



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2024 – 03:11 PM JST

PDB ID : 8IR7
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-nanosecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

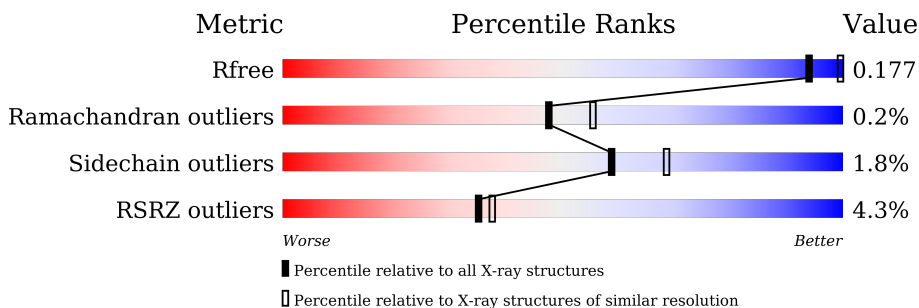
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



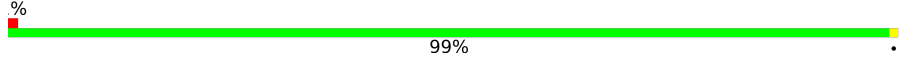
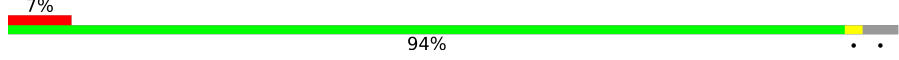
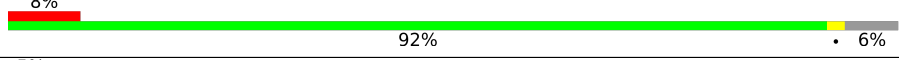


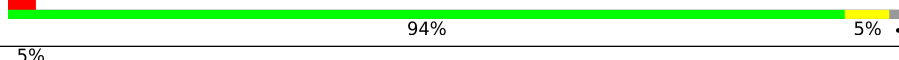
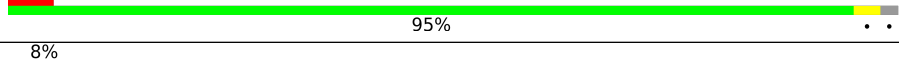
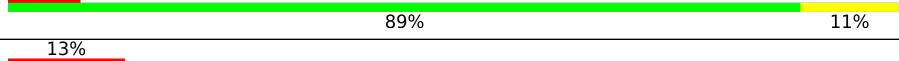
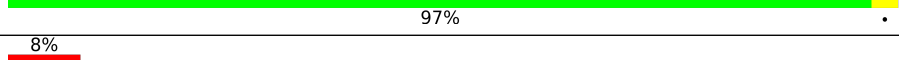
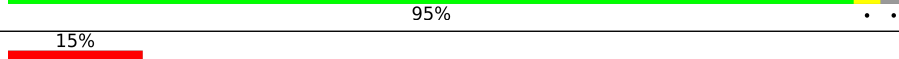
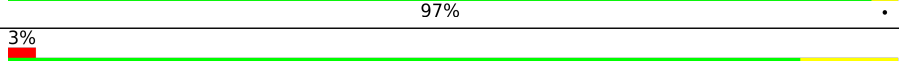
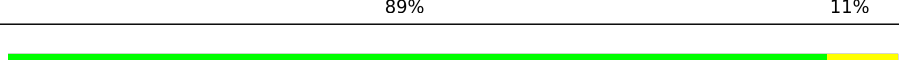
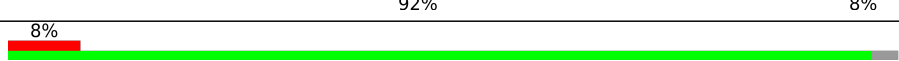
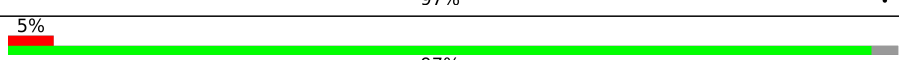
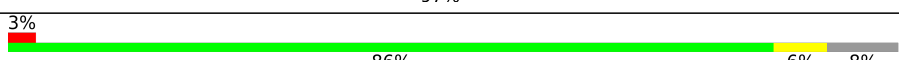
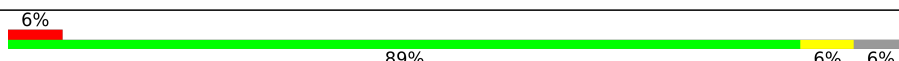
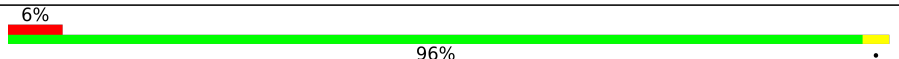
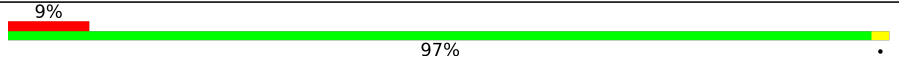

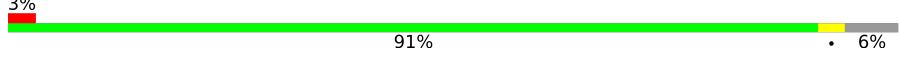
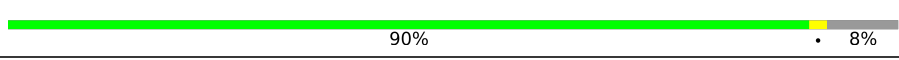
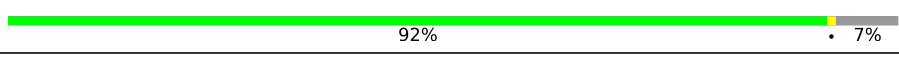
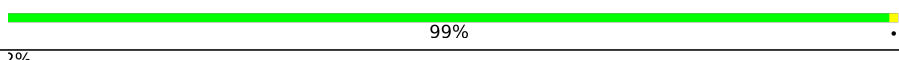
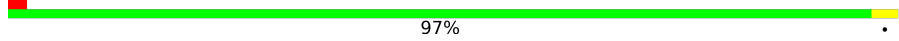

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1377 (2.26-2.26) |
| Ramachandran outliers | 138981 | 1449 (2.26-2.26) |
| Sidechain outliers | 138945 | 1450 (2.26-2.26) |
| RSRZ outliers | 127900 | 1356 (2.26-2.26) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 344 | 97% |
| 1 | a | 344 | 97% |
| 2 | B | 505 | 99% |
| 2 | b | 505 | 99% |
| 3 | C | 455 | 98% |
| 3 | c | 455 | 99% |
| 4 | D | 342 | 99% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | d | 342 |  99% |
| 5 | E | 84 |  94% |
| 5 | e | 84 |  92% 6% |
| 6 | F | 44 |  77% 23% |
| 6 | f | 44 |  70% 30% |
| 7 | H | 65 |  94% 5% |
| 7 | h | 65 |  95% |
| 8 | I | 38 |  89% 11% |
| 8 | i | 38 |  97% |
| 9 | J | 39 |  95% |
| 9 | j | 39 |  97% |
| 10 | K | 37 |  89% 11% |
| 10 | k | 37 |  92% 8% |
| 11 | L | 37 |  97% |
| 11 | l | 37 |  97% |
| 12 | M | 36 |  86% 6% 8% |
| 12 | m | 36 |  89% 6% 6% |
| 13 | O | 244 |  96% |
| 13 | o | 244 |  97% |
| 14 | T | 32 |  88% 6% 6% |
| 14 | t | 32 |  91% 6% |
| 15 | U | 104 |  90% 8% |
| 15 | u | 104 |  92% 7% |
| 16 | V | 137 |  99% |
| 16 | v | 137 |  97% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 17 | X | 40 | |
| 17 | x | 40 | |
| 18 | Y | 30 | |
| 18 | y | 30 | |
| 19 | Z | 62 | |
| 19 | z | 62 | |
| 20 | R | 34 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23 | CLA | A | 404[A] | X | - | - | - |
| 23 | CLA | A | 404[B] | X | - | - | - |
| 23 | CLA | A | 405[B] | X | - | - | - |
| 23 | CLA | A | 408 | X | - | - | - |
| 23 | CLA | B | 601 | X | - | - | - |
| 23 | CLA | B | 602 | X | - | - | - |
| 23 | CLA | B | 603 | X | - | - | - |
| 23 | CLA | B | 604 | X | - | - | - |
| 23 | CLA | B | 605 | X | - | - | - |
| 23 | CLA | B | 606 | X | - | - | - |
| 23 | CLA | B | 607 | X | - | - | - |
| 23 | CLA | B | 609 | X | - | - | - |
| 23 | CLA | B | 610 | X | - | - | - |
| 23 | CLA | B | 611 | X | - | - | - |
| 23 | CLA | B | 612 | X | - | - | - |
| 23 | CLA | B | 613 | X | - | - | - |
| 23 | CLA | B | 614 | X | - | - | - |
| 23 | CLA | B | 615 | X | - | - | - |
| 23 | CLA | B | 616 | X | - | - | - |
| 23 | CLA | C | 501 | X | - | - | - |
| 23 | CLA | C | 502 | X | - | - | - |
| 23 | CLA | C | 503 | X | - | - | - |
| 23 | CLA | C | 504 | X | - | - | - |
| 23 | CLA | C | 505 | X | - | - | - |
| 23 | CLA | C | 506 | X | - | - | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23 | CLA | C | 507 | X | - | - | - |
| 23 | CLA | C | 509 | X | - | - | - |
| 23 | CLA | C | 510 | X | - | - | - |
| 23 | CLA | C | 511 | X | - | - | - |
| 23 | CLA | C | 512 | X | - | - | - |
| 23 | CLA | C | 513 | X | - | - | - |
| 23 | CLA | D | 403[A] | X | - | - | - |
| 23 | CLA | D | 403[B] | X | - | - | - |
| 23 | CLA | D | 404 | X | - | - | - |
| 23 | CLA | a | 404[A] | X | - | - | - |
| 23 | CLA | a | 404[B] | X | - | - | - |
| 23 | CLA | a | 407 | X | - | - | - |
| 23 | CLA | b | 601 | X | - | - | - |
| 23 | CLA | b | 602 | X | - | - | - |
| 23 | CLA | b | 603 | X | - | - | - |
| 23 | CLA | b | 604 | X | - | - | - |
| 23 | CLA | b | 605 | X | - | - | - |
| 23 | CLA | b | 606 | X | - | - | - |
| 23 | CLA | b | 607 | X | - | - | - |
| 23 | CLA | b | 609 | X | - | - | - |
| 23 | CLA | b | 610 | X | - | - | - |
| 23 | CLA | b | 611 | X | - | - | - |
| 23 | CLA | b | 612 | X | - | - | - |
| 23 | CLA | b | 613 | X | - | - | - |
| 23 | CLA | b | 614 | X | - | - | - |
| 23 | CLA | b | 615 | X | - | - | - |
| 23 | CLA | b | 616 | X | - | - | - |
| 23 | CLA | c | 502 | X | - | - | - |
| 23 | CLA | c | 503 | X | - | - | - |
| 23 | CLA | c | 504 | X | - | - | - |
| 23 | CLA | c | 505 | X | - | - | - |
| 23 | CLA | c | 506 | X | - | - | - |
| 23 | CLA | c | 507 | X | - | - | - |
| 23 | CLA | c | 508 | X | - | - | - |
| 23 | CLA | c | 509 | X | - | - | - |
| 23 | CLA | c | 510 | X | - | - | - |
| 23 | CLA | c | 511 | X | - | - | - |
| 23 | CLA | c | 512 | X | - | - | - |
| 23 | CLA | c | 513 | X | - | - | - |
| 23 | CLA | c | 514 | X | - | - | - |
| 23 | CLA | d | 402[A] | X | - | - | - |
| 23 | CLA | d | 402[B] | X | - | - | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 23 | CLA | d | 403[A] | X | - | - | - |
| 23 | CLA | d | 403[B] | X | - | - | - |
| 23 | CLA | d | 404 | X | - | - | - |
| 27 | GOL | D | 413 | - | X | - | - |
| 27 | GOL | a | 416 | - | - | - | X |
| 31 | LMT | F | 101 | - | - | - | X |
| 31 | LMT | e | 101 | - | - | - | X |
| 34 | HTG | b | 623 | - | - | - | X |

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 334 | 4338 | 2836 | 717 | 760 | 25 | 0 | 222 | 0 |
| 1 | a | 334 | 4318 | 2821 | 715 | 757 | 25 | 0 | 220 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 279 | PRO | ARG | conflict | UNP P51765 |
| a | 279 | PRO | ARG | conflict | UNP P51765 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 504 | 4166 | 2735 | 694 | 724 | 13 | 0 | 22 | 0 |
| 2 | b | 504 | 4134 | 2718 | 687 | 716 | 13 | 0 | 19 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | C | 451 | 4272 | 2796 | 715 | 743 | 18 | 0 | 99 | 0 |
| 3 | c | 455 | 4316 | 2827 | 720 | 751 | 18 | 0 | 101 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 19 | ASN | - | expression tag | UNP D0VWR7 |
| C | 20 | SER | - | expression tag | UNP D0VWR7 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 21 | ILE | - | expression tag | UNP D0VWR7 |
| C | 22 | PHE | - | expression tag | UNP D0VWR7 |
| c | 19 | ASN | - | expression tag | UNP D0VWR7 |
| c | 20 | SER | - | expression tag | UNP D0VWR7 |
| c | 21 | ILE | - | expression tag | UNP D0VWR7 |
| c | 22 | PHE | - | expression tag | UNP D0VWR7 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 342 | Total | C | N | O | S | 0 | 115 | 0 |
| | | | 3625 | 2390 | 597 | 623 | 15 | | | |
| 4 | d | 341 | Total | C | N | O | S | 0 | 119 | 0 |
| | | | 3658 | 2412 | 605 | 626 | 15 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 432 | 107 | 123 | | | | |
| 5 | e | 79 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 670 | 439 | 110 | 121 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6 | F | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |
| 6 | f | 31 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 261 | 179 | 43 | 38 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | H | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 506 | 339 | 81 | 84 | 2 | | | |
| 7 | h | 64 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 517 | 345 | 85 | 85 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | I | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 314 | 211 | 48 | 54 | 1 | | | |
| 8 | i | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 314 | 211 | 48 | 54 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | J | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 272 | 182 | 42 | 47 | 1 | | | |
| 9 | j | 39 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 277 | 185 | 43 | 48 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | K | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |
| 10 | k | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K | 33 | LEU | PHE | conflict | UNP P19054 |
| K | 39 | TRP | VAL | conflict | UNP P19054 |
| k | 33 | LEU | PHE | conflict | UNP P19054 |
| k | 39 | TRP | VAL | conflict | UNP P19054 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11 | L | 36 | Total | C | N | O | 0 | 2 | 0 |
| | | | 311 | 207 | 49 | 55 | | | |
| 11 | l | 36 | Total | C | N | O | 0 | 2 | 0 |
| | | | 311 | 207 | 49 | 55 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | M | 33 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 268 | 179 | 39 | 49 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | m | 34 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 286 | 190 | 43 | 52 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| M | 8 | LEU | PHE | conflict | UNP P12312 |
| m | 8 | LEU | PHE | conflict | UNP P12312 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | O | 243 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1958 | 1221 | 335 | 398 | 4 | | | |
| 13 | o | 243 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1933 | 1207 | 330 | 392 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | T | 30 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 311 | 213 | 48 | 48 | 2 | | | |
| 14 | t | 30 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 302 | 208 | 47 | 45 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | U | 96 | Total | C | N | O | 0 | 4 | 0 |
| | | | 800 | 508 | 133 | 159 | | | |
| 15 | u | 97 | Total | C | N | O | 0 | 5 | 0 |
| | | | 815 | 519 | 135 | 161 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | V | 137 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 1120 | 711 | 185 | 220 | 4 | | | |
| 16 | v | 137 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 1117 | 712 | 185 | 216 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | X | 38 | Total | C | N | O | 0 | 1 | 0 |
| | | | 289 | 194 | 46 | 49 | | | |
| 17 | x | 38 | Total | C | N | O | 0 | 0 | 0 |
| | | | 281 | 188 | 45 | 48 | | | |

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18 | Y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |
| 18 | y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |

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

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

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

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

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | A | 1 | Total | Fe | 0 | 1 |
| | | | 2 | 2 | | |
| 21 | a | 1 | Total | Fe | 0 | 1 |
| | | | 2 | 2 | | |

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

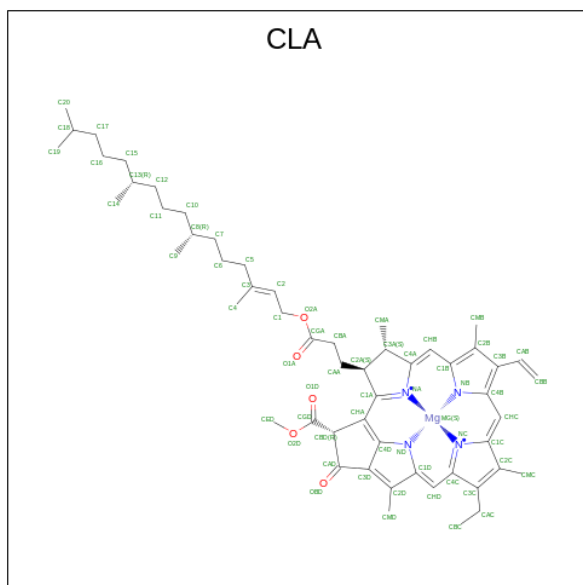
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | A | 2 | Total | Cl | 0 | 2 |
| | | | 4 | 4 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 22 | a | 2 | Total Cl 4 4 | 0 | 2 |

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|---------|
| | | | Total | C | Mg | N | O | | |
| 23 | A | 1 | Total 130 | C 110 | Mg 2 | N 8 | O 10 | 0 | 1 |
| 23 | A | 1 | Total 130 | C 110 | Mg 2 | N 8 | O 10 | 0 | 1 |
| 23 | A | 1 | Total 130 | C 110 | Mg 2 | N 8 | O 10 | 0 | 1 |
| 23 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 23 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| | | | Total | C | Mg | N | O | | |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| 23 | C | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |

Continued on next page...

Continued from previous page...

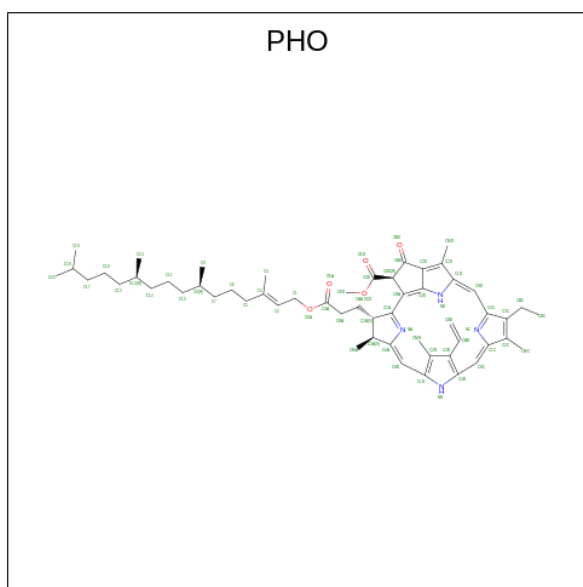
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|---------|
| 23 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | D | 1 | Total | C | Mg | N | O | 0 | 1 |
| | | | 130 | 110 | 2 | 8 | 10 | | |
| 23 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | a | 1 | Total | C | Mg | N | O | 0 | 1 |
| | | | 130 | 110 | 2 | 8 | 10 | | |
| 23 | a | 1 | Total | C | Mg | N | O | 0 | 1 |
| | | | 130 | 110 | 2 | 8 | 10 | | |
| 23 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

Continued on next page...

Continued from previous page...

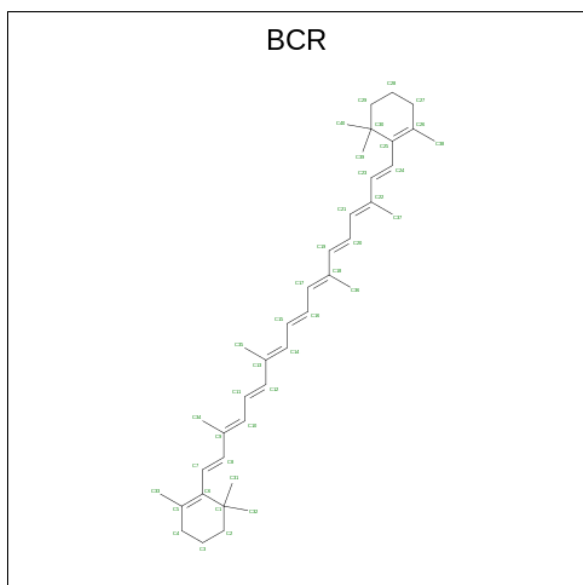
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|---------|
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 23 | d | 1 | Total | C | Mg | N | O | 0 | 1 |
| | | | 130 | 110 | 2 | 8 | 10 | | |
| 23 | d | 1 | Total | C | Mg | N | O | 0 | 1 |
| | | | 130 | 110 | 2 | 8 | 10 | | |
| 23 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



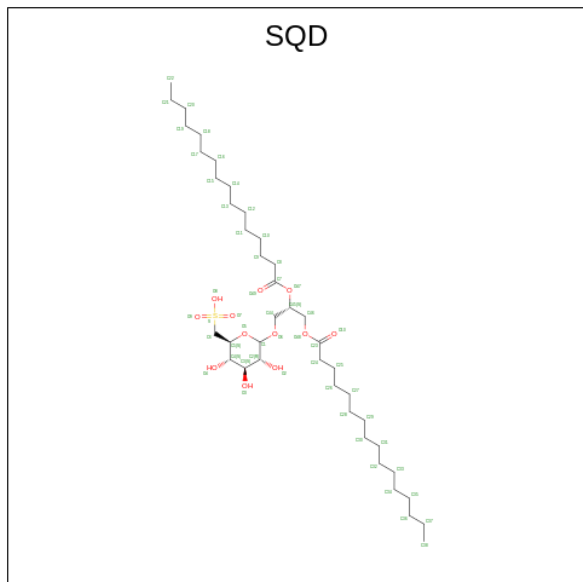
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|----|---------|---------|
| | | | Total | C | N | O | | |
| 24 | A | 1 | Total | C | N | O | 0 | 1 |
| | | | 128 | 110 | 8 | 10 | | |
| 24 | A | 1 | Total | C | N | O | 0 | 1 |
| | | | 128 | 110 | 8 | 10 | | |
| 24 | a | 1 | Total | C | N | O | 0 | 1 |
| | | | 128 | 110 | 8 | 10 | | |
| 24 | a | 1 | Total | C | N | O | 0 | 1 |
| | | | 128 | 110 | 8 | 10 | | |

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



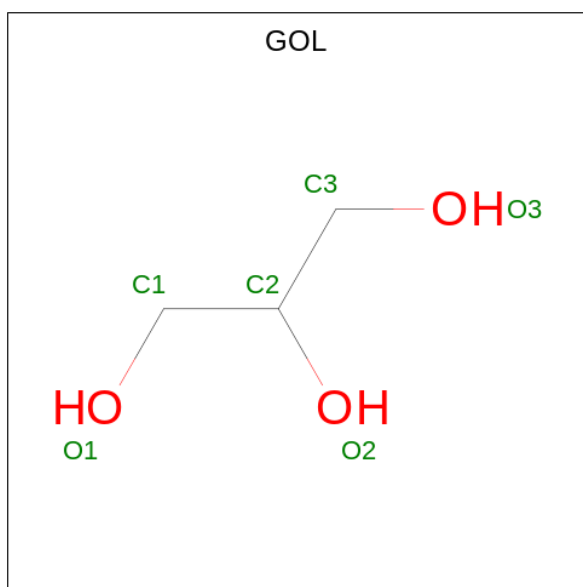
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25 | A | 1 | Total C 40 40 | 0 | 0 |
| 25 | B | 1 | Total C 40 40 | 0 | 0 |
| 25 | B | 1 | Total C 40 40 | 0 | 0 |
| 25 | B | 1 | Total C 40 40 | 0 | 0 |
| 25 | C | 1 | Total C 40 40 | 0 | 0 |
| 25 | C | 1 | Total C 40 40 | 0 | 0 |
| 25 | D | 1 | Total C 40 40 | 0 | 0 |
| 25 | H | 1 | Total C 40 40 | 0 | 0 |
| 25 | K | 1 | Total C 40 40 | 0 | 0 |
| 25 | T | 1 | Total C 40 40 | 0 | 0 |
| 25 | Y | 1 | Total C 40 40 | 0 | 0 |
| 25 | a | 1 | Total C 40 40 | 0 | 0 |
| 25 | b | 1 | Total C 40 40 | 0 | 0 |
| 25 | b | 1 | Total C 40 40 | 0 | 0 |
| 25 | b | 1 | Total C 40 40 | 0 | 0 |
| 25 | c | 1 | Total C 40 40 | 0 | 0 |
| 25 | c | 1 | Total C 40 40 | 0 | 0 |
| 25 | d | 1 | Total C 40 40 | 0 | 0 |
| 25 | h | 1 | Total C 40 40 | 0 | 0 |
| 25 | k | 1 | Total C 40 40 | 0 | 0 |
| 25 | t | 1 | Total C 40 40 | 0 | 0 |
| 25 | y | 1 | Total C 40 40 | 0 | 0 |

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|--------|---------|---------|
| | | | Total | C | O | S | | |
| 26 | A | 1 | Total 108 | C 82 | O 24 | S 2 | 0 | 1 |
| 26 | A | 1 | Total 54 | C 41 | O 12 | S 1 | 0 | 0 |
| 26 | B | 1 | Total 54 | C 41 | O 12 | S 1 | 0 | 0 |
| 26 | F | 1 | Total 43 | C 30 | O 12 | S 1 | 0 | 0 |
| 26 | a | 1 | Total 108 | C 82 | O 24 | S 2 | 0 | 1 |
| 26 | a | 1 | Total 54 | C 41 | O 12 | S 1 | 0 | 0 |
| 26 | b | 1 | Total 54 | C 41 | O 12 | S 1 | 0 | 0 |
| 26 | f | 1 | Total 43 | C 30 | O 12 | S 1 | 0 | 0 |

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



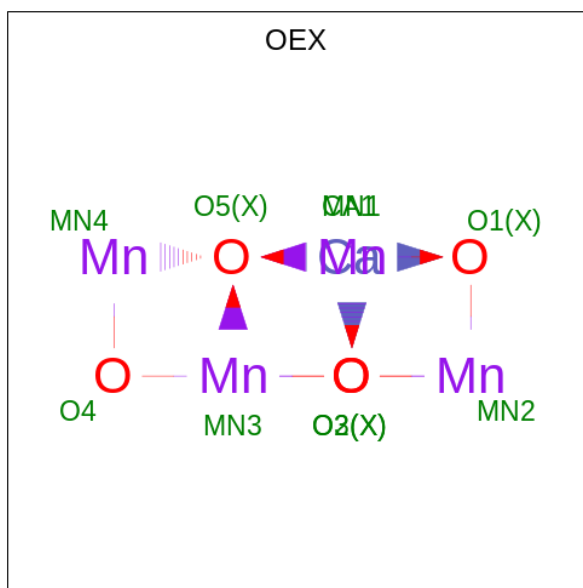
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 27 | A | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | B | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | B | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | B | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | C | 1 | Total C O 12 6 6 | 0 | 1 |
| 27 | D | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | D | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | O | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | O | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | V | 1 | Total C O 12 6 6 | 0 | 1 |
| 27 | a | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | a | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | b | 1 | Total C O 6 3 3 | 0 | 0 |
| 27 | b | 1 | Total C O 6 3 3 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 27 | c | 1 | Total | C | O | 0 | 1 |
| | | | 12 | 6 | 6 | | |
| 27 | c | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 27 | d | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 27 | l | 1 | Total | C | O | 0 | 1 |
| | | | 12 | 6 | 6 | | |
| 27 | o | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 27 | o | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 27 | v | 1 | Total | C | O | 0 | 1 |
| | | | 12 | 6 | 6 | | |

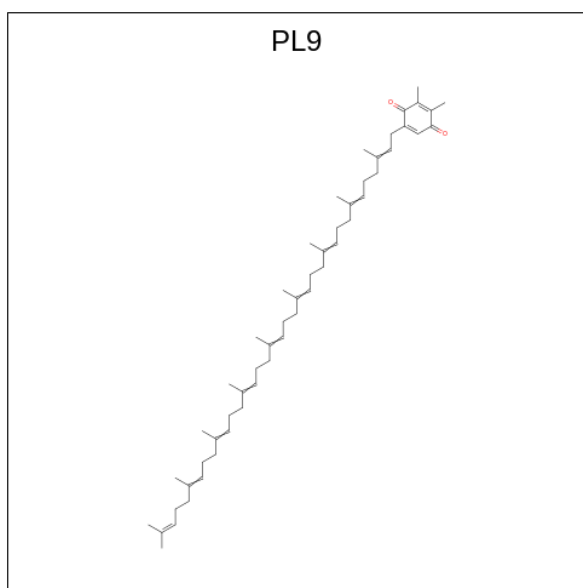
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 28 | A | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 20 | 2 | 8 | 10 | | |
| 28 | a | 1 | Total | Ca | Mn | O | 0 | 1 |
| | | | 20 | 2 | 8 | 10 | | |

- Molecule 29 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:

C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|---------|---------|
| 29 | A | 1 | Total | C | O | 0 | 1 |
| | | | 110 | 106 | 4 | | |
| 29 | D | 1 | Total | C | O | 0 | 1 |
| | | | 110 | 106 | 4 | | |
| 29 | a | 1 | Total | C | O | 0 | 1 |
| | | | 110 | 106 | 4 | | |
| 29 | d | 1 | Total | C | O | 0 | 1 |
| | | | 110 | 106 | 4 | | |

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

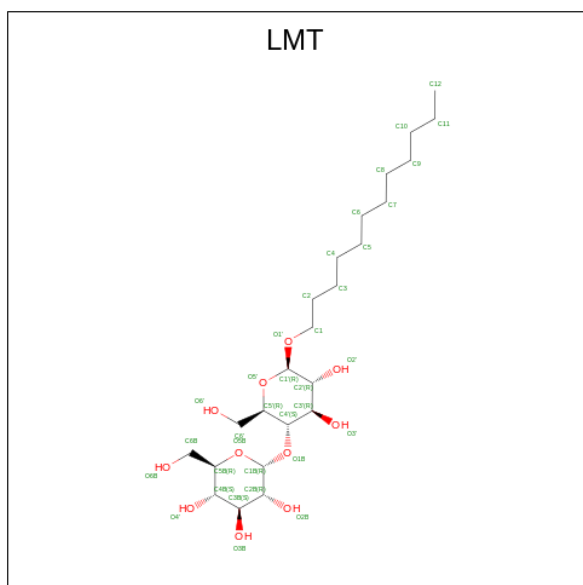
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30 | A | 1 | Total | C | O | 0 | 0 |
| | | | 28 | 23 | 5 | | |
| 30 | B | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 28 | 5 | | |
| 30 | D | 2 | Total | C | O | 0 | 0 |
| | | | 57 | 51 | 6 | | |
| 30 | I | 1 | Total | C | O | 0 | 0 |
| | | | 40 | 35 | 5 | | |
| 30 | J | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 30 | K | 1 | Total | C | O | 0 | 1 |
| | | | 68 | 58 | 10 | | |
| 30 | X | 1 | Total | C | O | 0 | 0 |
| | | | 18 | 16 | 2 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| | | | Total | C | O | | |
| 30 | a | 1 | 30 | 25 | 5 | 0 | 0 |
| 30 | b | 1 | 33 | 28 | 5 | 0 | 0 |
| 30 | c | 1 | 64 | 54 | 10 | 0 | 1 |
| 30 | d | 2 | 53 | 47 | 6 | 0 | 0 |
| 30 | i | 1 | 40 | 35 | 5 | 0 | 0 |
| 30 | j | 1 | 10 | 10 | | 0 | 0 |
| 30 | l | 1 | 10 | 10 | | 0 | 0 |
| 30 | m | 1 | 10 | 10 | | 0 | 0 |
| 30 | x | 1 | 18 | 16 | 2 | 0 | 0 |

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



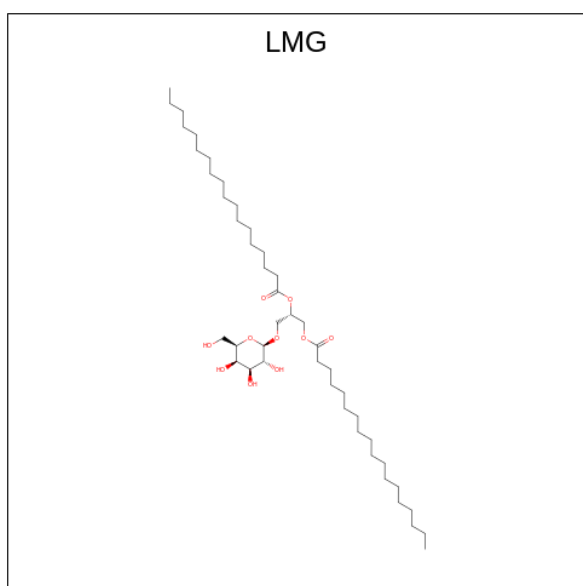
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| | | | Total | C | O | | |
| 31 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 31 | A | 1 | 35 | 24 | 11 | 0 | 0 |

Continued on next page...

Continued from previous page...

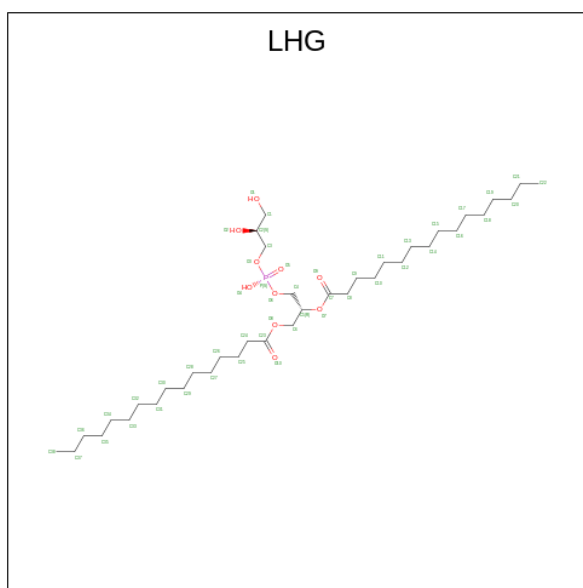
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 31 | B | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | B | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | B | 1 | Total | C | O | 0 | 0 |
| | | | 25 | 19 | 6 | | |
| 31 | F | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | M | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | M | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | a | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | b | 1 | Total | C | O | 0 | 0 |
| | | | 25 | 19 | 6 | | |
| 31 | b | 1 | Total | C | O | 0 | 0 |
| | | | 25 | 19 | 6 | | |
| 31 | e | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | m | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 31 | t | 1 | Total | C | O | 0 | 0 |
| | | | 26 | 19 | 7 | | |

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



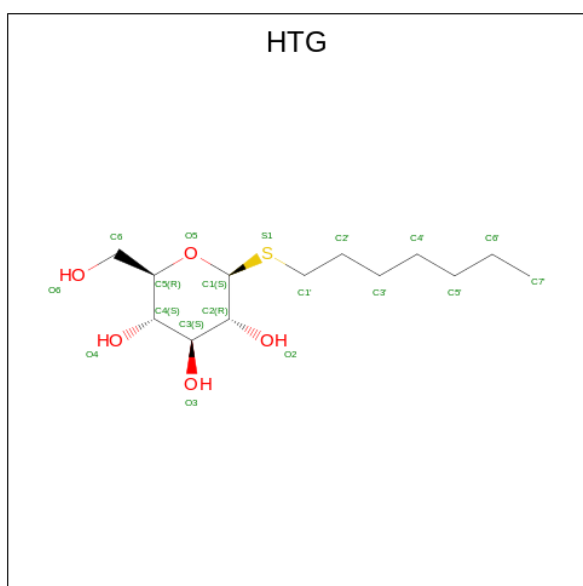
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32 | A | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | B | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | D | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | d | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | m | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 32 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 37 | 27 | 10 | | |
| 32 | z | 1 | Total | C | O | 0 | 0 |
| | | | 39 | 29 | 10 | | |

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33 | A | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | D | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | D | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | E | 1 | Total | C | O | P | 0 | 1 |
| | | | 84 | 62 | 20 | 2 | | |
| 33 | L | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | a | 1 | Total | C | O | P | 0 | 1 |
| | | | 84 | 62 | 20 | 2 | | |
| 33 | b | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | d | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | d | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |
| 33 | d | 1 | Total | C | O | P | 0 | 1 |
| | | | 98 | 76 | 20 | 2 | | |

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



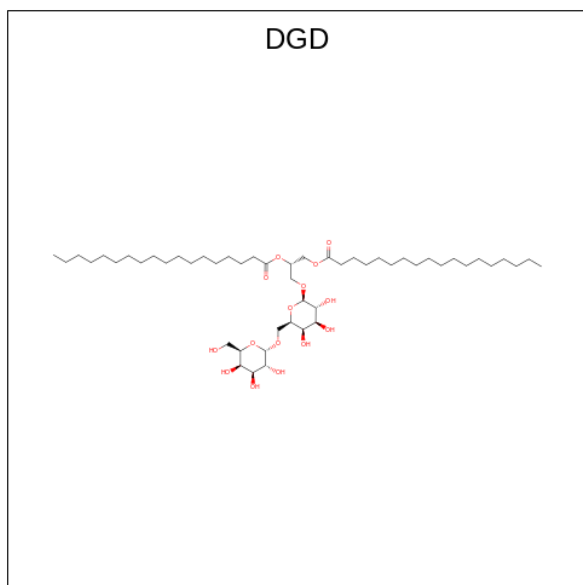
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 34 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| | | | Total | C | O | S | | |
| 34 | B | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | B | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | C | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | D | 1 | Total 16 | C 10 | O 5 | S 1 | 0 | 0 |
| 34 | V | 1 | Total 11 | C 6 | O 5 | | 0 | 0 |
| 34 | b | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | b | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | b | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | c | 1 | Total 19 | C 13 | O 5 | S 1 | 0 | 0 |
| 34 | d | 1 | Total 16 | C 10 | O 5 | S 1 | 0 | 0 |

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGD) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|---------|---------|
| | | | Total | C | O | | |
| 35 | C | 1 | Total 124 | C 94 | O 30 | 0 | 1 |

Continued on next page...

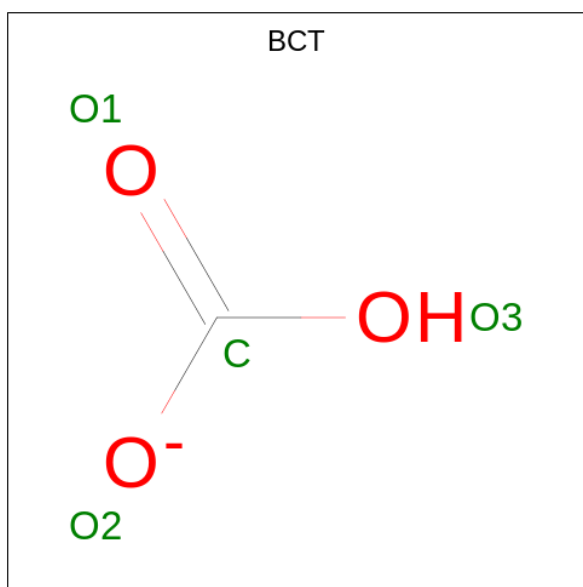
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35 | C | 1 | Total | C | O | 0 | 1 |
| | | | 124 | 94 | 30 | | |
| 35 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 35 | H | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 35 | c | 1 | Total | C | O | 0 | 1 |
| | | | 124 | 94 | 30 | | |
| 35 | c | 1 | Total | C | O | 0 | 1 |
| | | | 124 | 94 | 30 | | |
| 35 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 35 | h | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

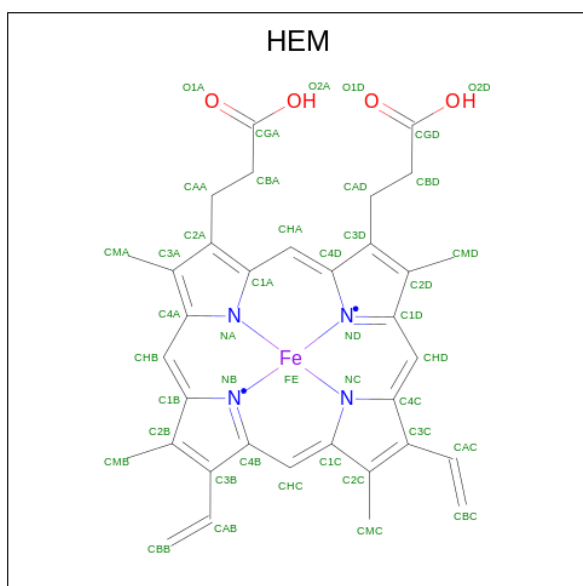
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 36 | C | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | F | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | O | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | c | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 36 | f | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 36 | o | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 37 | D | 1 | Total | C | O | 0 | 1 |
| | | | 8 | 2 | 6 | | |
| 37 | d | 1 | Total | C | O | 0 | 1 |
| | | | 8 | 2 | 6 | | |

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 38 | F | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

Continued on next page...

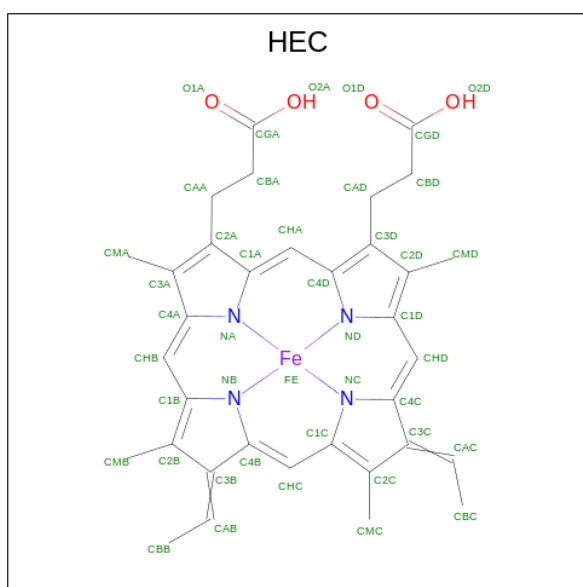
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 38 | f | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 39 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 39 | j | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 40 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 40 | V | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 40 | v | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 41 | A | 136 | Total | O | 0 | 86 |
| | | | 221 | 221 | | |
| 41 | B | 189 | Total | O | 0 | 2 |
| | | | 191 | 191 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | C | 169 | Total O 206 206 | 0 | 38 |
| 41 | D | 123 | Total O 157 157 | 0 | 34 |
| 41 | E | 15 | Total O 15 15 | 0 | 0 |
| 41 | F | 6 | Total O 6 6 | 0 | 0 |
| 41 | H | 23 | Total O 23 23 | 0 | 0 |
| 41 | I | 4 | Total O 4 4 | 0 | 0 |
| 41 | J | 7 | Total O 7 7 | 0 | 0 |
| 41 | K | 6 | Total O 6 6 | 0 | 0 |
| 41 | L | 9 | Total O 10 10 | 0 | 1 |
| 41 | M | 5 | Total O 5 5 | 0 | 0 |
| 41 | O | 106 | Total O 111 111 | 0 | 5 |
| 41 | T | 11 | Total O 14 14 | 0 | 3 |
| 41 | U | 42 | Total O 44 44 | 0 | 2 |
| 41 | V | 80 | Total O 81 81 | 0 | 1 |
| 41 | X | 7 | Total O 7 7 | 0 | 0 |
| 41 | a | 129 | Total O 209 209 | 0 | 81 |
| 41 | b | 199 | Total O 202 202 | 0 | 3 |
| 41 | c | 158 | Total O 191 191 | 0 | 34 |
| 41 | d | 121 | Total O 153 153 | 0 | 32 |
| 41 | e | 9 | Total O 9 9 | 0 | 0 |
| 41 | f | 3 | Total O 3 3 | 0 | 0 |

Continued on next page...

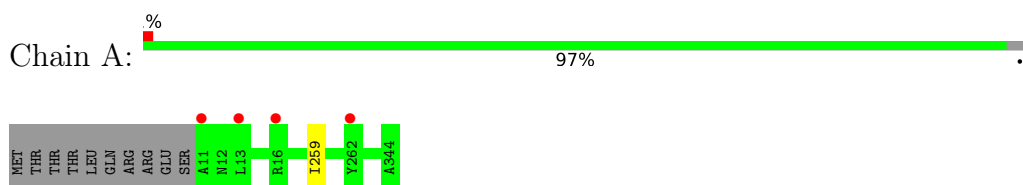
Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | h | 16 | Total O 16 16 | 0 | 0 |
| 41 | i | 2 | Total O 2 2 | 0 | 0 |
| 41 | j | 2 | Total O 2 2 | 0 | 0 |
| 41 | k | 3 | Total O 3 3 | 0 | 0 |
| 41 | l | 8 | Total O 10 10 | 0 | 2 |
| 41 | m | 13 | Total O 13 13 | 0 | 0 |
| 41 | o | 100 | Total O 104 104 | 0 | 4 |
| 41 | t | 7 | Total O 10 10 | 0 | 3 |
| 41 | u | 49 | Total O 50 50 | 0 | 1 |
| 41 | v | 59 | Total O 61 61 | 0 | 2 |
| 41 | x | 7 | Total O 7 7 | 0 | 0 |
| 41 | y | 2 | Total O 2 2 | 0 | 0 |

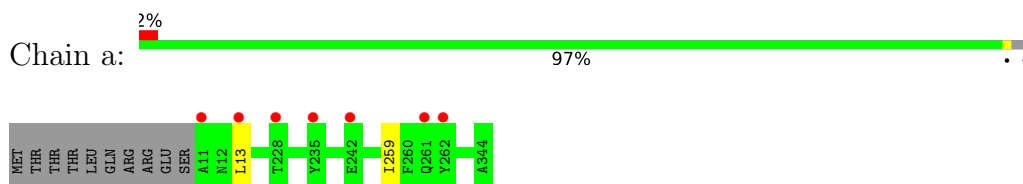
3 Residue-property plots [i](#)

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

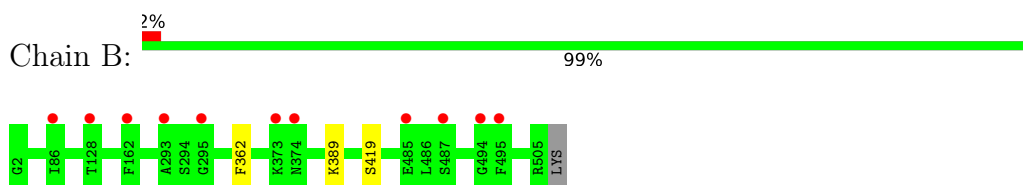
- Molecule 1: Photosystem II protein D1



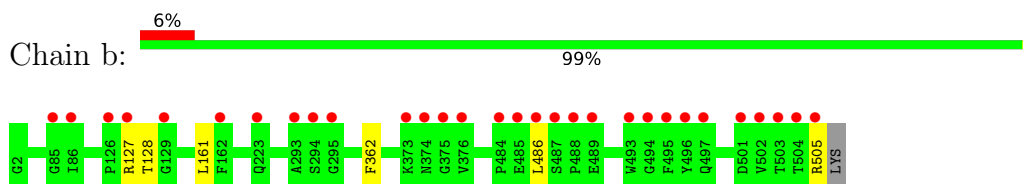
- Molecule 1: Photosystem II protein D1



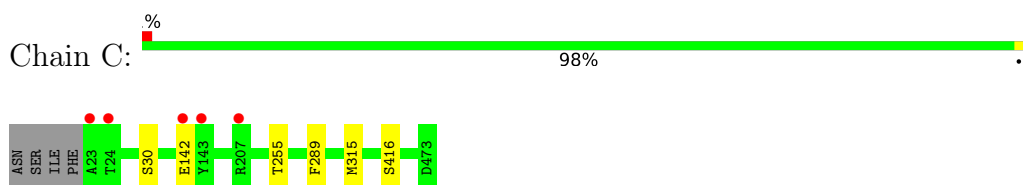
- Molecule 2: Photosystem II CP47 reaction center protein



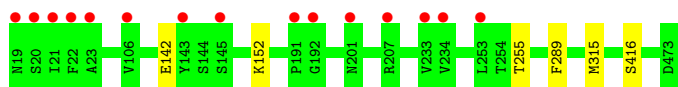
- Molecule 2: Photosystem II CP47 reaction center protein



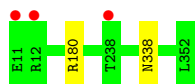
- Molecule 3: Photosystem II CP43 reaction center protein



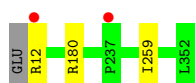
- Molecule 3: Photosystem II CP43 reaction center protein



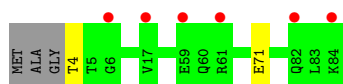
- Molecule 4: Photosystem II D2 protein



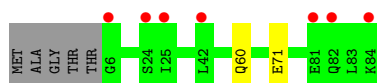
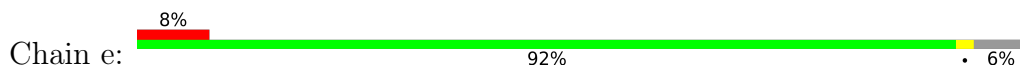
- Molecule 4: Photosystem II D2 protein



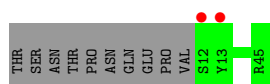
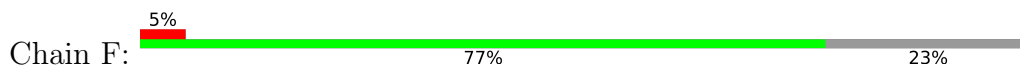
- Molecule 5: Cytochrome b559 subunit alpha



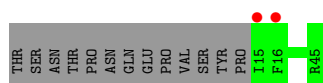
- Molecule 5: Cytochrome b559 subunit alpha



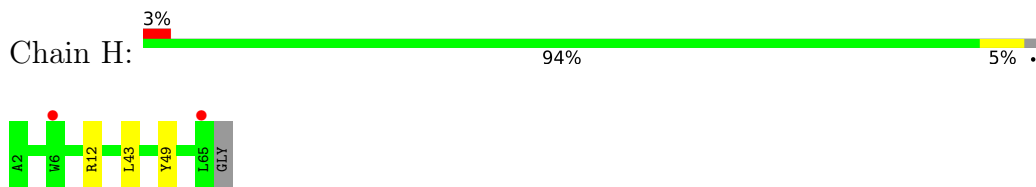
- Molecule 6: Cytochrome b559 subunit beta



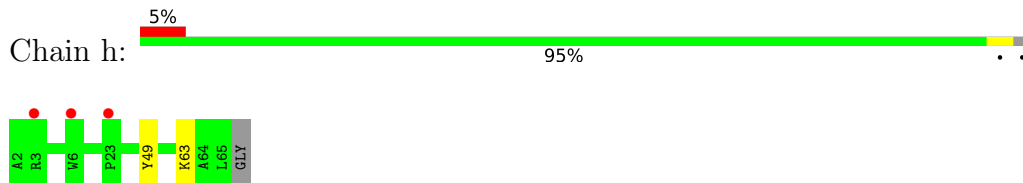
- Molecule 6: Cytochrome b559 subunit beta



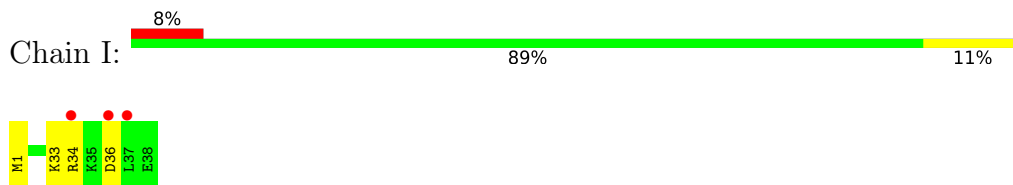
- Molecule 7: Photosystem II reaction center protein H



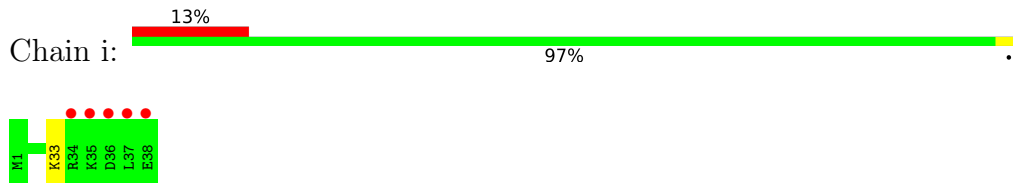
- Molecule 7: Photosystem II reaction center protein H



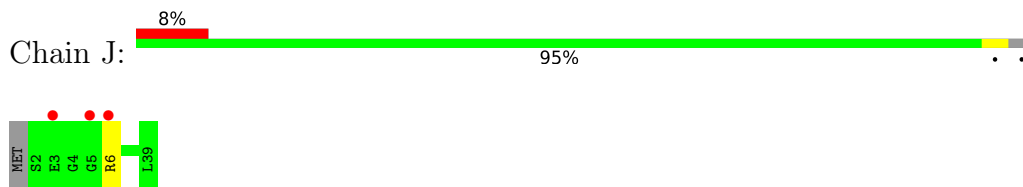
- Molecule 8: Photosystem II reaction center protein I



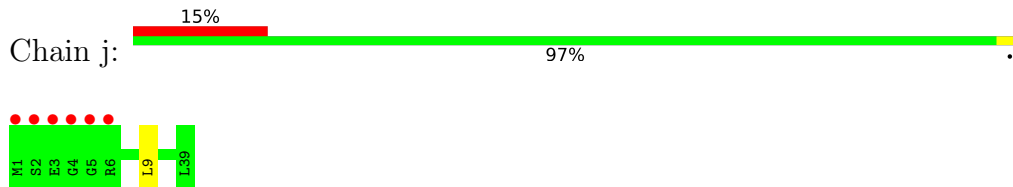
- Molecule 8: Photosystem II reaction center protein I



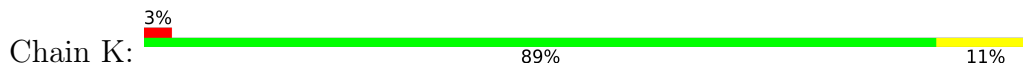
- Molecule 9: Photosystem II reaction center protein J

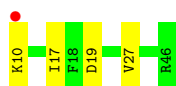


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

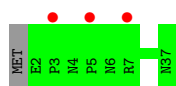




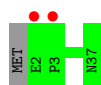
- Molecule 10: Photosystem II reaction center protein K



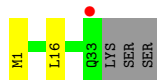
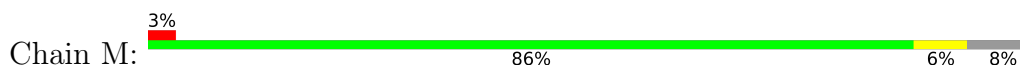
- Molecule 11: Photosystem II reaction center protein L



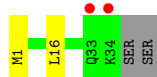
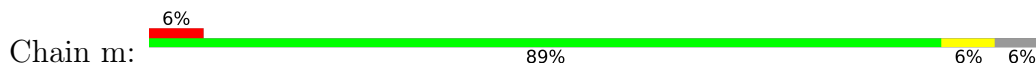
- Molecule 11: Photosystem II reaction center protein L



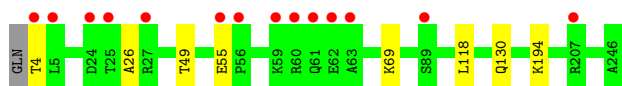
- Molecule 12: Photosystem II reaction center protein M



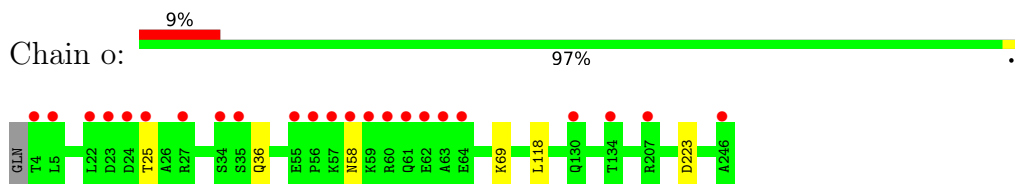
- Molecule 12: Photosystem II reaction center protein M



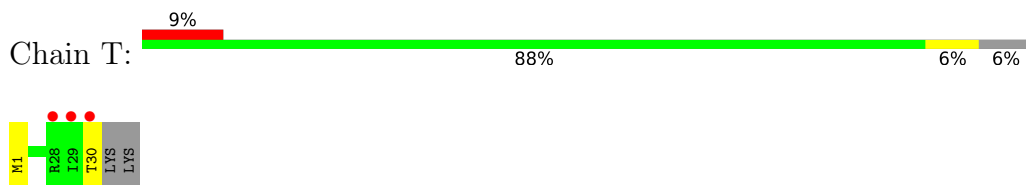
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



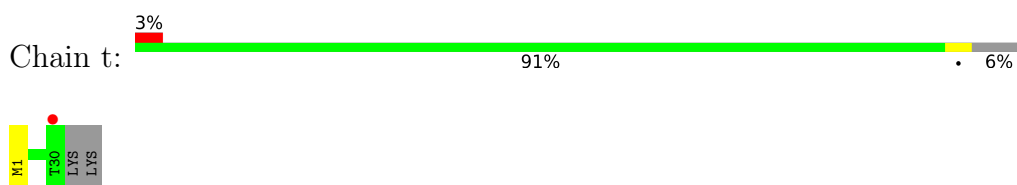
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



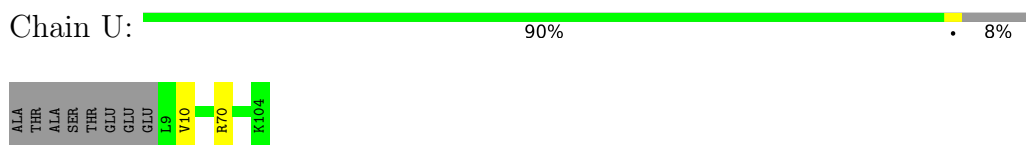
- Molecule 14: Photosystem II reaction center protein T



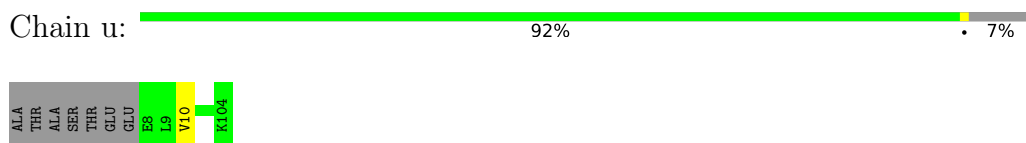
- Molecule 14: Photosystem II reaction center protein T



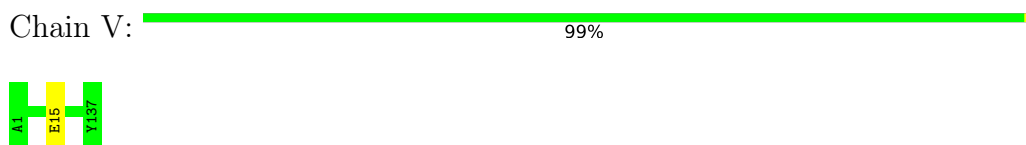
- Molecule 15: Photosystem II 12 kDa extrinsic protein



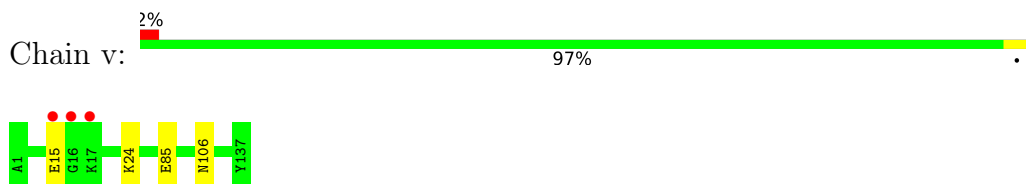
- Molecule 15: Photosystem II 12 kDa extrinsic protein



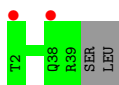
- Molecule 16: Cytochrome c-550



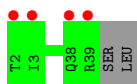
- Molecule 16: Cytochrome c-550



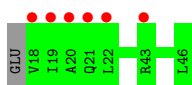
- Molecule 17: Photosystem II reaction center protein X



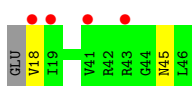
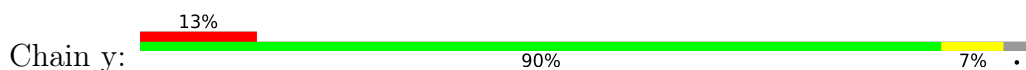
- Molecule 17: Photosystem II reaction center protein X



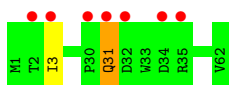
- Molecule 18: Photosystem II reaction center protein Ycf12



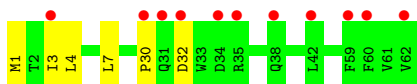
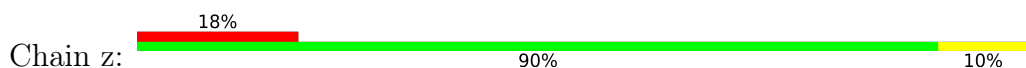
- Molecule 18: Photosystem II reaction center protein Ycf12



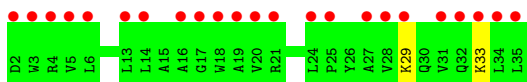
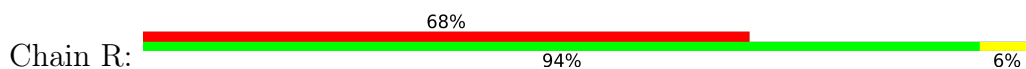
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 19.98 – 2.25 19.98 – 2.25 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (19.98-2.25) 99.9 (19.98-2.25) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.69 (at 2.26Å) | Xtrriage |
| Refinement program | PHENIX (1.19.2_4158: ???) | Depositor |
| R, R_{free} | 0.140 , 0.177 0.140 , 0.177 | Depositor DCC |
| R_{free} test set | 19819 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 50.3 | Xtrriage |
| Anisotropy | 0.516 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 86.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.98 | EDS |
| Total number of atoms | 62674 | wwPDB-VP |
| Average B, all atoms (Å ²) | 65.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.42 | 0/4478 | 0.58 | 0/6098 |
| 1 | a | 0.42 | 0/4457 | 0.56 | 0/6069 |
| 2 | B | 0.43 | 0/4314 | 0.58 | 0/5879 |
| 2 | b | 0.41 | 0/4285 | 0.57 | 0/5841 |
| 3 | C | 0.40 | 0/4416 | 0.56 | 0/6013 |
| 3 | c | 0.40 | 0/4467 | 0.54 | 0/6082 |
| 4 | D | 0.45 | 0/3746 | 0.60 | 0/5102 |
| 4 | d | 0.44 | 0/3780 | 0.57 | 0/5147 |
| 5 | E | 0.40 | 0/681 | 0.57 | 0/928 |
| 5 | e | 0.38 | 0/690 | 0.54 | 0/939 |
| 6 | F | 0.38 | 0/284 | 0.55 | 0/387 |
| 6 | f | 0.37 | 0/269 | 0.50 | 0/365 |
| 7 | H | 0.38 | 0/519 | 0.60 | 0/708 |
| 7 | h | 0.36 | 0/530 | 0.57 | 0/722 |
| 8 | I | 0.35 | 0/311 | 0.53 | 0/419 |
| 8 | i | 0.40 | 0/311 | 0.55 | 0/419 |
| 9 | J | 0.38 | 0/278 | 0.53 | 0/376 |
| 9 | j | 0.36 | 0/283 | 0.55 | 0/383 |
| 10 | K | 0.39 | 0/303 | 0.52 | 0/416 |
| 10 | k | 0.39 | 0/303 | 0.51 | 0/416 |
| 11 | L | 0.41 | 0/318 | 0.56 | 0/433 |
| 11 | l | 0.43 | 0/318 | 0.55 | 0/433 |
| 12 | M | 0.45 | 0/261 | 0.51 | 0/357 |
| 12 | m | 0.39 | 0/279 | 0.51 | 0/380 |
| 13 | O | 0.42 | 0/1991 | 0.64 | 0/2698 |
| 13 | o | 0.39 | 0/1966 | 0.63 | 1/2665 (0.0%) |
| 14 | T | 0.45 | 0/310 | 0.62 | 0/419 |
| 14 | t | 0.43 | 0/301 | 0.58 | 0/406 |
| 15 | U | 0.43 | 0/811 | 0.62 | 0/1095 |
| 15 | u | 0.44 | 0/826 | 0.62 | 0/1116 |
| 16 | V | 0.40 | 0/1142 | 0.58 | 0/1545 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | v | 0.37 | 0/1139 | 0.55 | 0/1542 |
| 17 | X | 0.32 | 0/292 | 0.47 | 0/395 |
| 17 | x | 0.32 | 0/284 | 0.48 | 0/384 |
| 18 | Y | 0.33 | 0/216 | 0.52 | 0/289 |
| 18 | y | 0.30 | 0/216 | 0.50 | 0/289 |
| 19 | Z | 0.31 | 0/490 | 0.44 | 0/669 |
| 19 | z | 0.31 | 0/490 | 0.43 | 0/669 |
| 20 | R | 0.33 | 0/279 | 0.52 | 0/383 |
| All | All | 0.41 | 0/50634 | 0.57 | 1/68876 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 13 | o | 223 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

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 | 553/344 (161%) | 544 (98%) | 7 (1%) | 2 (0%) | 34 | 37 |
| 1 | a | 551/344 (160%) | 539 (98%) | 10 (2%) | 2 (0%) | 34 | 37 |
| 2 | B | 524/505 (104%) | 516 (98%) | 8 (2%) | 0 | 100 | 100 |
| 2 | b | 521/505 (103%) | 510 (98%) | 11 (2%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 3 | C | 548/455 (120%) | 537 (98%) | 10 (2%) | 1 (0%) | 47 | 55 |
| 3 | c | 554/455 (122%) | 543 (98%) | 10 (2%) | 1 (0%) | 47 | 55 |
| 4 | D | 454/342 (133%) | 440 (97%) | 14 (3%) | 0 | 100 | 100 |
| 4 | d | 457/342 (134%) | 444 (97%) | 13 (3%) | 0 | 100 | 100 |
| 5 | E | 79/84 (94%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 79/84 (94%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 32/44 (73%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 30/44 (68%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 7 | h | 63/65 (97%) | 59 (94%) | 3 (5%) | 1 (2%) | 9 | 5 |
| 8 | I | 36/38 (95%) | 33 (92%) | 2 (6%) | 1 (3%) | 5 | 2 |
| 8 | i | 36/38 (95%) | 32 (89%) | 4 (11%) | 0 | 100 | 100 |
| 9 | J | 36/39 (92%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 9 | j | 37/39 (95%) | 37 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 11 | L | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 32/36 (89%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 34/36 (94%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 251/244 (103%) | 242 (96%) | 8 (3%) | 1 (0%) | 34 | 37 |
| 13 | o | 249/244 (102%) | 243 (98%) | 6 (2%) | 0 | 100 | 100 |
| 14 | T | 33/32 (103%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 32/32 (100%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 15 | U | 97/104 (93%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | u | 99/104 (95%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 16 | V | 140/137 (102%) | 137 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | v | 140/137 (102%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 17 | X | 37/40 (92%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 17 | x | 36/40 (90%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 18 | Y | 27/30 (90%) | 24 (89%) | 3 (11%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 18 | y | 27/30 (90%) | 26 (96%) | 1 (4%) | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 58 (97%) | 1 (2%) | 1 (2%) | 9 | 4 |
| 19 | z | 60/62 (97%) | 59 (98%) | 0 | 1 (2%) | 9 | 4 |
| 20 | R | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 6180/5384 (115%) | 6036 (98%) | 133 (2%) | 11 (0%) | 47 | 55 |

5 of 11 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 416 | SER |
| 8 | I | 36 | ASP |
| 3 | c | 416 | SER |
| 19 | Z | 31 | GLN |
| 13 | O | 26 | ALA |

5.3.2 Protein sidechains [i](#)

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 | 444/279 (159%) | 444 (100%) | 0 | 100 | 100 |
| 1 | a | 442/279 (158%) | 441 (100%) | 1 (0%) | 93 | 96 |
| 2 | B | 423/403 (105%) | 420 (99%) | 3 (1%) | 84 | 90 |
| 2 | b | 420/403 (104%) | 413 (98%) | 7 (2%) | 60 | 71 |
| 3 | C | 431/356 (121%) | 425 (99%) | 6 (1%) | 67 | 76 |
| 3 | c | 437/356 (123%) | 431 (99%) | 6 (1%) | 67 | 76 |
| 4 | D | 368/277 (133%) | 366 (100%) | 2 (0%) | 88 | 92 |
| 4 | d | 372/277 (134%) | 368 (99%) | 4 (1%) | 73 | 82 |
| 5 | E | 72/73 (99%) | 70 (97%) | 2 (3%) | 43 | 52 |
| 5 | e | 72/73 (99%) | 70 (97%) | 2 (3%) | 43 | 52 |
| 6 | F | 28/38 (74%) | 28 (100%) | 0 | 100 | 100 |
| 6 | f | 26/38 (68%) | 26 (100%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 7 | H | 54/54 (100%) | 51 (94%) | 3 (6%) | 21 | 21 |
| 7 | h | 55/54 (102%) | 54 (98%) | 1 (2%) | 59 | 68 |
| 8 | I | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 19 |
| 8 | i | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 51 |
| 9 | J | 26/27 (96%) | 25 (96%) | 1 (4%) | 33 | 39 |
| 9 | j | 26/27 (96%) | 25 (96%) | 1 (4%) | 33 | 39 |
| 10 | K | 30/30 (100%) | 26 (87%) | 4 (13%) | 4 | 2 |
| 10 | k | 30/30 (100%) | 27 (90%) | 3 (10%) | 7 | 5 |
| 11 | L | 36/35 (103%) | 36 (100%) | 0 | 100 | 100 |
| 11 | l | 36/35 (103%) | 36 (100%) | 0 | 100 | 100 |
| 12 | M | 30/32 (94%) | 28 (93%) | 2 (7%) | 16 | 15 |
| 12 | m | 32/32 (100%) | 30 (94%) | 2 (6%) | 18 | 17 |
| 13 | O | 216/207 (104%) | 209 (97%) | 7 (3%) | 39 | 47 |
| 13 | o | 213/207 (103%) | 208 (98%) | 5 (2%) | 50 | 59 |
| 14 | T | 32/28 (114%) | 30 (94%) | 2 (6%) | 18 | 17 |
| 14 | t | 31/28 (111%) | 31 (100%) | 0 | 100 | 100 |
| 15 | U | 86/89 (97%) | 84 (98%) | 2 (2%) | 50 | 59 |
| 15 | u | 88/89 (99%) | 86 (98%) | 2 (2%) | 50 | 59 |
| 16 | V | 123/117 (105%) | 122 (99%) | 1 (1%) | 81 | 88 |
| 16 | v | 123/117 (105%) | 119 (97%) | 4 (3%) | 38 | 46 |
| 17 | X | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 17 | x | 31/33 (94%) | 31 (100%) | 0 | 100 | 100 |
| 18 | Y | 22/23 (96%) | 22 (100%) | 0 | 100 | 100 |
| 18 | y | 22/23 (96%) | 20 (91%) | 2 (9%) | 9 | 7 |
| 19 | Z | 52/52 (100%) | 50 (96%) | 2 (4%) | 33 | 39 |
| 19 | z | 52/52 (100%) | 47 (90%) | 5 (10%) | 8 | 6 |
| 20 | R | 29/29 (100%) | 27 (93%) | 2 (7%) | 15 | 14 |
| All | All | 5110/4403 (116%) | 5023 (98%) | 87 (2%) | 59 | 71 |

5 of 87 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | h | 49 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 15 | u | 10[B] | VAL |
| 9 | j | 9 | LEU |
| 13 | o | 25 | THR |
| 16 | v | 106 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 60 | GLN |
| 13 | o | 58 | ASN |
| 16 | v | 86 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 12 | FME | m | 1 | 12 | 8,9,10 | 0.53 | 0 | 7,9,11 | 1.44 | 2 (28%) |
| 14 | FME | T | 1 | 14 | 8,9,10 | 0.72 | 0 | 7,9,11 | 1.64 | 1 (14%) |
| 14 | FME | t | 1 | 14 | 8,9,10 | 0.73 | 0 | 7,9,11 | 1.39 | 1 (14%) |
| 12 | FME | M | 1 | 12 | 8,9,10 | 0.61 | 0 | 7,9,11 | 1.13 | 1 (14%) |
| 8 | FME | i | 1 | 8 | 8,9,10 | 0.65 | 0 | 7,9,11 | 1.24 | 0 |
| 8 | FME | I | 1 | 8 | 8,9,10 | 0.59 | 0 | 7,9,11 | 1.32 | 2 (28%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 14 | t | 1 | FME | O-C-CA | -2.74 | 117.60 | 124.78 |
| 14 | T | 1 | FME | CG-CB-CA | 2.53 | 119.98 | 112.95 |
| 12 | m | 1 | FME | O1-CN-N | -2.45 | 118.81 | 125.27 |
| 8 | I | 1 | FME | O-C-CA | -2.28 | 118.80 | 124.78 |
| 12 | M | 1 | FME | O-C-CA | -2.19 | 119.05 | 124.78 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 8 | i | 1 | FME | O-C-CA-CB |
| 12 | m | 1 | FME | O1-CN-N-CA |
| 12 | m | 1 | FME | O-C-CA-CB |
| 14 | T | 1 | FME | C-CA-CB-CG |
| 8 | I | 1 | FME | O1-CN-N-CA |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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 |
| 25 | BCR | B | 617 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.28 | 7 (12%) |
| 33 | LHG | D | 408[A] | - | 48,48,48 | 0.92 | 2 (4%) | 51,54,54 | 0.99 | 4 (7%) |
| 26 | SQD | B | 620 | - | 53,54,54 | 1.07 | 4 (7%) | 62,65,65 | 1.74 | 12 (19%) |
| 23 | CLA | B | 604 | - | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.65 | 26 (34%) |
| 27 | GOL | c | 526[B] | - | 5,5,5 | 0.84 | 0 | 5,5,5 | 0.97 | 0 |
| 35 | DGD | C | 517[A] | - | 63,63,67 | 0.89 | 3 (4%) | 77,77,81 | 1.02 | 5 (6%) |
| 31 | LMT | m | 103 | - | 36,36,36 | 1.08 | 3 (8%) | 47,47,47 | 1.08 | 3 (6%) |
| 23 | CLA | a | 405[A] | 41 | 65,73,73 | 1.94 | 16 (24%) | 76,113,113 | 2.81 | 27 (35%) |
| 26 | SQD | b | 620 | - | 53,54,54 | 1.05 | 3 (5%) | 62,65,65 | 1.69 | 12 (19%) |
| 28 | OEX | A | 413[B] | 3,41,1 | 0,15,15 | - | - | - | - | - |
| 33 | LHG | D | 407[A] | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 0.99 | 3 (5%) |
| 23 | CLA | A | 406[B] | 41 | 65,73,73 | 2.06 | 16 (24%) | 76,113,113 | 2.78 | 28 (36%) |
| 35 | DGD | C | 518 | - | 63,63,67 | 0.88 | 3 (4%) | 77,77,81 | 0.99 | 4 (5%) |
| 31 | LMT | M | 102 | - | 36,36,36 | 1.09 | 3 (8%) | 47,47,47 | 1.07 | 2 (4%) |
| 28 | OEX | a | 411[A] | 3,41,1 | 0,15,15 | - | - | - | - | - |
| 28 | OEX | a | 411[B] | 3,41,1 | 0,15,15 | - | - | - | - | - |
| 25 | BCR | B | 618 | - | 41,41,41 | 0.98 | 1 (2%) | 56,56,56 | 1.40 | 7 (12%) |
| 33 | LHG | A | 419[B] | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 1.22 | 6 (11%) |
| 33 | LHG | d | 408[A] | - | 48,48,48 | 0.92 | 2 (4%) | 51,54,54 | 0.99 | 3 (5%) |
| 33 | LHG | d | 408[B] | - | 48,48,48 | 0.92 | 2 (4%) | 51,54,54 | 1.01 | 2 (3%) |
| 34 | HTG | b | 625 | - | 19,19,19 | 0.97 | 2 (10%) | 23,24,24 | 1.50 | 3 (13%) |
| 29 | PL9 | a | 412[A] | - | 55,55,55 | 0.65 | 2 (3%) | 68,69,69 | 2.00 | 22 (32%) |
| 27 | GOL | D | 413 | - | 5,5,5 | 1.45 | 2 (40%) | 5,5,5 | 0.81 | 0 |
| 25 | BCR | T | 101 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.64 | 15 (26%) |
| 25 | BCR | a | 408 | - | 41,41,41 | 1.05 | 1 (2%) | 56,56,56 | 1.40 | 6 (10%) |
| 29 | PL9 | d | 406[B] | - | 55,55,55 | 0.68 | 1 (1%) | 68,69,69 | 1.60 | 19 (27%) |
| 23 | CLA | B | 606 | - | 65,73,73 | 1.96 | 15 (23%) | 76,113,113 | 3.00 | 26 (34%) |
| 32 | LMG | C | 520 | - | 51,51,55 | 1.06 | 3 (5%) | 59,59,63 | 1.34 | 6 (10%) |
| 23 | CLA | c | 514 | - | 65,73,73 | 2.12 | 17 (26%) | 76,113,113 | 2.77 | 28 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | BCR | k | 101 | - | 41,41,41 | 1.05 | 1 (2%) | 56,56,56 | 1.46 | 12 (21%) |
| 29 | PL9 | A | 414[A] | - | 55,55,55 | 0.68 | 2 (3%) | 68,69,69 | 2.08 | 25 (36%) |
| 29 | PL9 | A | 414[B] | - | 55,55,55 | 0.65 | 2 (3%) | 68,69,69 | 1.98 | 24 (35%) |
| 23 | CLA | b | 606 | - | 65,73,73 | 1.99 | 15 (23%) | 76,113,113 | 2.82 | 28 (36%) |
| 33 | LHG | E | 101[B] | - | 41,41,48 | 1.06 | 2 (4%) | 44,47,54 | 1.10 | 4 (9%) |
| 37 | BCT | d | 401[A] | 21 | 2,3,3 | 0.57 | 0 | 2,3,3 | 1.58 | 1 (50%) |
| 23 | CLA | a | 404[A] | - | 65,73,73 | 1.99 | 15 (23%) | 76,113,113 | 2.87 | 32 (42%) |
| 23 | CLA | a | 404[B] | - | 65,73,73 | 2.05 | 16 (24%) | 76,113,113 | 2.85 | 32 (42%) |
| 37 | BCT | d | 401[B] | 21 | 2,3,3 | 0.64 | 0 | 2,3,3 | 1.22 | 0 |
| 23 | CLA | B | 605 | - | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.88 | 27 (35%) |
| 37 | BCT | D | 401[B] | 21 | 2,3,3 | 0.65 | 0 | 2,3,3 | 1.24 | 0 |
| 33 | LHG | a | 418[A] | - | 41,41,48 | 1.04 | 2 (4%) | 44,47,54 | 0.92 | 2 (4%) |
| 23 | CLA | b | 604 | - | 65,73,73 | 1.98 | 16 (24%) | 76,113,113 | 2.81 | 27 (35%) |
| 26 | SQD | F | 103 | - | 42,43,54 | 1.22 | 4 (9%) | 51,54,65 | 2.18 | 14 (27%) |
| 23 | CLA | A | 405[A] | 41 | 65,73,73 | 1.90 | 16 (24%) | 76,113,113 | 2.85 | 30 (39%) |
| 23 | CLA | d | 402[A] | 41 | 65,73,73 | 2.00 | 14 (21%) | 76,113,113 | 2.75 | 26 (34%) |
| 35 | DGD | h | 102 | - | 63,63,67 | 0.87 | 3 (4%) | 77,77,81 | 1.08 | 5 (6%) |
| 27 | GOL | a | 417 | - | 5,5,5 | 1.08 | 0 | 5,5,5 | 0.95 | 0 |
| 32 | LMG | A | 418 | - | 51,51,55 | 0.91 | 2 (3%) | 59,59,63 | 1.49 | 8 (13%) |
| 23 | CLA | b | 613 | - | 65,73,73 | 1.98 | 16 (24%) | 76,113,113 | 2.76 | 28 (36%) |
| 23 | CLA | C | 504 | 41 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.76 | 25 (32%) |
| 25 | BCR | b | 619 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.42 | 8 (14%) |
| 27 | GOL | d | 413 | - | 5,5,5 | 1.07 | 0 | 5,5,5 | 0.92 | 0 |
| 35 | DGD | C | 516[B] | - | 63,63,67 | 0.84 | 2 (3%) | 77,77,81 | 1.10 | 7 (9%) |
| 23 | CLA | D | 403[A] | - | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.87 | 29 (38%) |
| 27 | GOL | b | 624 | - | 5,5,5 | 1.20 | 1 (20%) | 5,5,5 | 0.79 | 0 |
| 27 | GOL | b | 628 | - | 5,5,5 | 0.50 | 0 | 5,5,5 | 1.34 | 1 (20%) |
| 23 | CLA | C | 512 | - | 65,73,73 | 2.04 | 15 (23%) | 76,113,113 | 2.78 | 31 (40%) |
| 24 | PHO | A | 407[B] | - | 51,69,69 | 1.80 | 8 (15%) | 47,99,99 | 1.70 | 11 (23%) |
| 23 | CLA | d | 404 | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.85 | 28 (36%) |
| 24 | PHO | a | 406[B] | - | 51,69,69 | 1.83 | 8 (15%) | 47,99,99 | 1.83 | 11 (23%) |
| 23 | CLA | c | 511 | - | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.79 | 31 (40%) |
| 27 | GOL | c | 526[A] | - | 5,5,5 | 0.94 | 0 | 5,5,5 | 0.95 | 0 |
| 31 | LMT | A | 420 | - | 36,36,36 | 1.06 | 2 (5%) | 47,47,47 | 1.15 | 4 (8%) |
| 23 | CLA | C | 511 | 3 | 65,73,73 | 2.07 | 17 (26%) | 76,113,113 | 2.71 | 26 (34%) |
| 25 | BCR | C | 514 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.46 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | OEX | A | 413[A] | 3,41,1 | 0,15,15 | - | - | - | - | - |
| 23 | CLA | A | 406[A] | 41 | 65,73,73 | 1.96 | 16 (24%) | 76,113,113 | 2.81 | 29 (38%) |
| 23 | CLA | c | 504 | - | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.78 | 27 (35%) |
| 34 | HTG | C | 521 | - | 19,19,19 | 0.86 | 1 (5%) | 23,24,24 | 1.37 | 2 (8%) |
| 31 | LMT | e | 101 | - | 36,36,36 | 1.02 | 4 (11%) | 47,47,47 | 1.02 | 1 (2%) |
| 25 | BCR | D | 405 | - | 41,41,41 | 1.10 | 1 (2%) | 56,56,56 | 1.84 | 16 (28%) |
| 27 | GOL | V | 203[B] | - | 5,5,5 | 1.06 | 0 | 5,5,5 | 0.85 | 0 |
| 33 | LHG | A | 419[A] | - | 48,48,48 | 0.84 | 2 (4%) | 51,54,54 | 1.31 | 6 (11%) |
| 35 | DGD | H | 102 | - | 63,63,67 | 0.88 | 3 (4%) | 77,77,81 | 1.07 | 6 (7%) |
| 31 | LMT | B | 628 | - | 36,36,36 | 1.17 | 4 (11%) | 47,47,47 | 1.37 | 6 (12%) |
| 23 | CLA | c | 512 | 3 | 65,73,73 | 2.08 | 17 (26%) | 76,113,113 | 2.80 | 29 (38%) |
| 29 | PL9 | d | 406[A] | - | 55,55,55 | 0.65 | 1 (1%) | 68,69,69 | 1.63 | 17 (25%) |
| 31 | LMT | M | 101 | - | 36,36,36 | 1.13 | 4 (11%) | 47,47,47 | 1.22 | 4 (8%) |
| 25 | BCR | B | 619 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 1.37 | 12 (21%) |
| 23 | CLA | C | 506 | - | 65,73,73 | 2.03 | 18 (27%) | 76,113,113 | 2.80 | 29 (38%) |
| 23 | CLA | b | 603 | - | 65,73,73 | 2.03 | 16 (24%) | 76,113,113 | 2.83 | 31 (40%) |
| 33 | LHG | E | 101[A] | - | 41,41,48 | 1.06 | 2 (4%) | 44,47,54 | 1.11 | 3 (6%) |
| 31 | LMT | a | 415 | - | 36,36,36 | 1.01 | 1 (2%) | 47,47,47 | 1.04 | 2 (4%) |
| 23 | CLA | b | 610 | 41 | 65,73,73 | 2.05 | 16 (24%) | 76,113,113 | 2.89 | 29 (38%) |
| 23 | CLA | C | 503 | - | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.80 | 27 (35%) |
| 37 | BCT | D | 401[A] | 21 | 2,3,3 | 0.54 | 0 | 2,3,3 | 1.81 | 1 (50%) |
| 23 | CLA | B | 610 | 41 | 65,73,73 | 2.05 | 16 (24%) | 76,113,113 | 2.86 | 30 (39%) |
| 25 | BCR | b | 617 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.34 | 6 (10%) |
| 33 | LHG | d | 407[A] | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 1.08 | 4 (7%) |
| 33 | LHG | d | 407[B] | - | 48,48,48 | 0.88 | 2 (4%) | 51,54,54 | 1.05 | 4 (7%) |
| 33 | LHG | b | 629[B] | - | 48,48,48 | 0.87 | 2 (4%) | 51,54,54 | 1.03 | 4 (7%) |
| 25 | BCR | C | 515 | - | 41,41,41 | 1.05 | 1 (2%) | 56,56,56 | 1.39 | 9 (16%) |
| 25 | BCR | Y | 101 | - | 41,41,41 | 0.99 | 1 (2%) | 56,56,56 | 1.66 | 10 (17%) |
| 33 | LHG | L | 101[B] | - | 48,48,48 | 0.92 | 2 (4%) | 51,54,54 | 1.04 | 2 (3%) |
| 35 | DGD | C | 516[A] | - | 63,63,67 | 0.81 | 2 (3%) | 77,77,81 | 1.21 | 8 (10%) |
| 40 | HEC | v | 201 | 16 | 32,50,50 | 2.04 | 3 (9%) | 24,82,82 | 1.97 | 6 (25%) |
| 25 | BCR | c | 516 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.44 | 12 (21%) |
| 27 | GOL | o | 302 | - | 5,5,5 | 0.95 | 0 | 5,5,5 | 0.99 | 0 |
| 23 | CLA | B | 607 | 41 | 65,73,73 | 1.95 | 16 (24%) | 76,113,113 | 2.89 | 27 (35%) |
| 23 | CLA | b | 608 | - | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.78 | 30 (39%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | SQD | a | 409[B] | - | 53,54,54 | 0.97 | 3 (5%) | 62,65,65 | 1.64 | 11 (17%) |
| 26 | SQD | a | 410 | - | 53,54,54 | 1.07 | 4 (7%) | 62,65,65 | 1.25 | 8 (12%) |
| 27 | GOL | B | 624 | - | 5,5,5 | 0.95 | 0 | 5,5,5 | 1.17 | 1 (20%) |
| 23 | CLA | C | 513 | - | 65,73,73 | 2.07 | 15 (23%) | 76,113,113 | 2.77 | 28 (36%) |
| 31 | LMT | b | 621 | - | 25,25,36 | 0.96 | 2 (8%) | 30,30,47 | 1.19 | 3 (10%) |
| 24 | PHO | A | 416[B] | - | 51,69,69 | 1.87 | 8 (15%) | 47,99,99 | 1.90 | 10 (21%) |
| 35 | DGD | c | 517[B] | - | 63,63,67 | 0.86 | 2 (3%) | 77,77,81 | 1.10 | 5 (6%) |
| 31 | LMT | b | 627 | - | 25,25,36 | 0.88 | 1 (4%) | 30,30,47 | 1.13 | 1 (3%) |
| 32 | LMG | Z | 101 | - | 37,37,55 | 1.00 | 2 (5%) | 45,45,63 | 1.46 | 8 (17%) |
| 24 | PHO | A | 407[A] | - | 51,69,69 | 1.78 | 8 (15%) | 47,99,99 | 1.77 | 11 (23%) |
| 27 | GOL | A | 411 | - | 5,5,5 | 1.09 | 0 | 5,5,5 | 0.77 | 0 |
| 32 | LMG | D | 412 | 39 | 51,51,55 | 0.84 | 2 (3%) | 59,59,63 | 1.11 | 4 (6%) |
| 24 | PHO | a | 406[A] | - | 51,69,69 | 1.83 | 8 (15%) | 47,99,99 | 1.71 | 10 (21%) |
| 23 | CLA | c | 503 | - | 65,73,73 | 2.05 | 13 (20%) | 76,113,113 | 2.64 | 26 (34%) |
| 23 | CLA | d | 403[A] | - | 65,73,73 | 1.94 | 17 (26%) | 76,113,113 | 2.79 | 29 (38%) |
| 23 | CLA | d | 403[B] | - | 65,73,73 | 1.96 | 16 (24%) | 76,113,113 | 2.80 | 29 (38%) |
| 27 | GOL | o | 303 | - | 5,5,5 | 1.00 | 0 | 5,5,5 | 1.07 | 0 |
| 34 | HTG | c | 522 | - | 19,19,19 | 0.98 | 1 (5%) | 23,24,24 | 1.54 | 1 (4%) |
| 35 | DGD | c | 519 | - | 63,63,67 | 0.89 | 4 (6%) | 77,77,81 | 1.06 | 4 (5%) |
| 23 | CLA | B | 611 | - | 65,73,73 | 2.56 | 16 (24%) | 76,113,113 | 3.24 | 29 (38%) |
| 33 | LHG | d | 414[B] | - | 48,48,48 | 0.90 | 2 (4%) | 51,54,54 | 1.06 | 4 (7%) |
| 25 | BCR | H | 101 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.49 | 9 (16%) |
| 23 | CLA | B | 601 | 41 | 65,73,73 | 2.12 | 17 (26%) | 76,113,113 | 2.82 | 28 (36%) |
| 23 | CLA | c | 509 | - | 65,73,73 | 2.12 | 16 (24%) | 76,113,113 | 2.74 | 23 (30%) |
| 23 | CLA | C | 505 | - | 65,73,73 | 1.96 | 16 (24%) | 76,113,113 | 2.74 | 28 (36%) |
| 23 | CLA | C | 502 | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.63 | 26 (34%) |
| 27 | GOL | B | 627 | - | 5,5,5 | 0.89 | 0 | 5,5,5 | 1.04 | 1 (20%) |
| 27 | GOL | V | 203[A] | - | 5,5,5 | 1.22 | 0 | 5,5,5 | 0.91 | 0 |
| 23 | CLA | C | 507 | 41 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.74 | 24 (31%) |
| 23 | CLA | C | 509 | - | 65,73,73 | 2.11 | 17 (26%) | 76,113,113 | 2.82 | 29 (38%) |
| 25 | BCR | y | 101 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.60 | 11 (19%) |
| 23 | CLA | B | 616 | - | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.92 | 26 (34%) |
| 27 | GOL | O | 302 | - | 5,5,5 | 0.96 | 0 | 5,5,5 | 0.89 | 0 |
| 25 | BCR | d | 405 | - | 41,41,41 | 1.11 | 2 (4%) | 56,56,56 | 2.03 | 17 (30%) |
| 23 | CLA | c | 513 | - | 65,73,73 | 2.06 | 16 (24%) | 76,113,113 | 2.74 | 28 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | BCR | K | 102 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.40 | 10 (17%) |
| 23 | CLA | B | 615 | - | 65,73,73 | 2.03 | 15 (23%) | 76,113,113 | 2.84 | 28 (36%) |
| 34 | HTG | b | 622 | - | 19,19,19 | 1.22 | 2 (10%) | 23,24,24 | 1.98 | 7 (30%) |
| 31 | LMT | A | 417 | - | 36,36,36 | 0.93 | 2 (5%) | 47,47,47 | 1.01 | 1 (2%) |
| 23 | CLA | c | 506 | - | 65,73,73 | 2.00 | 16 (24%) | 76,113,113 | 2.74 | 25 (32%) |
| 32 | LMG | B | 621 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 1.31 | 4 (6%) |
| 31 | LMT | F | 101 | - | 36,36,36 | 1.07 | 1 (2%) | 47,47,47 | 1.05 | 2 (4%) |
| 34 | HTG | B | 625 | - | 19,19,19 | 1.06 | 2 (10%) | 23,24,24 | 1.21 | 3 (13%) |
| 23 | CLA | b | 615 | - | 65,73,73 | 1.99 | 17 (26%) | 76,113,113 | 2.76 | 30 (39%) |
| 31 | LMT | B | 631 | - | 25,25,36 | 0.88 | 1 (4%) | 30,30,47 | 1.19 | 3 (10%) |
| 32 | LMG | c | 501 | - | 51,51,55 | 0.92 | 2 (3%) | 59,59,63 | 1.17 | 4 (6%) |
| 31 | LMT | B | 630 | - | 36,36,36 | 1.04 | 3 (8%) | 47,47,47 | 1.14 | 4 (8%) |
| 23 | CLA | B | 613 | - | 65,73,73 | 2.03 | 17 (26%) | 76,113,113 | 2.70 | 30 (39%) |
| 34 | HTG | V | 202 | - | 11,11,19 | 0.26 | 0 | 15,15,24 | 1.20 | 1 (6%) |
| 23 | CLA | B | 608 | - | 65,73,73 | 1.93 | 17 (26%) | 76,113,113 | 2.87 | 31 (40%) |
| 23 | CLA | B | 614 | - | 65,73,73 | 2.04 | 17 (26%) | 76,113,113 | 2.97 | 29 (38%) |
| 26 | SQD | A | 412 | - | 53,54,54 | 1.01 | 3 (5%) | 62,65,65 | 1.21 | 7 (11%) |
| 23 | CLA | b | 607 | 41 | 65,73,73 | 1.95 | 17 (26%) | 76,113,113 | 2.77 | 26 (34%) |
| 26 | SQD | A | 410[B] | - | 53,54,54 | 0.94 | 3 (5%) | 62,65,65 | 1.76 | 11 (17%) |
| 23 | CLA | b | 609 | - | 65,73,73 | 2.01 | 15 (23%) | 76,113,113 | 2.83 | 29 (38%) |
| 34 | HTG | D | 411 | - | 16,16,19 | 1.04 | 1 (6%) | 20,21,24 | 1.54 | 1 (5%) |
| 33 | LHG | b | 629[A] | - | 48,48,48 | 0.85 | 3 (6%) | 51,54,54 | 1.03 | 4 (7%) |
| 33 | LHG | L | 101[A] | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 1.15 | 3 (5%) |
| 27 | GOL | l | 102[B] | - | 5,5,5 | 0.84 | 0 | 5,5,5 | 1.02 | 0 |
| 23 | CLA | C | 510 | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.92 | 30 (39%) |
| 23 | CLA | b | 602 | - | 65,73,73 | 2.05 | 17 (26%) | 76,113,113 | 2.91 | 34 (44%) |
| 23 | CLA | B | 612 | - | 65,73,73 | 2.03 | 17 (26%) | 76,113,113 | 2.94 | 27 (35%) |
| 34 | HTG | b | 623 | - | 19,19,19 | 1.07 | 1 (5%) | 23,24,24 | 1.87 | 2 (8%) |
| 24 | PHO | a | 414[B] | - | 51,69,69 | 1.91 | 8 (15%) | 47,99,99 | 1.97 | 11 (23%) |
| 32 | LMG | m | 101 | - | 51,51,55 | 0.89 | 2 (3%) | 59,59,63 | 1.23 | 4 (6%) |
| 26 | SQD | a | 409[A] | - | 53,54,54 | 0.95 | 3 (5%) | 62,65,65 | 1.77 | 13 (20%) |
| 27 | GOL | c | 527 | - | 5,5,5 | 1.12 | 0 | 5,5,5 | 0.97 | 0 |
| 23 | CLA | b | 612 | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.70 | 27 (35%) |
| 35 | DGD | c | 518[B] | - | 63,63,67 | 0.86 | 2 (3%) | 77,77,81 | 0.95 | 5 (6%) |
| 23 | CLA | D | 404 | - | 65,73,73 | 2.09 | 17 (26%) | 76,113,113 | 2.66 | 27 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 38 | HEM | F | 102 | 6,5 | 41,50,50 | 1.30 | 4 (9%) | 45,82,82 | 2.11 | 12 (26%) |
| 33 | LHG | D | 408[B] | - | 48,48,48 | 0.91 | 2 (4%) | 51,54,54 | 0.98 | 3 (5%) |
| 38 | HEM | f | 101 | 6,5 | 41,50,50 | 1.29 | 5 (12%) | 45,82,82 | 1.81 | 11 (24%) |
| 24 | PHO | A | 416[A] | - | 51,69,69 | 1.87 | 8 (15%) | 47,99,99 | 1.93 | 12 (25%) |
| 35 | DGD | c | 517[A] | - | 63,63,67 | 0.85 | 2 (3%) | 77,77,81 | 1.12 | 6 (7%) |
| 35 | DGD | C | 517[B] | - | 63,63,67 | 0.86 | 2 (3%) | 77,77,81 | 0.96 | 5 (6%) |
| 25 | BCR | t | 102 | - | 41,41,41 | 1.06 | 1 (2%) | 56,56,56 | 1.59 | 10 (17%) |
| 27 | GOL | v | 202[A] | - | 5,5,5 | 1.27 | 0 | 5,5,5 | 0.72 | 0 |
| 27 | GOL | v | 202[B] | - | 5,5,5 | 1.05 | 0 | 5,5,5 | 0.88 | 0 |
| 23 | CLA | a | 405[B] | 41 | 65,73,73 | 2.00 | 16 (24%) | 76,113,113 | 2.84 | 28 (36%) |
| 25 | BCR | A | 409 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.29 | 7 (12%) |
| 33 | LHG | D | 407[B] | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.98 | 3 (5%) |
| 23 | CLA | a | 407 | - | 65,73,73 | 1.95 | 17 (26%) | 76,113,113 | 2.85 | 29 (38%) |
| 32 | LMG | c | 521 | - | 51,51,55 | 1.01 | 2 (3%) | 59,59,63 | 1.36 | 7 (11%) |
| 32 | LMG | c | 520 | - | 51,51,55 | 0.90 | 2 (3%) | 59,59,63 | 1.12 | 6 (10%) |
| 34 | HTG | d | 411 | - | 16,16,19 | 0.96 | 1 (6%) | 20,21,24 | 1.64 | 1 (5%) |
| 23 | CLA | b | 614 | - | 65,73,73 | 2.00 | 16 (24%) | 76,113,113 | 2.84 | 28 (36%) |
| 23 | CLA | c | 508 | 41 | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.83 | 26 (34%) |
| 23 | CLA | A | 408 | - | 65,73,73 | 1.97 | 14 (21%) | 76,113,113 | 2.96 | 34 (44%) |
| 31 | LMT | t | 101 | - | 26,26,36 | 0.94 | 2 (7%) | 31,31,47 | 1.30 | 2 (6%) |
| 34 | HTG | B | 622 | - | 19,19,19 | 1.05 | 2 (10%) | 23,24,24 | 1.56 | 5 (21%) |
| 29 | PL9 | a | 412[B] | - | 55,55,55 | 0.64 | 2 (3%) | 68,69,69 | 1.97 | 22 (32%) |
| 23 | CLA | c | 505 | 41 | 65,73,73 | 2.10 | 17 (26%) | 76,113,113 | 2.71 | 27 (35%) |
| 33 | LHG | d | 414[A] | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 1.12 | 4 (7%) |
| 23 | CLA | c | 507 | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.79 | 29 (38%) |
| 23 | CLA | c | 502 | - | 65,73,73 | 2.03 | 17 (26%) | 76,113,113 | 2.84 | 26 (34%) |
| 23 | CLA | c | 510 | - | 65,73,73 | 2.06 | 16 (24%) | 76,113,113 | 2.80 | 29 (38%) |
| 26 | SQD | f | 102 | - | 42,43,54 | 1.19 | 3 (7%) | 51,54,65 | 1.52 | 11 (21%) |
| 27 | GOL | B | 629 | - | 5,5,5 | 0.99 | 0 | 5,5,5 | 0.96 | 0 |
| 23 | CLA | A | 404[A] | - | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.77 | 32 (42%) |
| 23 | CLA | A | 404[B] | - | 65,73,73 | 2.08 | 16 (24%) | 76,113,113 | 2.80 | 29 (38%) |
| 25 | BCR | c | 515 | - | 41,41,41 | 0.99 | 1 (2%) | 56,56,56 | 1.71 | 15 (26%) |
| 27 | GOL | O | 303 | - | 5,5,5 | 0.82 | 0 | 5,5,5 | 1.14 | 1 (20%) |
| 29 | PL9 | D | 406[A] | - | 55,55,55 | 0.62 | 2 (3%) | 68,69,69 | 1.64 | 18 (26%) |
| 29 | PL9 | D | 406[B] | - | 55,55,55 | 0.61 | 1 (1%) | 68,69,69 | 1.68 | 15 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 33 | LHG | a | 418[B] | - | 41,41,48 | 1.04 | 2 (4%) | 44,47,54 | 0.93 | 2 (4%) |
| 23 | CLA | C | 501 | - | 65,73,73 | 1.95 | 16 (24%) | 76,113,113 | 2.85 | 30 (39%) |
| 23 | CLA | B | 602 | - | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.78 | 26 (34%) |
| 23 | CLA | d | 402[B] | 41 | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.87 | 28 (36%) |
| 23 | CLA | A | 405[B] | 41 | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.84 | 29 (38%) |
| 32 | LMG | z | 101 | - | 39,39,55 | 1.09 | 2 (5%) | 47,47,63 | 1.06 | 3 (6%) |
| 23 | CLA | B | 609 | - | 65,73,73 | 1.99 | 15 (23%) | 76,113,113 | 2.74 | 26 (34%) |
| 27 | GOL | D | 402 | - | 5,5,5 | 1.64 | 2 (40%) | 5,5,5 | 1.01 | 1 (20%) |
| 27 | GOL | a | 416 | - | 5,5,5 | 1.03 | 0 | 5,5,5 | 1.02 | 0 |
| 26 | SQD | A | 410[A] | - | 53,54,54 | 0.93 | 3 (5%) | 62,65,65 | 1.81 | 10 (16%) |
| 27 | GOL | C | 522[A] | - | 5,5,5 | 1.18 | 0 | 5,5,5 | 0.83 | 0 |
| 27 | GOL | C | 522[B] | - | 5,5,5 | 1.08 | 0 | 5,5,5 | 0.86 | 0 |
| 23 | CLA | B | 603 | - | 65,73,73 | 2.05 | 16 (24%) | 76,113,113 | 2.92 | 29 (38%) |
| 32 | LMG | C | 519 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 1.11 | 4 (6%) |
| 23 | CLA | C | 508 | - | 65,73,73 | 2.13 | 17 (26%) | 76,113,113 | 2.79 | 25 (32%) |
| 23 | CLA | b | 605 | - | 65,73,73 | 1.94 | 15 (23%) | 76,113,113 | 2.94 | 28 (36%) |
| 23 | CLA | b | 611 | - | 65,73,73 | 1.95 | 17 (26%) | 76,113,113 | 2.92 | 27 (35%) |
| 25 | BCR | b | 618 | - | 41,41,41 | 0.98 | 1 (2%) | 56,56,56 | 1.27 | 7 (12%) |
| 34 | HTG | B | 623 | - | 19,19,19 | 0.83 | 2 (10%) | 23,24,24 | 1.46 | 1 (4%) |
| 23 | CLA | D | 403[B] | - | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.80 | 29 (38%) |
| 25 | BCR | h | 101 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.46 | 10 (17%) |
| 23 | CLA | b | 601 | 41 | 65,73,73 | 2.12 | 15 (23%) | 76,113,113 | 2.76 | 27 (35%) |
| 27 | GOL | l | 102[A] | - | 5,5,5 | 0.96 | 0 | 5,5,5 | 0.97 | 0 |
| 40 | HEC | V | 201 | 16 | 32,50,50 | 1.99 | 4 (12%) | 24,82,82 | 2.11 | 7 (29%) |
| 24 | PHO | a | 414[A] | - | 51,69,69 | 1.86 | 9 (17%) | 47,99,99 | 1.99 | 13 (27%) |
| 32 | LMG | d | 412 | 39 | 51,51,55 | 0.89 | 2 (3%) | 59,59,63 | 1.11 | 4 (6%) |
| 23 | CLA | b | 616 | - | 65,73,73 | 2.00 | 15 (23%) | 76,113,113 | 2.89 | 29 (38%) |
| 35 | DGD | c | 518[A] | - | 63,63,67 | 0.84 | 2 (3%) | 77,77,81 | 0.97 | 5 (6%) |

