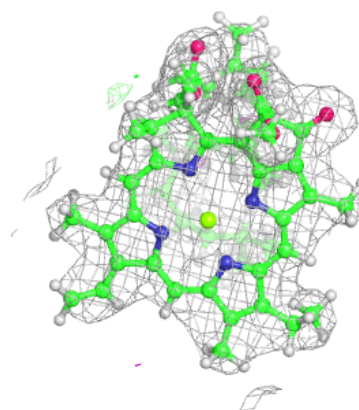
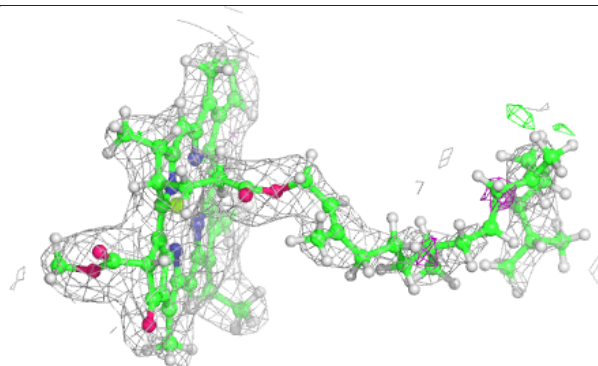
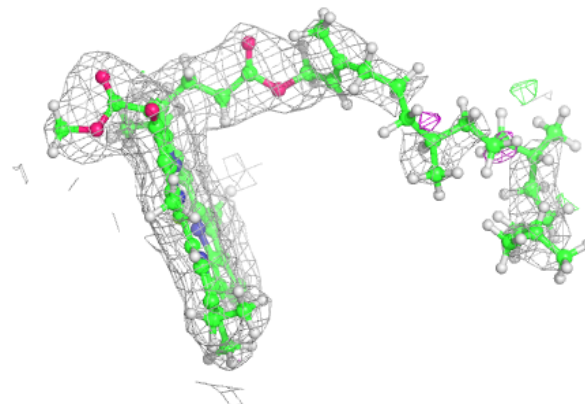
Electron density around CLA C 504:

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



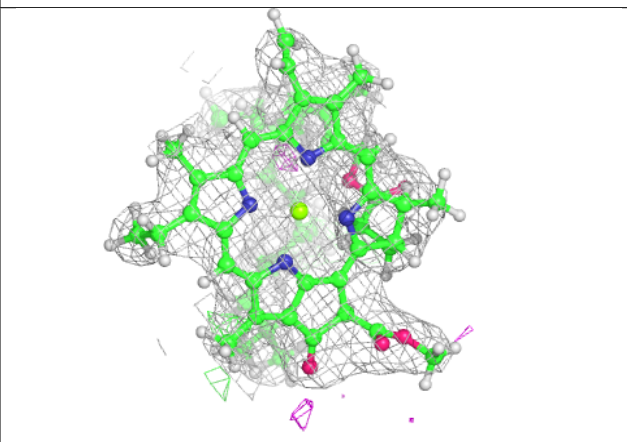
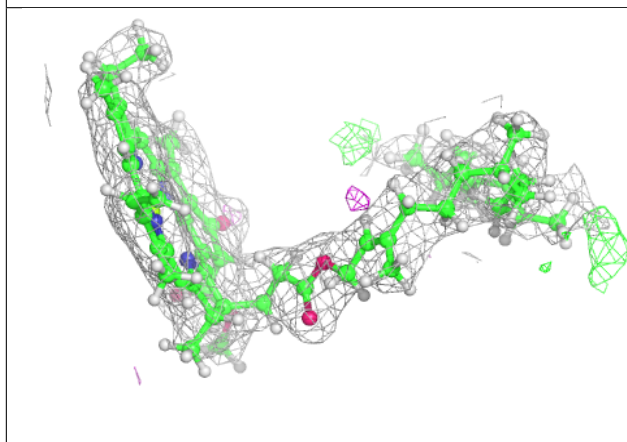
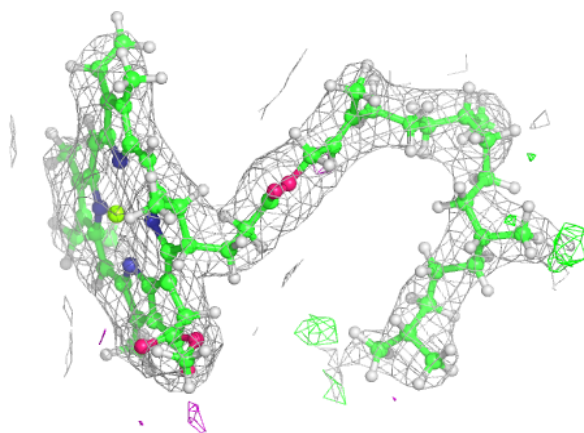
Electron density around CLA C 506:

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

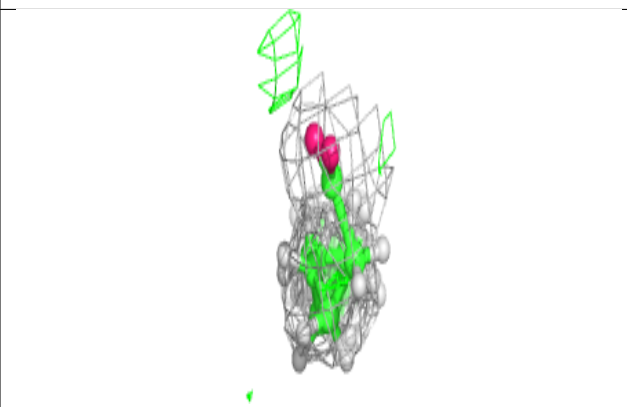
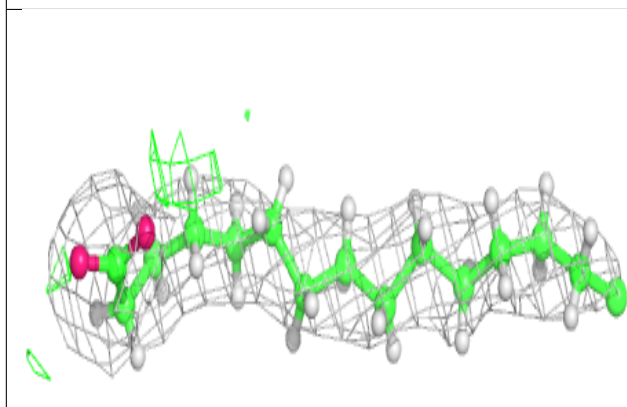
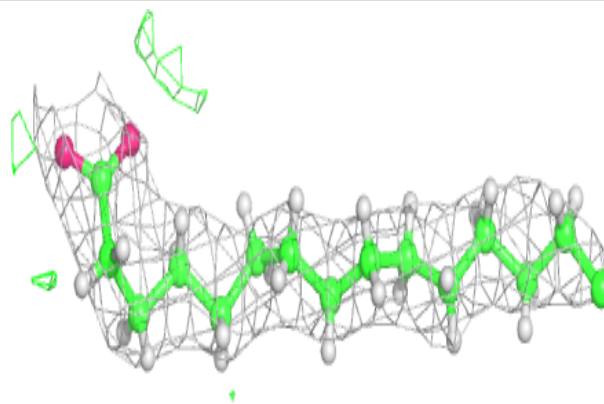


Electron density around CLA B 606:

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

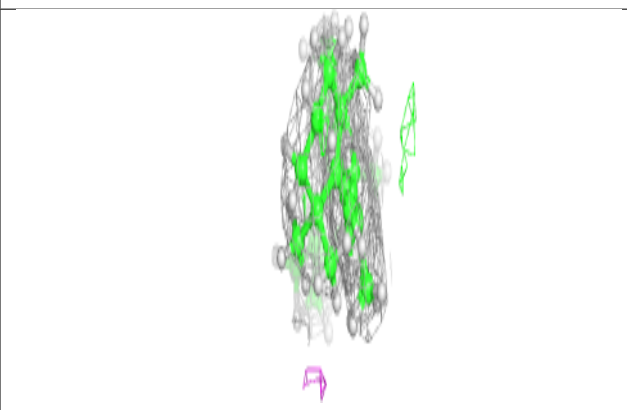
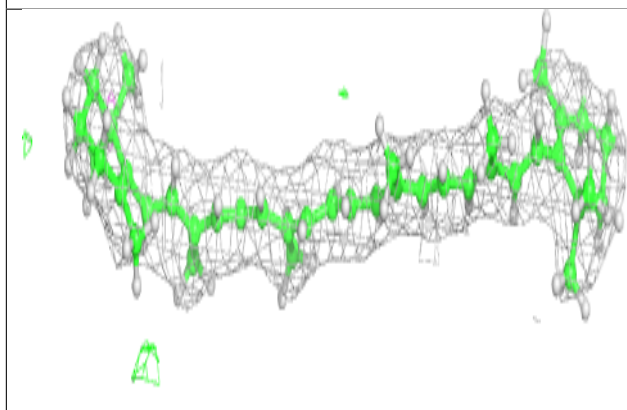
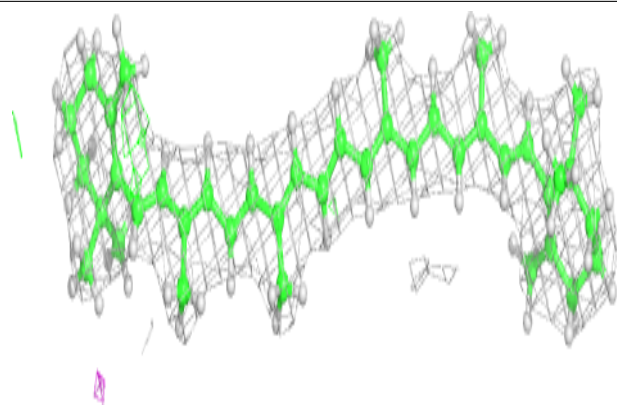
**Electron density around STE d 410:**

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



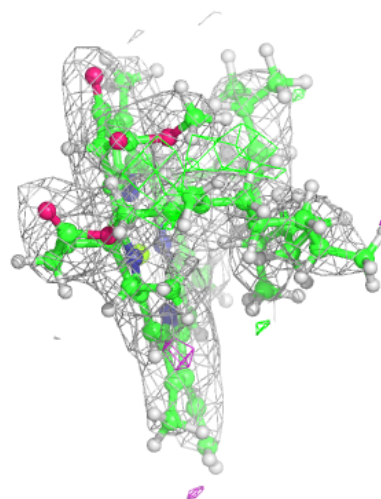
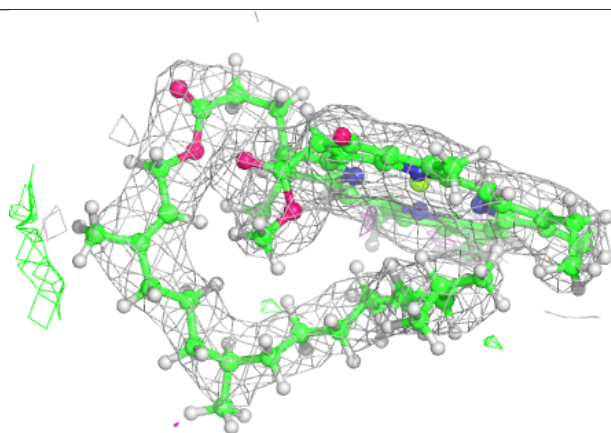
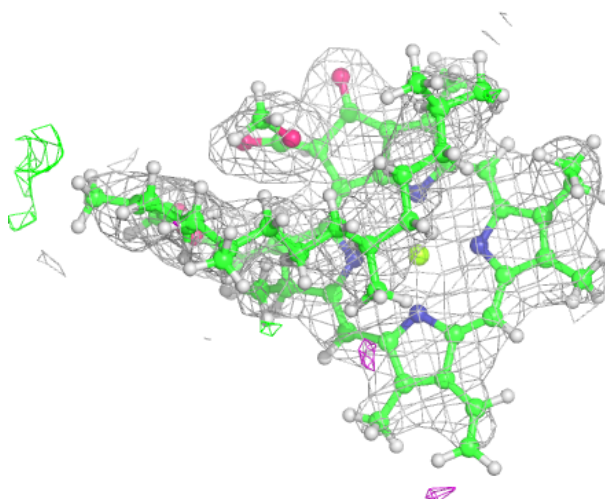
Electron density around BCR B 619:

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



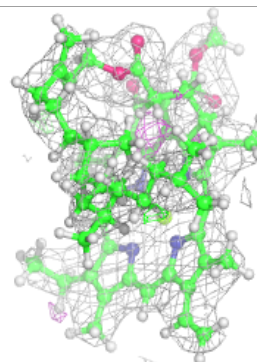
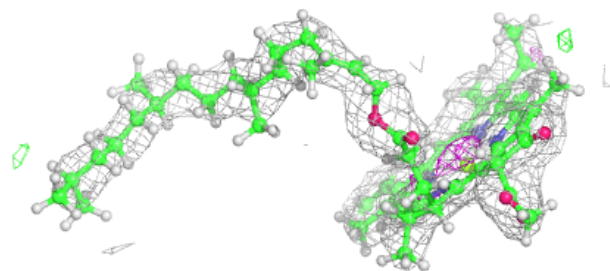
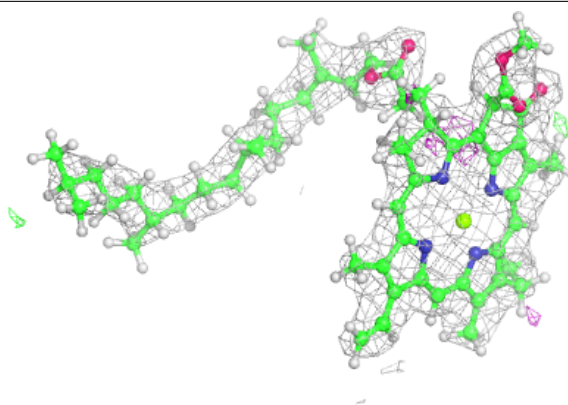
Electron density around CLA C 510:

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



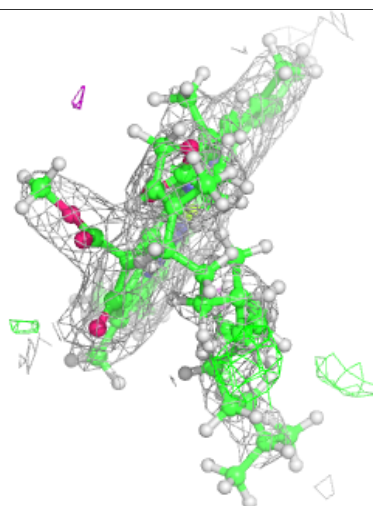
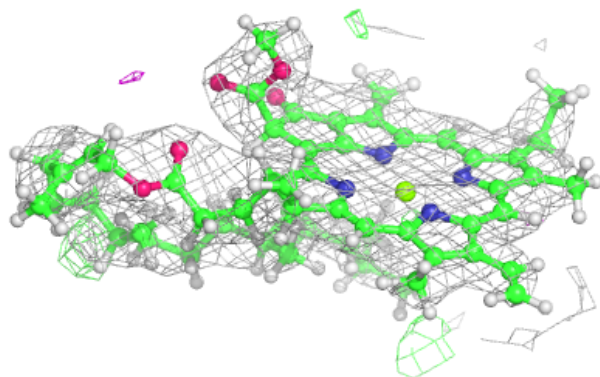
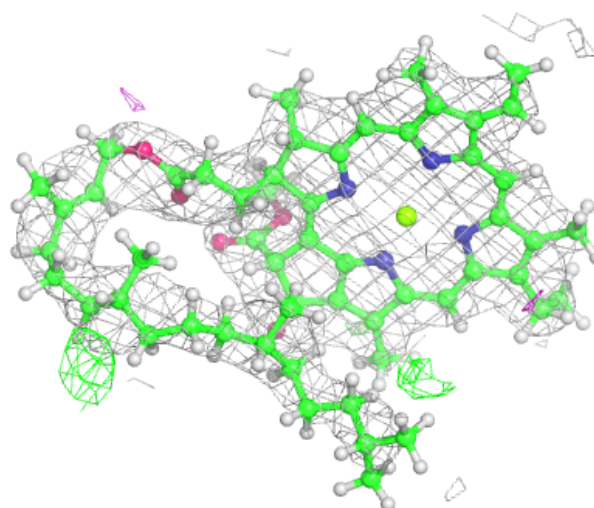
Electron density around CLA C 511:

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



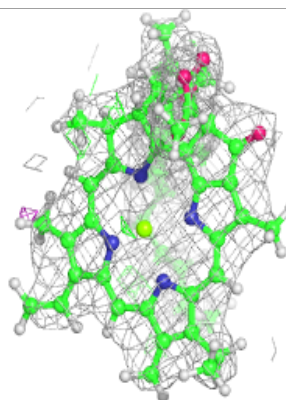
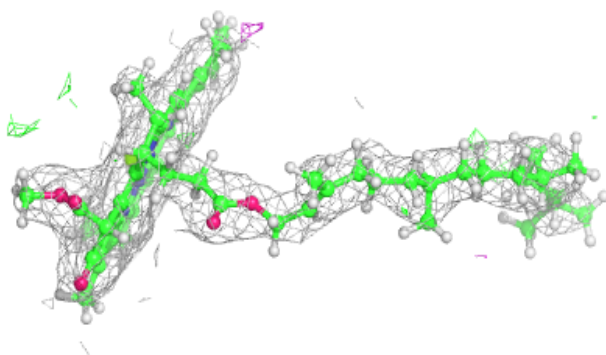
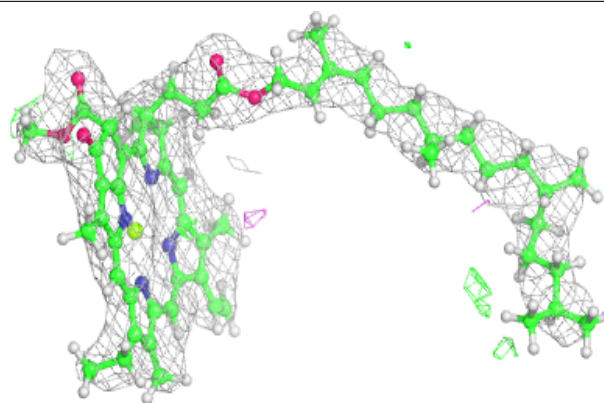
Electron density around CLA C 509:

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

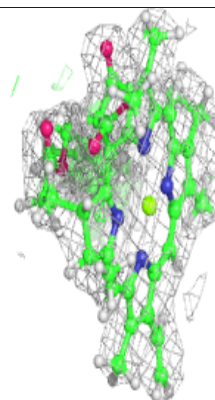
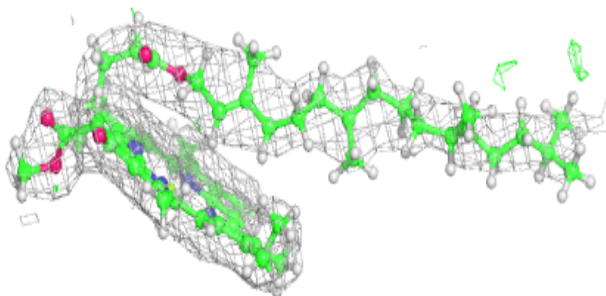
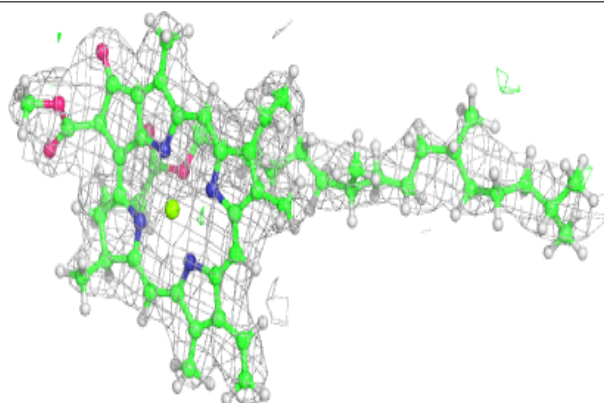


Electron density around CLA b 609:

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

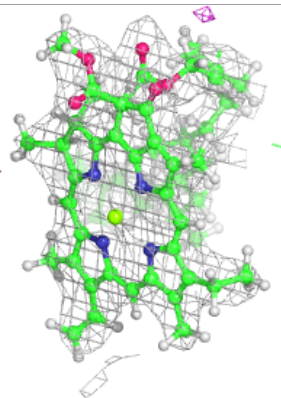
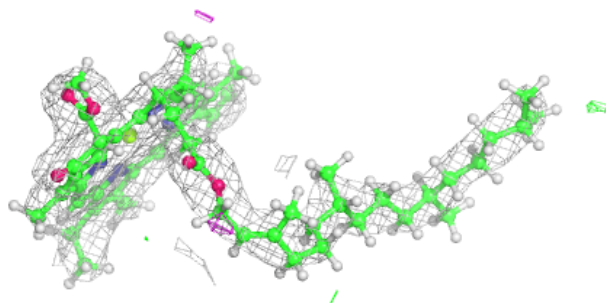
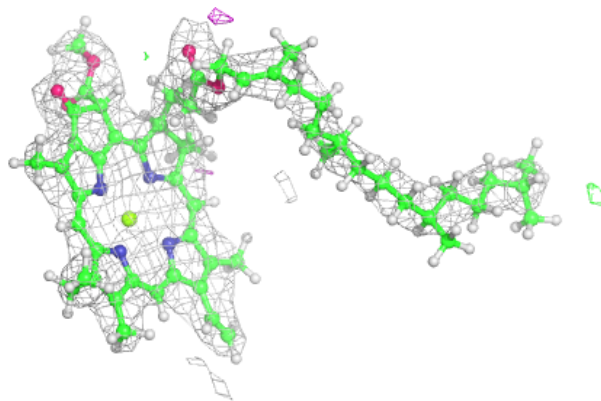
**Electron density around CLA b 614:**

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

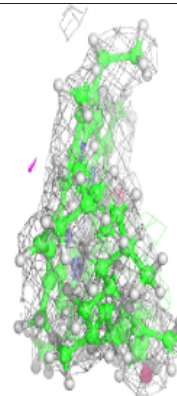
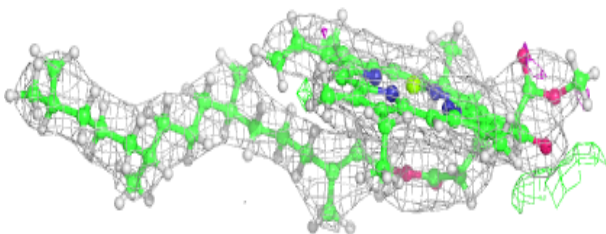
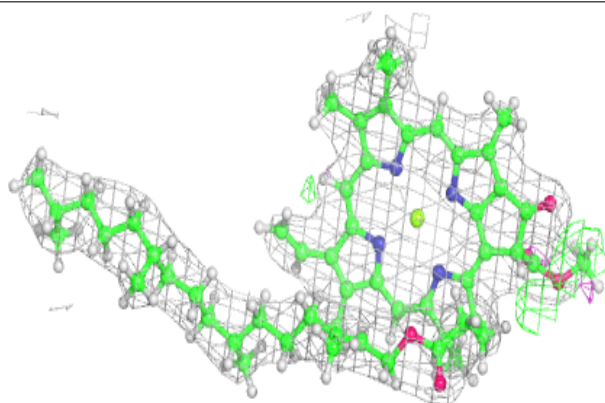


Electron density around CLA c 512:

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

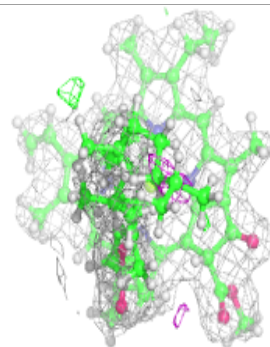
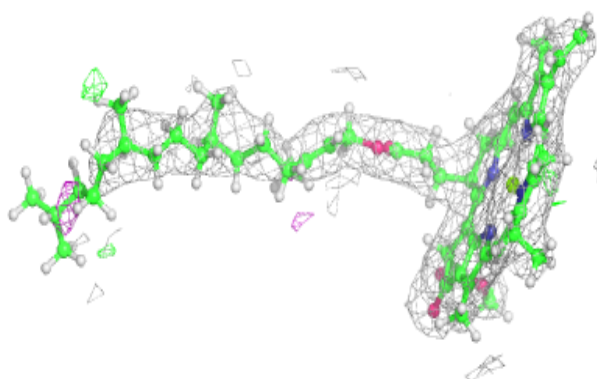
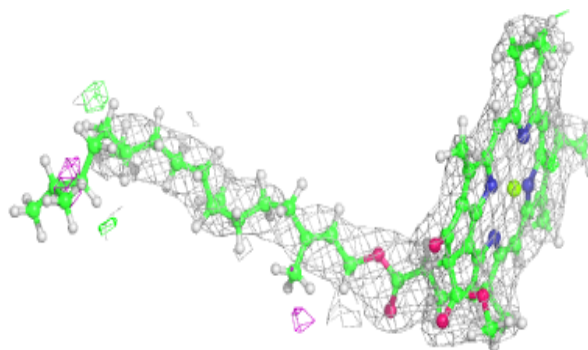
**Electron density around CLA C 501:**

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

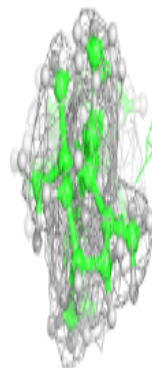
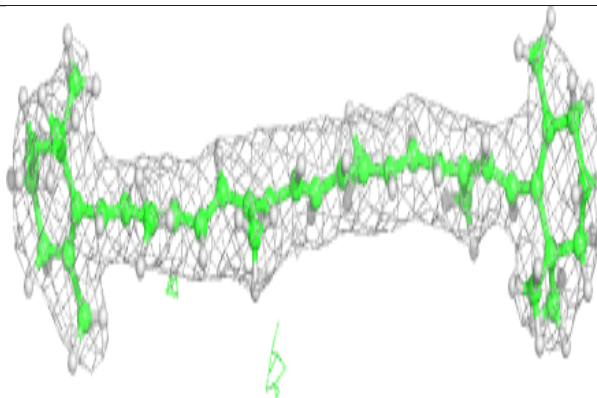
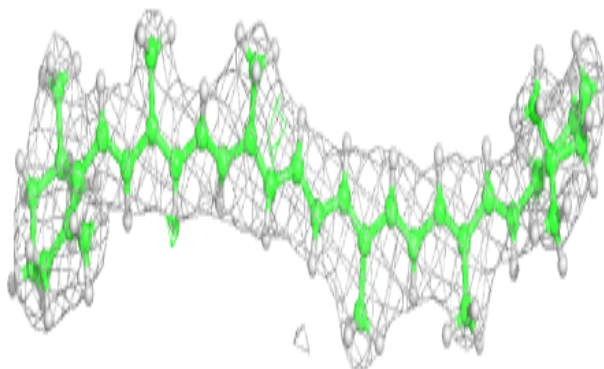


Electron density around CLA b 604:

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

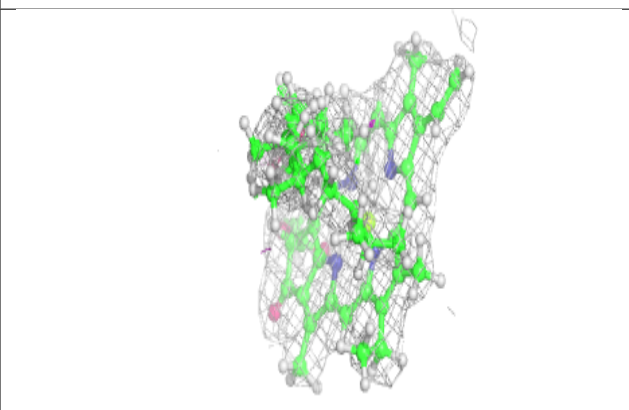
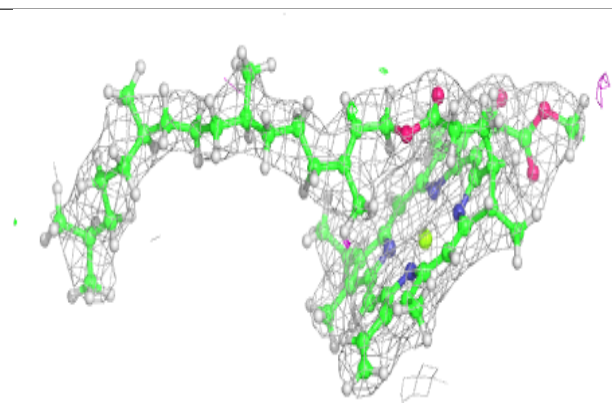
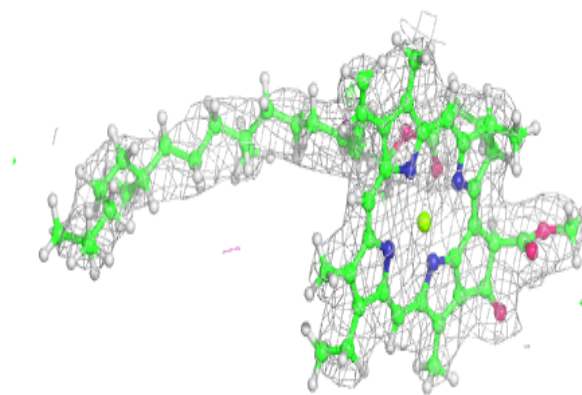
**Electron density around BCR A 405:**

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



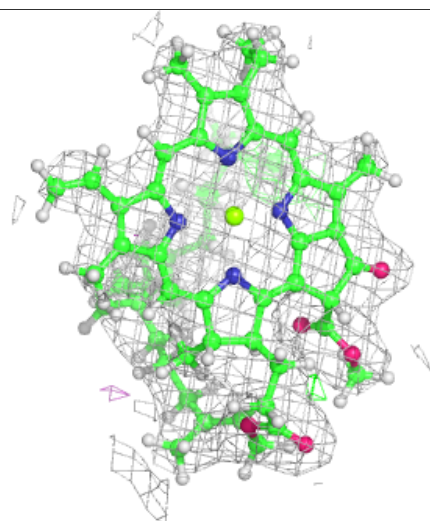
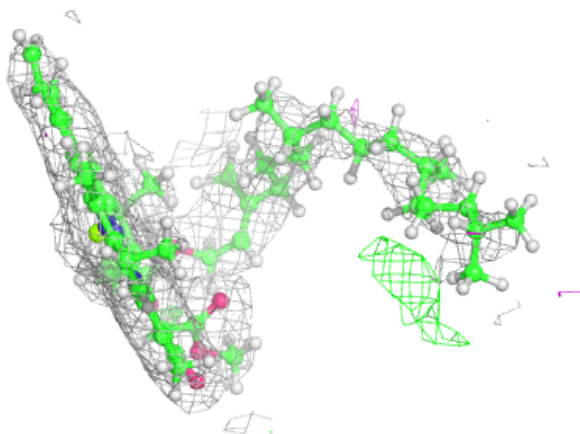
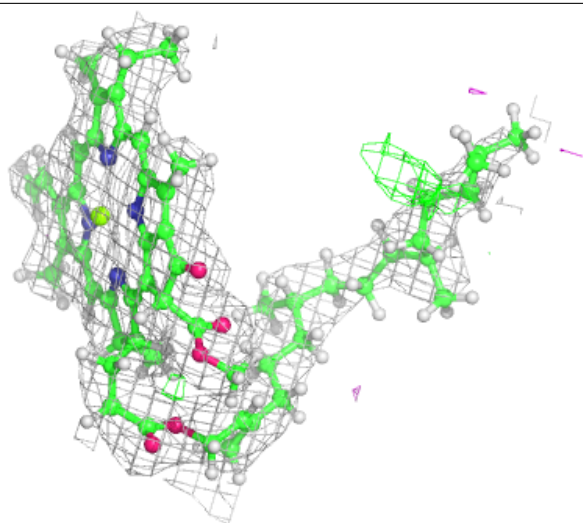
Electron density around CLA b 608:

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



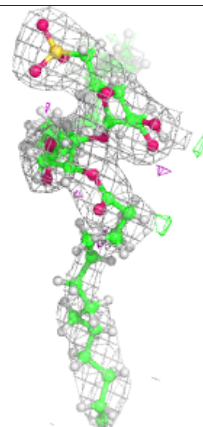
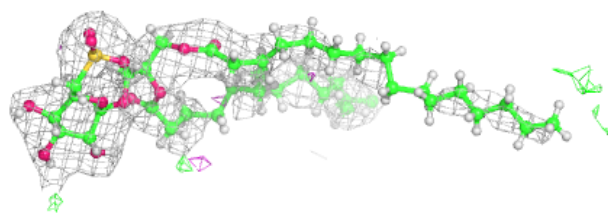
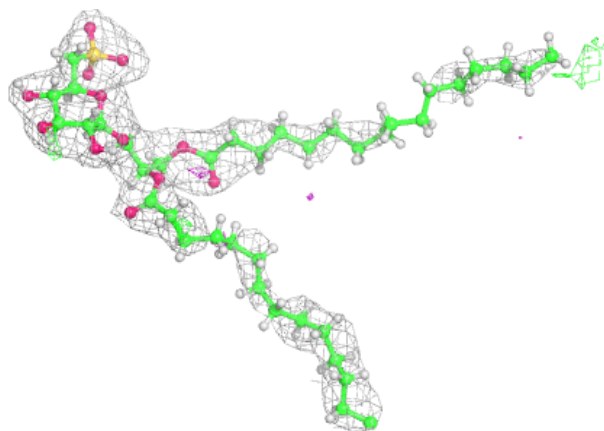
Electron density around CLA b 613:

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



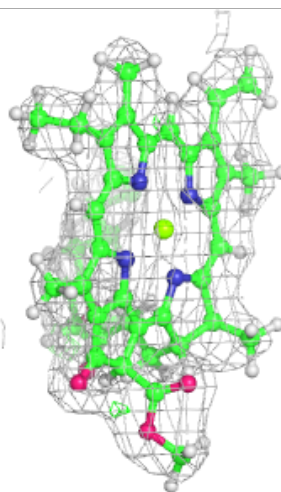
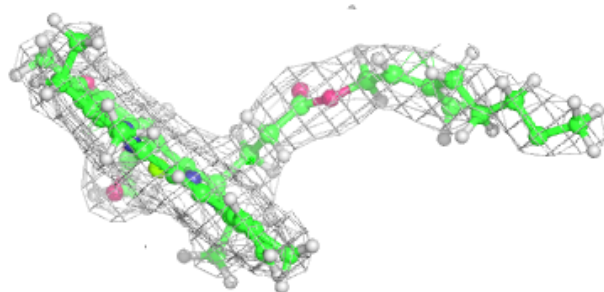
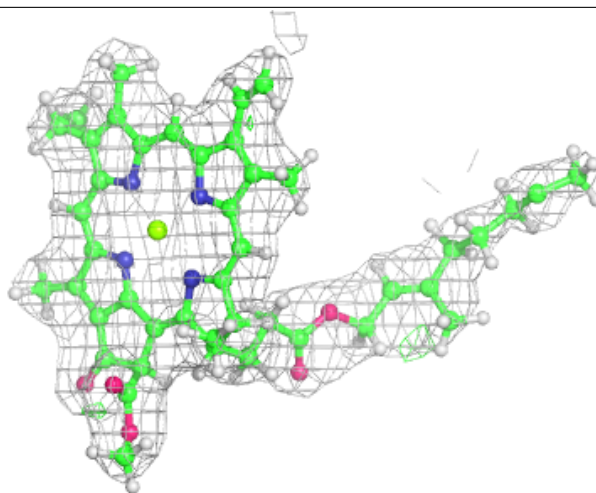
Electron density around SQD A 411:

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



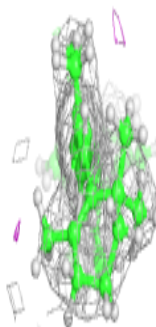
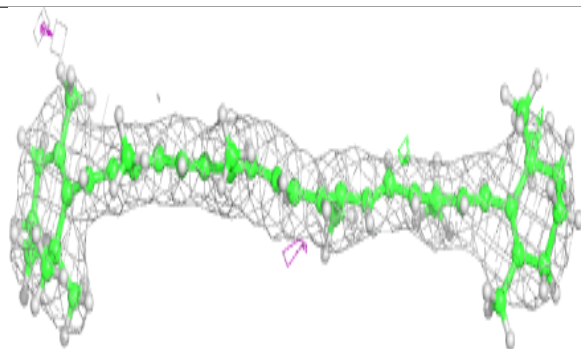
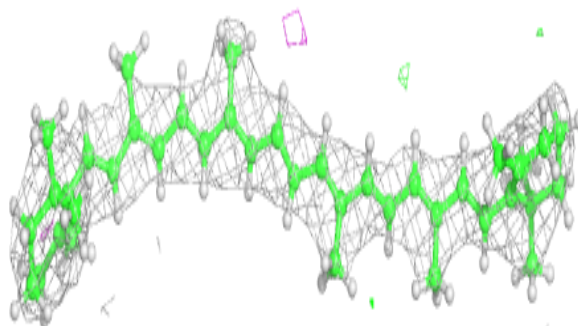
Electron density around CLA A 404:

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

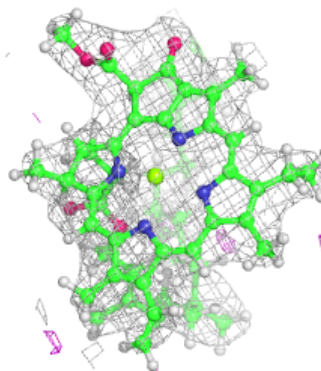
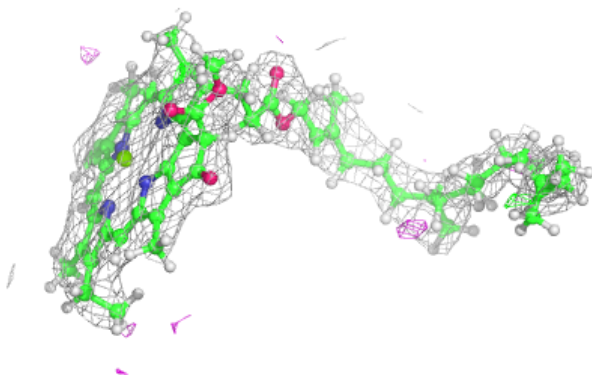
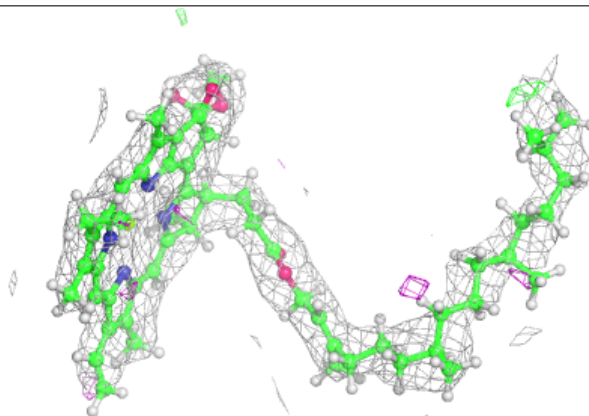


Electron density around BCR c 516:

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

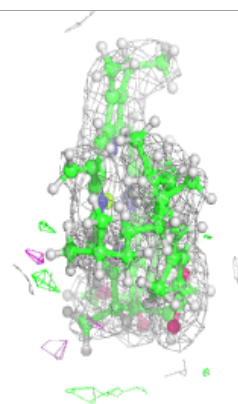
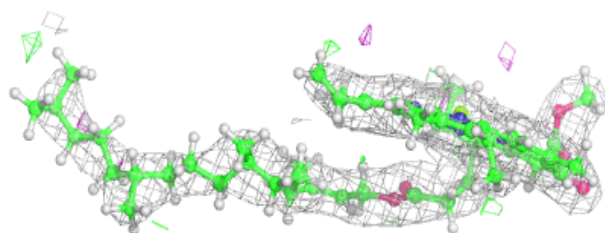
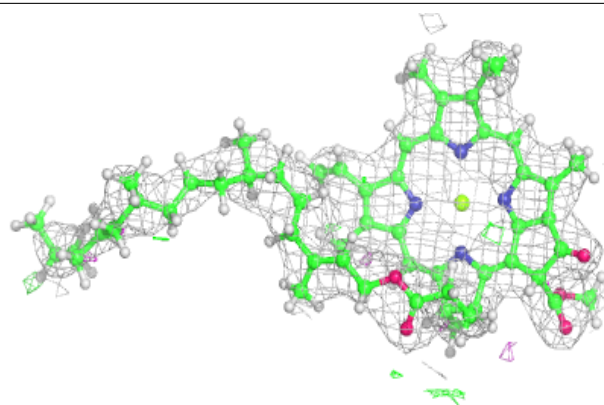
**Electron density around CLA b 606:**

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

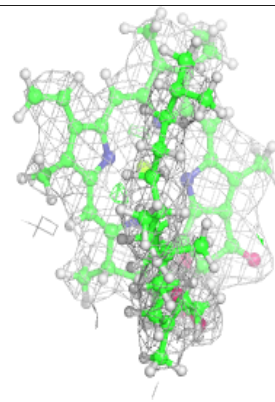
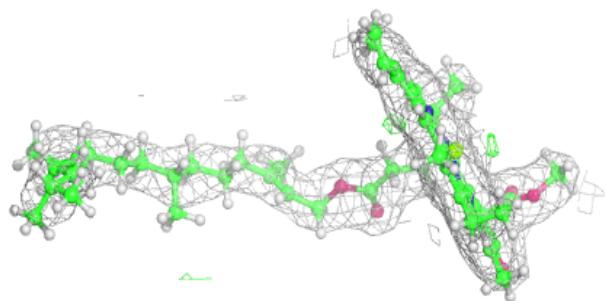
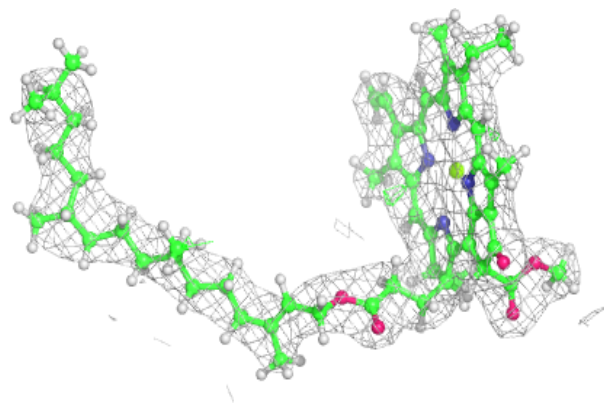


Electron density around CLA B 603:

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

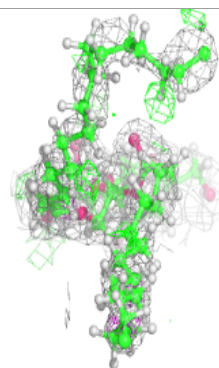
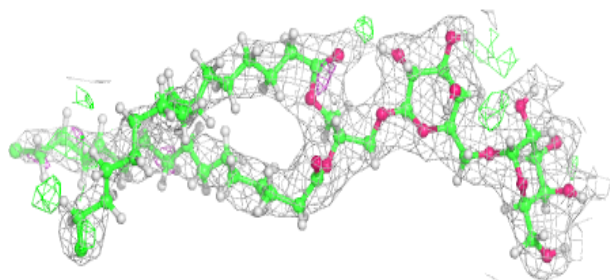
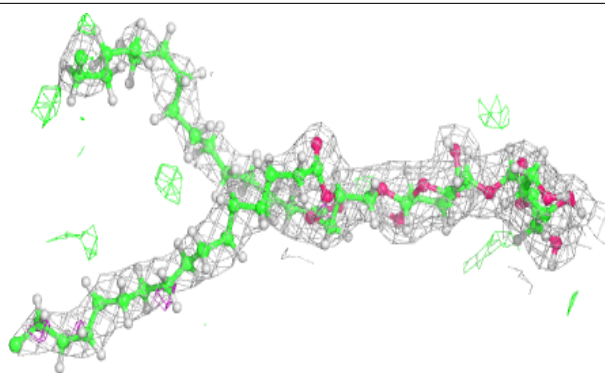
**Electron density around CLA B 609:**

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



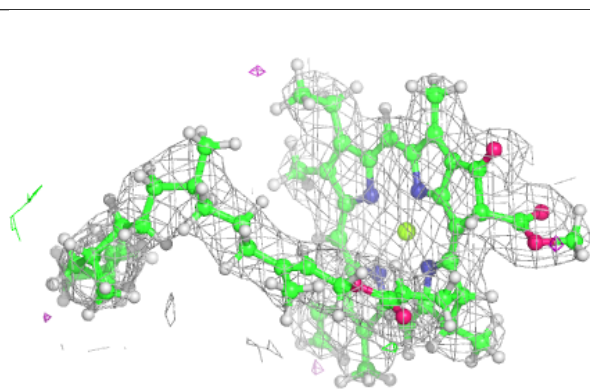
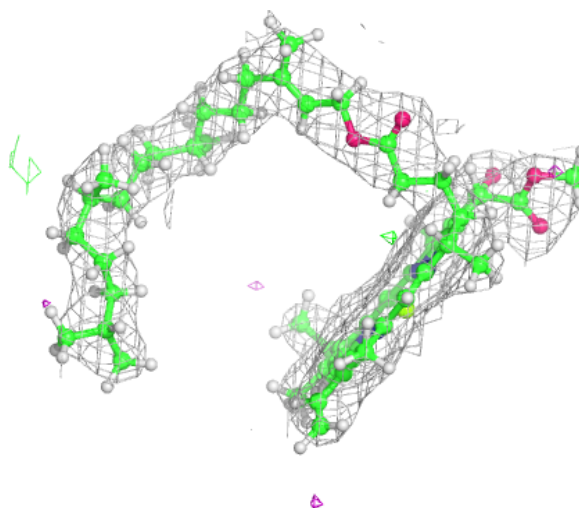
Electron density around DGD C 517:

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



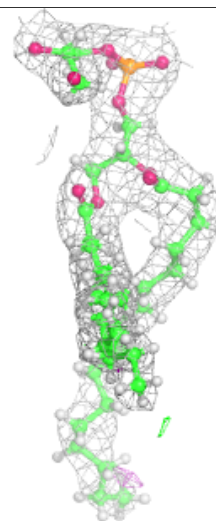
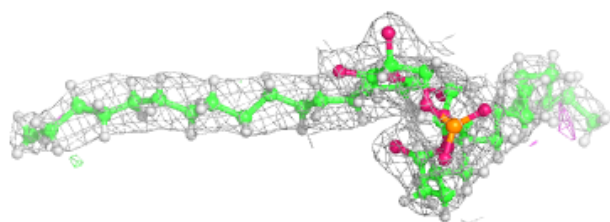
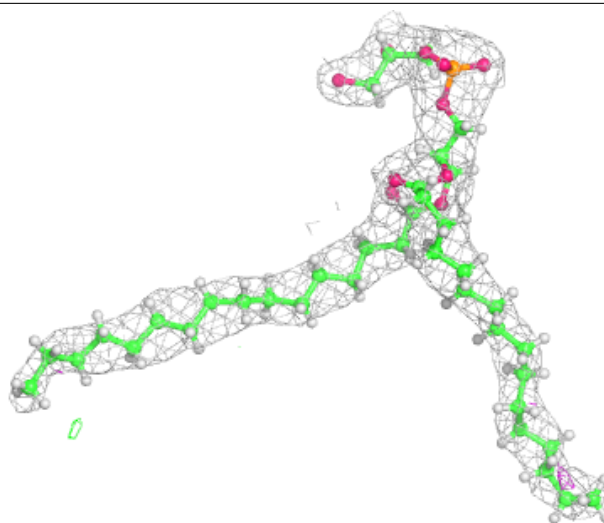
Electron density around CLA b 611:

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



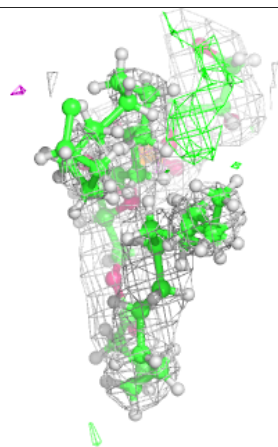
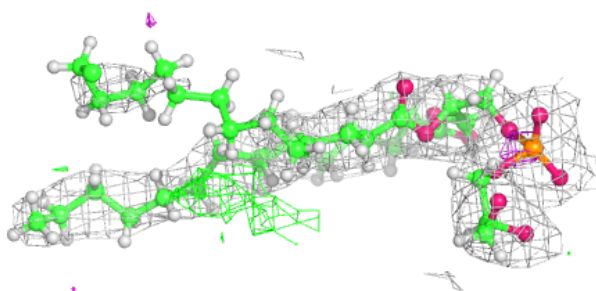
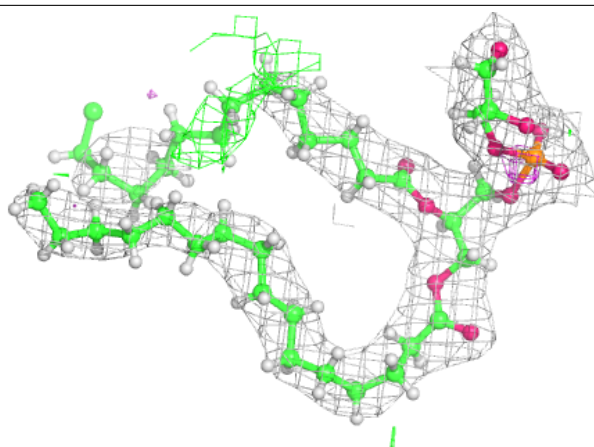
Electron density around LHG 1 101:

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



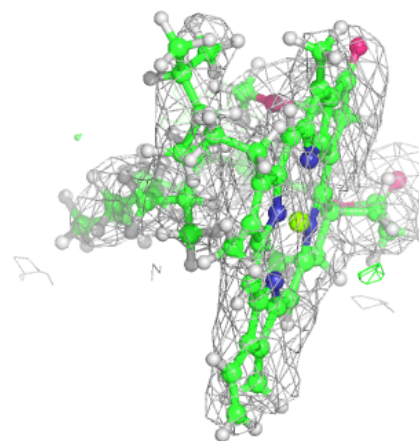
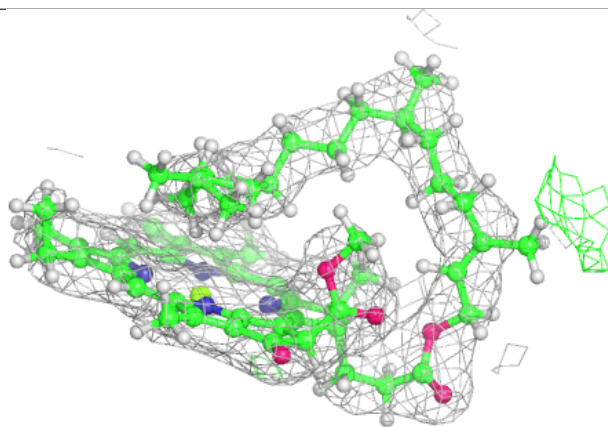
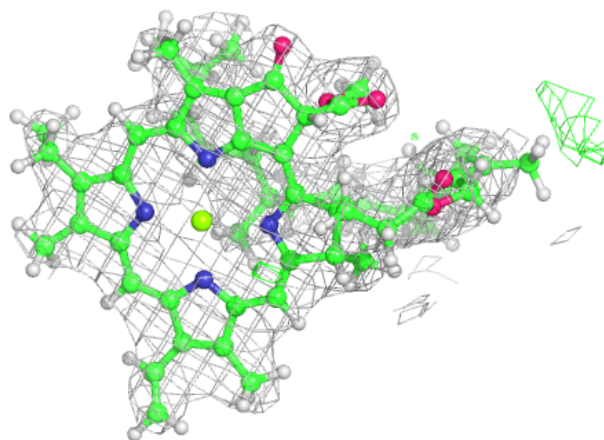
Electron density around LHG A 410:

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



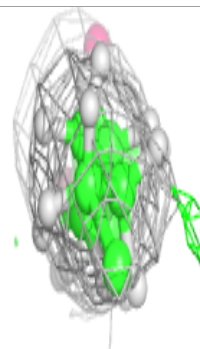
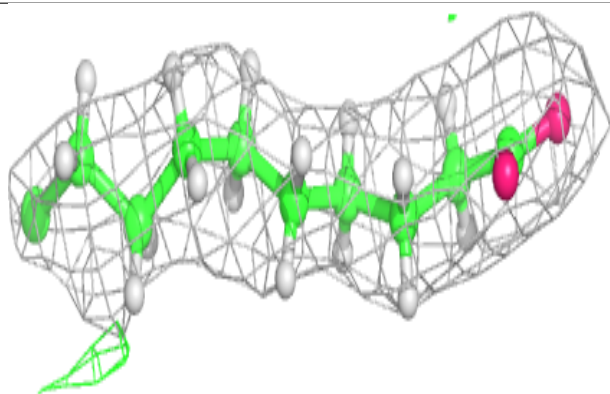
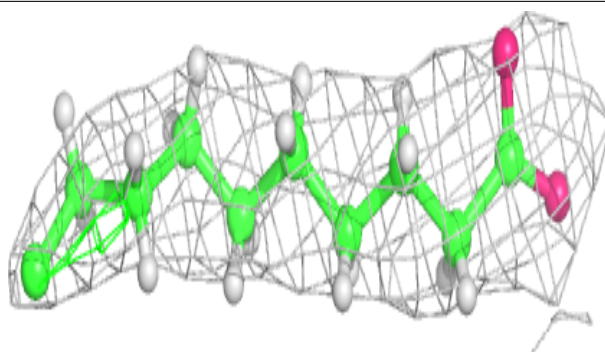
Electron density around CLA c 511:

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

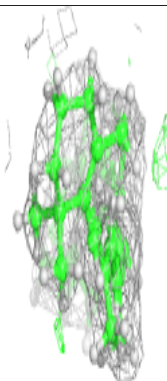
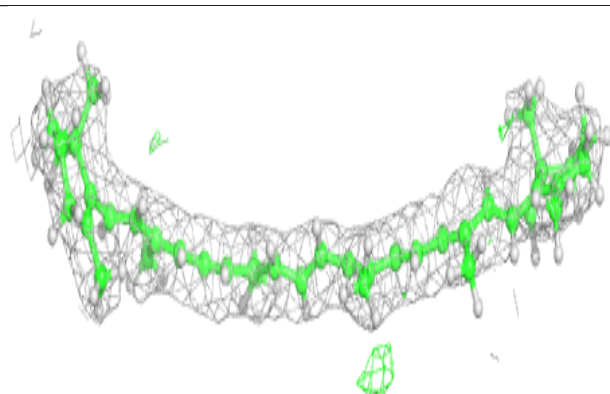
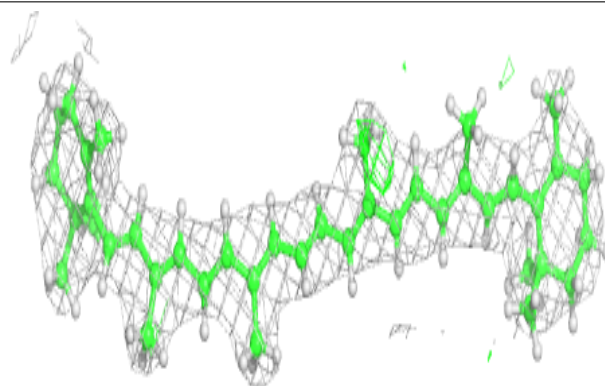


Electron density around STE J 101:

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

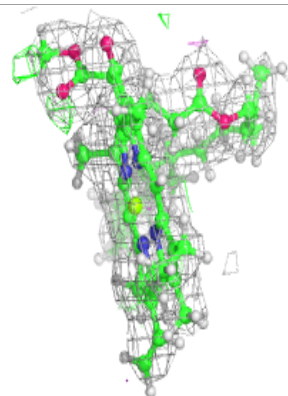
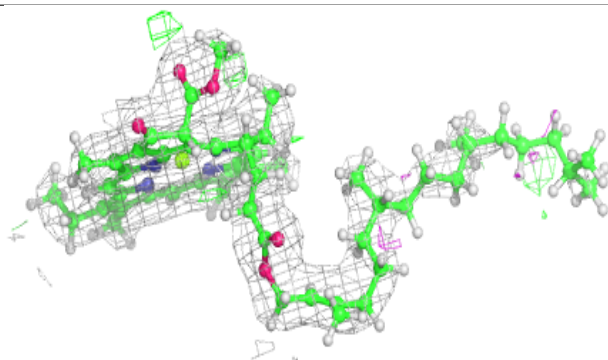
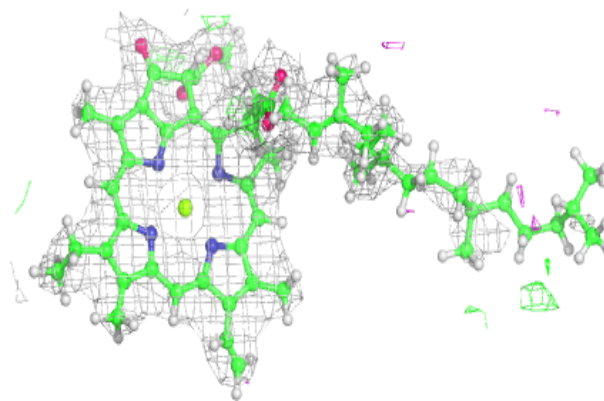
**Electron density around BCR T 101:**

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

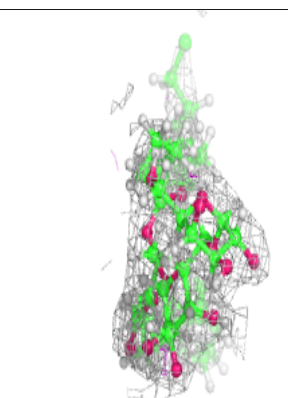
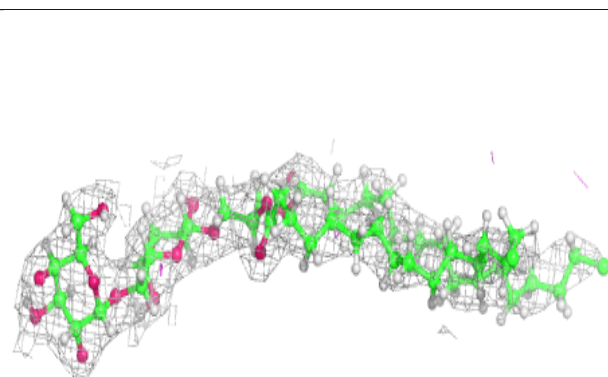
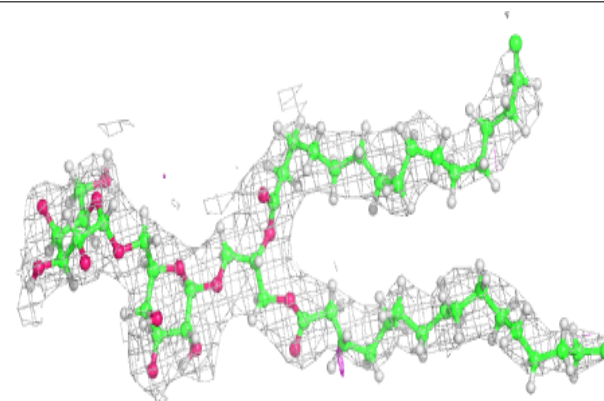


Electron density around CLA A 403:

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

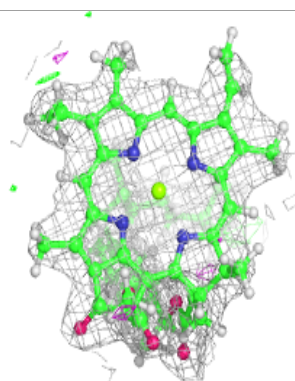
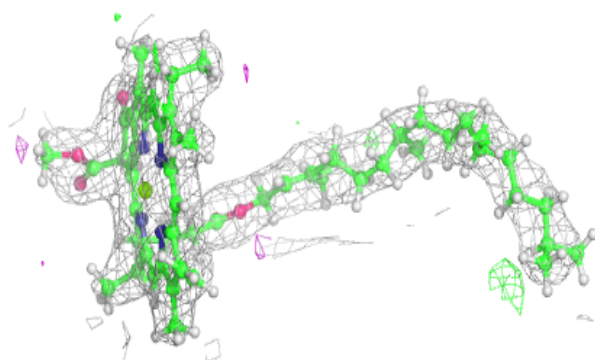
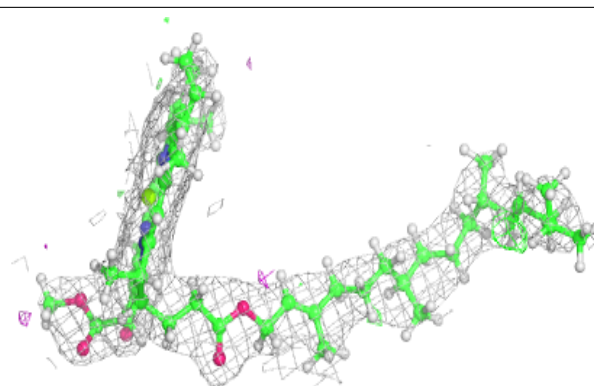
**Electron density around DGD C 519:**

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

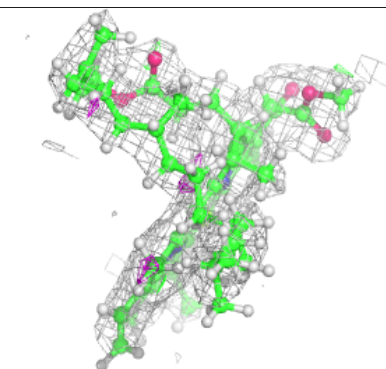
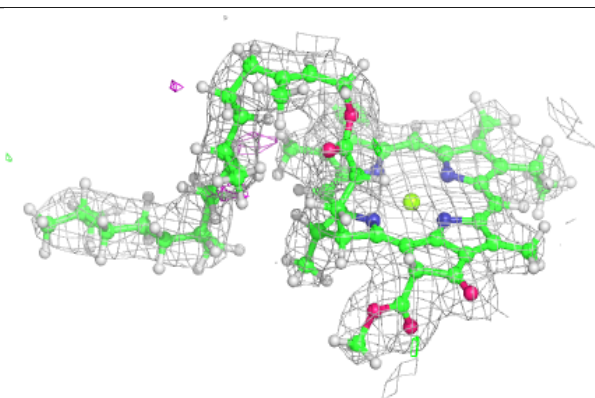
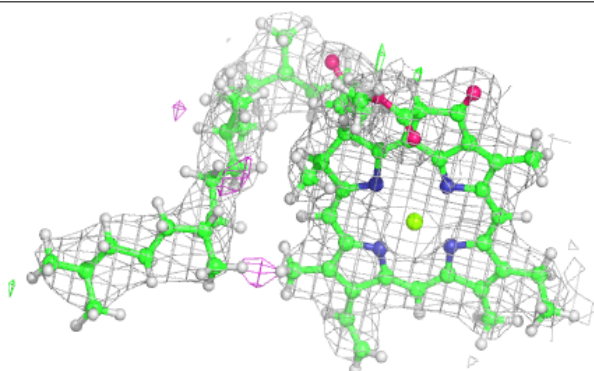


Electron density around CLA b 605:

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

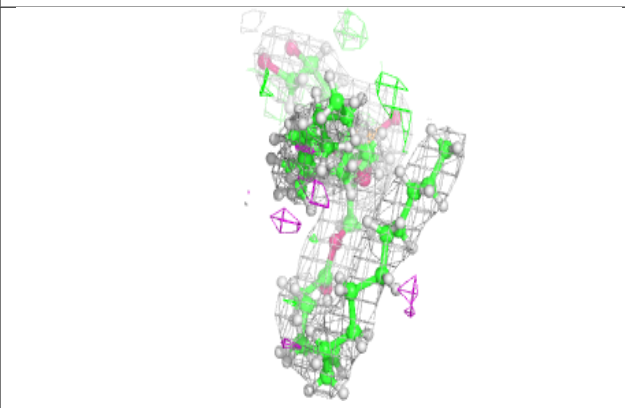
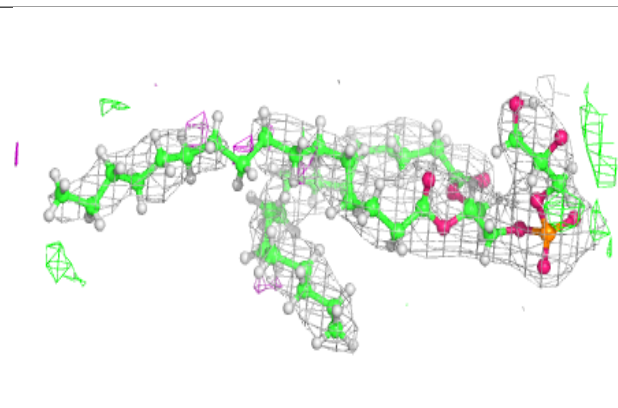
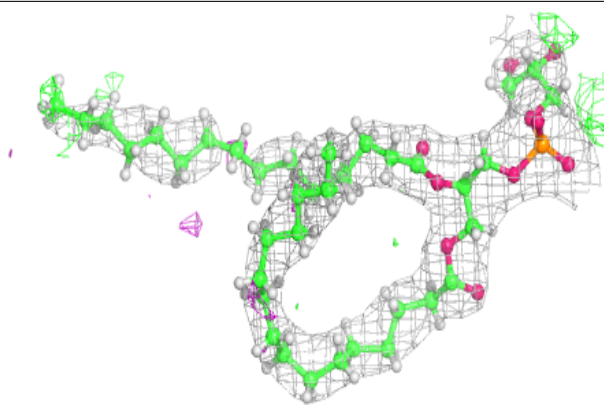
**Electron density around CLA a 411:**