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 |
|-----|------|-------|--------|------|---------|-------------|---------|
| 25 | BCR | B | 617 | - | - | 2/29/63/63 | 0/2/2/2 |
| 33 | LHG | D | 408[A] | - | - | 14/53/53/53 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 26 | SQD | B | 620 | - | - | 14/49/69/69 | 0/1/1/1 |
| 23 | CLA | B | 604 | - | 1/1/15/20 | 1/37/115/115 | - |
| 27 | GOL | c | 526[B] | - | - | 0/4/4/4 | - |
| 35 | DGD | C | 517[A] | - | - | 15/51/91/95 | 0/2/2/2 |
| 31 | LMT | m | 103 | - | - | 5/21/61/61 | 0/2/2/2 |
| 23 | CLA | a | 405[A] | 41 | - | 5/37/115/115 | - |
| 26 | SQD | b | 620 | - | - | 16/49/69/69 | 0/1/1/1 |
| 33 | LHG | D | 407[A] | - | - | 16/53/53/53 | - |
| 35 | DGD | C | 518 | - | - | 19/51/91/95 | 0/2/2/2 |
| 23 | CLA | A | 406[B] | 41 | - | 4/37/115/115 | - |
| 31 | LMT | M | 102 | - | - | 6/21/61/61 | 0/2/2/2 |
| 25 | BCR | B | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | LHG | A | 419[B] | - | - | 14/53/53/53 | - |
| 33 | LHG | d | 408[A] | - | - | 11/53/53/53 | - |
| 33 | LHG | d | 408[B] | - | - | 14/53/53/53 | - |
| 34 | HTG | b | 625 | - | - | 3/10/30/30 | 0/1/1/1 |
| 29 | PL9 | a | 412[A] | - | - | 14/53/73/73 | 0/1/1/1 |
| 27 | GOL | D | 413 | - | - | 4/4/4/4 | - |
| 25 | BCR | T | 101 | - | - | 1/29/63/63 | 0/2/2/2 |
| 25 | BCR | a | 408 | - | - | 2/29/63/63 | 0/2/2/2 |
| 29 | PL9 | d | 406[B] | - | - | 6/53/73/73 | 0/1/1/1 |
| 23 | CLA | B | 606 | - | 1/1/15/20 | 9/37/115/115 | - |
| 32 | LMG | C | 520 | - | - | 13/46/66/70 | 0/1/1/1 |
| 23 | CLA | c | 514 | - | 1/1/15/20 | 10/37/115/115 | - |
| 25 | BCR | k | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | PL9 | A | 414[A] | - | - | 15/53/73/73 | 0/1/1/1 |
| 29 | PL9 | A | 414[B] | - | - | 15/53/73/73 | 0/1/1/1 |
| 23 | CLA | b | 606 | - | 1/1/15/20 | 11/37/115/115 | - |
| 33 | LHG | E | 101[B] | - | - | 22/46/46/53 | - |
| 23 | CLA | a | 404[A] | - | 1/1/15/20 | 3/37/115/115 | - |
| 23 | CLA | a | 404[B] | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | B | 605 | - | 1/1/15/20 | 5/37/115/115 | - |
| 33 | LHG | a | 418[A] | - | - | 16/46/46/53 | - |
| 23 | CLA | b | 604 | - | 1/1/15/20 | 8/37/115/115 | - |
| 26 | SQD | F | 103 | - | - | 14/38/58/69 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23 | CLA | d | 402[A] | 41 | 1/1/15/20 | 8/37/115/115 | - |
| 23 | CLA | A | 405[A] | 41 | - | 4/37/115/115 | - |
| 35 | DGD | h | 102 | - | - | 15/51/91/95 | 0/2/2/2 |
| 27 | GOL | a | 417 | - | - | 0/4/4/4 | - |
| 32 | LMG | A | 418 | - | - | 14/46/66/70 | 0/1/1/1 |
| 23 | CLA | b | 613 | - | 1/1/15/20 | 3/37/115/115 | - |
| 23 | CLA | C | 504 | 41 | 1/1/15/20 | 6/37/115/115 | - |
| 25 | BCR | b | 619 | - | - | 2/29/63/63 | 0/2/2/2 |
| 27 | GOL | d | 413 | - | - | 4/4/4/4 | - |
| 35 | DGD | C | 516[B] | - | - | 14/51/91/95 | 0/2/2/2 |
| 23 | CLA | D | 403[A] | - | 1/1/15/20 | 0/37/115/115 | - |
| 27 | GOL | b | 624 | - | - | 2/4/4/4 | - |
| 27 | GOL | b | 628 | - | - | 0/4/4/4 | - |
| 23 | CLA | C | 512 | - | 1/1/15/20 | 9/37/115/115 | - |
| 24 | PHO | A | 407[B] | - | - | 2/37/103/103 | 0/5/6/6 |
| 23 | CLA | d | 404 | - | 1/1/15/20 | 8/37/115/115 | - |
| 24 | PHO | a | 406[B] | - | - | 5/37/103/103 | 0/5/6/6 |
| 23 | CLA | c | 511 | - | 1/1/15/20 | 10/37/115/115 | - |
| 27 | GOL | c | 526[A] | - | - | 0/4/4/4 | - |
| 31 | LMT | A | 420 | - | - | 16/21/61/61 | 0/2/2/2 |
| 23 | CLA | C | 511 | 3 | 1/1/15/20 | 4/37/115/115 | - |
| 25 | BCR | C | 514 | - | - | 1/29/63/63 | 0/2/2/2 |
| 23 | CLA | c | 504 | - | 1/1/15/20 | 1/37/115/115 | - |
| 23 | CLA | A | 406[A] | 41 | - | 5/37/115/115 | - |
| 34 | HTG | C | 521 | - | - | 0/10/30/30 | 0/1/1/1 |
| 31 | LMT | e | 101 | - | - | 15/21/61/61 | 0/2/2/2 |
| 25 | BCR | D | 405 | - | - | 4/29/63/63 | 0/2/2/2 |
| 27 | GOL | V | 203[B] | - | - | 2/4/4/4 | - |
| 33 | LHG | A | 419[A] | - | - | 10/53/53/53 | - |
| 35 | DGD | H | 102 | - | - | 9/51/91/95 | 0/2/2/2 |
| 31 | LMT | B | 628 | - | - | 12/21/61/61 | 0/2/2/2 |
| 23 | CLA | c | 512 | 3 | 1/1/15/20 | 6/37/115/115 | - |
| 29 | PL9 | d | 406[A] | - | - | 6/53/73/73 | 0/1/1/1 |
| 31 | LMT | M | 101 | - | - | 4/21/61/61 | 0/2/2/2 |
| 25 | BCR | B | 619 | - | - | 0/29/63/63 | 0/2/2/2 |
| 23 | CLA | C | 506 | - | 1/1/15/20 | 12/37/115/115 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|--------------|---------|
| 23 | CLA | b | 603 | - | 1/1/15/20 | 6/37/115/115 | - |
| 33 | LHG | E | 101[A] | - | - | 22/46/46/53 | - |
| 31 | LMT | a | 415 | - | - | 10/21/61/61 | 0/2/2/2 |
| 23 | CLA | b | 610 | 41 | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | C | 503 | - | 1/1/15/20 | 2/37/115/115 | - |
| 23 | CLA | B | 610 | 41 | 1/1/15/20 | 8/37/115/115 | - |
| 25 | BCR | b | 617 | - | - | 2/29/63/63 | 0/2/2/2 |
| 33 | LHG | d | 407[A] | - | - | 13/53/53/53 | - |
| 33 | LHG | d | 407[B] | - | - | 15/53/53/53 | - |
| 33 | LHG | b | 629[B] | - | - | 19/53/53/53 | - |
| 25 | BCR | C | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | BCR | Y | 101 | - | - | 2/29/63/63 | 0/2/2/2 |
| 33 | LHG | L | 101[B] | - | - | 17/53/53/53 | - |
| 35 | DGD | C | 516[A] | - | - | 11/51/91/95 | 0/2/2/2 |
| 40 | HEC | v | 201 | 16 | - | 2/10/54/54 | - |
| 25 | BCR | c | 516 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | GOL | o | 302 | - | - | 2/4/4/4 | - |
| 23 | CLA | B | 607 | 41 | 1/1/15/20 | 3/37/115/115 | - |
| 23 | CLA | b | 608 | - | - | 5/37/115/115 | - |
| 26 | SQD | a | 409[B] | - | - | 10/49/69/69 | 0/1/1/1 |
| 26 | SQD | a | 410 | - | - | 13/49/69/69 | 0/1/1/1 |
| 27 | GOL | B | 624 | - | - | 3/4/4/4 | - |
| 23 | CLA | C | 513 | - | 1/1/15/20 | 7/37/115/115 | - |
| 31 | LMT | b | 621 | - | - | 8/17/37/61 | 0/1/1/2 |
| 24 | PHO | A | 416[B] | - | - | 2/37/103/103 | 0/5/6/6 |
| 35 | DGD | c | 517[B] | - | - | 19/51/91/95 | 0/2/2/2 |
| 31 | LMT | b | 627 | - | - | 11/17/37/61 | 0/1/1/2 |
| 32 | LMG | Z | 101 | - | - | 10/31/51/70 | 0/1/1/1 |
| 24 | PHO | A | 407[A] | - | - | 4/37/103/103 | 0/5/6/6 |
| 27 | GOL | A | 411 | - | - | 2/4/4/4 | - |
| 32 | LMG | D | 412 | 39 | - | 8/46/66/70 | 0/1/1/1 |
| 24 | PHO | a | 406[A] | - | - | 6/37/103/103 | 0/5/6/6 |
| 23 | CLA | c | 503 | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | d | 403[A] | - | 1/1/15/20 | 2/37/115/115 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23 | CLA | d | 403[B] | - | 1/1/15/20 | 4/37/115/115 | - |
| 27 | GOL | o | 303 | - | - | 3/4/4/4 | - |
| 34 | HTG | c | 522 | - | - | 2/10/30/30 | 0/1/1/1 |
| 35 | DGD | c | 519 | - | - | 12/51/91/95 | 0/2/2/2 |
| 23 | CLA | B | 611 | - | 1/1/15/20 | 1/37/115/115 | - |
| 33 | LHG | d | 414[B] | - | - | 12/53/53/53 | - |
| 25 | BCR | H | 101 | - | - | 3/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 601 | 41 | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CLA | c | 509 | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | C | 505 | - | 1/1/15/20 | 6/37/115/115 | - |
| 23 | CLA | C | 502 | - | 1/1/15/20 | 9/37/115/115 | - |
| 27 | GOL | B | 627 | - | - | 0/4/4/4 | - |
| 27 | GOL | V | 203[A] | - | - | 2/4/4/4 | - |
| 23 | CLA | C | 507 | 41 | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | C | 509 | - | 1/1/15/20 | 9/37/115/115 | - |
| 25 | BCR | y | 101 | - | - | 4/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 616 | - | 1/1/15/20 | 5/37/115/115 | - |
| 27 | GOL | O | 302 | - | - | 2/4/4/4 | - |
| 25 | BCR | d | 405 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CLA | c | 513 | - | 1/1/15/20 | 14/37/115/115 | - |
| 25 | BCR | K | 102 | - | - | 2/29/63/63 | 0/2/2/2 |
| 23 | CLA | B | 615 | - | 1/1/15/20 | 8/37/115/115 | - |
| 34 | HTG | b | 622 | - | - | 5/10/30/30 | 0/1/1/1 |
| 31 | LMT | A | 417 | - | - | 7/21/61/61 | 0/2/2/2 |
| 23 | CLA | c | 506 | - | 1/1/15/20 | 7/37/115/115 | - |
| 32 | LMG | B | 621 | - | - | 18/46/66/70 | 0/1/1/1 |
| 31 | LMT | F | 101 | - | - | 8/21/61/61 | 0/2/2/2 |
| 34 | HTG | B | 625 | - | - | 4/10/30/30 | 0/1/1/1 |
| 23 | CLA | b | 615 | - | 1/1/15/20 | 7/37/115/115 | - |
| 31 | LMT | B | 631 | - | - | 11/17/37/61 | 0/1/1/2 |
| 32 | LMG | c | 501 | - | - | 13/46/66/70 | 0/1/1/1 |
| 31 | LMT | B | 630 | - | - | 10/21/61/61 | 0/2/2/2 |
| 23 | CLA | B | 613 | - | 1/1/15/20 | 9/37/115/115 | - |
| 34 | HTG | V | 202 | - | - | 0/2/19/30 | 0/1/1/1 |
| 23 | CLA | B | 608 | - | - | 3/37/115/115 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23 | CLA | B | 614 | - | 1/1/15/20 | 14/37/115/115 | - |
| 26 | SQD | A | 412 | - | - | 16/49/69/69 | 0/1/1/1 |
| 23 | CLA | b | 607 | 41 | 1/1/15/20 | 4/37/115/115 | - |
| 26 | SQD | A | 410[B] | - | - | 12/49/69/69 | 0/1/1/1 |
| 23 | CLA | b | 609 | - | 1/1/15/20 | 1/37/115/115 | - |
| 34 | HTG | D | 411 | - | - | 3/7/27/30 | 0/1/1/1 |
| 33 | LHG | b | 629[A] | - | - | 20/53/53/53 | - |
| 33 | LHG | L | 101[A] | - | - | 19/53/53/53 | - |
| 27 | GOL | l | 102[B] | - | - | 1/4/4/4 | - |
| 23 | CLA | C | 510 | - | 1/1/15/20 | 13/37/115/115 | - |
| 23 | CLA | b | 602 | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | B | 612 | - | 1/1/15/20 | 4/37/115/115 | - |
| 34 | HTG | b | 623 | - | - | 4/10/30/30 | 0/1/1/1 |
| 24 | PHO | a | 414[B] | - | - | 0/37/103/103 | 0/5/6/6 |
| 32 | LMG | m | 101 | - | - | 11/46/66/70 | 0/1/1/1 |
| 26 | SQD | a | 409[A] | - | - | 10/49/69/69 | 0/1/1/1 |
| 27 | GOL | c | 527 | - | - | 3/4/4/4 | - |
| 23 | CLA | b | 612 | - | 1/1/15/20 | 3/37/115/115 | - |
| 35 | DGD | c | 518[B] | - | - | 17/51/91/95 | 0/2/2/2 |
| 23 | CLA | D | 404 | - | 1/1/15/20 | 12/37/115/115 | - |
| 38 | HEM | F | 102 | 6,5 | - | 4/12/54/54 | - |
| 33 | LHG | D | 408[B] | - | - | 13/53/53/53 | - |
| 38 | HEM | f | 101 | 6,5 | - | 6/12/54/54 | - |
| 24 | PHO | A | 416[A] | - | - | 1/37/103/103 | 0/5/6/6 |
| 35 | DGD | c | 517[A] | - | - | 20/51/91/95 | 0/2/2/2 |
| 35 | DGD | C | 517[B] | - | - | 14/51/91/95 | 0/2/2/2 |
| 25 | BCR | t | 102 | - | - | 5/29/63/63 | 0/2/2/2 |
| 27 | GOL | v | 202[A] | - | - | 1/4/4/4 | - |
| 27 | GOL | v | 202[B] | - | - | 2/4/4/4 | - |
| 23 | CLA | a | 405[B] | 41 | - | 5/37/115/115 | - |
| 25 | BCR | A | 409 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | LHG | D | 407[B] | - | - | 16/53/53/53 | - |
| 23 | CLA | a | 407 | - | 1/1/15/20 | 9/37/115/115 | - |
| 32 | LMG | c | 521 | - | - | 12/46/66/70 | 0/1/1/1 |
| 32 | LMG | c | 520 | - | - | 12/46/66/70 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 34 | HTG | d | 411 | - | - | 1/7/27/30 | 0/1/1/1 |
| 23 | CLA | b | 614 | - | 1/1/15/20 | 15/37/115/115 | - |
| 23 | CLA | c | 508 | 41 | 1/1/15/20 | 7/37/115/115 | - |
| 23 | CLA | A | 408 | - | 1/1/15/20 | 8/37/115/115 | - |
| 31 | LMT | t | 101 | - | - | 10/17/38/61 | 0/1/1/2 |
| 34 | HTG | B | 622 | - | - | 3/10/30/30 | 0/1/1/1 |
| 29 | PL9 | a | 412[B] | - | - | 15/53/73/73 | 0/1/1/1 |
| 23 | CLA | c | 505 | 41 | 1/1/15/20 | 6/37/115/115 | - |
| 33 | LHG | d | 414[A] | - | - | 13/53/53/53 | - |
| 23 | CLA | c | 507 | - | 1/1/15/20 | 6/37/115/115 | - |
| 23 | CLA | c | 502 | - | 1/1/15/20 | 2/37/115/115 | - |
| 23 | CLA | c | 510 | - | 1/1/15/20 | 15/37/115/115 | - |
| 26 | SQD | f | 102 | - | - | 13/38/58/69 | 0/1/1/1 |
| 27 | GOL | B | 629 | - | - | 4/4/4/4 | - |
| 23 | CLA | A | 404[A] | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | A | 404[B] | - | 1/1/15/20 | 7/37/115/115 | - |
| 25 | BCR | c | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | GOL | O | 303 | - | - | 2/4/4/4 | - |
| 29 | PL9 | D | 406[A] | - | - | 8/53/73/73 | 0/1/1/1 |
| 29 | PL9 | D | 406[B] | - | - | 9/53/73/73 | 0/1/1/1 |
| 33 | LHG | a | 418[B] | - | - | 16/46/46/53 | - |
| 23 | CLA | C | 501 | - | 1/1/15/20 | 5/37/115/115 | - |
| 23 | CLA | B | 602 | - | 1/1/15/20 | 7/37/115/115 | - |
| 23 | CLA | A | 405[B] | 41 | 1/1/15/20 | 3/37/115/115 | - |
| 23 | CLA | d | 402[B] | 41 | 1/1/15/20 | 3/37/115/115 | - |
| 32 | LMG | z | 101 | - | - | 9/34/54/70 | 0/1/1/1 |
| 23 | CLA | B | 609 | - | 1/1/15/20 | 1/37/115/115 | - |
| 27 | GOL | D | 402 | - | - | 2/4/4/4 | - |
| 27 | GOL | a | 416 | - | - | 2/4/4/4 | - |
| 26 | SQD | A | 410[A] | - | - | 12/49/69/69 | 0/1/1/1 |
| 27 | GOL | C | 522[A] | - | - | 0/4/4/4 | - |
| 27 | GOL | C | 522[B] | - | - | 0/4/4/4 | - |
| 23 | CLA | B | 603 | - | 1/1/15/20 | 6/37/115/115 | - |
| 32 | LMG | C | 519 | - | - | 10/46/66/70 | 0/1/1/1 |
| 23 | CLA | b | 605 | - | 1/1/15/20 | 7/37/115/115 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23 | CLA | C | 508 | - | - | 3/37/115/115 | - |
| 23 | CLA | b | 611 | - | 1/1/15/20 | 3/37/115/115 | - |
| 25 | BCR | b | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 34 | HTG | B | 623 | - | - | 2/10/30/30 | 0/1/1/1 |
| 23 | CLA | D | 403[B] | - | 1/1/15/20 | 2/37/115/115 | - |
| 25 | BCR | h | 101 | - | - | 1/29/63/63 | 0/2/2/2 |
| 23 | CLA | b | 601 | 41 | 1/1/15/20 | 18/37/115/115 | - |
| 27 | GOL | l | 102[A] | - | - | 2/4/4/4 | - |
| 40 | HEC | V | 201 | 16 | - | 2/10/54/54 | - |
| 24 | PHO | a | 414[A] | - | - | 2/37/103/103 | 0/5/6/6 |
| 32 | LMG | d | 412 | 39 | - | 10/46/66/70 | 0/1/1/1 |
| 23 | CLA | b | 616 | - | 1/1/15/20 | 9/37/115/115 | - |
| 35 | DGD | c | 518[A] | - | - | 17/51/91/95 | 0/2/2/2 |

The worst 5 of 1554 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | B | 611 | CLA | C3B-C2B | 10.49 | 1.54 | 1.40 |
| 23 | B | 612 | CLA | C3B-C2B | 7.21 | 1.50 | 1.40 |
| 23 | C | 508 | CLA | C3B-C2B | 6.98 | 1.50 | 1.40 |
| 23 | C | 511 | CLA | C3B-C2B | 6.66 | 1.49 | 1.40 |
| 23 | C | 509 | CLA | C3B-C2B | 6.63 | 1.49 | 1.40 |

The worst 5 of 3086 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 23 | B | 611 | CLA | C1D-ND-C4D | -12.14 | 97.71 | 106.33 |
| 23 | B | 612 | CLA | C1D-ND-C4D | -10.81 | 98.65 | 106.33 |
| 23 | b | 605 | CLA | C1D-ND-C4D | -10.51 | 98.87 | 106.33 |
| 23 | B | 611 | CLA | C2D-C1D-ND | 10.51 | 117.85 | 110.10 |
| 23 | a | 405[B] | CLA | C1D-ND-C4D | -10.23 | 99.07 | 106.33 |

5 of 70 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|--------|------|------|
| 23 | A | 404[A] | CLA | ND |
| 23 | A | 404[B] | CLA | ND |
| 23 | A | 405[B] | CLA | ND |
| 23 | A | 408 | CLA | ND |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | B | 601 | CLA | ND |

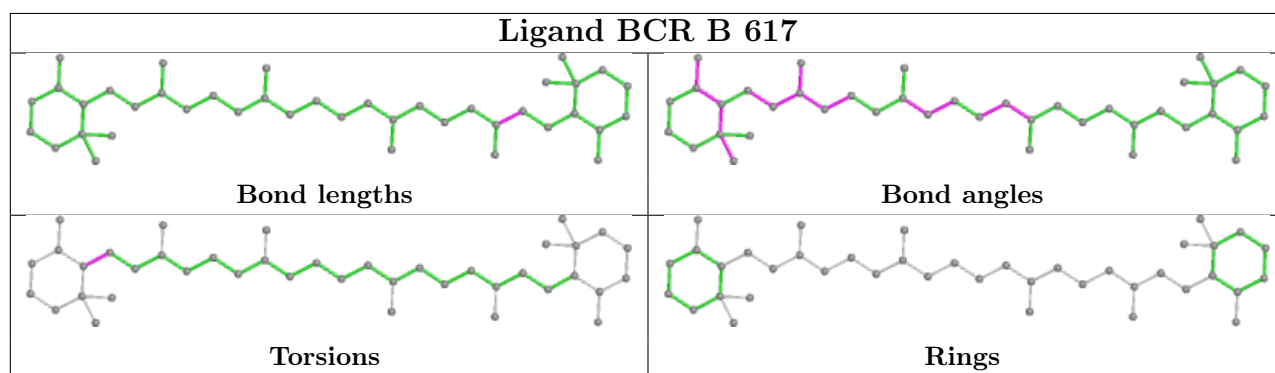
5 of 1620 torsion outliers are listed below:

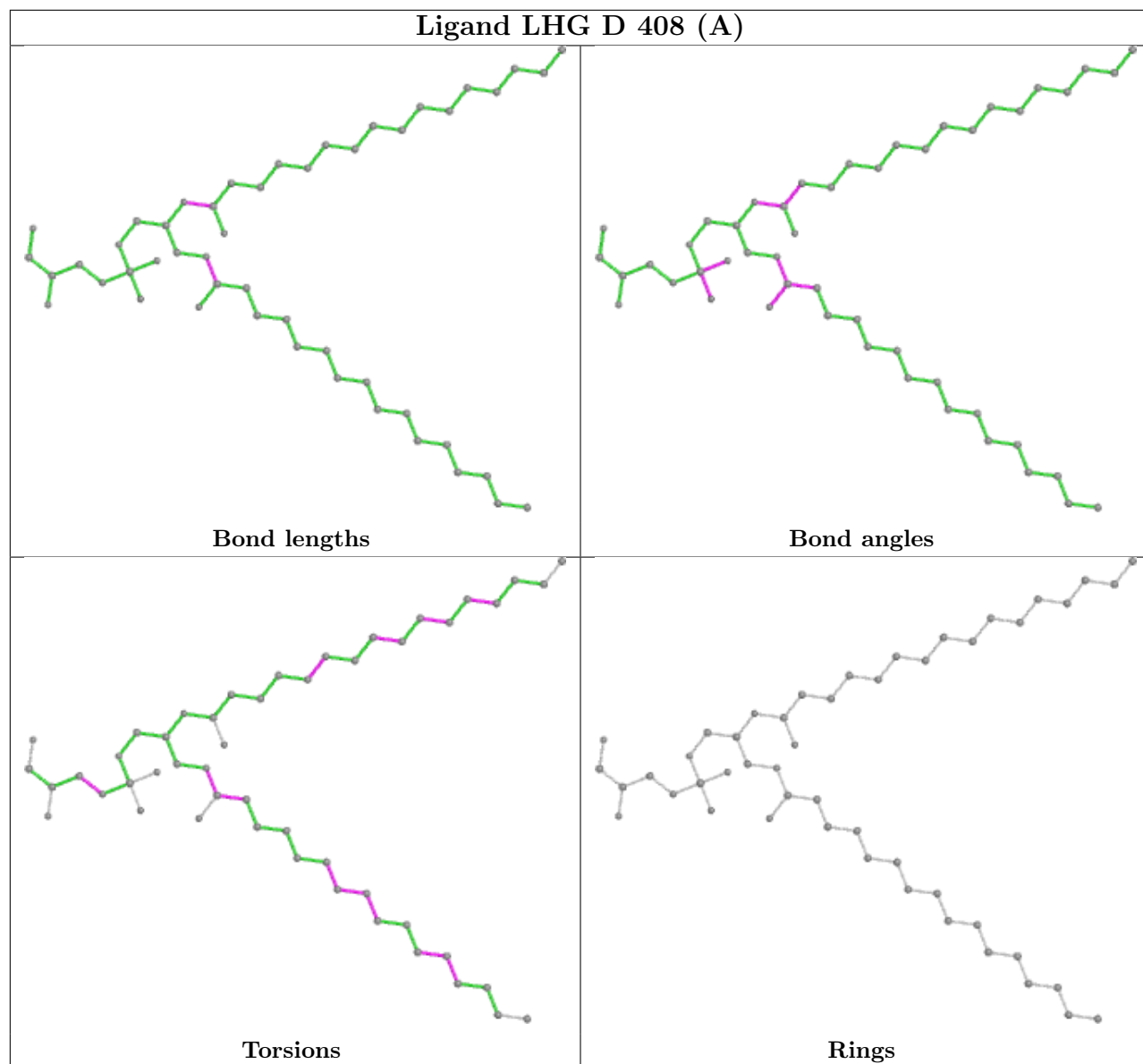
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | A | 408 | CLA | C4-C3-C5-C6 |
| 23 | B | 614 | CLA | CHA-CBD-CGD-O1D |
| 23 | B | 614 | CLA | CHA-CBD-CGD-O2D |
| 23 | B | 614 | CLA | CAD-CBD-CGD-O1D |
| 23 | B | 614 | CLA | CAD-CBD-CGD-O2D |

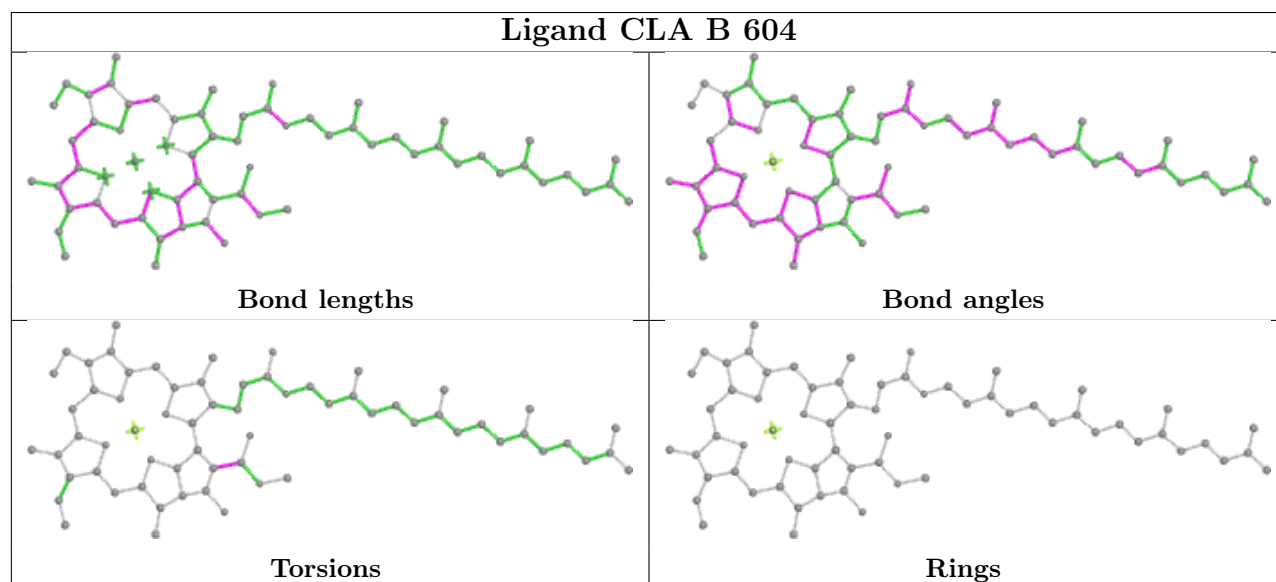
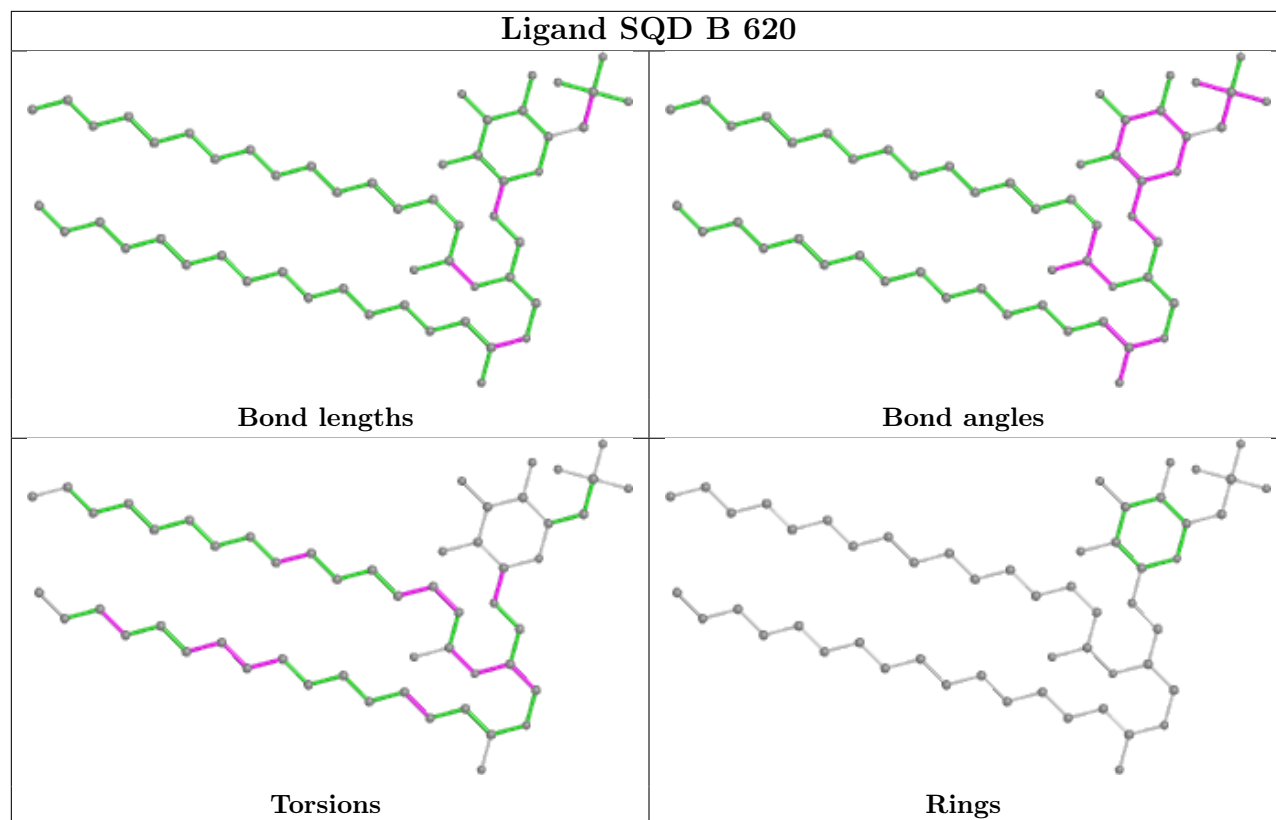
There are no ring outliers.

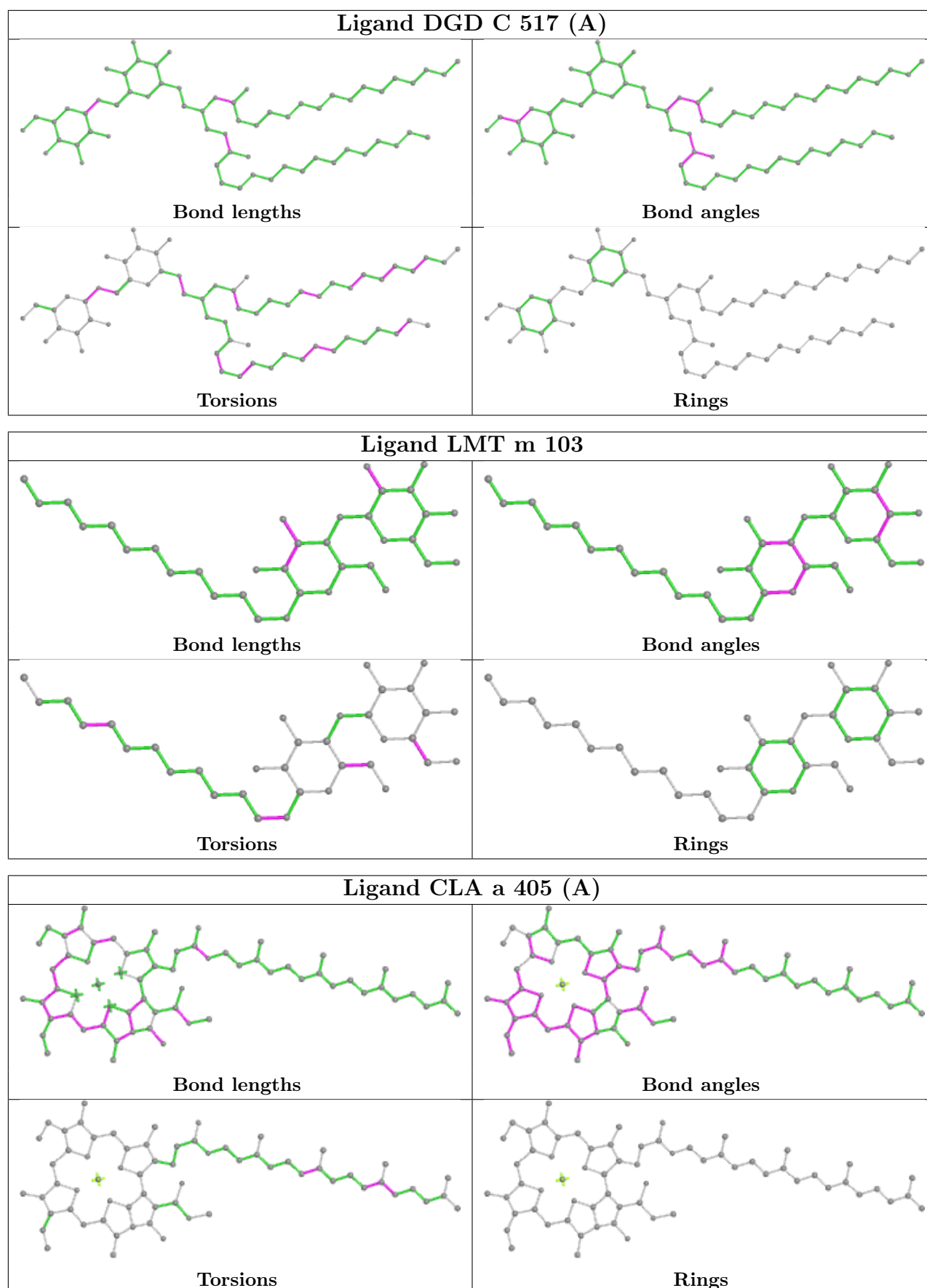
No monomer is involved in short contacts.

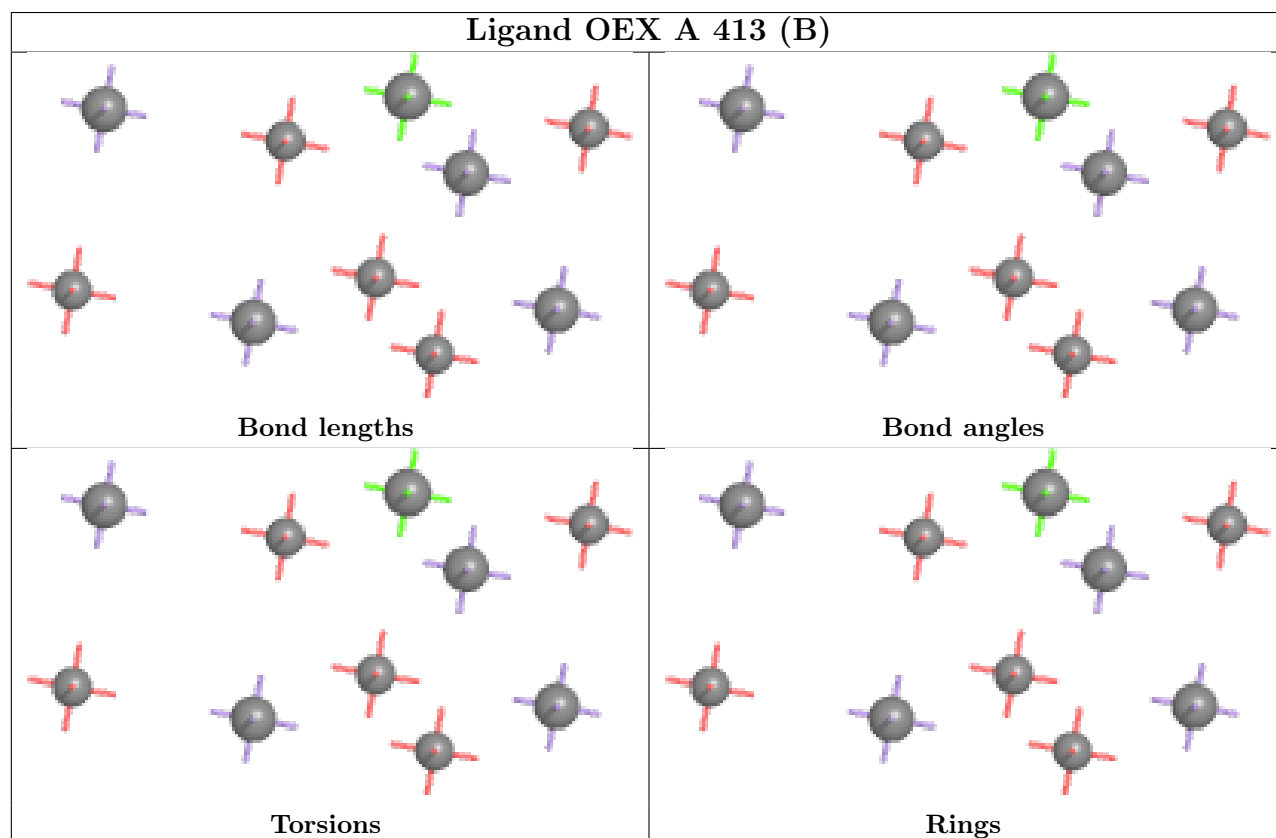
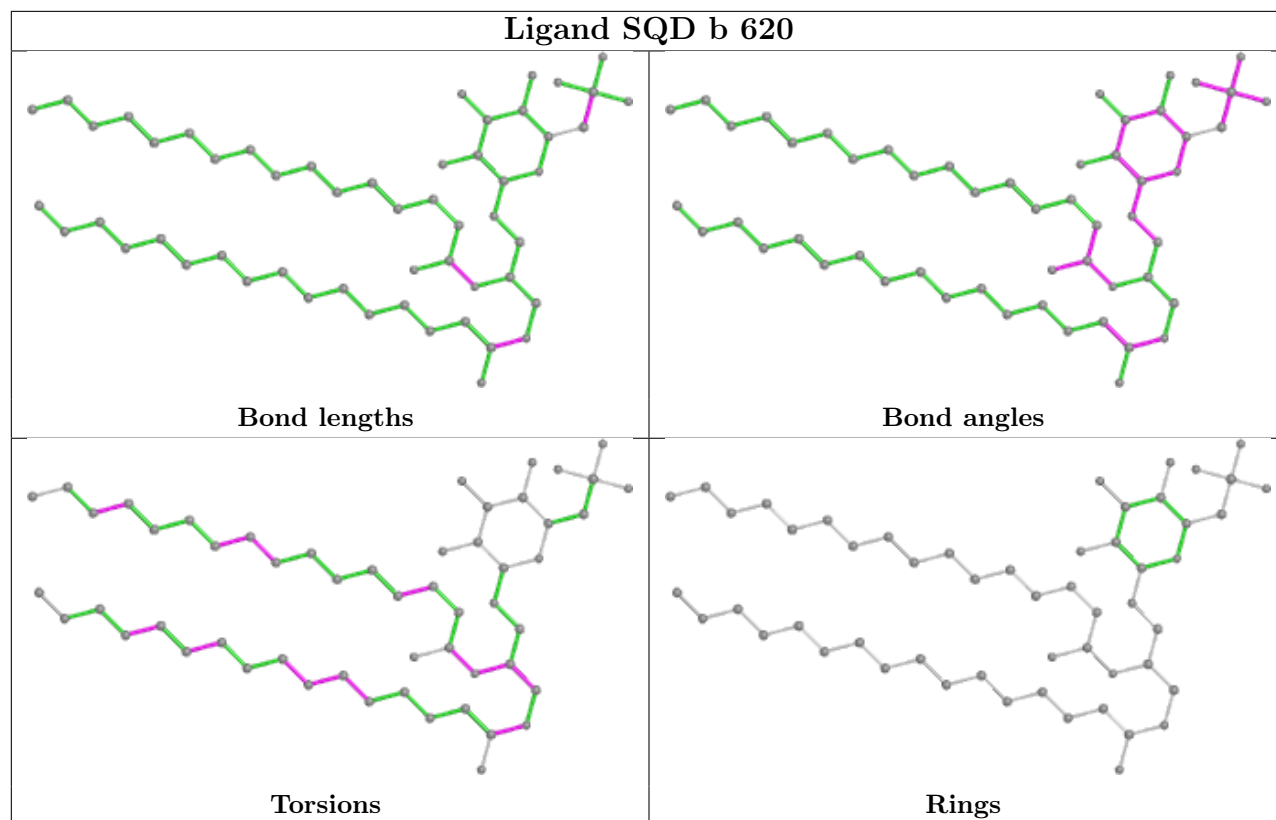
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

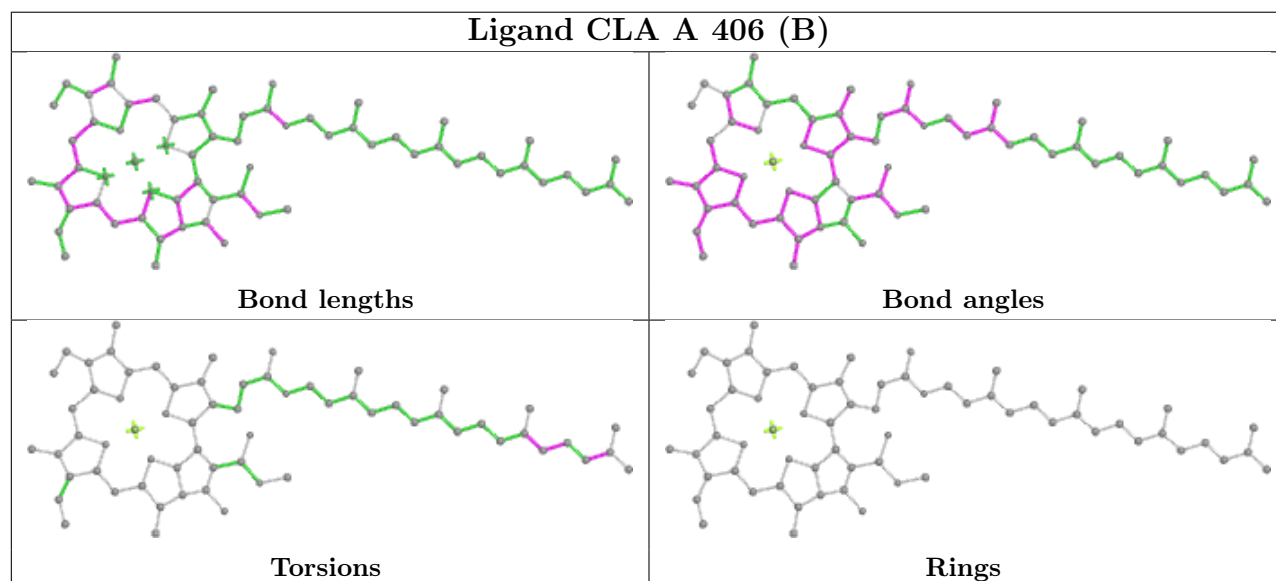
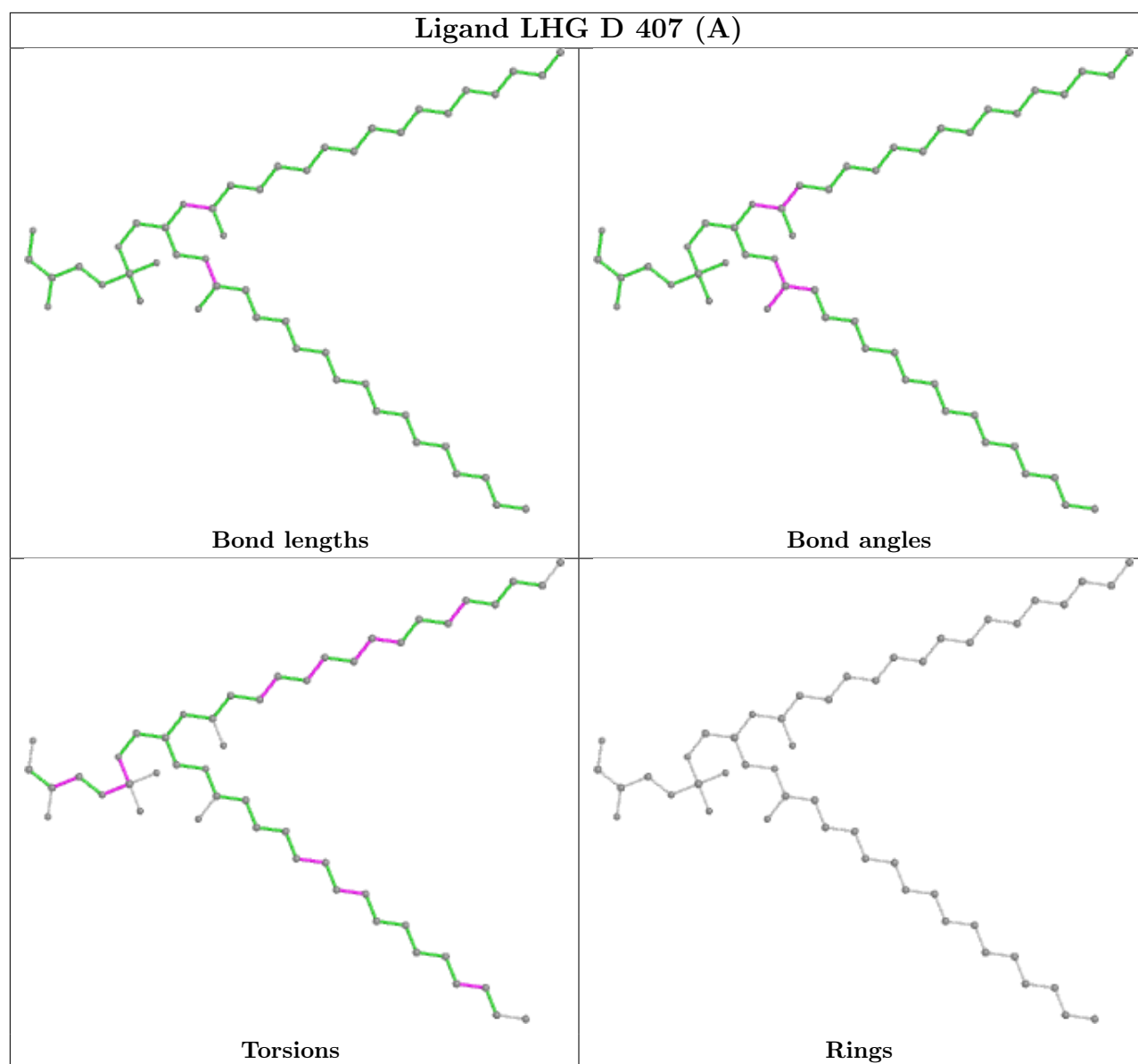


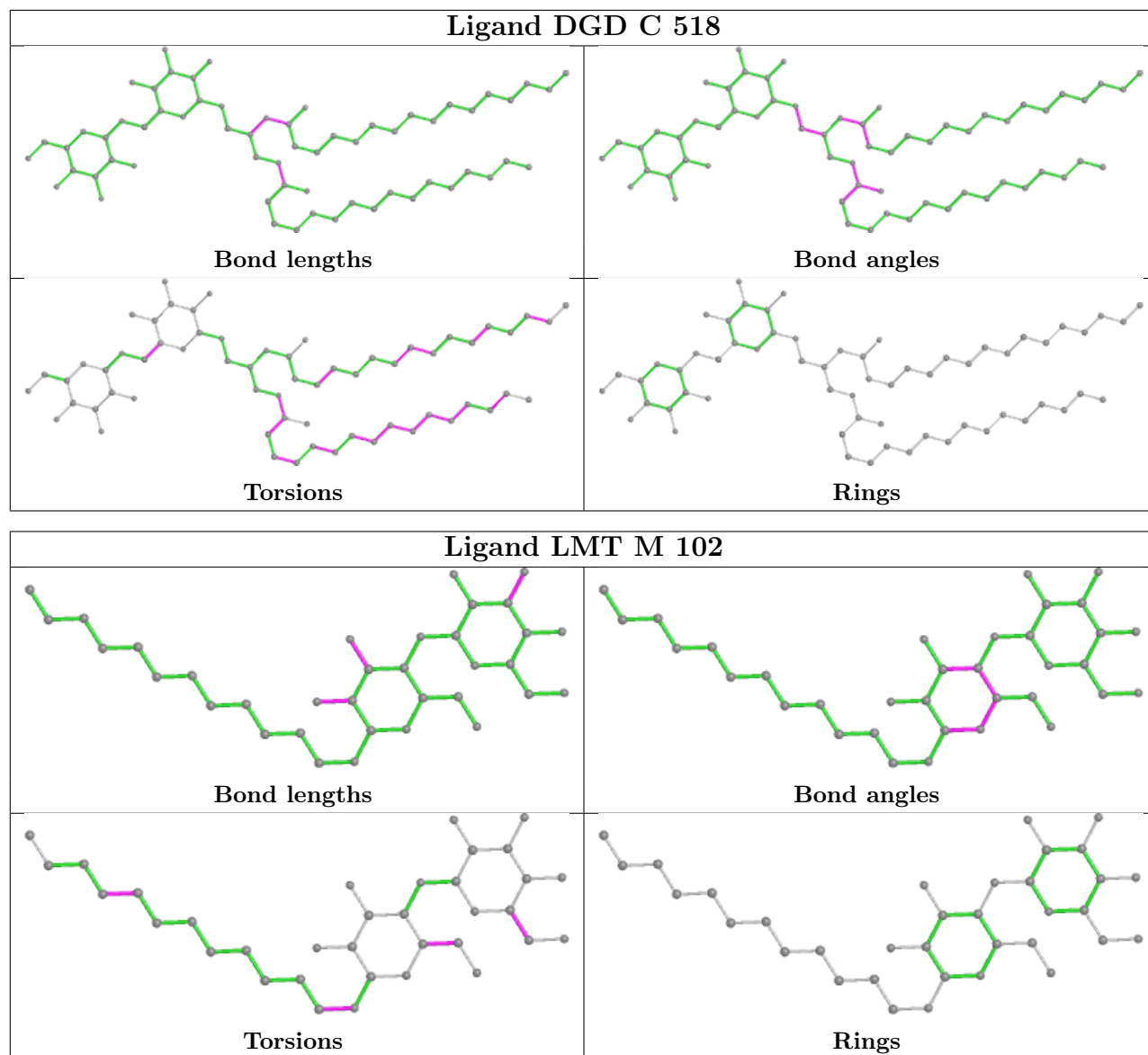


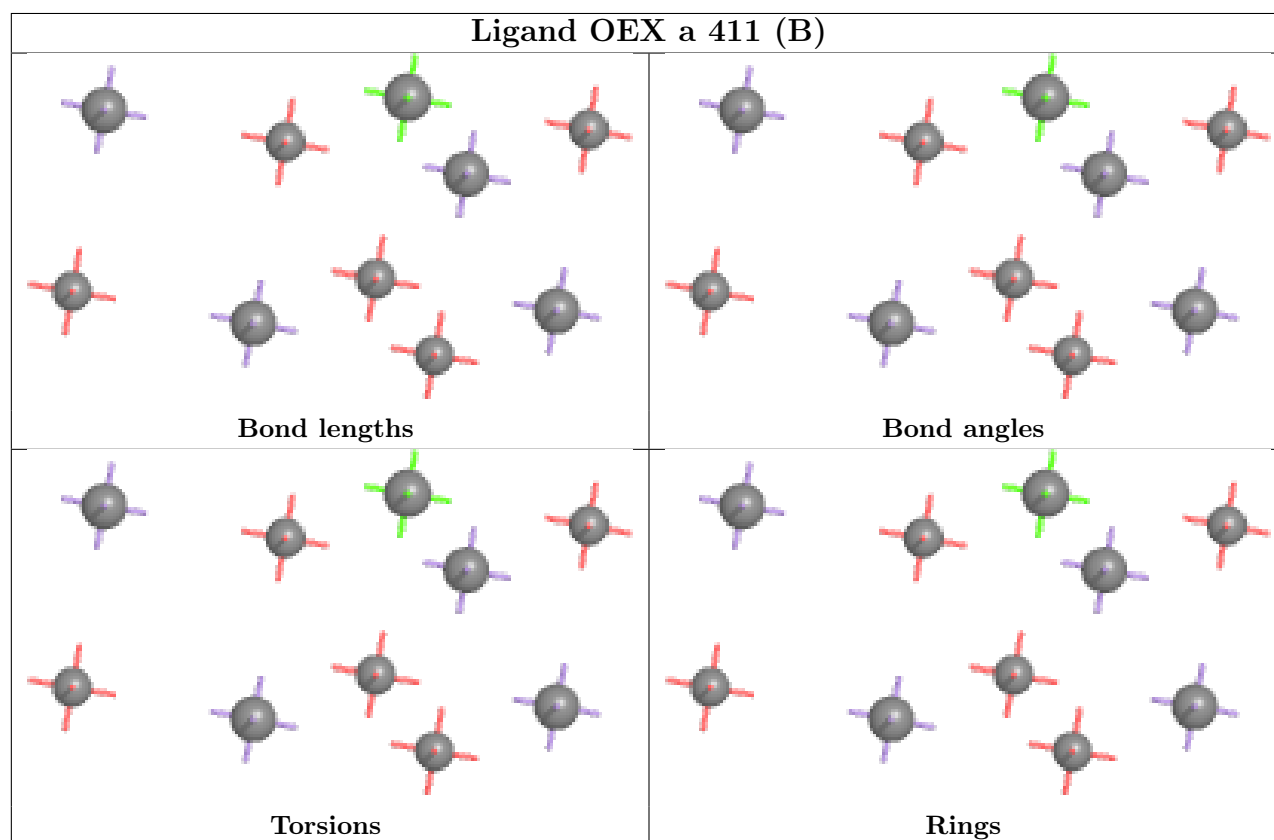
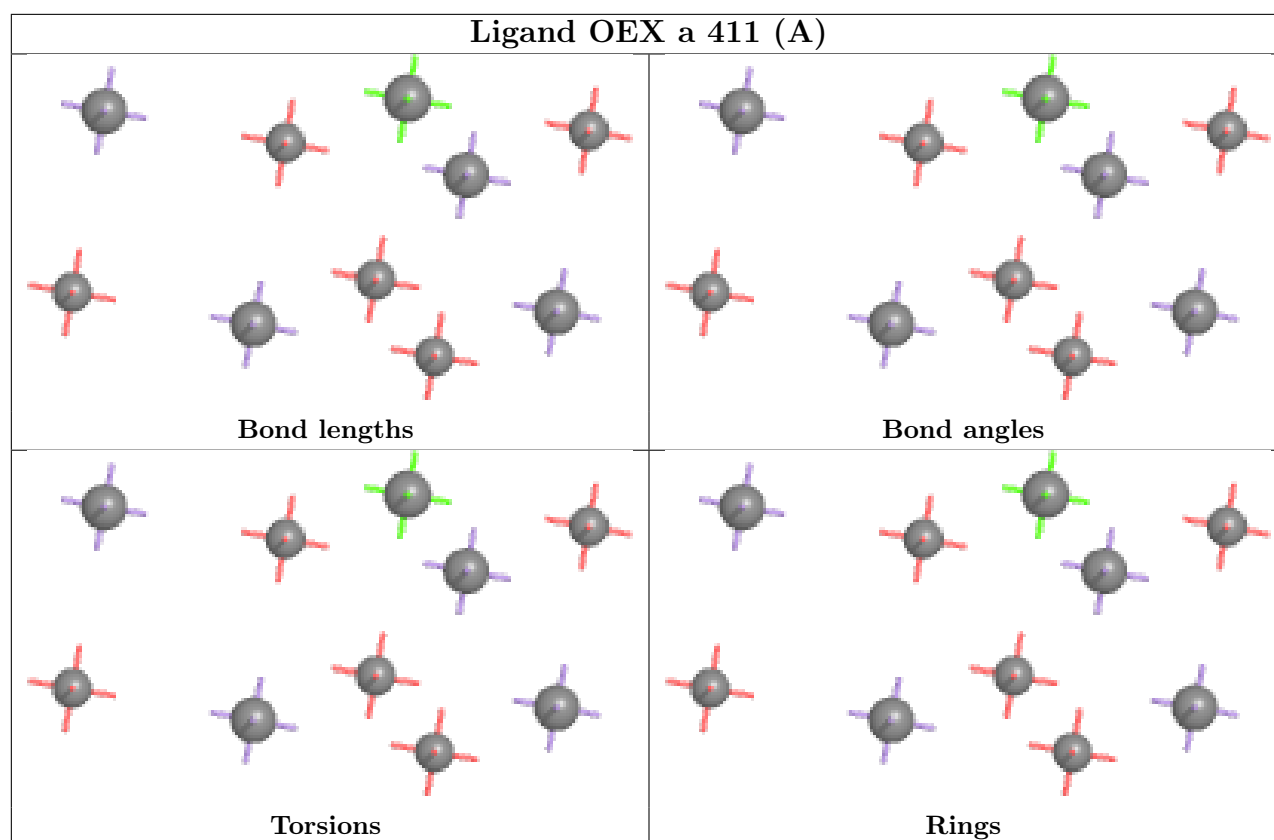


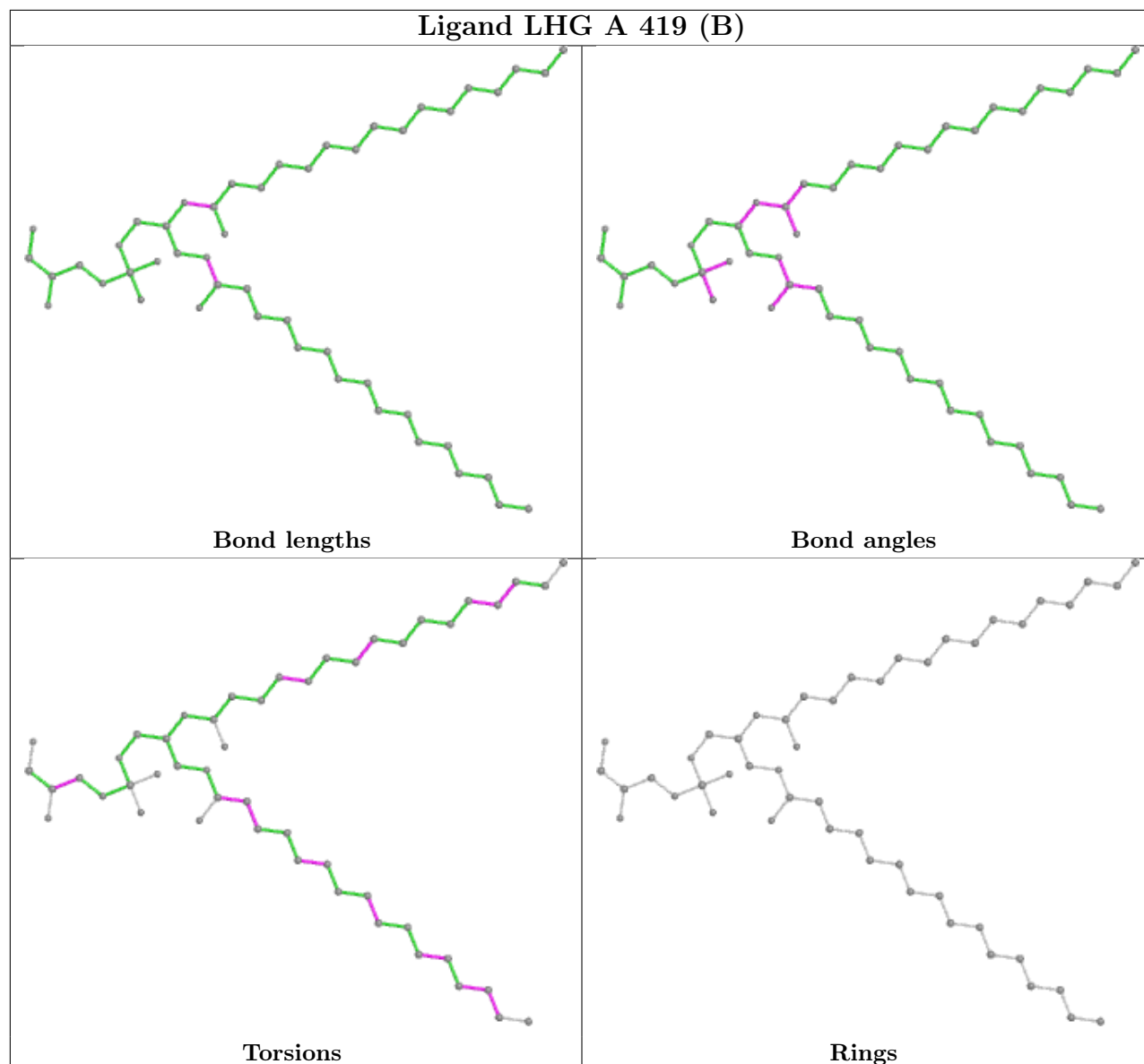
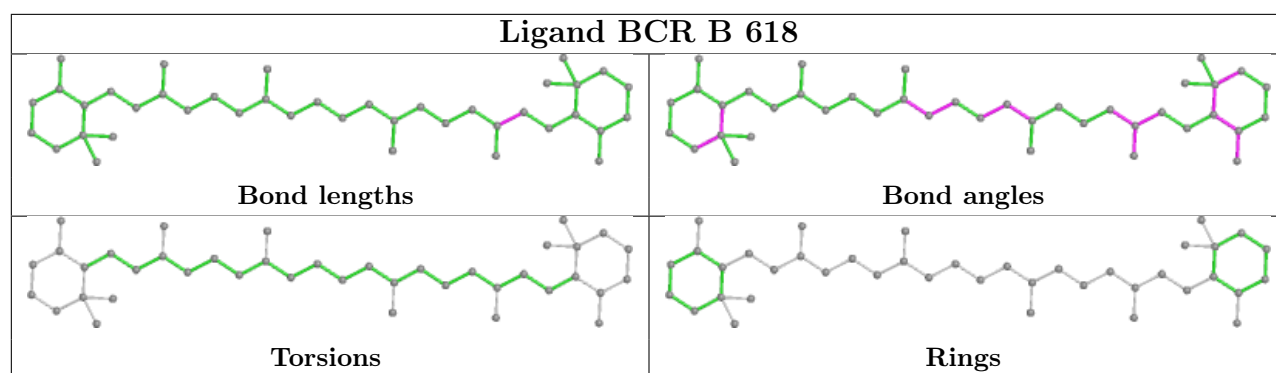


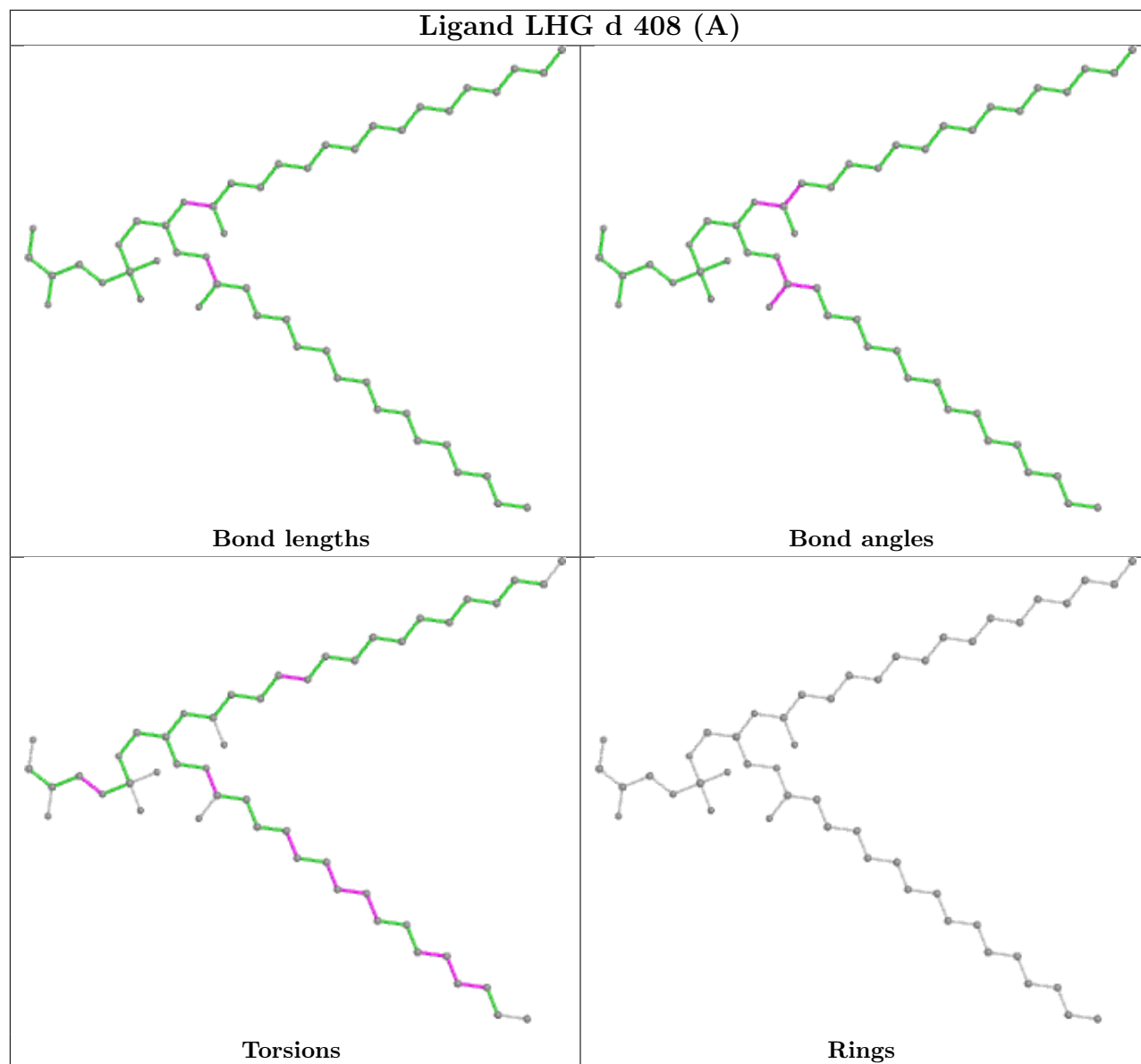


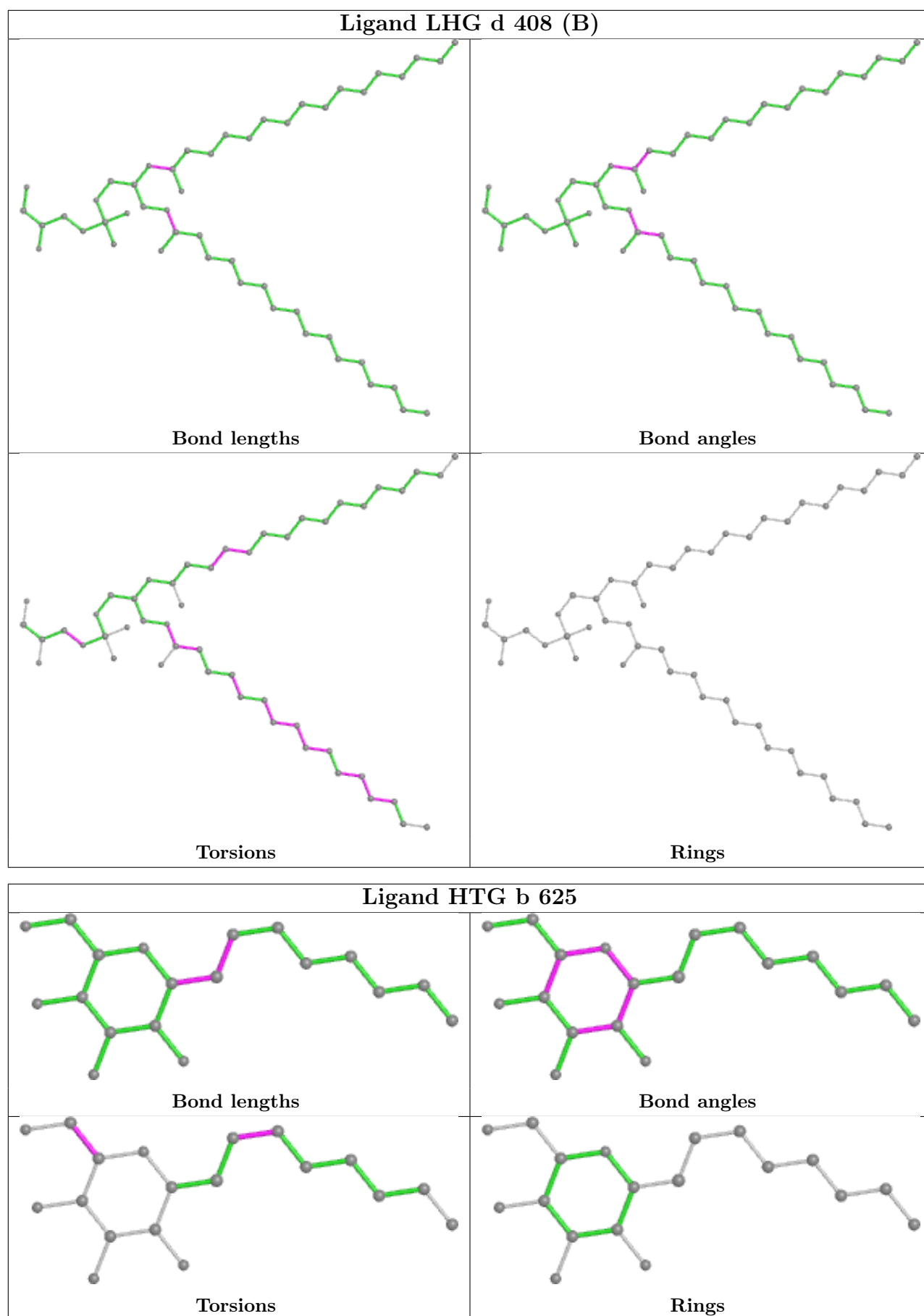




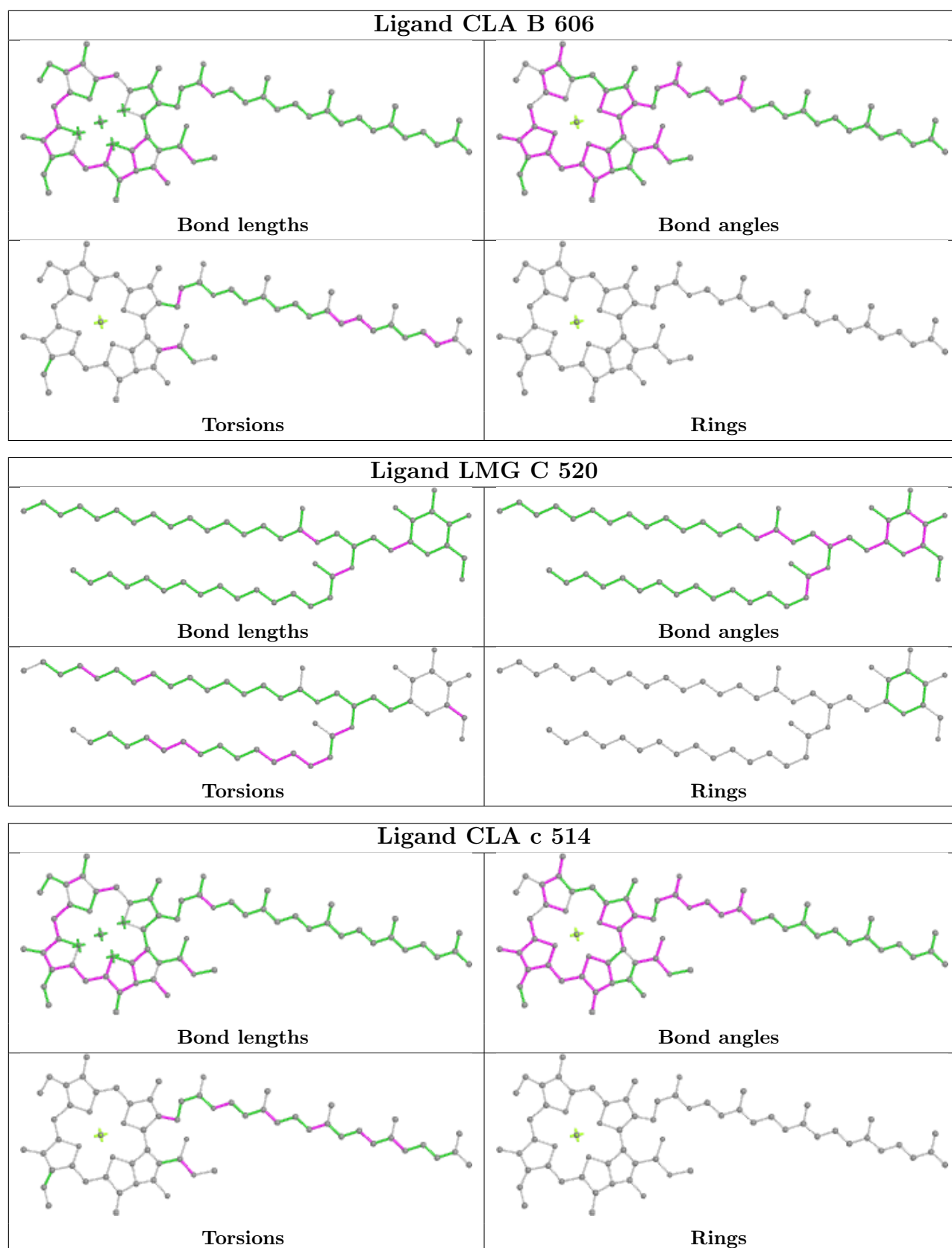


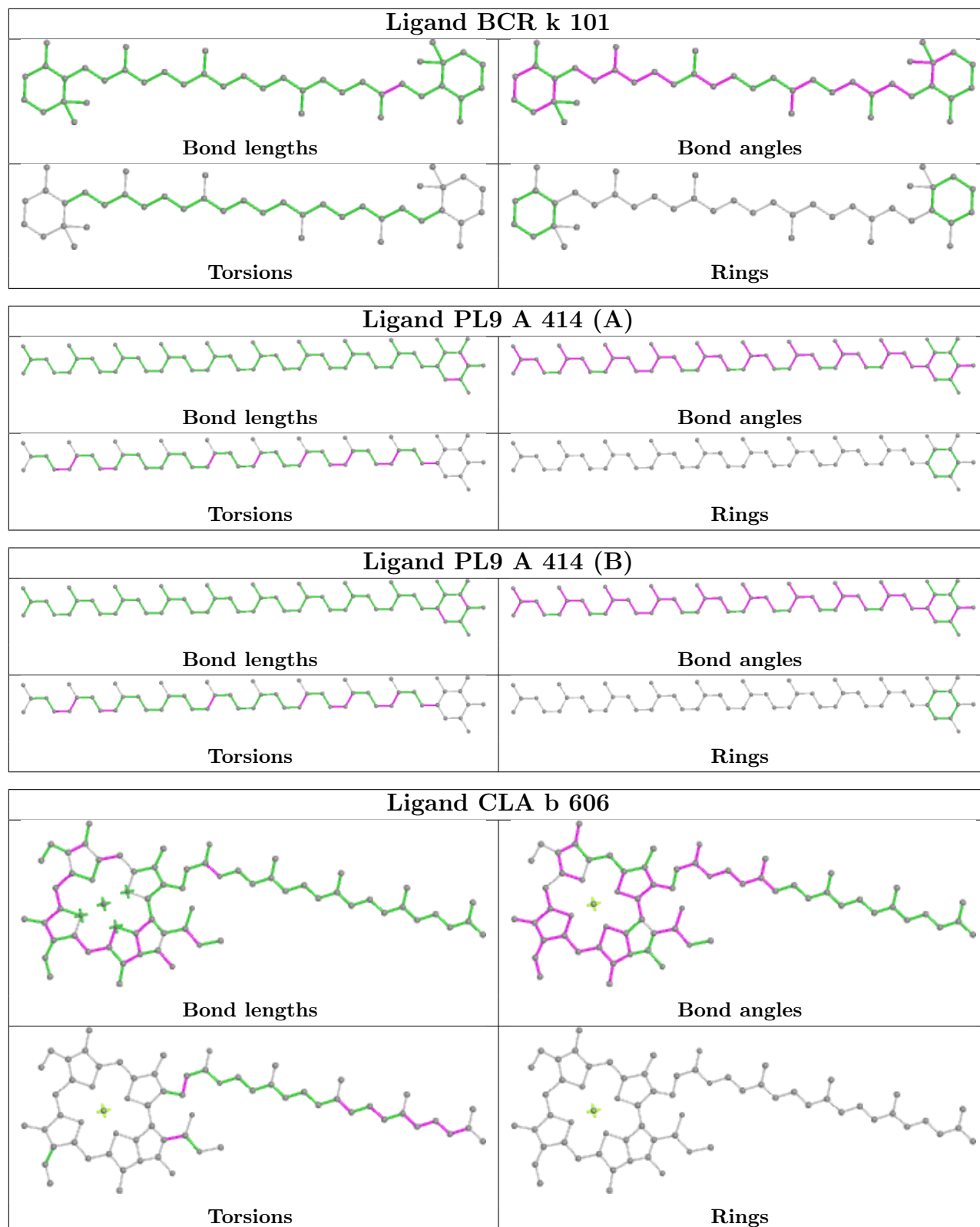


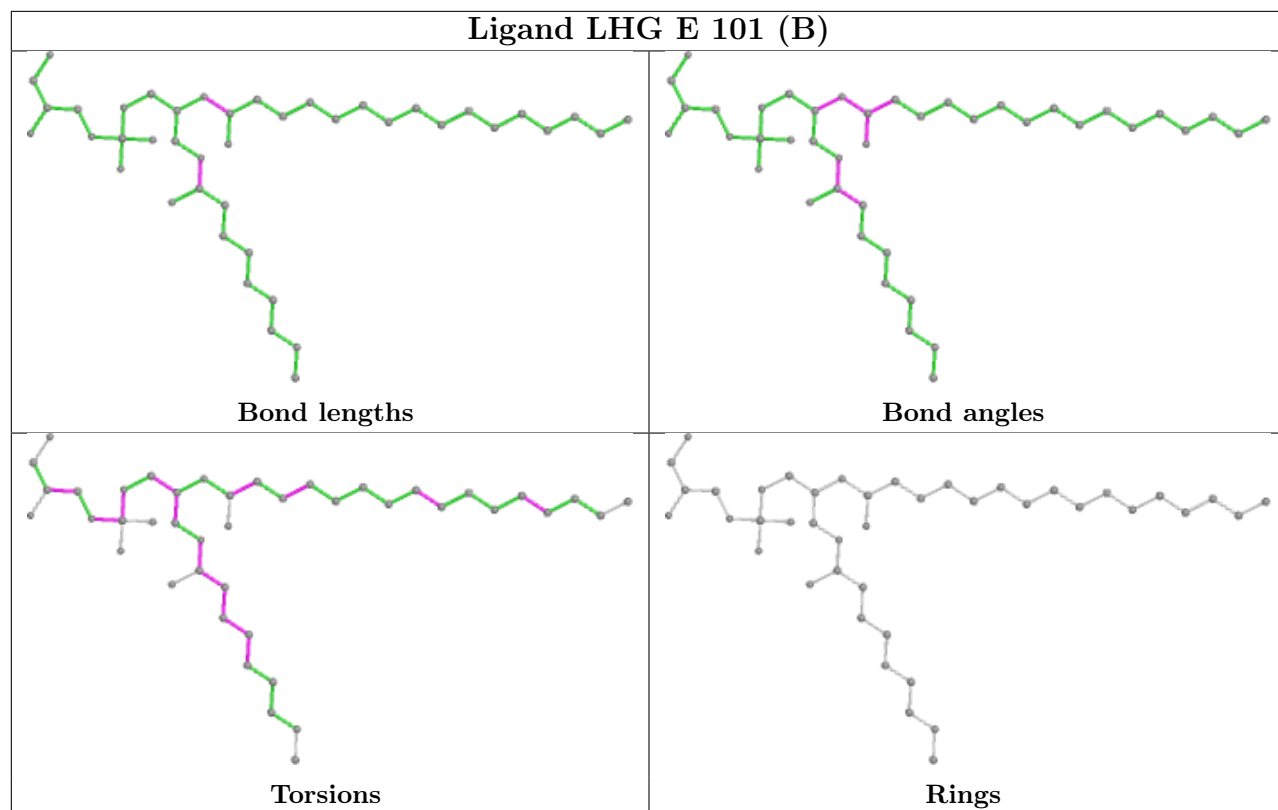


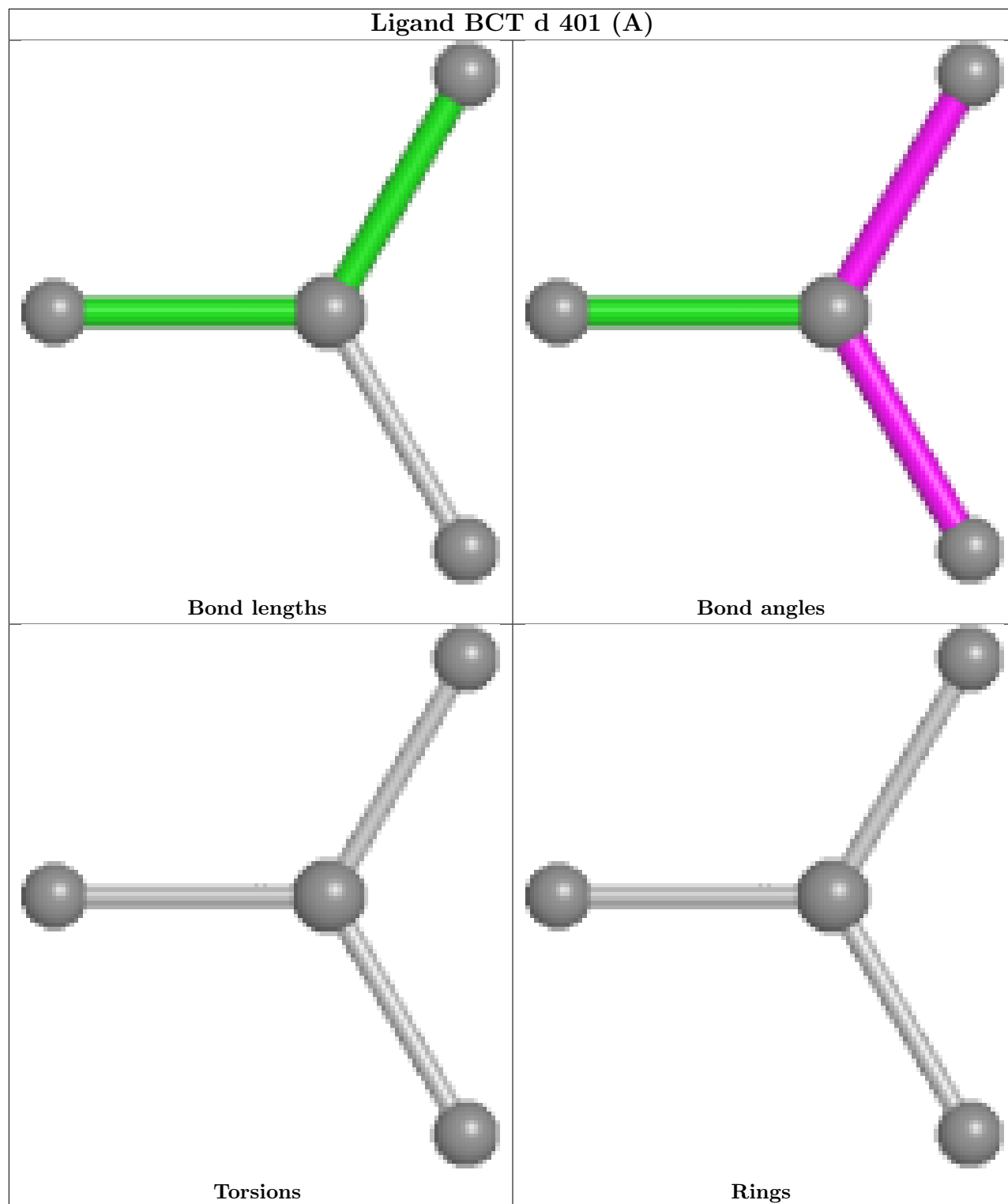


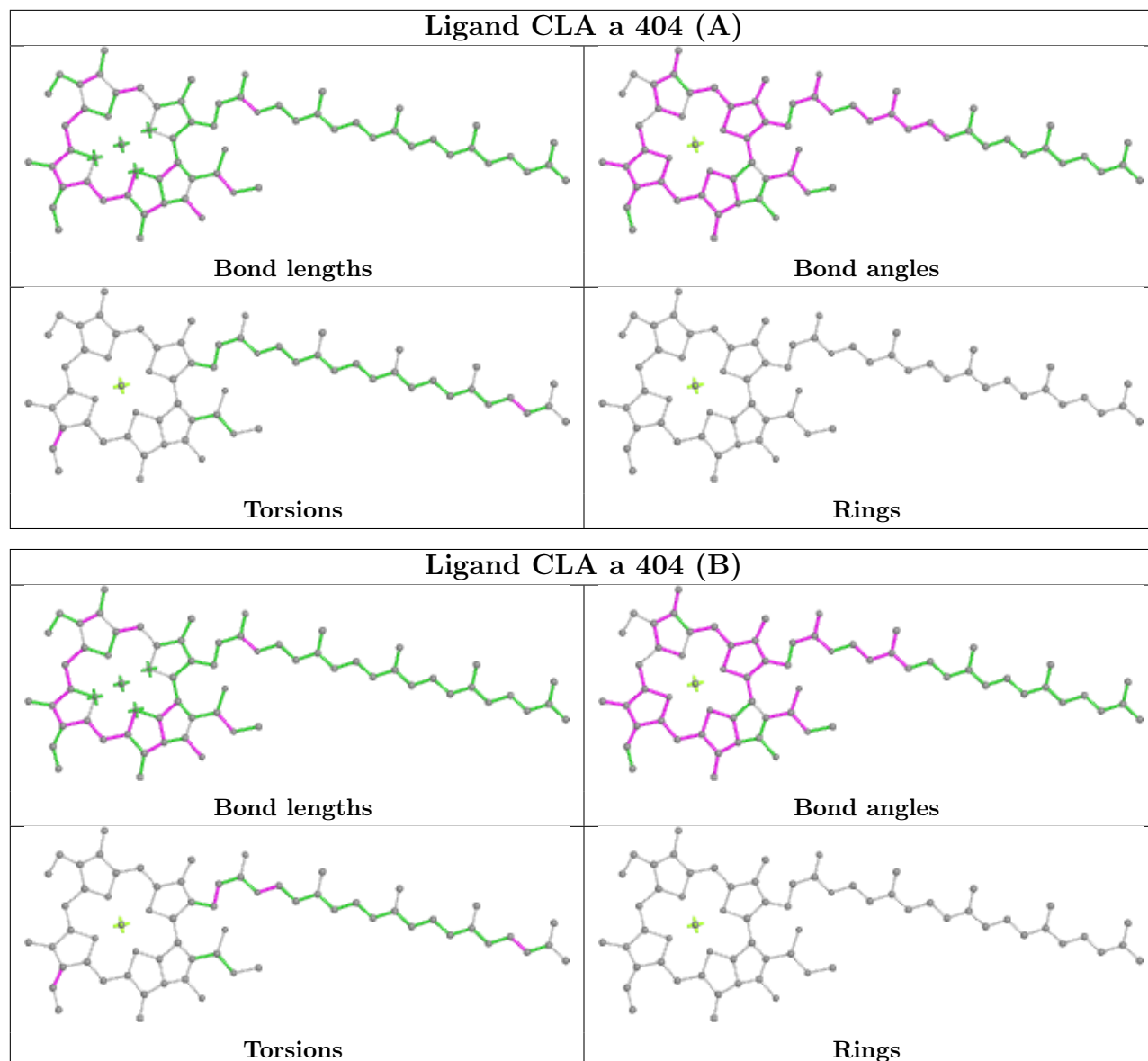
| Ligand PL9 a 412 (A) | |
|----------------------|--------------------|
| <p>Bond lengths</p> | <p>Bond angles</p> |
| <p>Torsions</p> | <p>Rings</p> |
| Ligand BCR T 101 | |
| <p>Bond lengths</p> | <p>Bond angles</p> |
| <p>Torsions</p> | <p>Rings</p> |
| Ligand BCR a 408 | |
| <p>Bond lengths</p> | <p>Bond angles</p> |
| <p>Torsions</p> | <p>Rings</p> |
| Ligand PL9 d 406 (B) | |
| <p>Bond lengths</p> | <p>Bond angles</p> |
| <p>Torsions</p> | <p>Rings</p> |

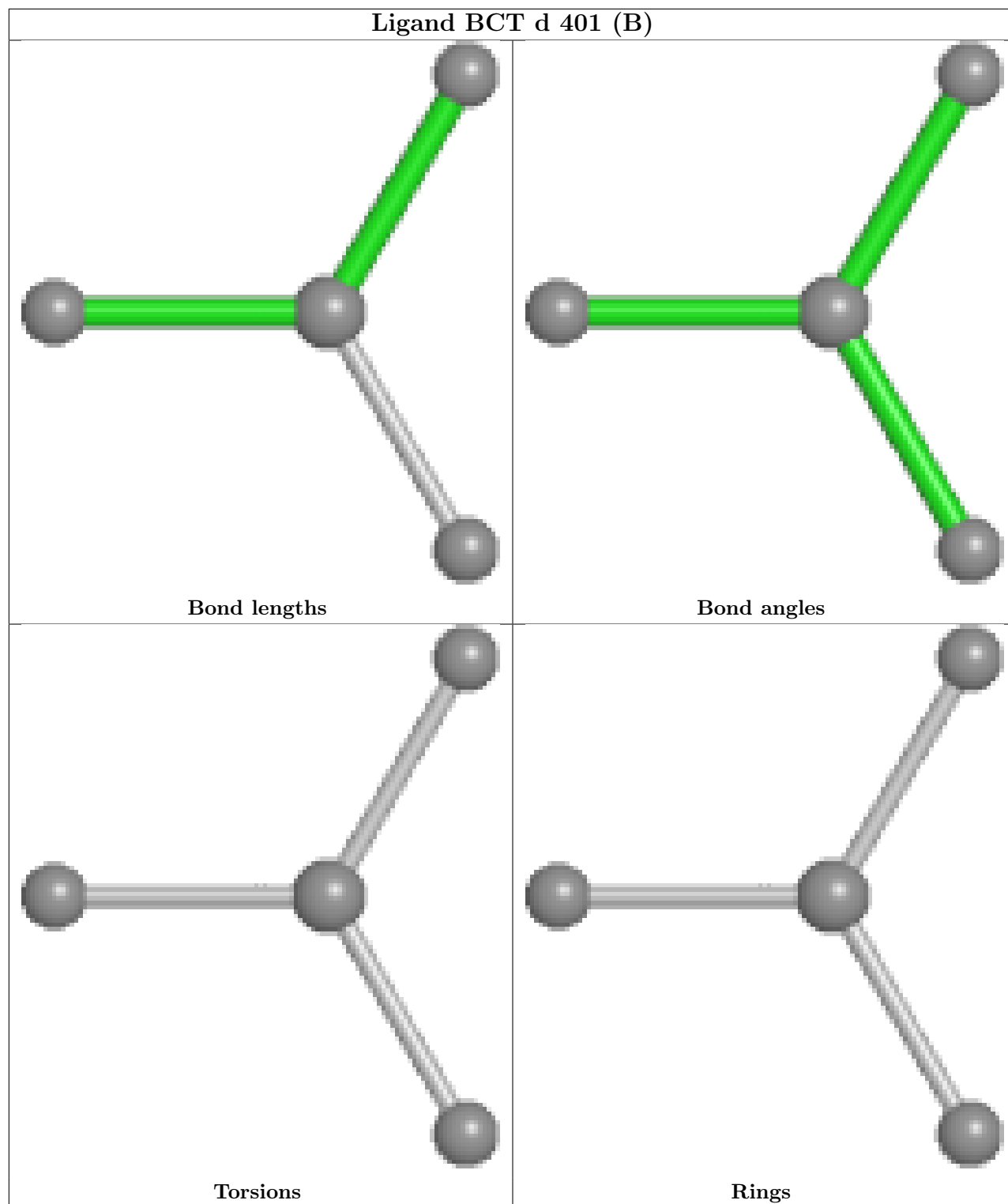


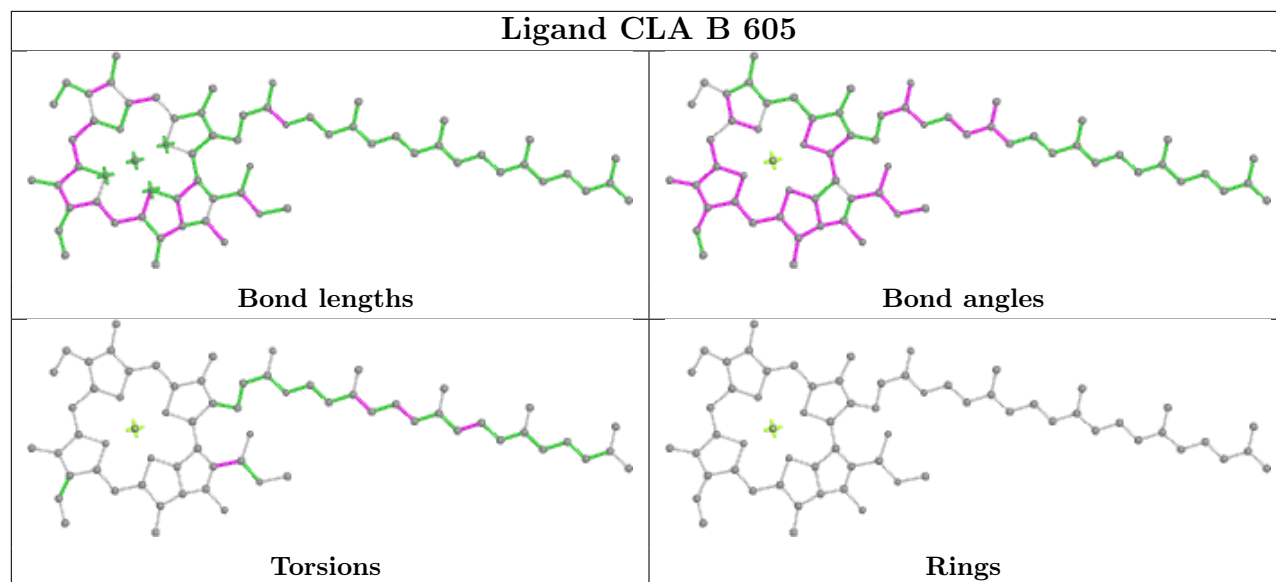


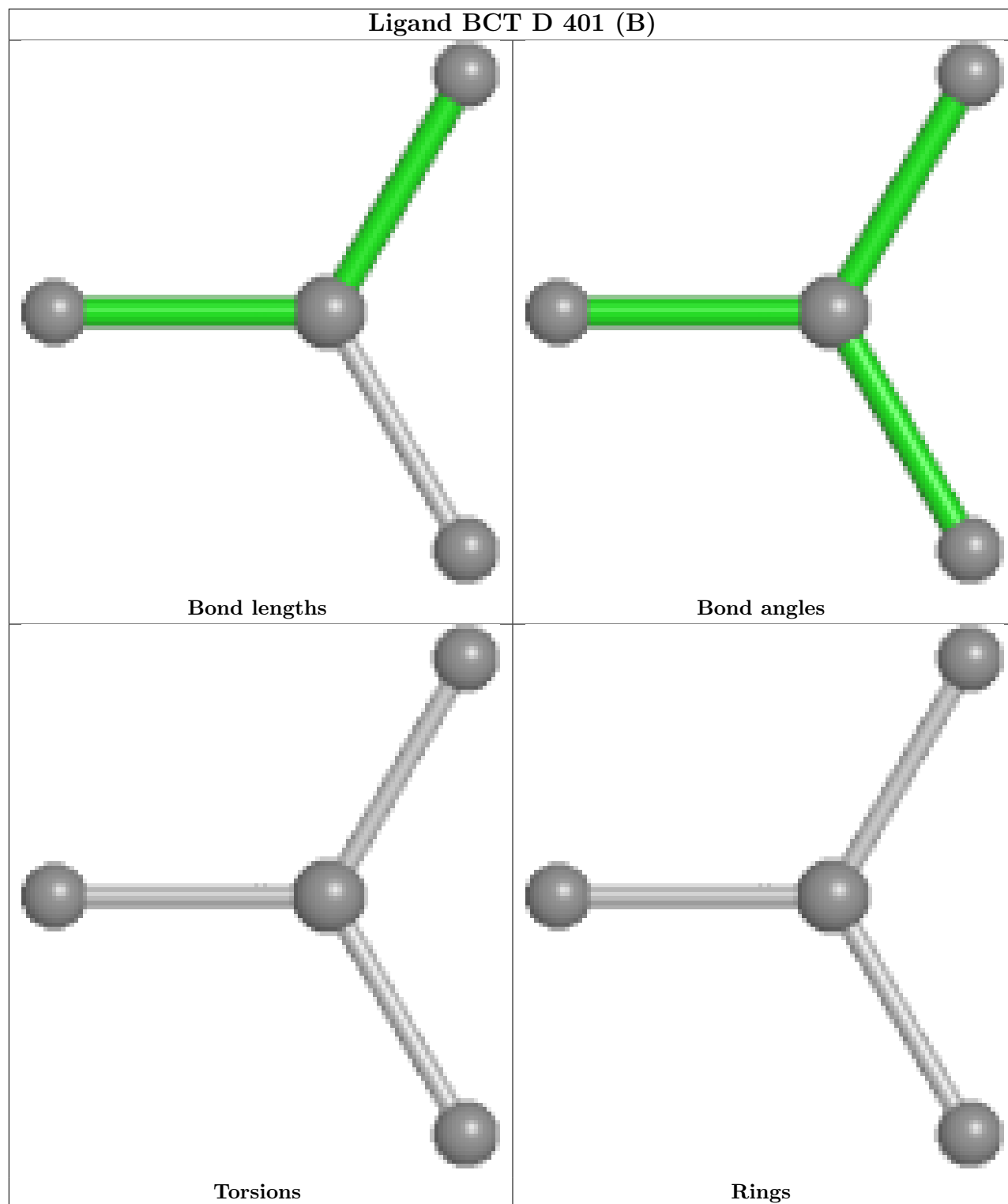


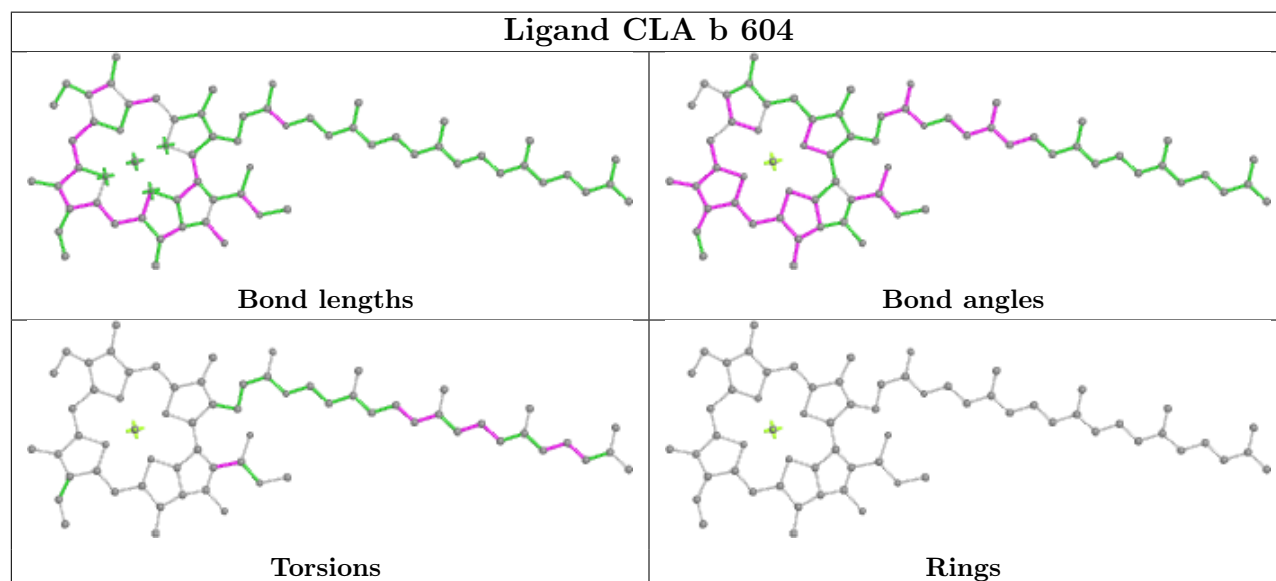
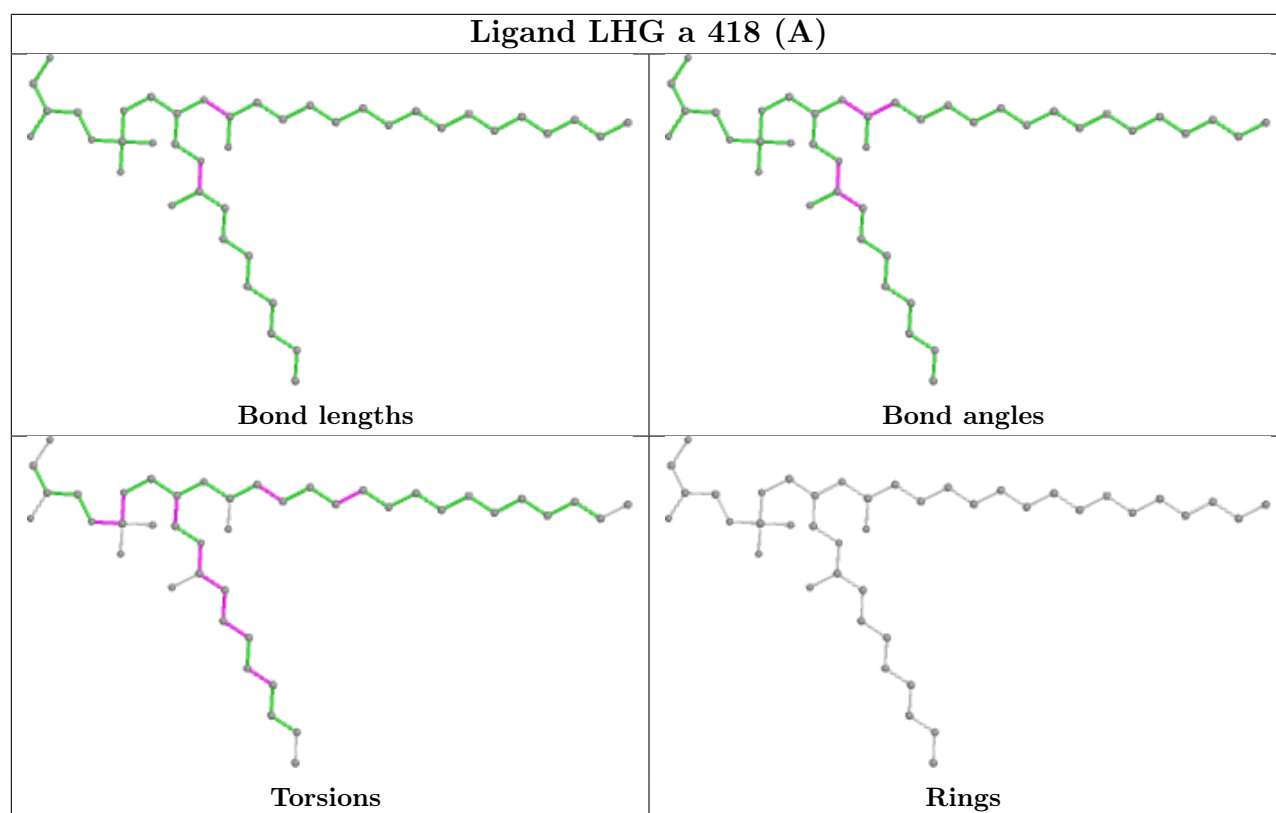


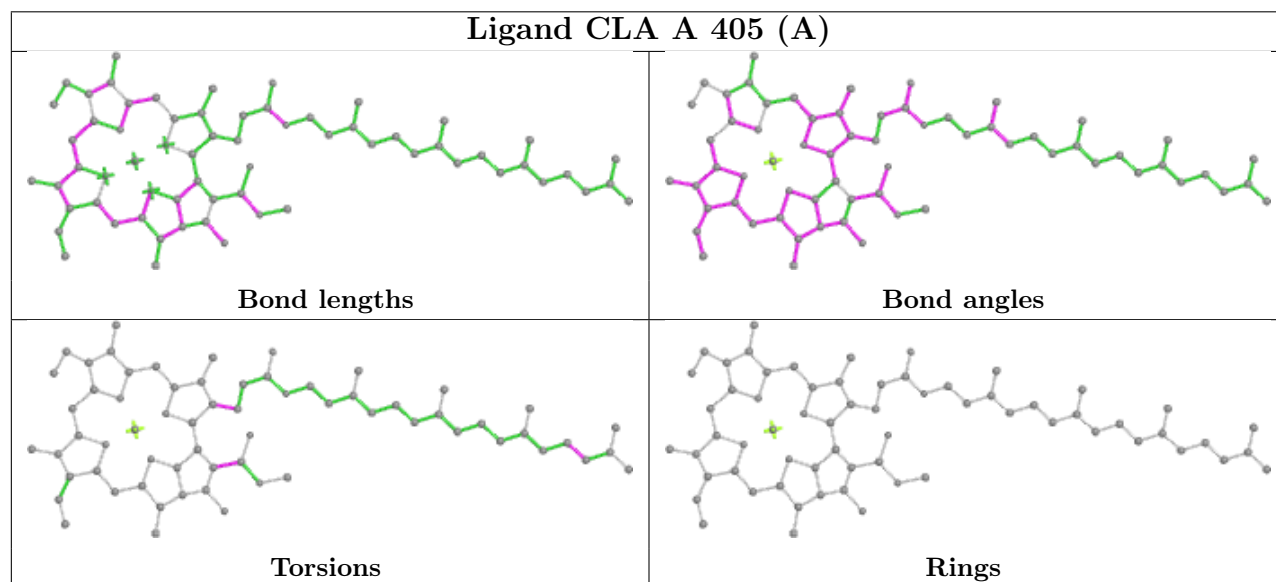
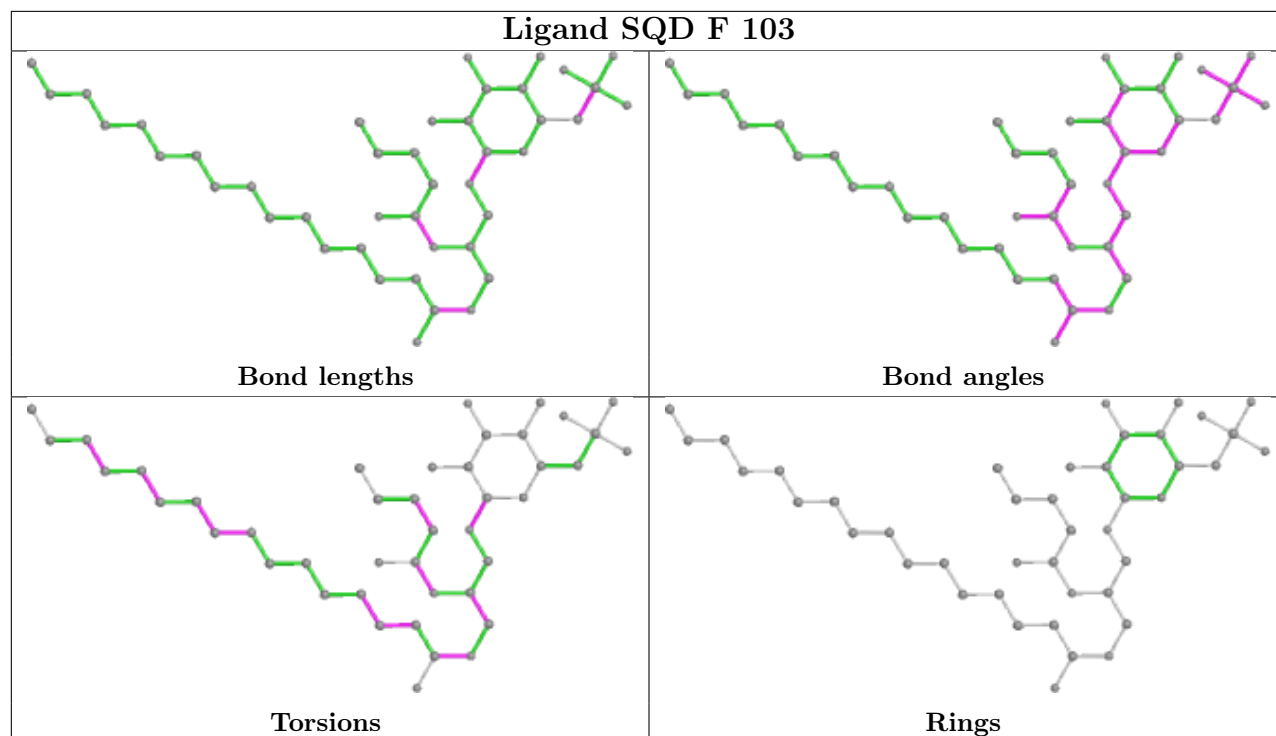


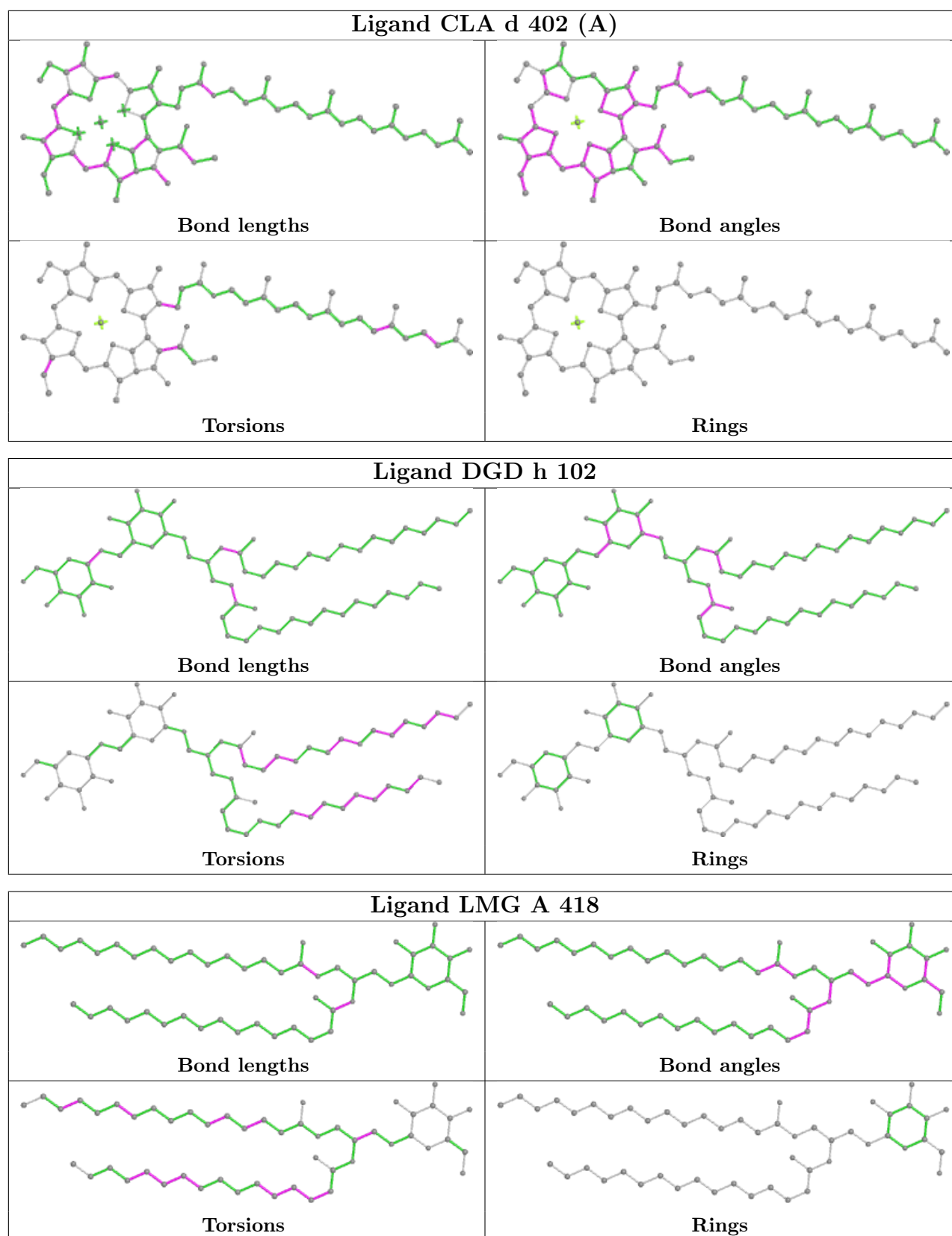


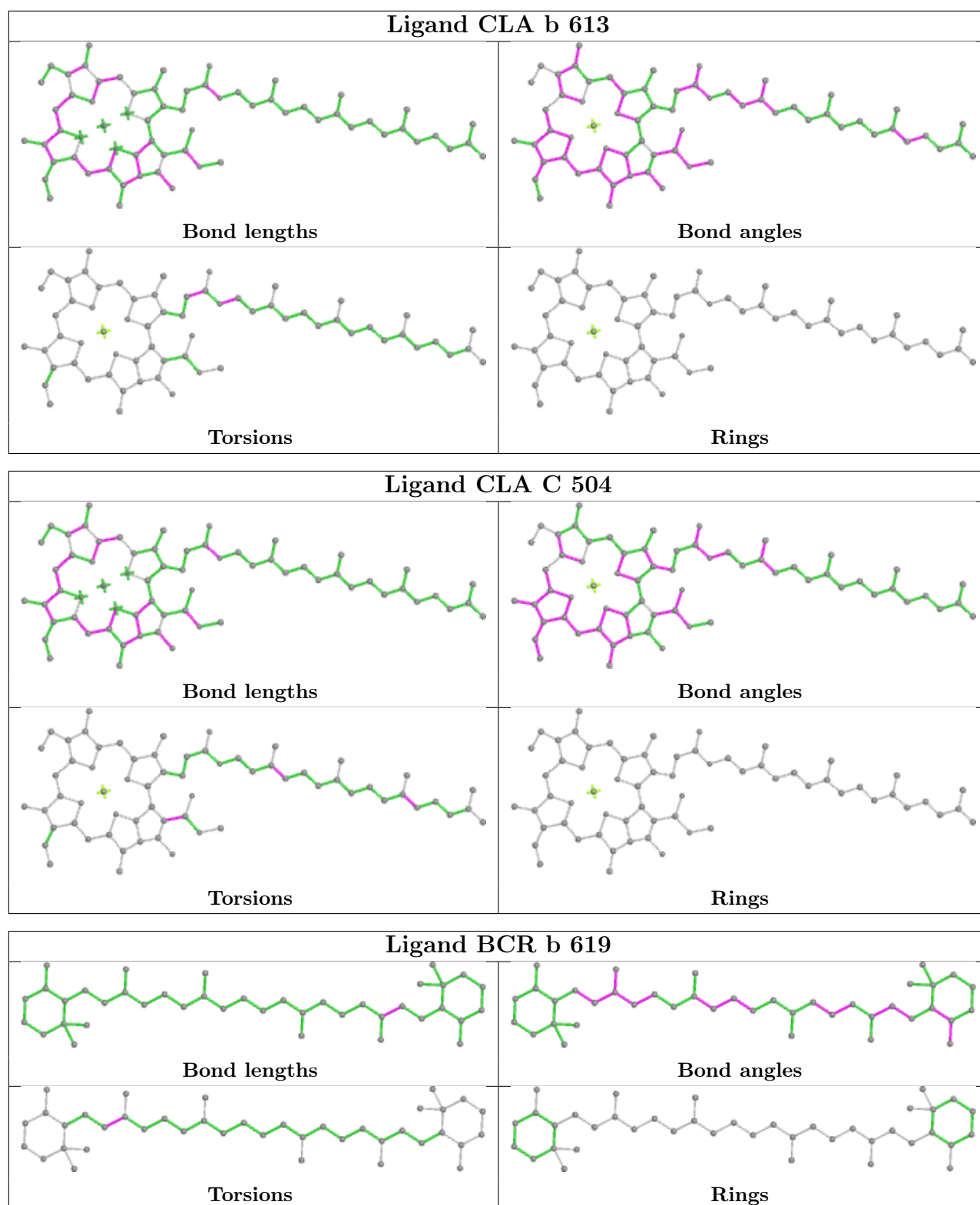


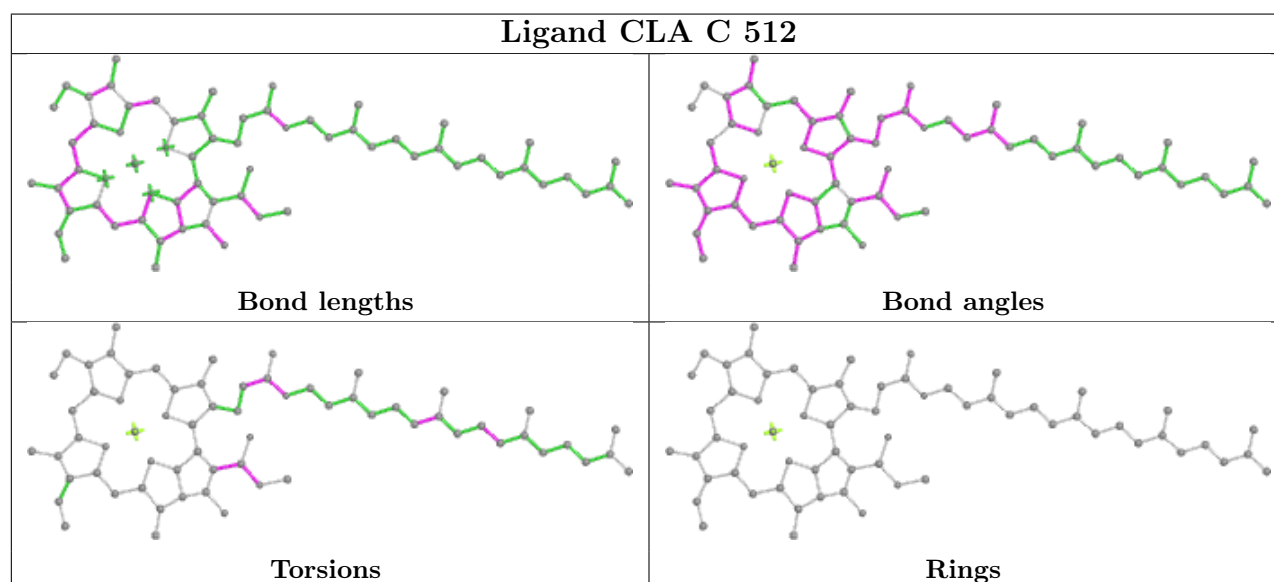
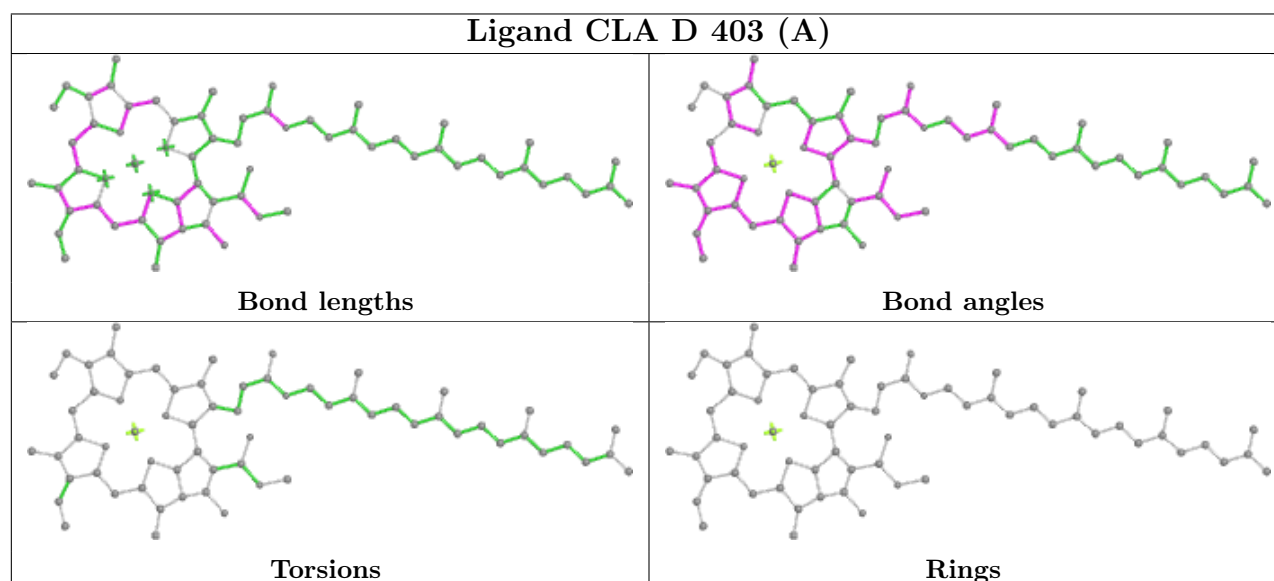
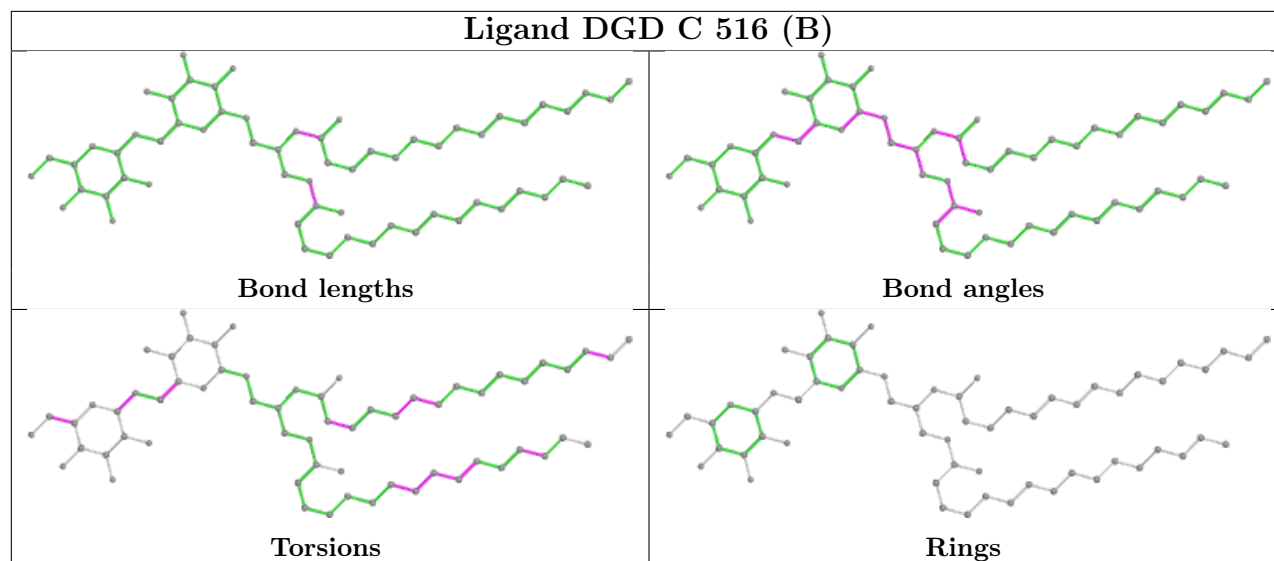


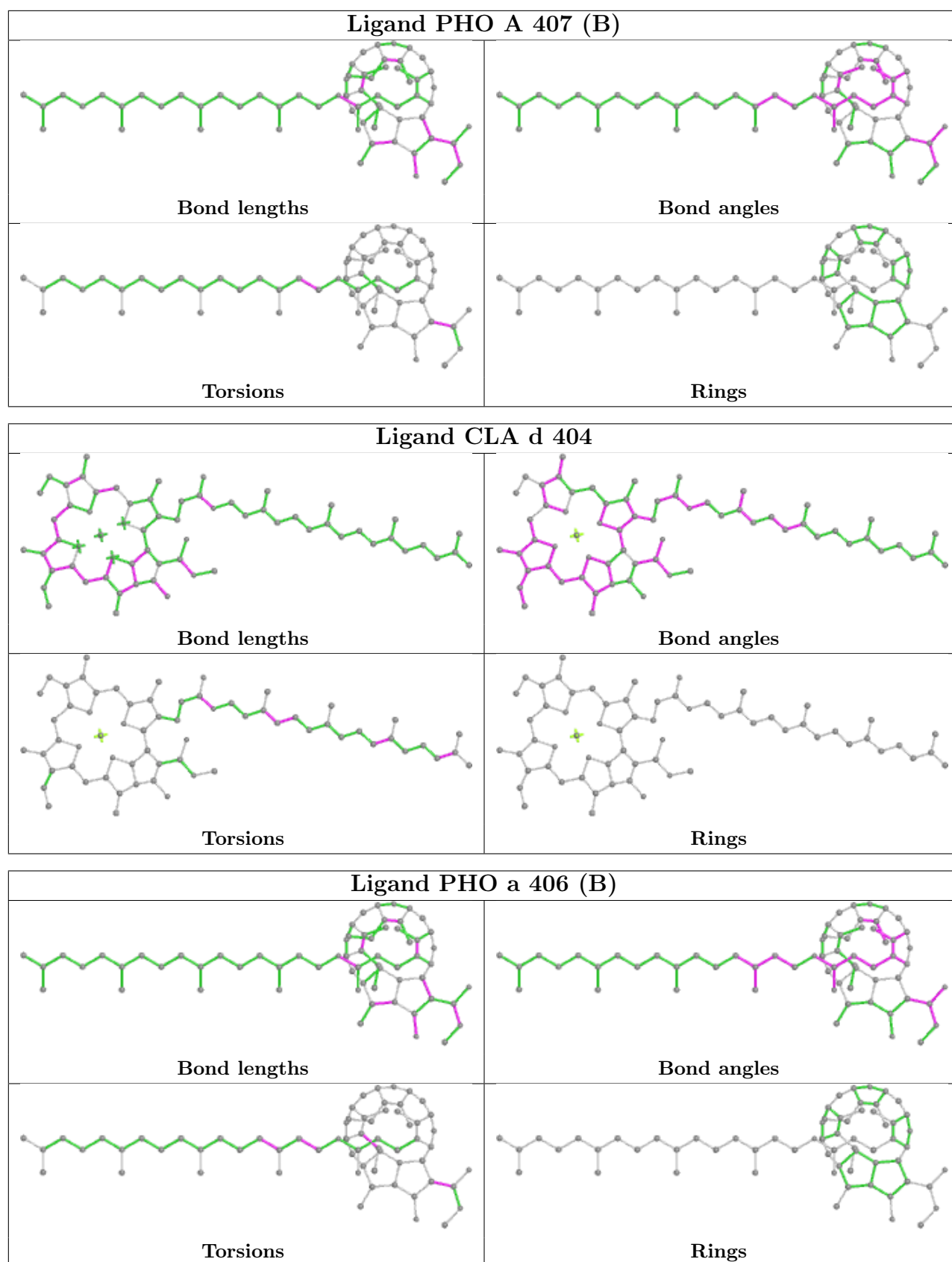


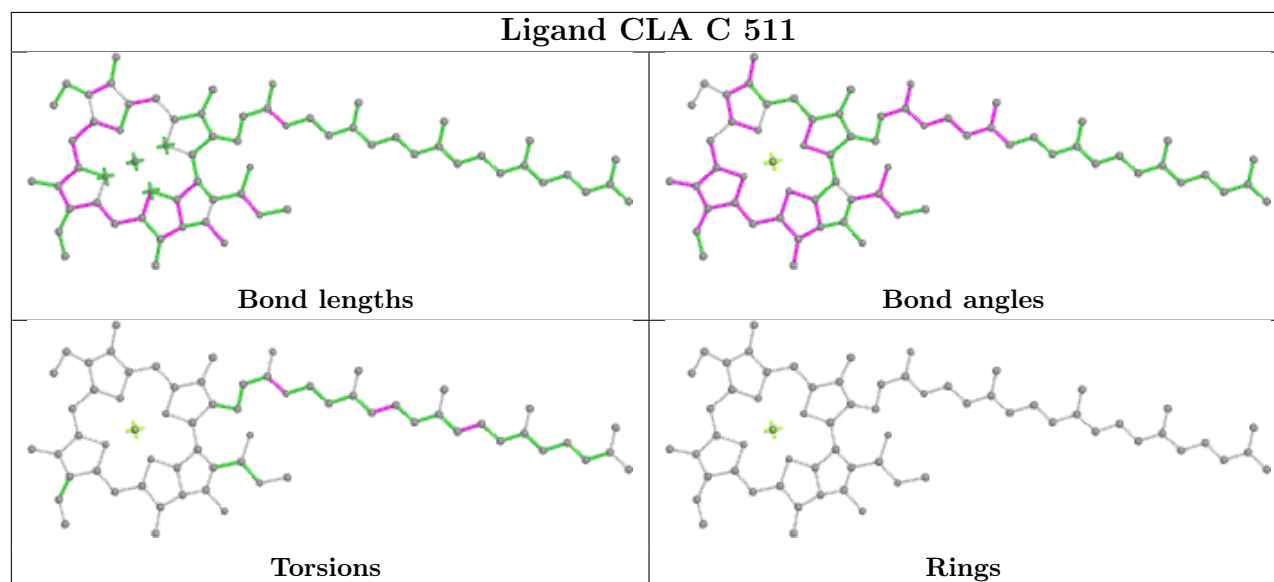
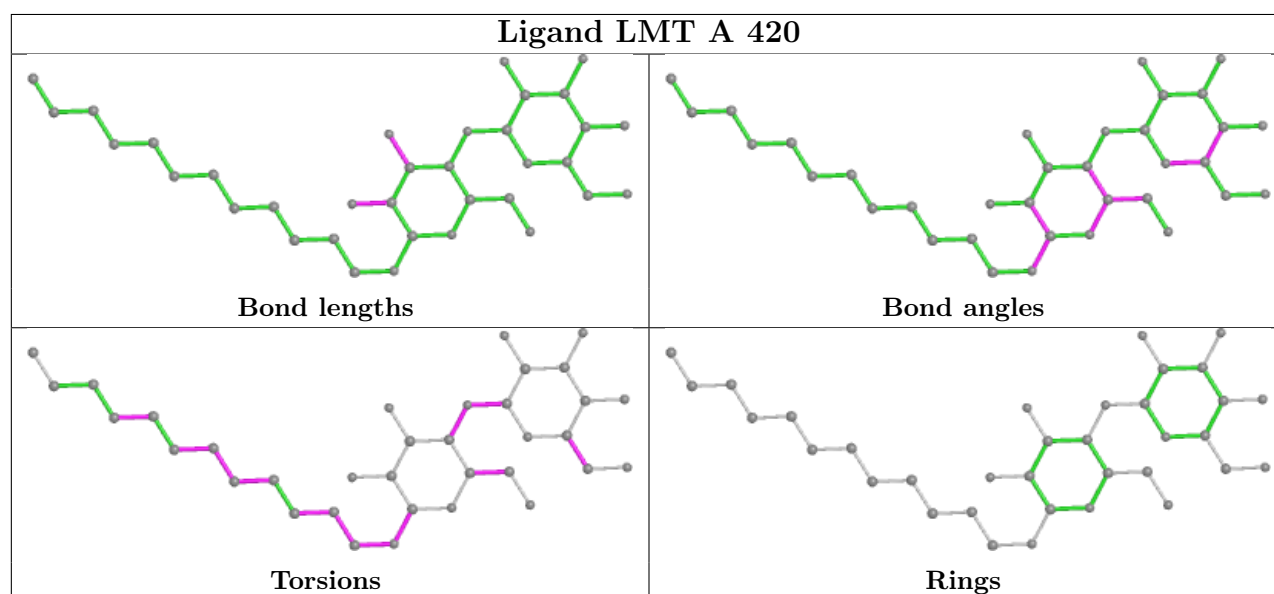
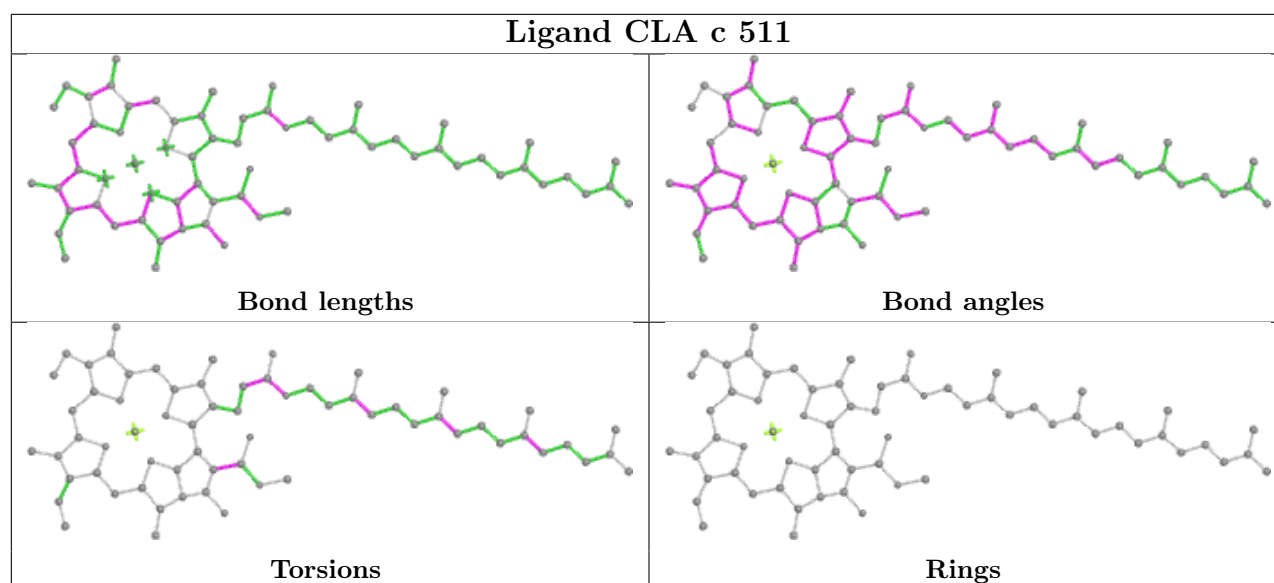


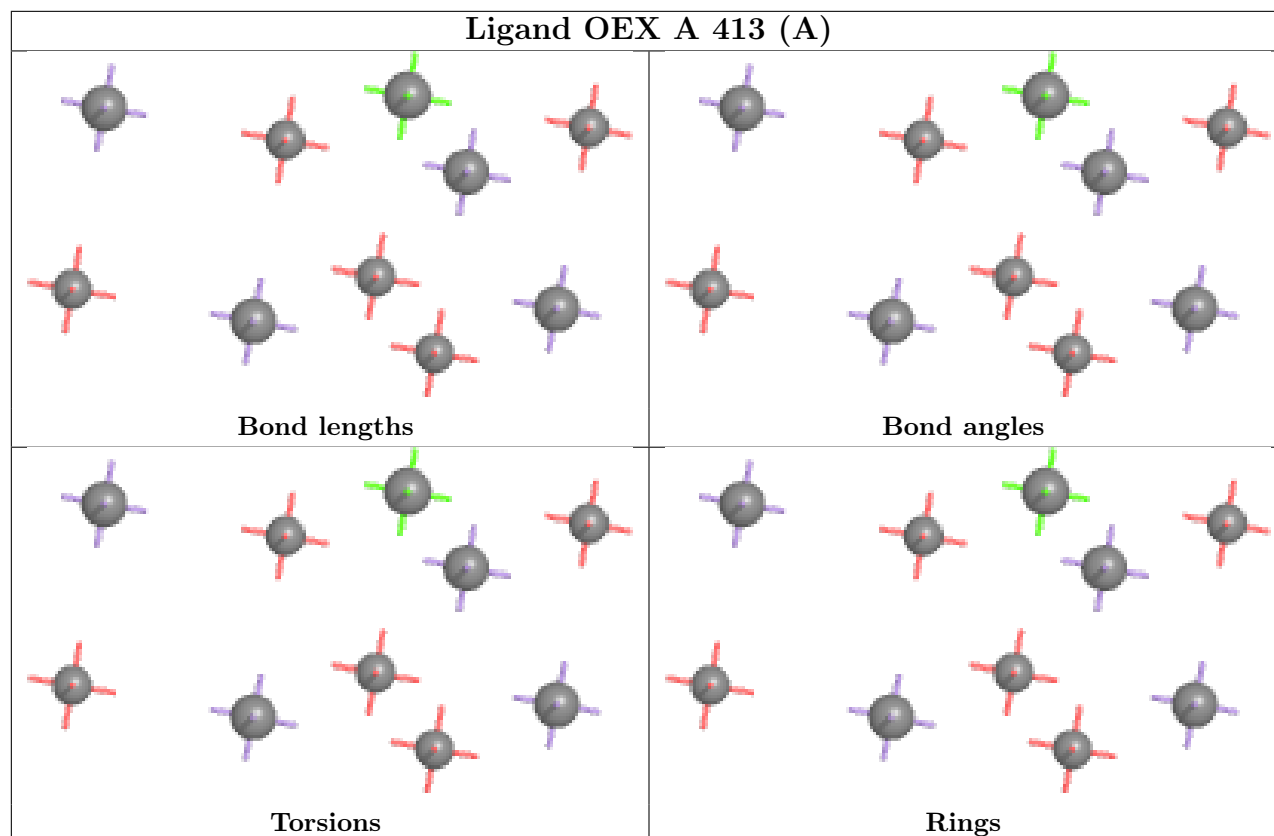
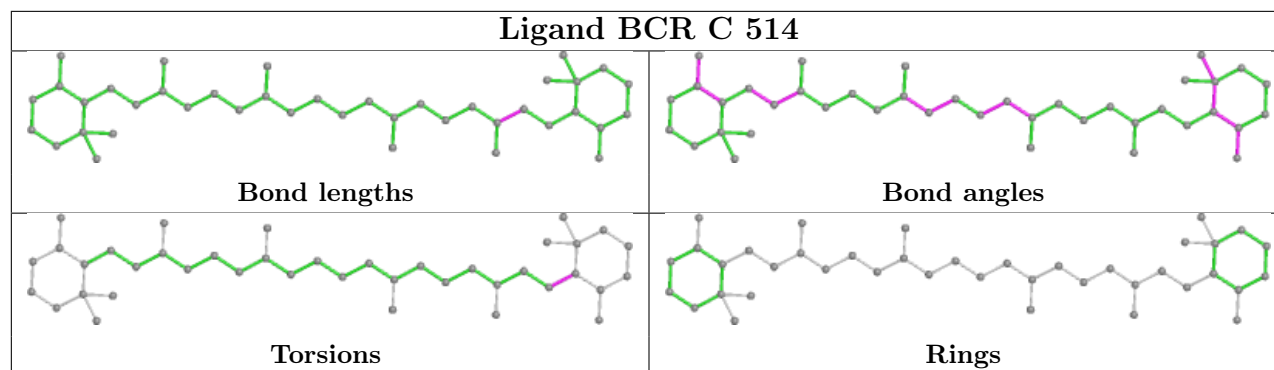


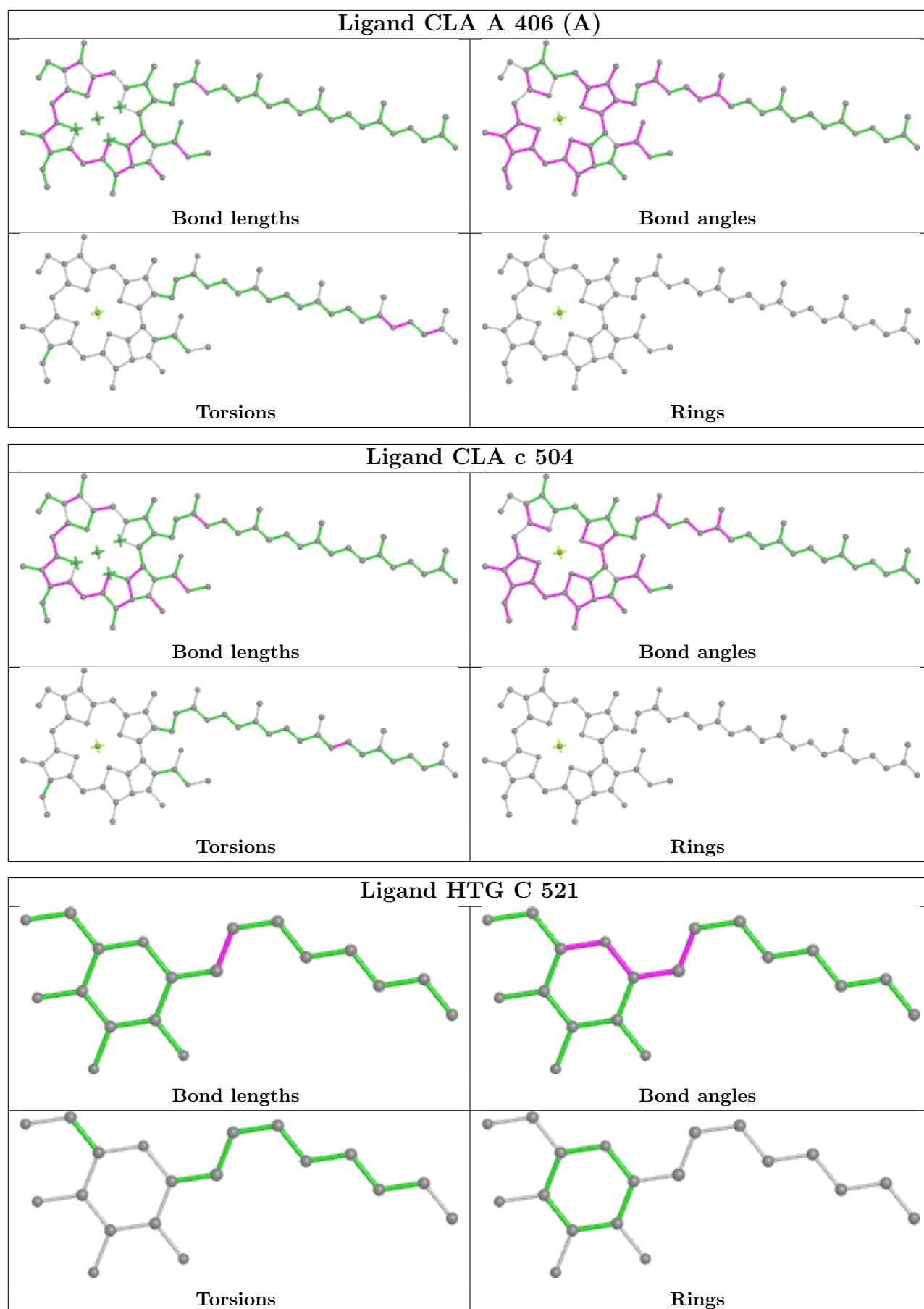


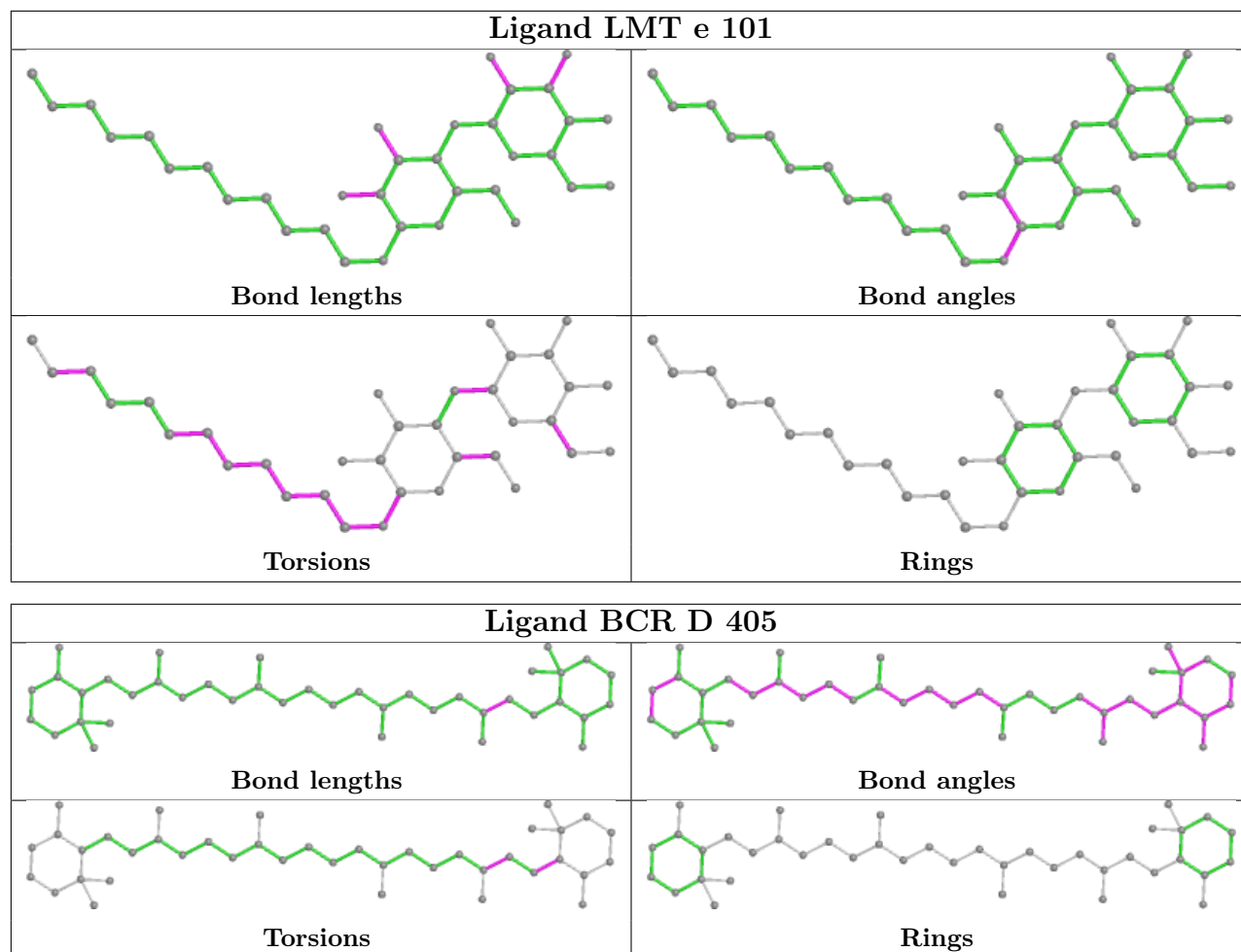


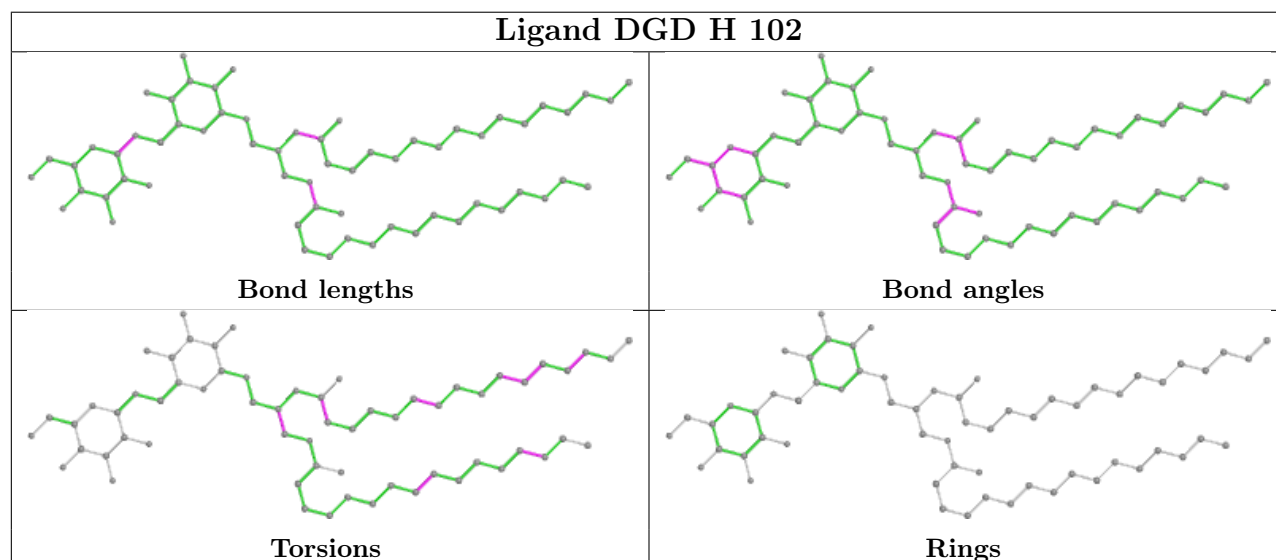
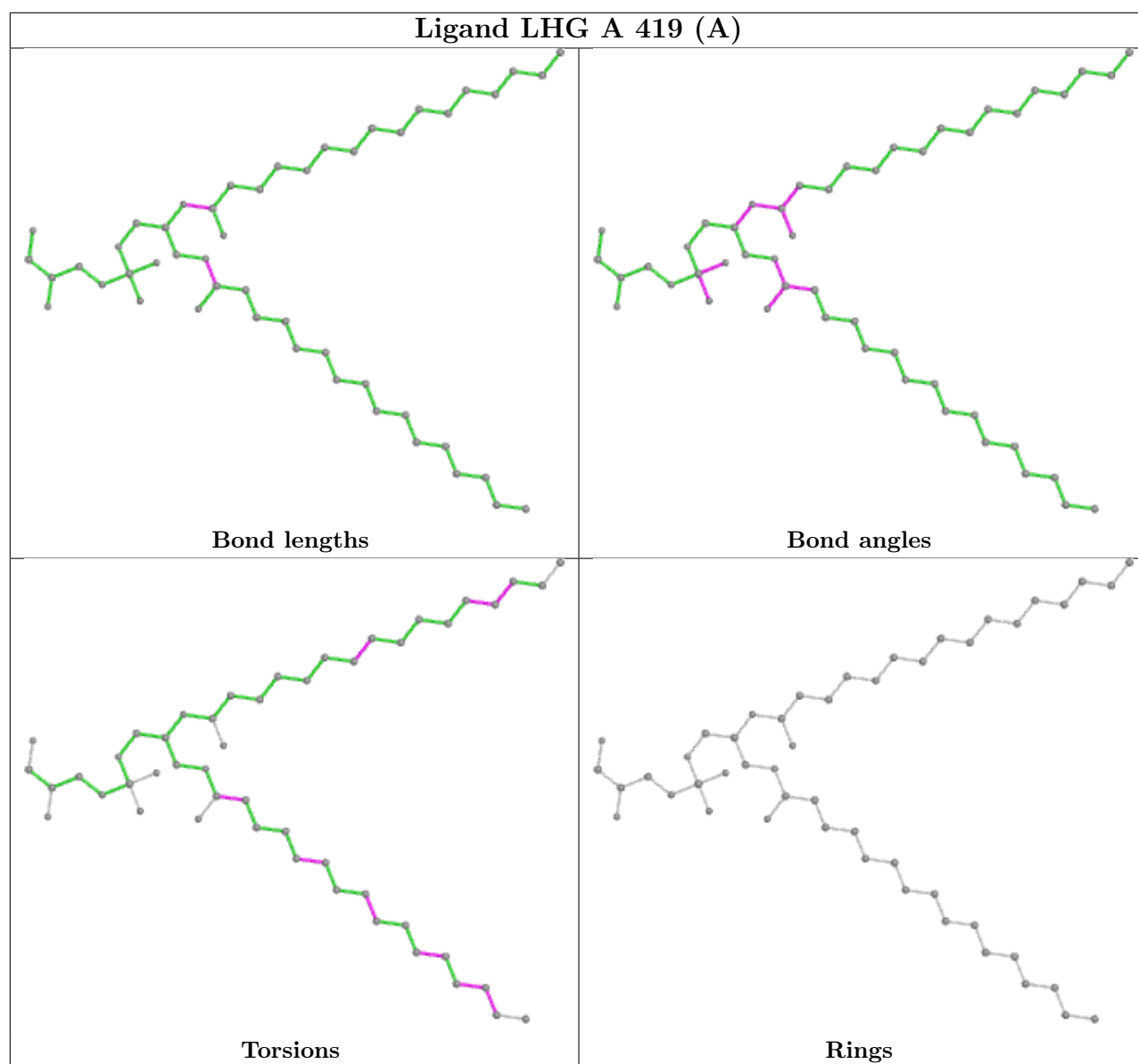


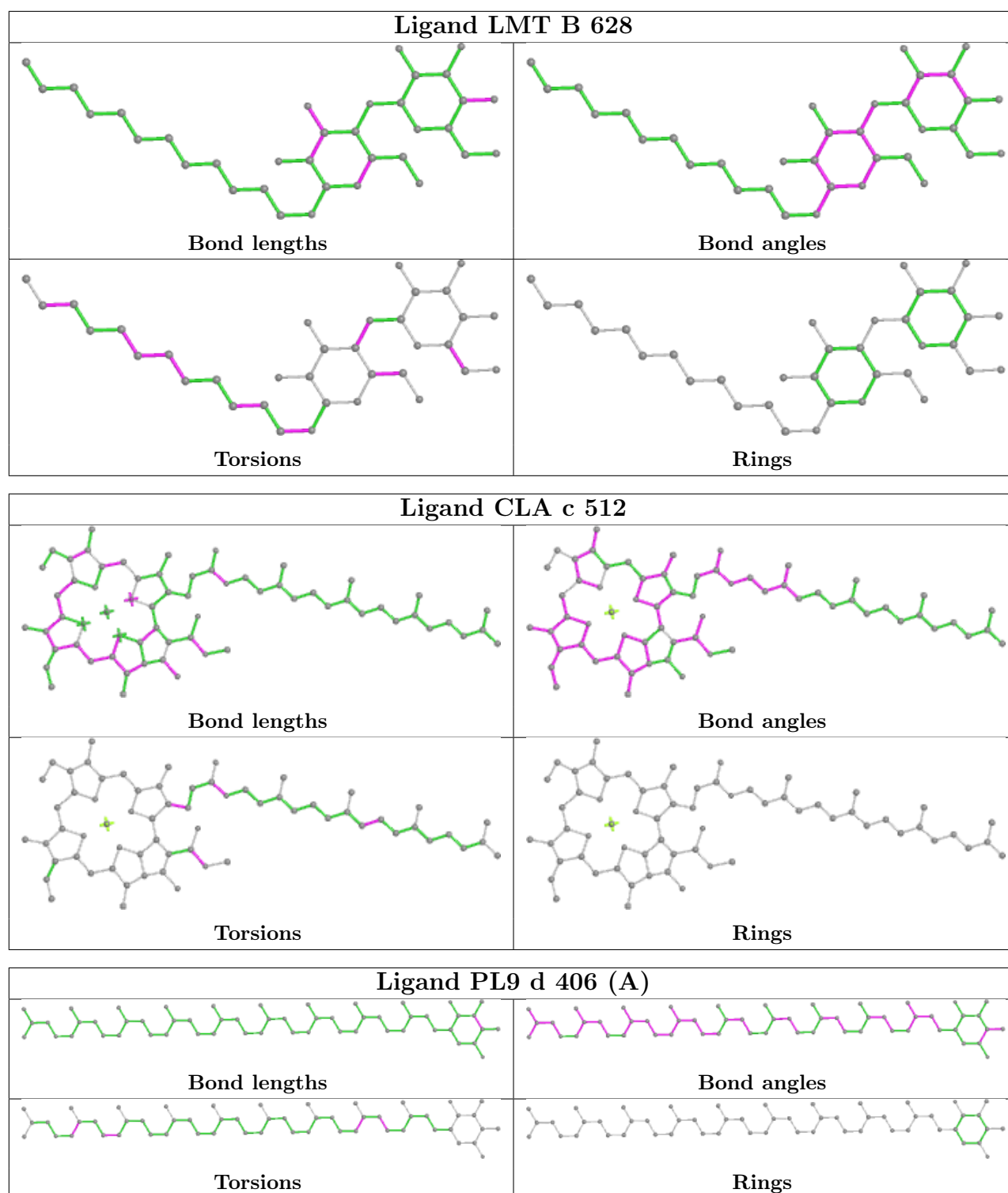


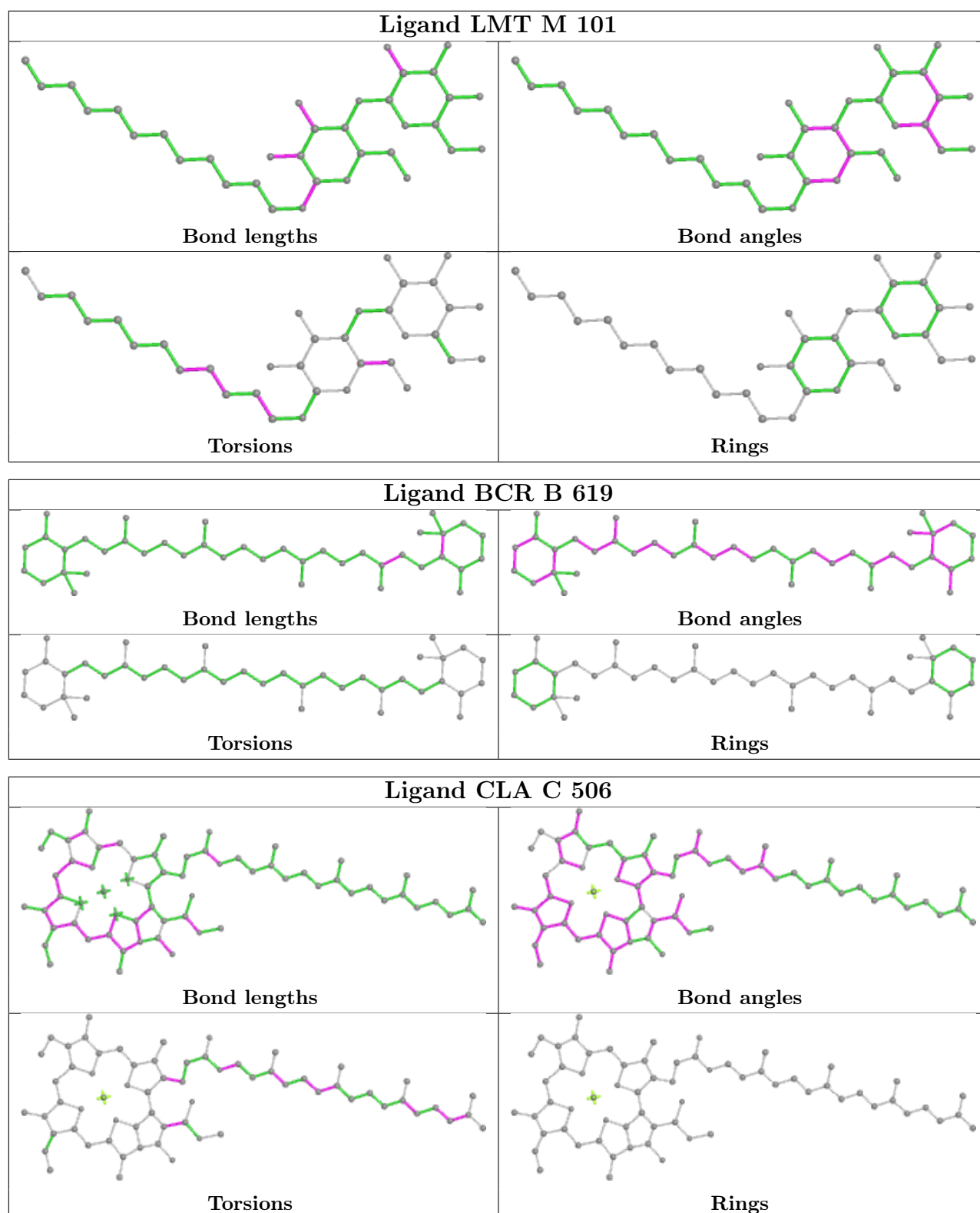


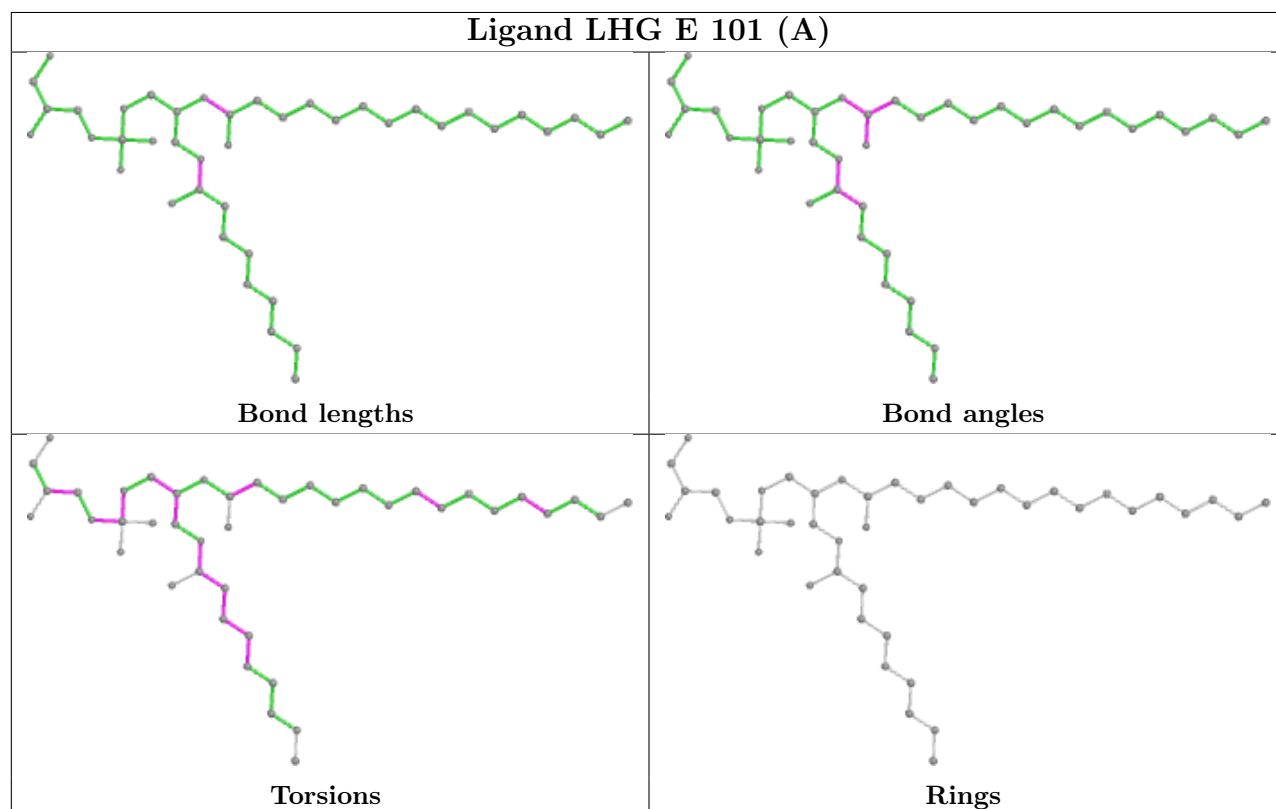
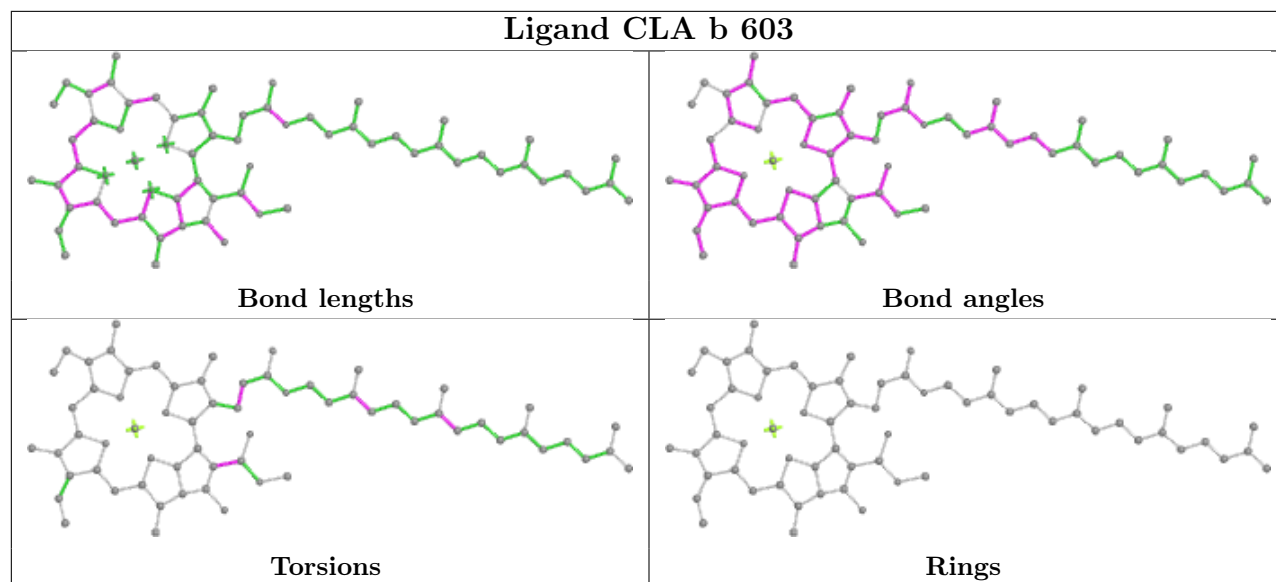


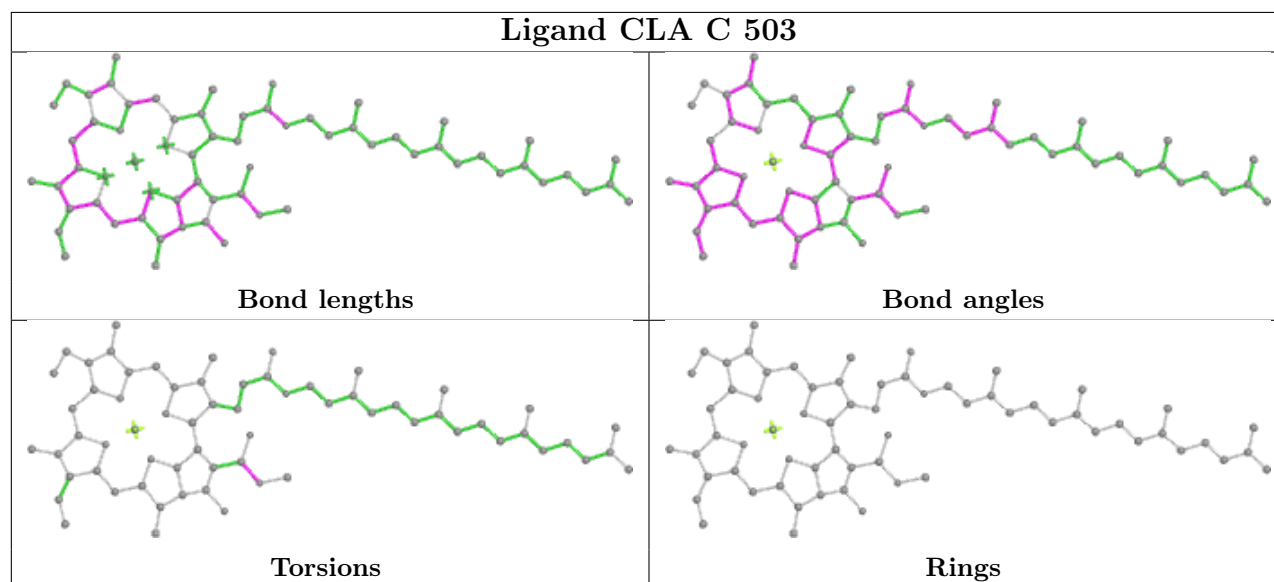
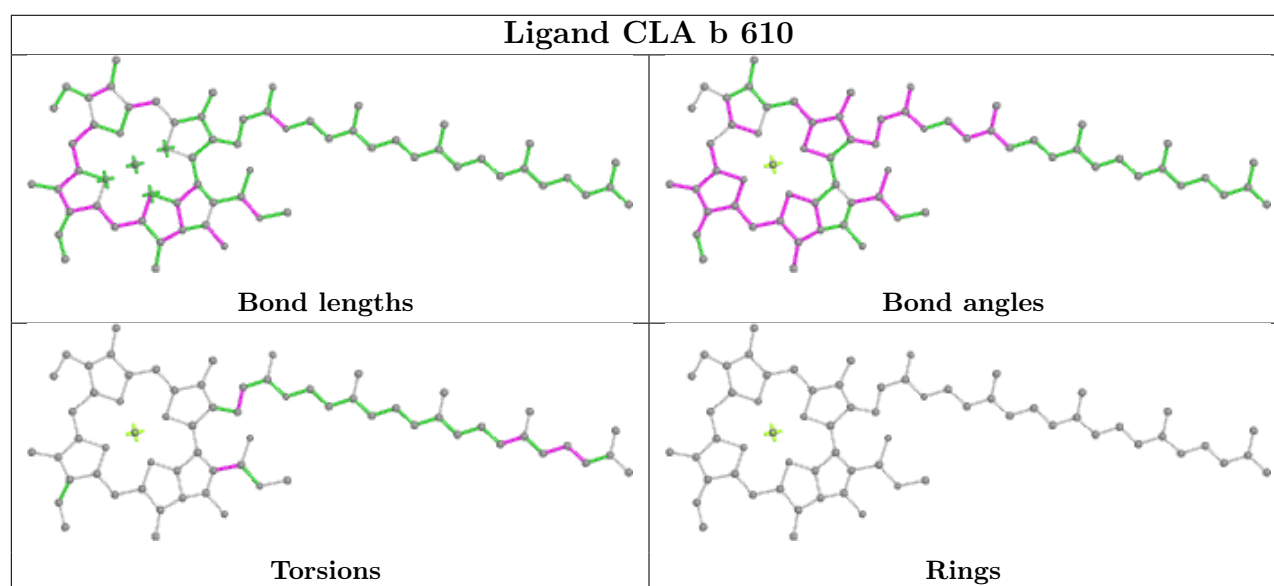
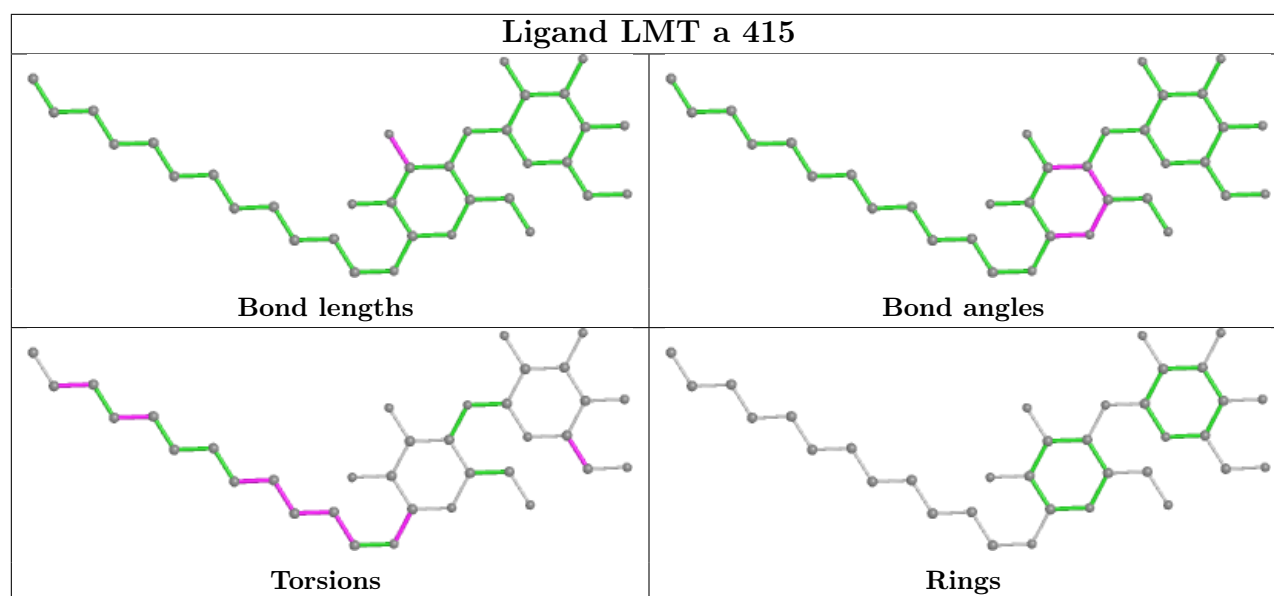