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

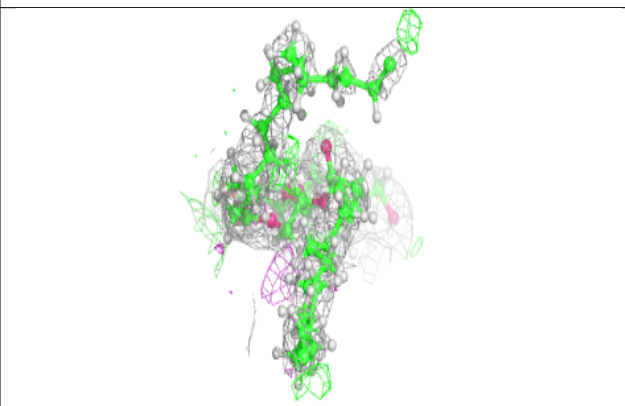
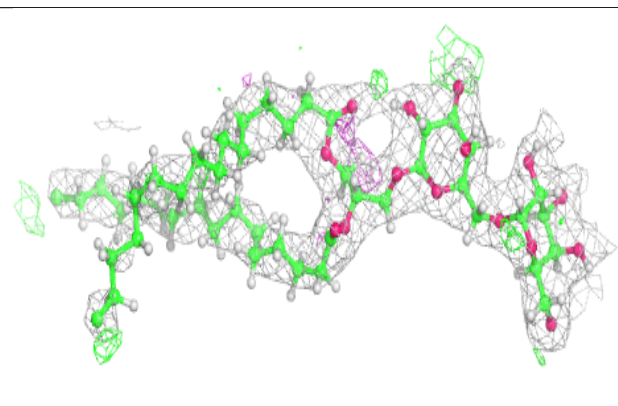
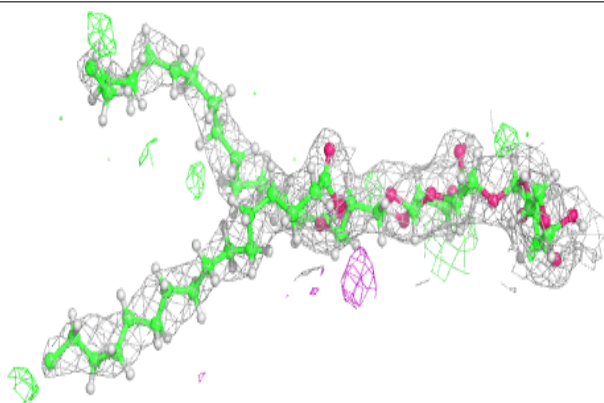


Electron density around LHG a 412:

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

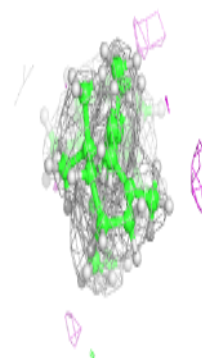
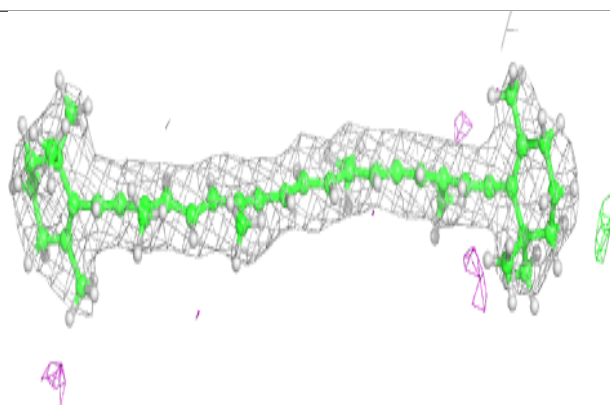
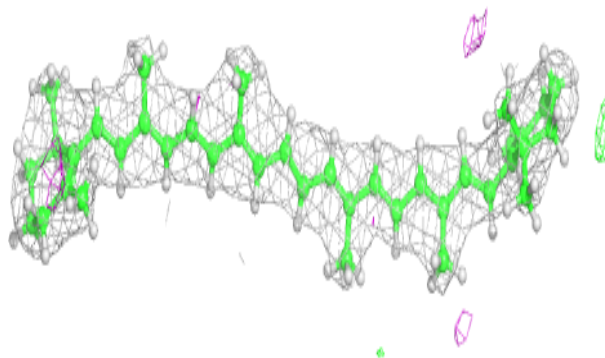
**Electron density around DGD c 517:**

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



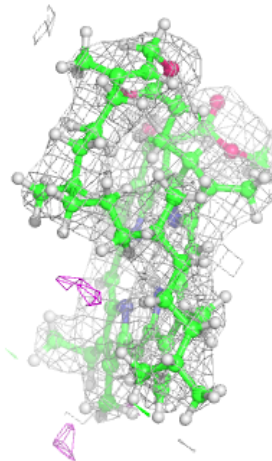
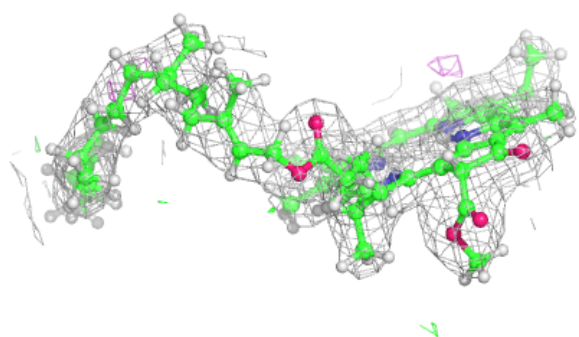
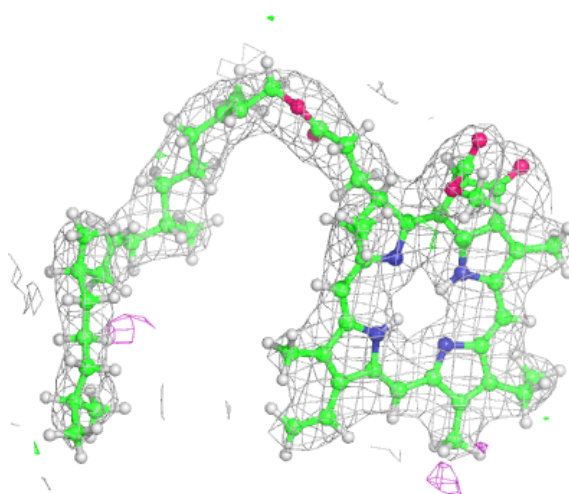
Electron density around BCR a 406:

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



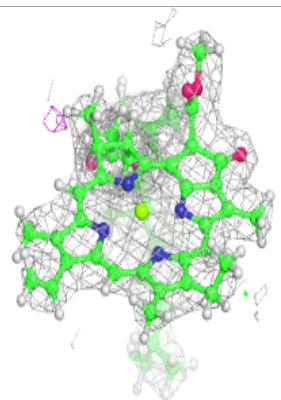
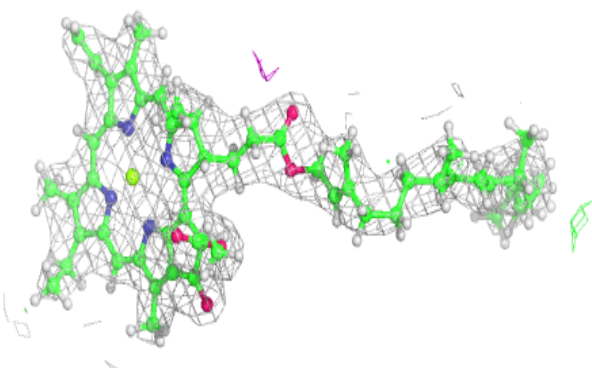
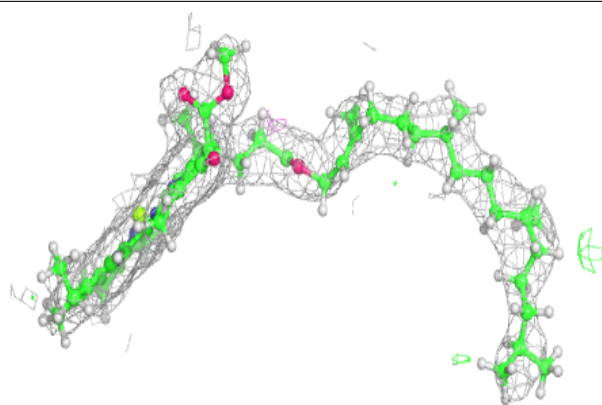
Electron density around PHO d 401:

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

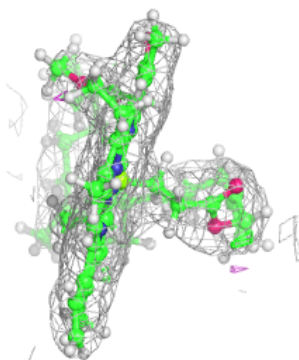
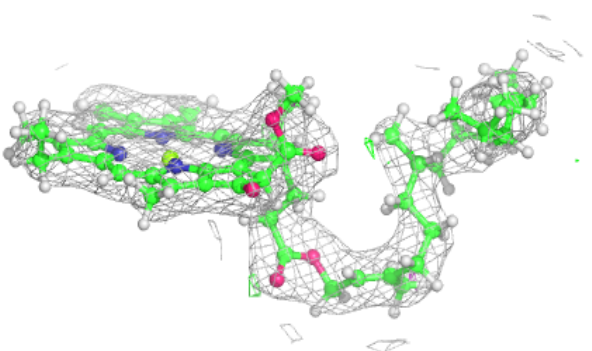
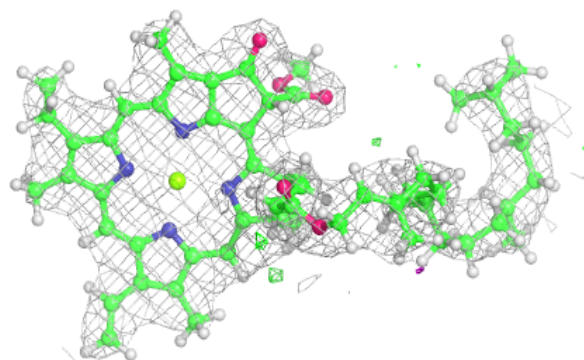


Electron density around CLA d 402:

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

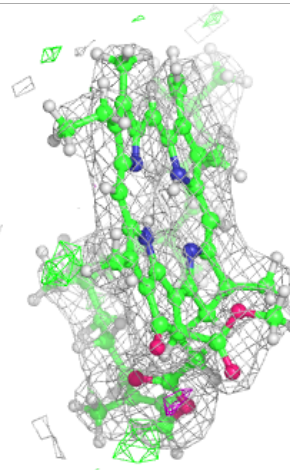
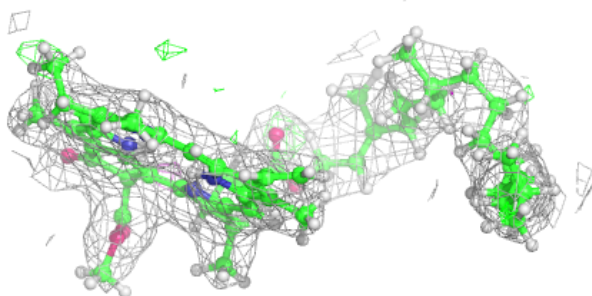
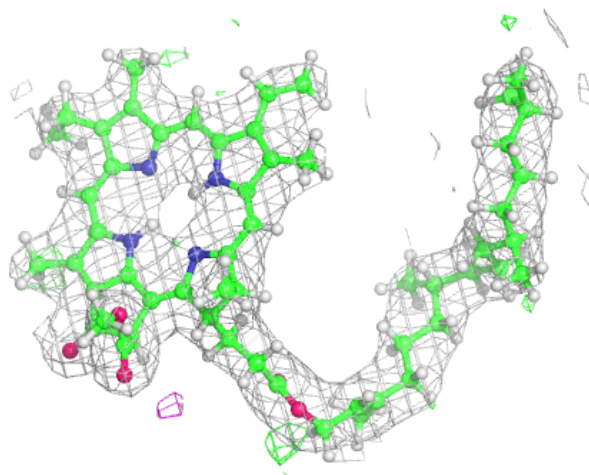
**Electron density around CLA b 612:**

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



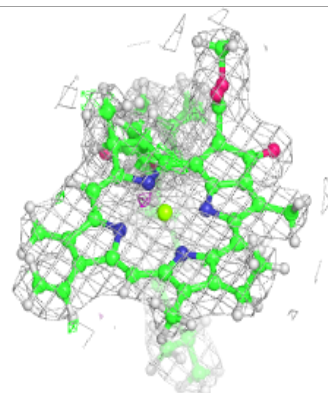
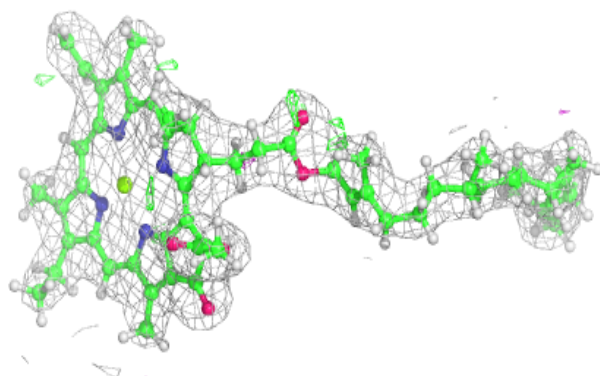
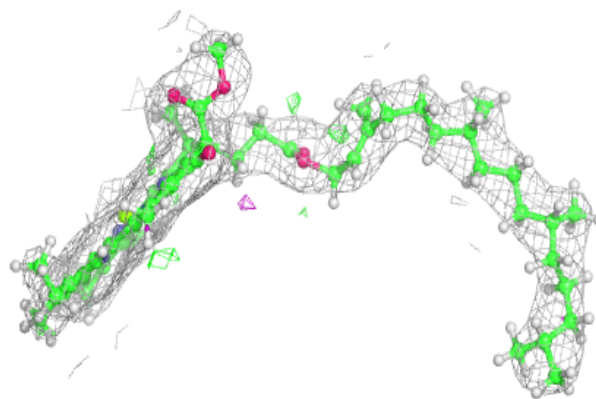
Electron density around PHO D 402:

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

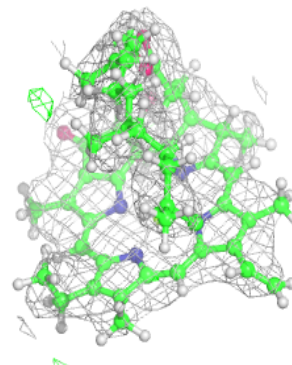
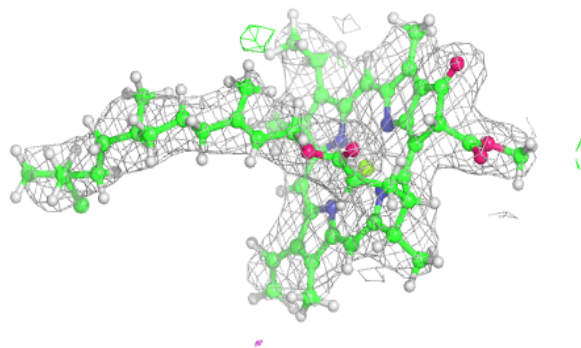
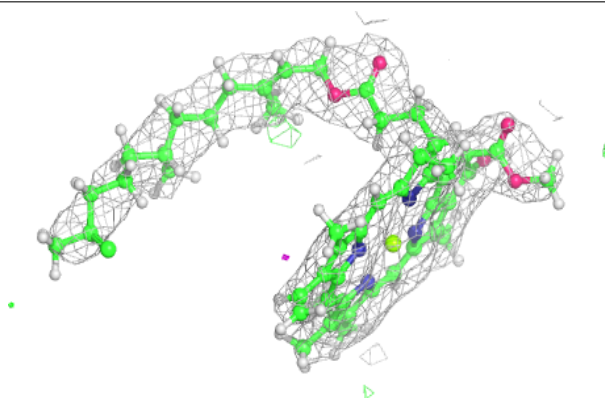


Electron density around CLA D 404:

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

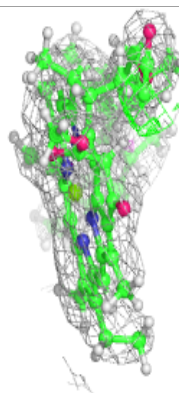
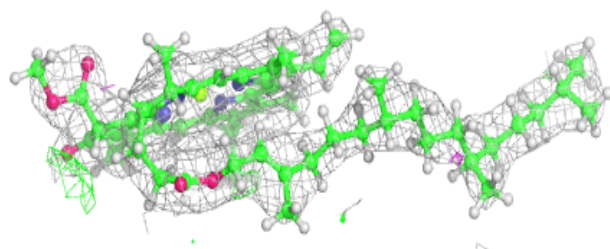
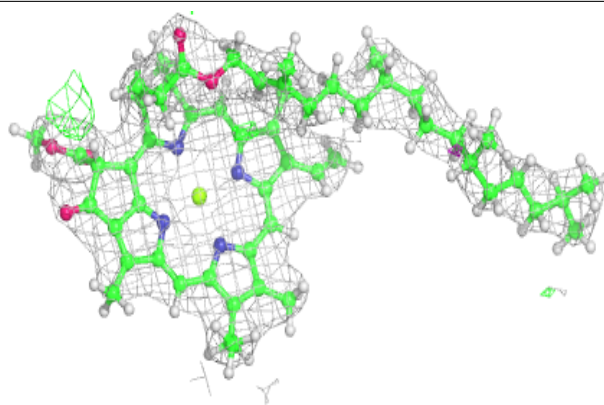
**Electron density around CLA c 505:**