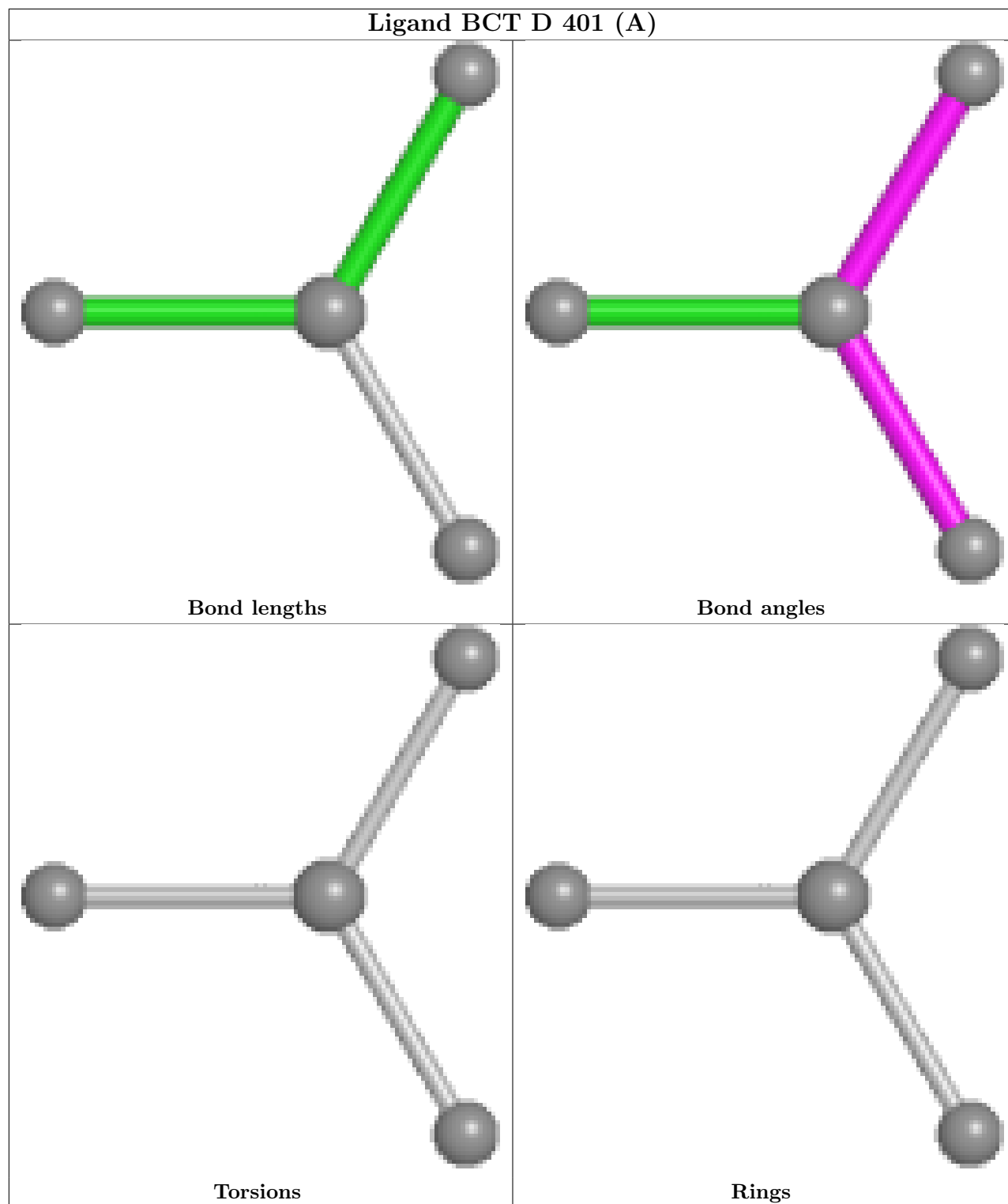


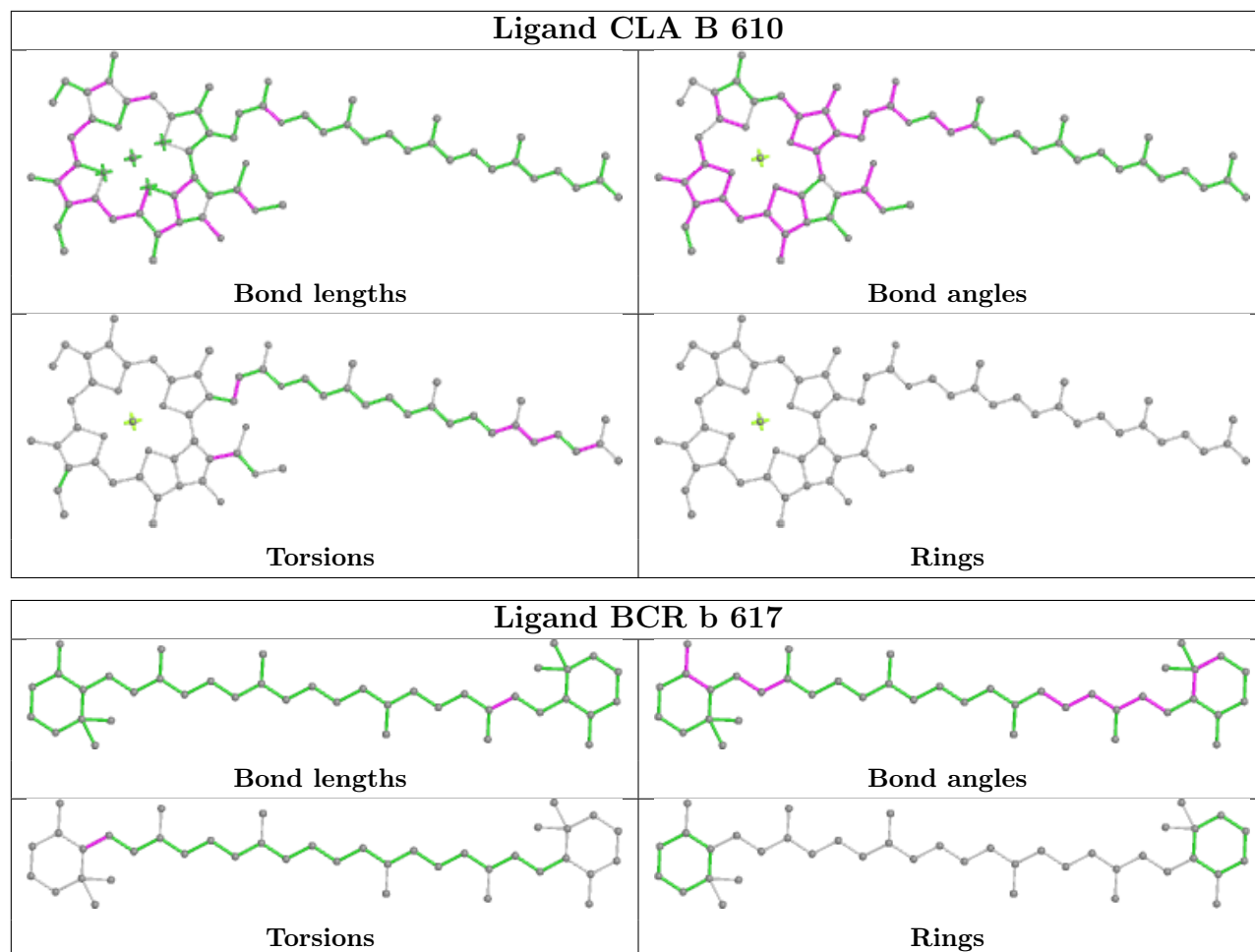


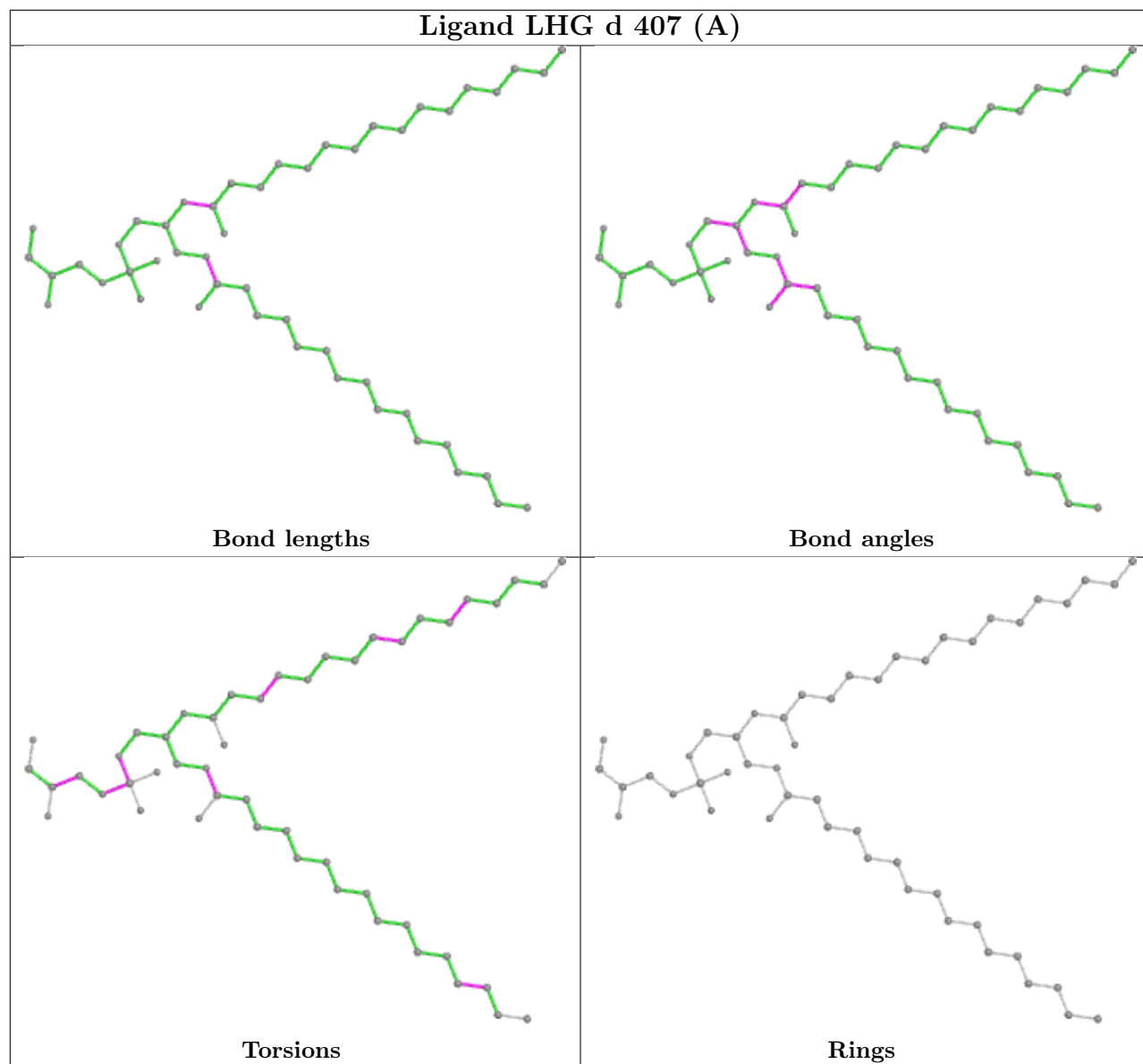


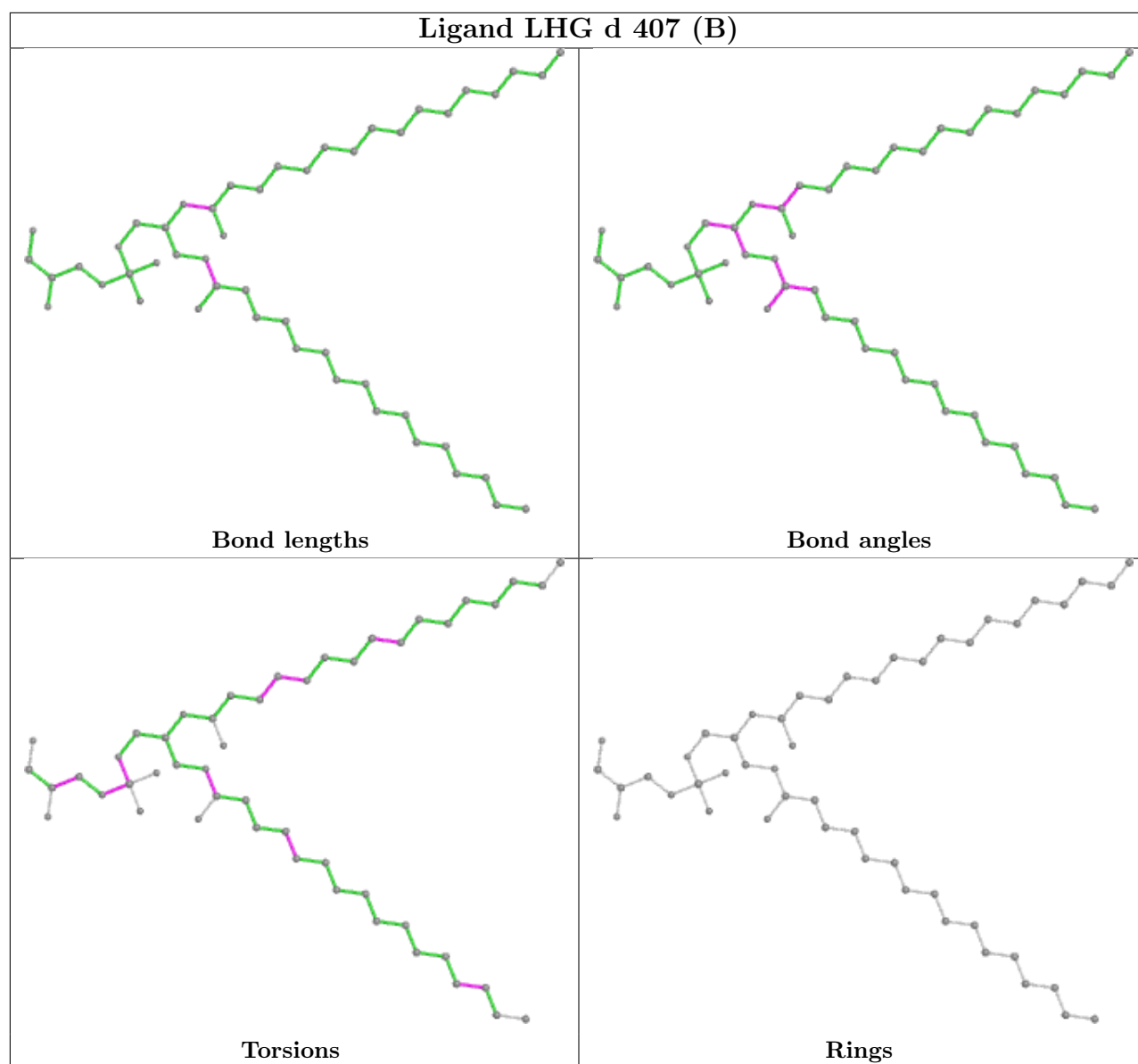


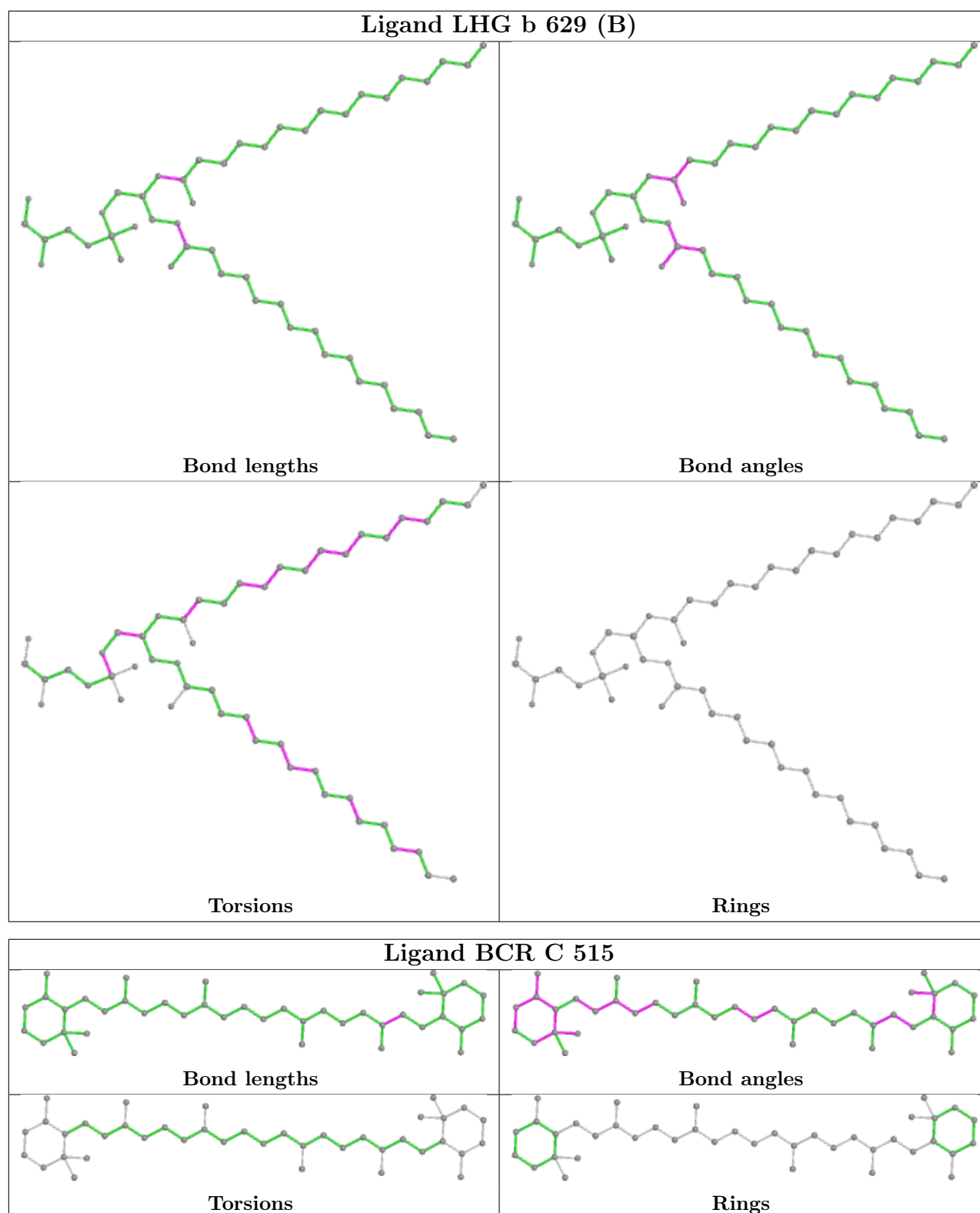


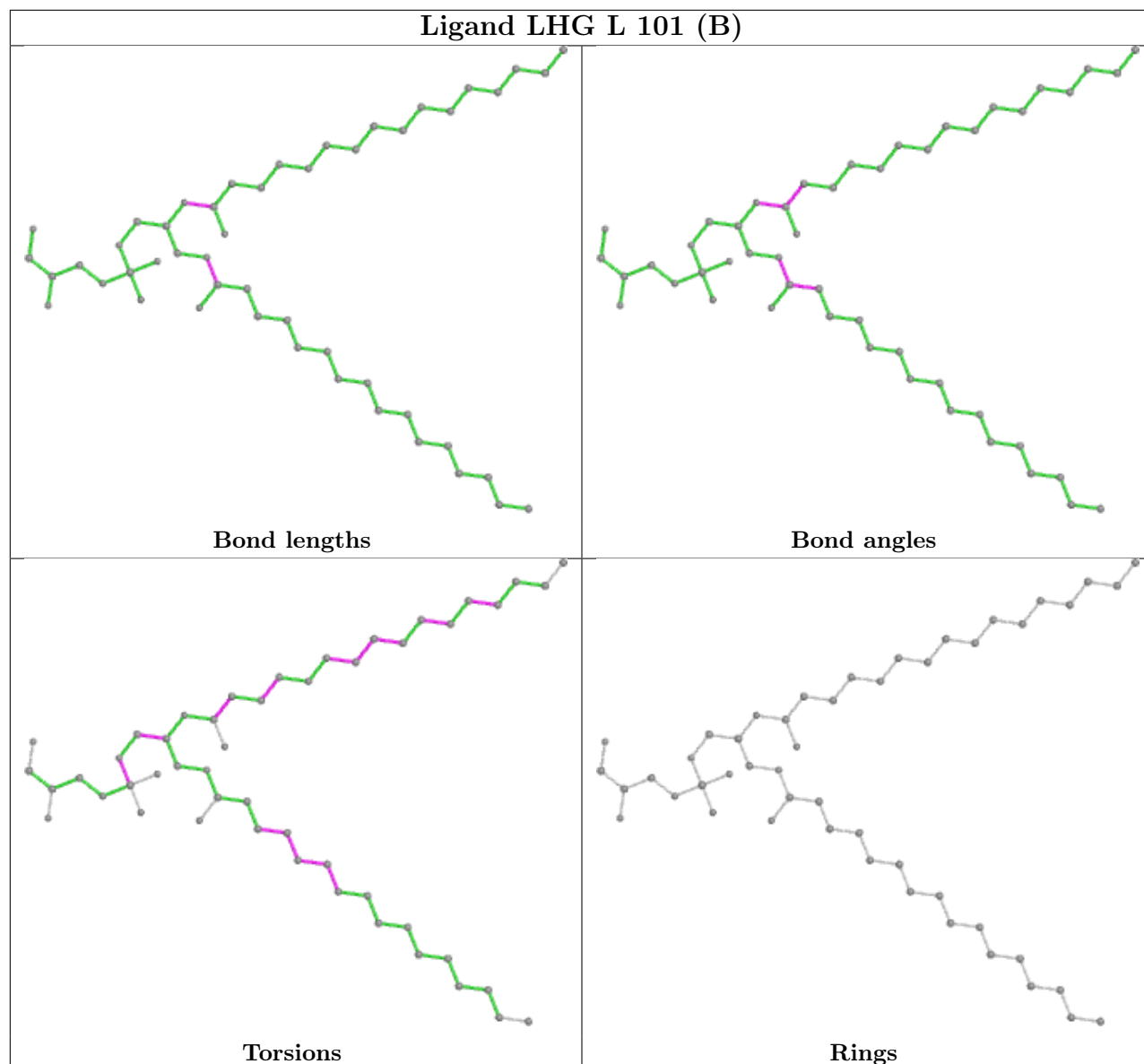
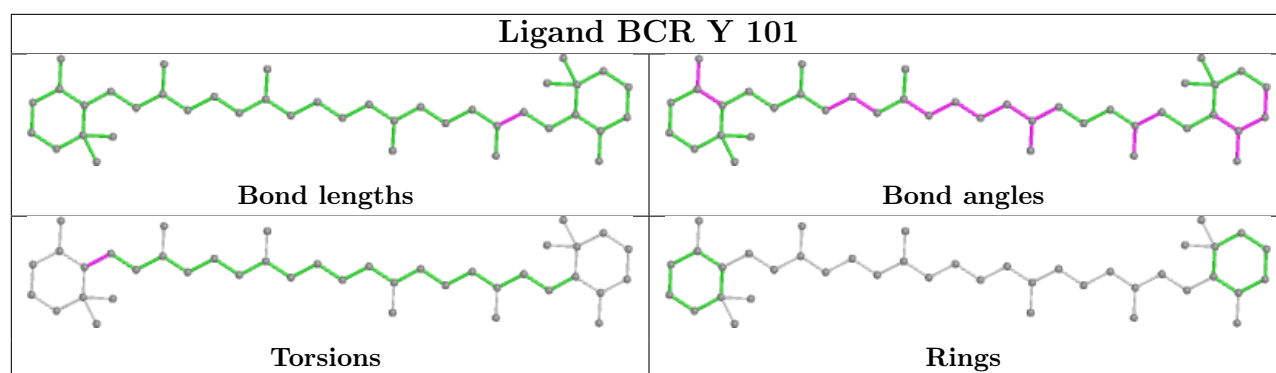


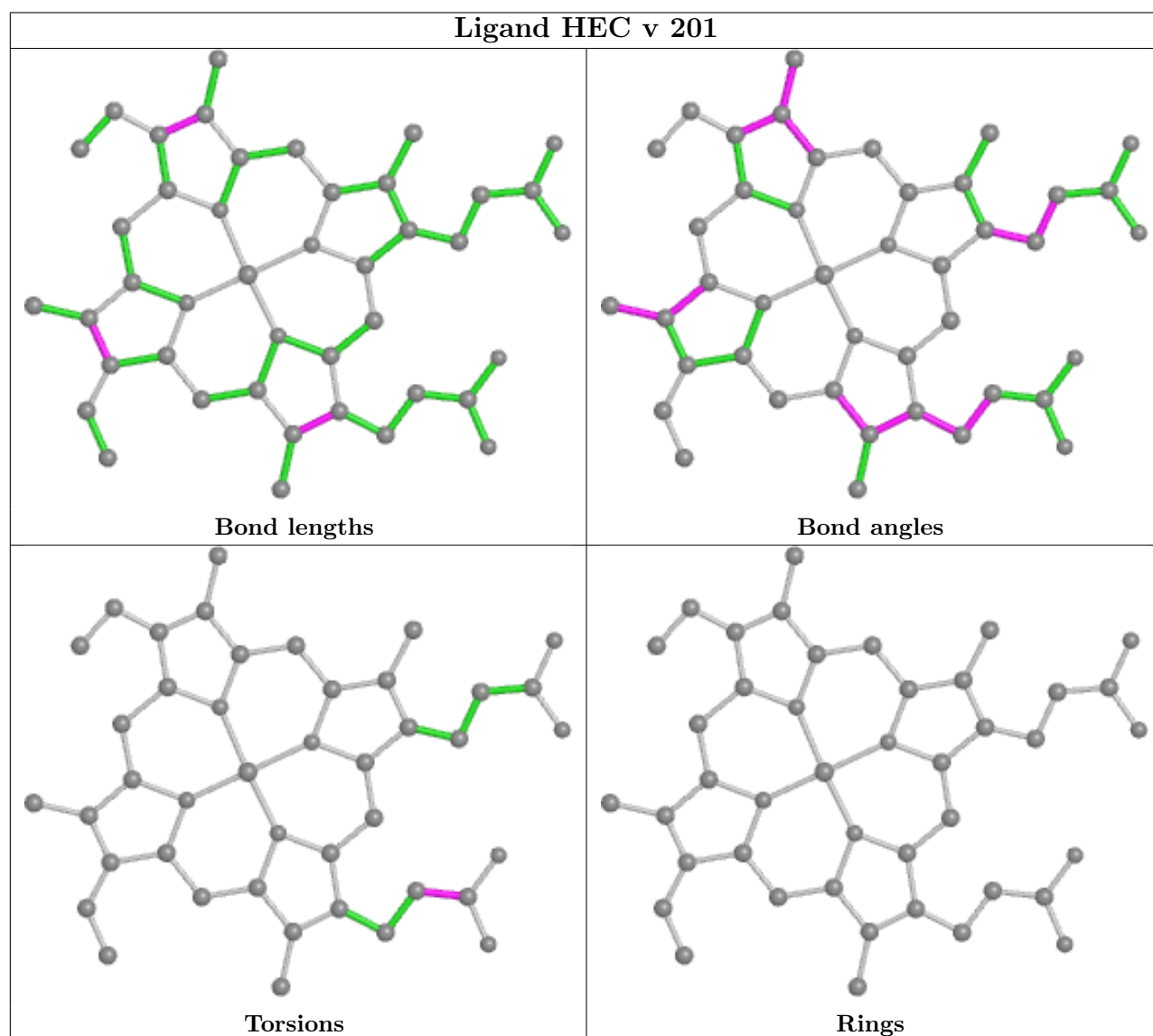
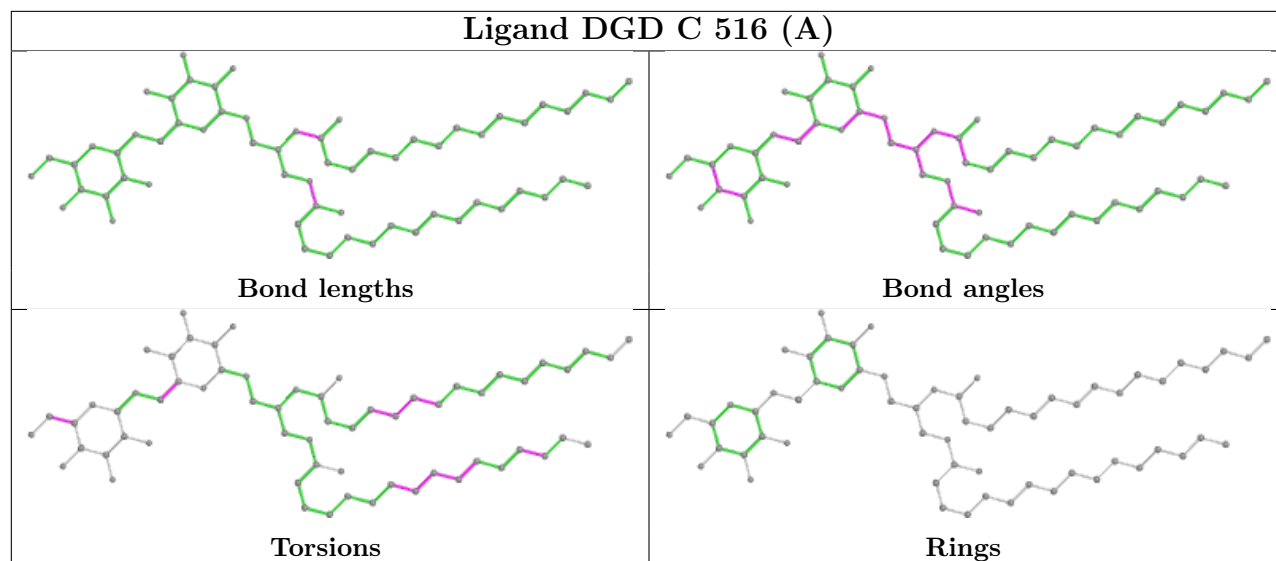


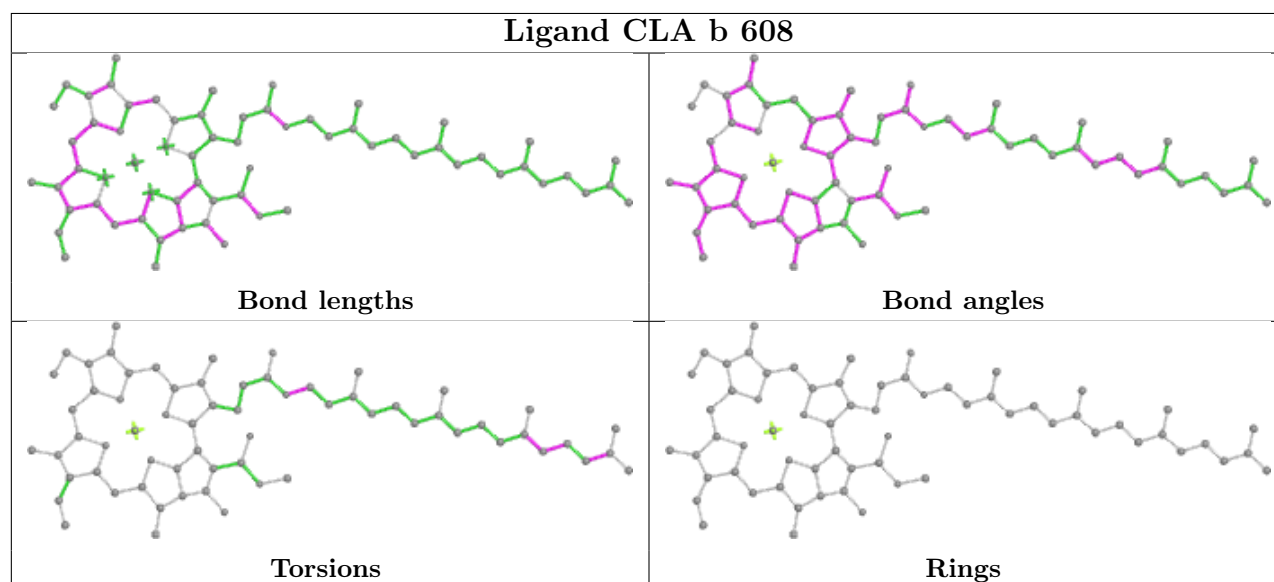
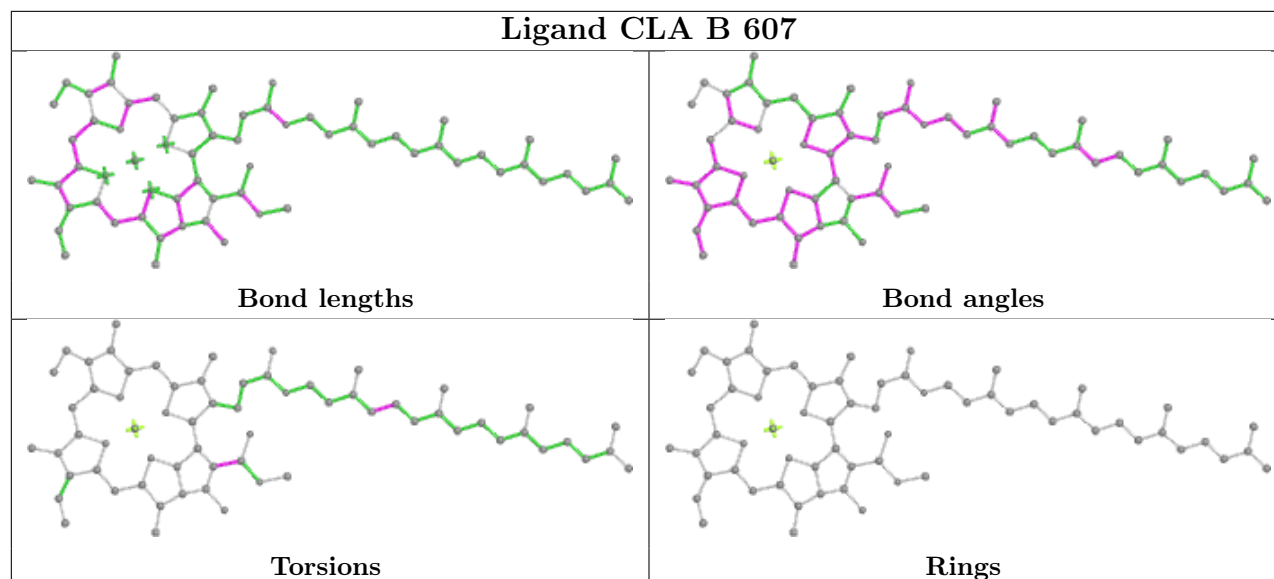
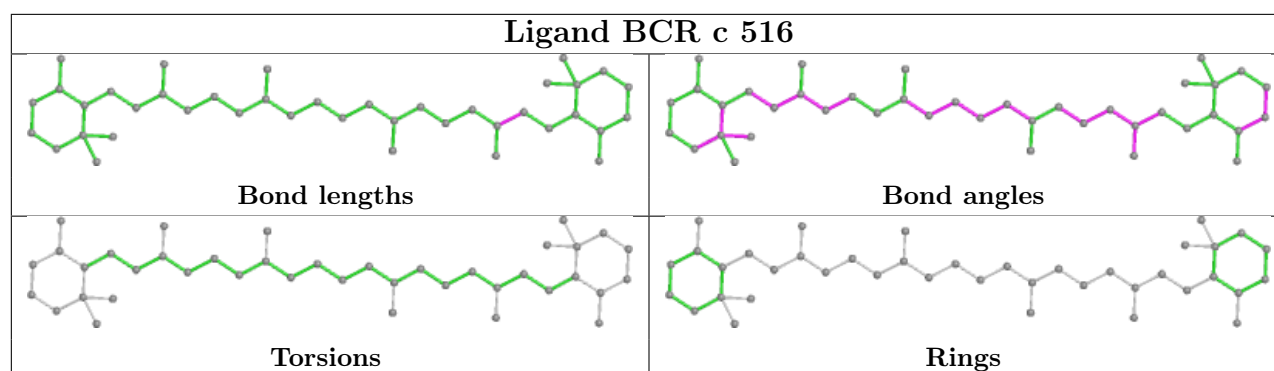


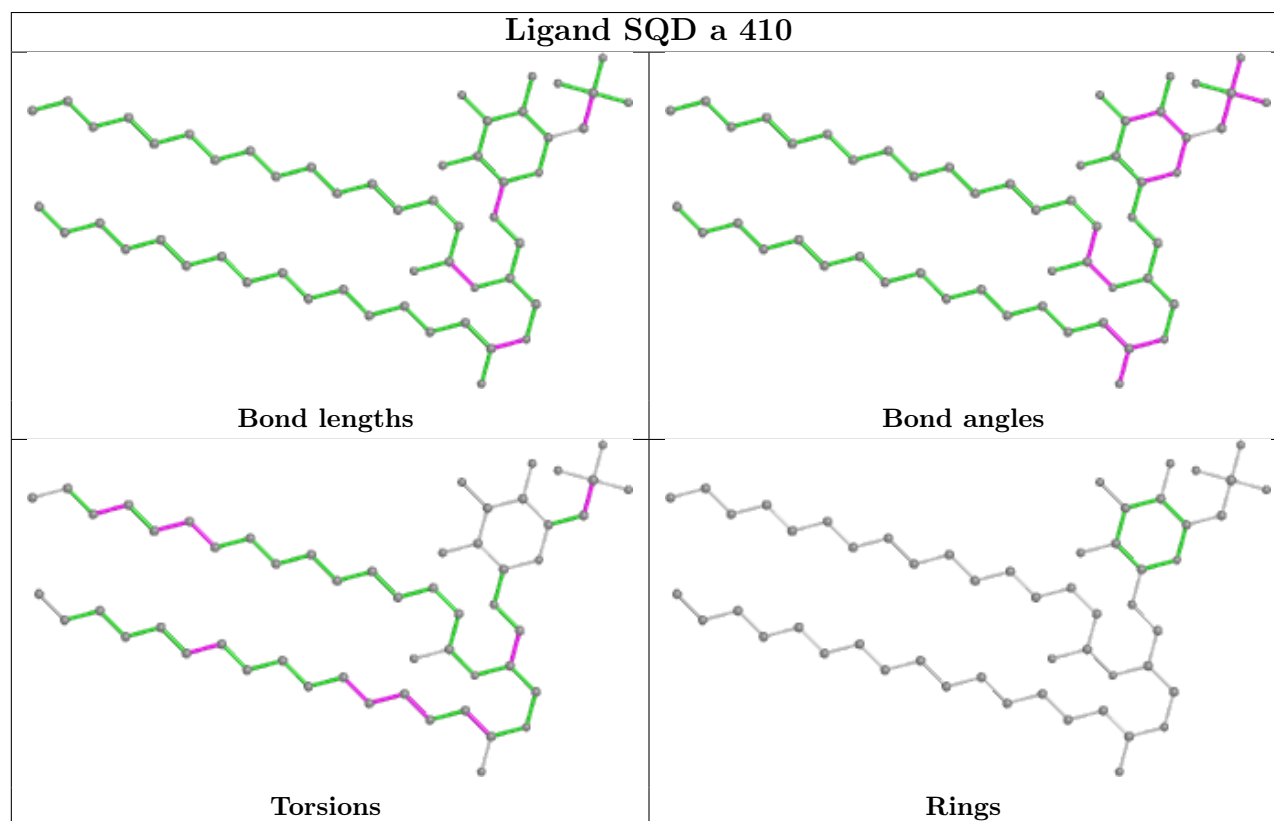
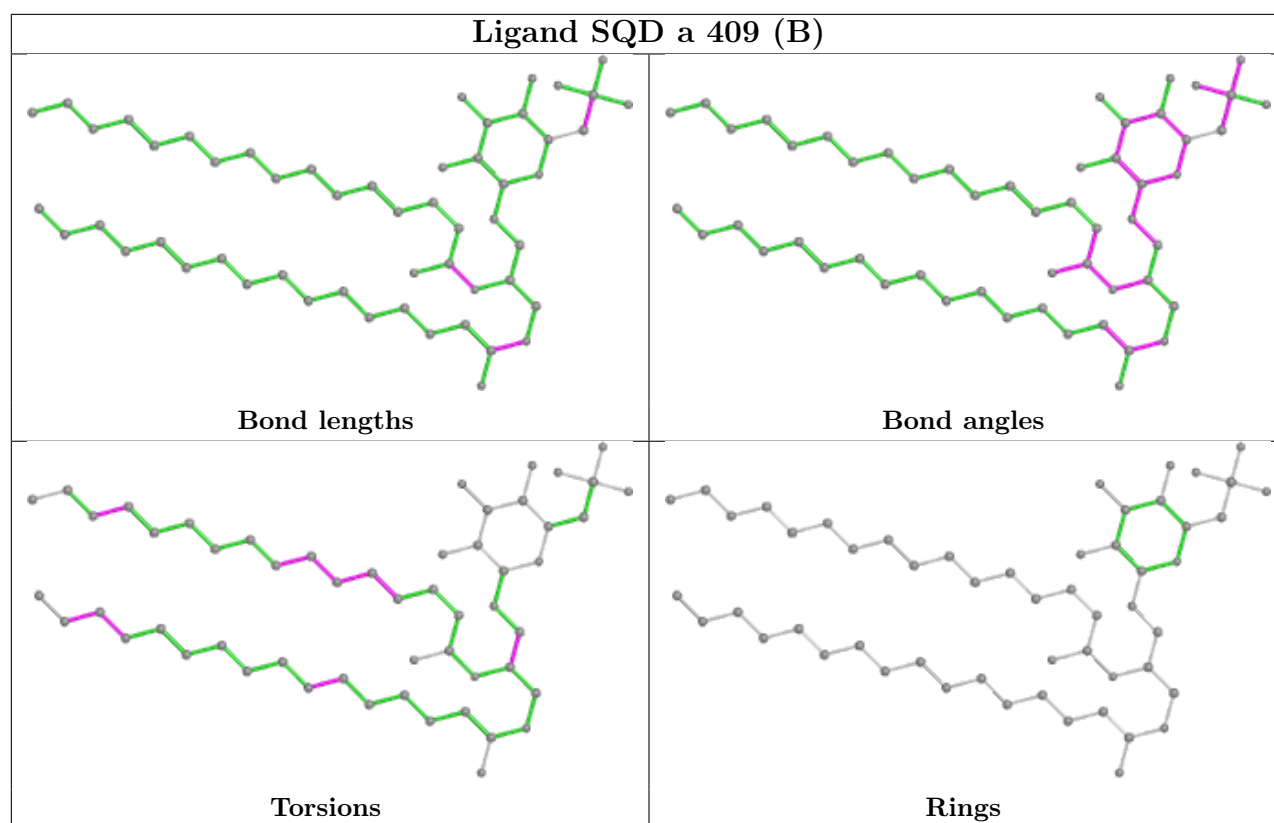


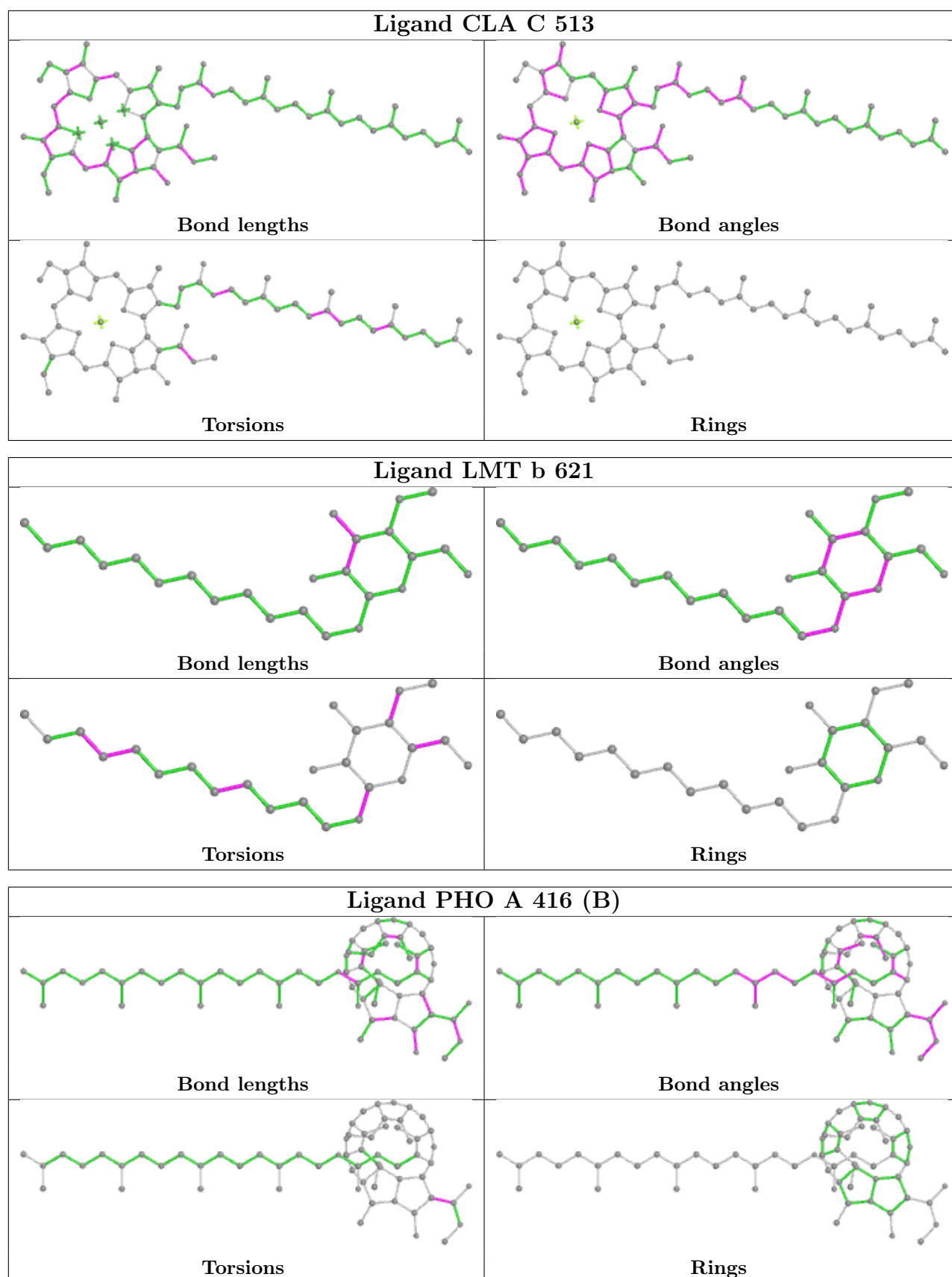


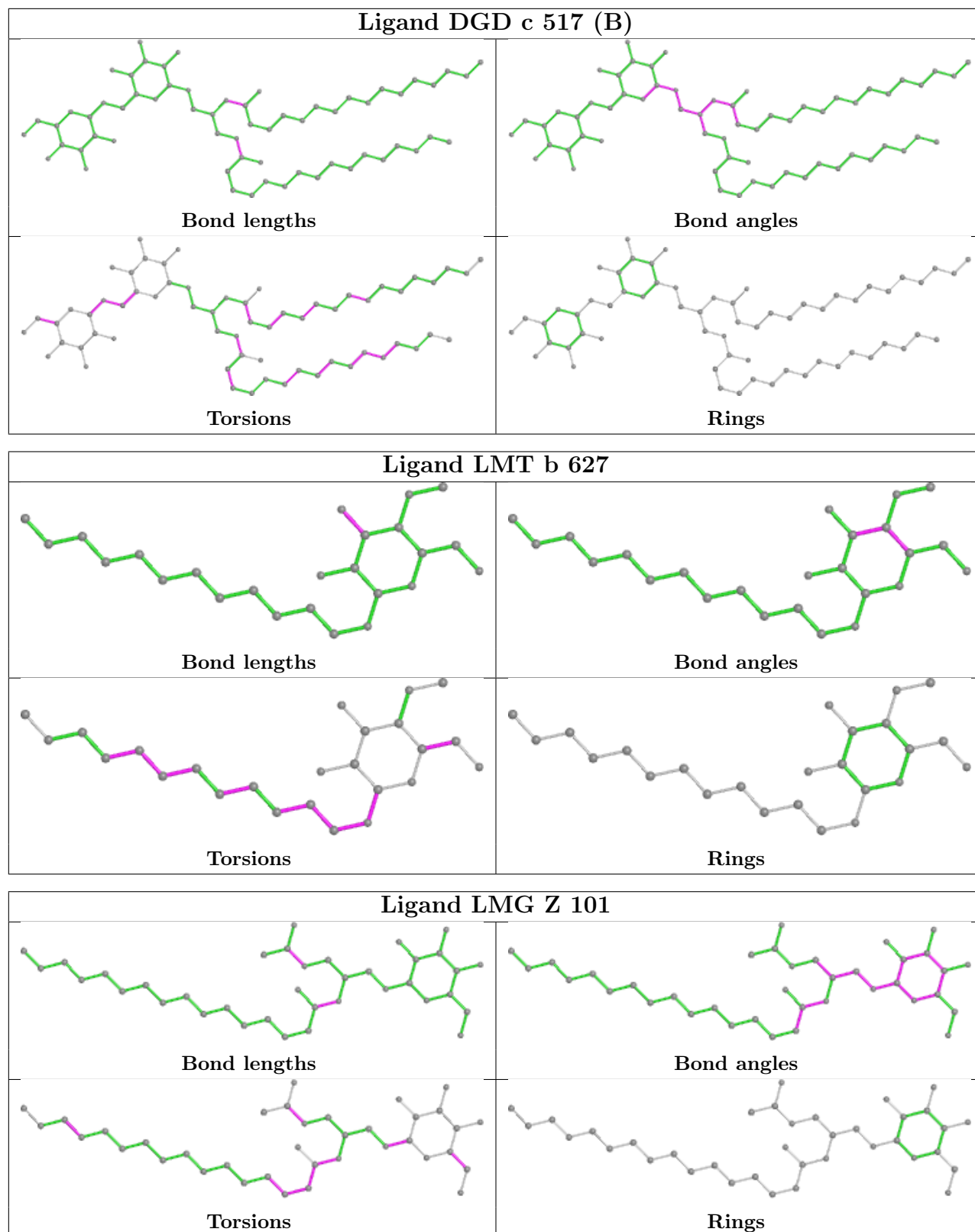


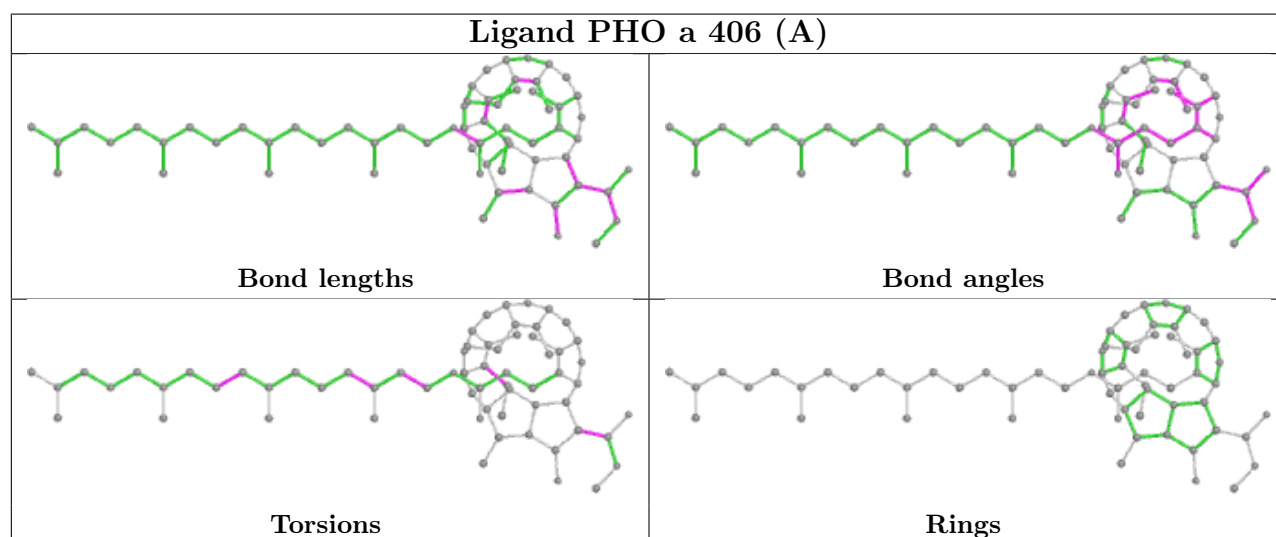
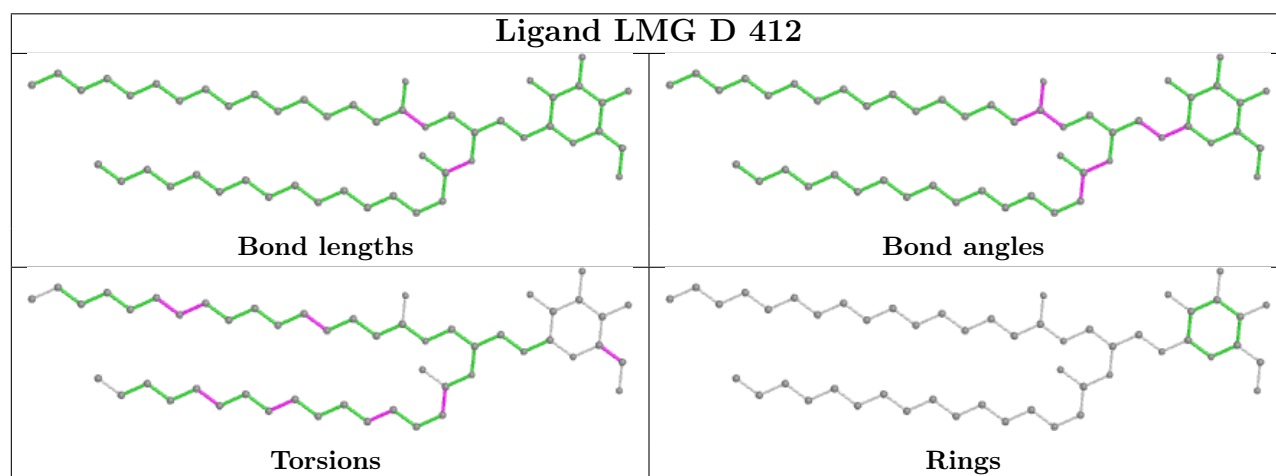
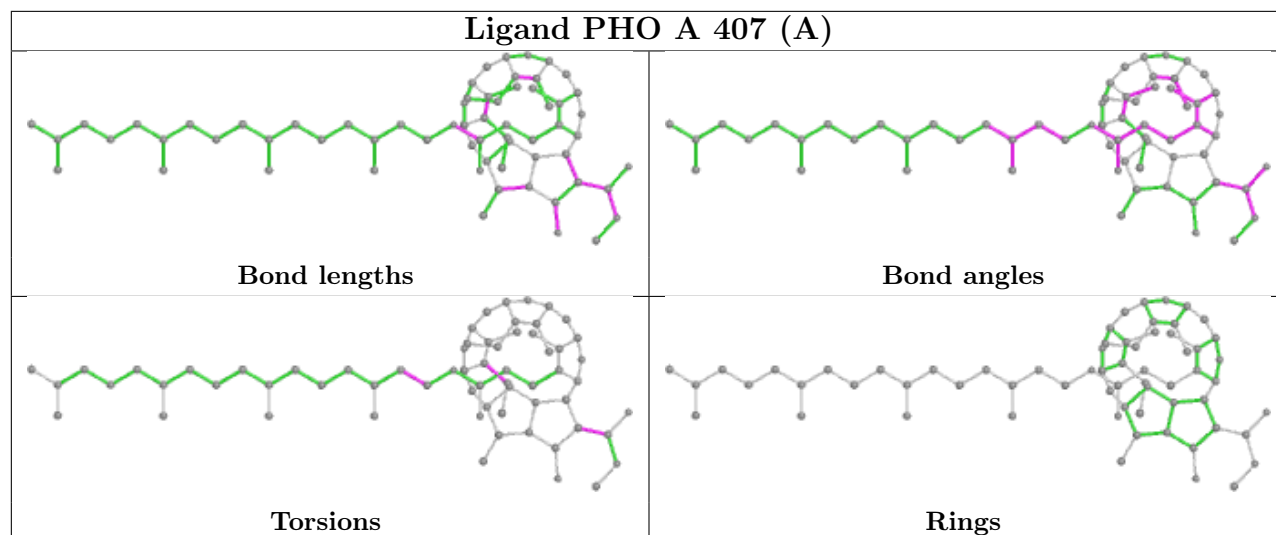


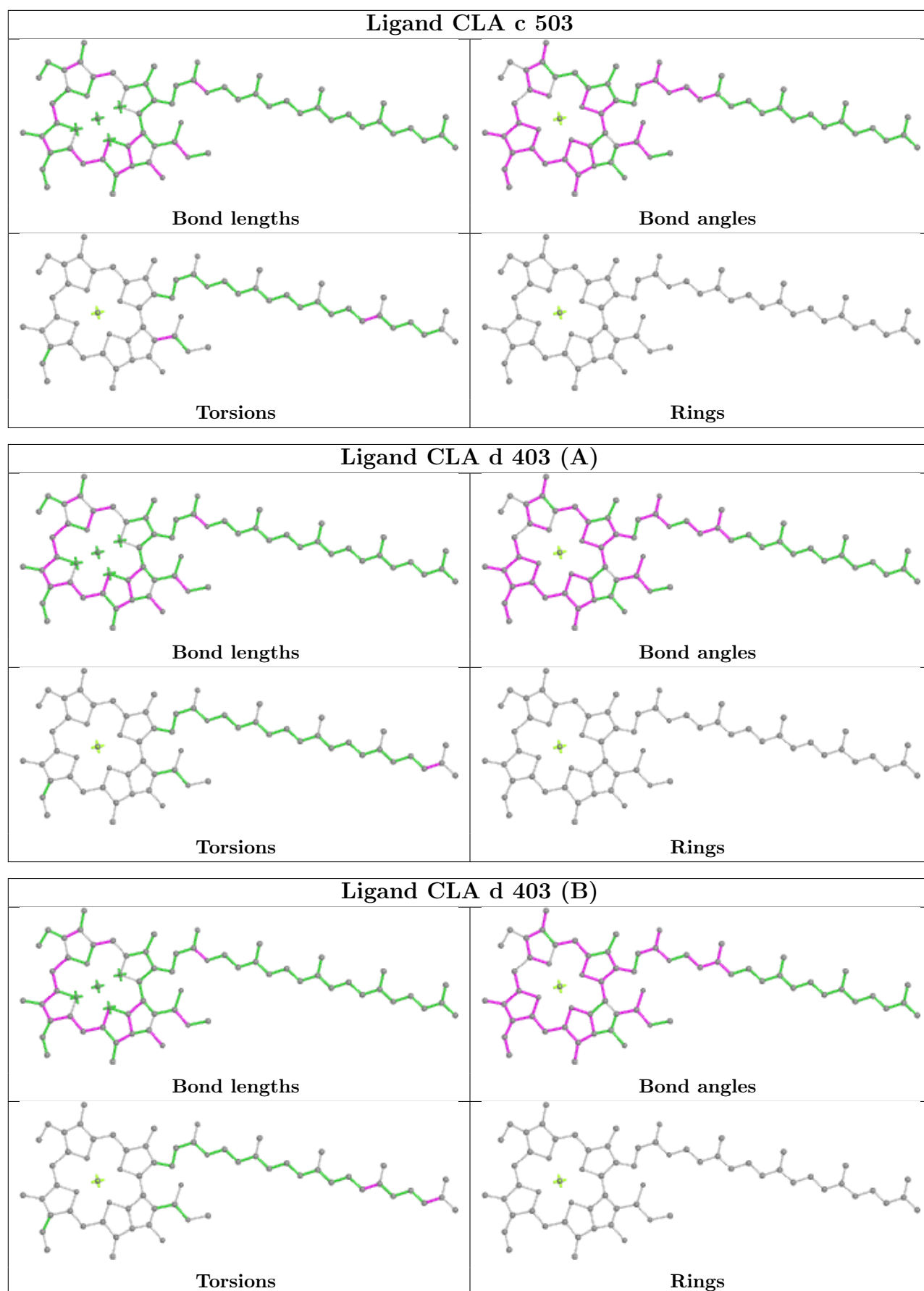


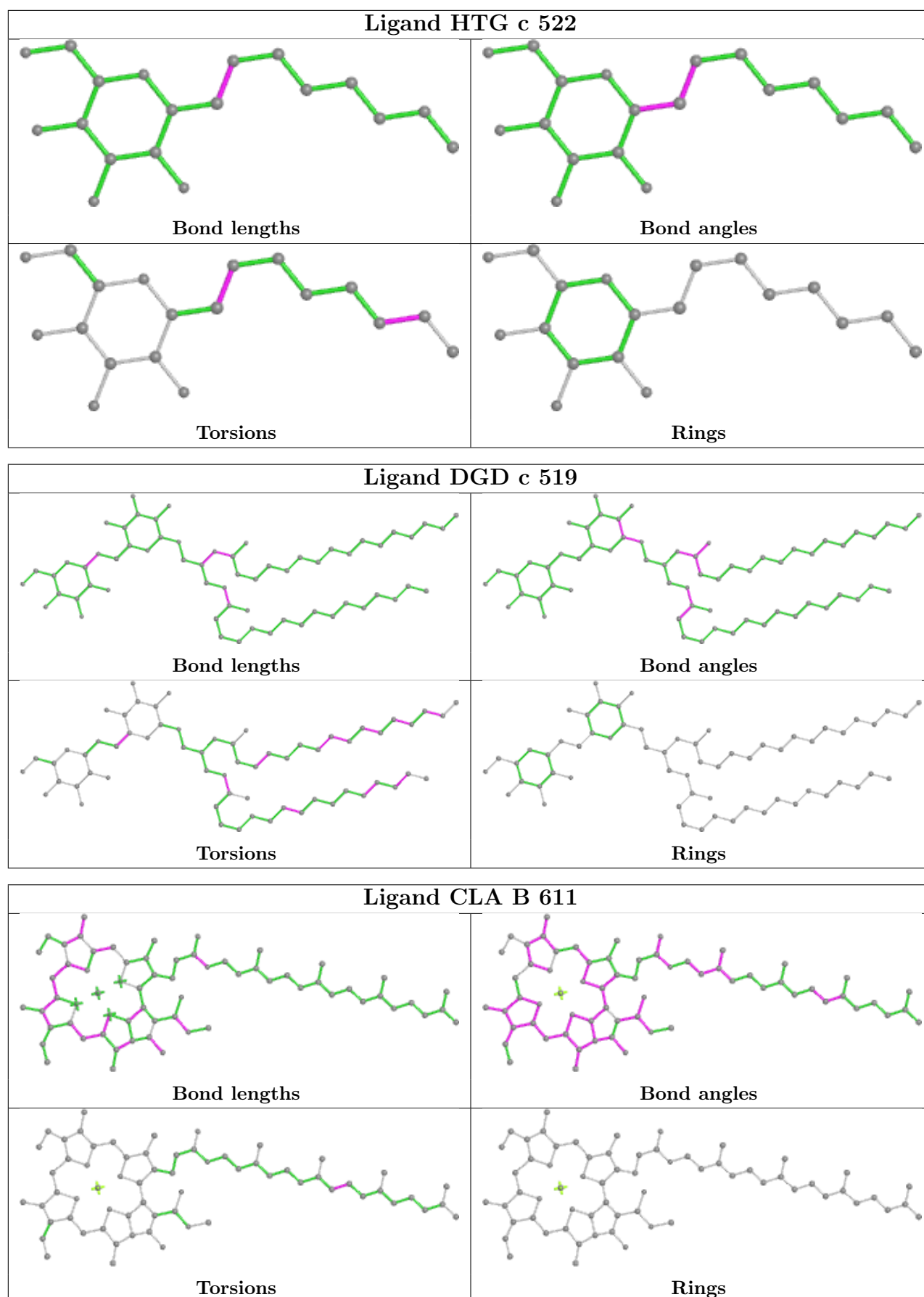


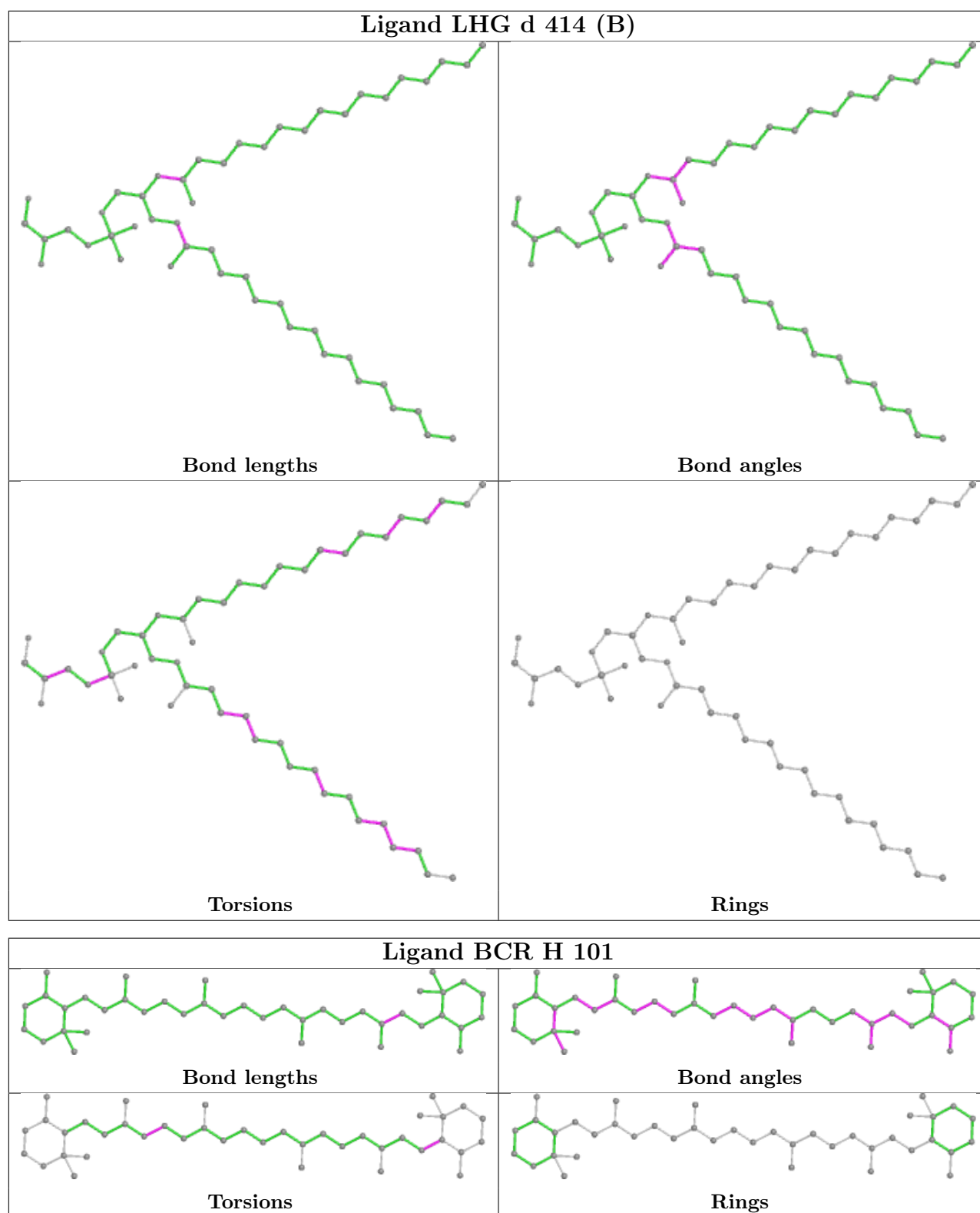


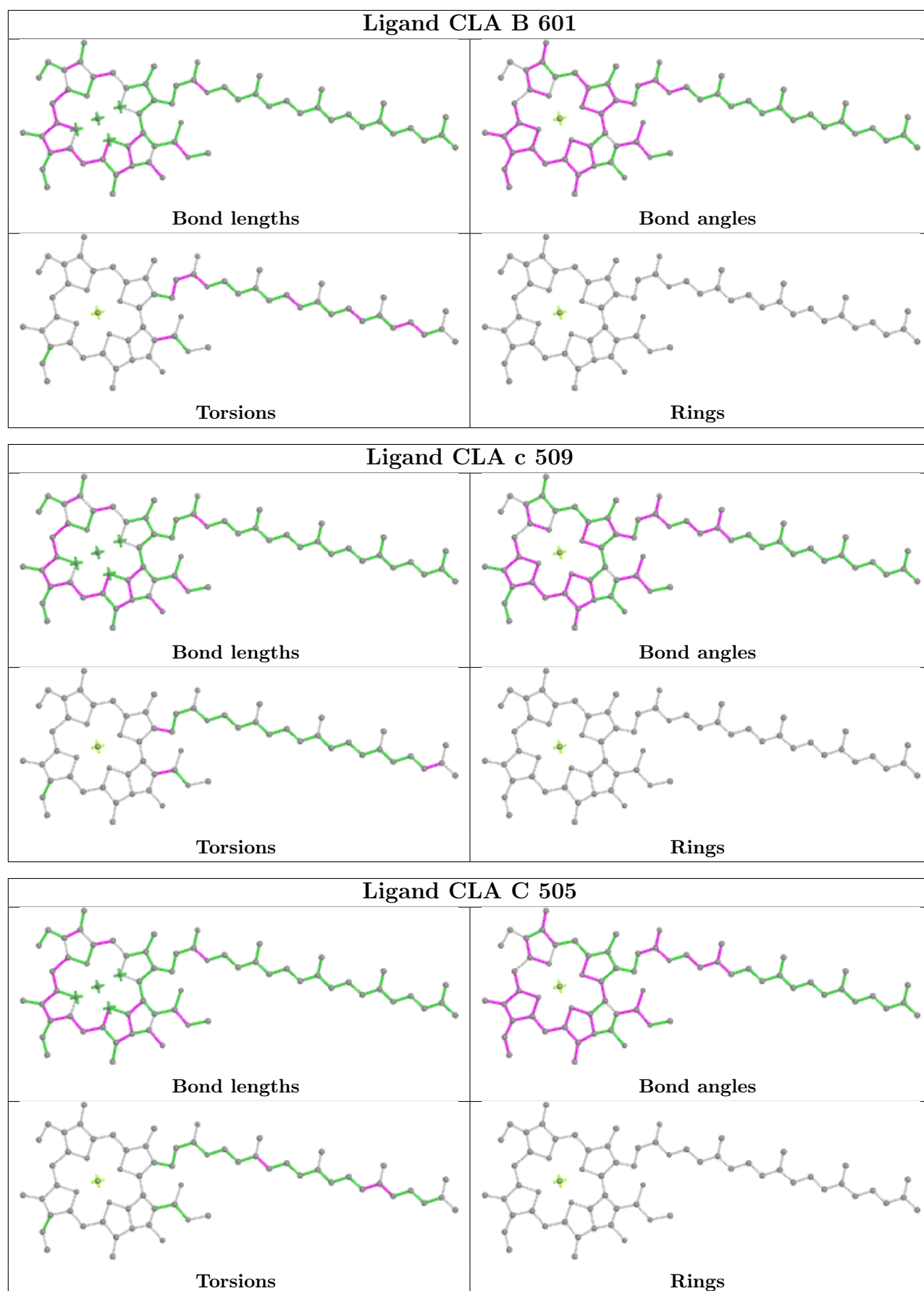


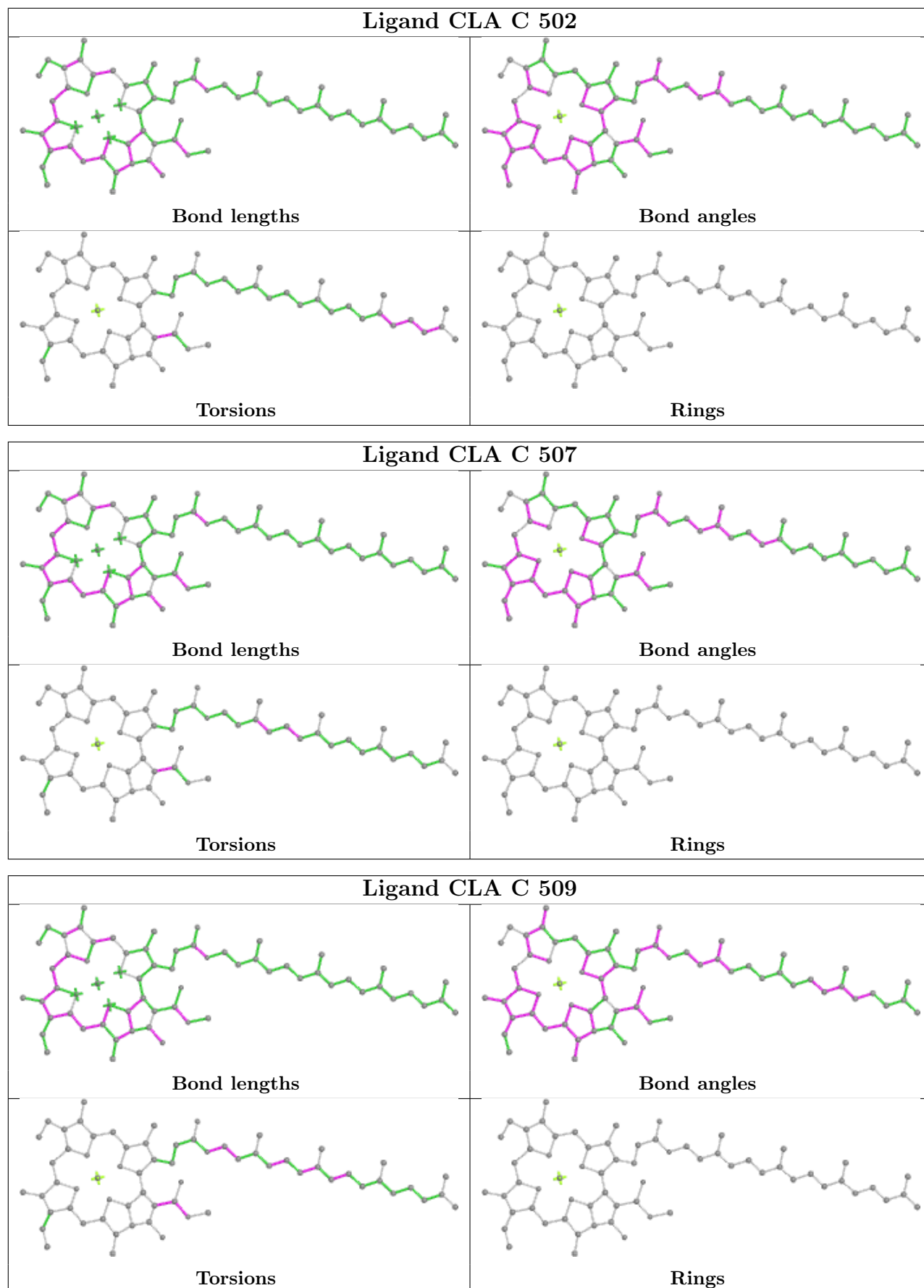


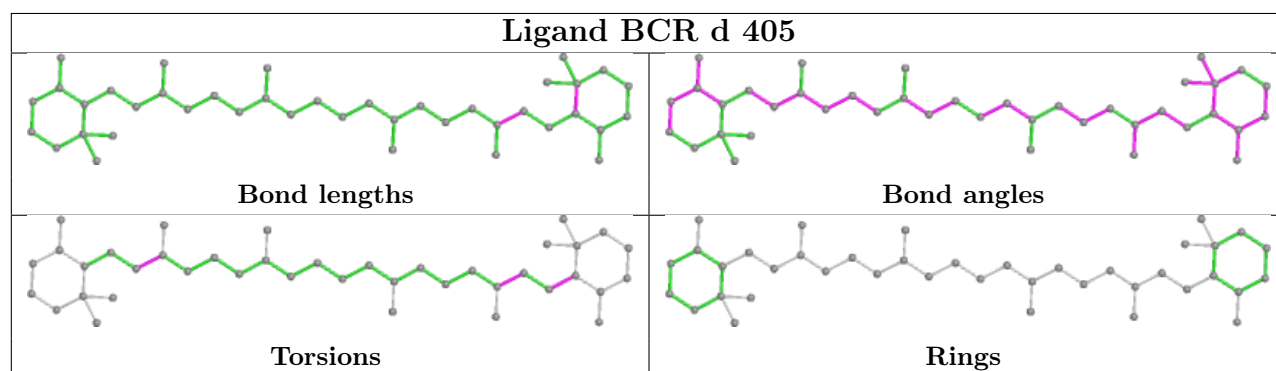
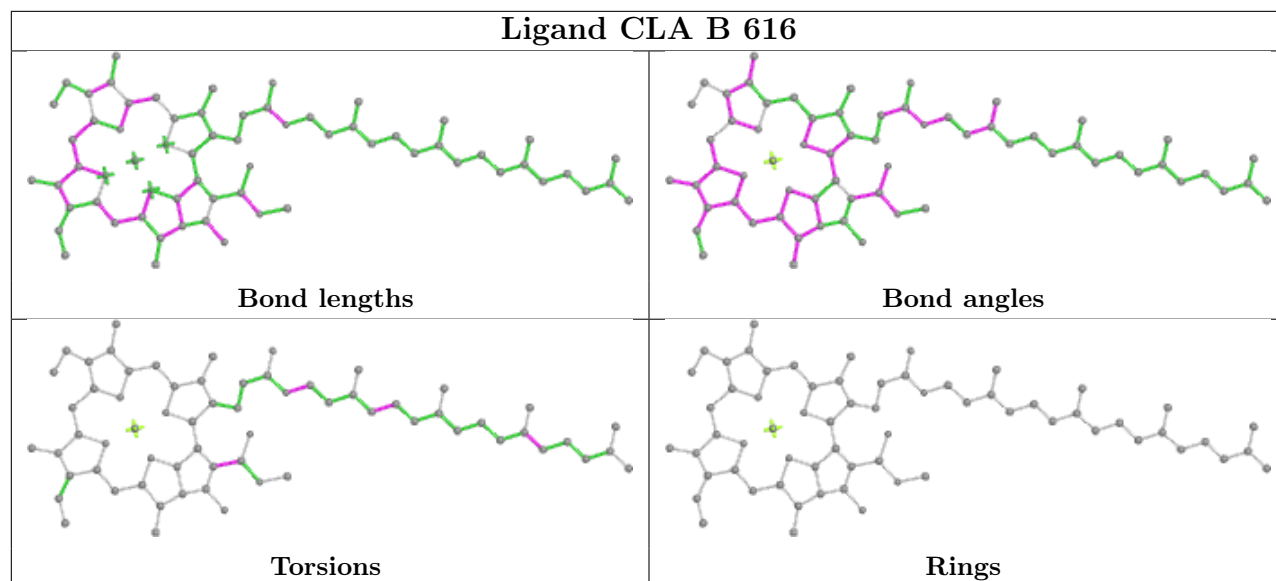
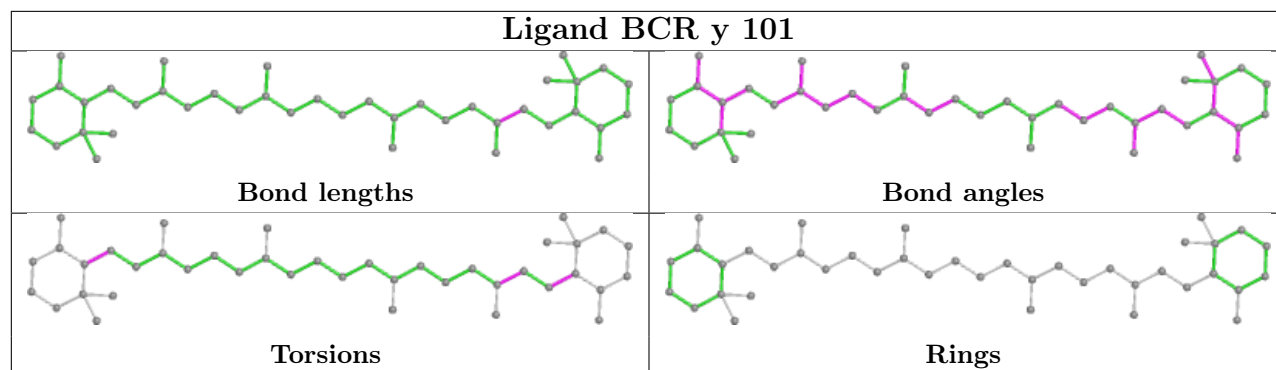


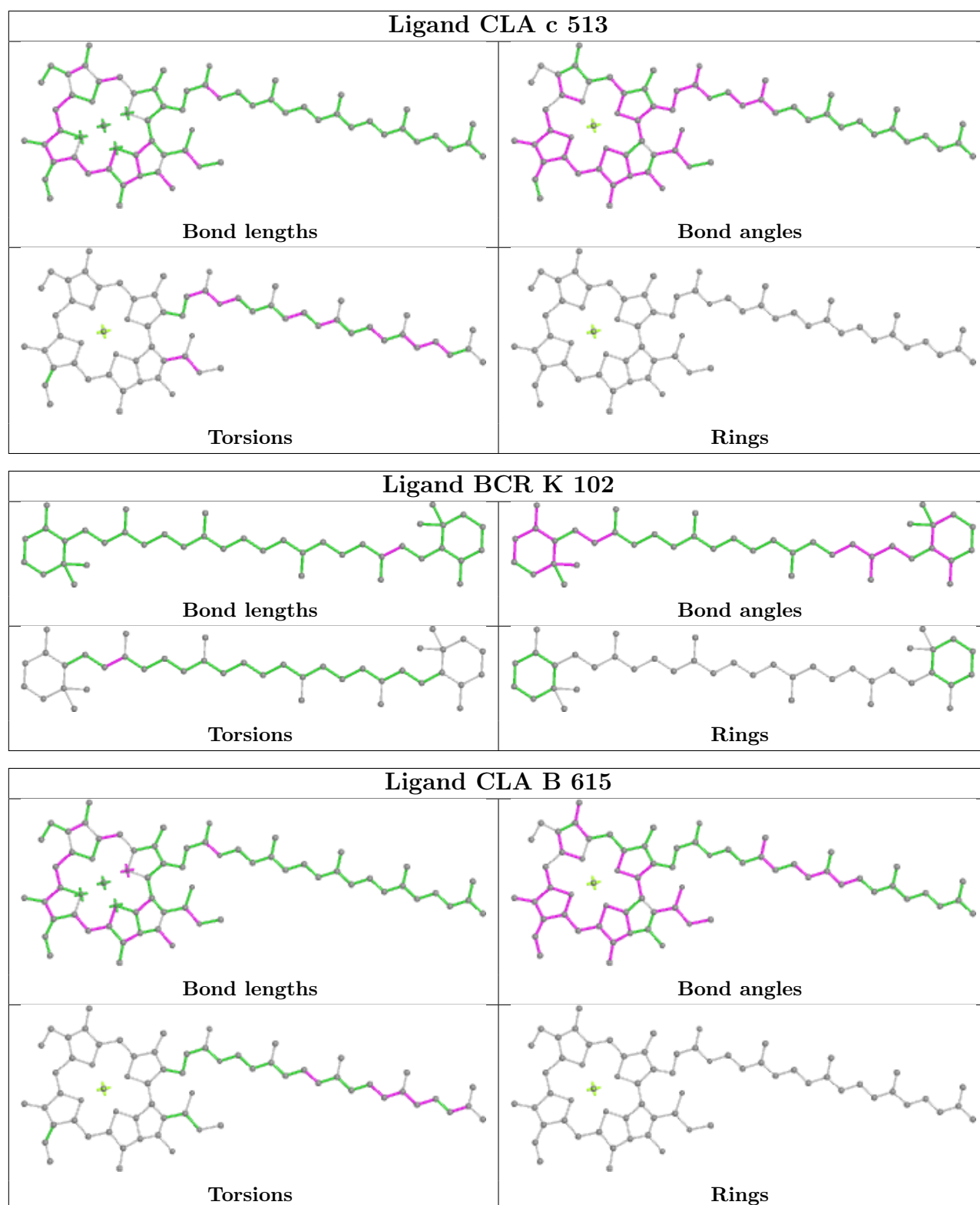


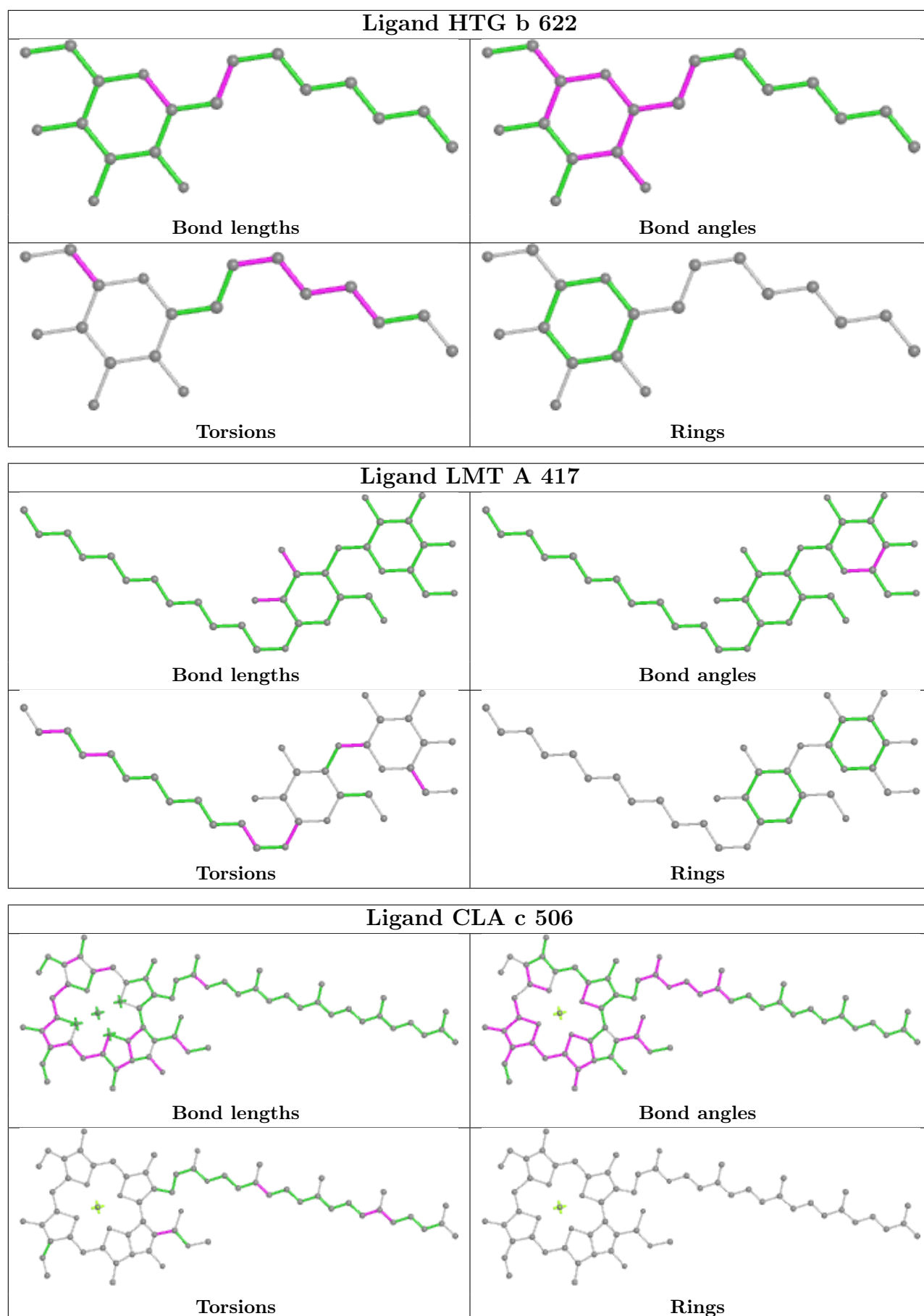


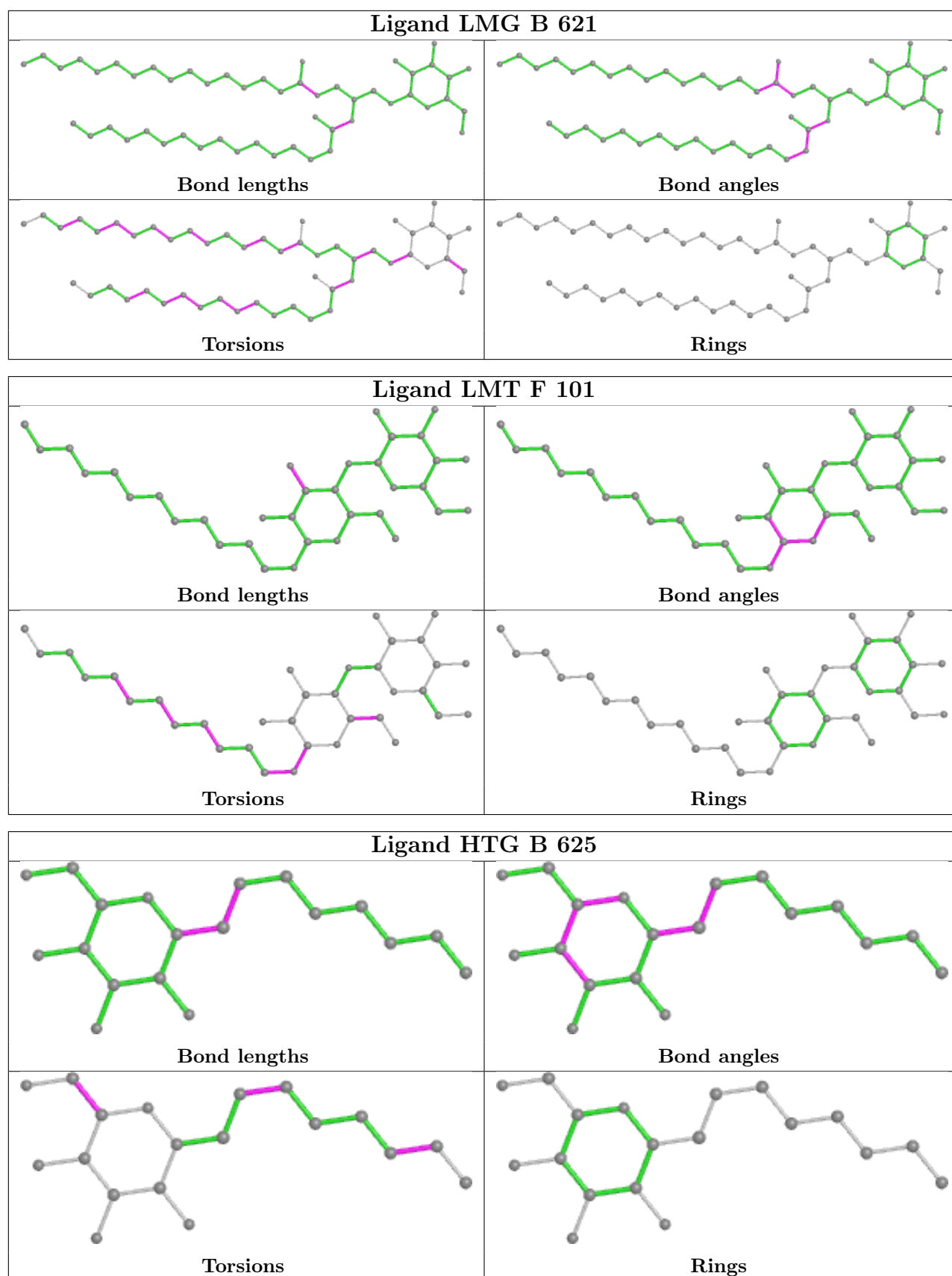


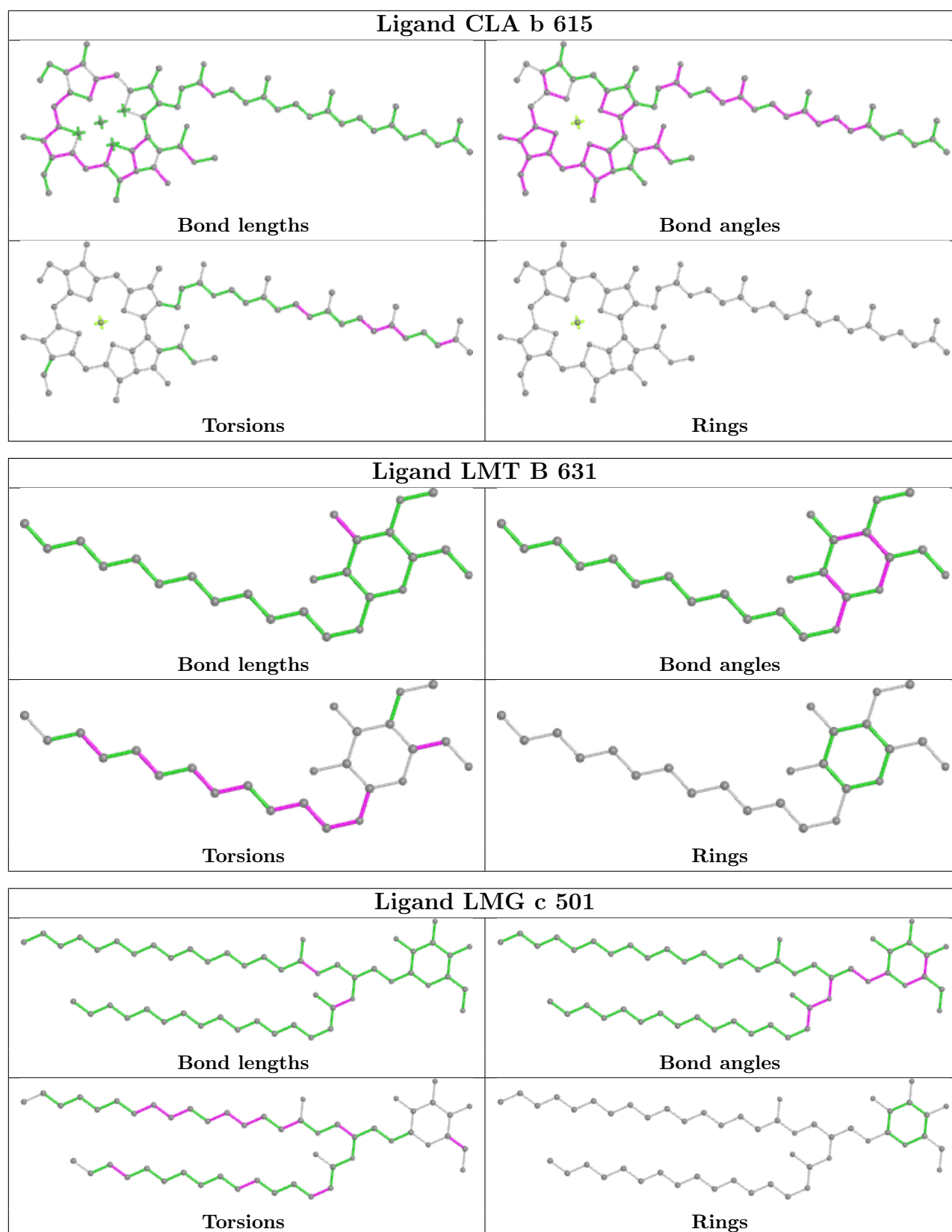


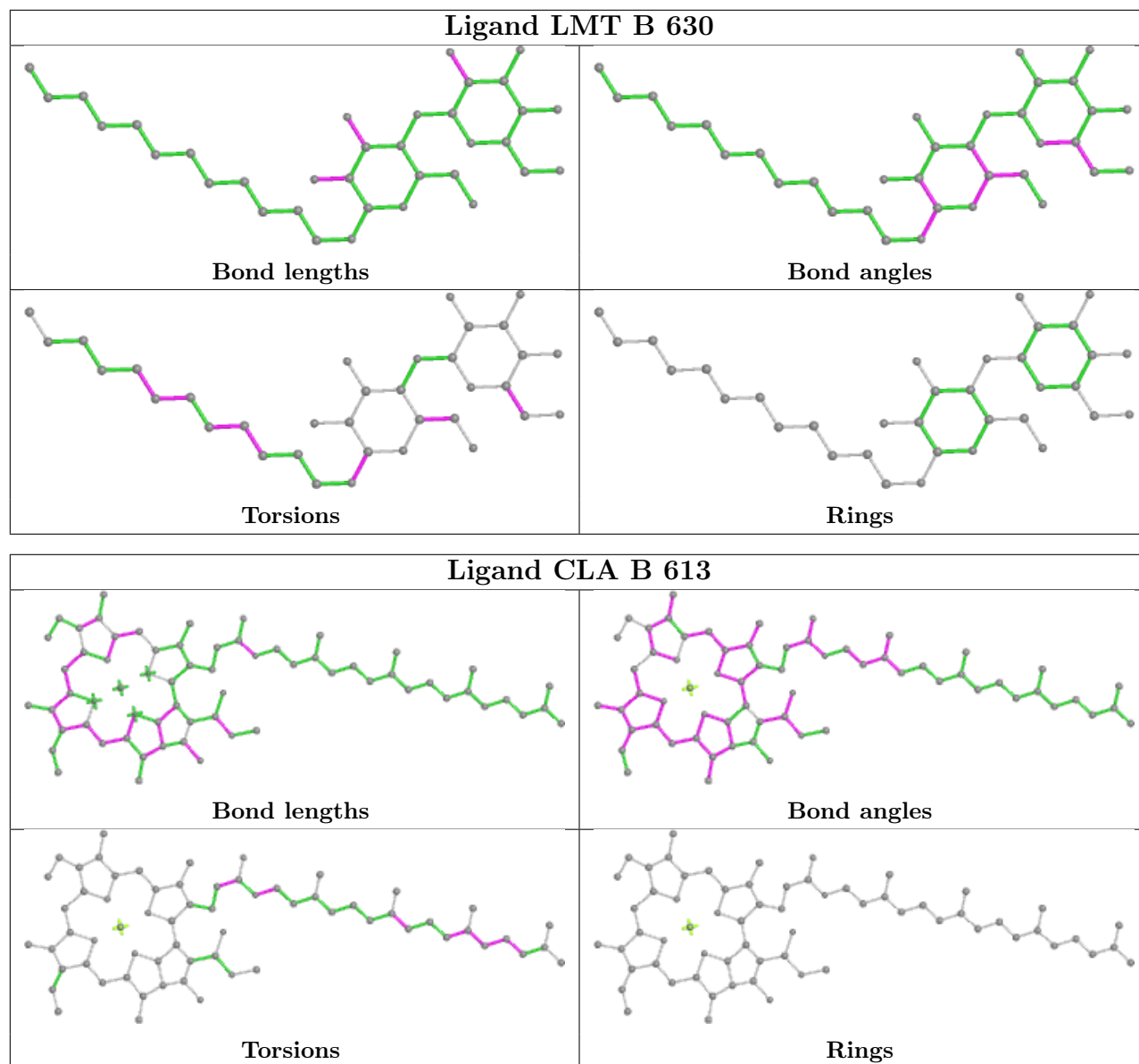


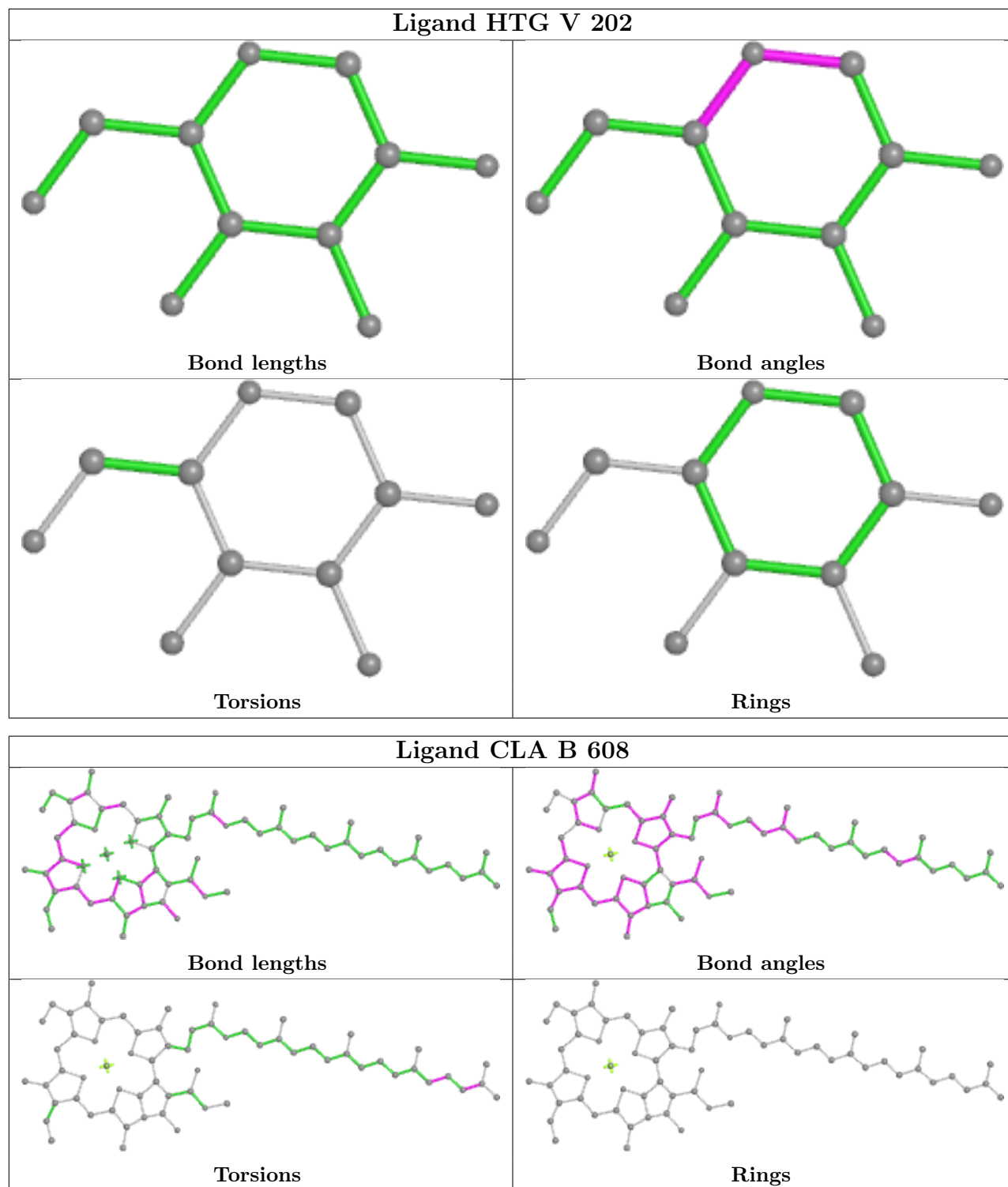


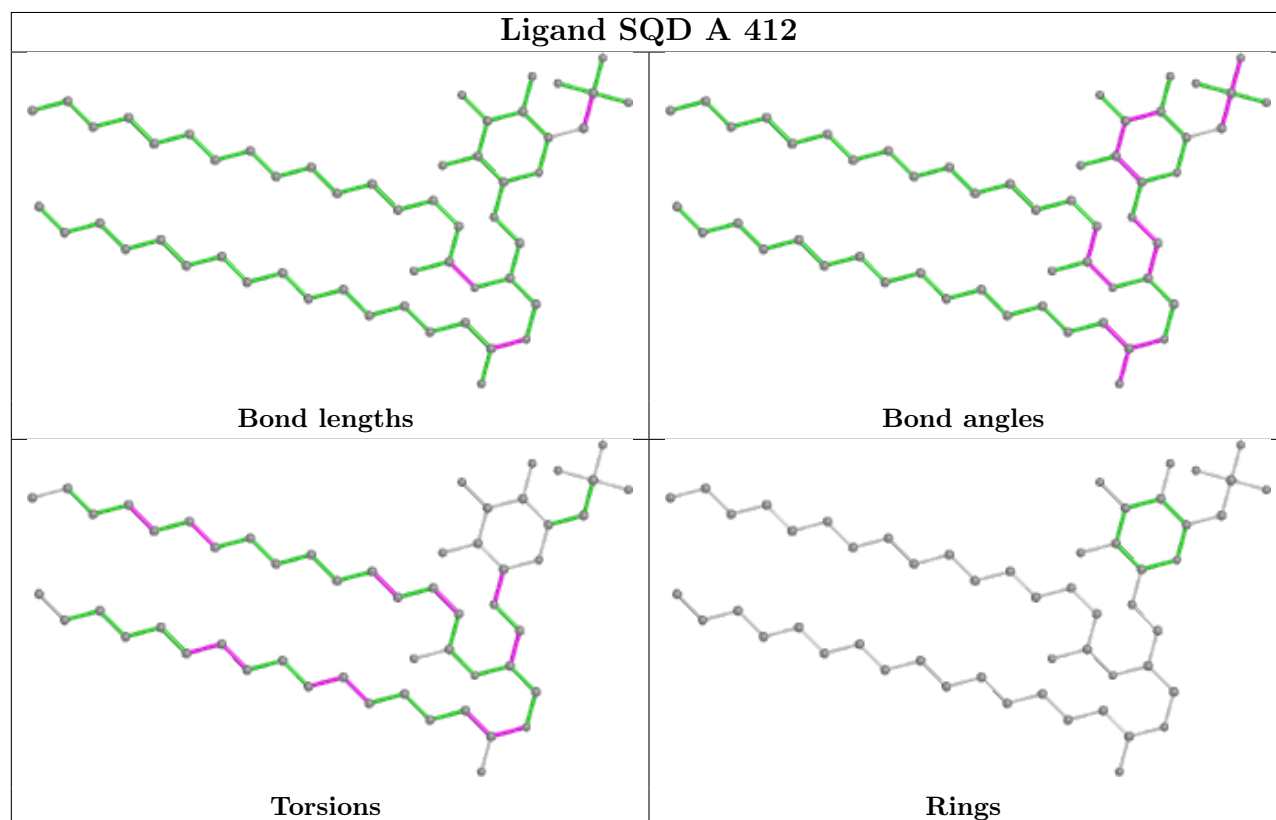
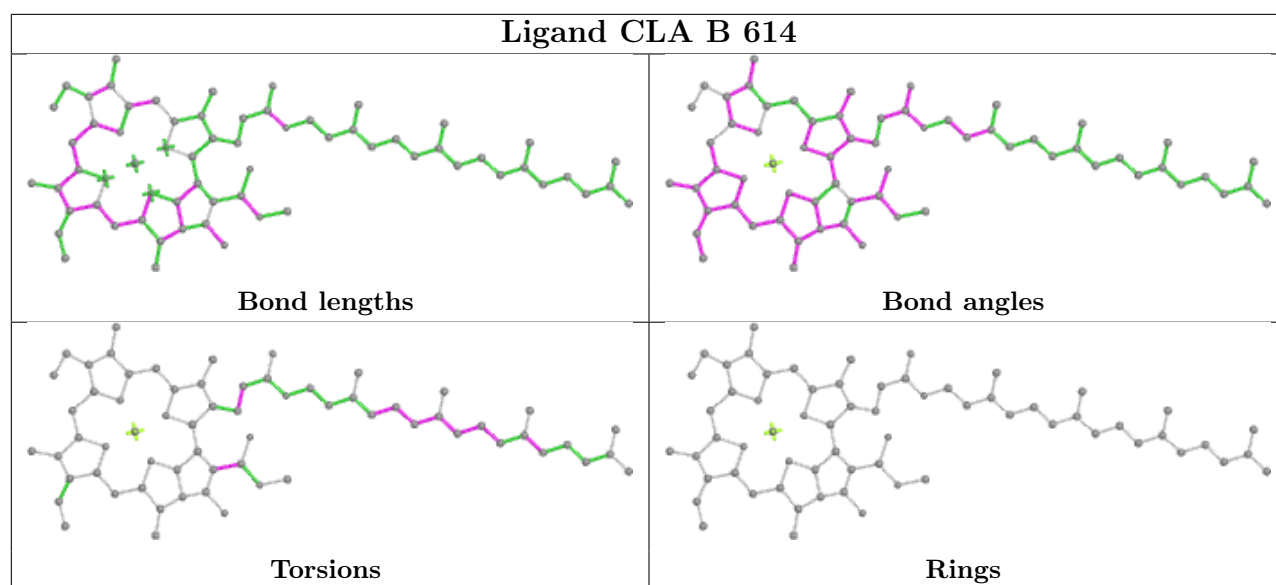


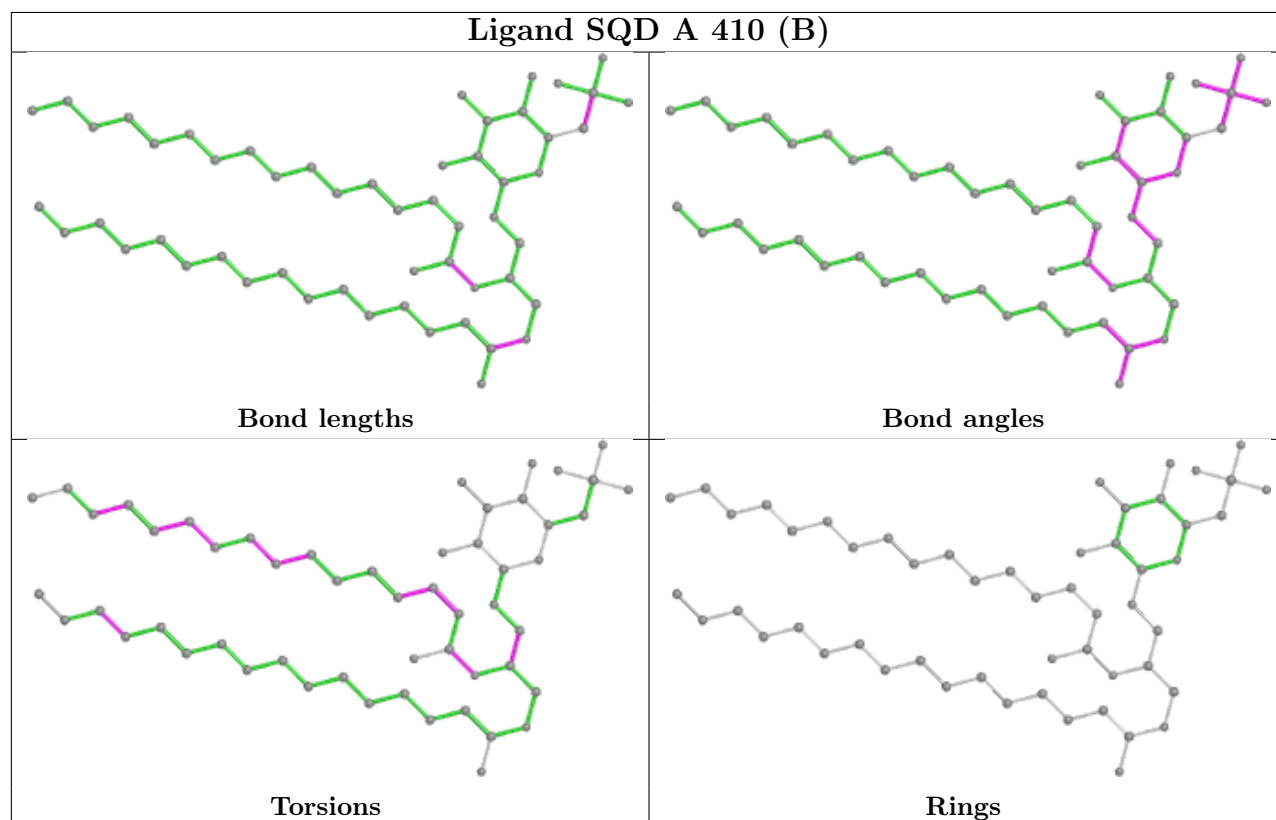
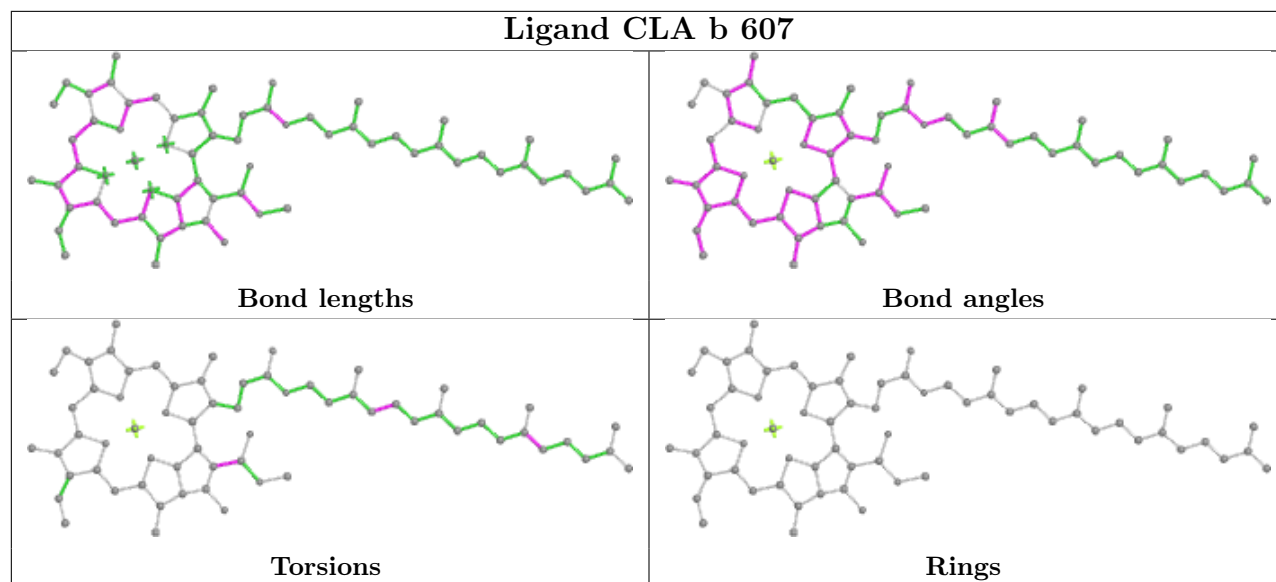


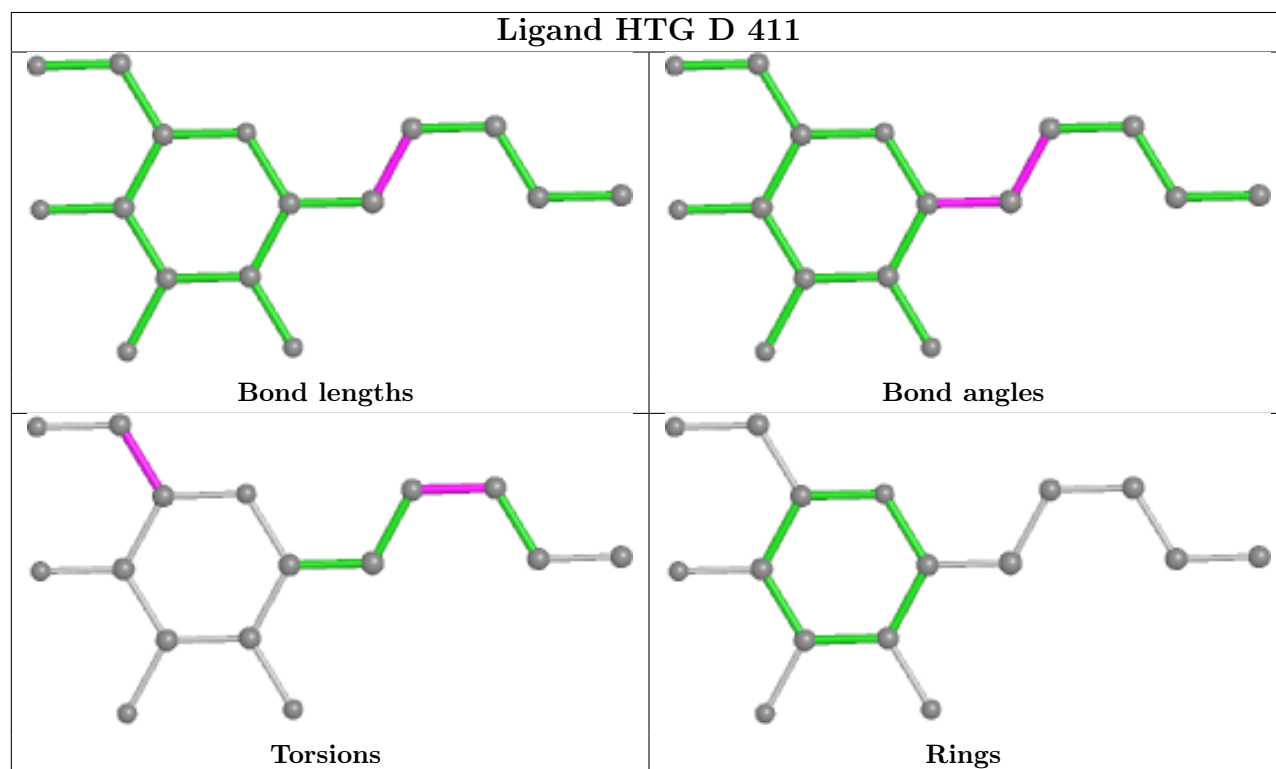
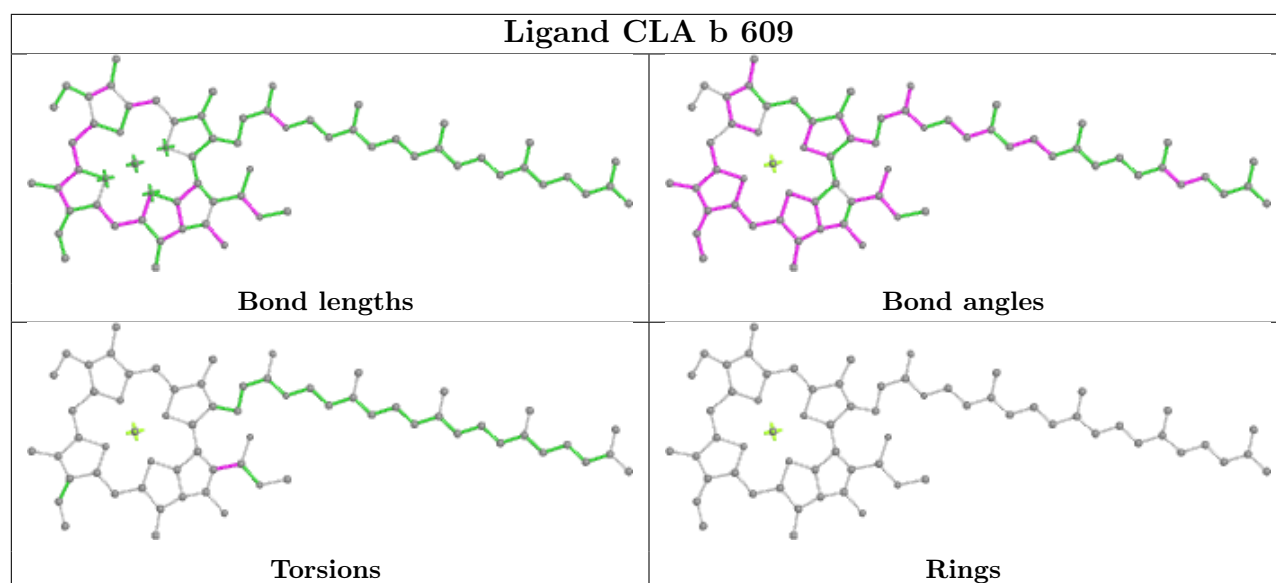


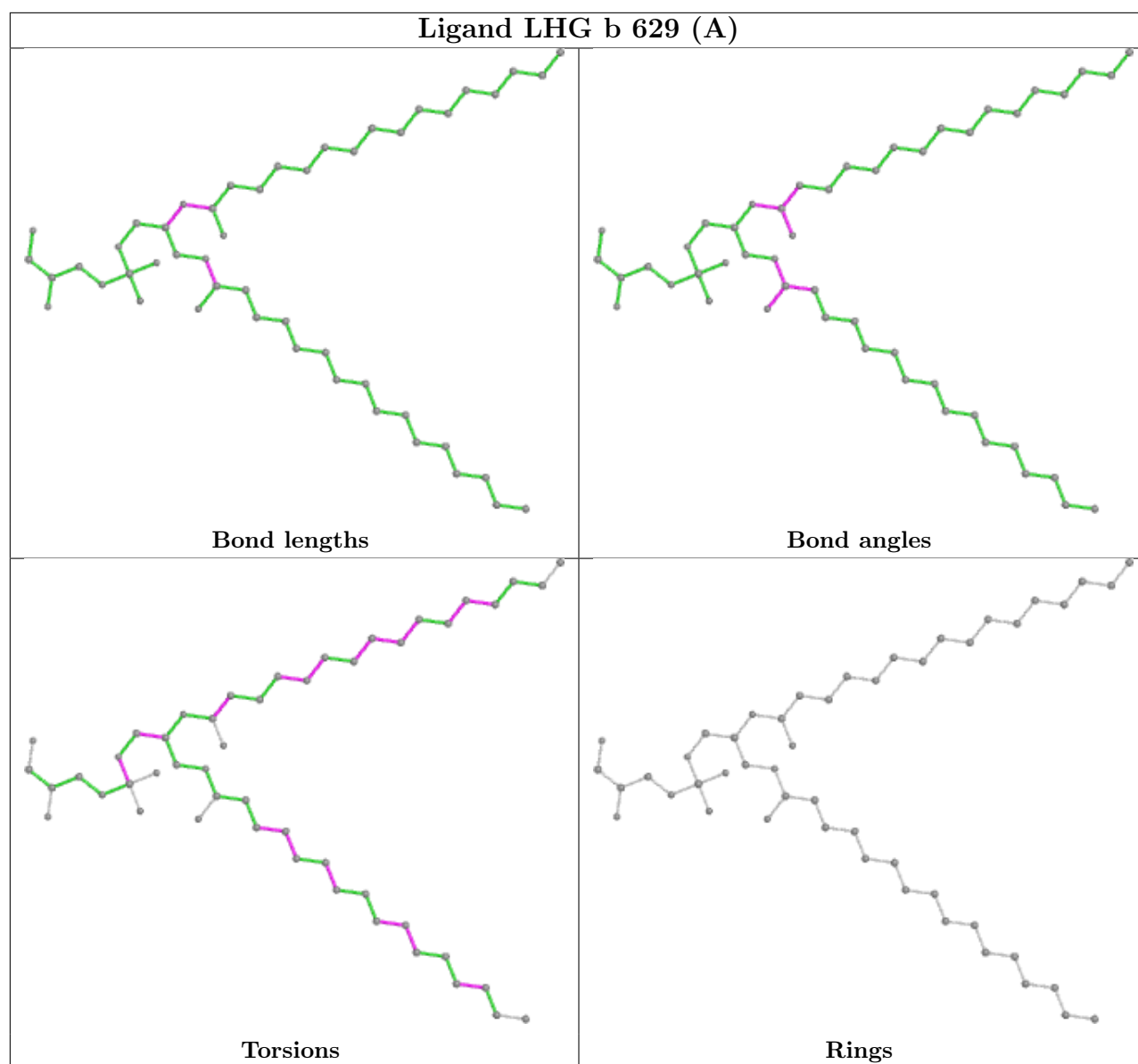


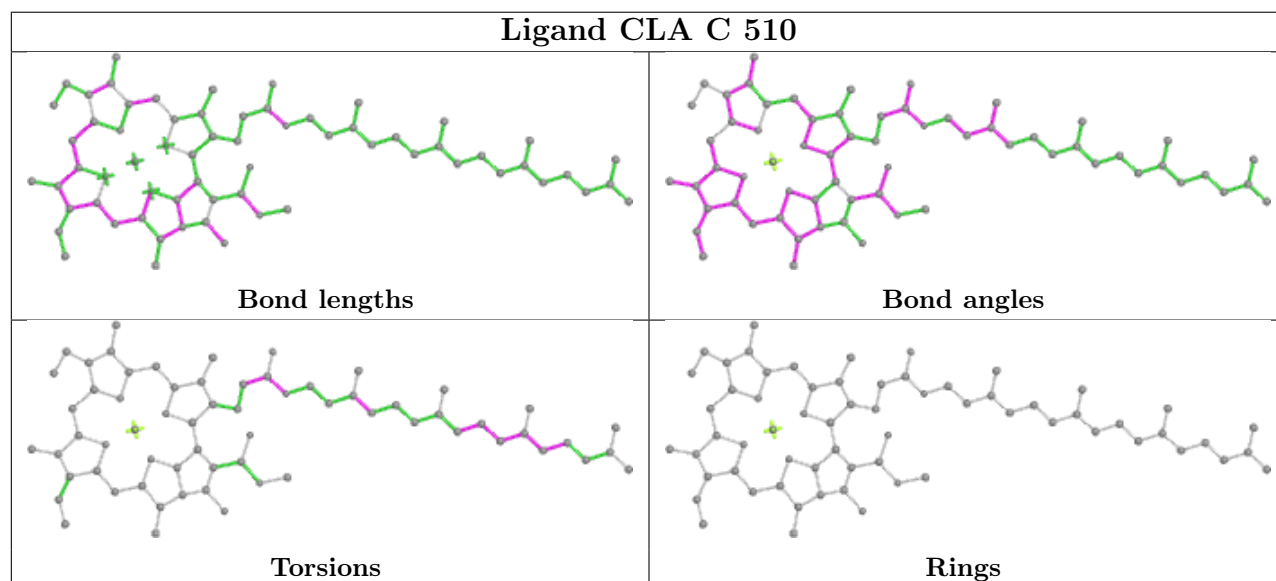
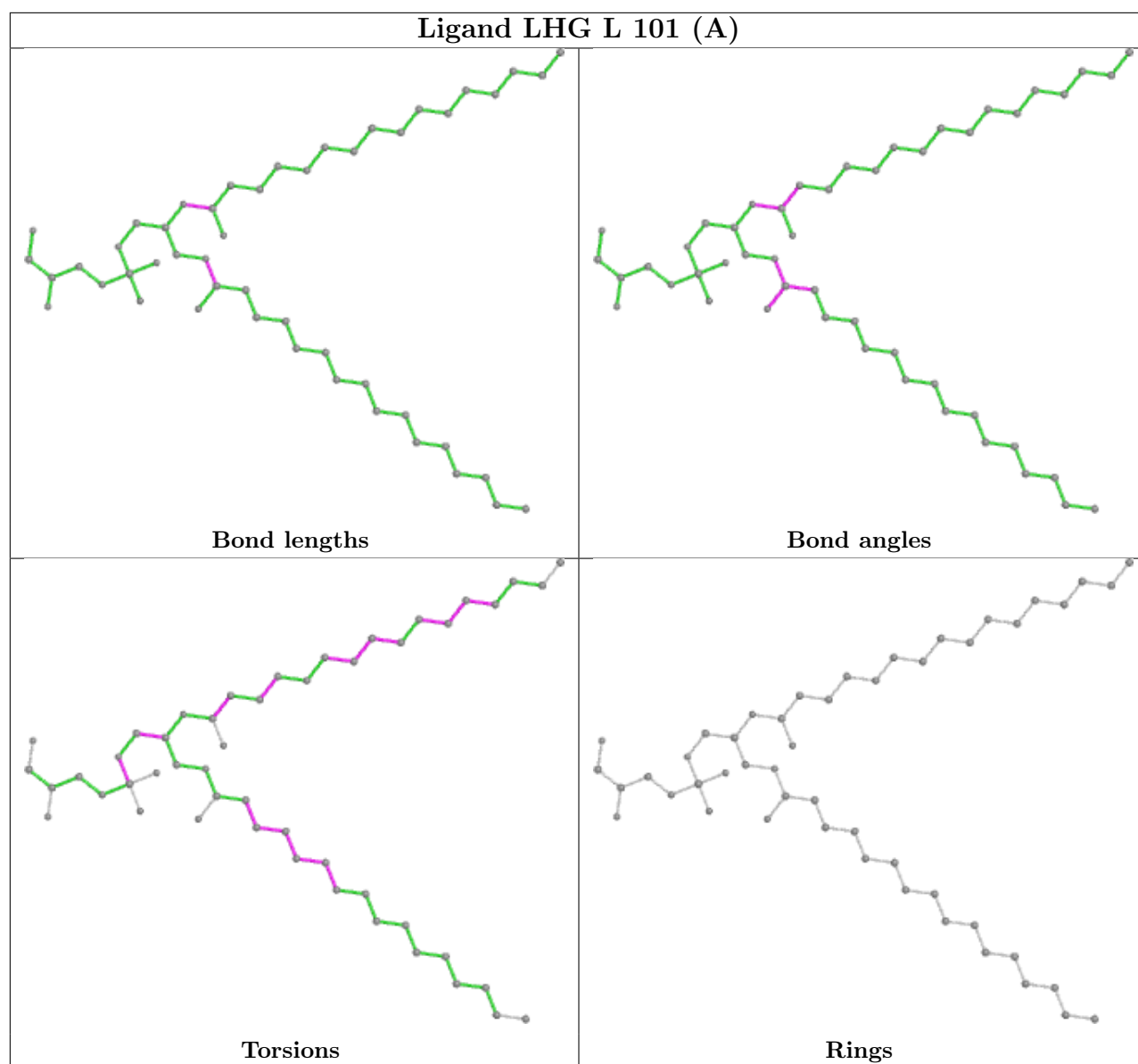


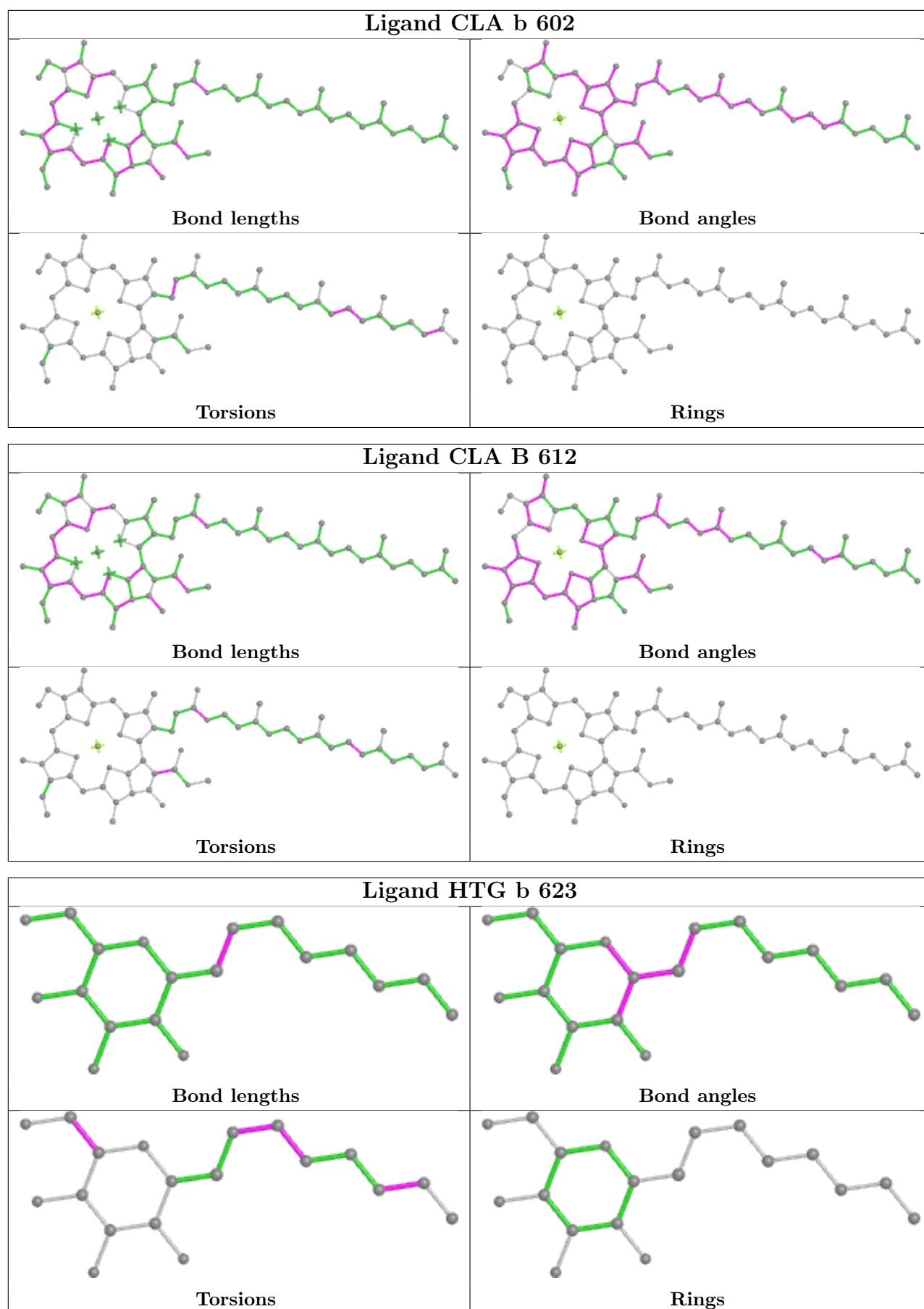


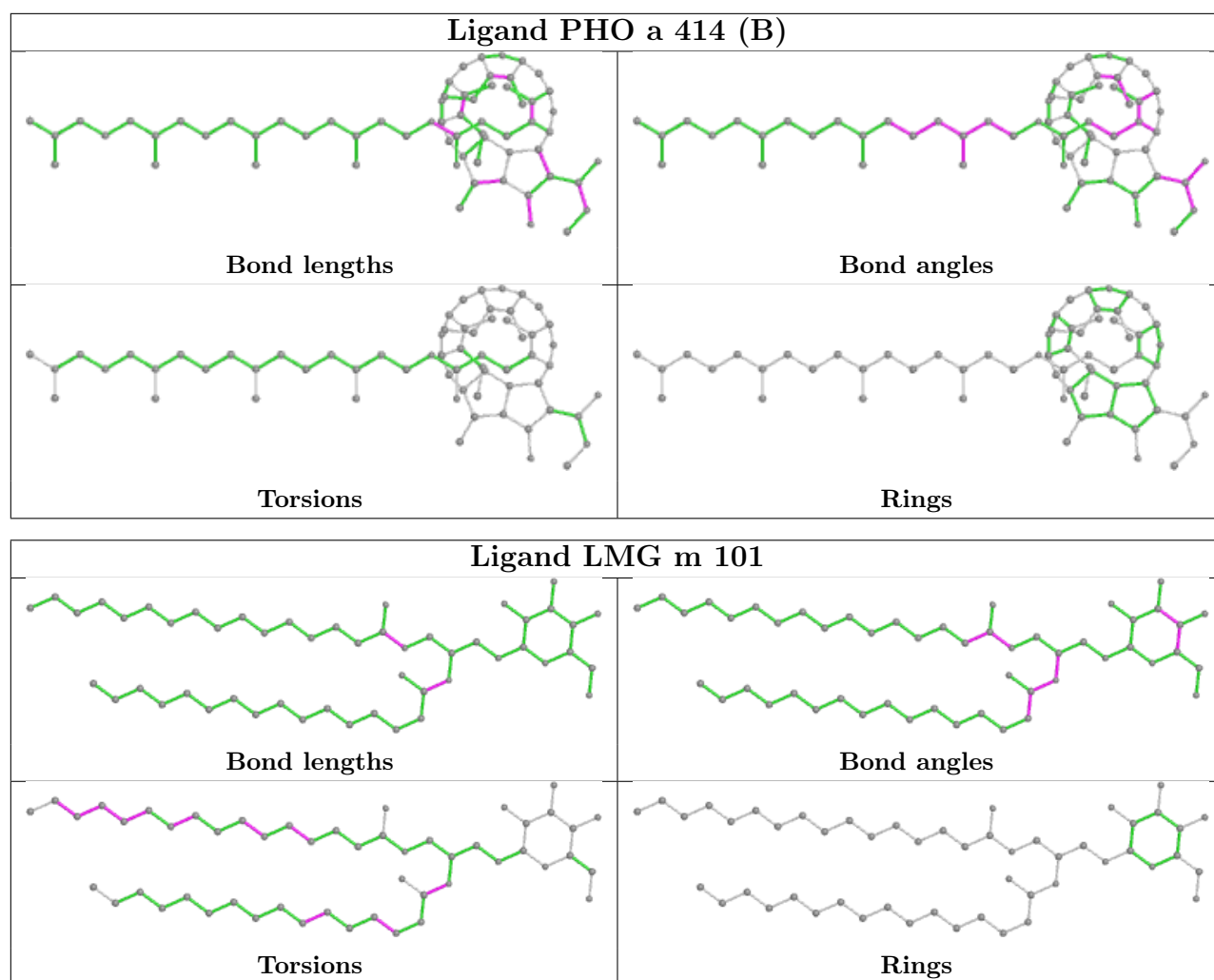


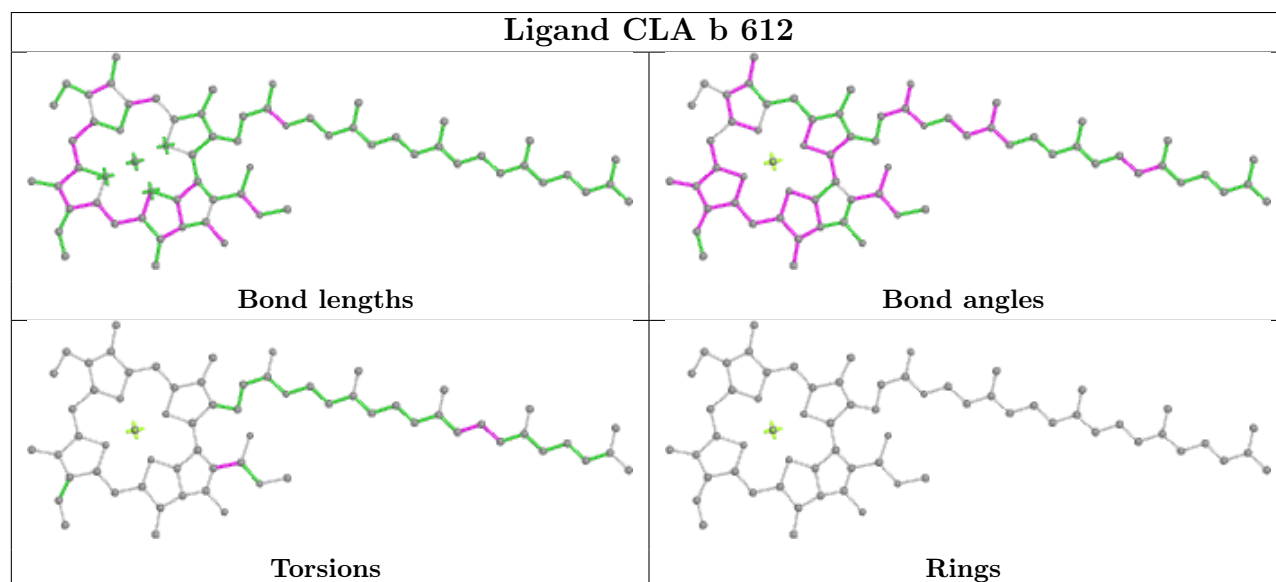
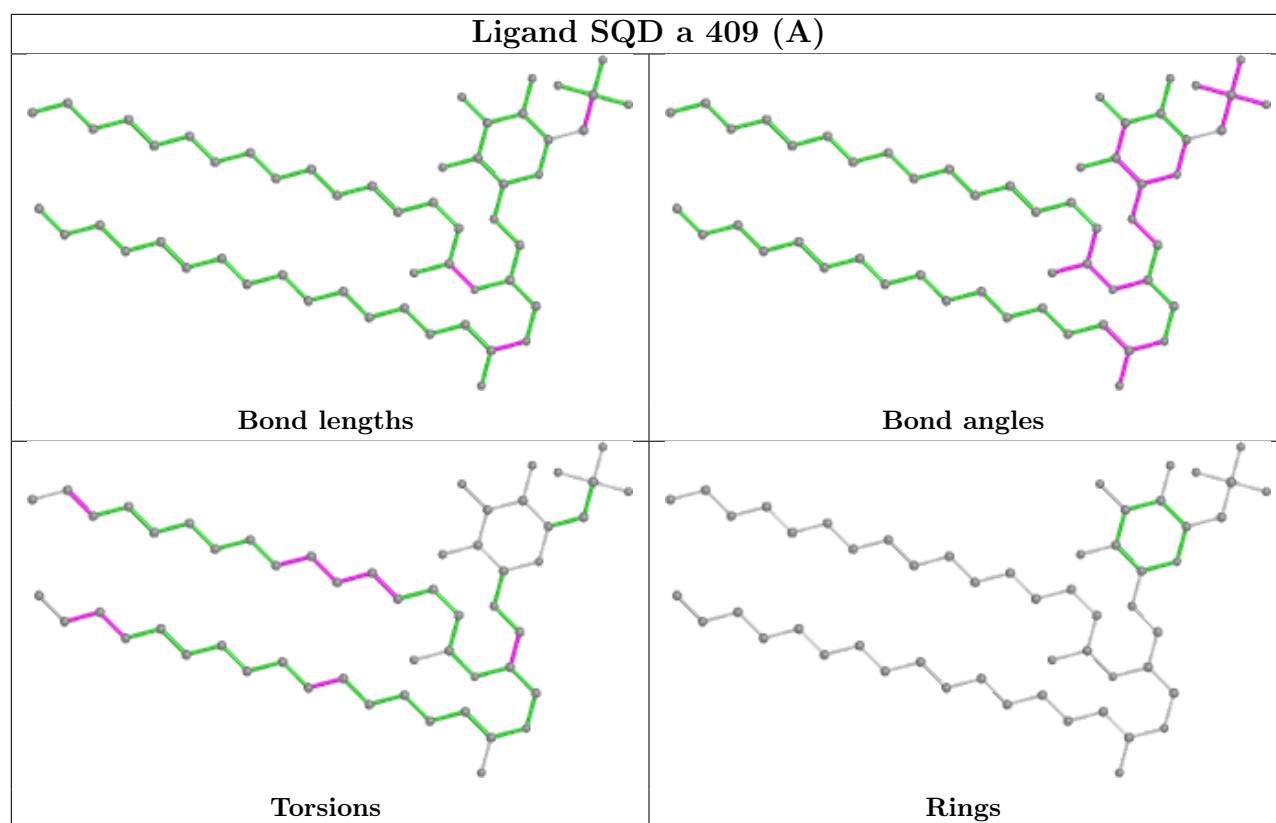


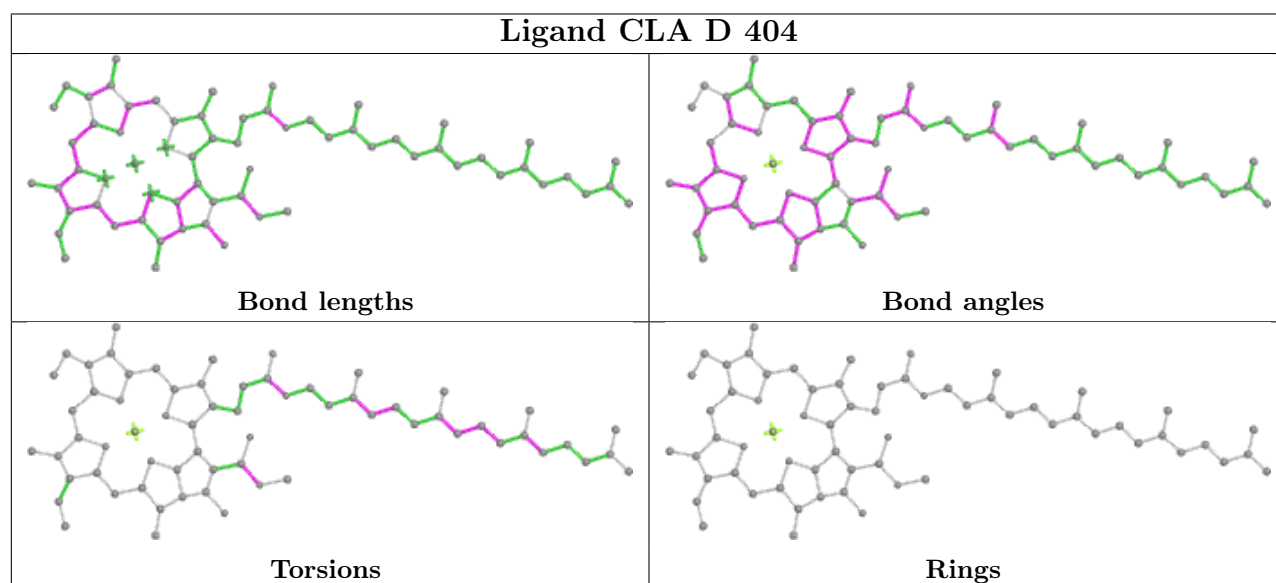
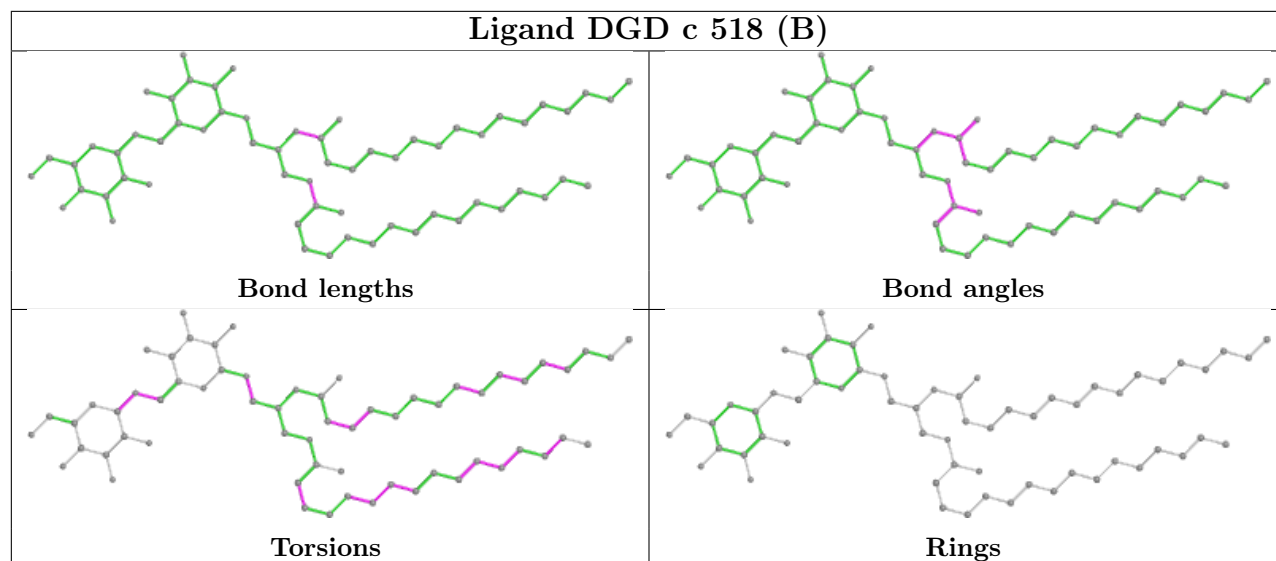


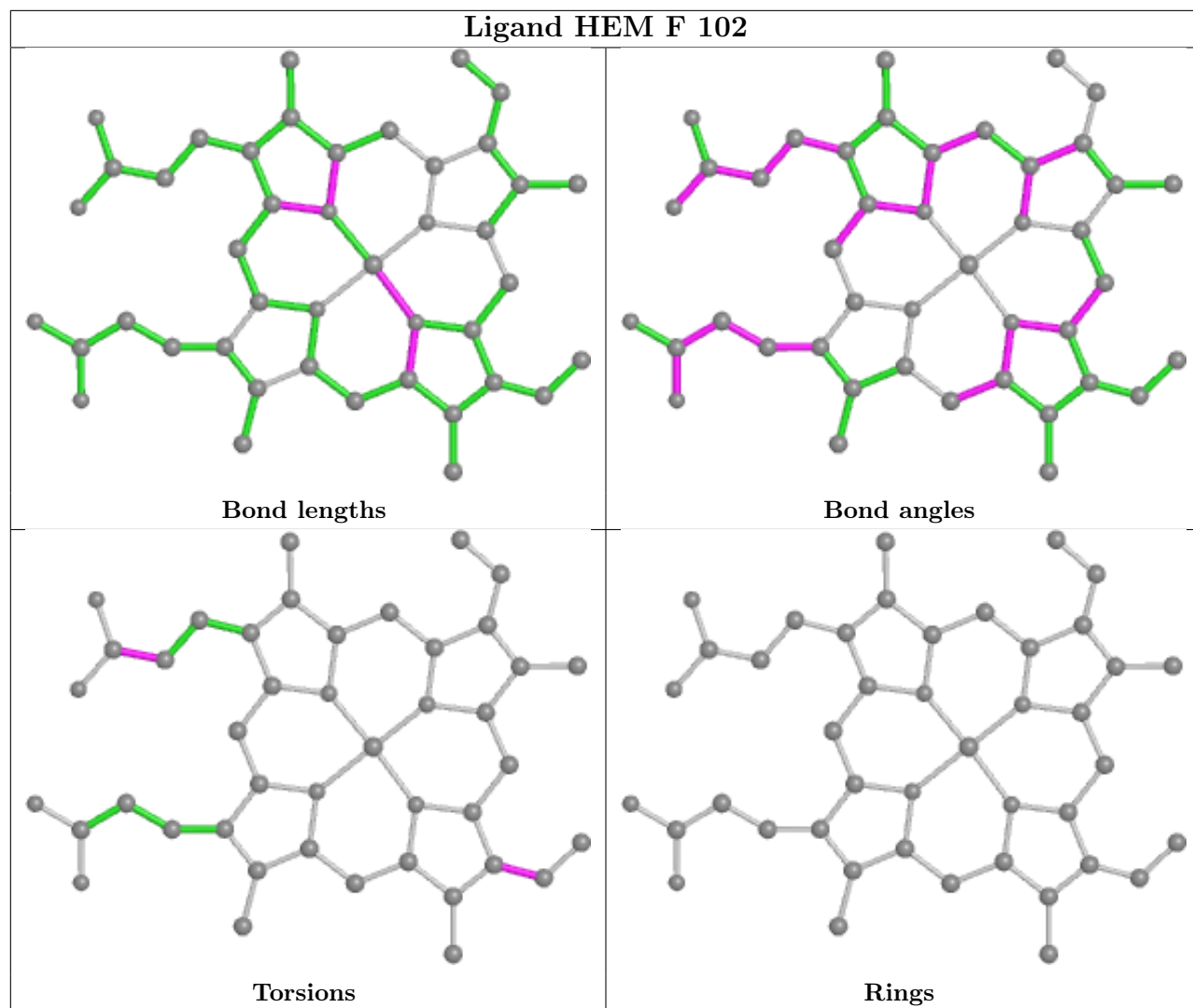


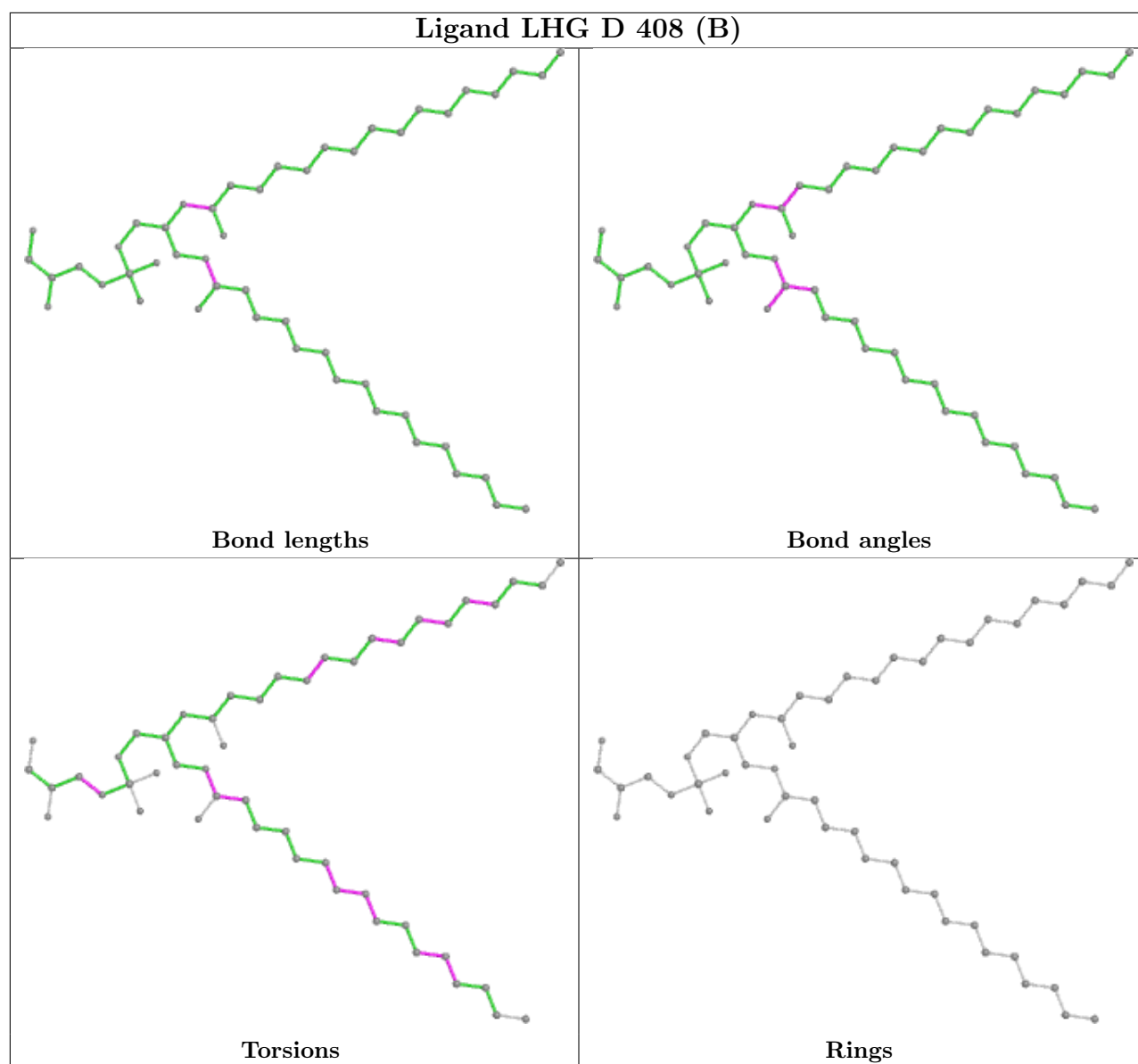


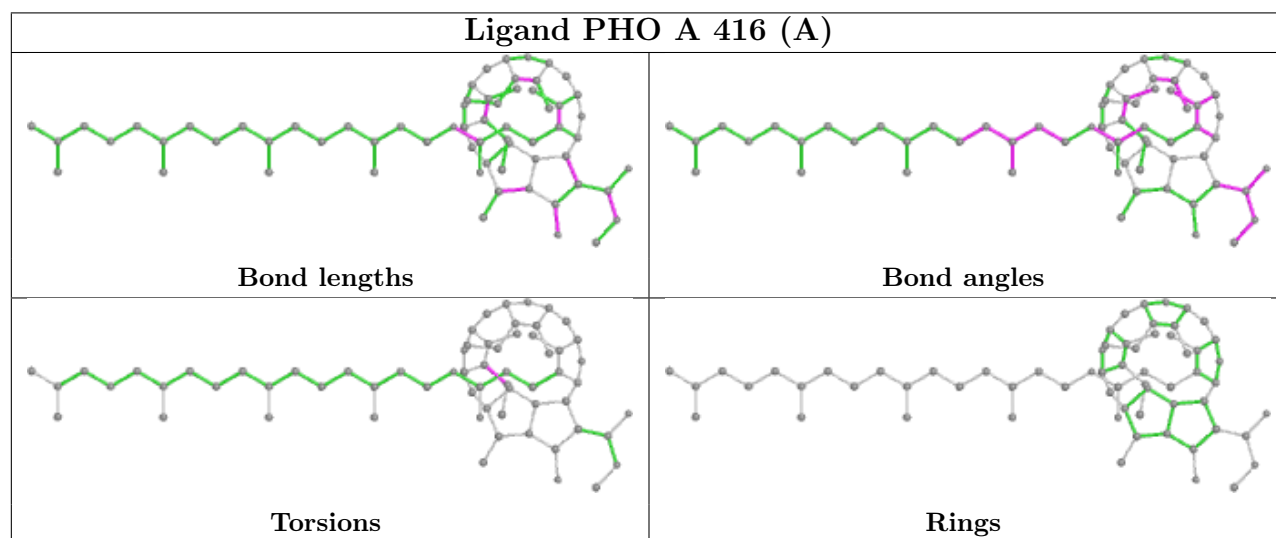
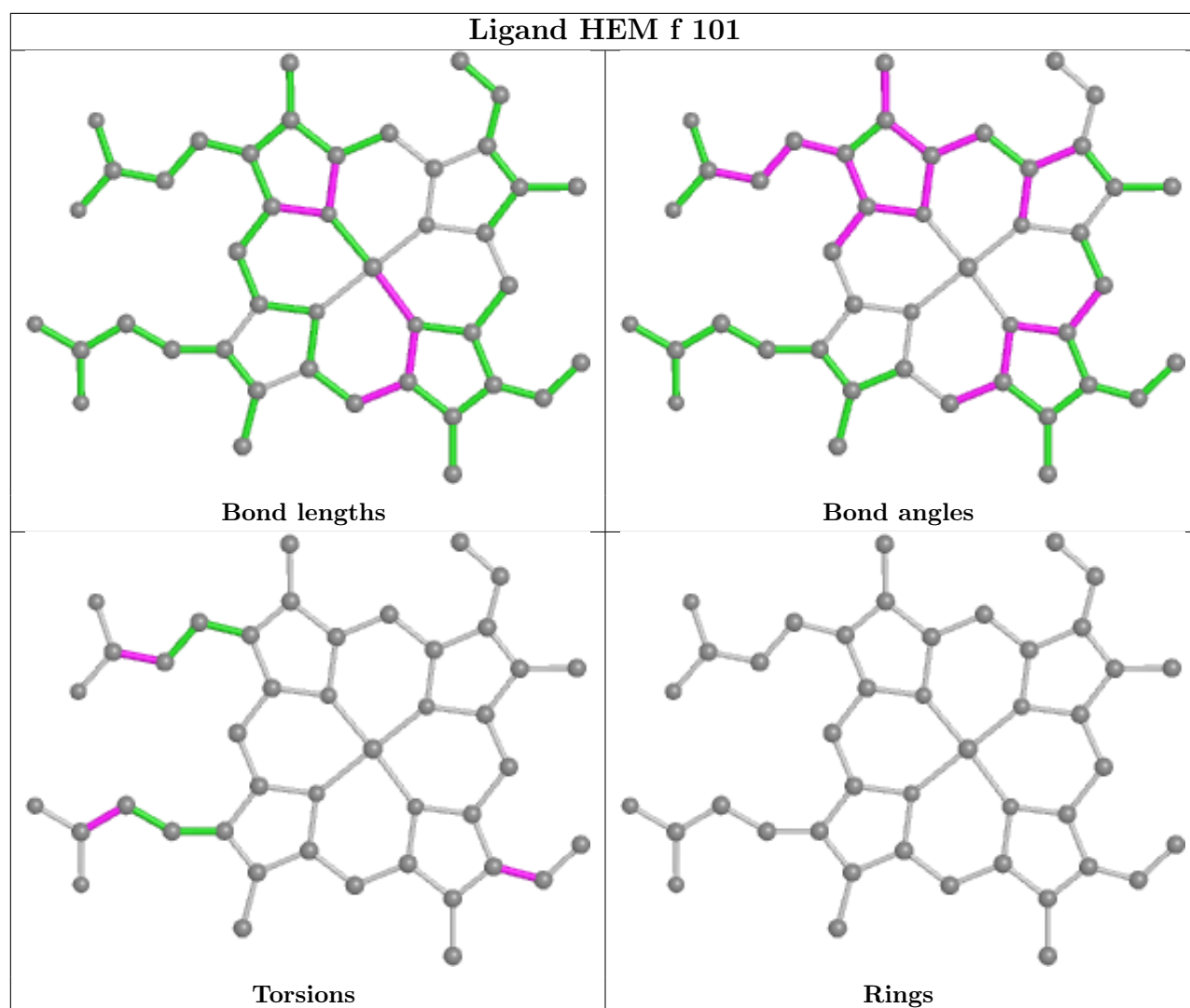


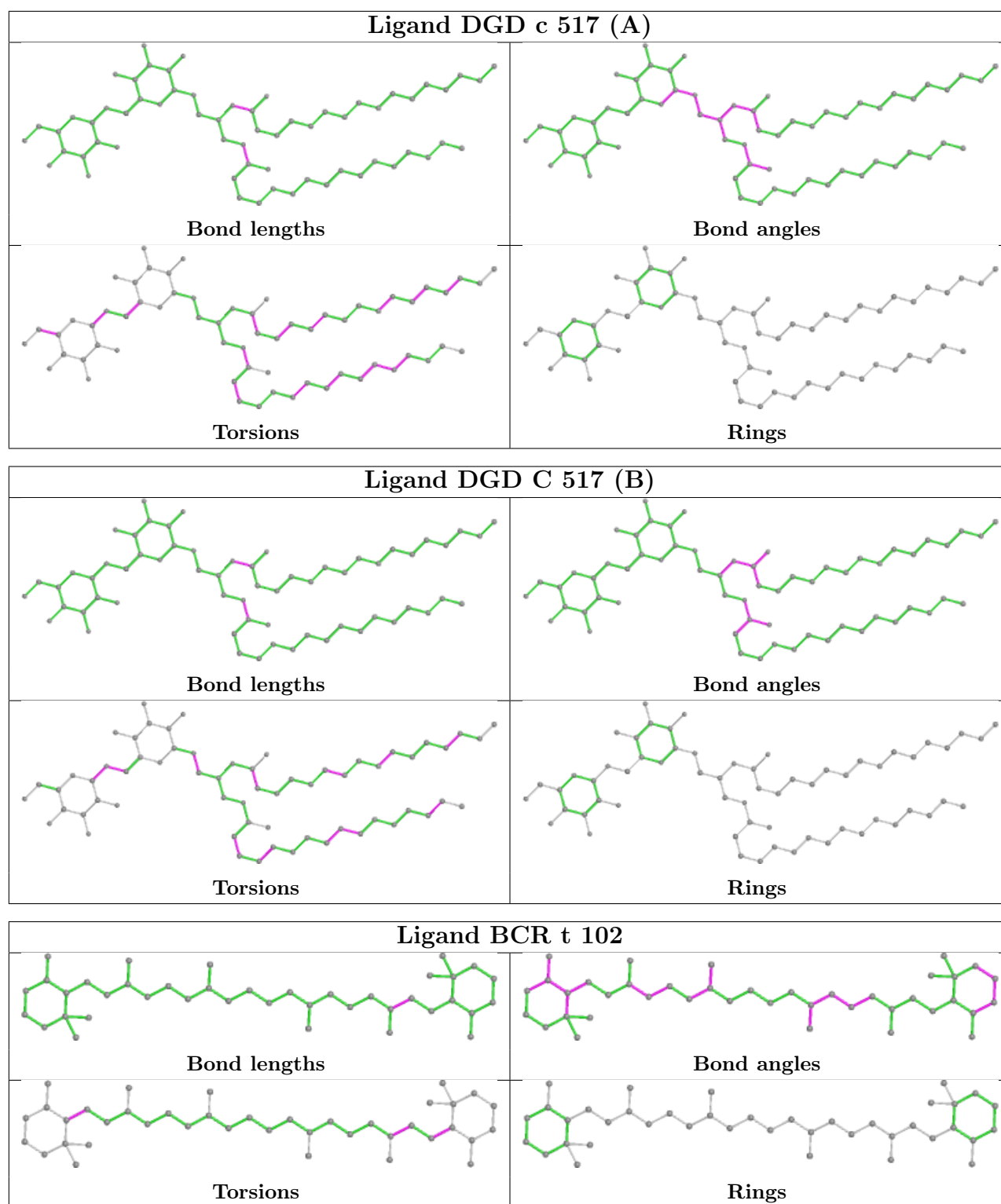


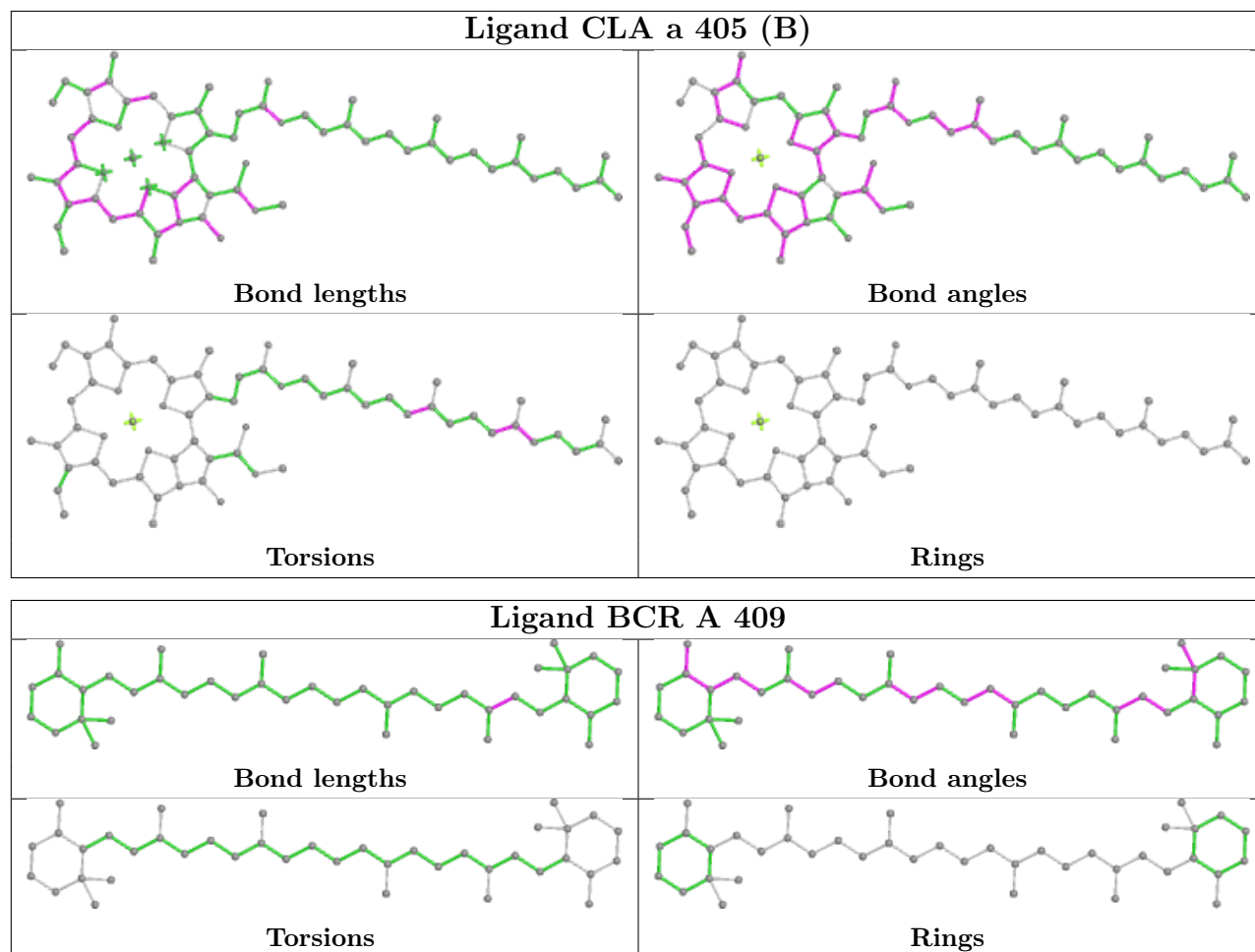


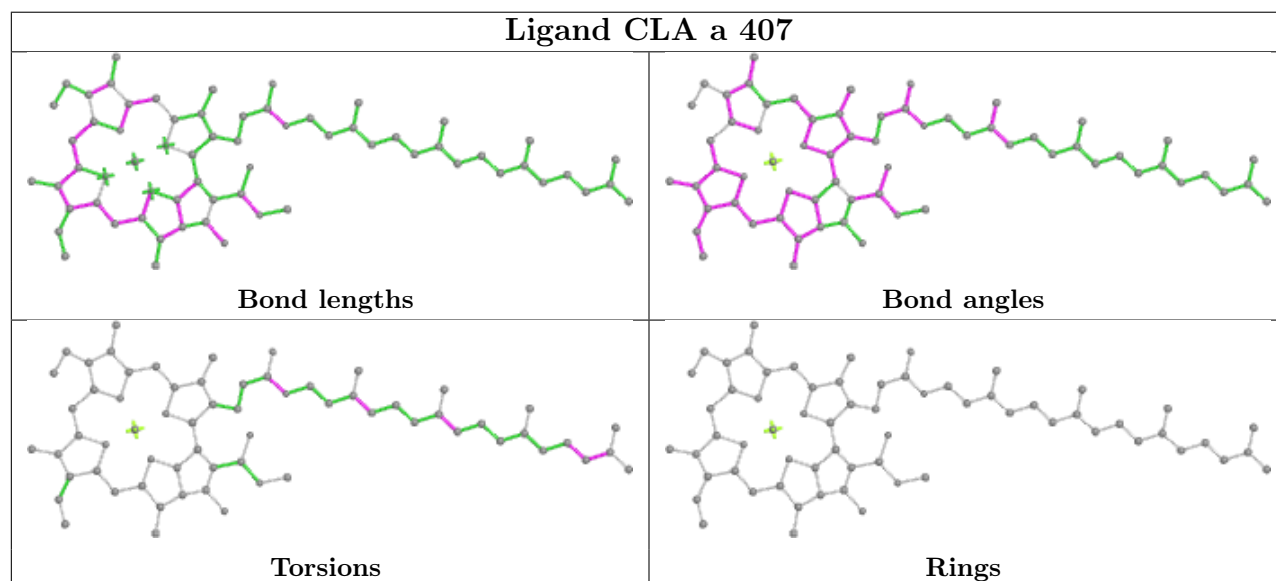
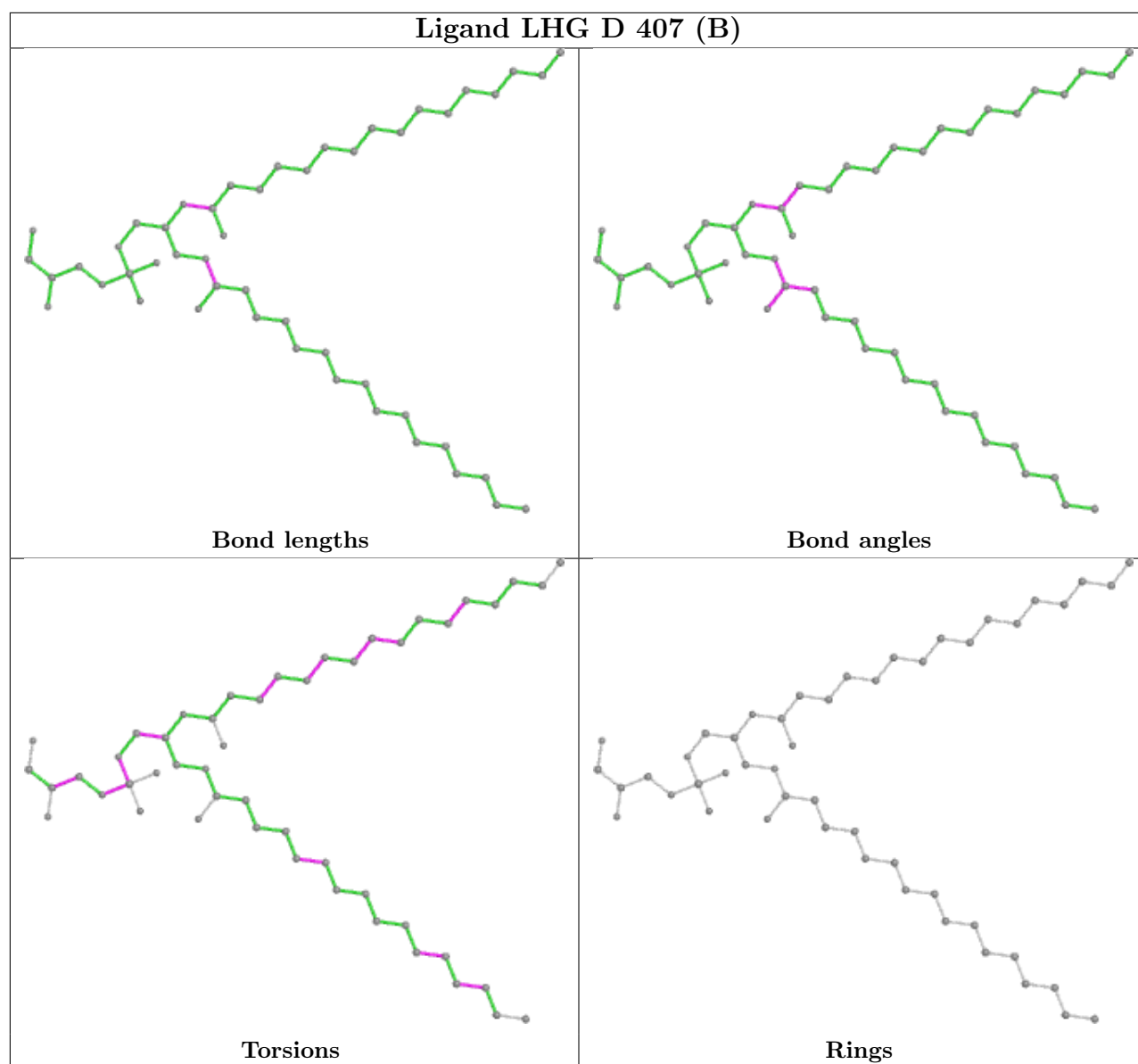


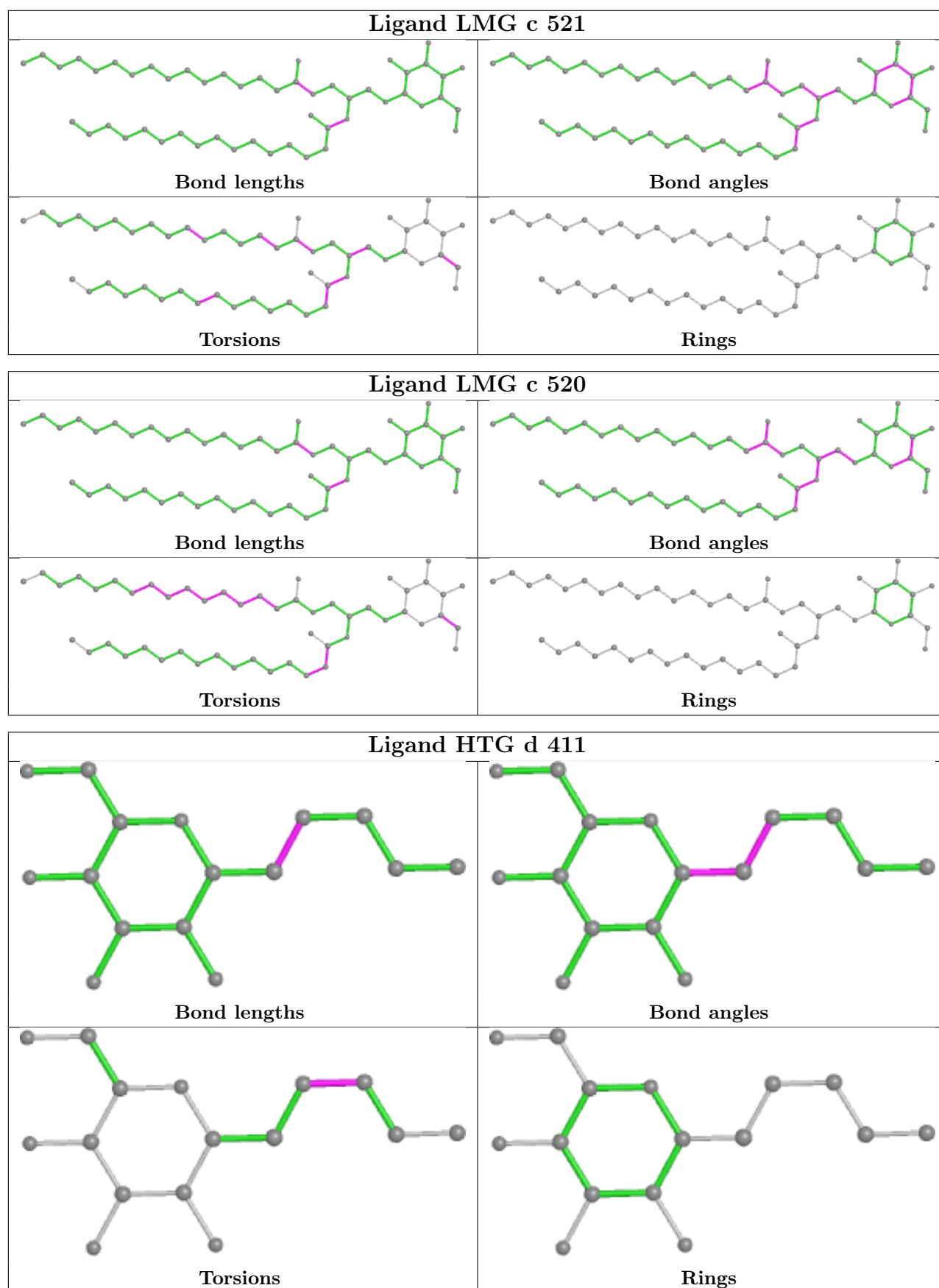


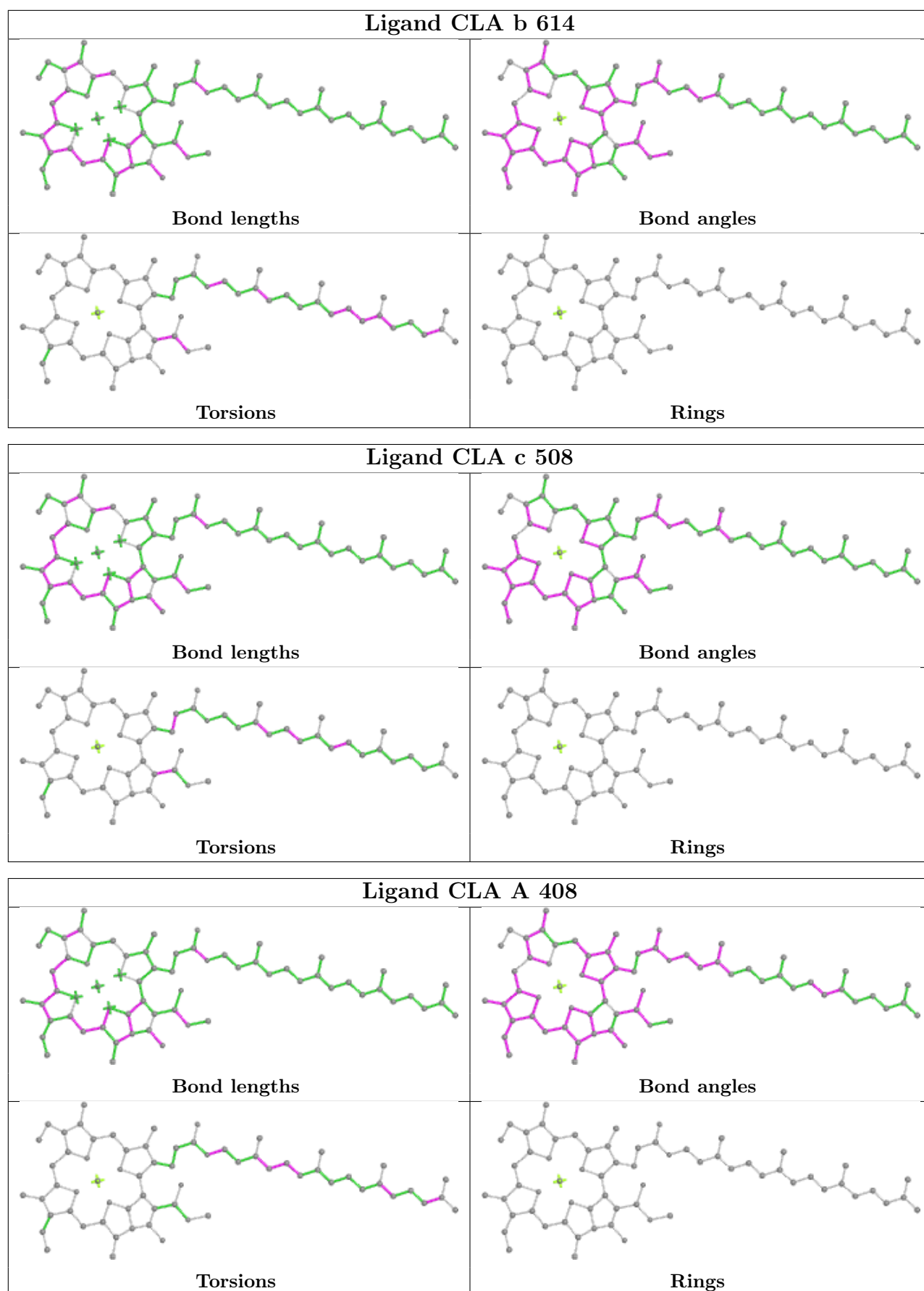


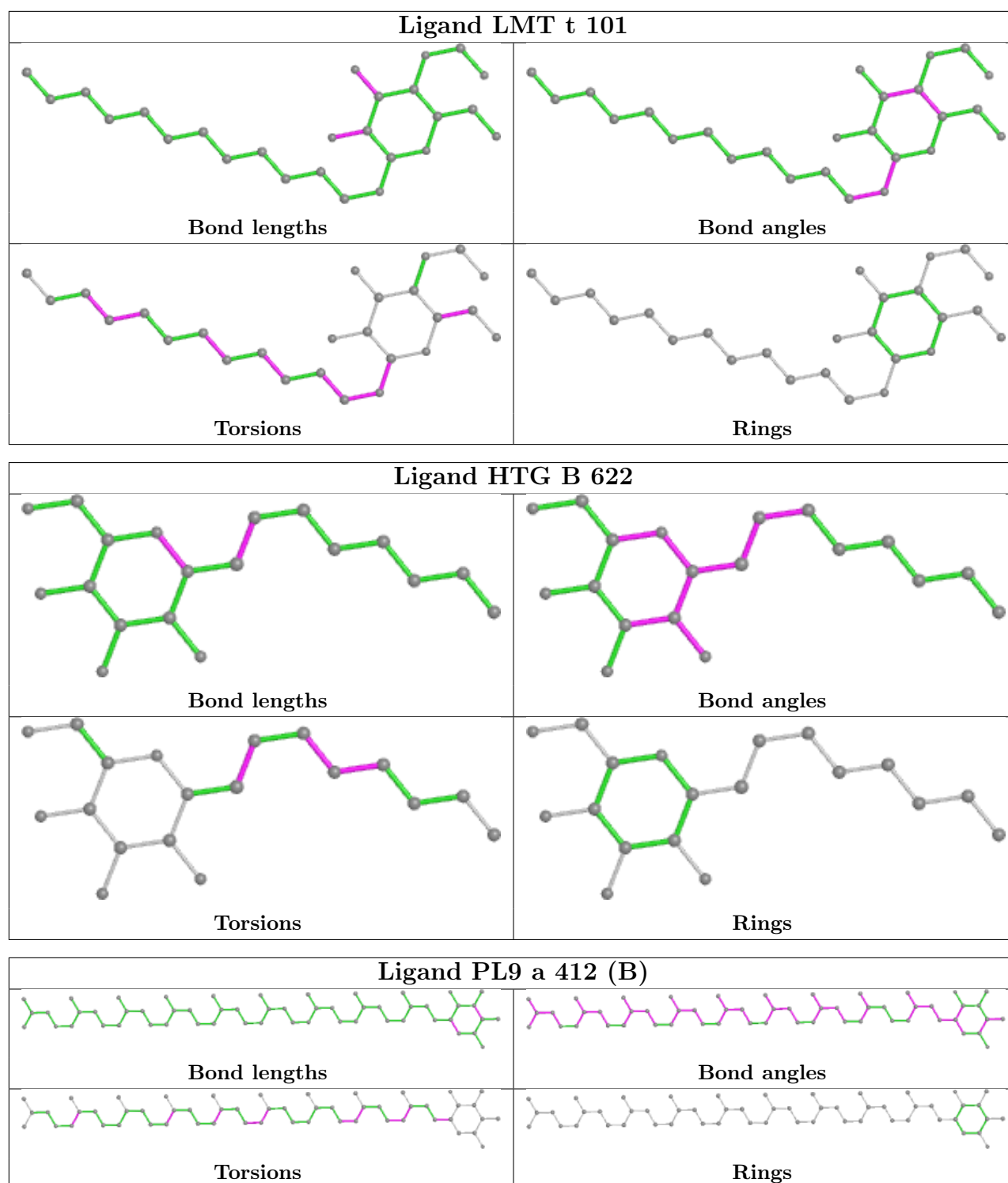


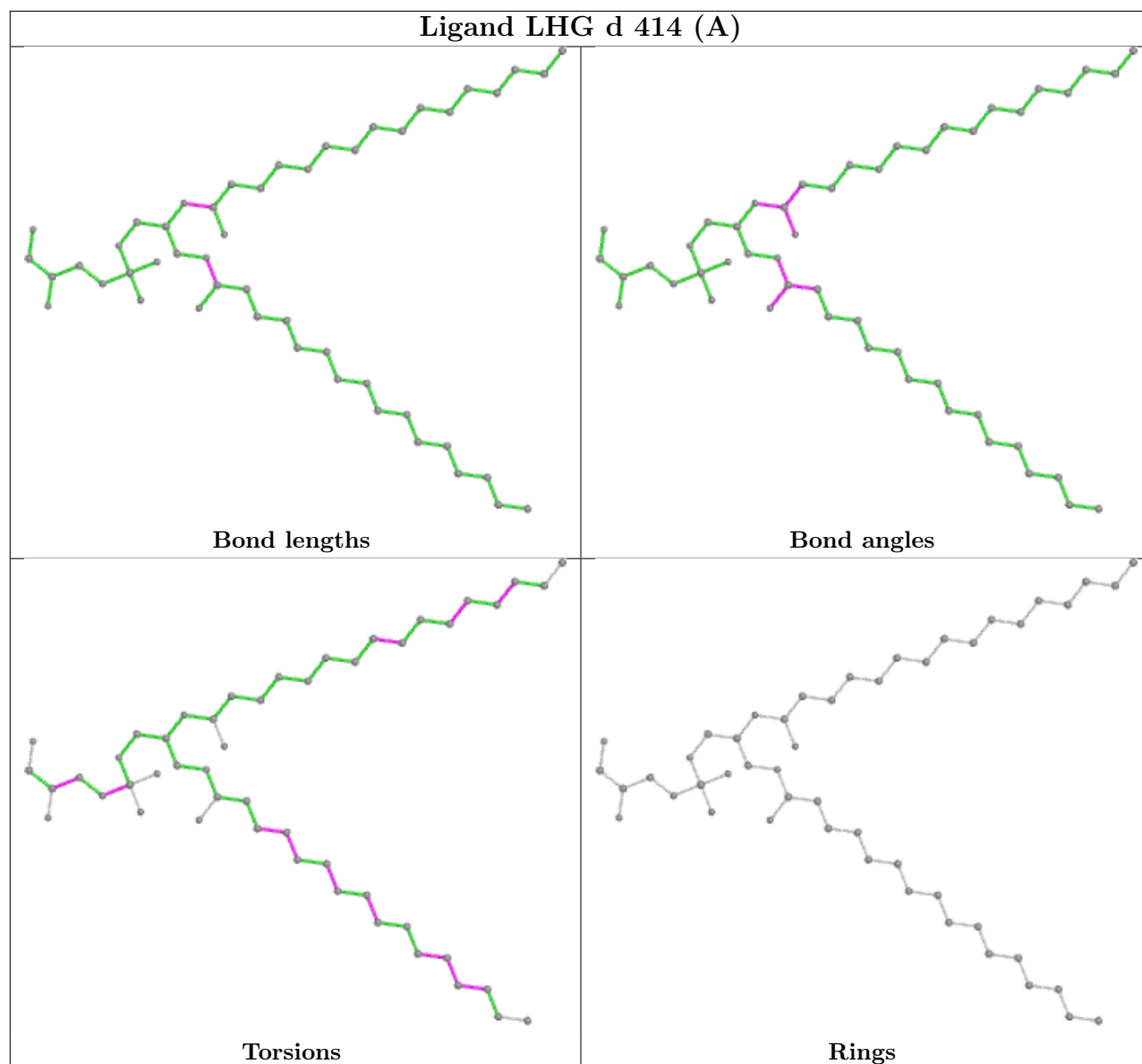
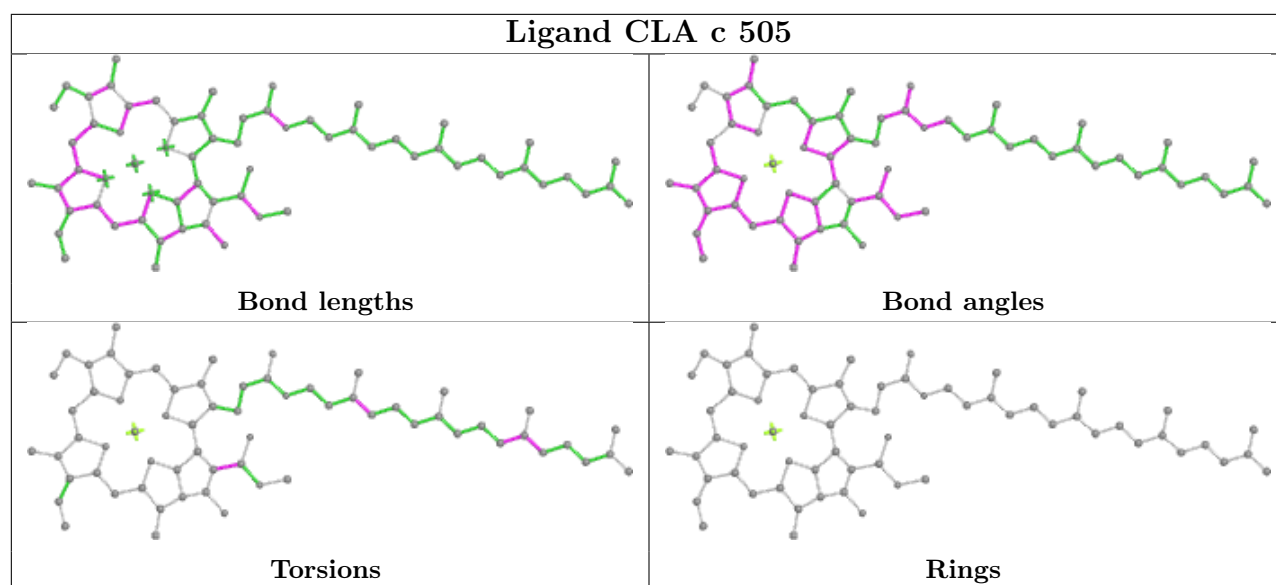