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

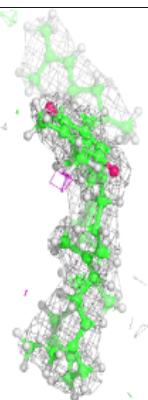
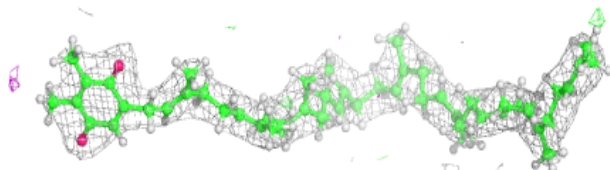
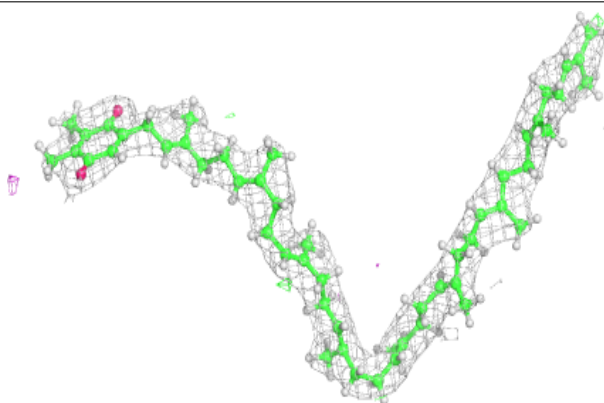


Electron density around CLA c 502:

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

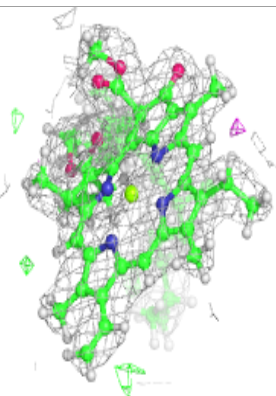
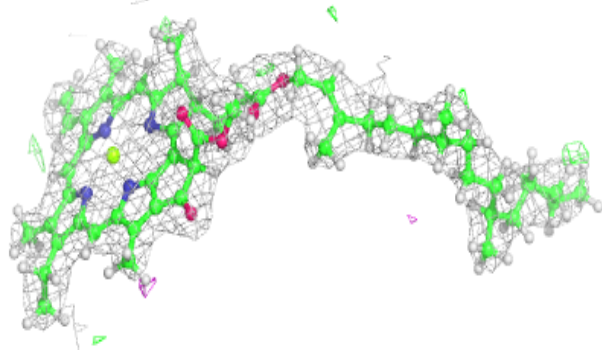
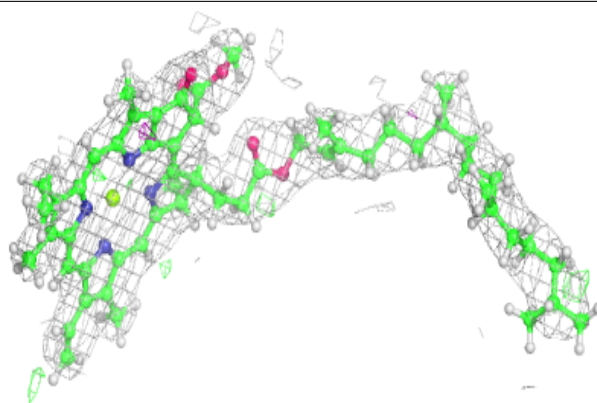
**Electron density around PL9 d 405:**

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

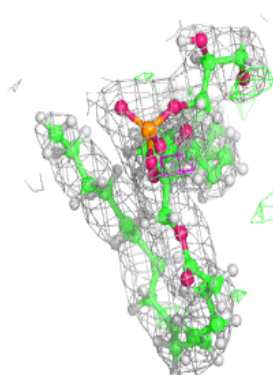
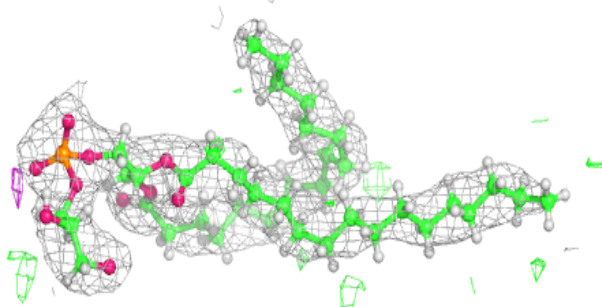
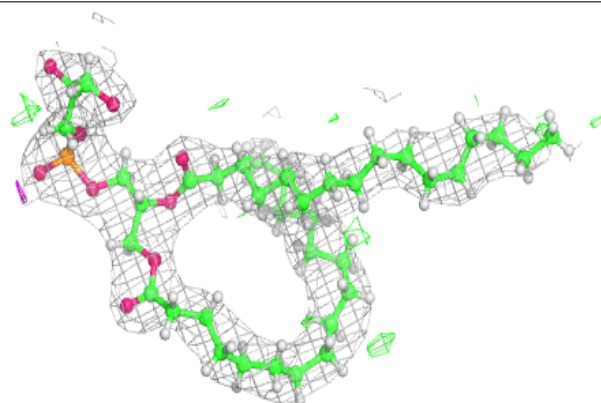


Electron density around CLA A 402:

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

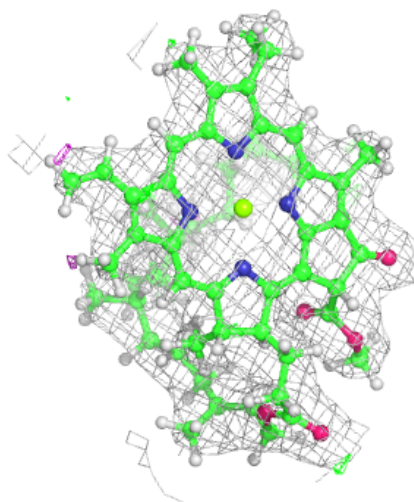
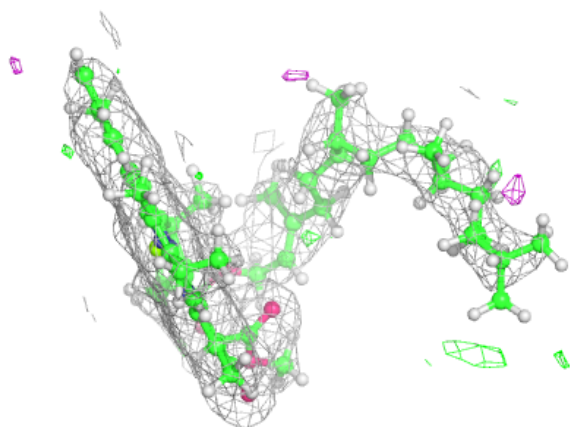
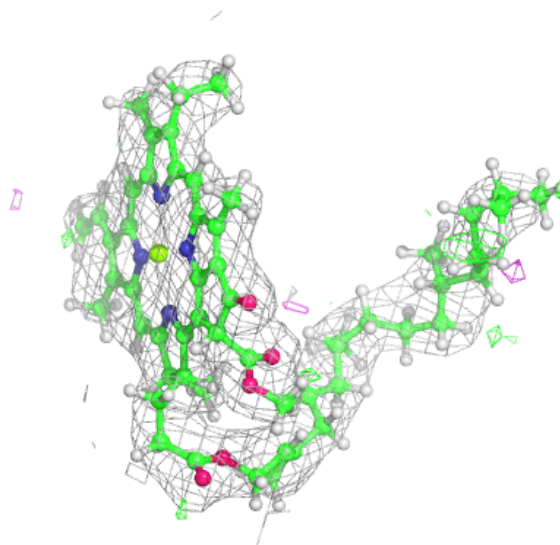
**Electron density around LHG D 412:**

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



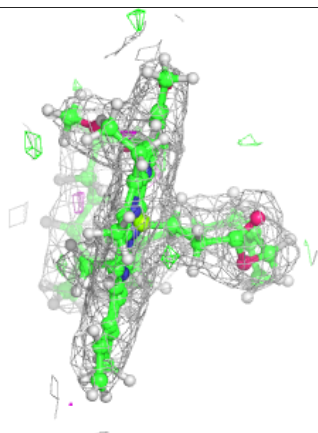
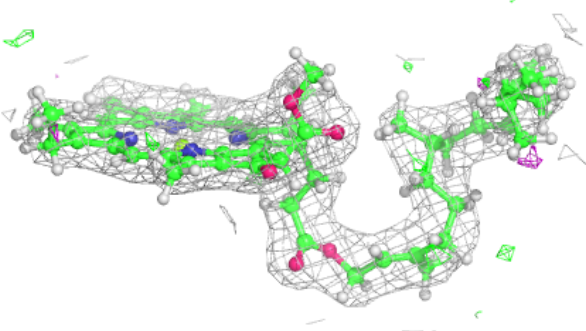
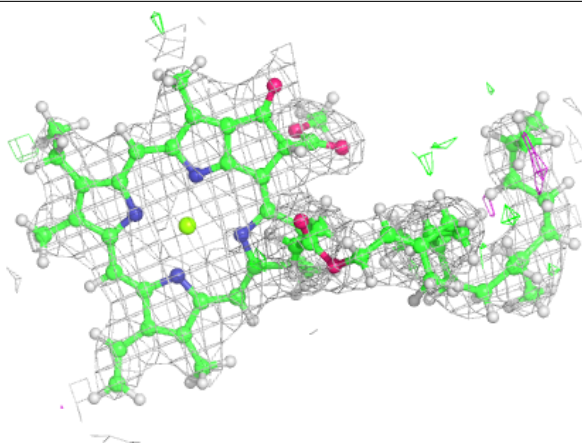
Electron density around CLA B 613:

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



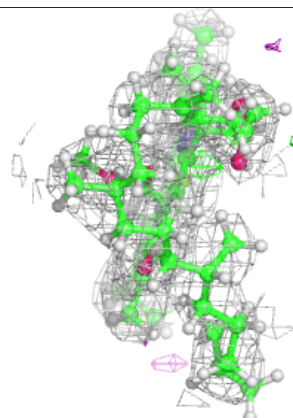
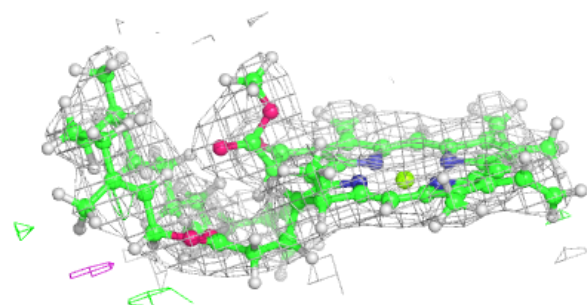
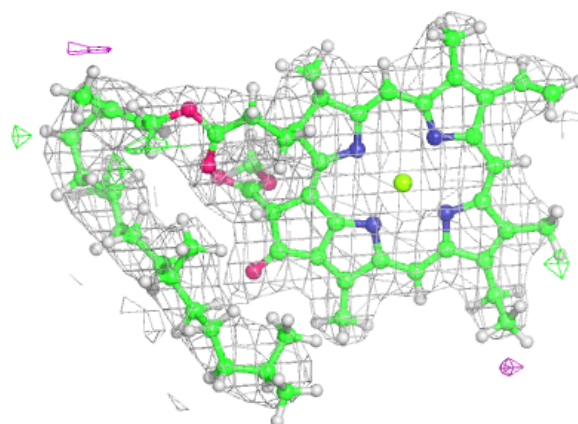
Electron density around CLA B 612:

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

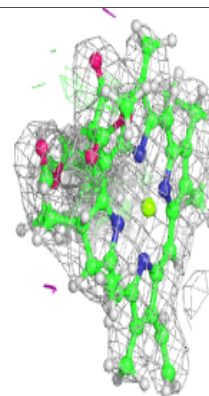
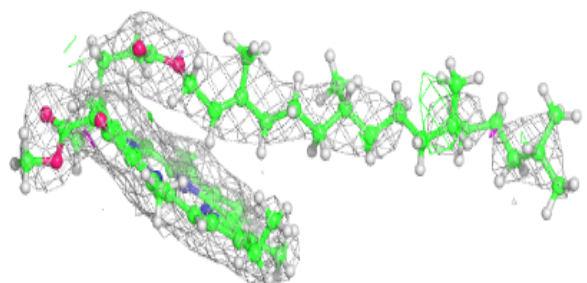
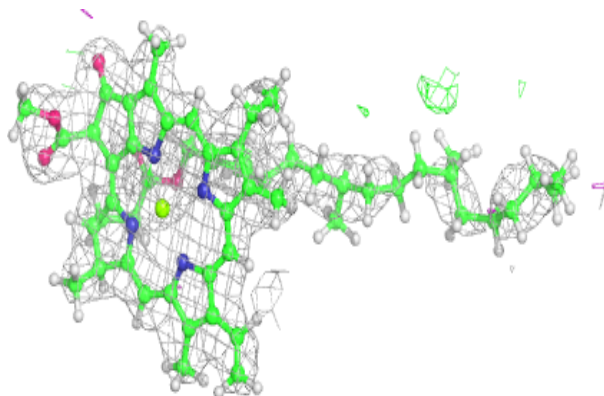


Electron density around CLA B 610:

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

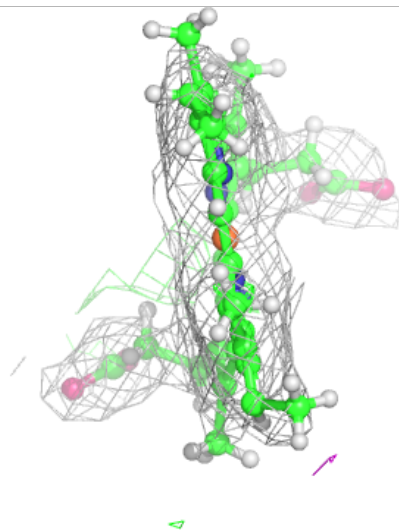
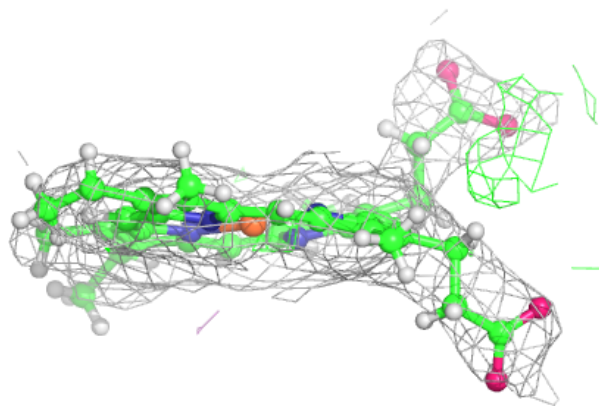
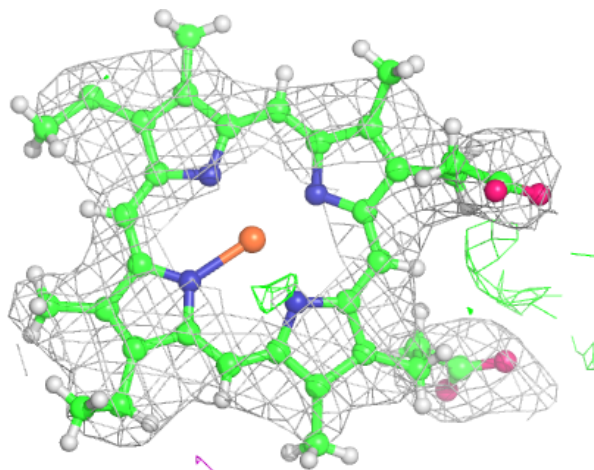
**Electron density around CLA B 614:**

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



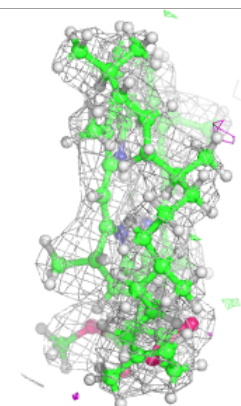
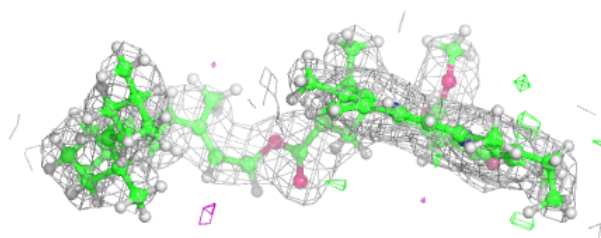
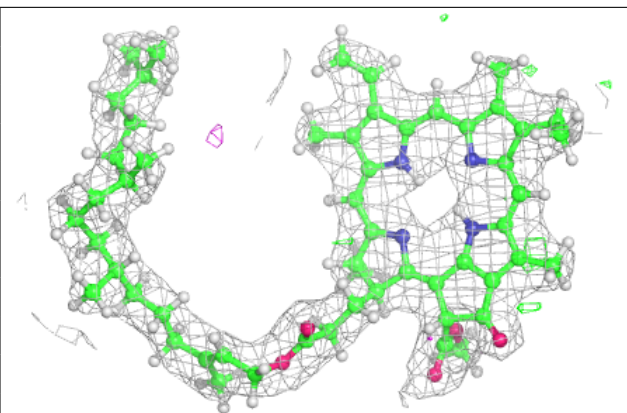
Electron density around HEC f 101:

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

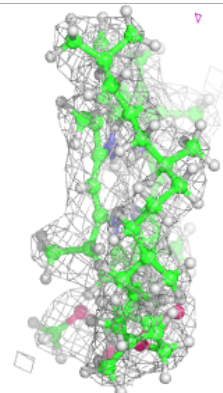
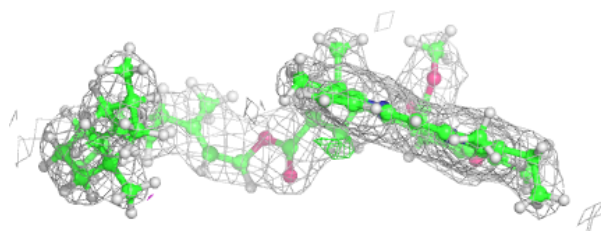
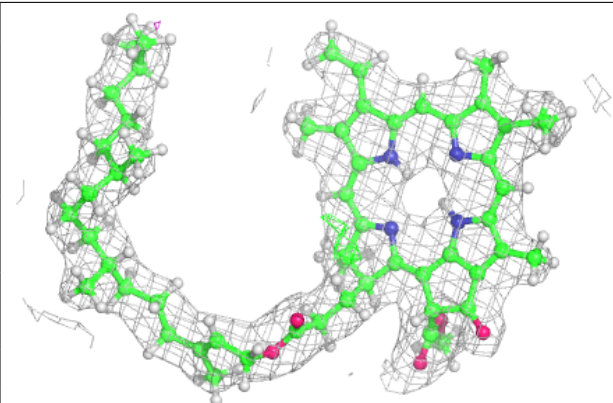


Electron density around PHO D 401:

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

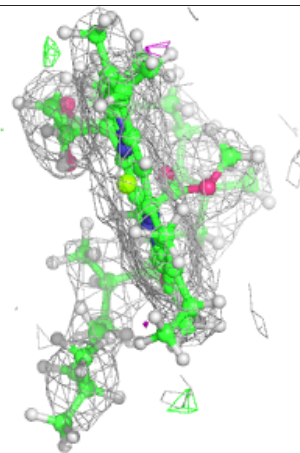
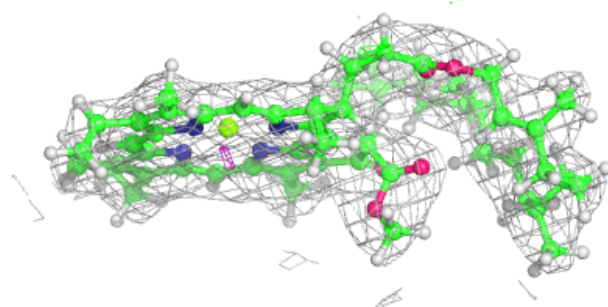
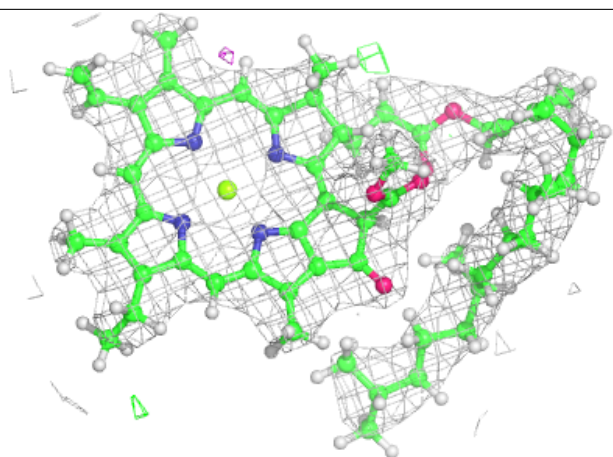
**Electron density around PHO a 404:**

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



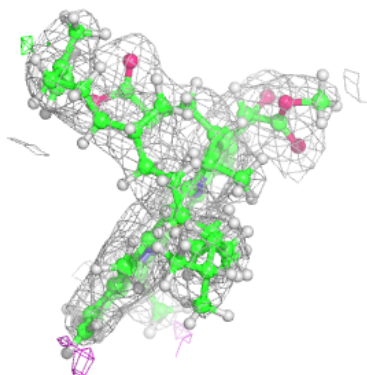
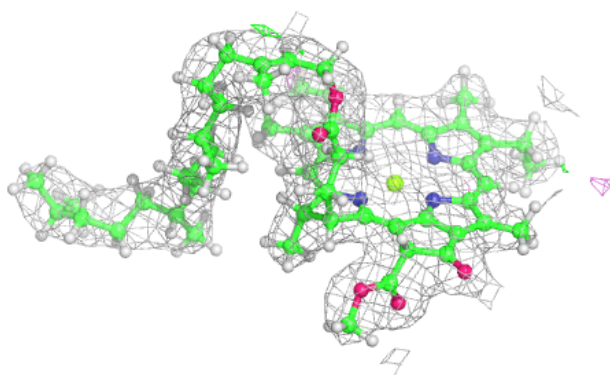
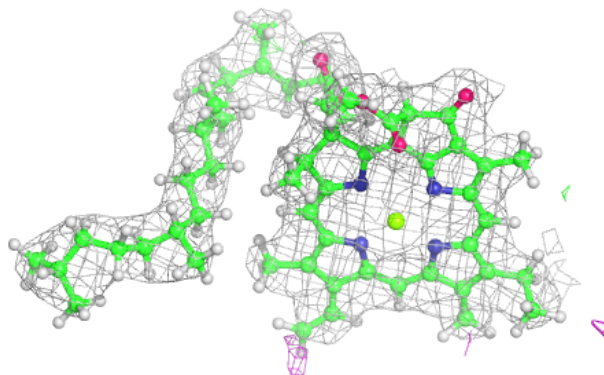
Electron density around CLA b 610:

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

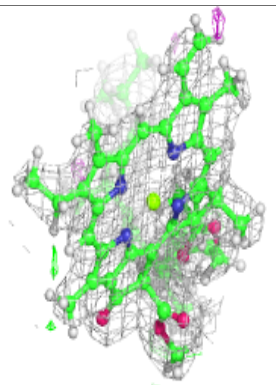
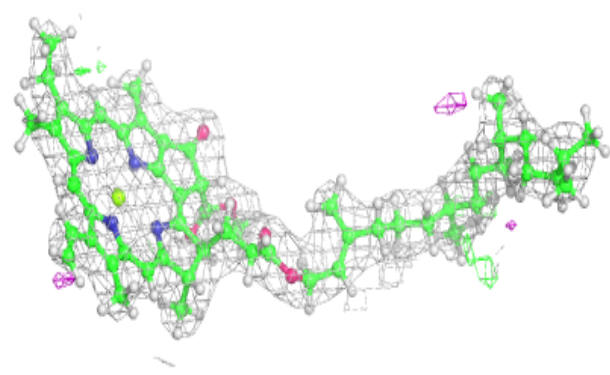
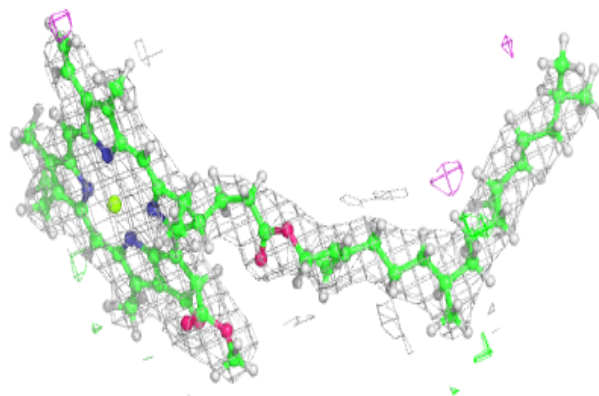


Electron density around CLA A 409:

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

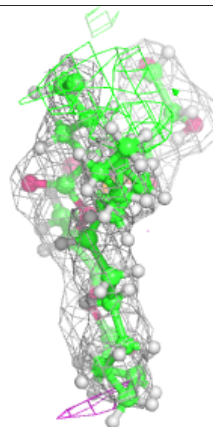
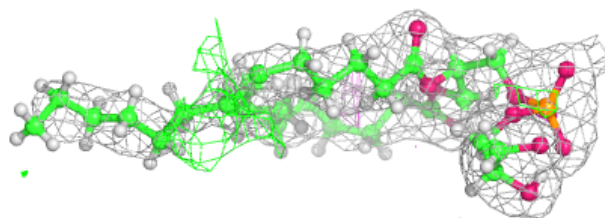
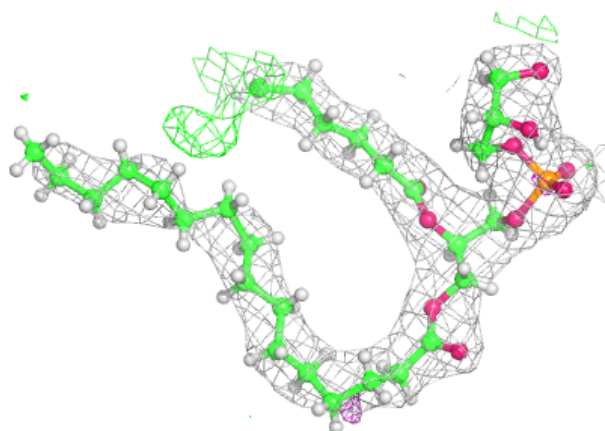
**Electron density around CLA a 402:**

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

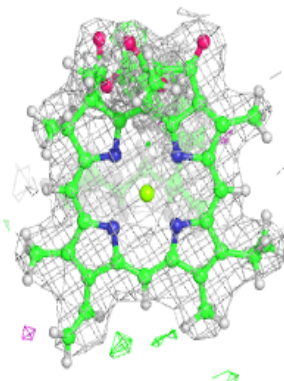
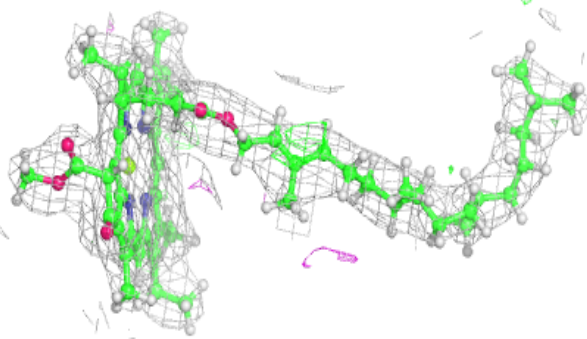
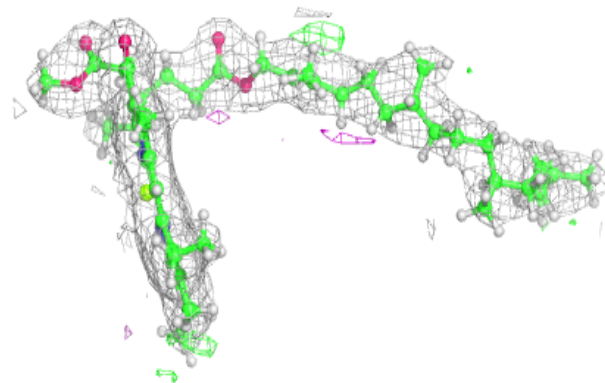


Electron density around LHG d 407:

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

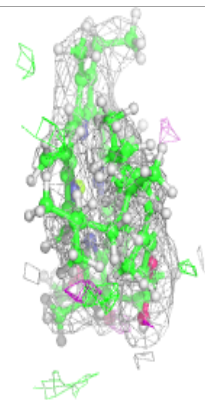
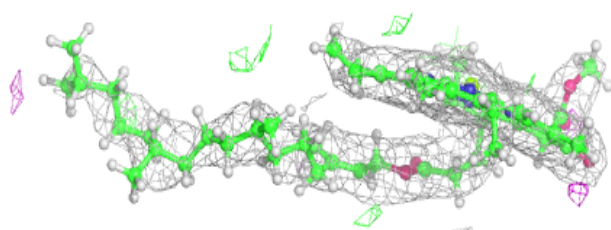
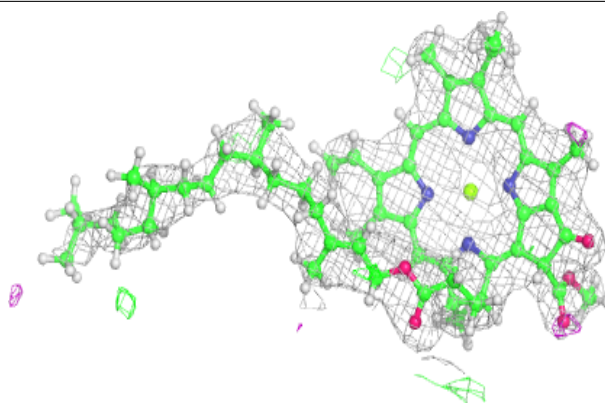
**Electron density around CLA B 605:**

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

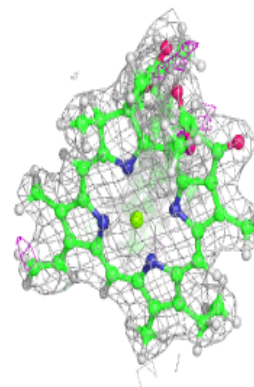
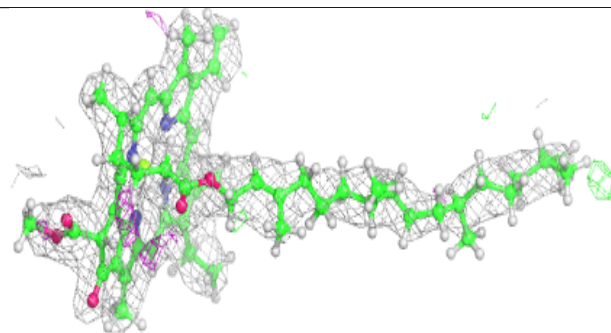
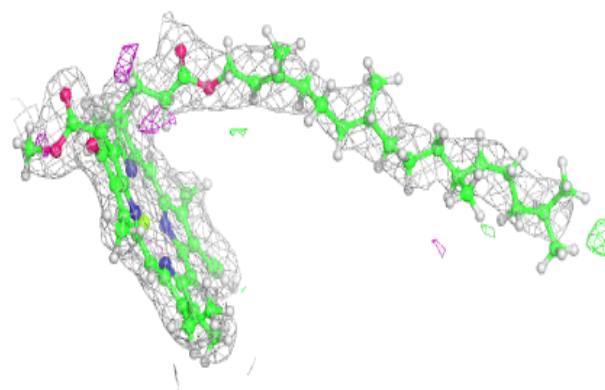


Electron density around CLA b 603:

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

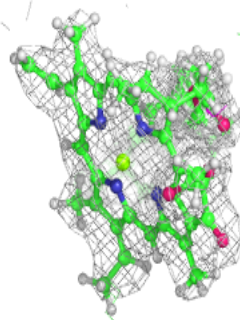
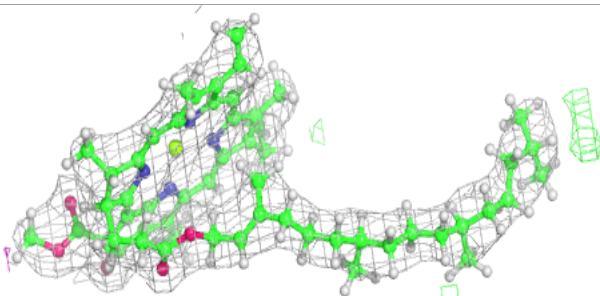
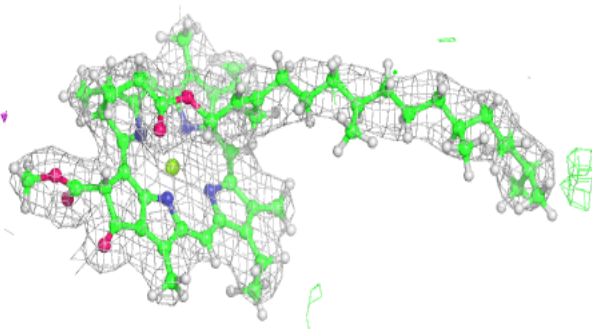
**Electron density around CLA B 607:**