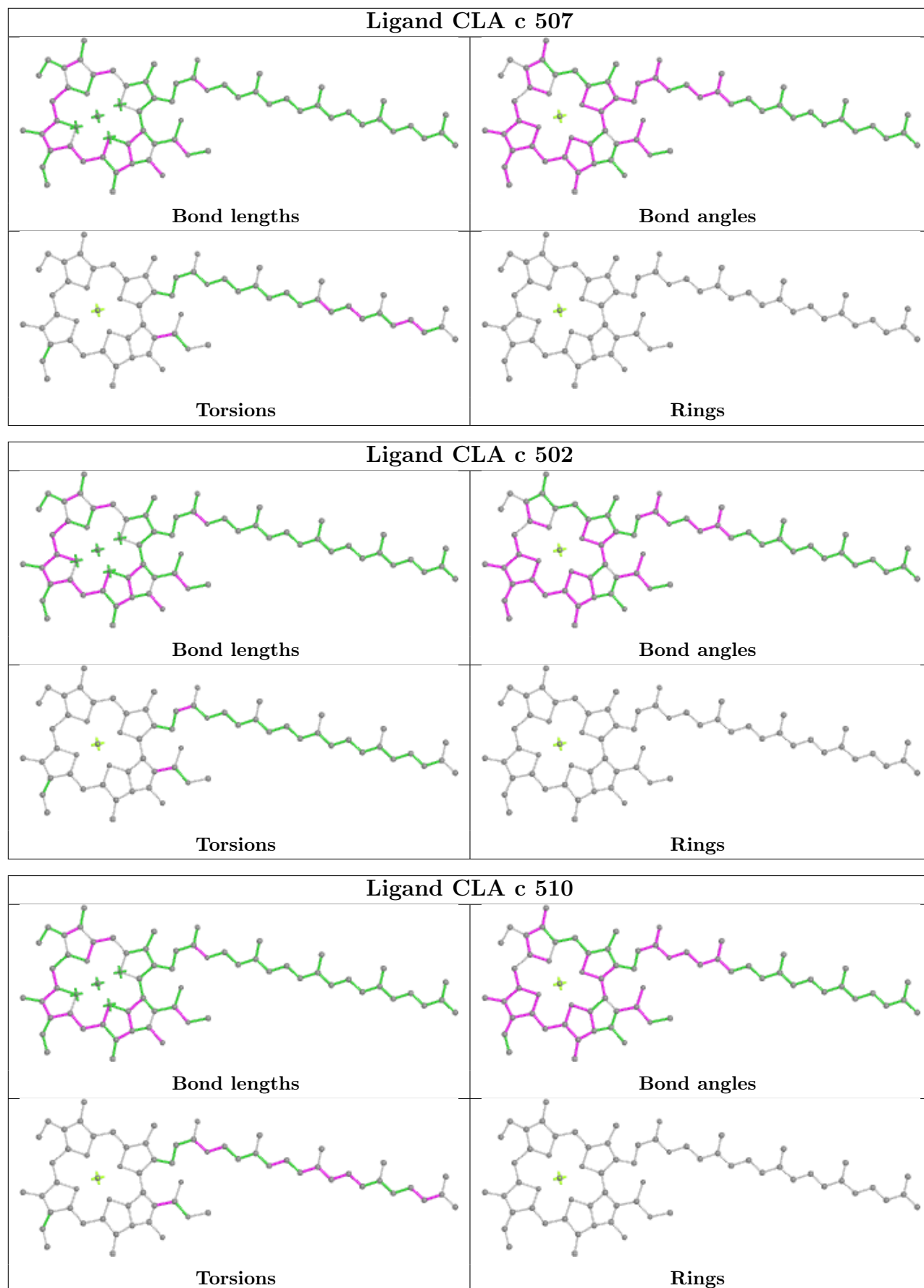


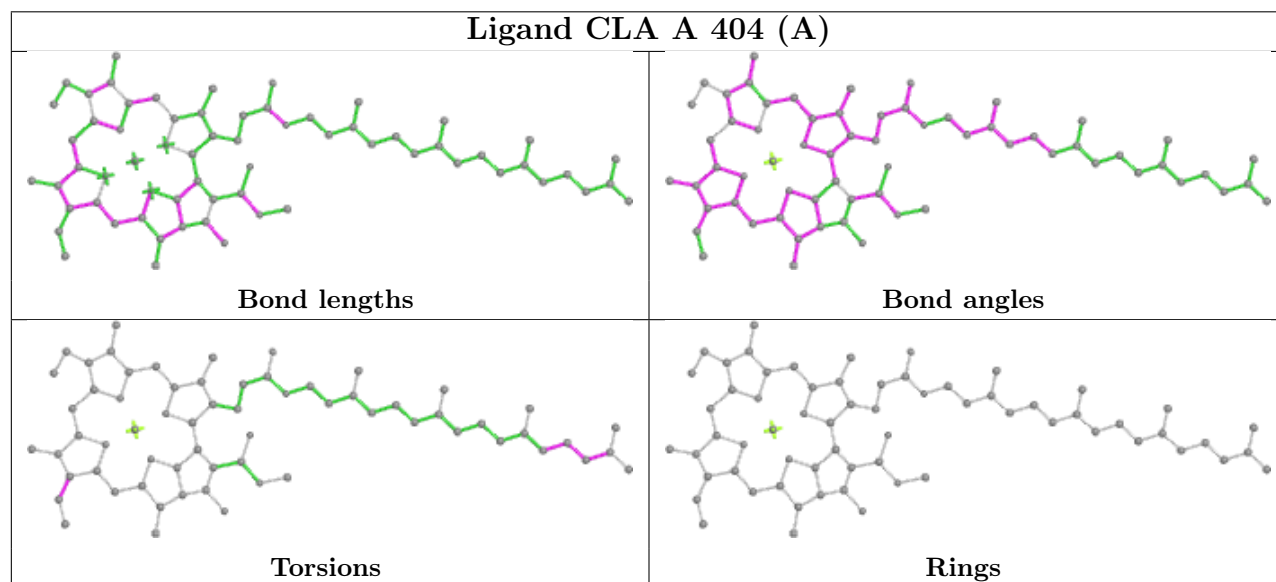
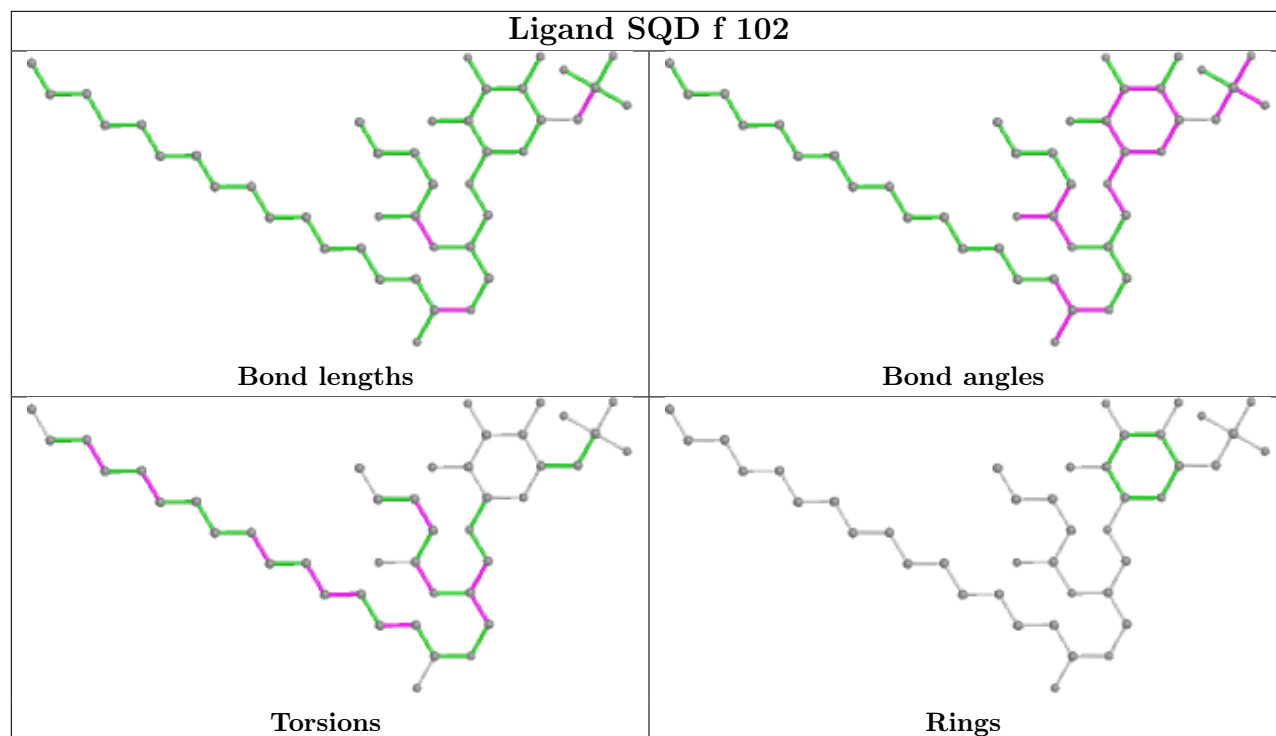


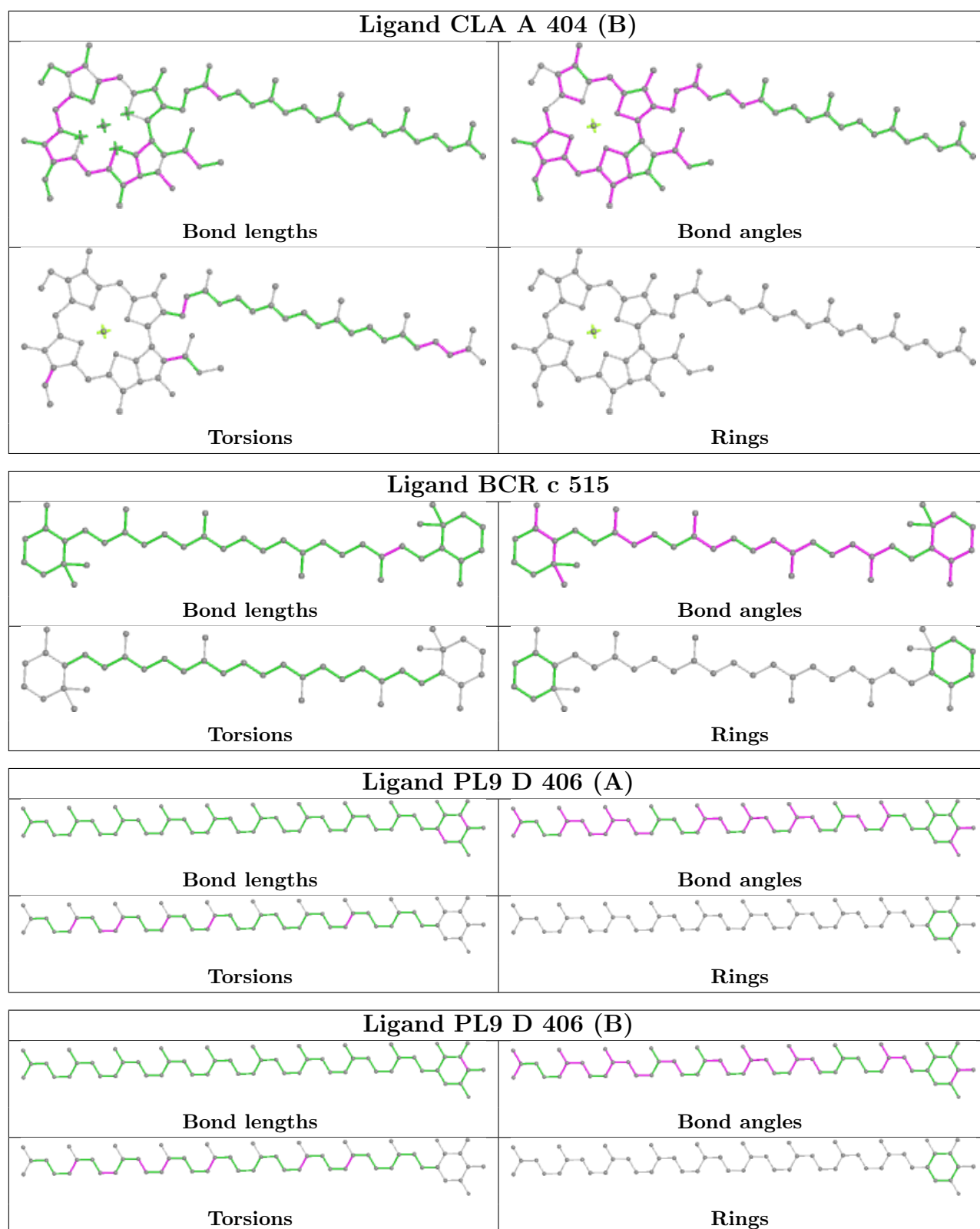


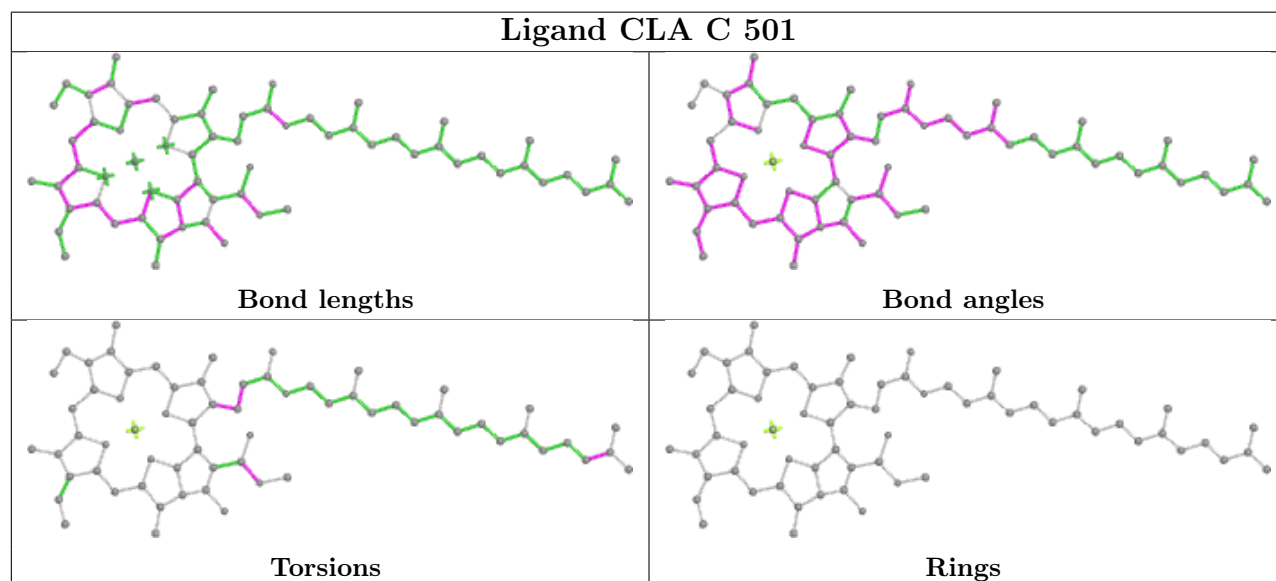
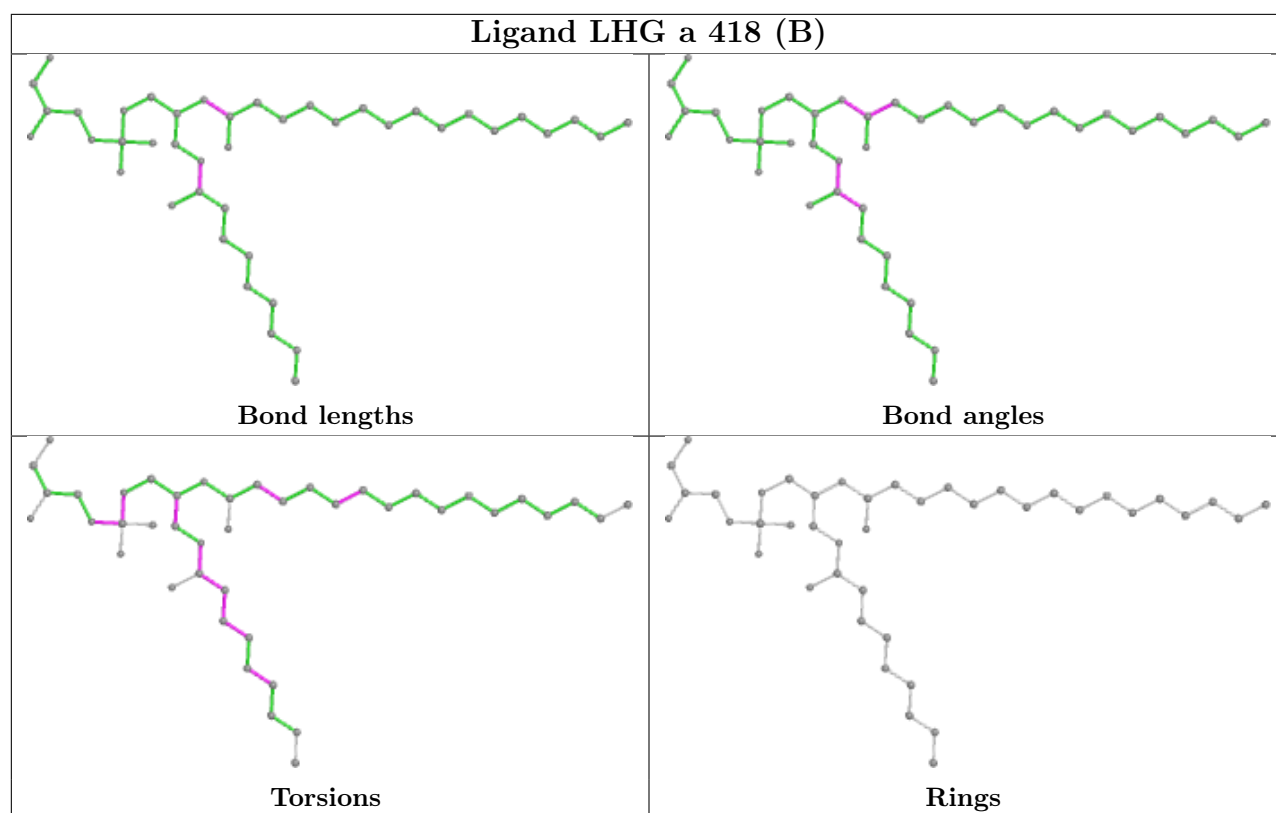


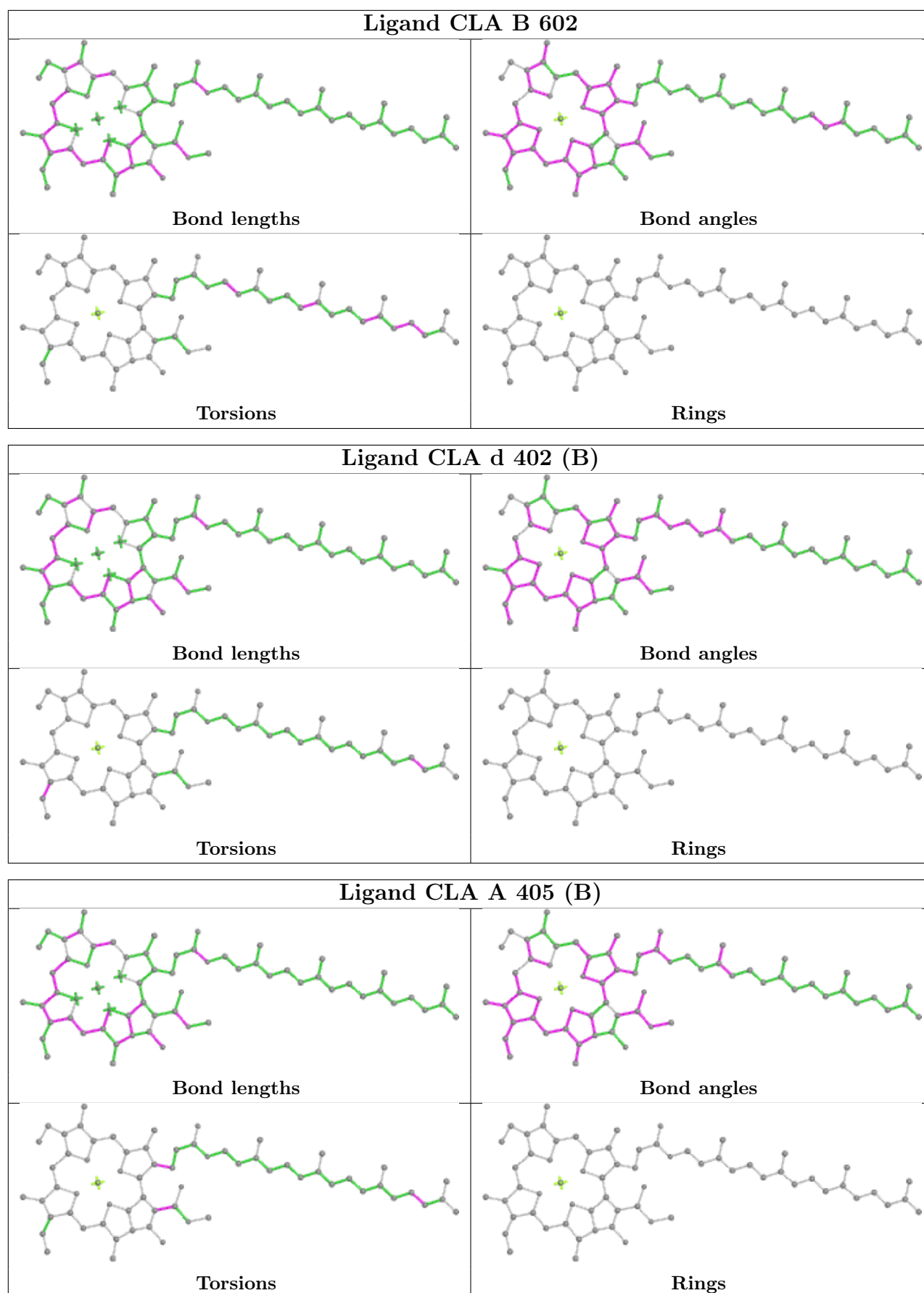


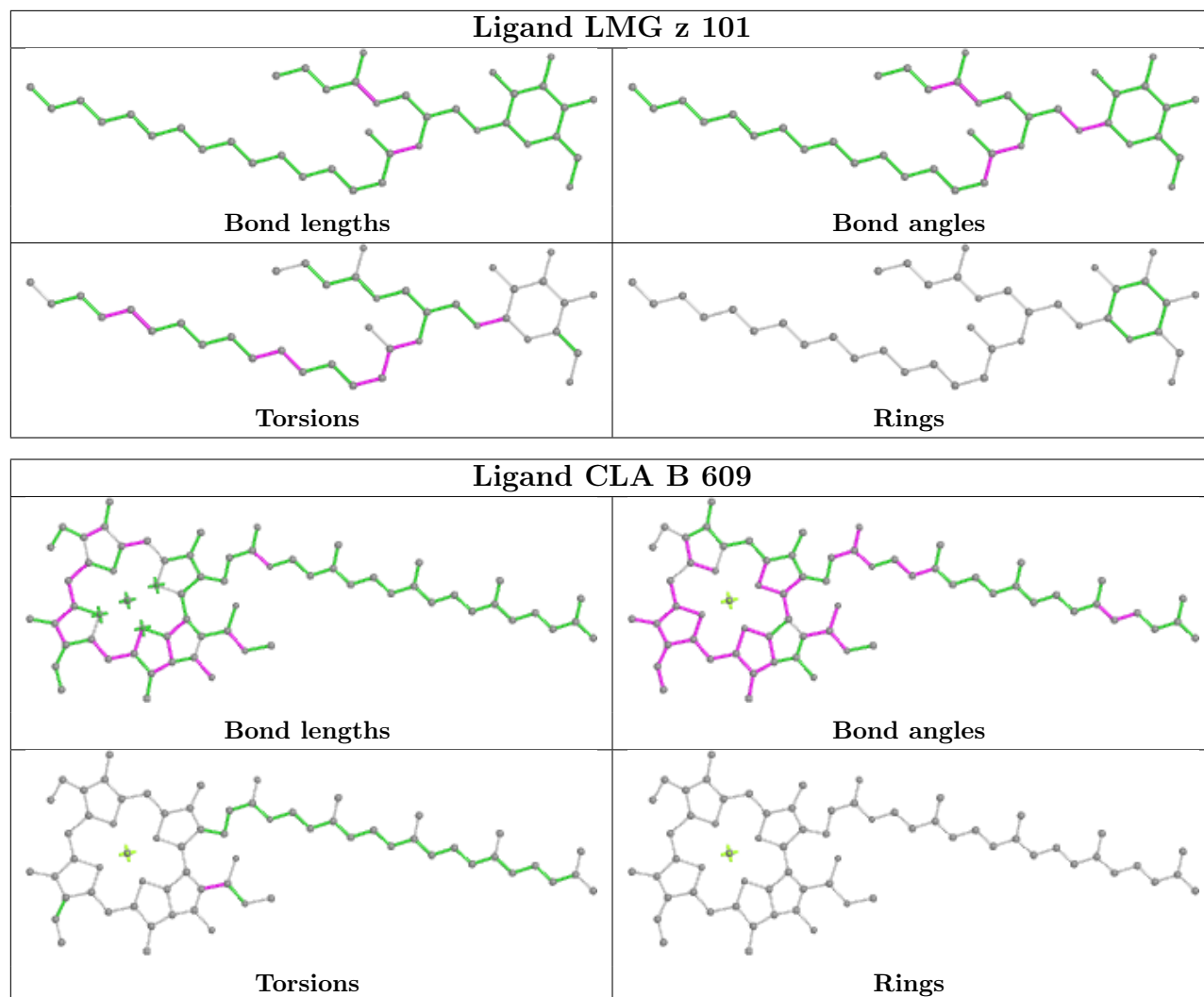


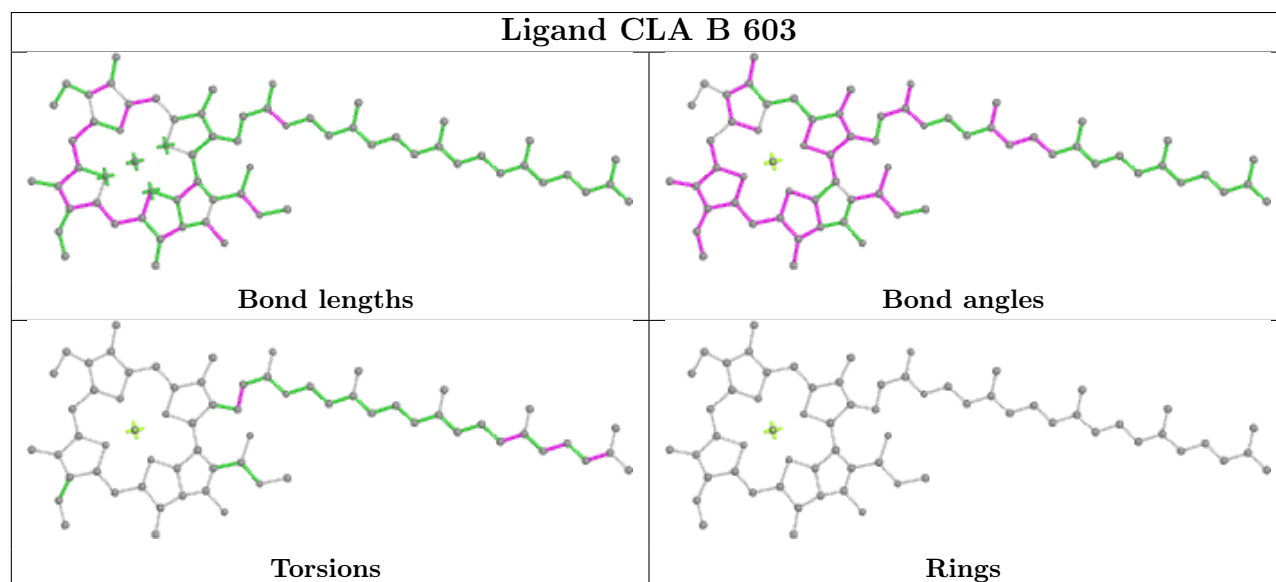
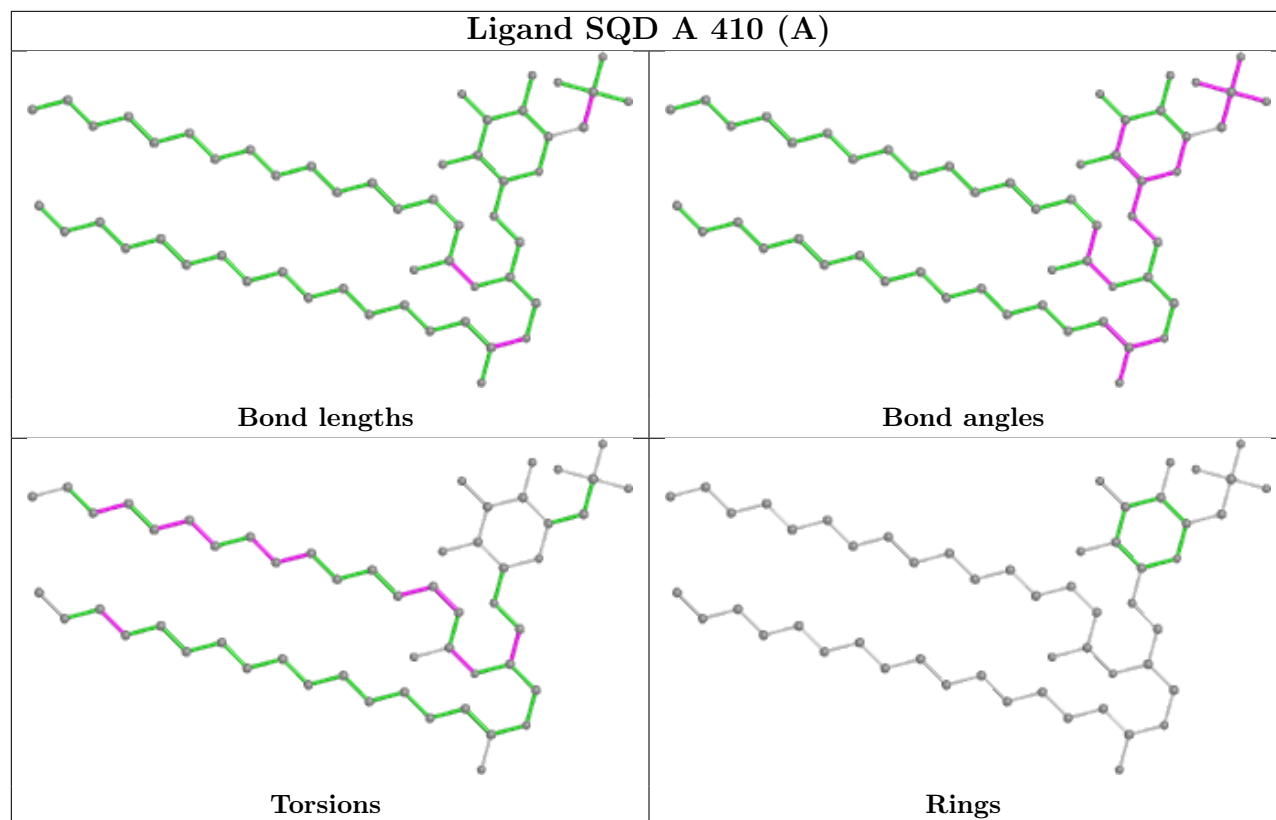


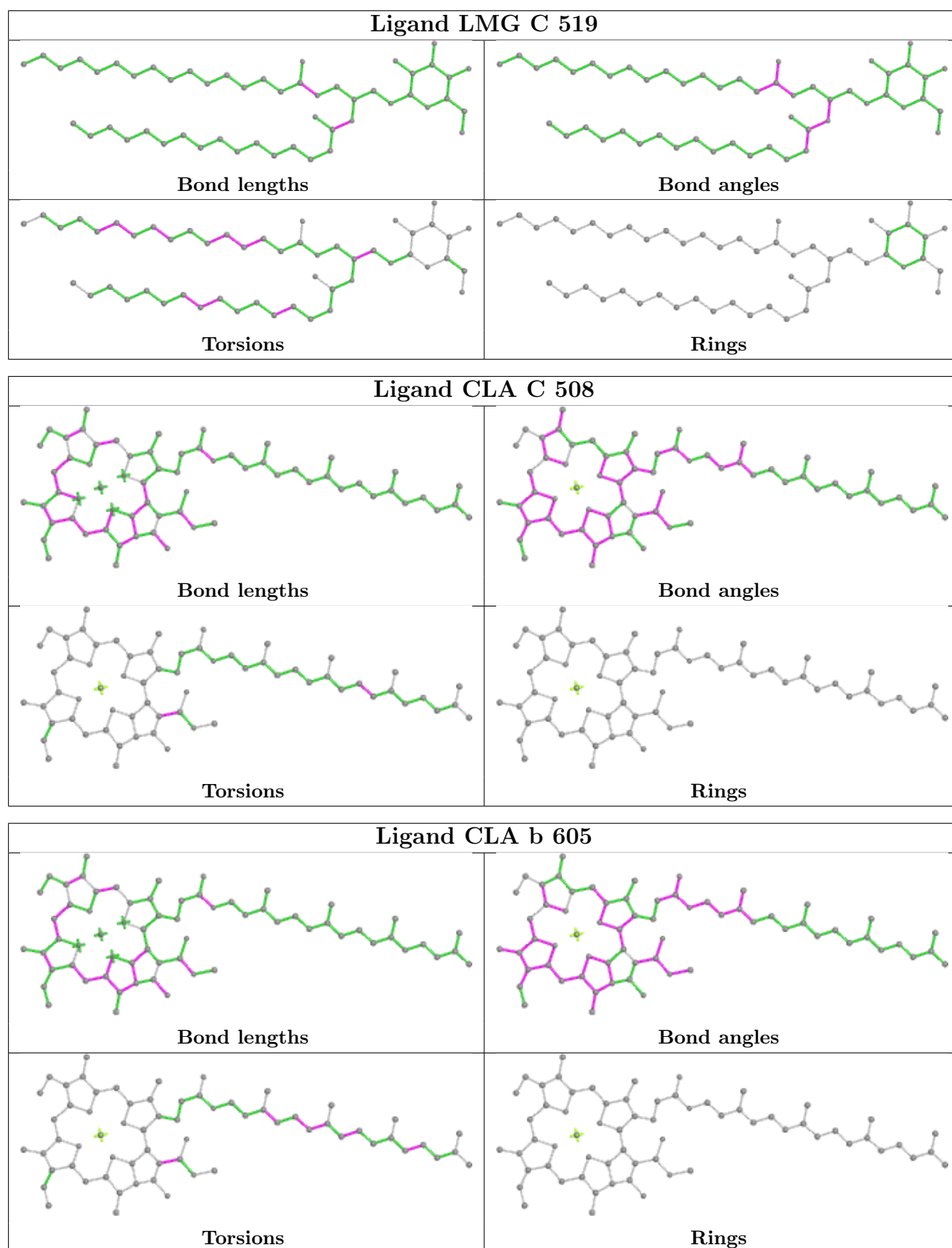


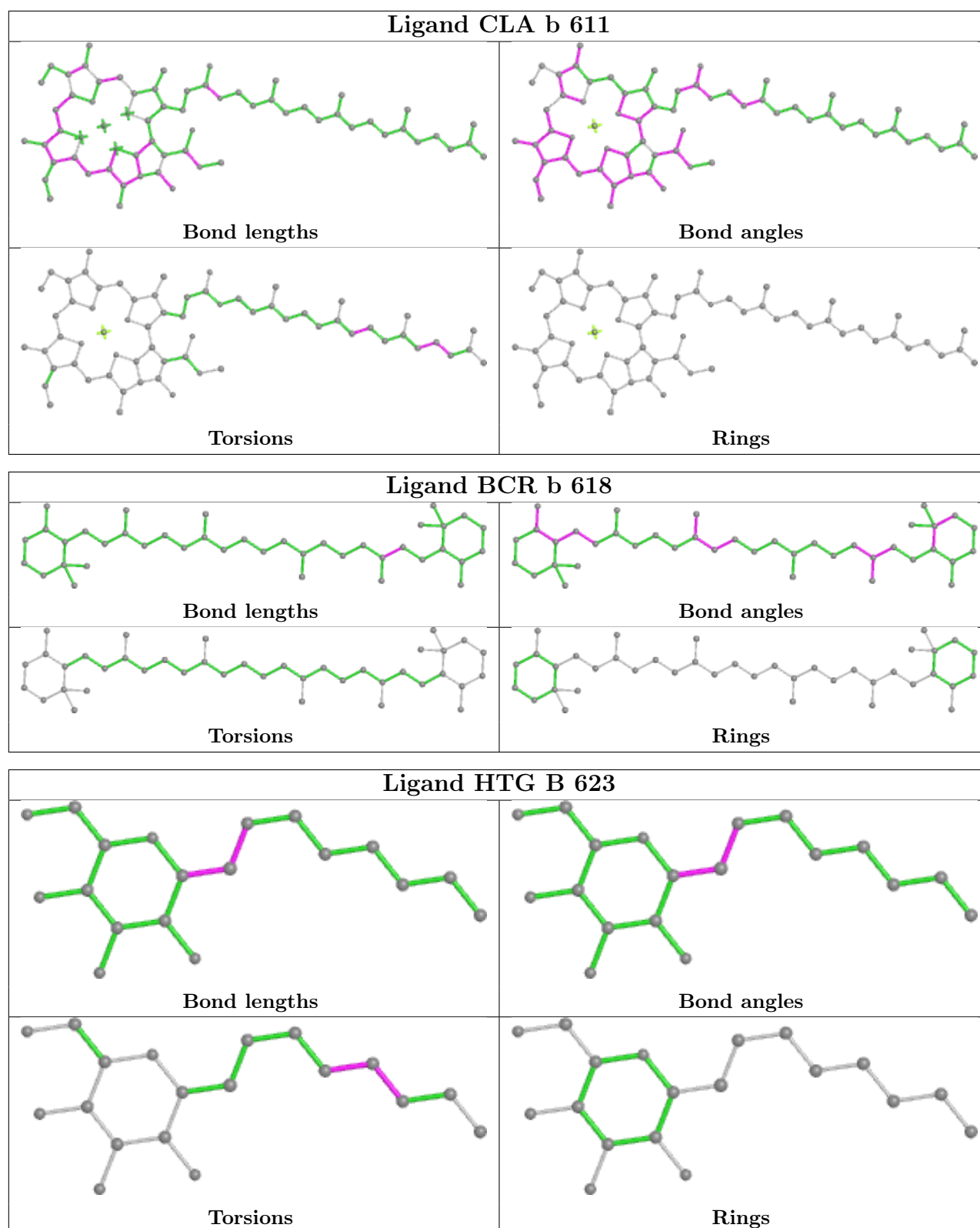


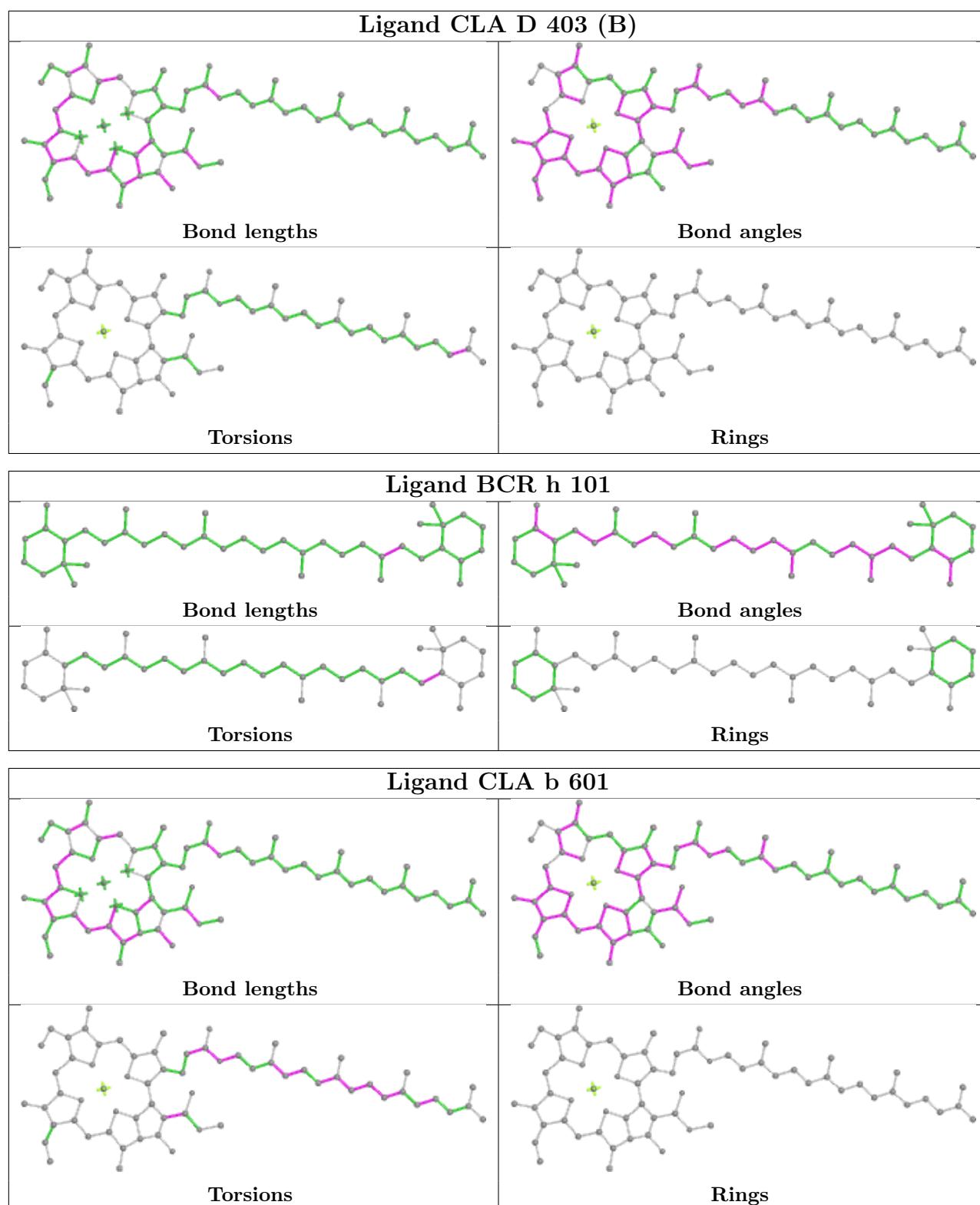


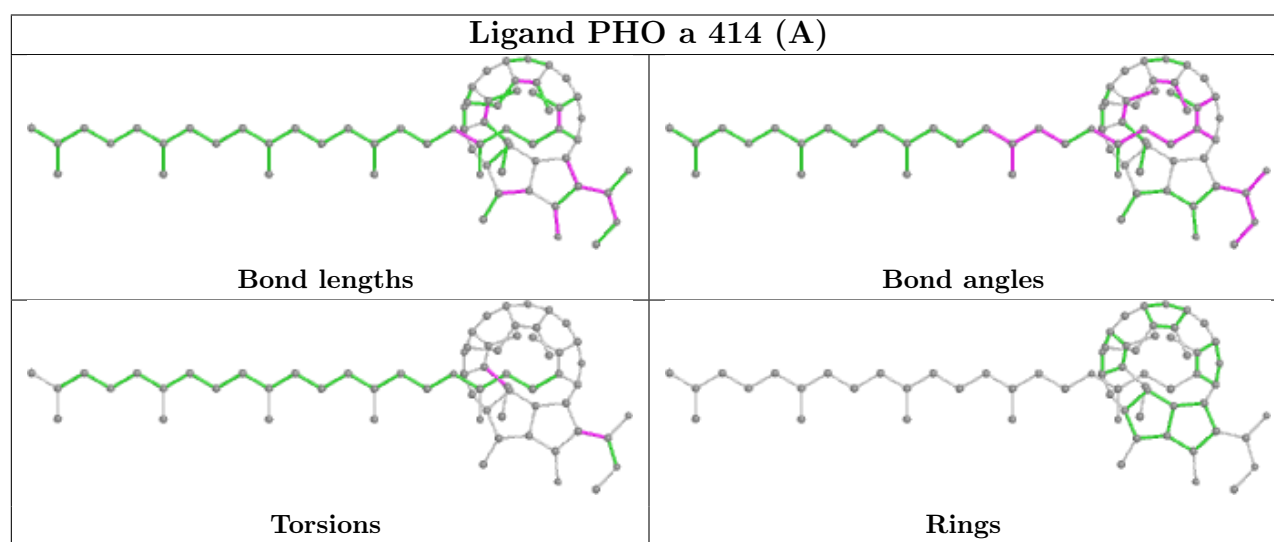
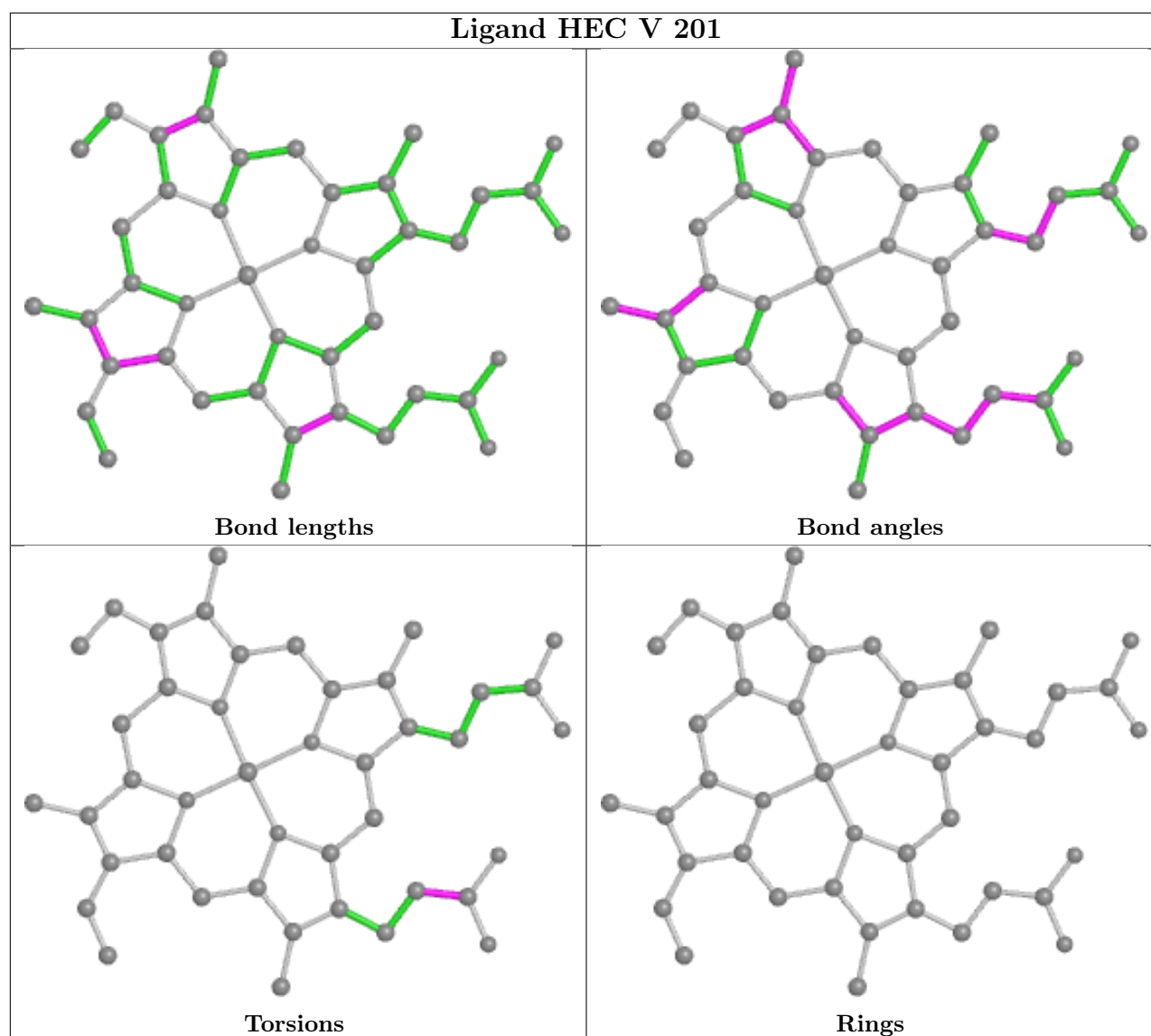


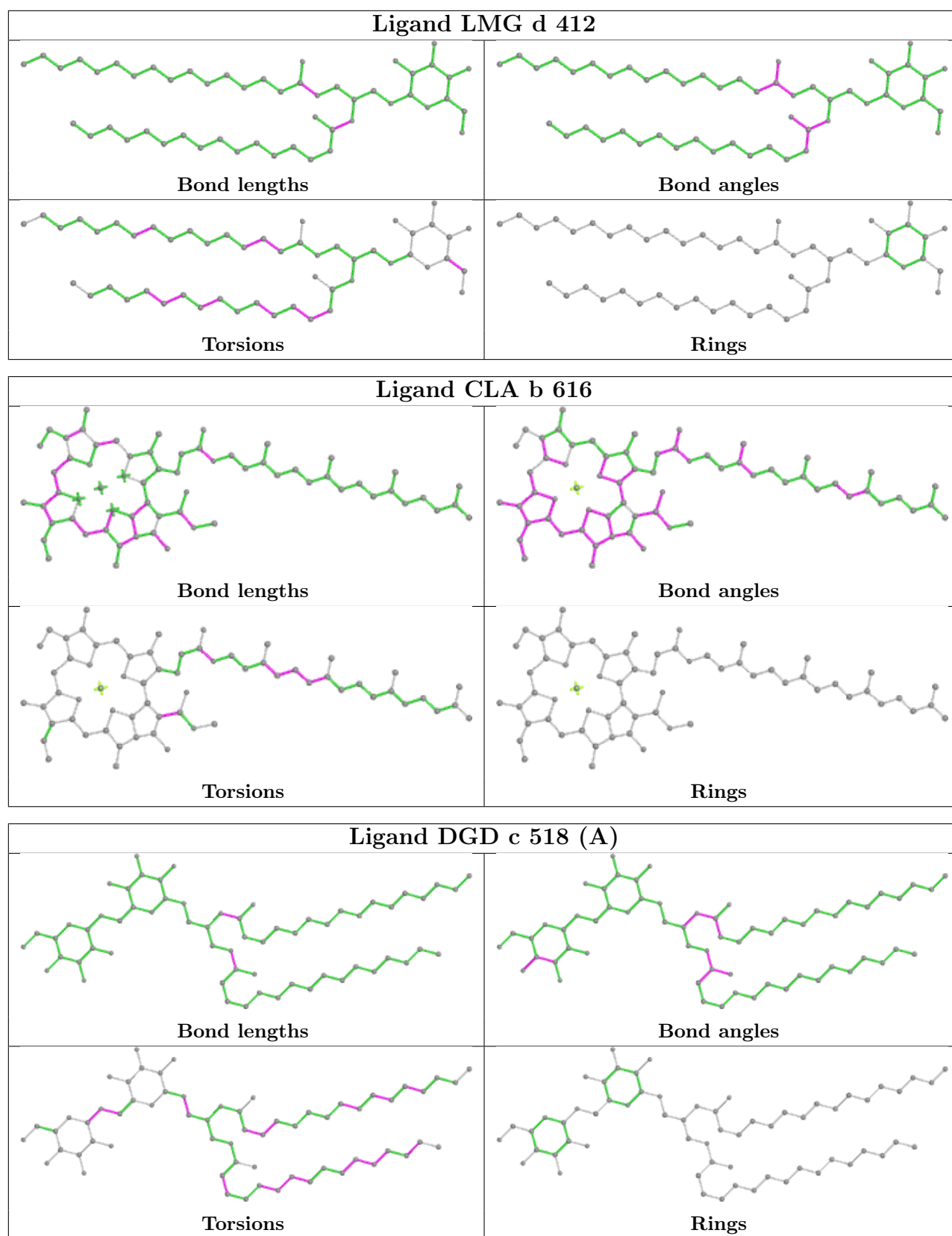












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%) | -0.77 | 4 (1%) 79 81 | 41, 48, 71, 127 | 0 |
| 1 | a | 334/344 (97%) | -0.68 | 7 (2%) 63 66 | 42, 52, 80, 127 | 0 |
| 2 | B | 504/505 (99%) | -0.53 | 11 (2%) 62 65 | 42, 54, 83, 117 | 0 |
| 2 | b | 504/505 (99%) | -0.36 | 30 (5%) 21 23 | 45, 58, 99, 162 | 1 (0%) |
| 3 | C | 451/455 (99%) | -0.56 | 5 (1%) 80 82 | 45, 60, 81, 158 | 0 |
| 3 | c | 455/455 (100%) | -0.48 | 15 (3%) 46 48 | 48, 66, 87, 124 | 2 (0%) |
| 4 | D | 342/342 (100%) | -0.70 | 3 (0%) 84 85 | 40, 50, 67, 138 | 0 |
| 4 | d | 341/342 (99%) | -0.68 | 2 (0%) 89 89 | 44, 54, 77, 134 | 0 |
| 5 | E | 81/84 (96%) | -0.10 | 6 (7%) 14 15 | 52, 71, 98, 166 | 0 |
| 5 | e | 79/84 (94%) | 0.19 | 7 (8%) 9 10 | 63, 76, 119, 150 | 0 |
| 6 | F | 34/44 (77%) | -0.48 | 2 (5%) 22 24 | 54, 62, 88, 115 | 0 |
| 6 | f | 31/44 (70%) | -0.30 | 2 (6%) 18 20 | 59, 67, 99, 152 | 0 |
| 7 | H | 64/65 (98%) | -0.31 | 2 (3%) 49 52 | 51, 63, 84, 112 | 0 |
| 7 | h | 64/65 (98%) | -0.34 | 3 (4%) 31 34 | 57, 69, 94, 111 | 0 |
| 8 | I | 37/38 (97%) | -0.12 | 3 (8%) 12 13 | 56, 63, 127, 163 | 0 |
| 8 | i | 37/38 (97%) | -0.07 | 5 (13%) 3 2 | 56, 63, 124, 148 | 0 |
| 9 | J | 38/39 (97%) | -0.25 | 3 (7%) 12 14 | 53, 71, 122, 182 | 0 |
| 9 | j | 39/39 (100%) | 0.19 | 6 (15%) 2 2 | 60, 75, 131, 175 | 0 |
| 10 | K | 37/37 (100%) | -0.61 | 1 (2%) 54 57 | 59, 69, 88, 110 | 0 |
| 10 | k | 37/37 (100%) | -0.51 | 0 100 100 | 69, 75, 98, 113 | 0 |
| 11 | L | 36/37 (97%) | -0.36 | 3 (8%) 11 12 | 40, 47, 105, 144 | 0 |
| 11 | l | 36/37 (97%) | -0.35 | 2 (5%) 24 26 | 43, 49, 97, 125 | 0 |
| 12 | M | 32/36 (88%) | -0.67 | 1 (3%) 49 52 | 44, 49, 77, 140 | 0 |
| 12 | m | 33/36 (91%) | -0.46 | 2 (6%) 21 23 | 43, 50, 72, 153 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 13 | O | 243/244 (99%) | -0.13 | 14 (5%) 23 25 | 44, 65, 119, 185 | 0 |
| 13 | o | 243/244 (99%) | -0.03 | 23 (9%) 8 8 | 45, 67, 128, 169 | 0 |
| 14 | T | 29/32 (90%) | -0.61 | 3 (10%) 6 6 | 44, 49, 78, 116 | 0 |
| 14 | t | 29/32 (90%) | -0.67 | 1 (3%) 45 47 | 45, 51, 75, 128 | 0 |
| 15 | U | 96/104 (92%) | -0.47 | 0 100 100 | 49, 59, 92, 101 | 0 |
| 15 | u | 97/104 (93%) | -0.41 | 0 100 100 | 52, 63, 83, 135 | 0 |
| 16 | V | 137/137 (100%) | -0.61 | 0 100 100 | 48, 58, 82, 105 | 0 |
| 16 | v | 137/137 (100%) | -0.23 | 3 (2%) 62 65 | 54, 71, 104, 138 | 0 |
| 17 | X | 38/40 (95%) | -0.29 | 2 (5%) 26 29 | 62, 72, 94, 115 | 0 |
| 17 | x | 38/40 (95%) | 0.08 | 4 (10%) 6 6 | 65, 78, 119, 163 | 0 |
| 18 | Y | 29/30 (96%) | 0.91 | 6 (20%) 1 1 | 69, 85, 126, 135 | 0 |
| 18 | y | 29/30 (96%) | 0.24 | 4 (13%) 2 2 | 77, 90, 111, 120 | 0 |
| 19 | Z | 62/62 (100%) | 0.02 | 7 (11%) 5 4 | 67, 80, 140, 163 | 0 |
| 19 | z | 62/62 (100%) | 0.36 | 11 (17%) 1 1 | 80, 95, 144, 189 | 0 |
| 20 | R | 34/34 (100%) | 2.44 | 23 (67%) 0 0 | 85, 109, 136, 155 | 0 |
| All | All | 5283/5384 (98%) | -0.41 | 226 (4%) 35 37 | 40, 60, 101, 189 | 3 (0%) |

The worst 5 of 226 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | E | 84 | LYS | 8.4 |
| 1 | a | 11 | ALA | 8.1 |
| 2 | b | 495 | PHE | 7.9 |
| 3 | C | 23 | ALA | 7.7 |
| 3 | c | 20 | SER | 7.2 |

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 8 | FME | i | 1 | 10/11 | 0.91 | 0.17 | 53,71,78,80 | 0 |
| 14 | FME | T | 1 | 10/11 | 0.95 | 0.10 | 43,57,72,74 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 14 | FME | t | 1 | 10/11 | 0.96 | 0.10 | 46,50,59,77 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.97 | 0.14 | 48,60,93,98 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.97 | 0.08 | 61,69,76,80 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.99 | 0.12 | 50,64,86,115 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 30 | UNL | B | 626 | 33/- | 0.49 | 0.36 | 52,106,144,150 | 0 |
| 30 | UNL | b | 626 | 33/- | 0.52 | 0.38 | 72,98,155,160 | 0 |
| 30 | UNL | I | 101 | 40/- | 0.53 | 0.34 | 72,105,157,164 | 0 |
| 27 | GOL | a | 416 | 6/6 | 0.53 | 0.53 | 77,99,109,115 | 0 |
| 31 | LMT | M | 102 | 35/35 | 0.56 | 0.30 | 74,127,183,188 | 0 |
| 32 | LMG | C | 520 | 51/55 | 0.58 | 0.31 | 63,120,162,184 | 0 |
| 31 | LMT | b | 621 | 25/35 | 0.59 | 0.28 | 80,113,162,172 | 0 |
| 30 | UNL | K | 101[B] | 34/- | 0.60 | 0.37 | 89,111,127,127 | 34 |
| 30 | UNL | K | 101[A] | 34/- | 0.60 | 0.37 | 89,111,127,127 | 34 |
| 30 | UNL | i | 101 | 40/- | 0.60 | 0.31 | 78,107,158,162 | 0 |
| 31 | LMT | F | 101 | 35/35 | 0.64 | 0.51 | 101,134,184,188 | 0 |
| 31 | LMT | M | 101 | 35/35 | 0.65 | 0.25 | 60,98,124,133 | 0 |
| 30 | UNL | j | 101 | 10/- | 0.66 | 0.28 | 75,91,107,111 | 0 |
| 31 | LMT | B | 631 | 25/35 | 0.68 | 0.24 | 62,89,154,167 | 0 |
| 30 | UNL | A | 415 | 28/- | 0.69 | 0.35 | 89,114,133,157 | 0 |
| 30 | UNL | x | 101 | 18/- | 0.69 | 0.25 | 72,82,136,137 | 0 |
| 31 | LMT | B | 630 | 35/35 | 0.69 | 0.35 | 65,119,149,170 | 0 |
| 32 | LMG | Z | 101 | 37/55 | 0.70 | 0.29 | 70,121,155,172 | 0 |
| 36 | CA | F | 104 | 1/1 | 0.70 | 0.23 | 128,128,128,128 | 0 |
| 27 | GOL | b | 624 | 6/6 | 0.71 | 0.23 | 87,102,106,114 | 0 |
| 30 | UNL | c | 525[A] | 32/- | 0.71 | 0.40 | 97,116,129,140 | 32 |
| 32 | LMG | c | 521 | 51/55 | 0.71 | 0.29 | 74,136,164,192 | 0 |
| 30 | UNL | c | 525[B] | 32/- | 0.71 | 0.40 | 97,116,129,141 | 32 |
| 30 | UNL | d | 410 | 36/- | 0.71 | 0.20 | 72,94,131,144 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 31 | LMT | m | 103 | 35/35 | 0.72 | 0.26 | 59,91,108,120 | 0 |
| 31 | LMT | b | 627 | 25/35 | 0.73 | 0.23 | 60,99,146,162 | 0 |
| 31 | LMT | A | 417 | 35/35 | 0.75 | 0.29 | 67,117,141,143 | 0 |
| 30 | UNL | X | 101 | 18/- | 0.76 | 0.22 | 63,74,107,110 | 0 |
| 30 | UNL | a | 413 | 30/- | 0.76 | 0.31 | 91,122,144,152 | 0 |
| 33 | LHG | a | 418[A] | 42/49 | 0.76 | 0.36 | 99,142,159,169 | 42 |
| 33 | LHG | a | 418[B] | 42/49 | 0.76 | 0.36 | 99,142,160,170 | 42 |
| 34 | HTG | D | 411 | 16/19 | 0.76 | 0.25 | 85,109,138,155 | 0 |
| 31 | LMT | A | 420 | 35/35 | 0.76 | 0.35 | 98,138,160,173 | 0 |
| 31 | LMT | a | 415 | 35/35 | 0.77 | 0.40 | 108,136,150,161 | 0 |
| 27 | GOL | B | 627 | 6/6 | 0.77 | 0.26 | 67,92,106,120 | 0 |
| 30 | UNL | m | 102 | 10/- | 0.77 | 0.32 | 72,78,95,98 | 0 |
| 31 | LMT | e | 101 | 35/35 | 0.77 | 0.52 | 103,152,193,201 | 0 |
| 31 | LMT | B | 628 | 35/35 | 0.77 | 0.25 | 65,105,146,152 | 0 |
| 27 | GOL | o | 302 | 6/6 | 0.77 | 0.30 | 89,105,115,125 | 0 |
| 34 | HTG | b | 623 | 19/19 | 0.78 | 0.47 | 86,126,163,167 | 0 |
| 34 | HTG | d | 411 | 16/19 | 0.79 | 0.30 | 84,123,143,152 | 0 |
| 26 | SQD | f | 102 | 43/54 | 0.80 | 0.34 | 98,128,180,194 | 0 |
| 30 | UNL | l | 101 | 10/- | 0.80 | 0.28 | 72,84,95,97 | 0 |
| 32 | LMG | z | 101 | 39/55 | 0.80 | 0.24 | 76,128,154,167 | 0 |
| 27 | GOL | c | 527 | 6/6 | 0.81 | 0.25 | 106,114,129,130 | 0 |
| 34 | HTG | C | 521 | 19/19 | 0.81 | 0.34 | 105,130,146,146 | 0 |
| 27 | GOL | A | 411 | 6/6 | 0.82 | 0.18 | 65,81,86,86 | 0 |
| 26 | SQD | b | 620 | 54/54 | 0.82 | 0.18 | 66,95,127,132 | 0 |
| 27 | GOL | D | 402 | 6/6 | 0.82 | 0.41 | 53,80,82,89 | 0 |
| 27 | GOL | O | 302 | 6/6 | 0.82 | 0.23 | 76,91,103,107 | 0 |
| 27 | GOL | o | 303 | 6/6 | 0.82 | 0.20 | 84,94,101,105 | 0 |
| 27 | GOL | O | 303 | 6/6 | 0.83 | 0.23 | 85,103,105,108 | 0 |
| 27 | GOL | l | 102[A] | 6/6 | 0.83 | 0.88 | 70,103,107,112 | 6 |
| 27 | GOL | l | 102[B] | 6/6 | 0.83 | 0.88 | 69,103,108,112 | 6 |
| 31 | LMT | t | 101 | 26/35 | 0.84 | 0.17 | 72,104,148,156 | 0 |
| 27 | GOL | v | 202[A] | 6/6 | 0.84 | 0.17 | 67,80,85,87 | 6 |
| 27 | GOL | v | 202[B] | 6/6 | 0.84 | 0.17 | 67,80,85,87 | 6 |
| 29 | PL9 | A | 414[A] | 55/55 | 0.84 | 0.23 | 73,99,113,114 | 55 |
| 30 | UNL | J | 101 | 10/- | 0.84 | 0.16 | 74,84,93,99 | 0 |
| 29 | PL9 | A | 414[B] | 55/55 | 0.84 | 0.23 | 73,99,113,115 | 55 |
| 26 | SQD | A | 412 | 54/54 | 0.85 | 0.18 | 68,93,134,159 | 0 |
| 32 | LMG | c | 501 | 51/55 | 0.85 | 0.16 | 65,96,111,119 | 0 |
| 26 | SQD | B | 620 | 54/54 | 0.85 | 0.15 | 64,93,135,152 | 0 |
| 27 | GOL | a | 417 | 6/6 | 0.85 | 0.44 | 59,81,81,85 | 0 |
| 26 | SQD | a | 410 | 54/54 | 0.85 | 0.19 | 63,99,137,154 | 0 |
| 34 | HTG | c | 522 | 19/19 | 0.85 | 0.25 | 111,129,143,150 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 33 | LHG | E | 101[A] | 42/49 | 0.85 | 0.23 | 76,106,119,123 | 42 |
| 33 | LHG | E | 101[B] | 42/49 | 0.85 | 0.23 | 76,106,119,124 | 42 |
| 36 | CA | f | 103 | 1/1 | 0.85 | 0.09 | 124,124,124,124 | 0 |
| 32 | LMG | A | 418 | 51/55 | 0.86 | 0.16 | 67,91,119,134 | 0 |
| 30 | UNL | D | 410 | 40/- | 0.86 | 0.16 | 66,93,138,147 | 0 |
| 34 | HTG | B | 623 | 19/19 | 0.86 | 0.22 | 65,97,115,117 | 0 |
| 29 | PL9 | a | 412[A] | 55/55 | 0.86 | 0.21 | 89,110,123,125 | 55 |
| 29 | PL9 | a | 412[B] | 55/55 | 0.86 | 0.21 | 90,110,123,126 | 55 |
| 34 | HTG | b | 622 | 19/19 | 0.88 | 0.16 | 58,88,121,122 | 0 |
| 25 | BCR | C | 514 | 40/40 | 0.88 | 0.13 | 55,76,88,94 | 0 |
| 23 | CLA | c | 514 | 65/65 | 0.88 | 0.17 | 62,95,121,145 | 0 |
| 23 | CLA | b | 616 | 65/65 | 0.89 | 0.16 | 48,64,125,141 | 0 |
| 32 | LMG | D | 412 | 51/55 | 0.89 | 0.17 | 51,66,122,146 | 0 |
| 27 | GOL | d | 413 | 6/6 | 0.89 | 0.35 | 56,70,85,97 | 0 |
| 23 | CLA | d | 404 | 65/65 | 0.89 | 0.15 | 50,67,120,154 | 0 |
| 32 | LMG | d | 412 | 51/55 | 0.89 | 0.17 | 55,71,117,152 | 0 |
| 27 | GOL | B | 629 | 6/6 | 0.90 | 0.26 | 75,77,89,98 | 0 |
| 25 | BCR | K | 102 | 40/40 | 0.90 | 0.17 | 58,67,79,84 | 0 |
| 34 | HTG | B | 622 | 19/19 | 0.90 | 0.14 | 60,87,119,127 | 0 |
| 25 | BCR | h | 101 | 40/40 | 0.90 | 0.14 | 57,70,91,98 | 0 |
| 32 | LMG | c | 520 | 51/55 | 0.90 | 0.18 | 60,90,133,162 | 0 |
| 23 | CLA | b | 601 | 65/65 | 0.90 | 0.15 | 59,84,124,161 | 0 |
| 23 | CLA | B | 601 | 65/65 | 0.91 | 0.13 | 53,79,109,156 | 0 |
| 26 | SQD | F | 103 | 43/54 | 0.91 | 0.18 | 70,104,133,142 | 0 |
| 23 | CLA | C | 513 | 65/65 | 0.91 | 0.13 | 60,86,109,119 | 0 |
| 27 | GOL | V | 203[A] | 6/6 | 0.91 | 0.15 | 56,66,76,77 | 6 |
| 27 | GOL | V | 203[B] | 6/6 | 0.91 | 0.15 | 56,66,76,77 | 6 |
| 32 | LMG | C | 519 | 51/55 | 0.91 | 0.17 | 59,83,120,134 | 0 |
| 23 | CLA | c | 513 | 65/65 | 0.91 | 0.17 | 62,82,129,135 | 0 |
| 25 | BCR | d | 405 | 40/40 | 0.92 | 0.13 | 51,65,107,114 | 0 |
| 23 | CLA | C | 512 | 65/65 | 0.92 | 0.14 | 57,74,115,133 | 0 |
| 27 | GOL | D | 413 | 6/6 | 0.92 | 0.20 | 50,65,76,97 | 0 |
| 30 | UNL | d | 409 | 17/- | 0.92 | 0.12 | 67,83,114,117 | 0 |
| 23 | CLA | B | 606 | 65/65 | 0.92 | 0.14 | 44,59,106,130 | 0 |
| 23 | CLA | B | 616 | 65/65 | 0.92 | 0.17 | 46,60,132,143 | 0 |
| 25 | BCR | Y | 101 | 40/40 | 0.92 | 0.12 | 53,66,81,88 | 0 |
| 30 | UNL | D | 409 | 17/- | 0.92 | 0.14 | 59,77,102,118 | 0 |
| 23 | CLA | b | 606 | 65/65 | 0.93 | 0.13 | 45,60,112,121 | 0 |
| 32 | LMG | B | 621 | 51/55 | 0.93 | 0.12 | 55,73,94,118 | 0 |
| 35 | DGD | c | 518[A] | 62/66 | 0.93 | 0.12 | 53,68,119,132 | 62 |
| 35 | DGD | c | 518[B] | 62/66 | 0.93 | 0.12 | 53,68,119,133 | 62 |
| 23 | CLA | C | 506 | 65/65 | 0.93 | 0.13 | 57,71,122,143 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 32 | LMG | m | 101 | 51/55 | 0.93 | 0.12 | 57,77,101,118 | 0 |
| 36 | CA | o | 301 | 1/1 | 0.93 | 0.04 | 104,104,104,104 | 0 |
| 25 | BCR | c | 515 | 40/40 | 0.94 | 0.10 | 68,80,93,96 | 0 |
| 23 | CLA | a | 407 | 65/65 | 0.94 | 0.17 | 45,58,147,168 | 0 |
| 34 | HTG | b | 625 | 19/19 | 0.94 | 0.09 | 65,80,96,103 | 0 |
| 23 | CLA | c | 507 | 65/65 | 0.94 | 0.13 | 55,72,124,142 | 0 |
| 25 | BCR | k | 101 | 40/40 | 0.94 | 0.13 | 56,74,87,91 | 0 |
| 35 | DGD | C | 517[A] | 62/66 | 0.94 | 0.12 | 51,65,110,116 | 62 |
| 35 | DGD | C | 517[B] | 62/66 | 0.94 | 0.12 | 51,65,110,116 | 62 |
| 35 | DGD | C | 518 | 62/66 | 0.94 | 0.11 | 46,62,94,114 | 0 |
| 35 | DGD | H | 102 | 62/66 | 0.94 | 0.11 | 46,61,80,94 | 0 |
| 25 | BCR | D | 405 | 40/40 | 0.94 | 0.10 | 46,62,103,107 | 0 |
| 23 | CLA | B | 609 | 65/65 | 0.94 | 0.14 | 43,59,71,80 | 0 |
| 35 | DGD | c | 519 | 62/66 | 0.94 | 0.12 | 51,68,101,132 | 0 |
| 35 | DGD | h | 102 | 62/66 | 0.94 | 0.11 | 52,66,82,87 | 0 |
| 34 | HTG | B | 625 | 19/19 | 0.94 | 0.10 | 68,82,99,100 | 0 |
| 23 | CLA | C | 508 | 65/65 | 0.94 | 0.10 | 47,56,111,146 | 0 |
| 25 | BCR | b | 618 | 40/40 | 0.94 | 0.10 | 45,58,78,85 | 0 |
| 23 | CLA | b | 612 | 65/65 | 0.95 | 0.10 | 42,54,66,75 | 0 |
| 34 | HTG | V | 202 | 11/19 | 0.95 | 0.41 | 77,111,125,125 | 0 |
| 25 | BCR | t | 102 | 40/40 | 0.95 | 0.09 | 43,60,79,87 | 0 |
| 25 | BCR | y | 101 | 40/40 | 0.95 | 0.09 | 59,71,85,102 | 0 |
| 26 | SQD | A | 410[A] | 54/54 | 0.95 | 0.13 | 56,80,112,118 | 54 |
| 26 | SQD | A | 410[B] | 54/54 | 0.95 | 0.13 | 56,80,112,119 | 54 |
| 25 | BCR | C | 515 | 40/40 | 0.95 | 0.11 | 50,65,76,85 | 0 |
| 23 | CLA | a | 405[A] | 65/65 | 0.95 | 0.11 | 42,54,121,135 | 65 |
| 25 | BCR | H | 101 | 40/40 | 0.95 | 0.10 | 49,66,82,87 | 0 |
| 23 | CLA | a | 405[B] | 65/65 | 0.95 | 0.11 | 42,54,121,135 | 65 |
| 23 | CLA | B | 611 | 65/65 | 0.95 | 0.10 | 38,47,67,77 | 0 |
| 23 | CLA | A | 408 | 65/65 | 0.95 | 0.12 | 43,53,132,147 | 0 |
| 33 | LHG | d | 408[A] | 49/49 | 0.95 | 0.14 | 52,65,110,124 | 49 |
| 33 | LHG | d | 408[B] | 49/49 | 0.95 | 0.14 | 52,65,110,124 | 49 |
| 23 | CLA | D | 404 | 65/65 | 0.95 | 0.14 | 48,60,122,143 | 0 |
| 36 | CA | C | 523 | 1/1 | 0.95 | 0.07 | 75,75,75,75 | 0 |
| 27 | GOL | B | 624 | 6/6 | 0.95 | 0.22 | 73,81,88,89 | 0 |
| 25 | BCR | A | 409 | 40/40 | 0.95 | 0.10 | 40,52,65,71 | 0 |
| 25 | BCR | B | 618 | 40/40 | 0.95 | 0.09 | 44,57,74,83 | 0 |
| 33 | LHG | A | 419[B] | 49/49 | 0.96 | 0.12 | 50,65,85,90 | 49 |
| 33 | LHG | D | 408[A] | 49/49 | 0.96 | 0.14 | 49,62,111,112 | 49 |
| 33 | LHG | D | 408[B] | 49/49 | 0.96 | 0.14 | 49,62,111,113 | 49 |
| 26 | SQD | a | 409[A] | 54/54 | 0.96 | 0.13 | 58,83,118,125 | 54 |
| 26 | SQD | a | 409[B] | 54/54 | 0.96 | 0.13 | 58,83,119,125 | 54 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 23 | CLA | b | 614 | 65/65 | 0.96 | 0.09 | 42,51,101,119 | 0 |
| 23 | CLA | b | 615 | 65/65 | 0.96 | 0.11 | 46,59,79,92 | 0 |
| 33 | LHG | b | 629[A] | 49/49 | 0.96 | 0.13 | 50,59,71,93 | 49 |
| 33 | LHG | b | 629[B] | 49/49 | 0.96 | 0.13 | 50,59,71,94 | 49 |
| 33 | LHG | d | 407[A] | 49/49 | 0.96 | 0.15 | 49,57,71,77 | 49 |
| 33 | LHG | d | 407[B] | 49/49 | 0.96 | 0.15 | 49,57,72,78 | 49 |
| 23 | CLA | C | 501 | 65/65 | 0.96 | 0.08 | 49,61,72,80 | 0 |
| 23 | CLA | c | 502 | 65/65 | 0.96 | 0.10 | 56,68,81,89 | 0 |
| 33 | LHG | d | 414[A] | 49/49 | 0.96 | 0.14 | 55,68,80,91 | 49 |
| 33 | LHG | d | 414[B] | 49/49 | 0.96 | 0.14 | 55,69,80,91 | 49 |
| 29 | PL9 | D | 406[A] | 55/55 | 0.96 | 0.11 | 39,50,60,73 | 55 |
| 29 | PL9 | D | 406[B] | 55/55 | 0.96 | 0.11 | 39,50,60,73 | 55 |
| 25 | BCR | T | 101 | 40/40 | 0.96 | 0.08 | 45,60,73,80 | 0 |
| 23 | CLA | c | 505 | 65/65 | 0.96 | 0.10 | 50,65,107,140 | 0 |
| 23 | CLA | c | 506 | 65/65 | 0.96 | 0.09 | 49,65,91,99 | 0 |
| 27 | GOL | C | 522[A] | 6/6 | 0.96 | 0.12 | 58,61,63,72 | 6 |
| 27 | GOL | C | 522[B] | 6/6 | 0.96 | 0.12 | 58,62,63,72 | 6 |
| 25 | BCR | b | 619 | 40/40 | 0.96 | 0.08 | 50,66,88,92 | 0 |
| 23 | CLA | C | 509 | 65/65 | 0.96 | 0.10 | 46,60,85,93 | 0 |
| 25 | BCR | c | 516 | 40/40 | 0.96 | 0.11 | 55,67,77,93 | 0 |
| 23 | CLA | c | 508 | 65/65 | 0.96 | 0.10 | 54,69,86,92 | 0 |
| 23 | CLA | c | 509 | 65/65 | 0.96 | 0.12 | 47,63,123,148 | 0 |
| 23 | CLA | c | 512 | 65/65 | 0.96 | 0.10 | 57,68,88,104 | 0 |
| 23 | CLA | C | 511 | 65/65 | 0.96 | 0.12 | 49,65,83,87 | 0 |
| 23 | CLA | C | 504 | 65/65 | 0.96 | 0.10 | 39,58,107,136 | 0 |
| 35 | DGD | c | 517[A] | 62/66 | 0.96 | 0.11 | 50,65,99,107 | 62 |
| 35 | DGD | c | 517[B] | 62/66 | 0.96 | 0.11 | 50,65,100,107 | 62 |
| 23 | CLA | b | 604 | 65/65 | 0.96 | 0.11 | 39,52,101,120 | 0 |
| 27 | GOL | c | 526[A] | 6/6 | 0.96 | 0.25 | 66,69,73,74 | 6 |
| 27 | GOL | c | 526[B] | 6/6 | 0.96 | 0.25 | 66,69,73,74 | 6 |
| 23 | CLA | B | 614 | 65/65 | 0.96 | 0.10 | 41,50,106,118 | 0 |
| 23 | CLA | b | 609 | 65/65 | 0.96 | 0.13 | 47,65,78,89 | 0 |
| 25 | BCR | B | 619 | 40/40 | 0.96 | 0.08 | 48,60,92,98 | 0 |
| 23 | CLA | C | 507 | 65/65 | 0.96 | 0.11 | 49,64,82,96 | 0 |
| 33 | LHG | A | 419[A] | 49/49 | 0.96 | 0.12 | 50,65,85,89 | 49 |
| 38 | HEM | f | 101 | 43/43 | 0.96 | 0.14 | 61,82,118,133 | 0 |
| 23 | CLA | b | 613 | 65/65 | 0.97 | 0.08 | 42,50,90,102 | 0 |
| 23 | CLA | B | 613 | 65/65 | 0.97 | 0.08 | 40,47,94,117 | 0 |
| 29 | PL9 | d | 406[A] | 55/55 | 0.97 | 0.10 | 42,52,62,71 | 55 |
| 29 | PL9 | d | 406[B] | 55/55 | 0.97 | 0.10 | 42,53,62,71 | 55 |
| 23 | CLA | B | 603 | 65/65 | 0.97 | 0.10 | 45,53,72,83 | 0 |
| 23 | CLA | B | 605 | 65/65 | 0.97 | 0.11 | 40,49,66,84 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 25 | BCR | a | 408 | 40/40 | 0.97 | 0.07 | 46,55,66,71 | 0 |
| 25 | BCR | b | 617 | 40/40 | 0.97 | 0.08 | 46,55,65,68 | 0 |
| 23 | CLA | A | 406[A] | 65/65 | 0.97 | 0.09 | 41,48,114,126 | 65 |
| 23 | CLA | c | 504 | 65/65 | 0.97 | 0.09 | 51,71,84,98 | 0 |
| 23 | CLA | a | 404[A] | 65/65 | 0.97 | 0.13 | 39,48,64,75 | 65 |
| 23 | CLA | a | 404[B] | 65/65 | 0.97 | 0.13 | 39,48,65,75 | 65 |
| 23 | CLA | C | 502 | 65/65 | 0.97 | 0.08 | 45,56,83,92 | 0 |
| 23 | CLA | C | 503 | 65/65 | 0.97 | 0.08 | 51,61,72,78 | 0 |
| 23 | CLA | B | 607 | 65/65 | 0.97 | 0.09 | 36,49,73,84 | 0 |
| 27 | GOL | b | 628 | 6/6 | 0.97 | 0.20 | 78,86,89,89 | 0 |
| 23 | CLA | c | 510 | 65/65 | 0.97 | 0.10 | 47,63,88,100 | 0 |
| 35 | DGD | C | 516[A] | 62/66 | 0.97 | 0.10 | 48,59,99,107 | 62 |
| 35 | DGD | C | 516[B] | 62/66 | 0.97 | 0.10 | 48,59,99,107 | 62 |
| 23 | CLA | A | 406[B] | 65/65 | 0.97 | 0.09 | 41,48,114,126 | 65 |
| 23 | CLA | b | 602 | 65/65 | 0.97 | 0.12 | 48,60,80,86 | 0 |
| 23 | CLA | B | 610 | 65/65 | 0.97 | 0.11 | 43,56,67,85 | 0 |
| 23 | CLA | b | 605 | 65/65 | 0.97 | 0.11 | 39,51,72,81 | 0 |
| 24 | PHO | a | 414[A] | 64/64 | 0.97 | 0.11 | 45,55,62,67 | 64 |
| 24 | PHO | a | 414[B] | 64/64 | 0.97 | 0.11 | 45,55,62,67 | 64 |
| 23 | CLA | B | 602 | 65/65 | 0.97 | 0.11 | 45,57,73,89 | 0 |
| 25 | BCR | B | 617 | 40/40 | 0.97 | 0.09 | 42,53,64,66 | 0 |
| 23 | CLA | b | 607 | 65/65 | 0.97 | 0.08 | 38,49,81,92 | 0 |
| 33 | LHG | L | 101[A] | 49/49 | 0.97 | 0.11 | 50,58,71,92 | 49 |
| 33 | LHG | L | 101[B] | 49/49 | 0.97 | 0.11 | 49,58,71,92 | 49 |
| 23 | CLA | B | 612 | 65/65 | 0.97 | 0.07 | 37,50,64,71 | 0 |
| 36 | CA | O | 301 | 1/1 | 0.97 | 0.06 | 105,105,105,105 | 0 |
| 23 | CLA | b | 610 | 65/65 | 0.97 | 0.08 | 49,58,69,74 | 0 |
| 23 | CLA | b | 611 | 65/65 | 0.97 | 0.08 | 39,50,72,82 | 0 |
| 23 | CLA | C | 510 | 65/65 | 0.97 | 0.07 | 46,60,82,88 | 0 |
| 40 | HEC | V | 201 | 43/43 | 0.97 | 0.12 | 39,50,58,63 | 0 |
| 40 | HEC | v | 201 | 43/43 | 0.97 | 0.11 | 52,63,72,74 | 0 |
| 23 | CLA | D | 403[A] | 65/65 | 0.98 | 0.11 | 34,44,71,78 | 65 |
| 24 | PHO | A | 407[A] | 64/64 | 0.98 | 0.08 | 38,47,55,57 | 64 |
| 24 | PHO | A | 407[B] | 64/64 | 0.98 | 0.08 | 38,47,55,57 | 64 |
| 33 | LHG | D | 407[A] | 49/49 | 0.98 | 0.13 | 48,56,68,81 | 49 |
| 33 | LHG | D | 407[B] | 49/49 | 0.98 | 0.13 | 47,56,68,81 | 49 |
| 24 | PHO | A | 416[A] | 64/64 | 0.98 | 0.09 | 39,51,57,64 | 64 |
| 24 | PHO | A | 416[B] | 64/64 | 0.98 | 0.09 | 38,51,57,65 | 64 |
| 24 | PHO | a | 406[A] | 64/64 | 0.98 | 0.08 | 44,50,54,57 | 64 |
| 24 | PHO | a | 406[B] | 64/64 | 0.98 | 0.08 | 44,50,54,58 | 64 |
| 23 | CLA | D | 403[B] | 65/65 | 0.98 | 0.11 | 34,44,72,79 | 65 |
| 23 | CLA | c | 503 | 65/65 | 0.98 | 0.08 | 44,59,89,106 | 0 |

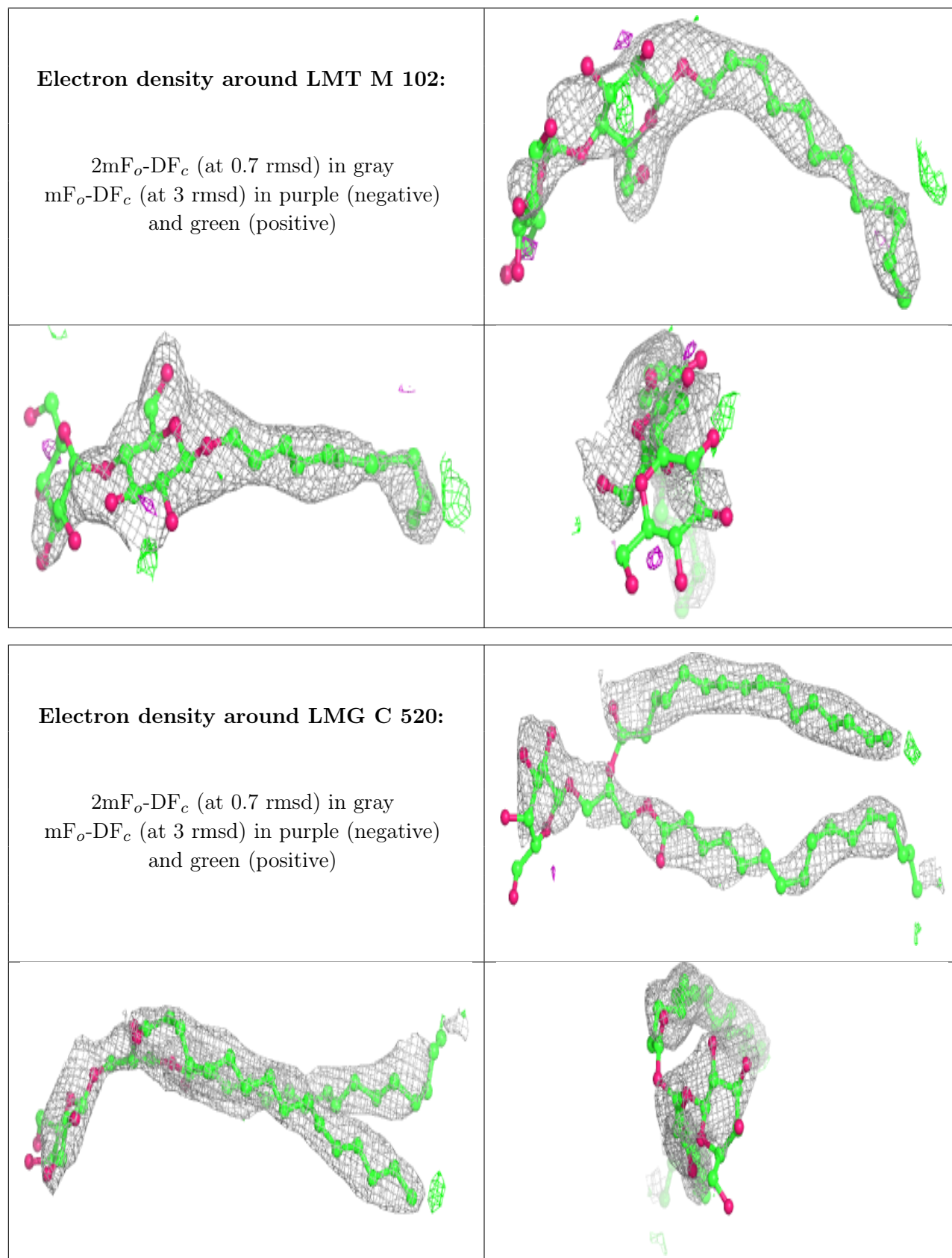
Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 23 | CLA | B | 608 | 65/65 | 0.98 | 0.07 | 43,51,71,83 | 0 |
| 23 | CLA | B | 615 | 65/65 | 0.98 | 0.10 | 43,54,80,90 | 0 |
| 23 | CLA | b | 608 | 65/65 | 0.98 | 0.07 | 43,57,78,91 | 0 |
| 23 | CLA | A | 404[B] | 65/65 | 0.98 | 0.12 | 37,44,63,70 | 65 |
| 23 | CLA | B | 604 | 65/65 | 0.98 | 0.09 | 38,48,111,141 | 0 |
| 23 | CLA | A | 405[A] | 65/65 | 0.98 | 0.10 | 38,45,56,70 | 65 |
| 23 | CLA | A | 405[B] | 65/65 | 0.98 | 0.10 | 37,45,56,70 | 65 |
| 23 | CLA | c | 511 | 65/65 | 0.98 | 0.09 | 51,65,80,93 | 0 |
| 23 | CLA | A | 404[A] | 65/65 | 0.98 | 0.12 | 37,44,62,70 | 65 |
| 23 | CLA | C | 505 | 65/65 | 0.98 | 0.08 | 48,60,89,106 | 0 |
| 36 | CA | c | 523 | 1/1 | 0.98 | 0.05 | 75,75,75,75 | 0 |
| 36 | CA | c | 524 | 1/1 | 0.98 | 0.07 | 77,77,77,77 | 0 |
| 23 | CLA | b | 603 | 65/65 | 0.98 | 0.07 | 45,57,81,98 | 0 |
| 23 | CLA | d | 402[A] | 65/65 | 0.98 | 0.08 | 40,45,63,73 | 65 |
| 37 | BCT | d | 401[A] | 4/4 | 0.98 | 0.09 | 59,63,67,79 | 4 |
| 37 | BCT | d | 401[B] | 4/4 | 0.98 | 0.09 | 59,64,67,80 | 4 |
| 38 | HEM | F | 102 | 43/43 | 0.98 | 0.09 | 55,69,84,89 | 0 |
| 23 | CLA | d | 402[B] | 65/65 | 0.98 | 0.08 | 40,45,64,73 | 65 |
| 23 | CLA | d | 403[A] | 65/65 | 0.98 | 0.11 | 39,47,77,91 | 65 |
| 23 | CLA | d | 403[B] | 65/65 | 0.98 | 0.11 | 39,47,77,91 | 65 |
| 28 | OEX | a | 411[A] | 10/10 | 0.99 | 0.06 | 46,49,51,56 | 10 |
| 28 | OEX | a | 411[B] | 10/10 | 0.99 | 0.06 | 46,50,54,56 | 10 |
| 21 | FE2 | A | 401[A] | 1/1 | 0.99 | 0.04 | 52,52,52,52 | 1 |
| 21 | FE2 | A | 401[B] | 1/1 | 0.99 | 0.04 | 52,52,52,52 | 1 |
| 21 | FE2 | a | 401[A] | 1/1 | 0.99 | 0.05 | 55,55,55,55 | 1 |
| 21 | FE2 | a | 401[B] | 1/1 | 0.99 | 0.05 | 55,55,55,55 | 1 |
| 22 | CL | A | 402[A] | 1/1 | 0.99 | 0.02 | 44,44,44,44 | 1 |
| 22 | CL | A | 402[B] | 1/1 | 0.99 | 0.02 | 44,44,44,44 | 1 |
| 22 | CL | A | 403[A] | 1/1 | 0.99 | 0.04 | 47,47,47,47 | 1 |
| 22 | CL | A | 403[B] | 1/1 | 0.99 | 0.04 | 47,47,47,47 | 1 |
| 37 | BCT | D | 401[A] | 4/4 | 0.99 | 0.13 | 55,60,61,68 | 4 |
| 37 | BCT | D | 401[B] | 4/4 | 0.99 | 0.13 | 55,57,62,72 | 4 |
| 22 | CL | a | 402[A] | 1/1 | 0.99 | 0.04 | 50,50,50,50 | 1 |
| 22 | CL | a | 402[B] | 1/1 | 0.99 | 0.04 | 50,50,50,50 | 1 |
| 22 | CL | a | 403[A] | 1/1 | 0.99 | 0.04 | 52,52,52,52 | 1 |
| 22 | CL | a | 403[B] | 1/1 | 0.99 | 0.04 | 52,52,52,52 | 1 |
| 39 | MG | J | 102 | 1/1 | 0.99 | 0.02 | 59,59,59,59 | 0 |
| 39 | MG | j | 102 | 1/1 | 0.99 | 0.07 | 63,63,63,63 | 0 |
| 28 | OEX | A | 413[A] | 10/10 | 0.99 | 0.06 | 40,44,50,50 | 10 |
| 28 | OEX | A | 413[B] | 10/10 | 0.99 | 0.06 | 40,44,50,51 | 10 |

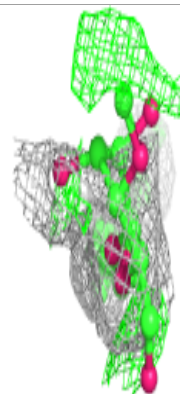
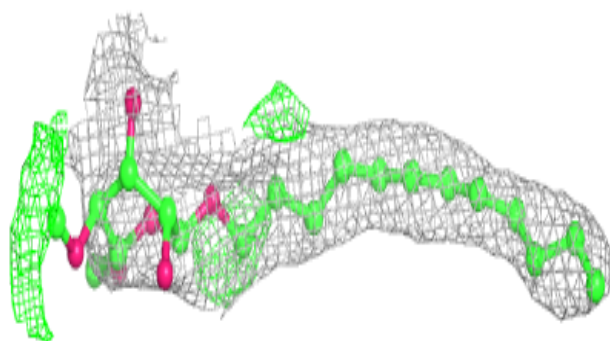
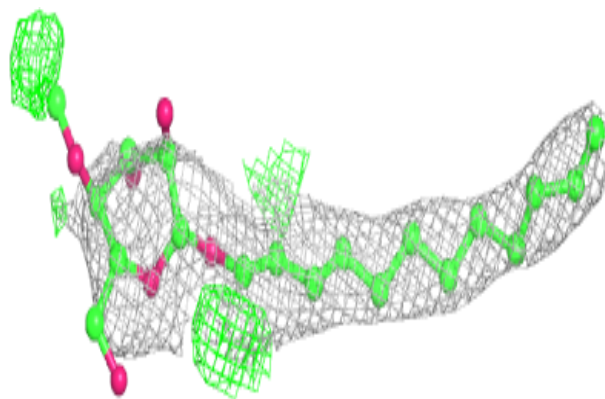
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

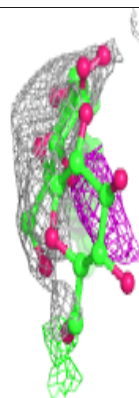
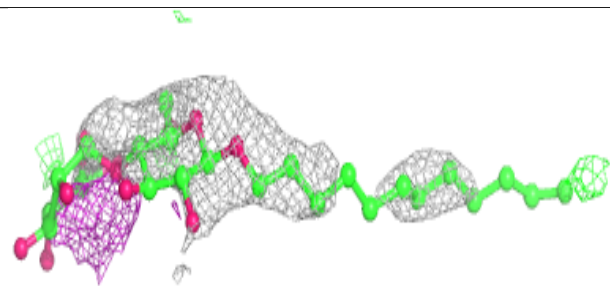
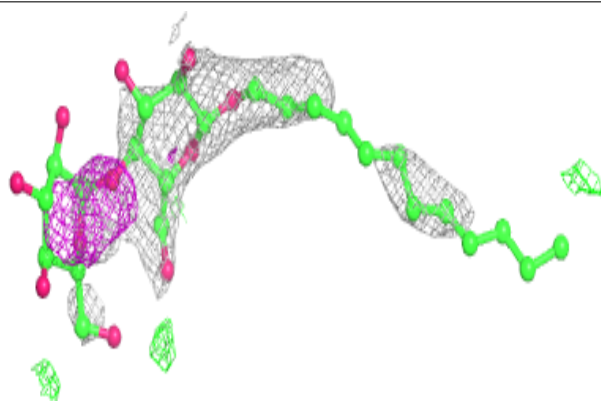


Electron density around LMT b 621:

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

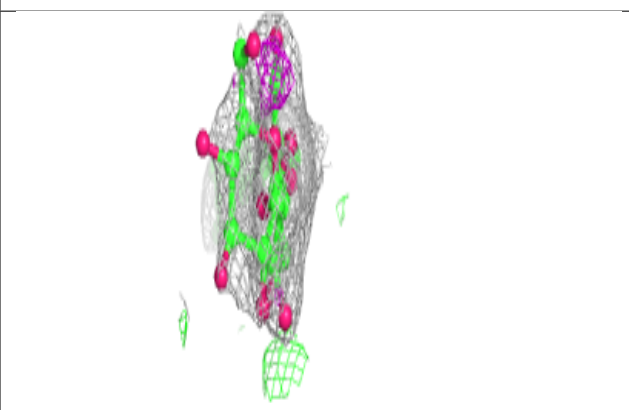
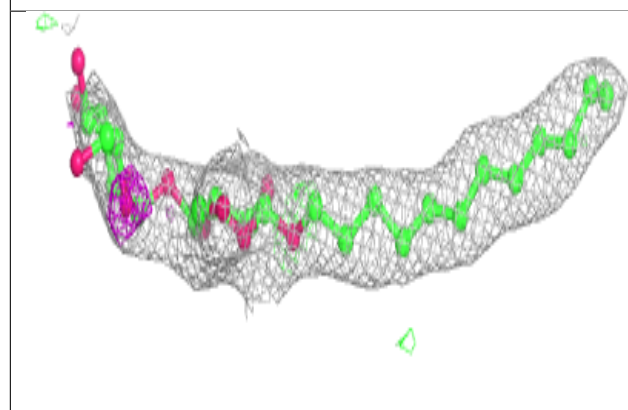
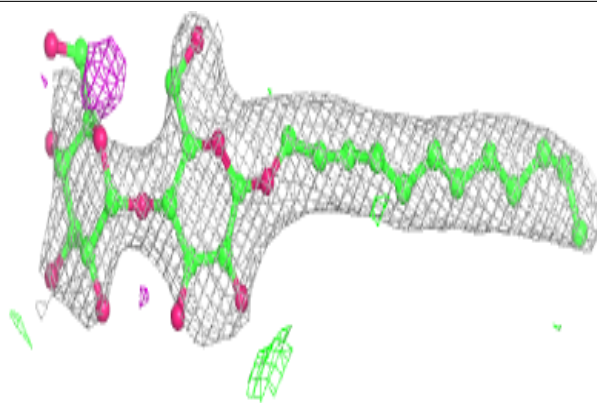
**Electron density around LMT F 101:**

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

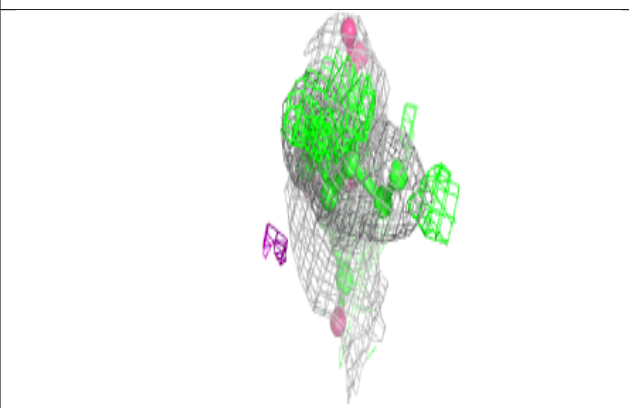
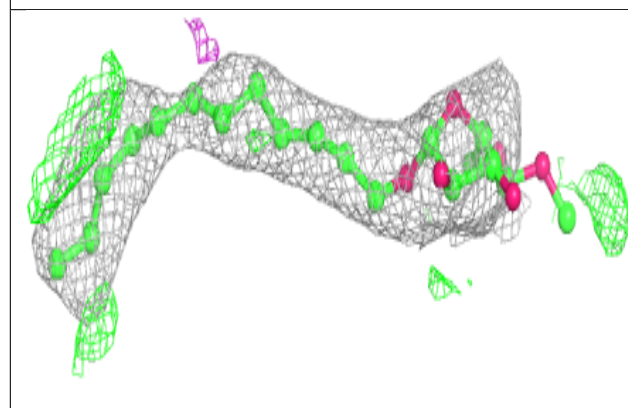
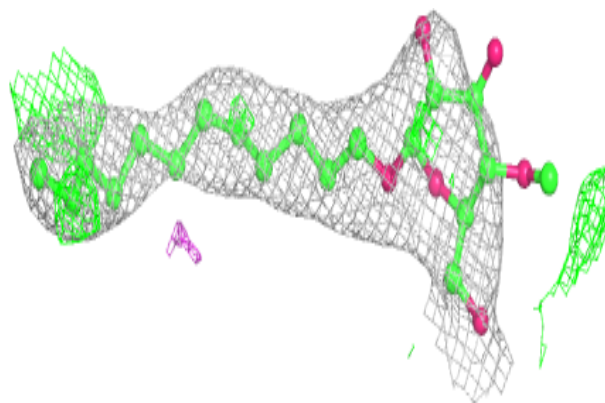


Electron density around LMT M 101:

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

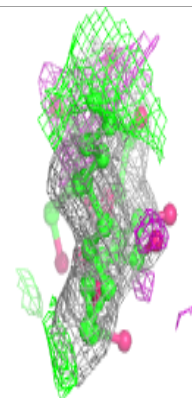
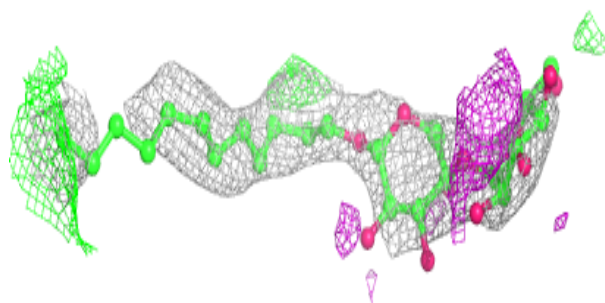
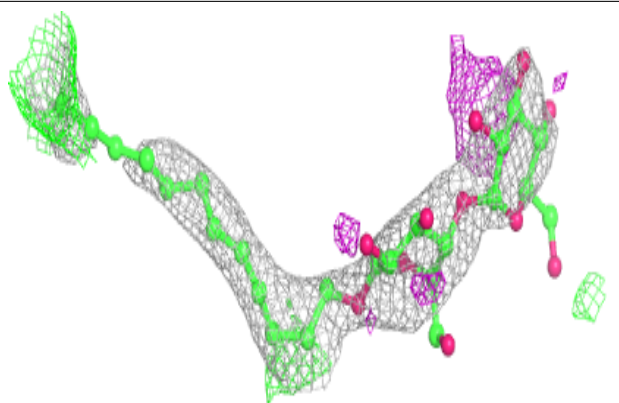
**Electron density around LMT B 631:**

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

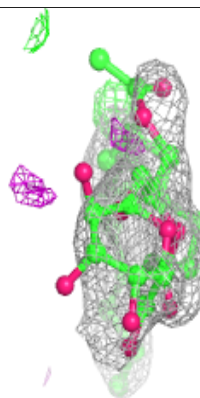
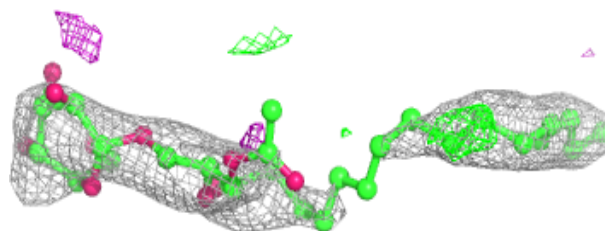
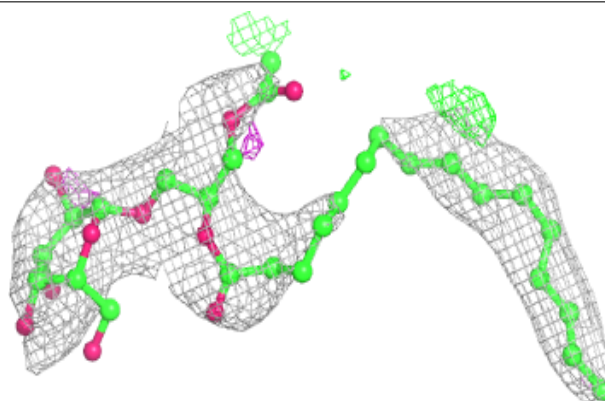


Electron density around LMT B 630:

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

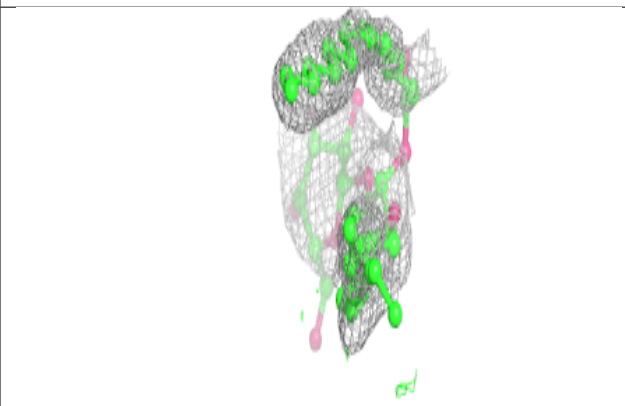
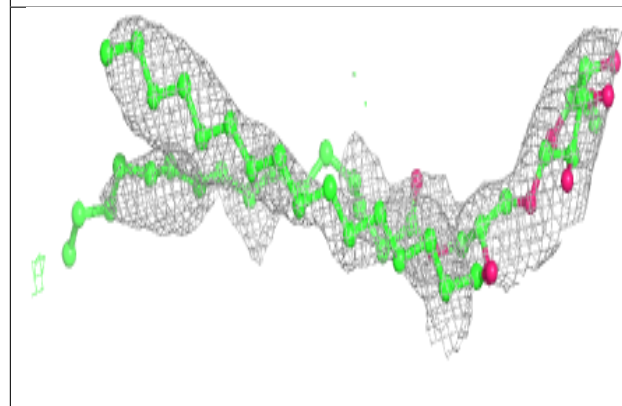
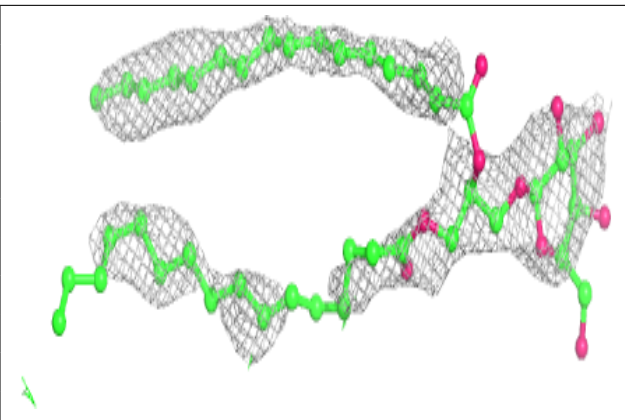
**Electron density around LMG Z 101:**

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

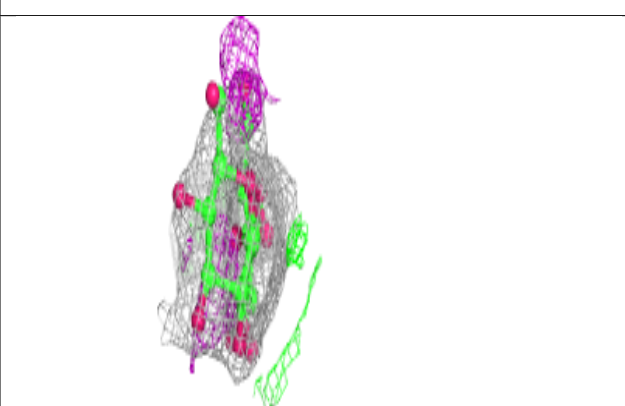
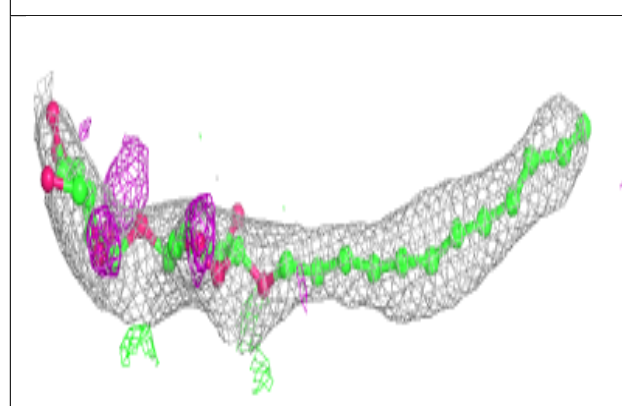
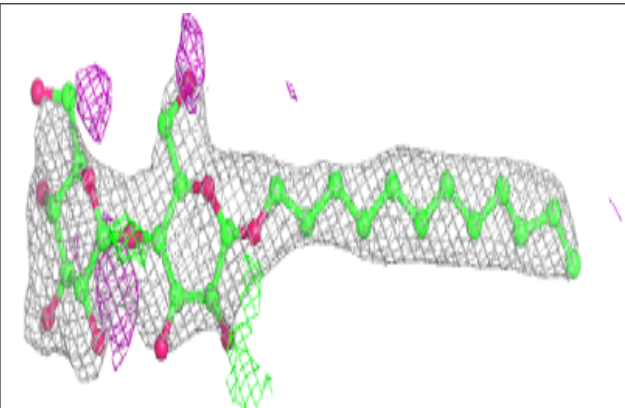


Electron density around LMG c 521:

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

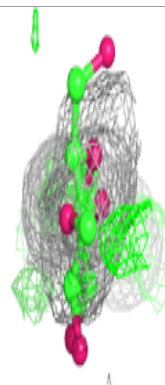
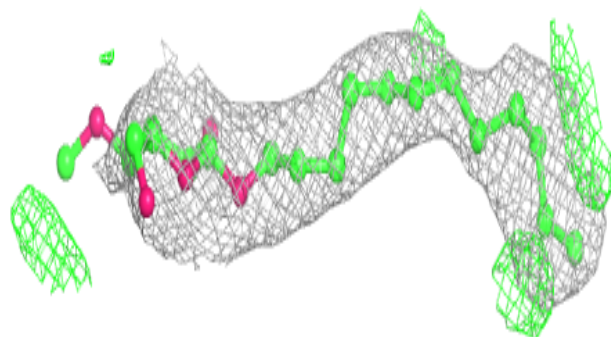
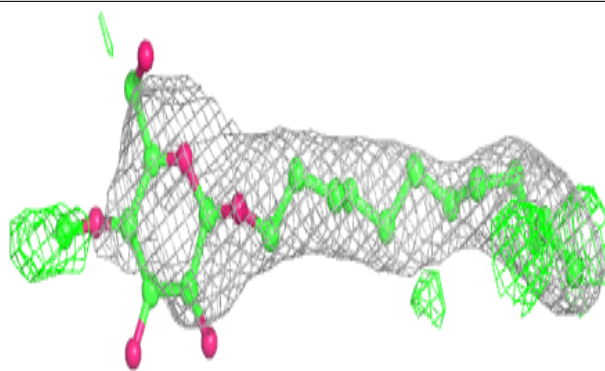
**Electron density around LMT m 103:**

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

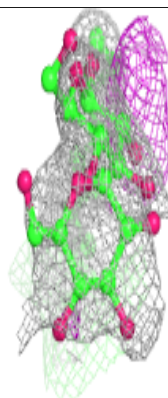
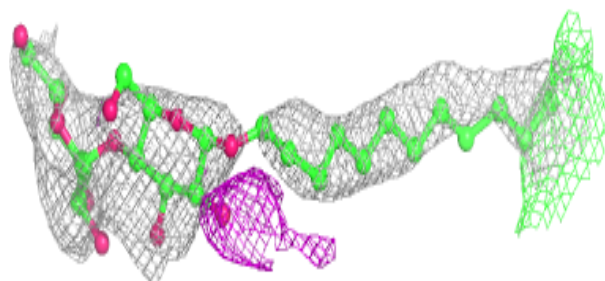
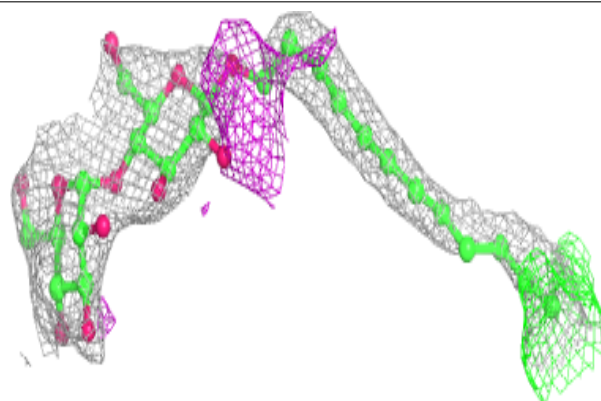


Electron density around LMT b 627:

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

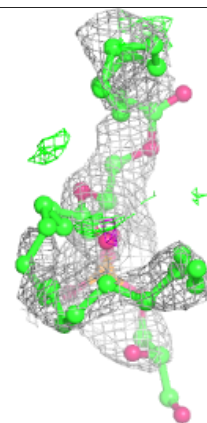
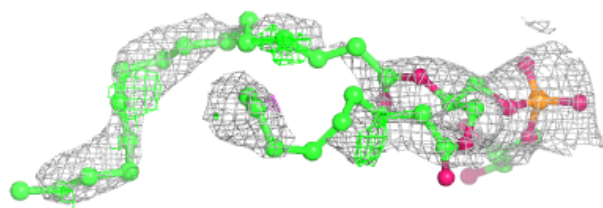
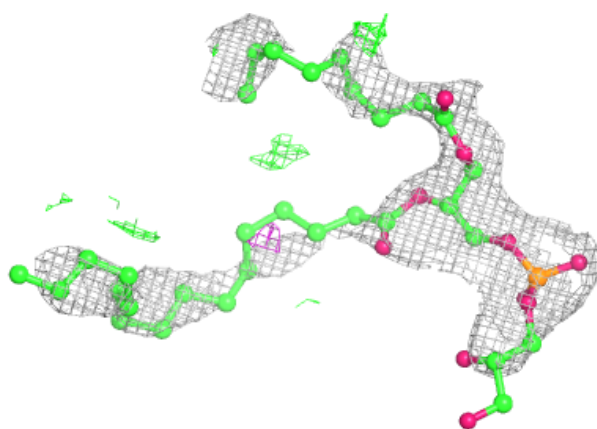
**Electron density around LMT A 417:**

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

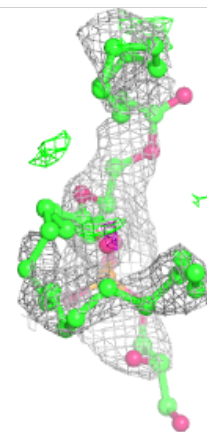
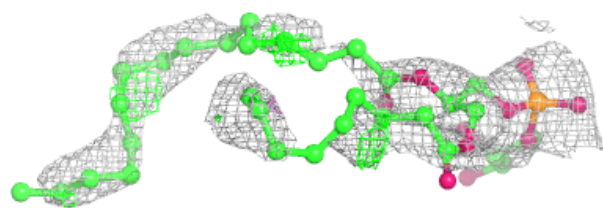
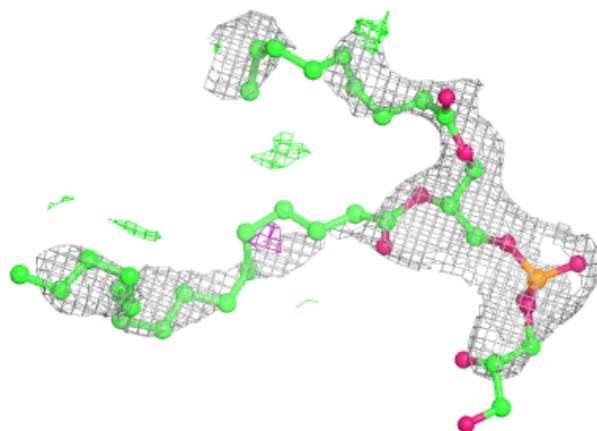


Electron density around LHG a 418 (A):

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

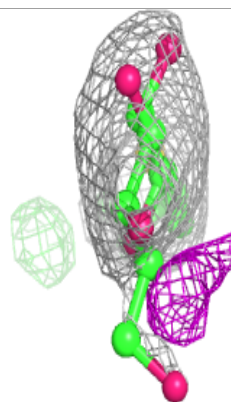
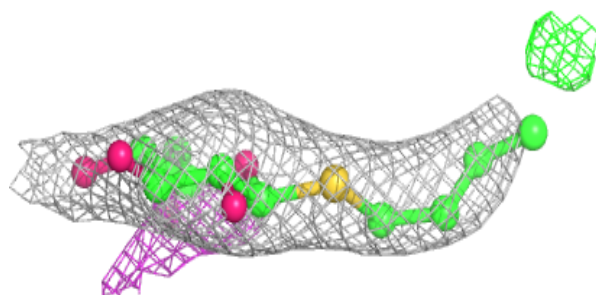
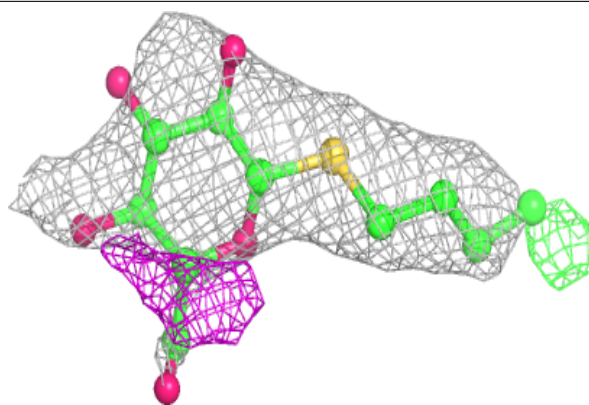
**Electron density around LHG a 418 (B):**

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

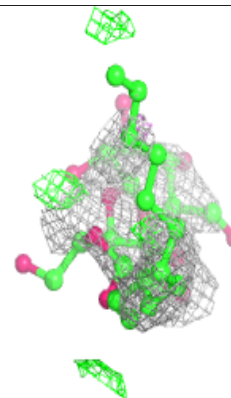
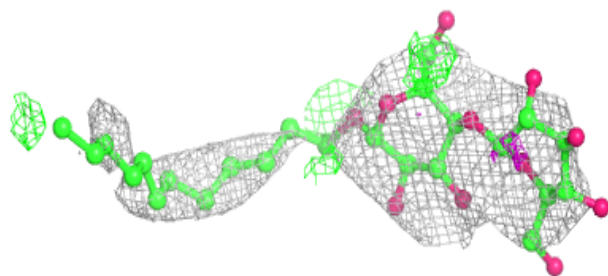
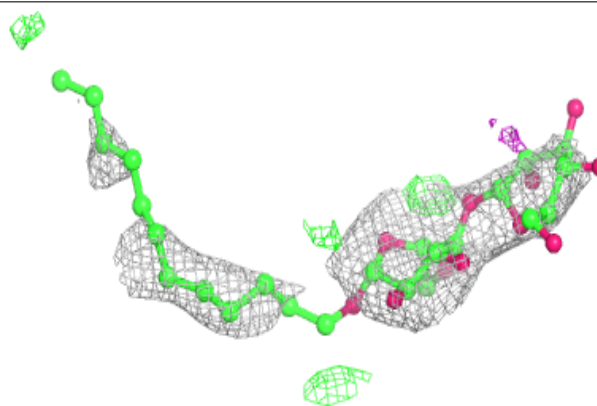


Electron density around HTG D 411:

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

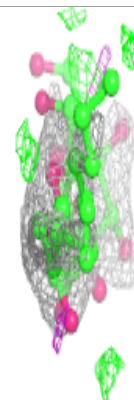
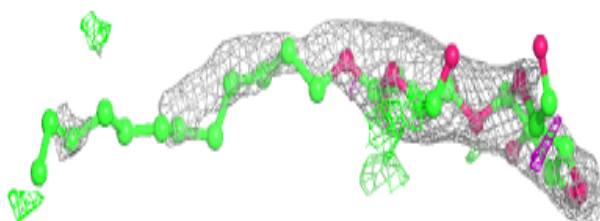
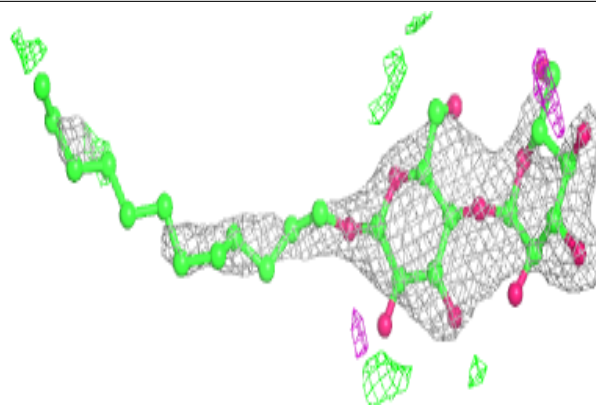
**Electron density around LMT A 420:**

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

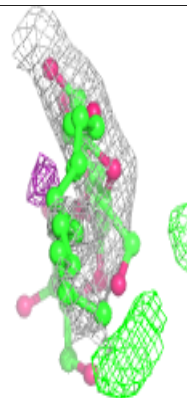
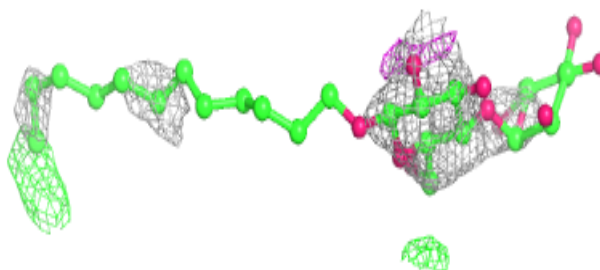
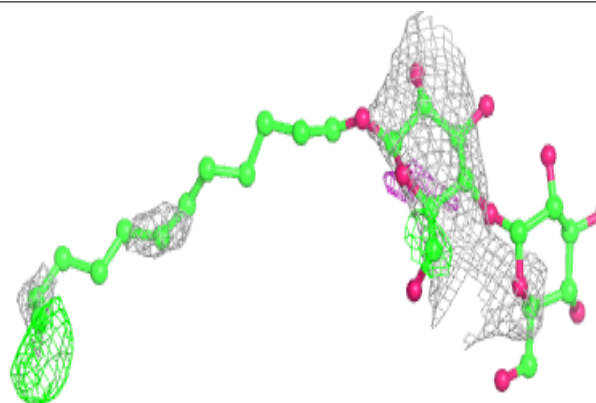


Electron density around LMT a 415:

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

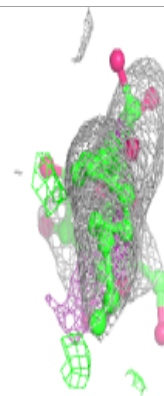
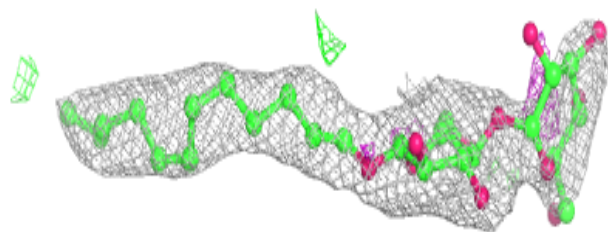
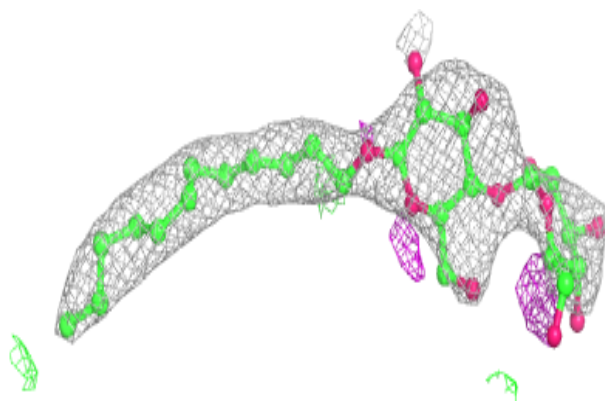
**Electron density around LMT e 101:**

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

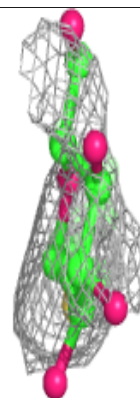
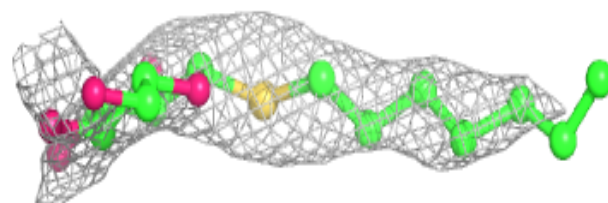
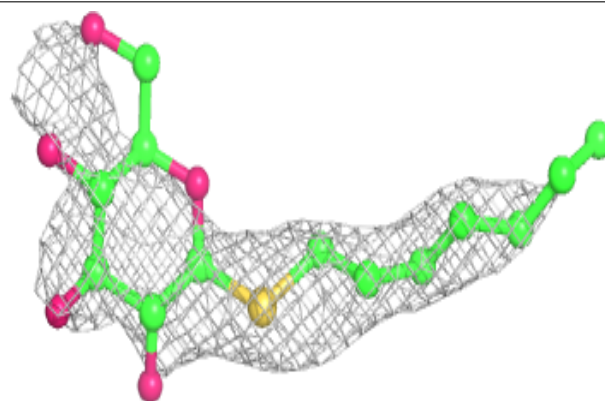


Electron density around LMT B 628:

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

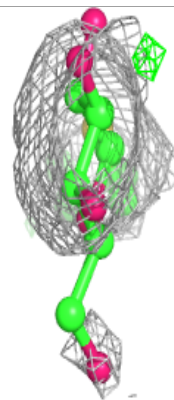
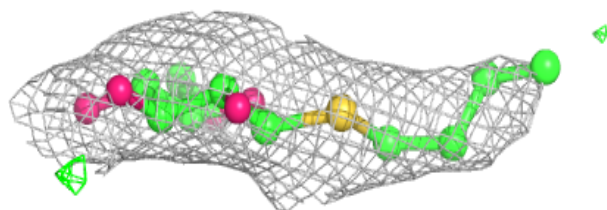
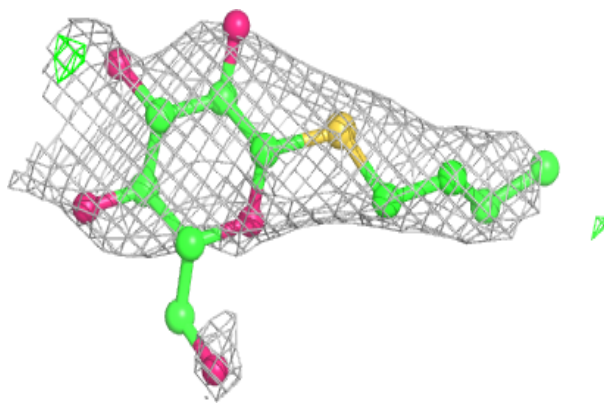
**Electron density around HTG b 623:**

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

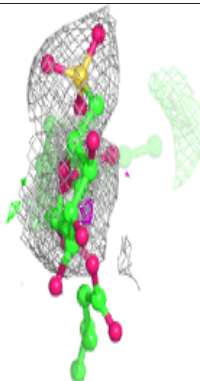
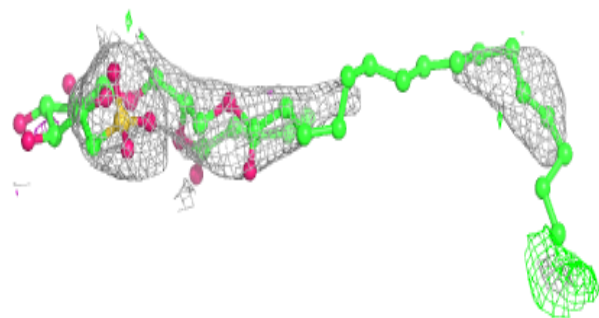
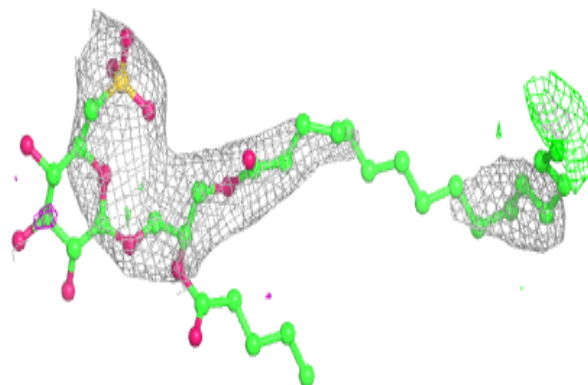


Electron density around HTG d 411:

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

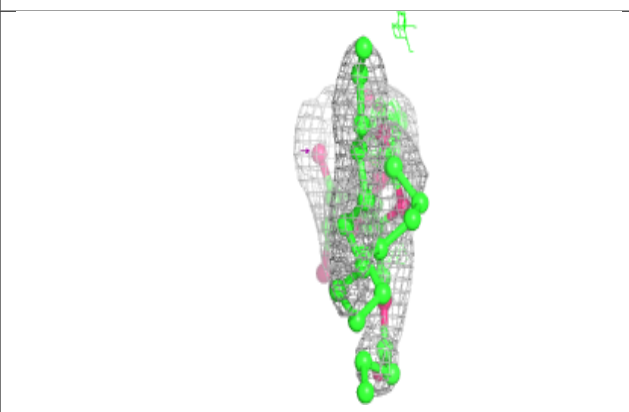
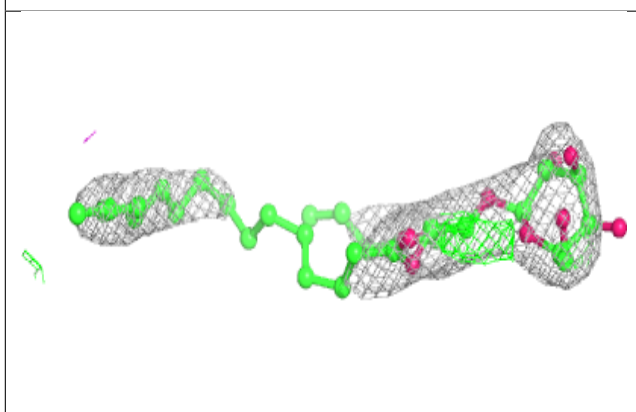
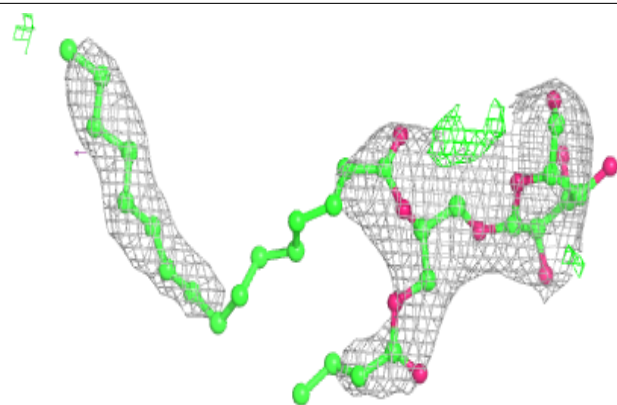
**Electron density around SQD f 102:**

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

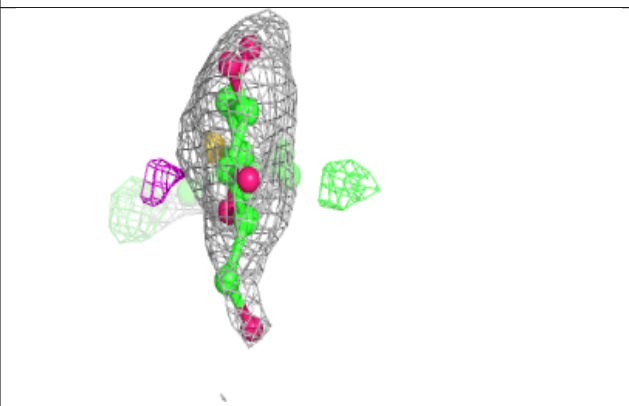
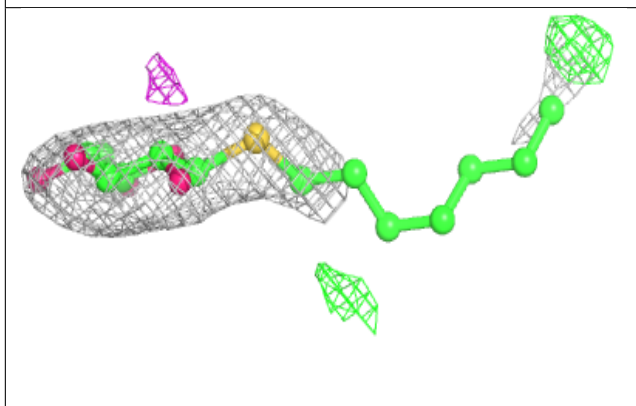
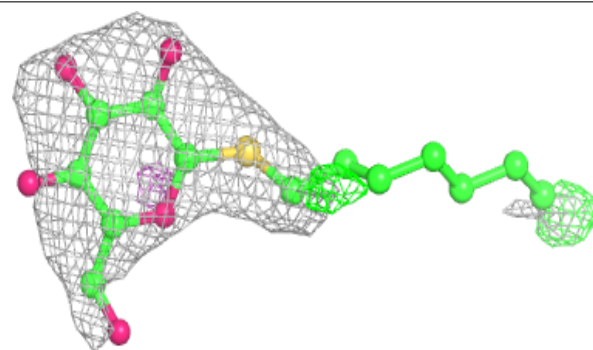


Electron density around LMG z 101:

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

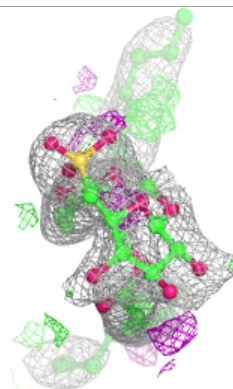
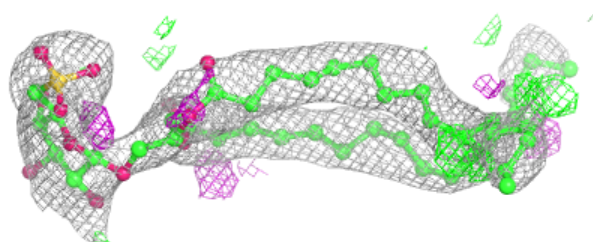
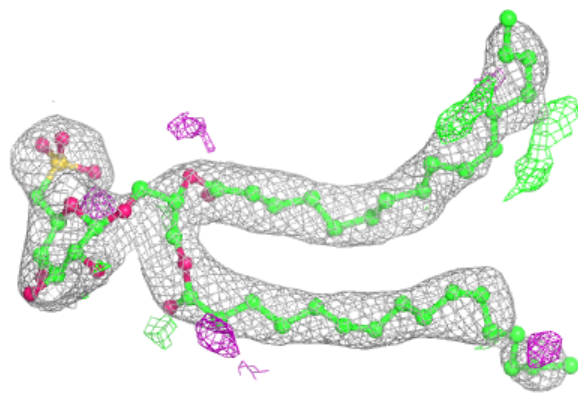
**Electron density around HTG C 521:**

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

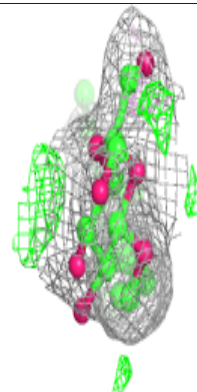
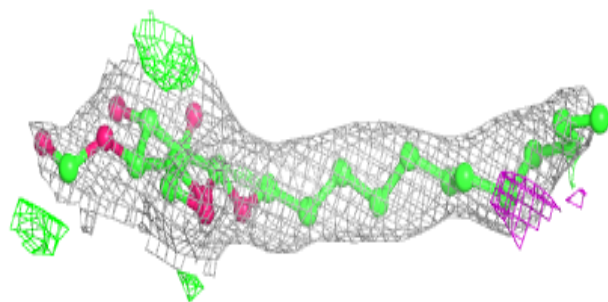
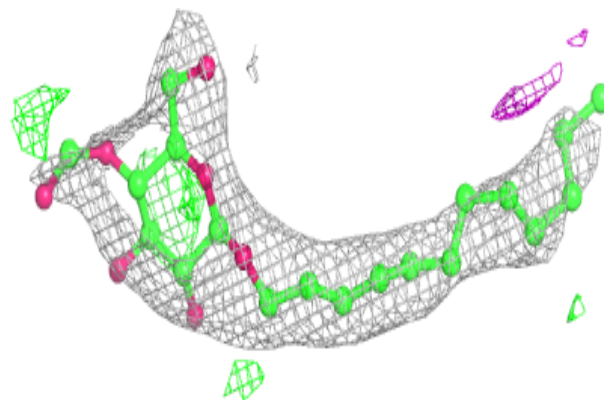


Electron density around SQD b 620:

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

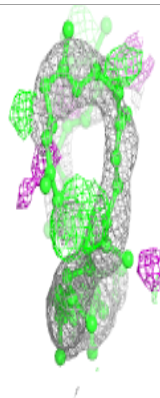
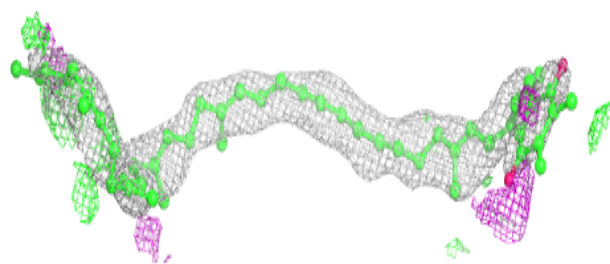
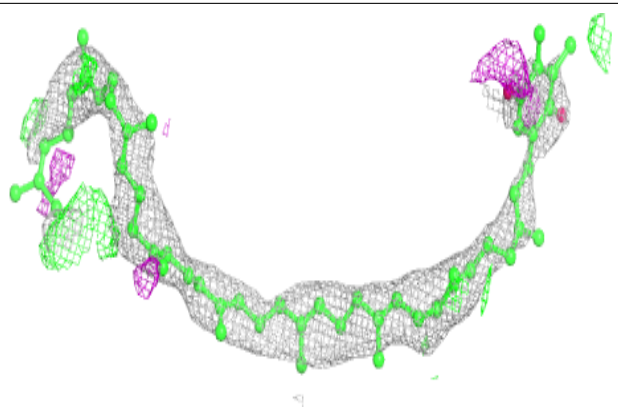
**Electron density around LMT t 101:**

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

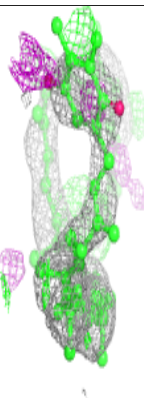
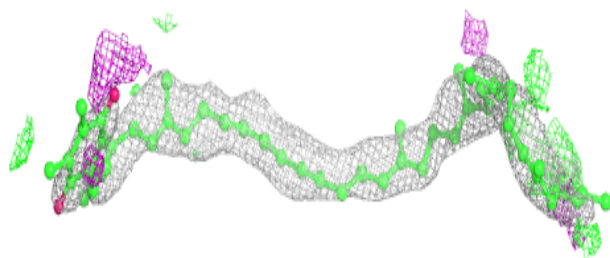
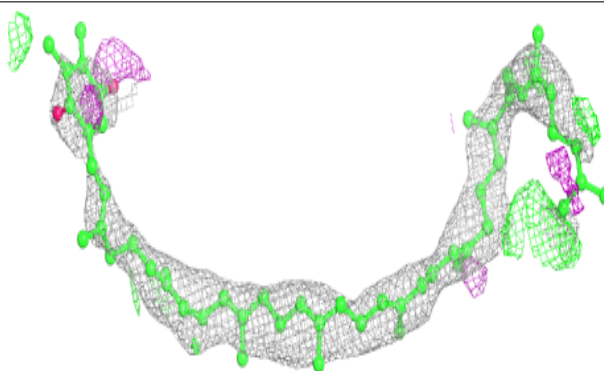


Electron density around PL9 A 414 (A):

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

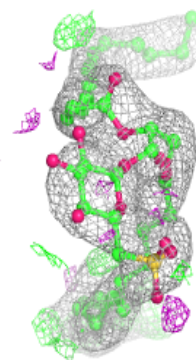
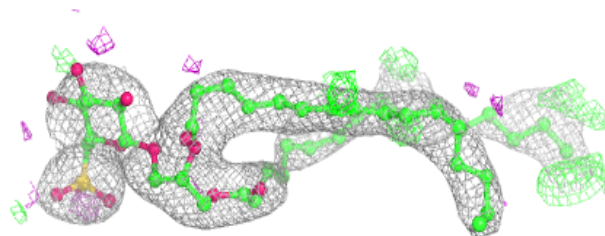
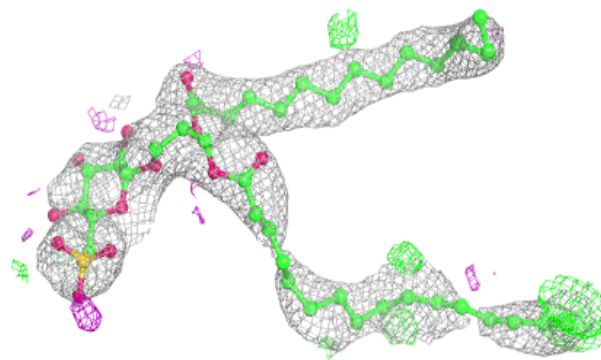
**Electron density around PL9 A 414 (B):**

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

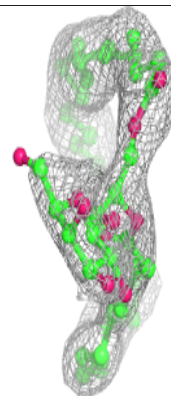
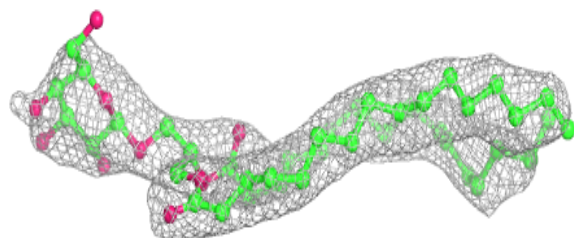
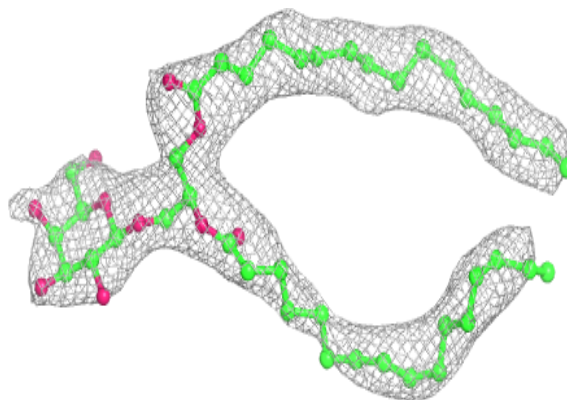


Electron density around SQD A 412:

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

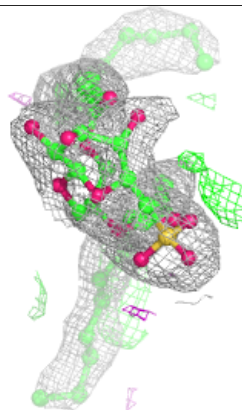
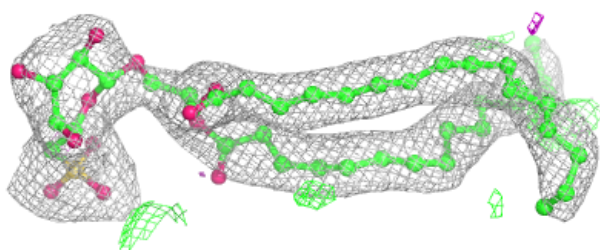
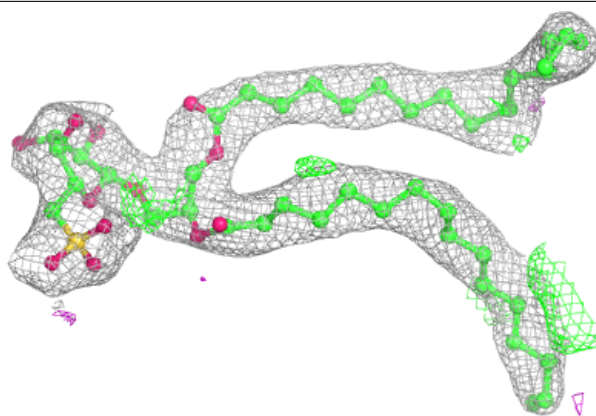
**Electron density around LMG c 501:**

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

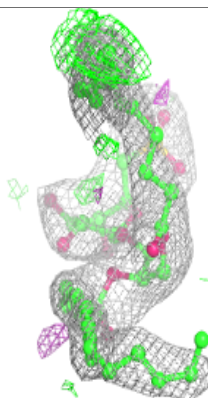
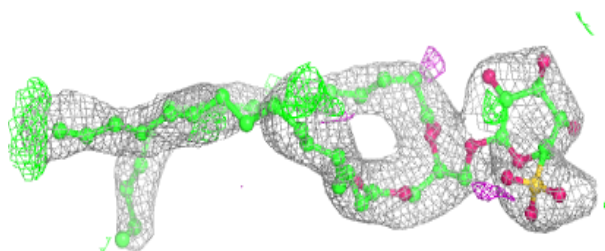
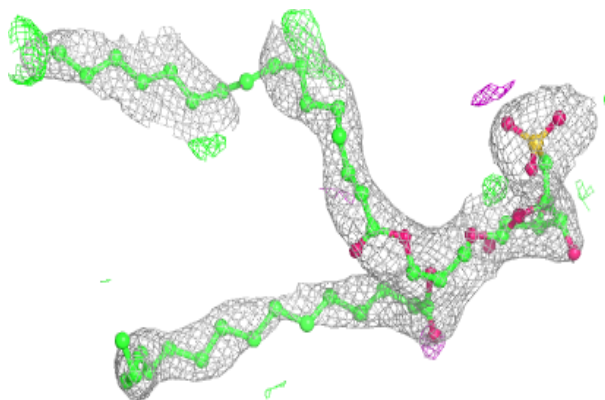


Electron density around SQD B 620:

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

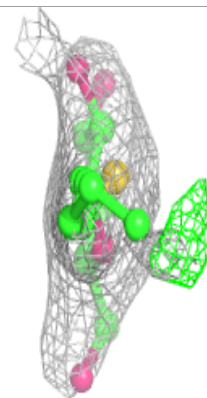
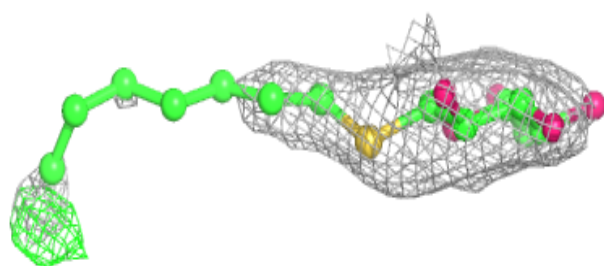
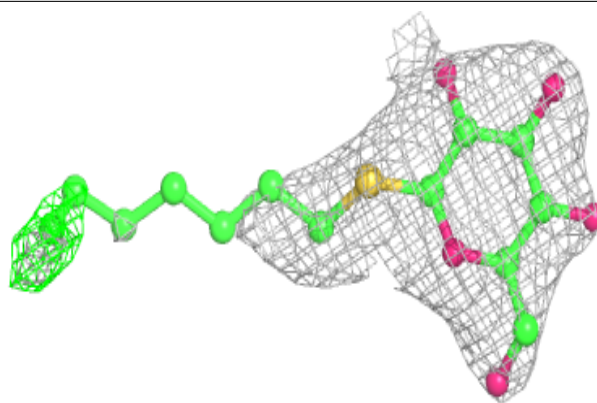
**Electron density around SQD a 410:**

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

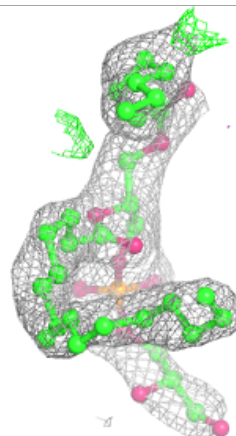
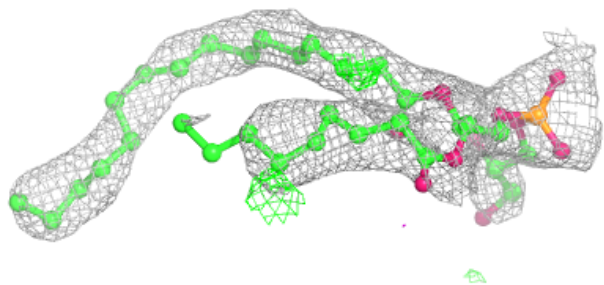
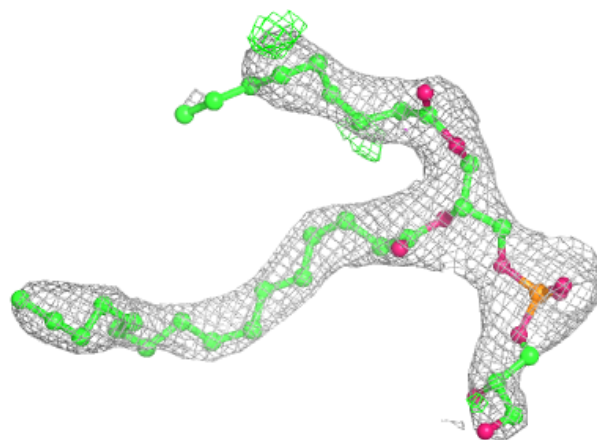


Electron density around HTG c 522:

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

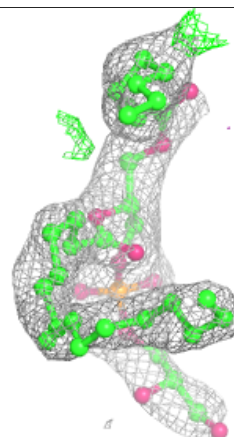
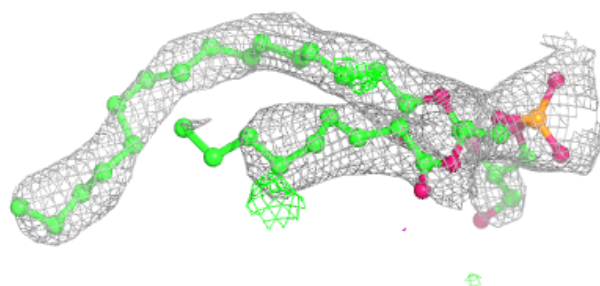
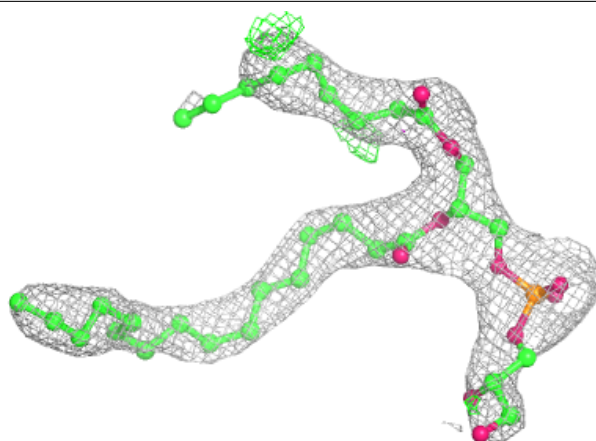
**Electron density around LHG E 101 (A):**

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

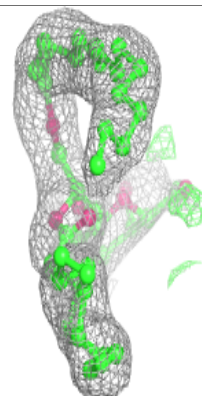
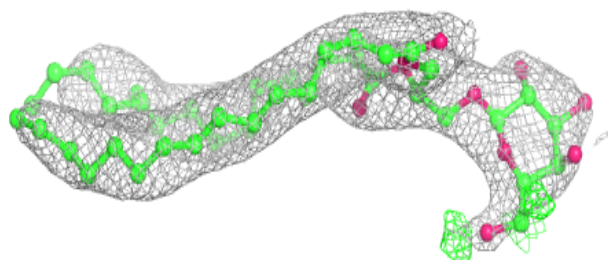
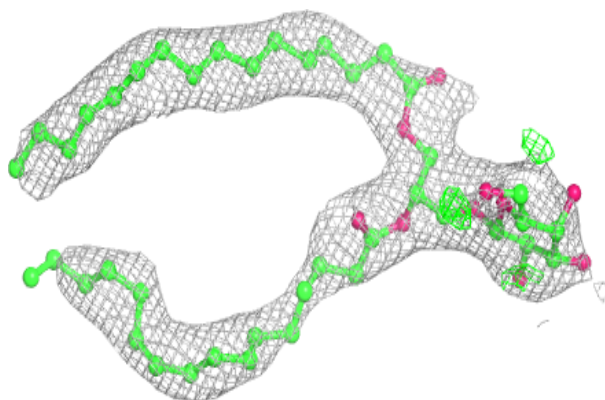


Electron density around LHG E 101 (B):

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

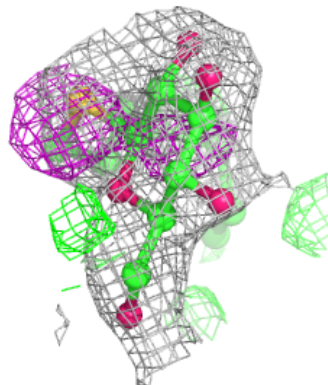
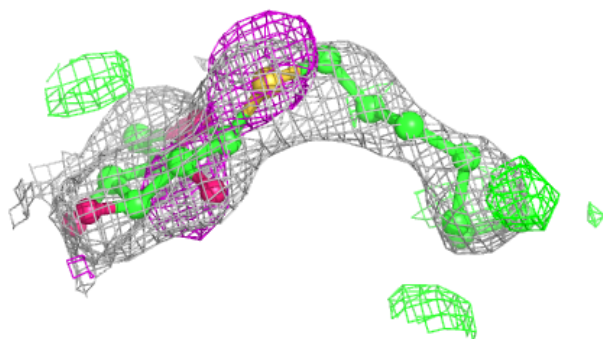
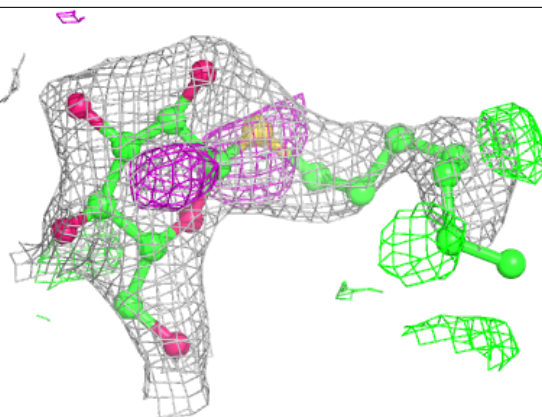
**Electron density around LMG A 418:**

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

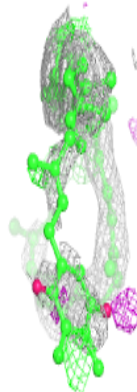
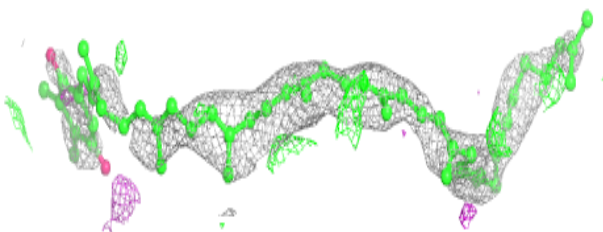
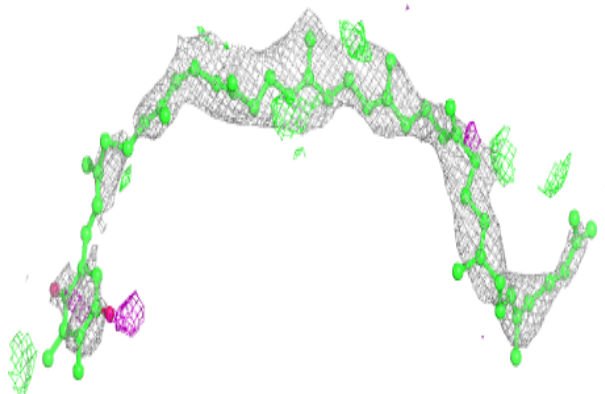


Electron density around HTG B 623:

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

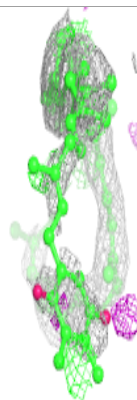
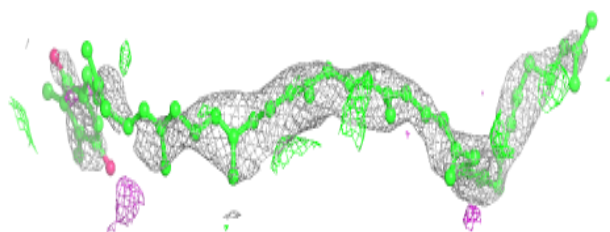
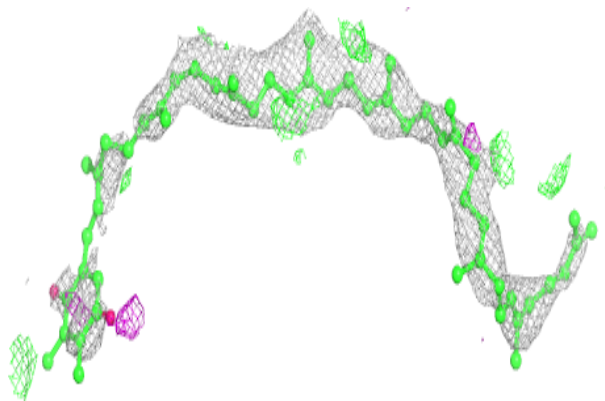
**Electron density around PL9 a 412 (A):**

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

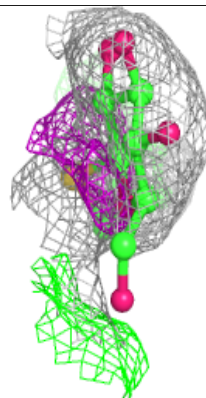
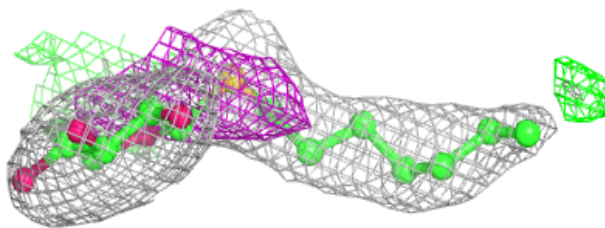
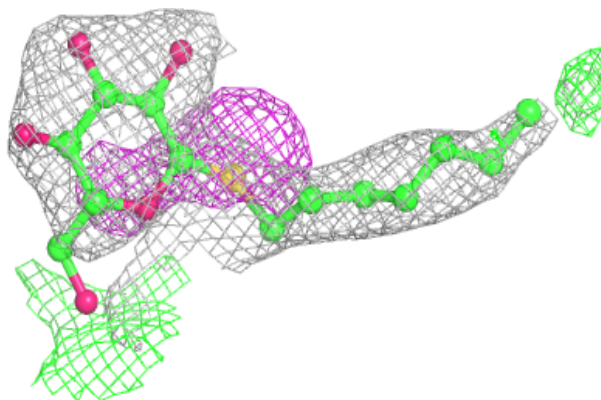


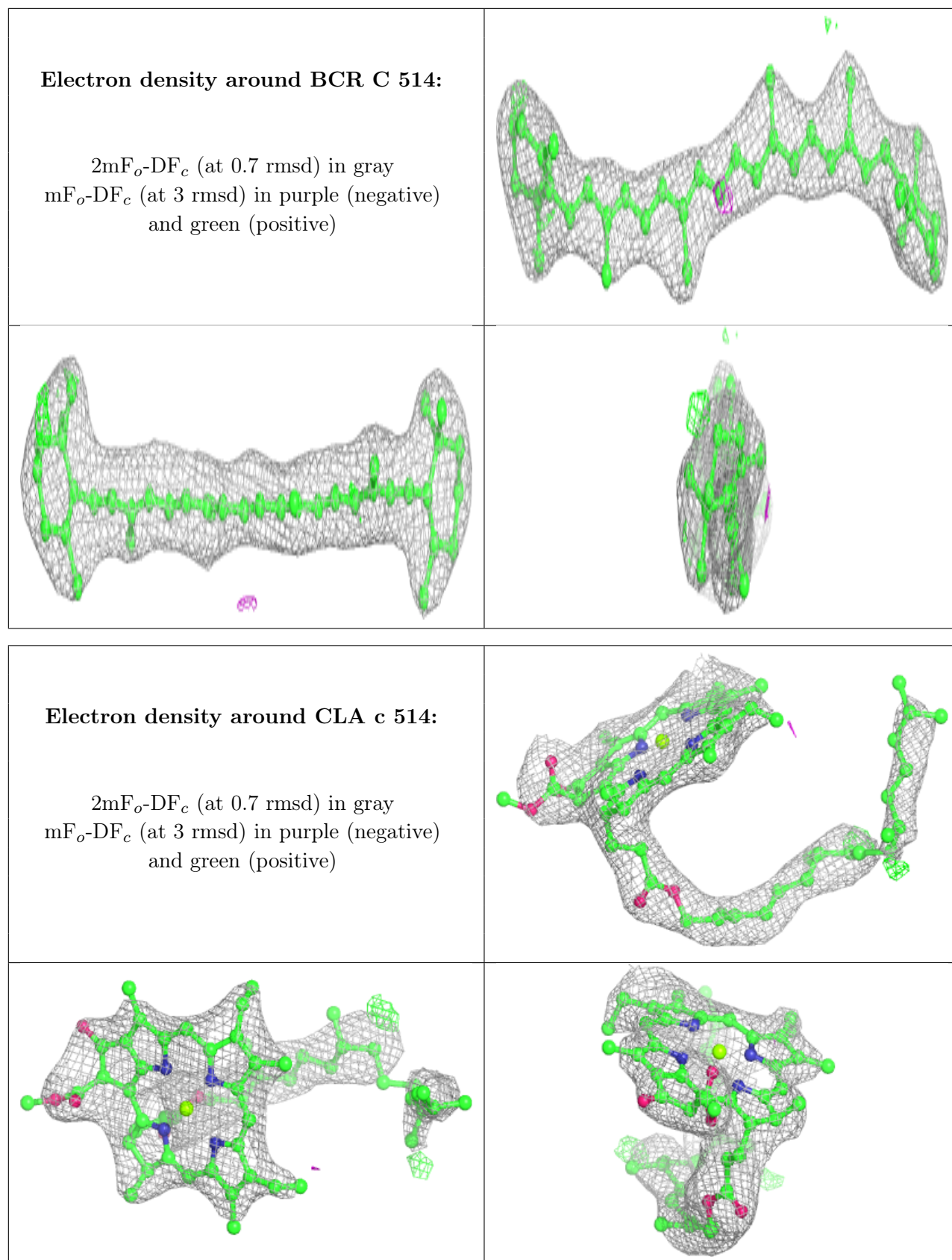
Electron density around PL9 a 412 (B):

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

**Electron density around HTG b 622:**

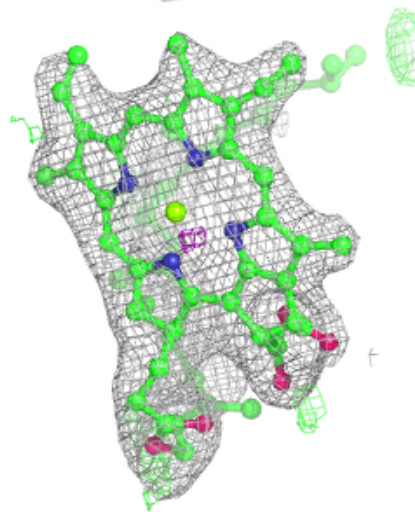
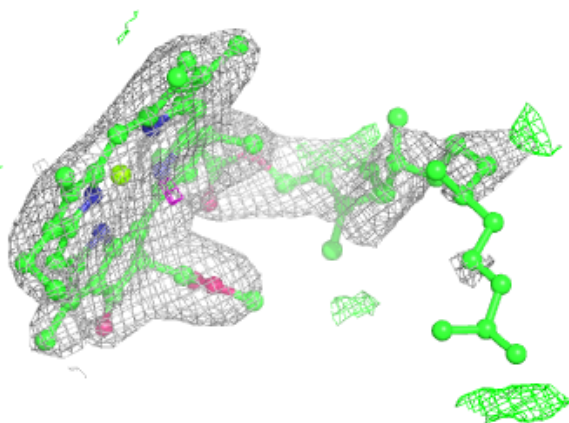
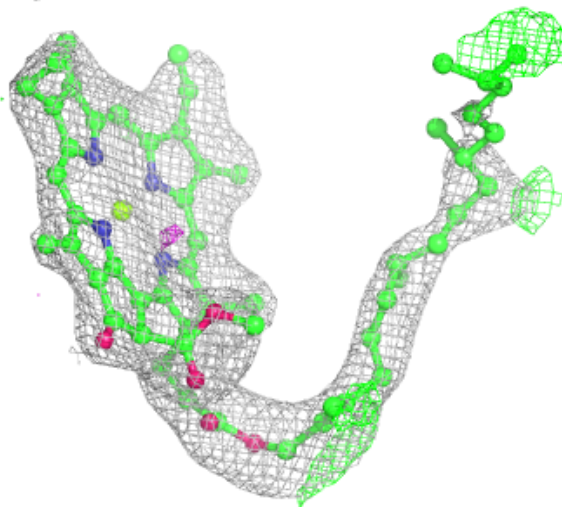
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





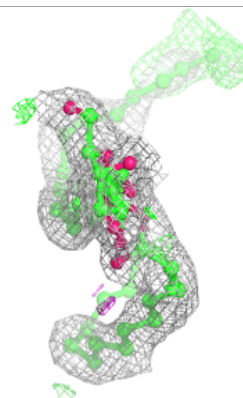
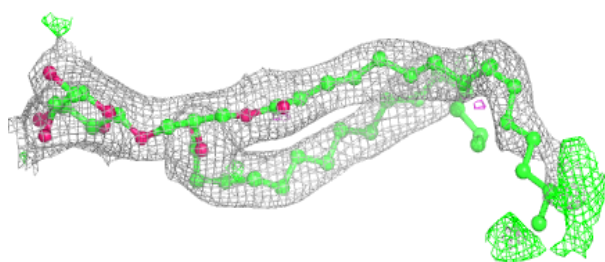
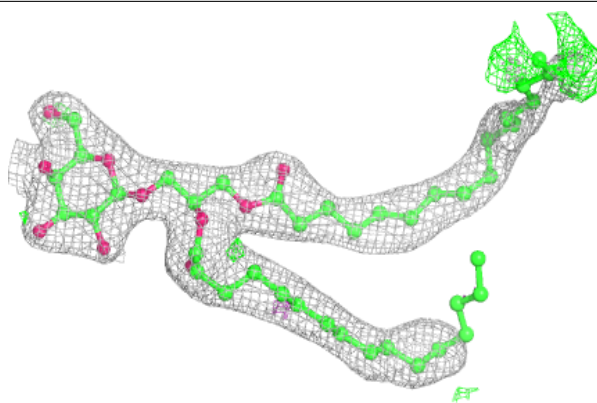
Electron density around CLA b 616:

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

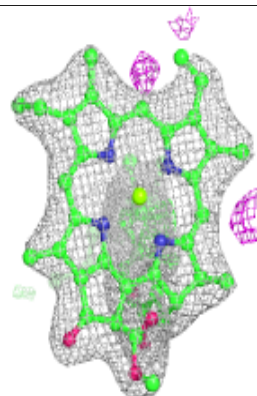
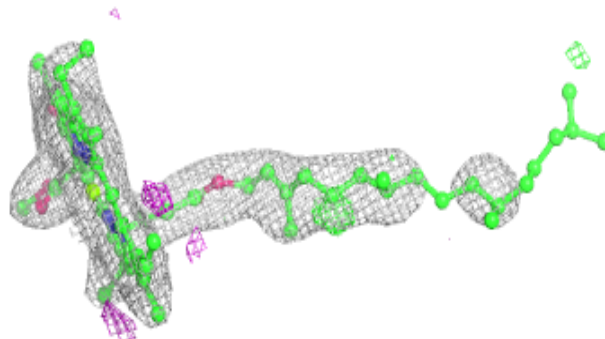
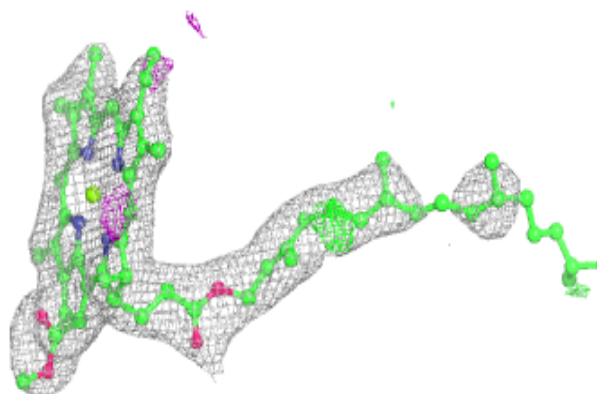


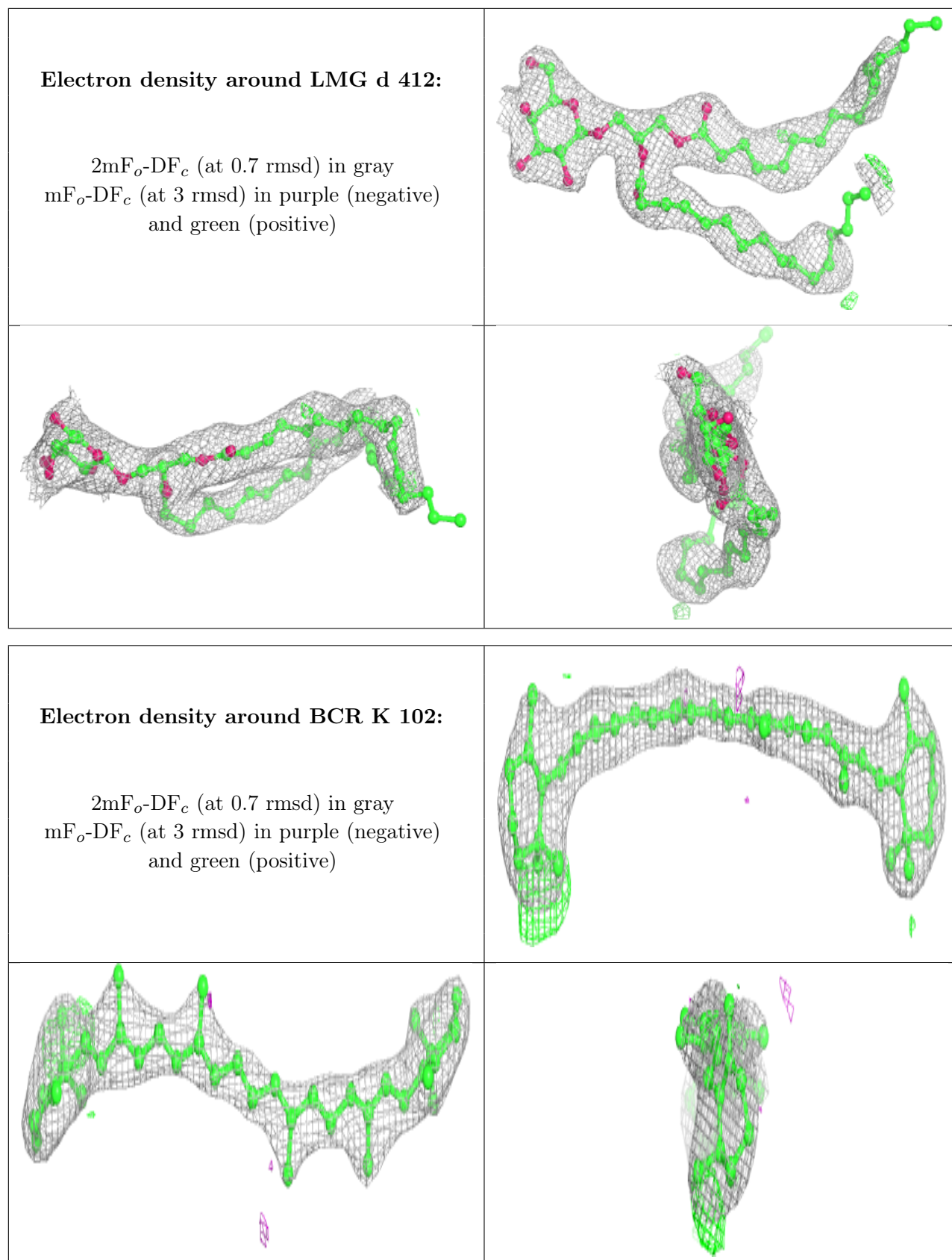
Electron density around LMG D 412:

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

**Electron density around CLA d 404:**

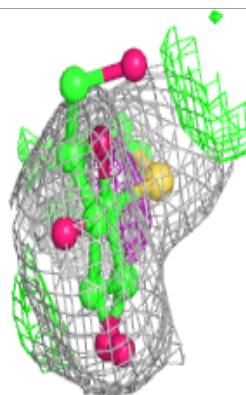
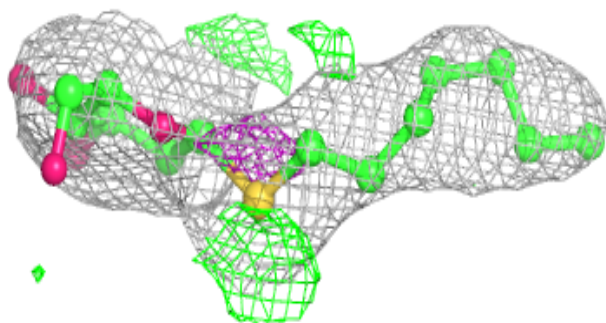
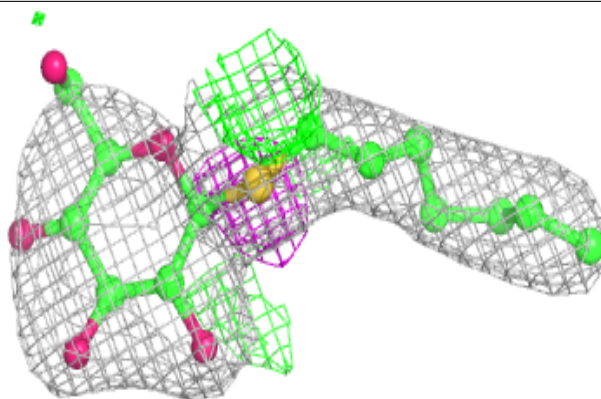
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



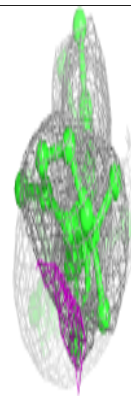
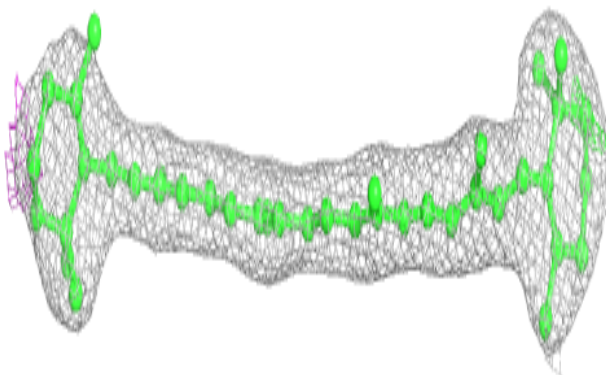
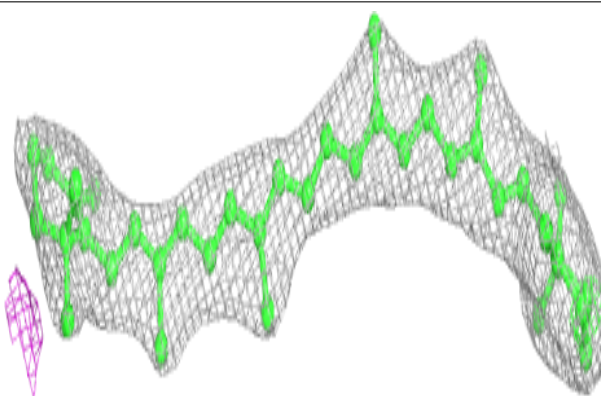


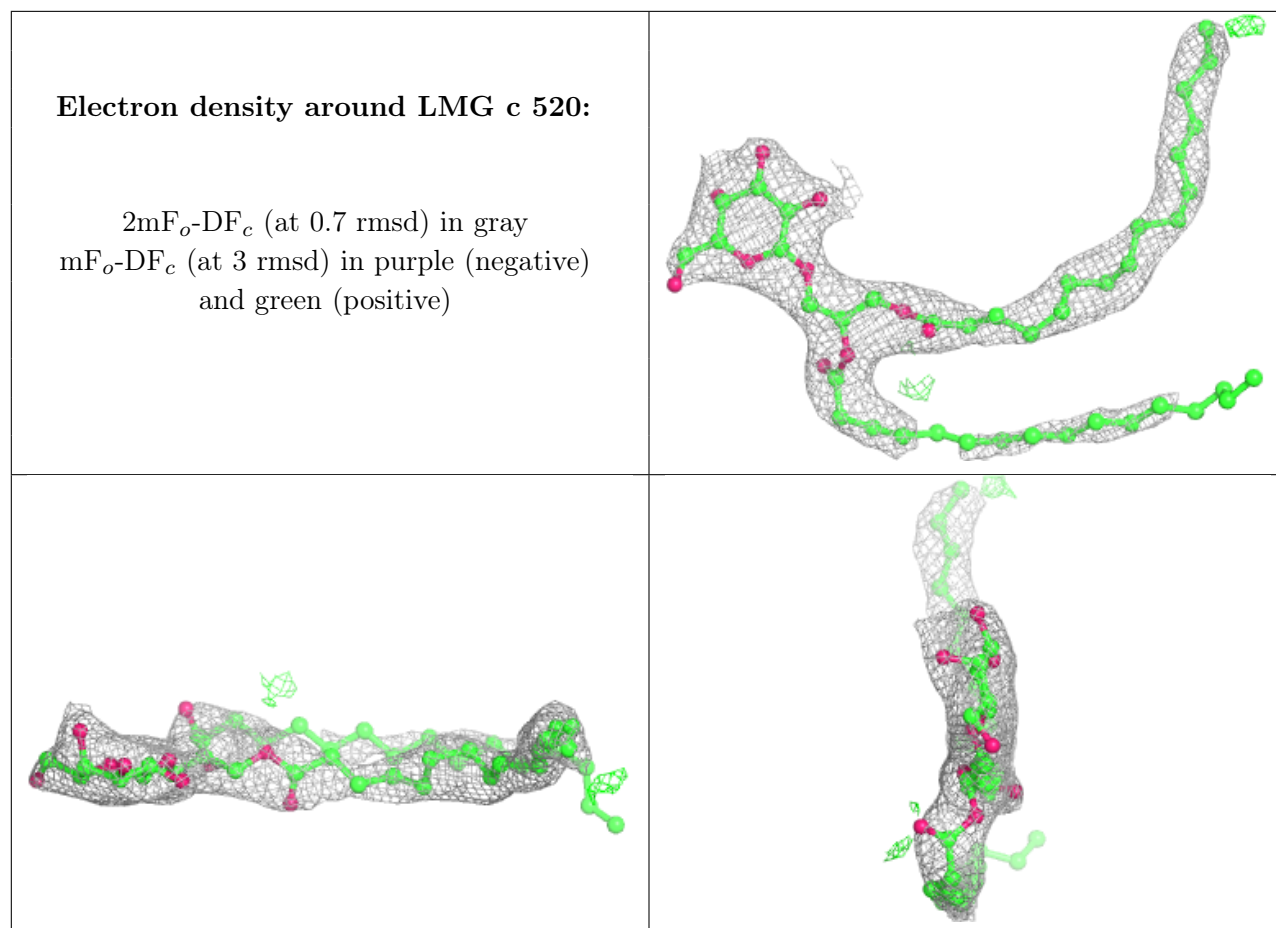
Electron density around HTG B 622:

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

**Electron density around BCR h 101:**

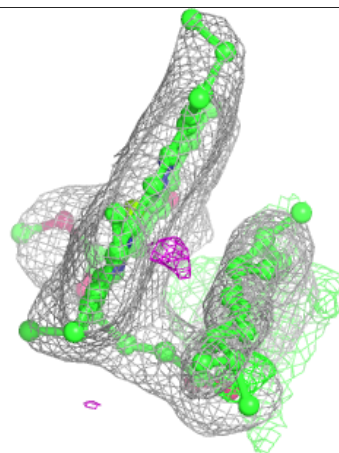
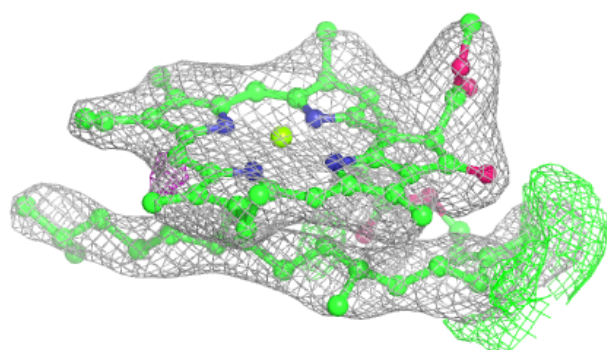
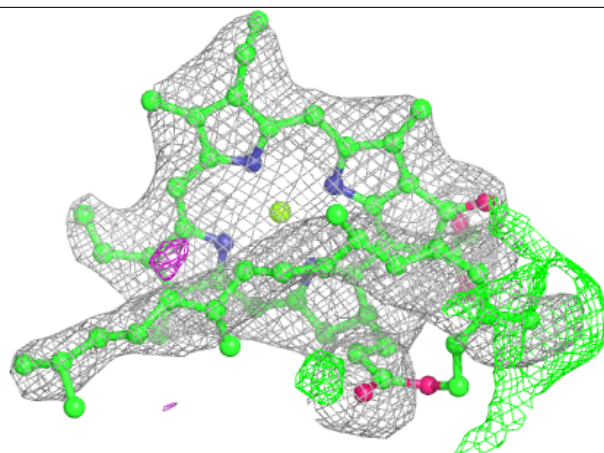
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



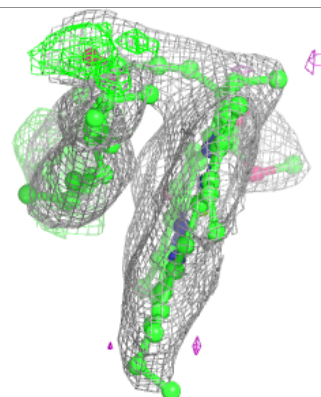
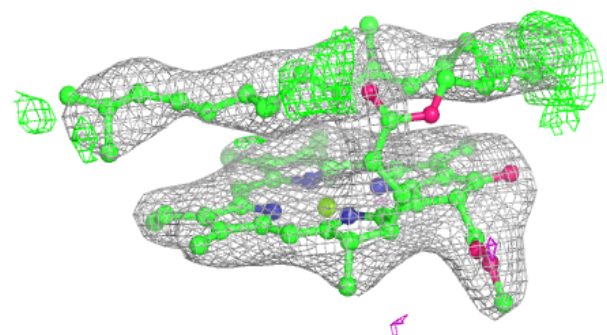
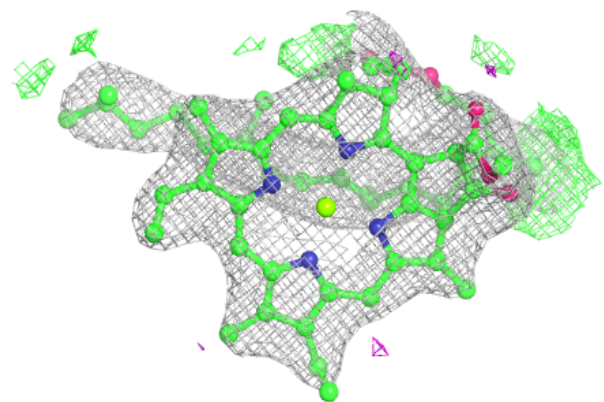


Electron density around CLA b 601:

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

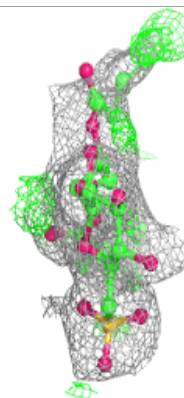
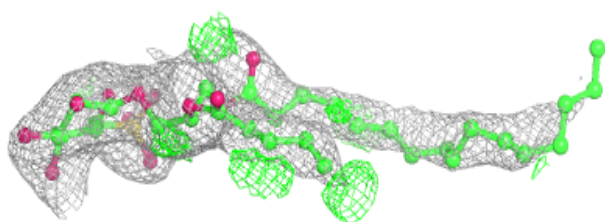
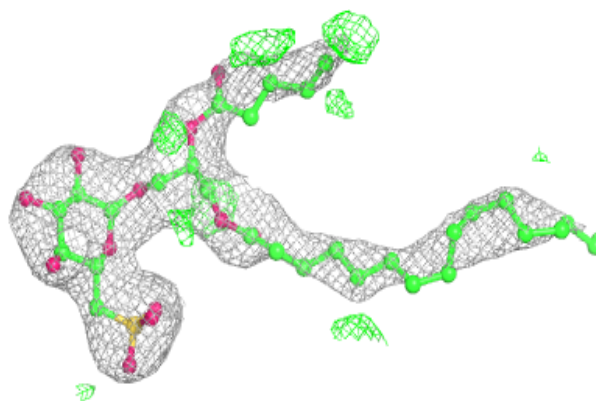
**Electron density around CLA B 601:**