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

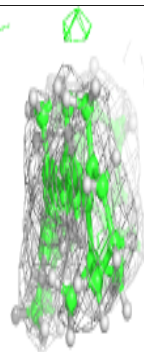
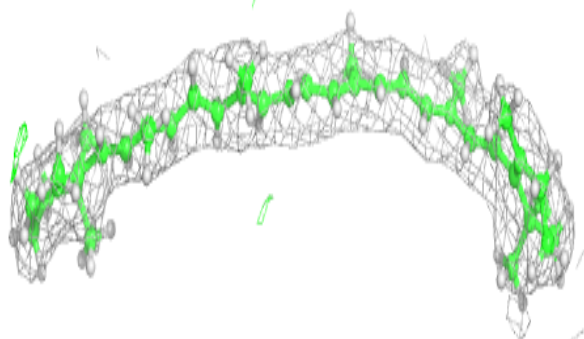
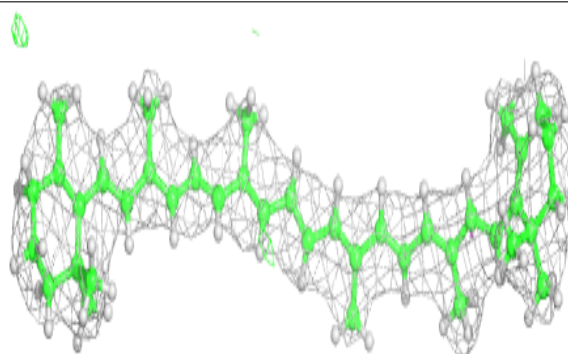


Electron density around CLA B 608:

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

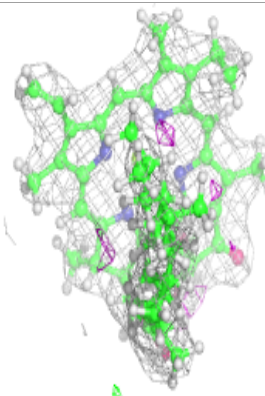
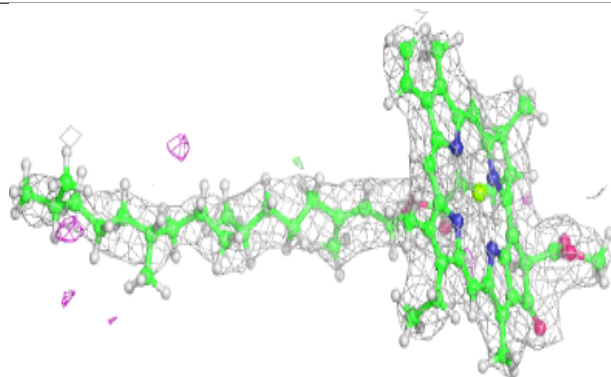
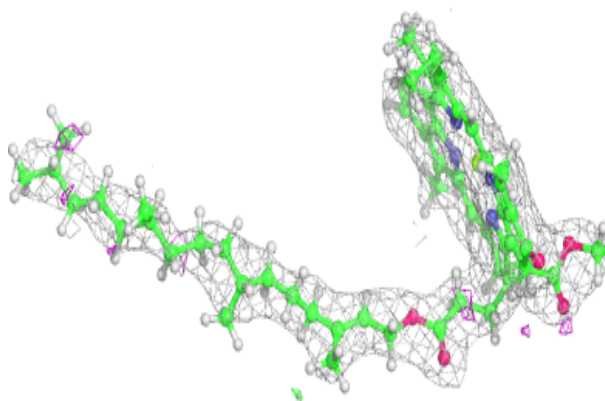
**Electron density around BCR t 101:**

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



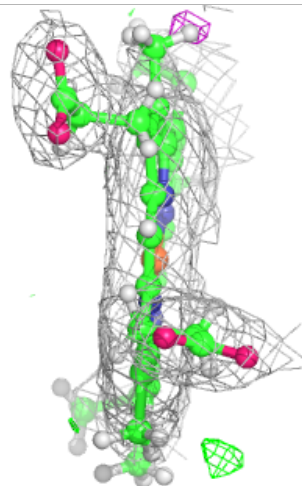
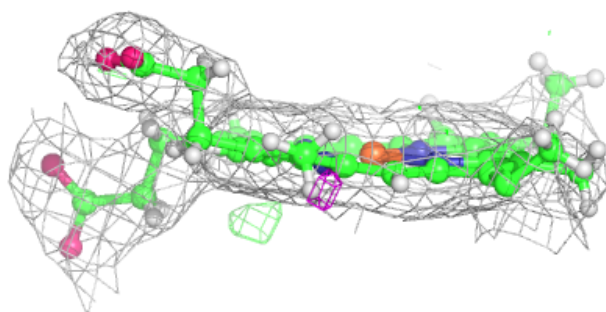
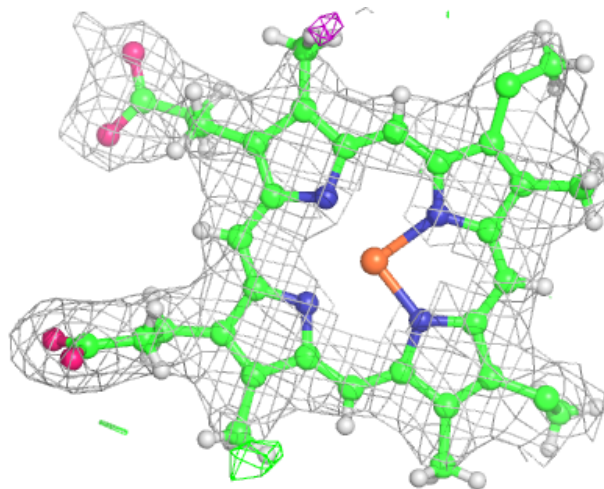
Electron density around CLA b 607:

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



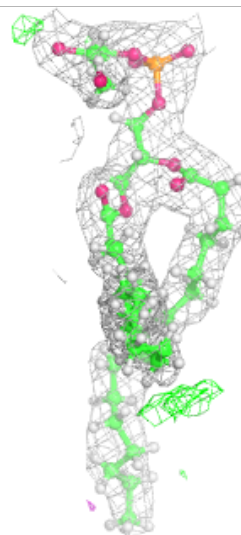
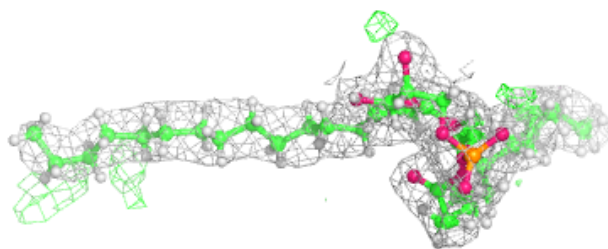
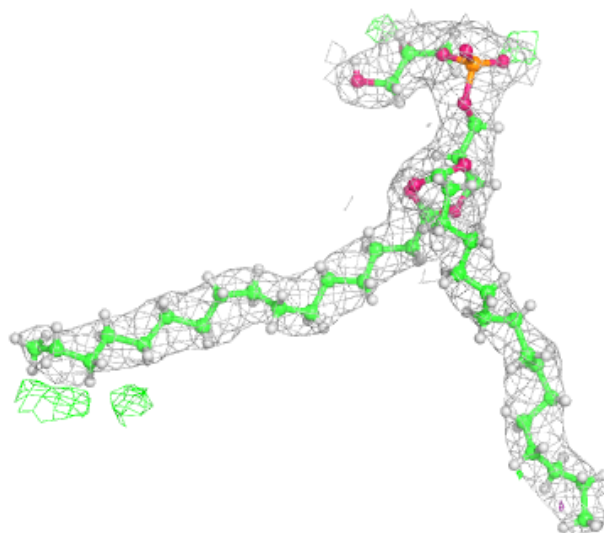
Electron density around HEC v 201:

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



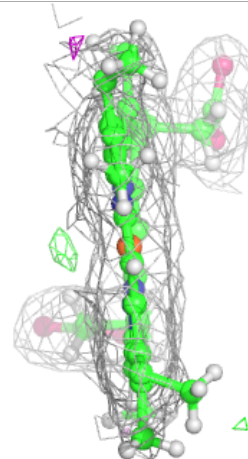
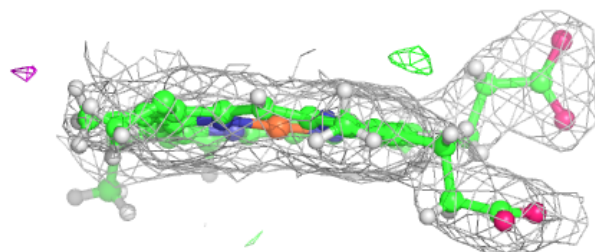
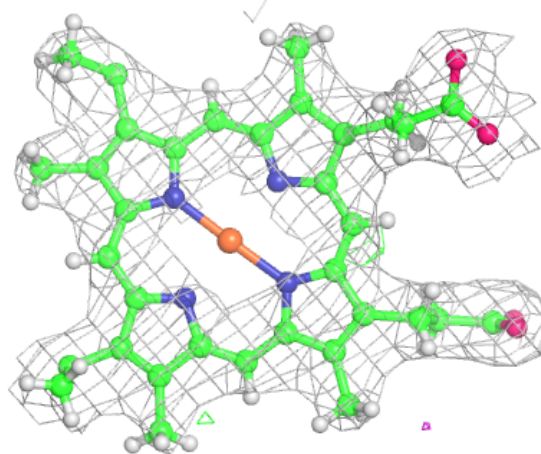
Electron density around LHG L 102:

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



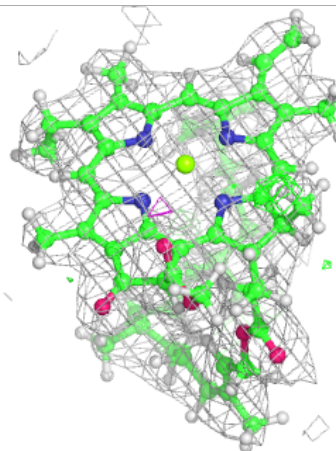
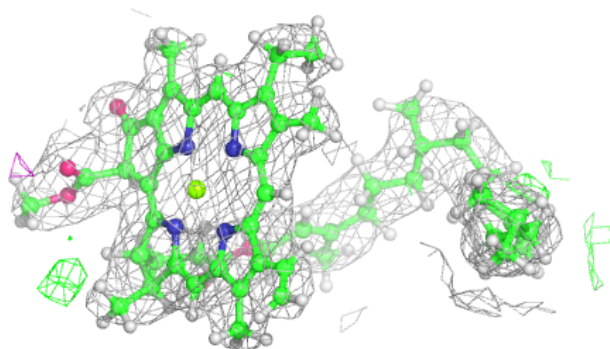
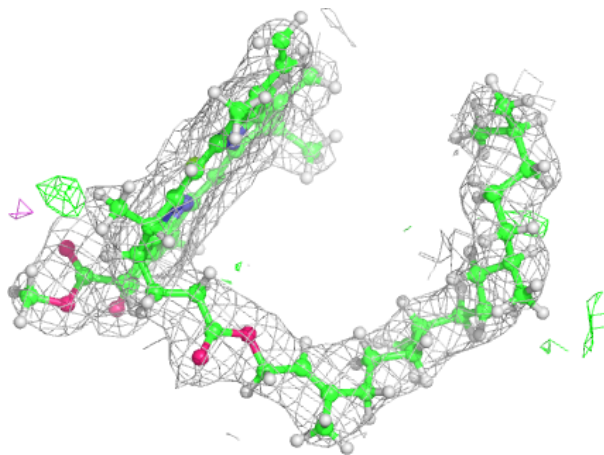
Electron density around HEC V 201:

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



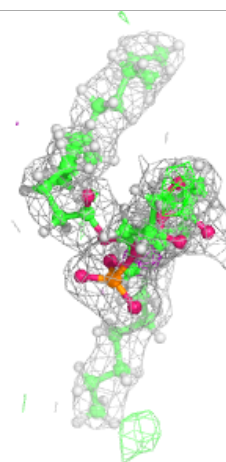
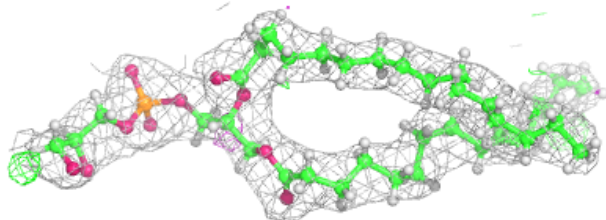
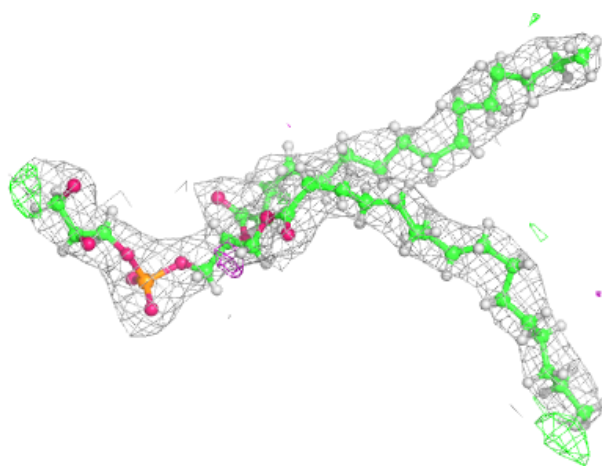
Electron density around CLA B 611:

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



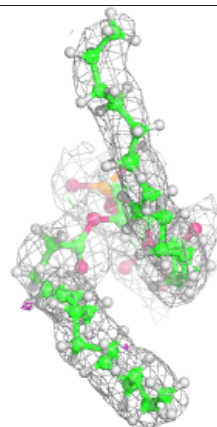
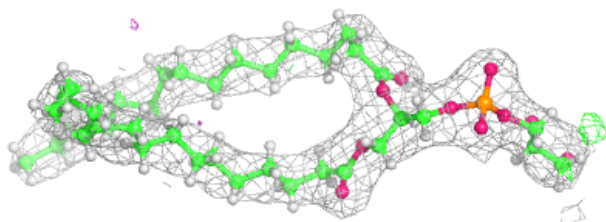
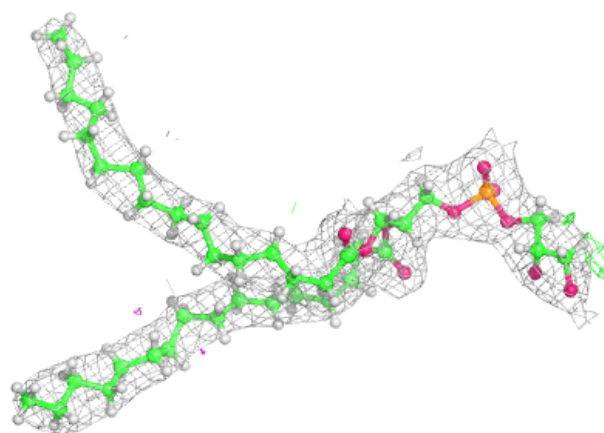
Electron density around LHG D 409:

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



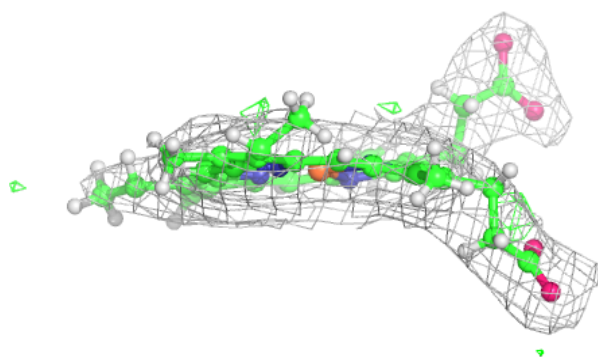
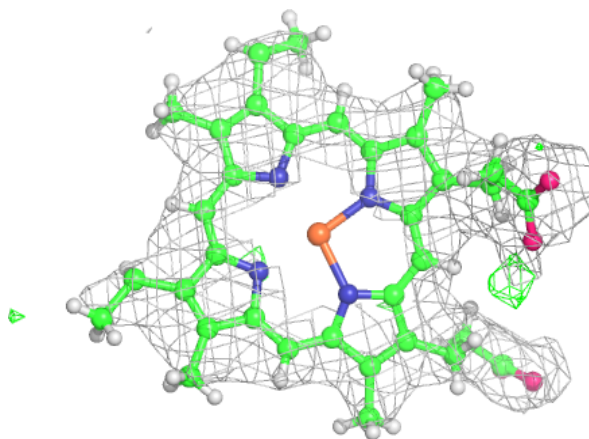
Electron density around LHG d 406:

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.