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

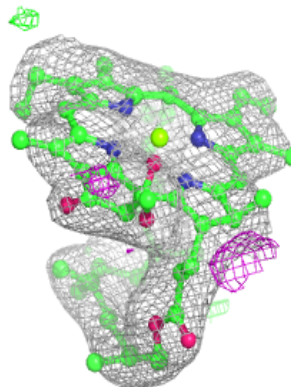
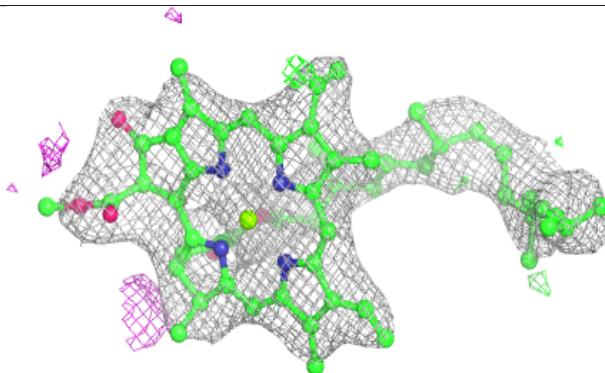
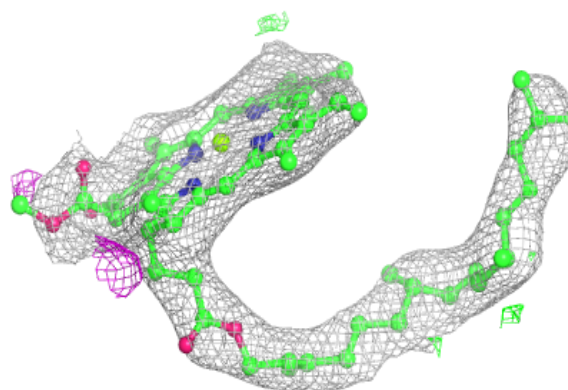


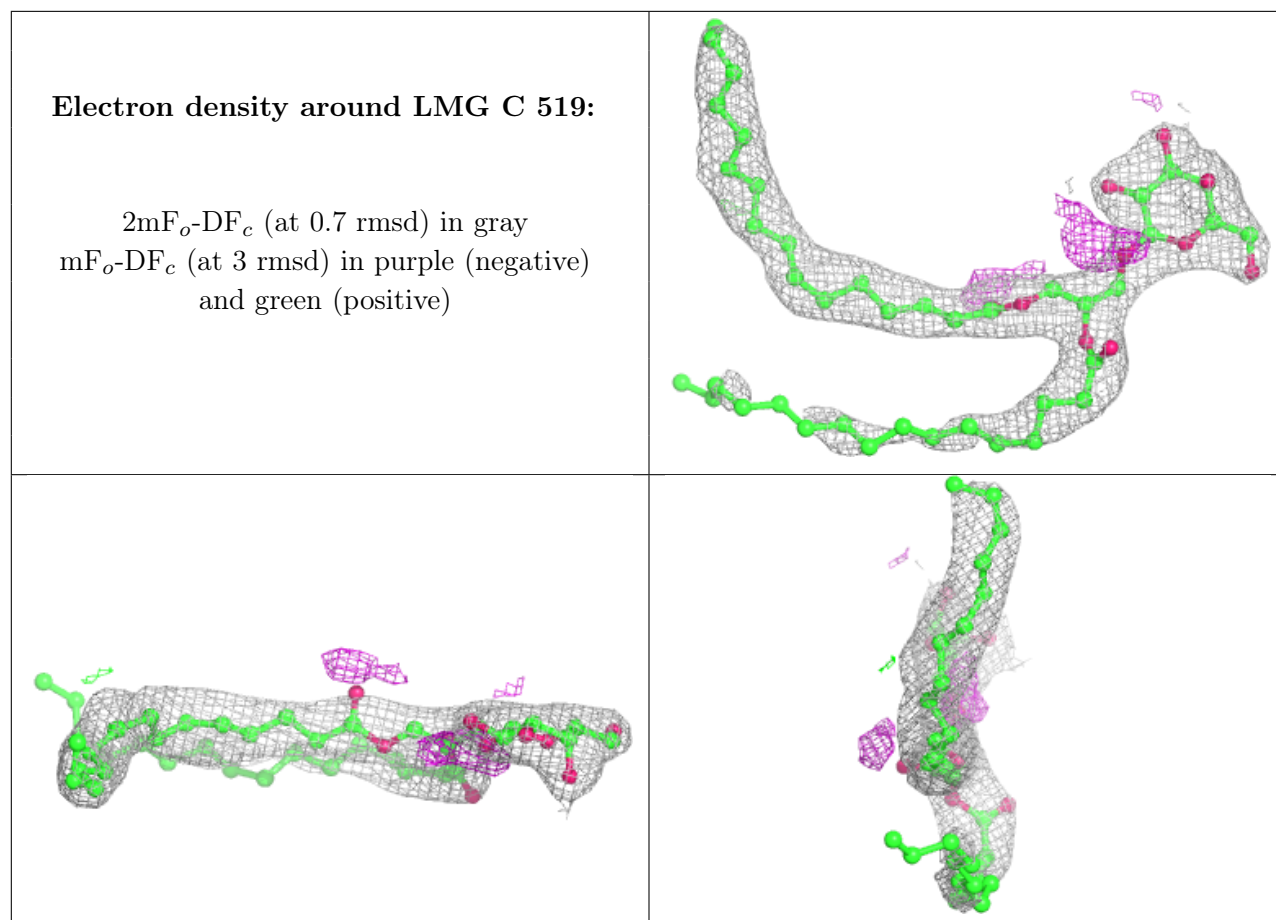
Electron density around SQD F 103:

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

**Electron density around CLA C 513:**

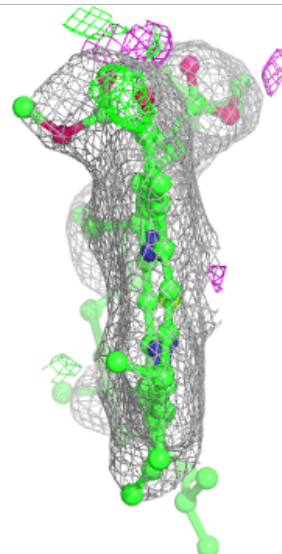
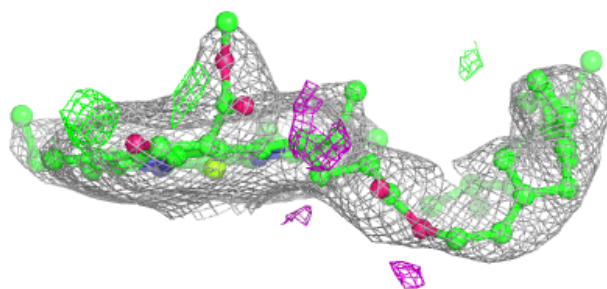
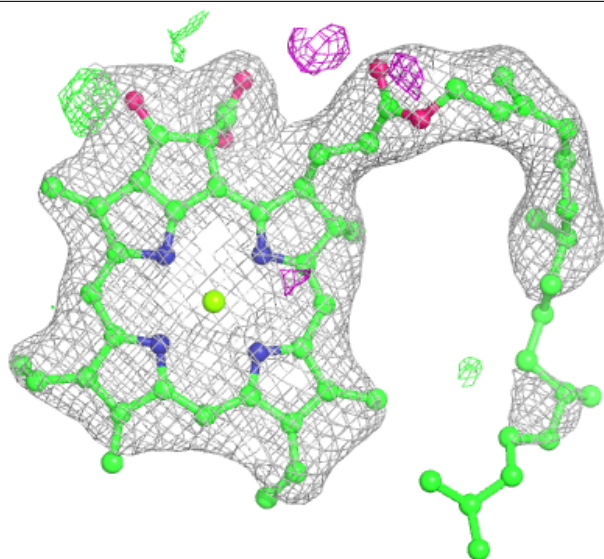
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

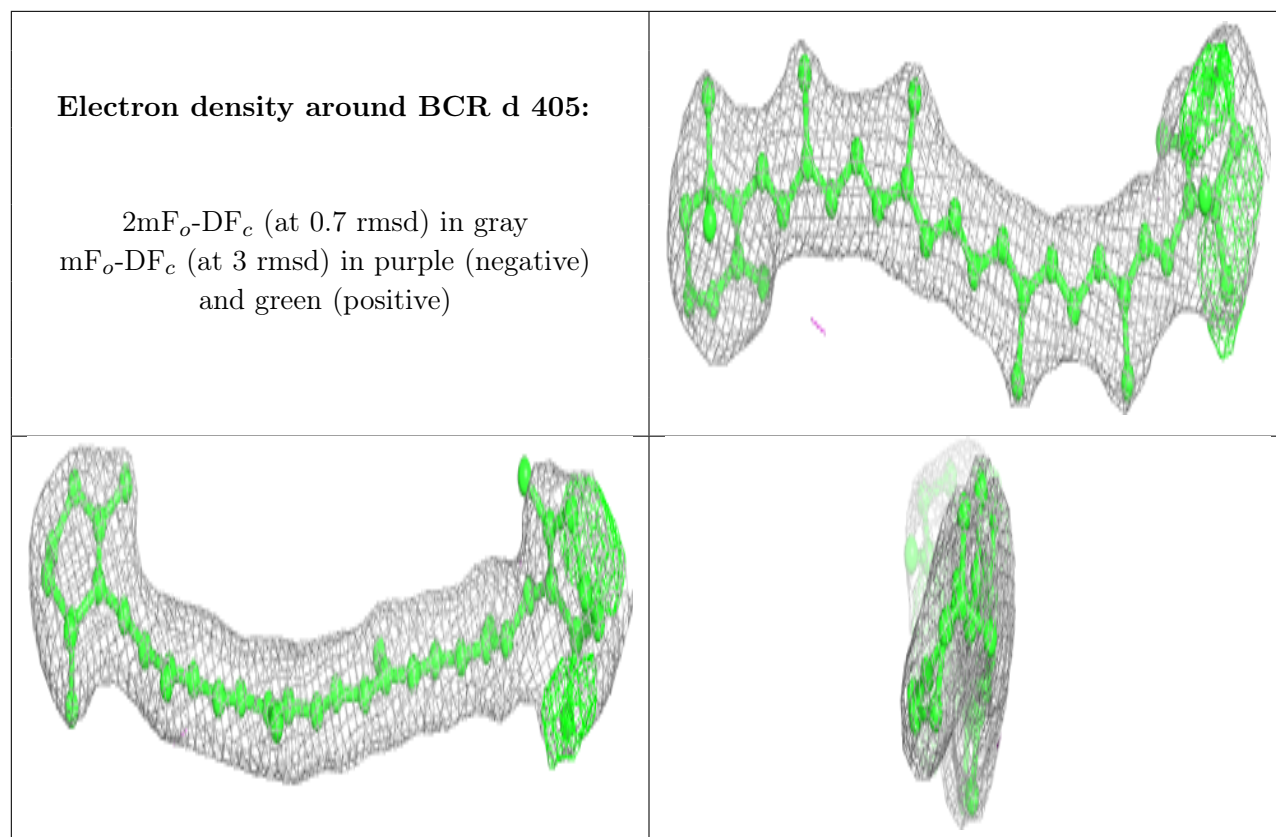




Electron density around CLA c 513:

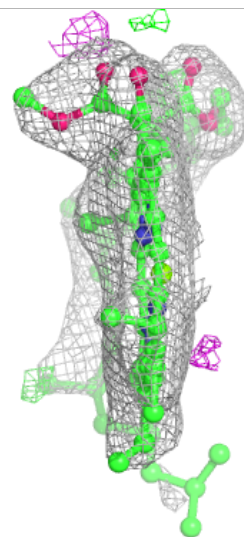
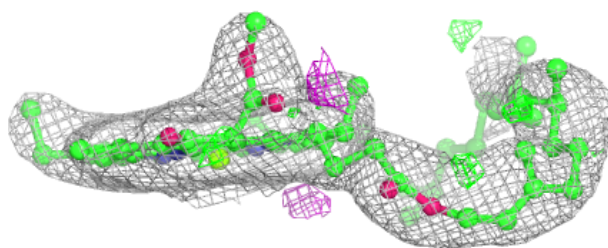
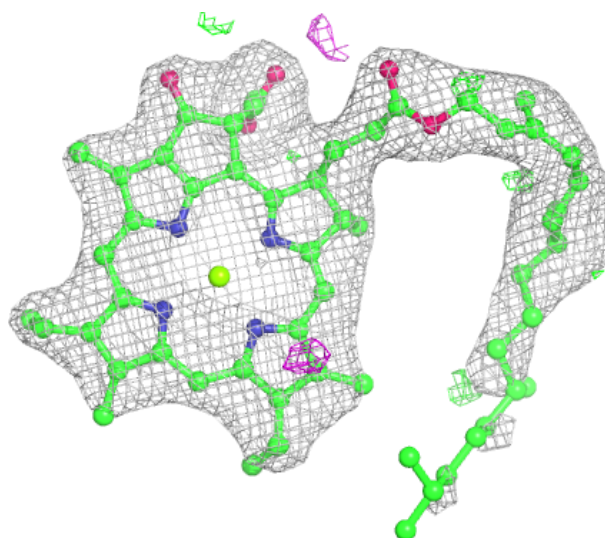
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

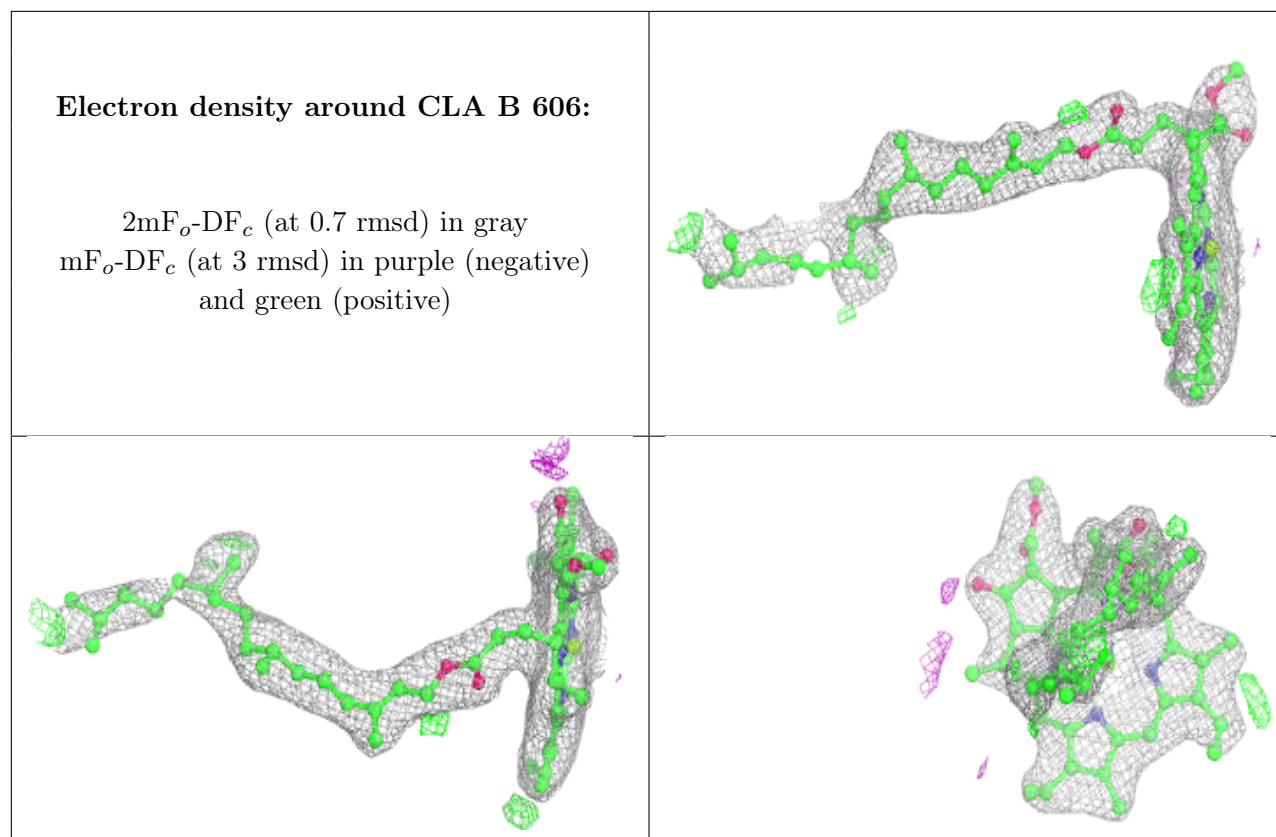




Electron density around CLA C 512:

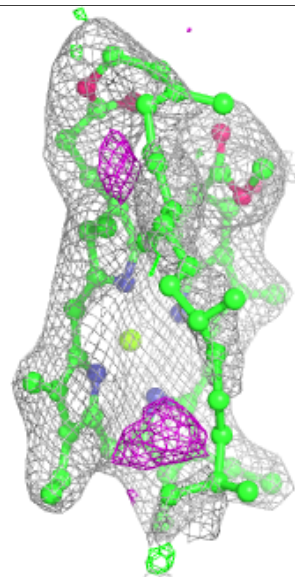
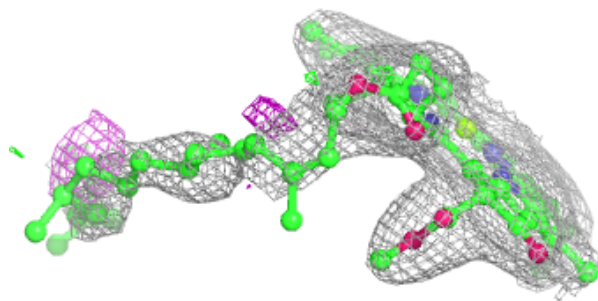
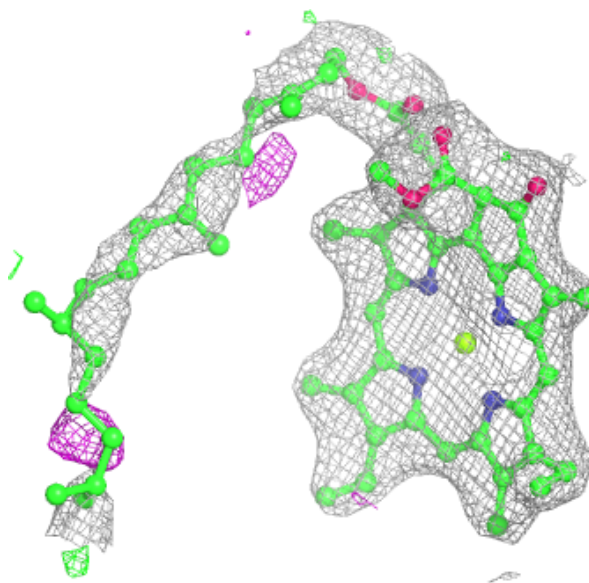
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

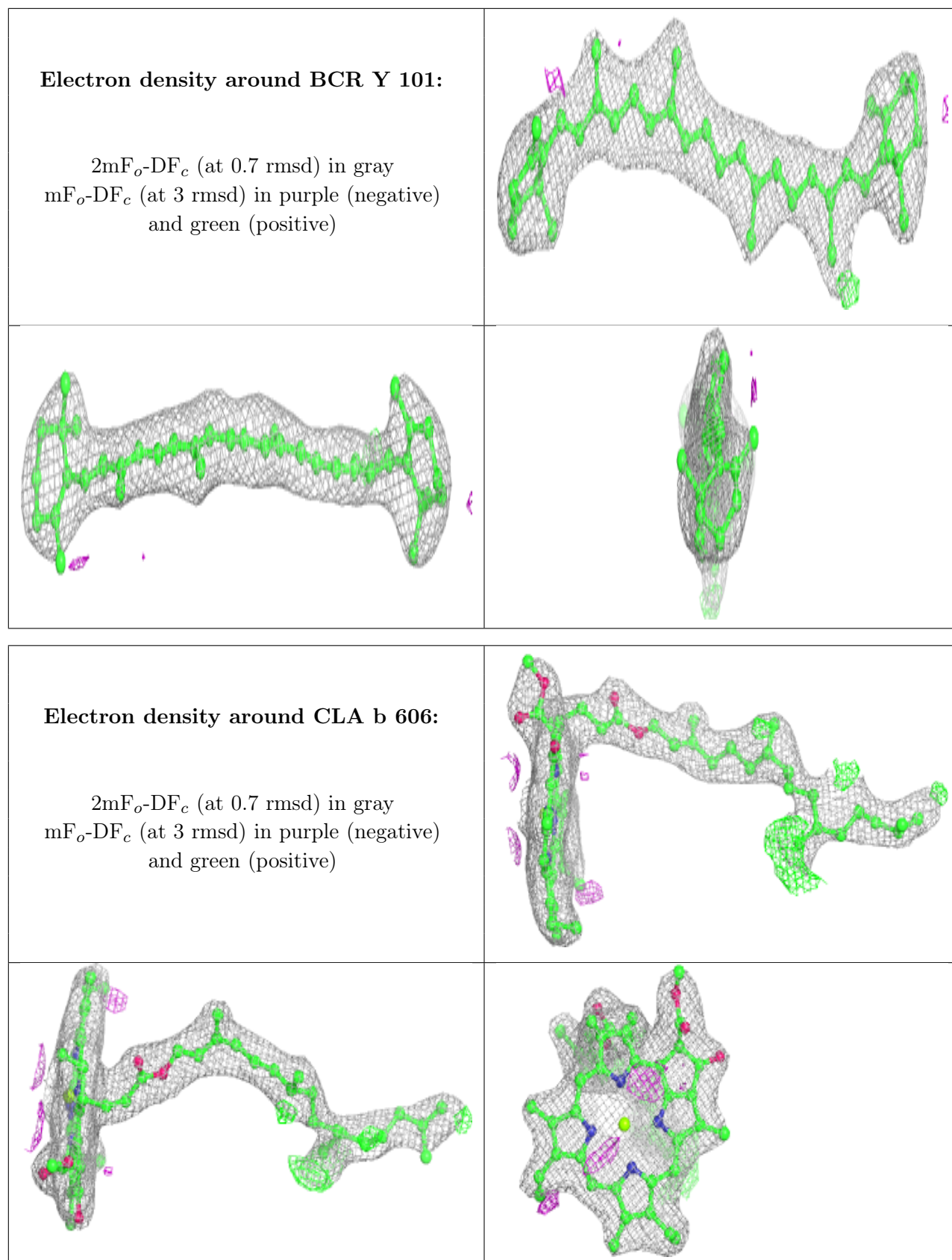




Electron density around CLA B 616:

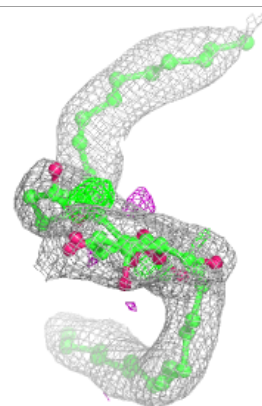
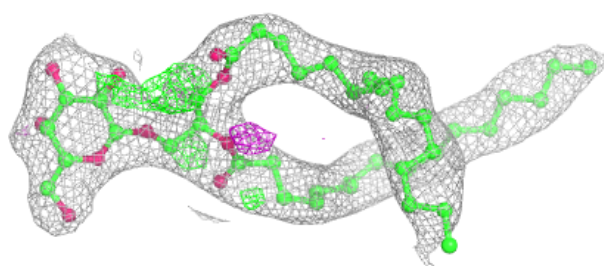
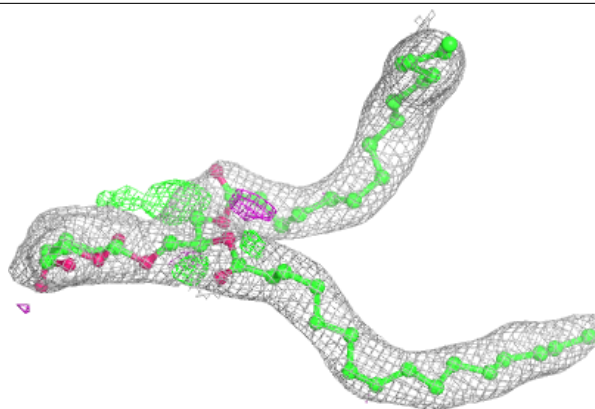
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



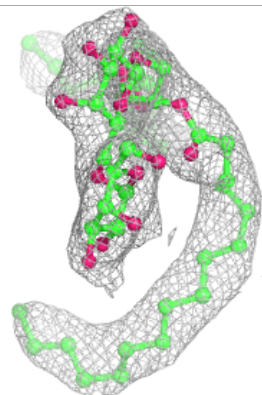
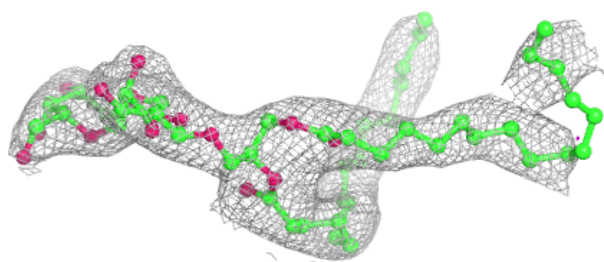
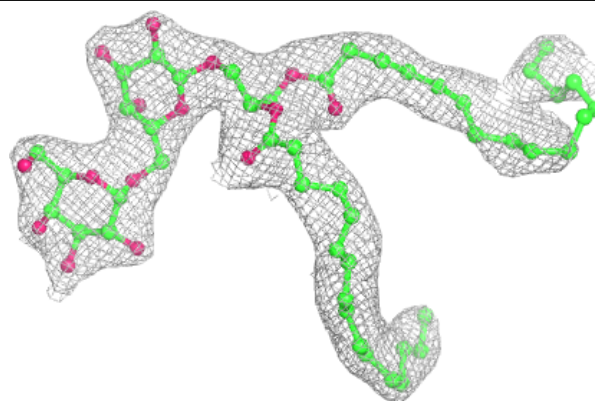


Electron density around LMG B 621:

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

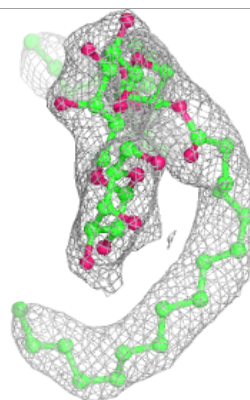
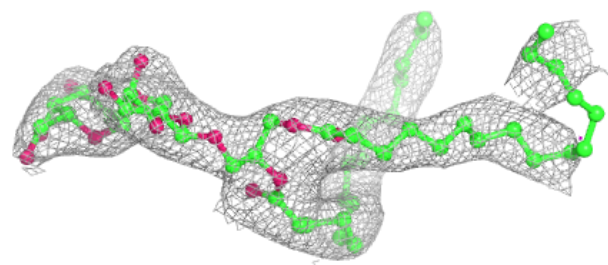
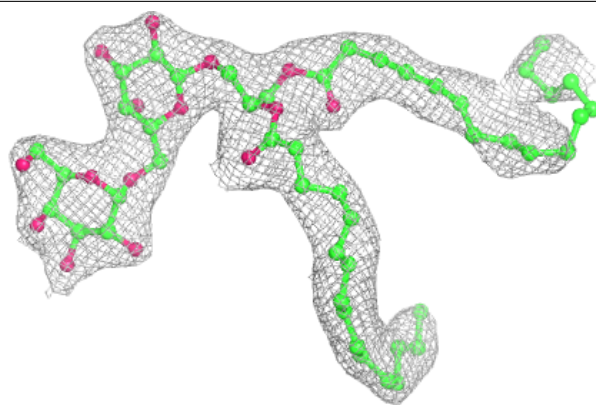
**Electron density around DGD c 518 (A):**

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

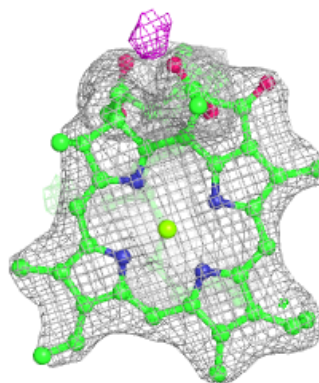
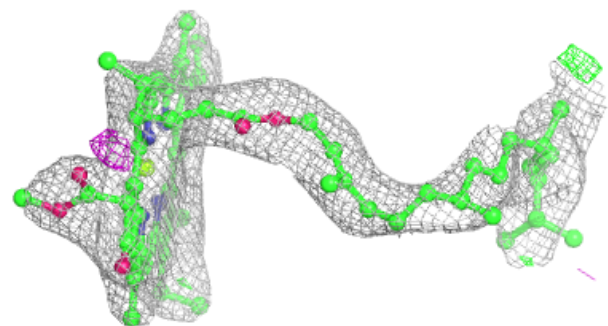
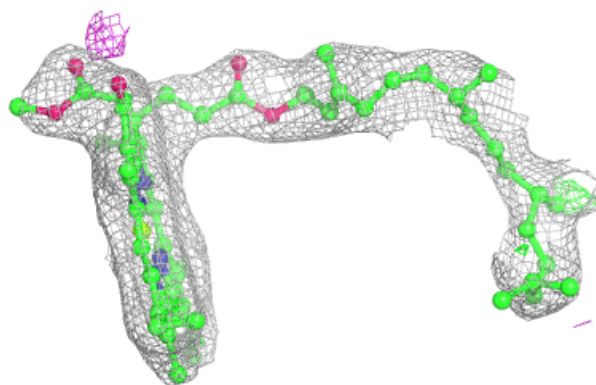


Electron density around DGD c 518 (B):

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

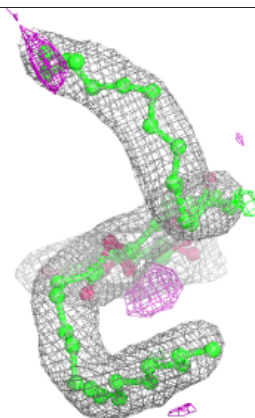
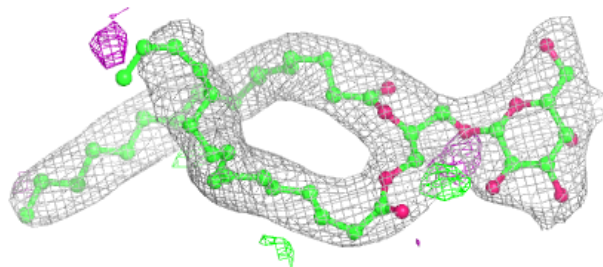
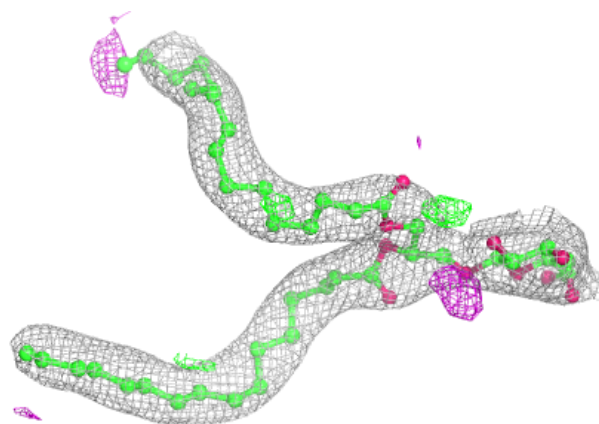
**Electron density around CLA C 506:**

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

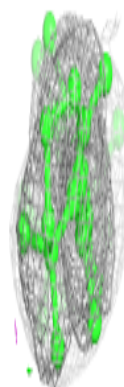
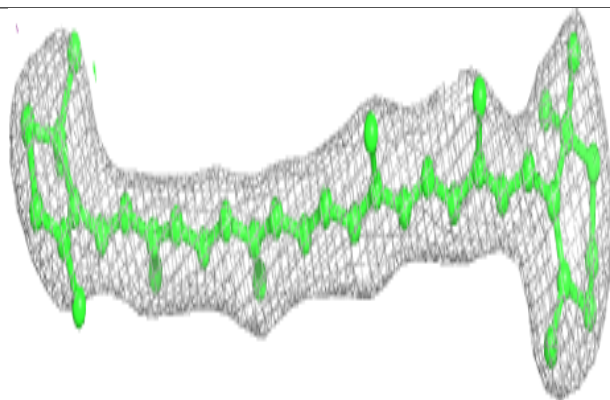
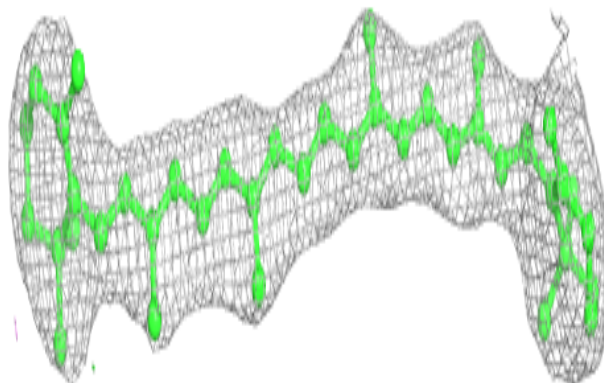


Electron density around LMG m 101:

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

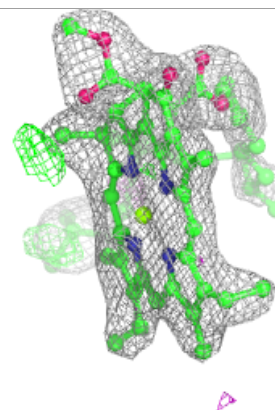
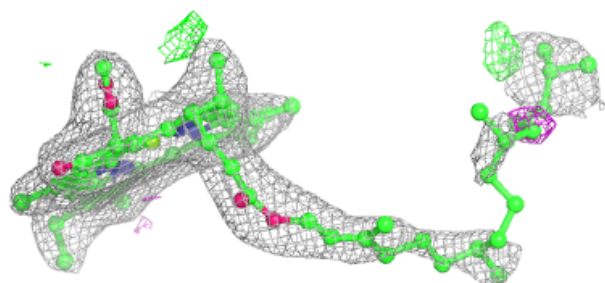
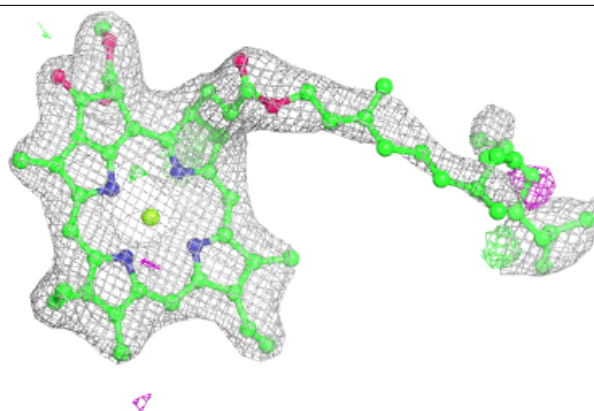
**Electron density around BCR c 515:**

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

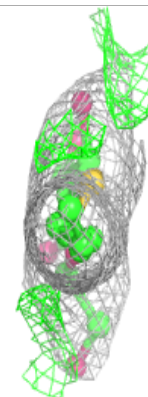
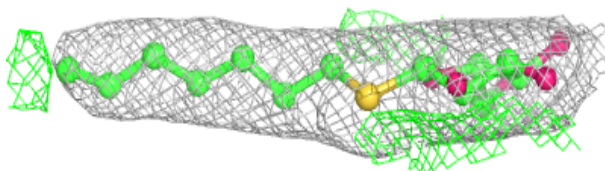
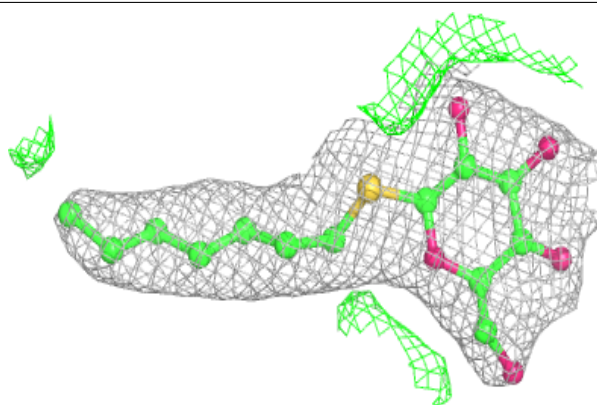


Electron density around CLA a 407:

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

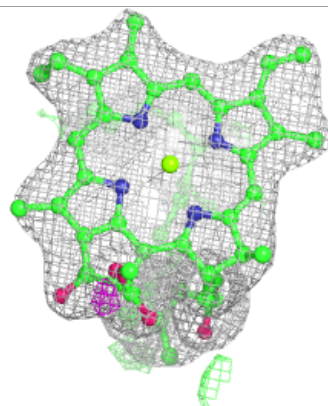
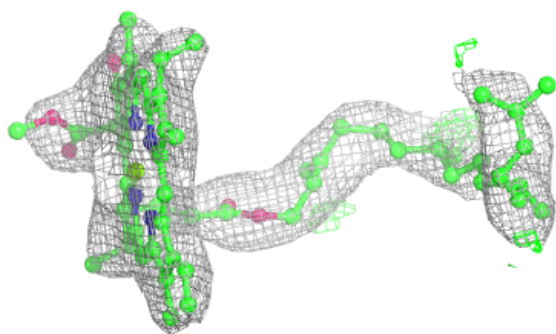
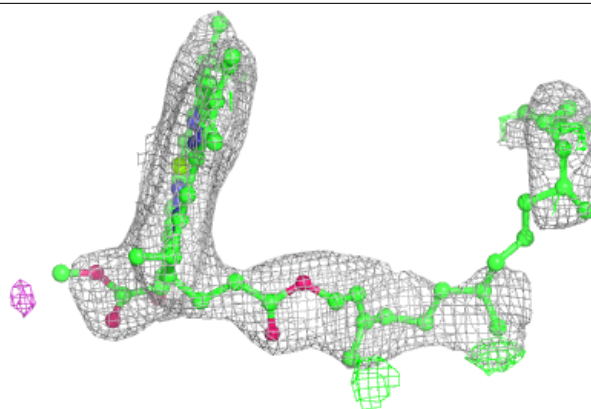
**Electron density around HTG b 625:**

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

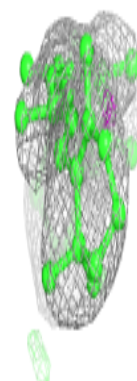
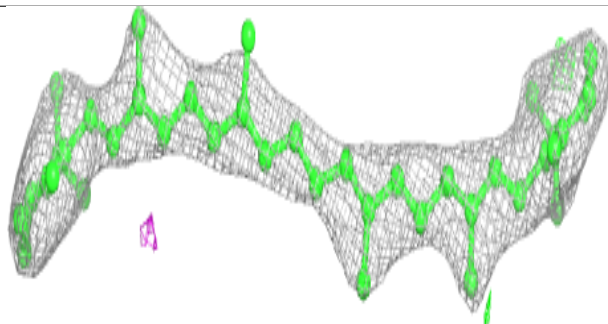
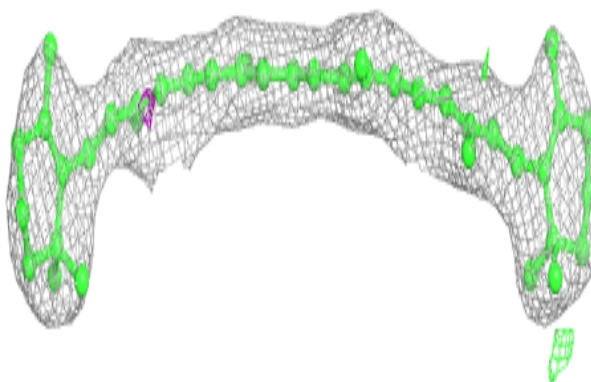


Electron density around CLA c 507:

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

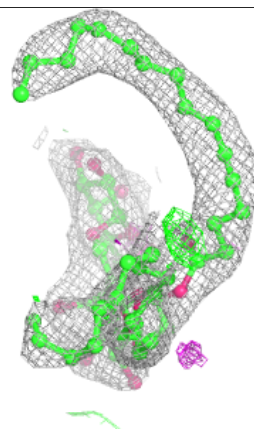
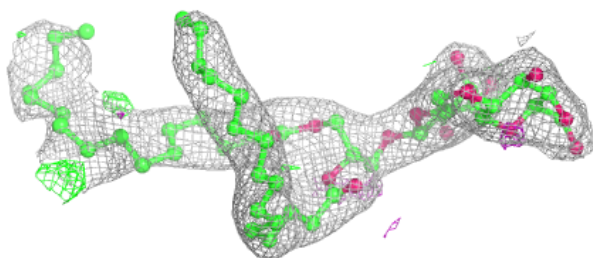
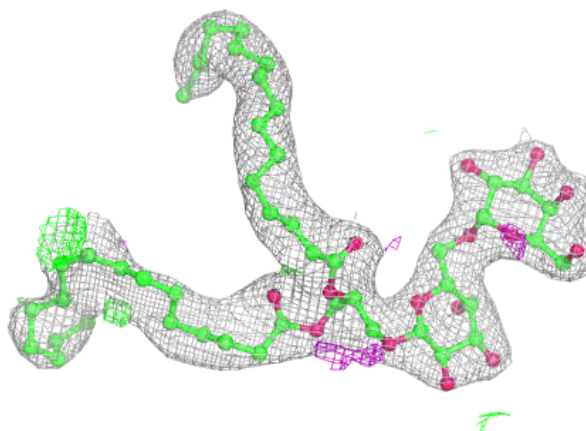
**Electron density around BCR k 101:**

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



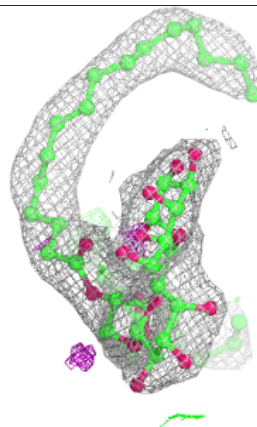
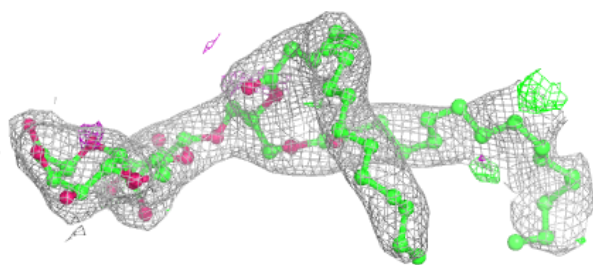
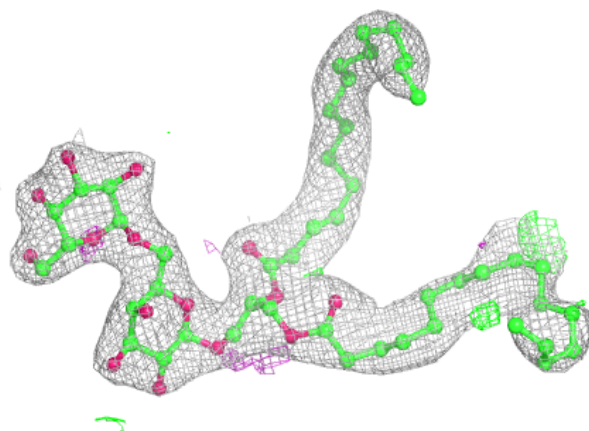
Electron density around DGD C 517 (A):

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

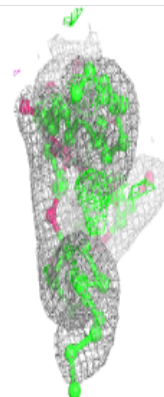
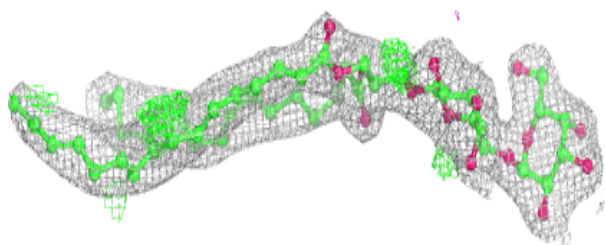
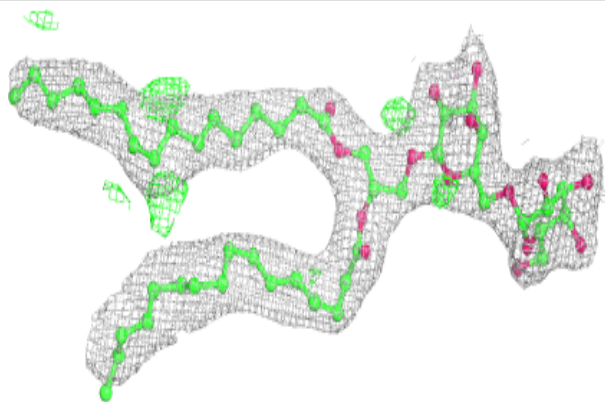


Electron density around DGD C 517 (B):

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

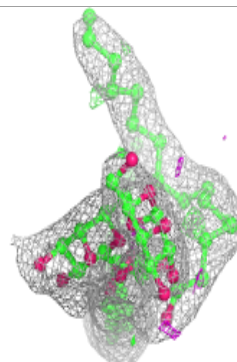
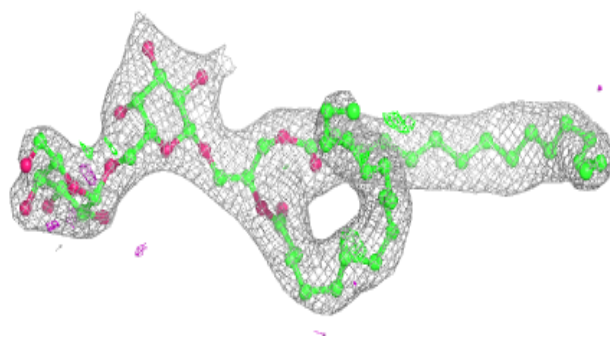
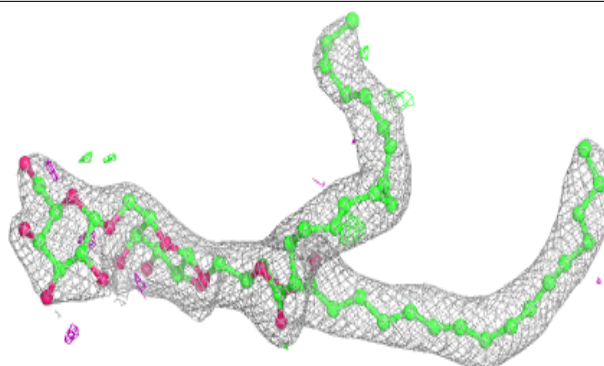
**Electron density around DGD C 518:**

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

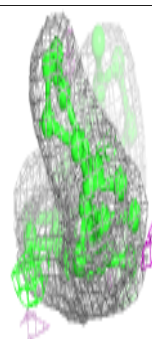
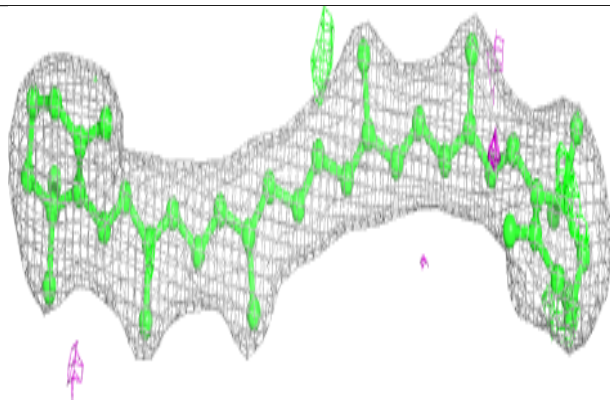
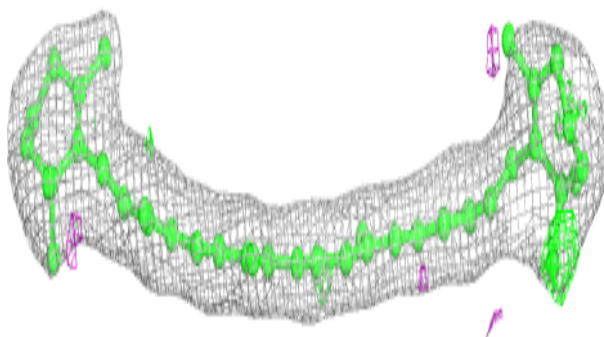


Electron density around DGD H 102:

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

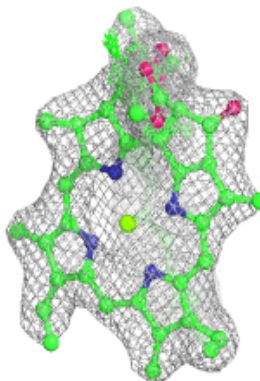
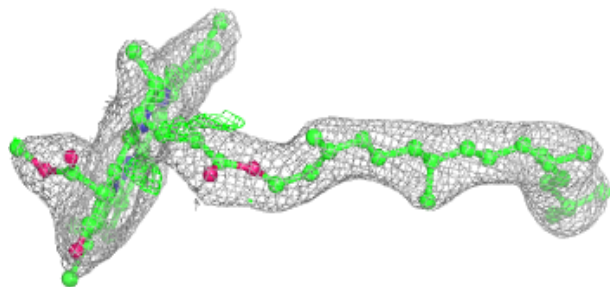
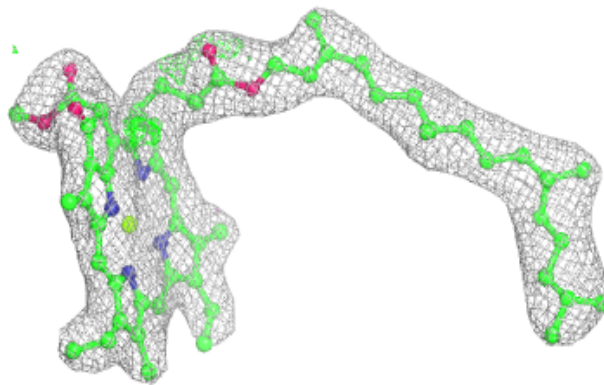
**Electron density around BCR D 405:**

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

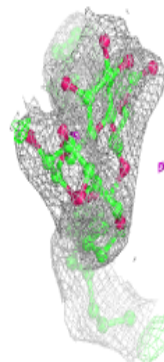
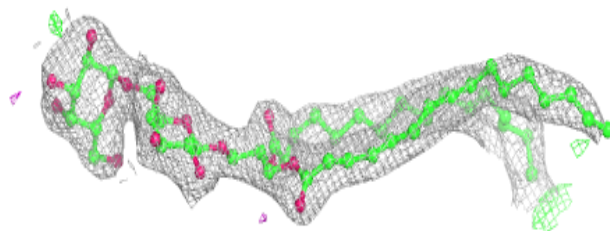
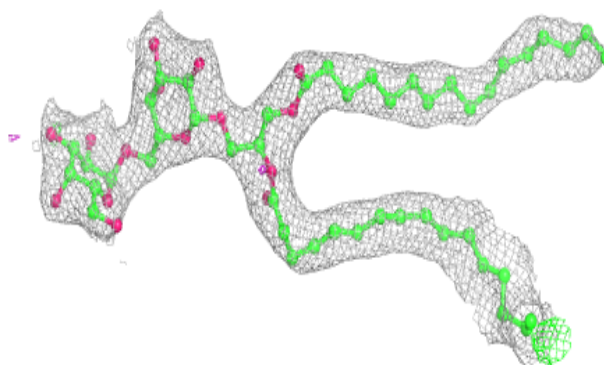


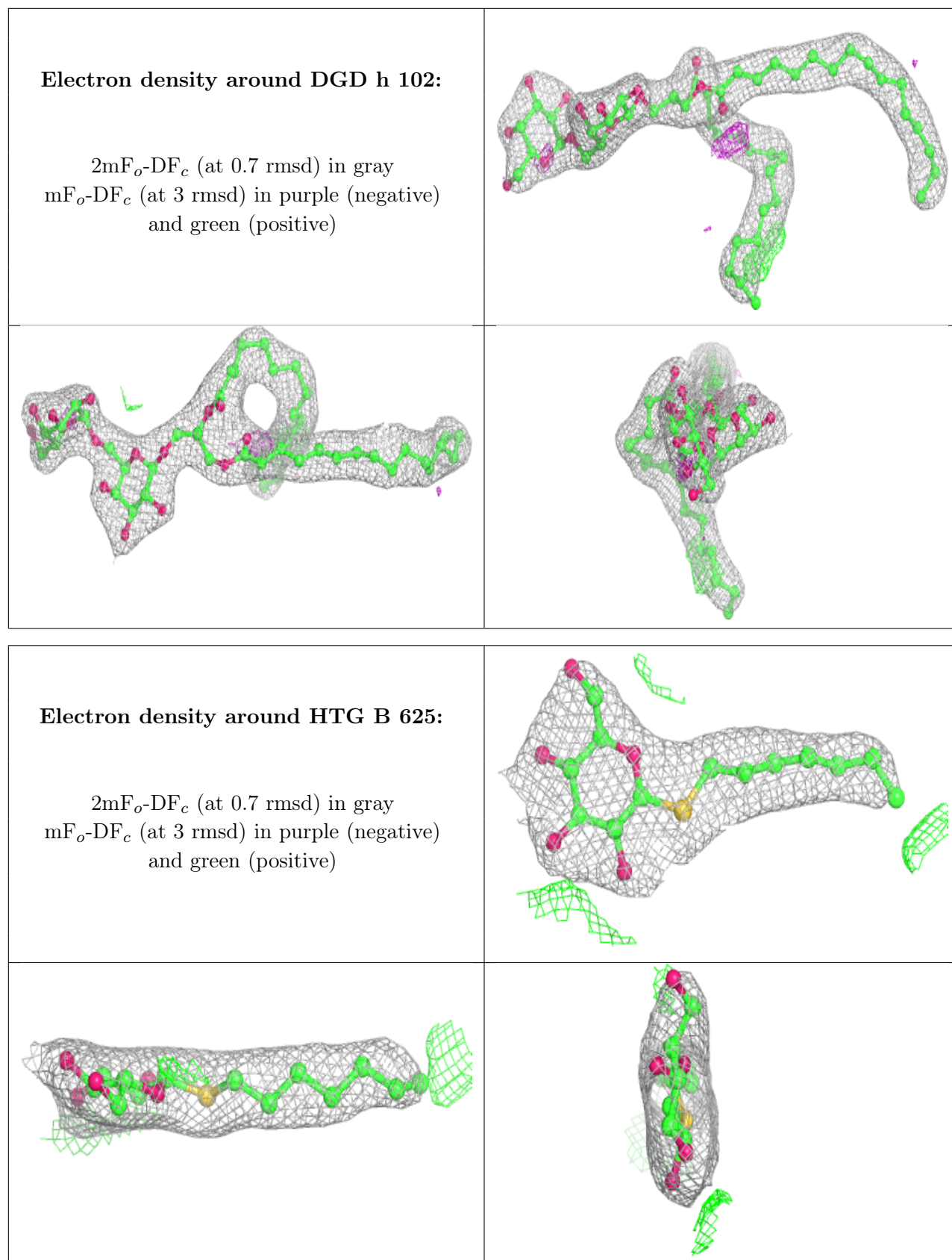
Electron density around CLA B 609:

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

**Electron density around DGD c 519:**

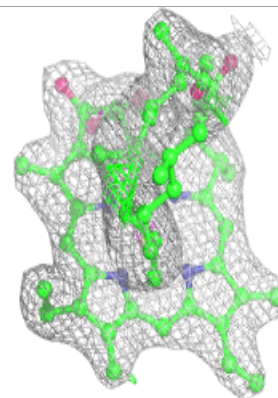
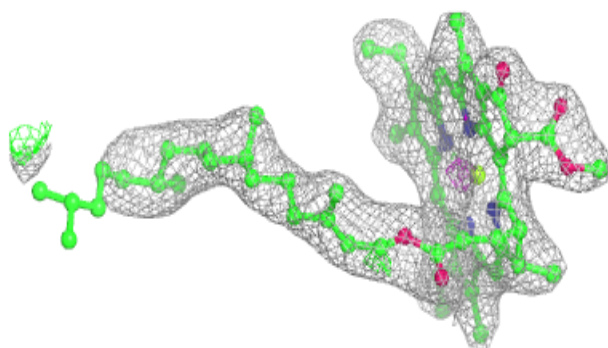
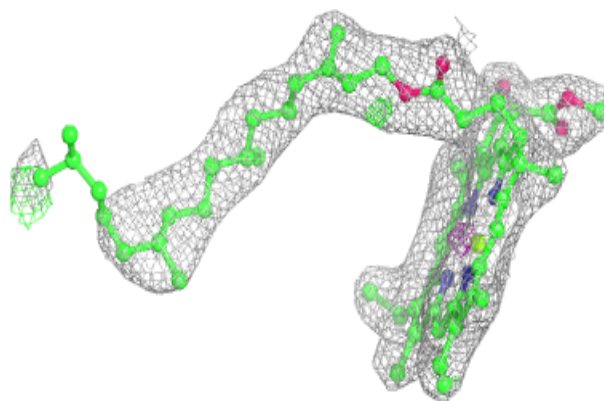
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



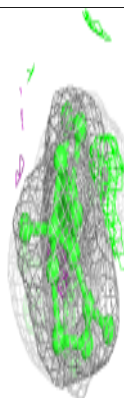
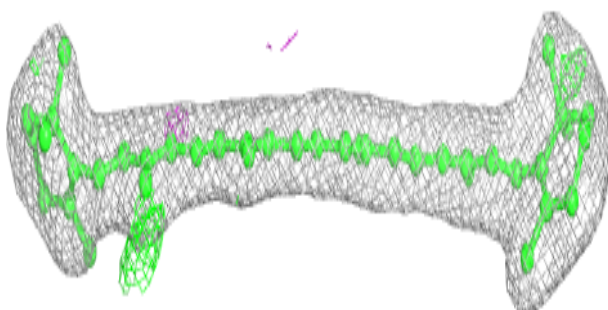
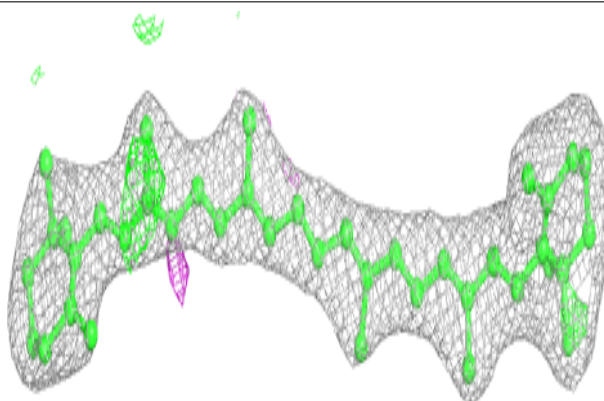


Electron density around CLA C 508:

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

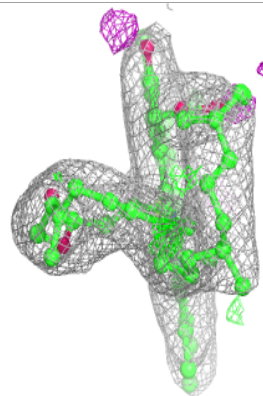
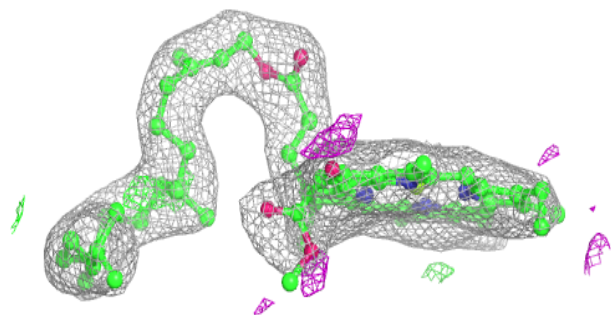
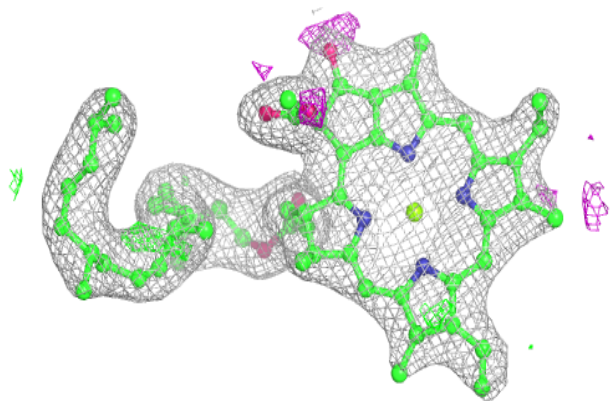
**Electron density around BCR b 618:**

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



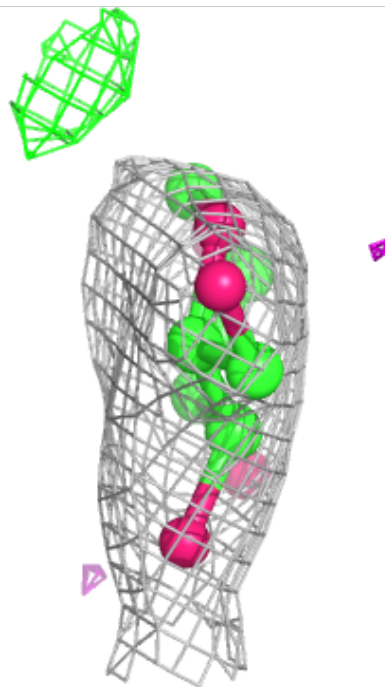
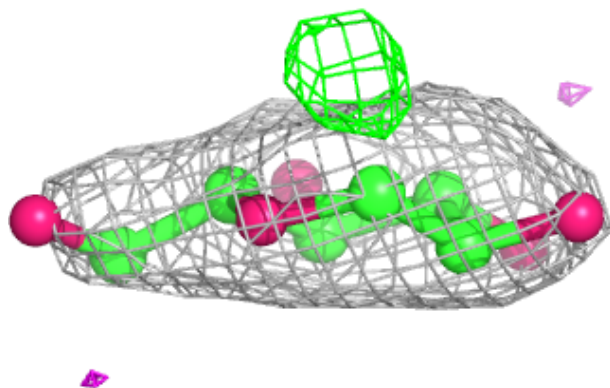
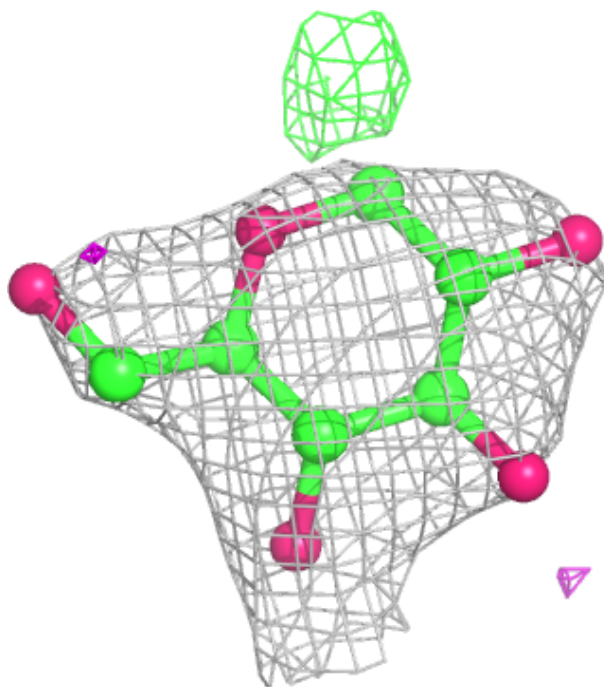
Electron density around CLA b 612:

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



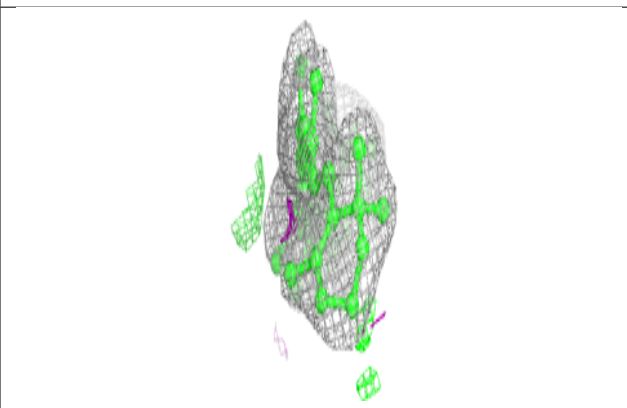
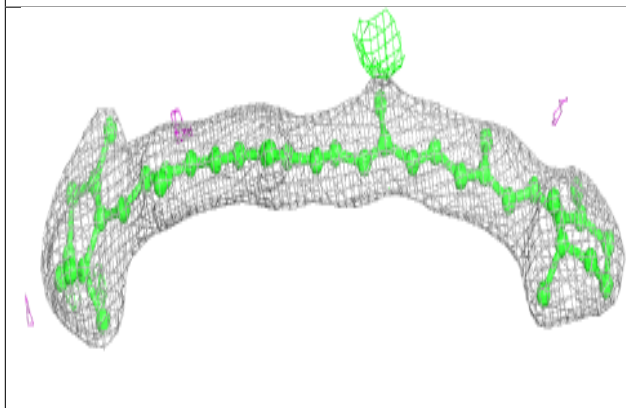
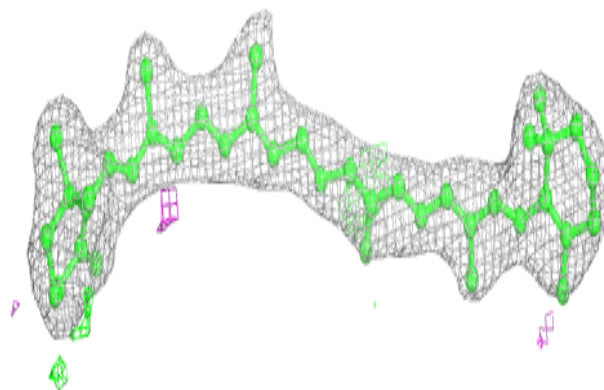
Electron density around HTG V 202:

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

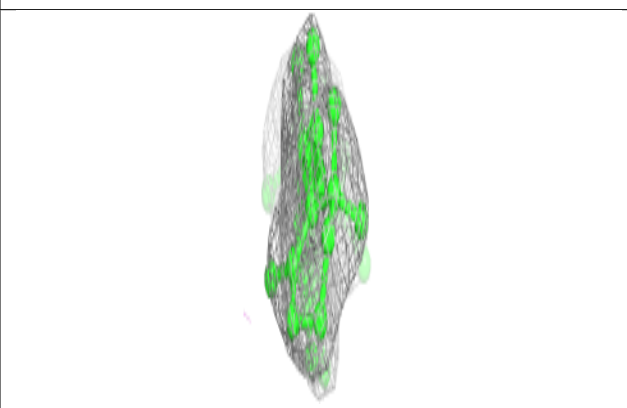
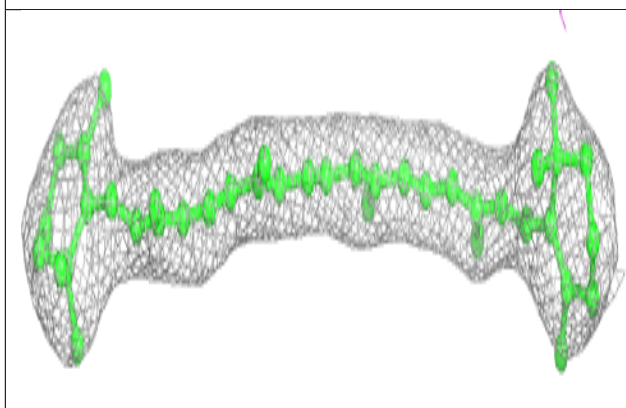
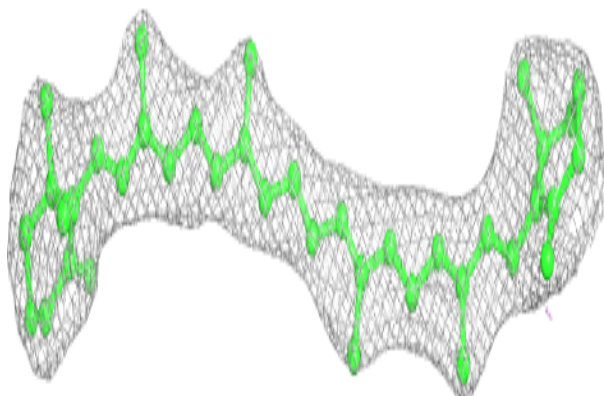


Electron density around BCR t 102:

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

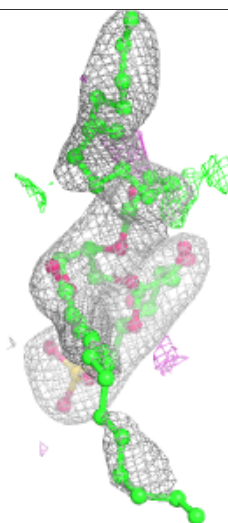
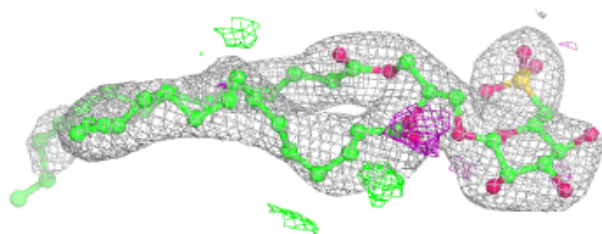
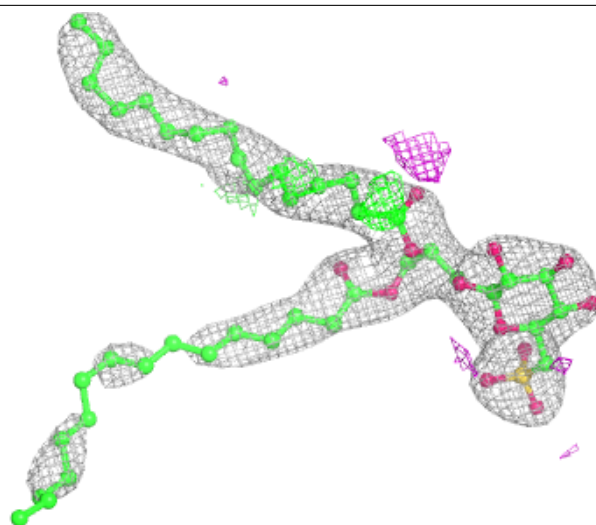
**Electron density around BCR y 101:**

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



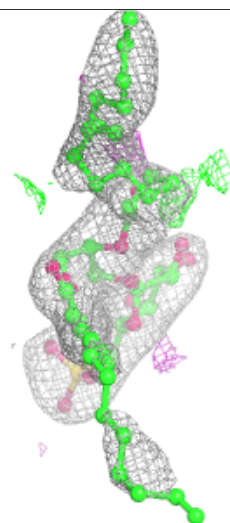
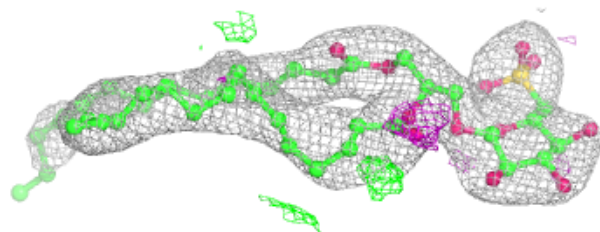
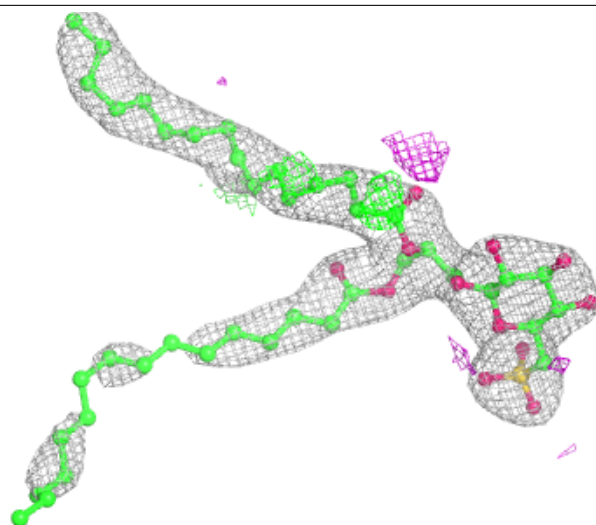
Electron density around SQD A 410 (A):

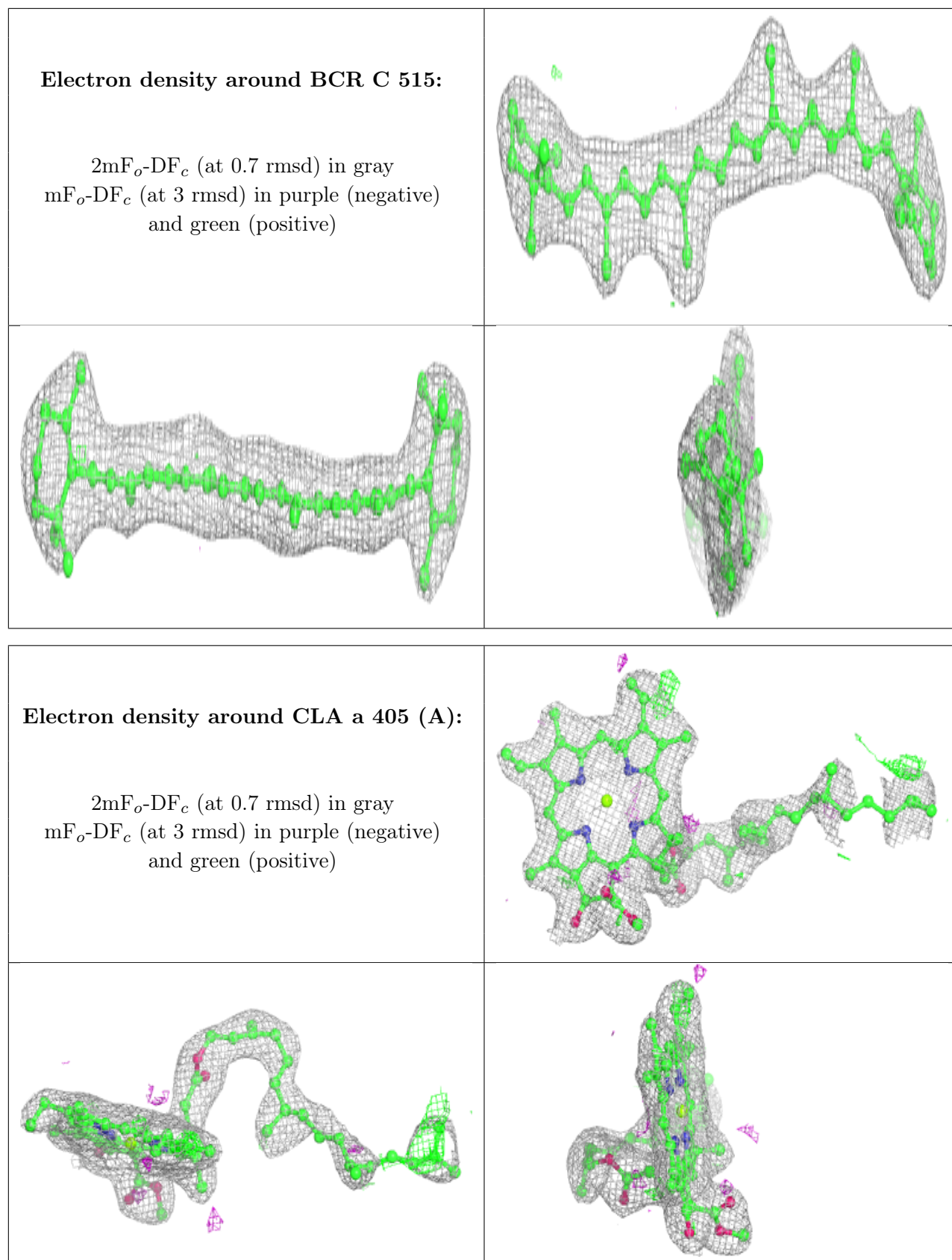
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

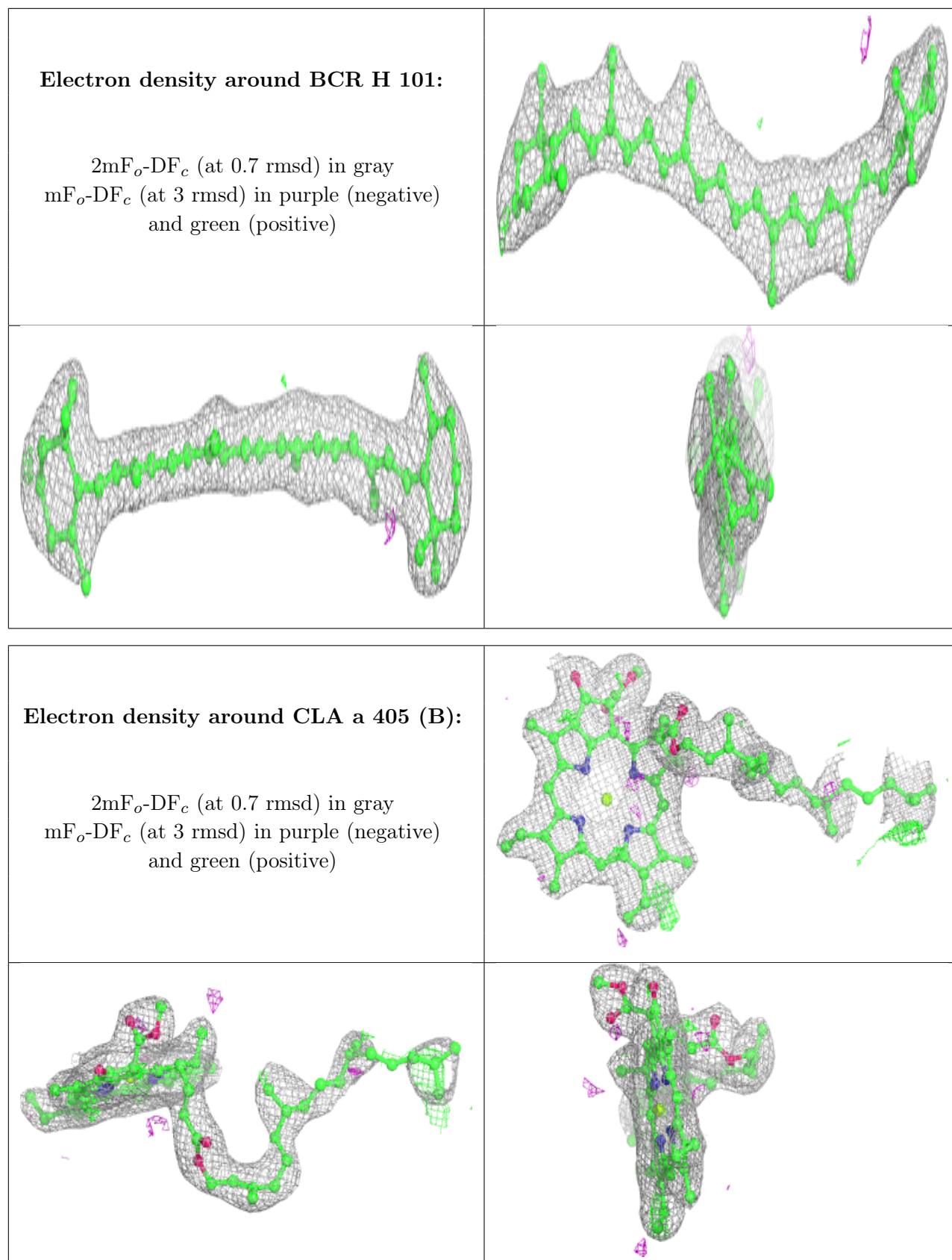


Electron density around SQD A 410 (B):

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

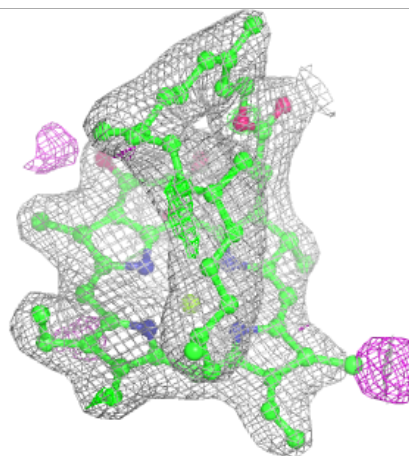
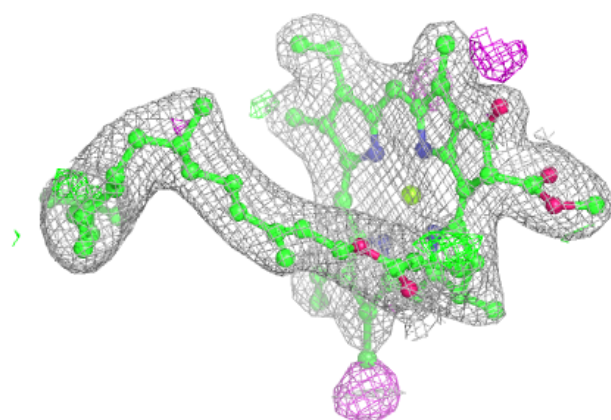
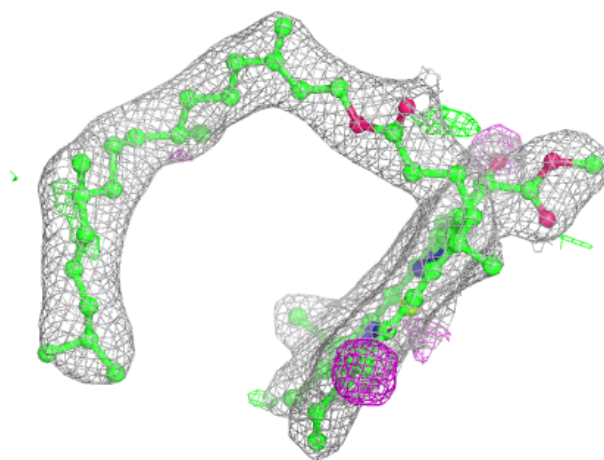






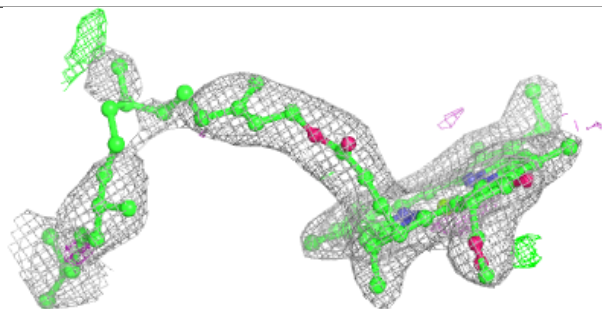
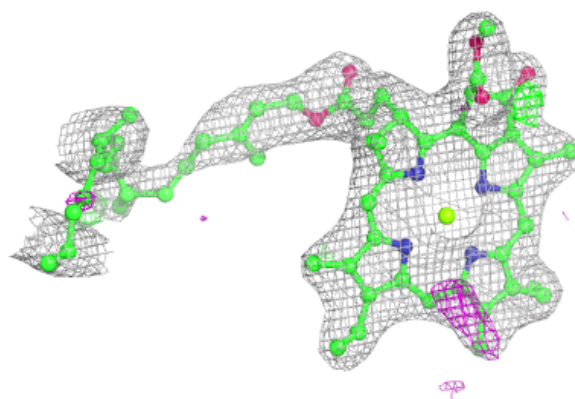
Electron density around CLA B 611:

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

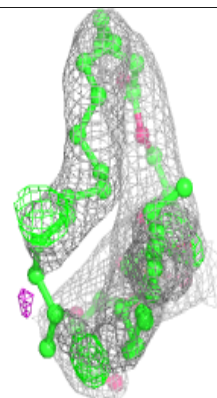
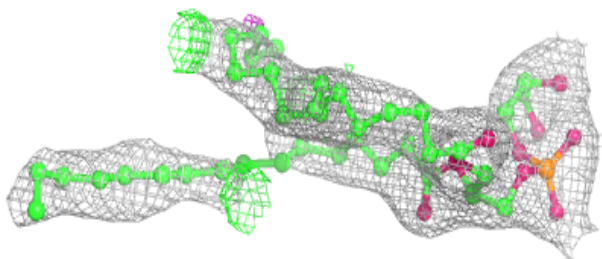
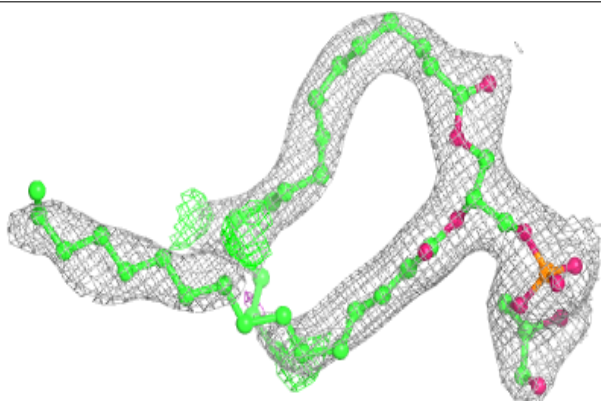


Electron density around CLA A 408:

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

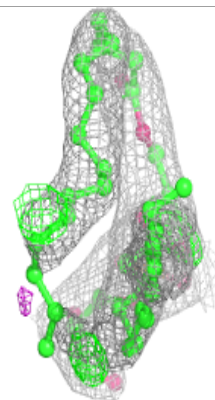
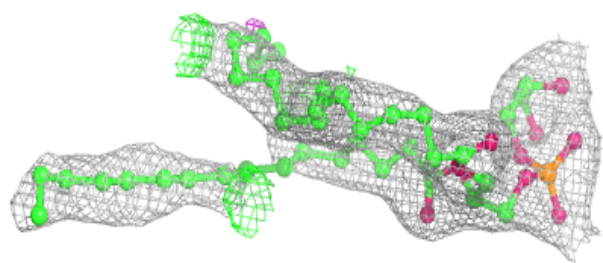
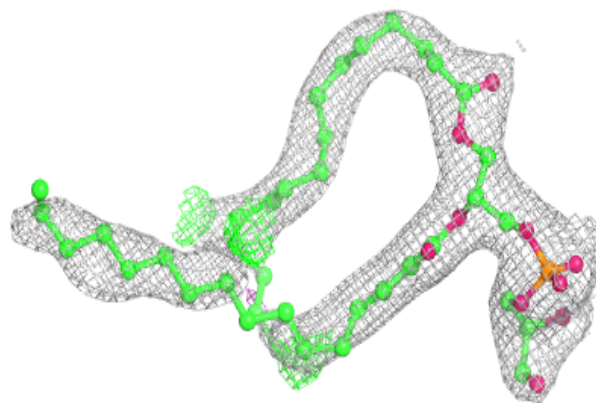
**Electron density around LHG d 408 (A):**

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

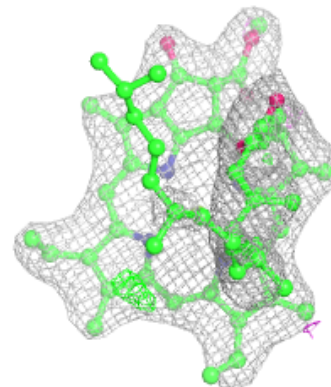
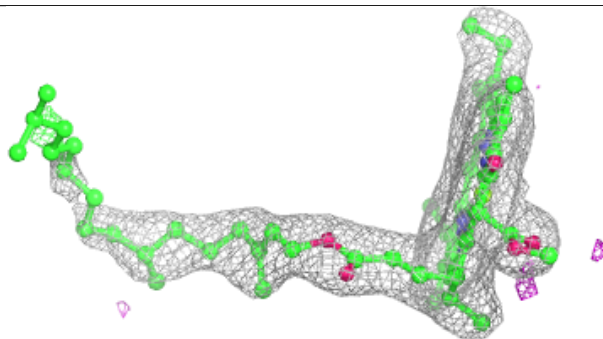
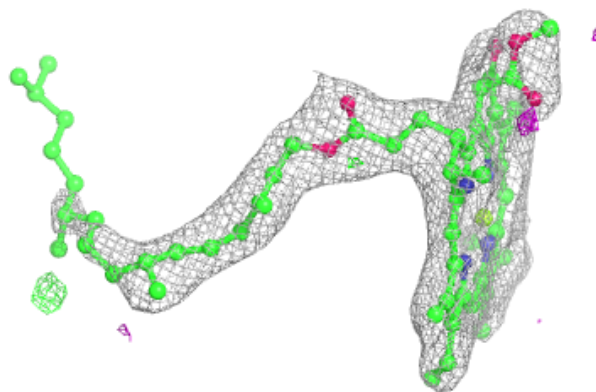


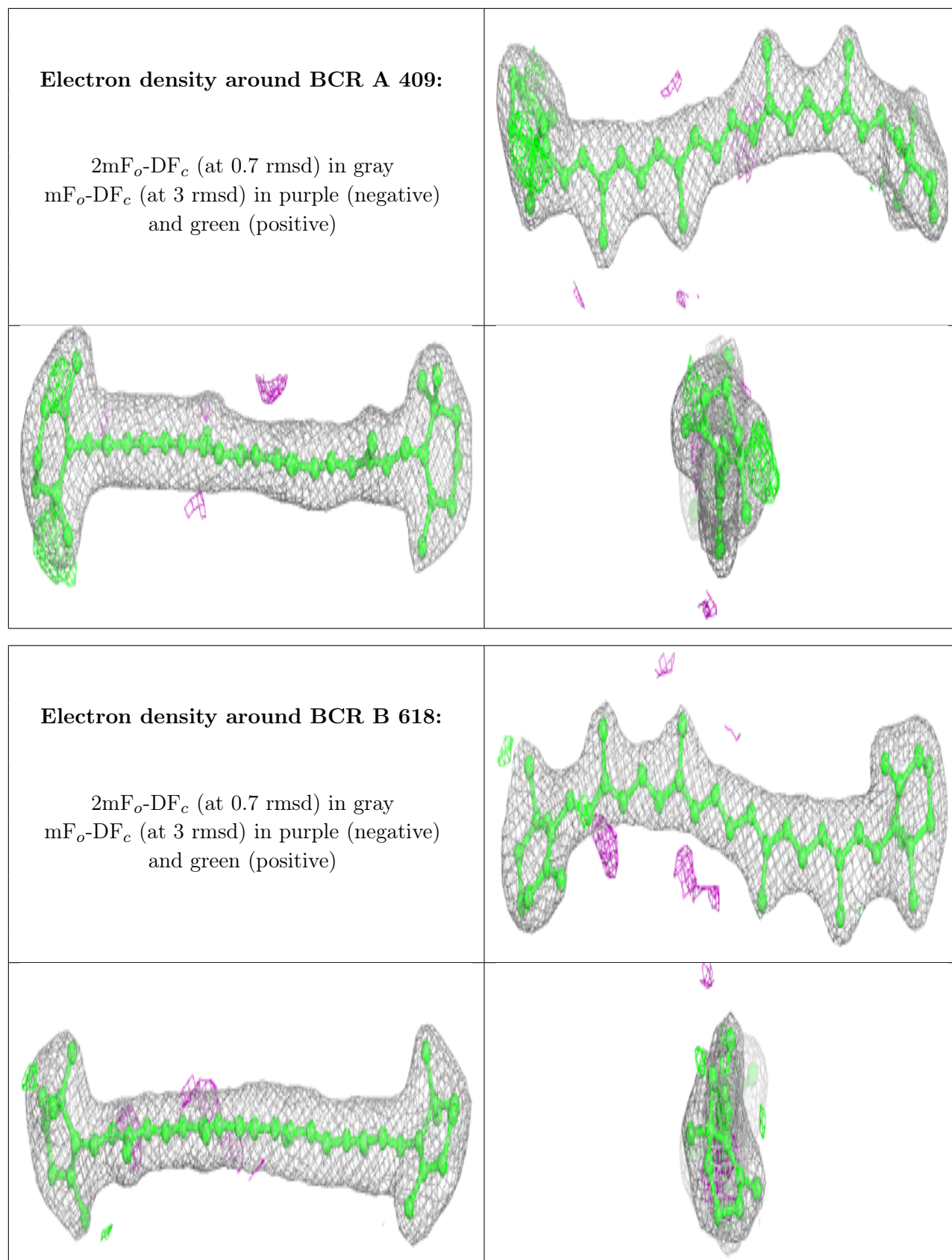
Electron density around LHG d 408 (B):

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

**Electron density around CLA D 404:**

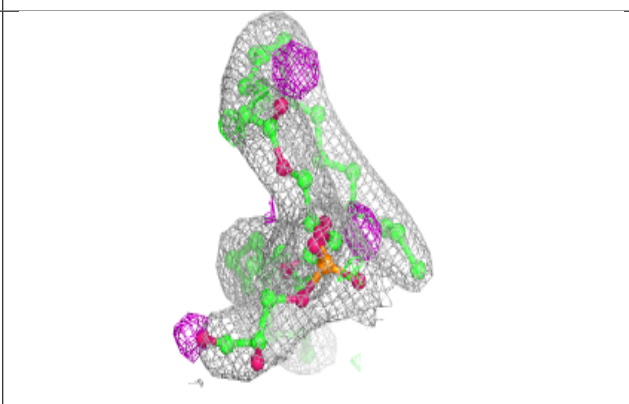
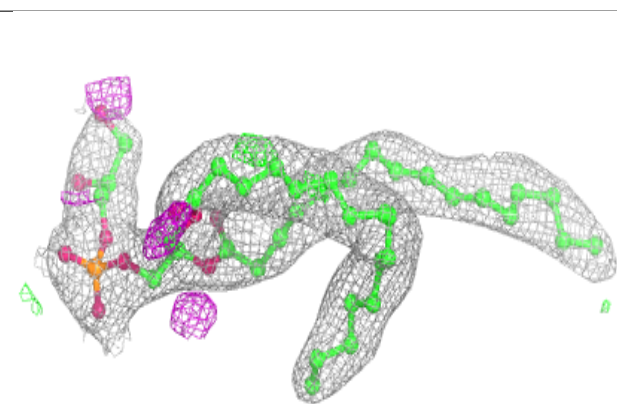
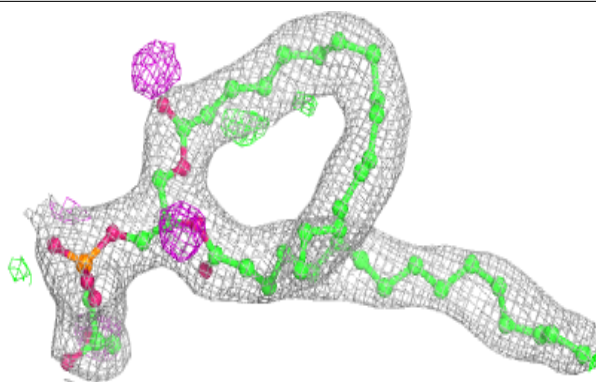
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



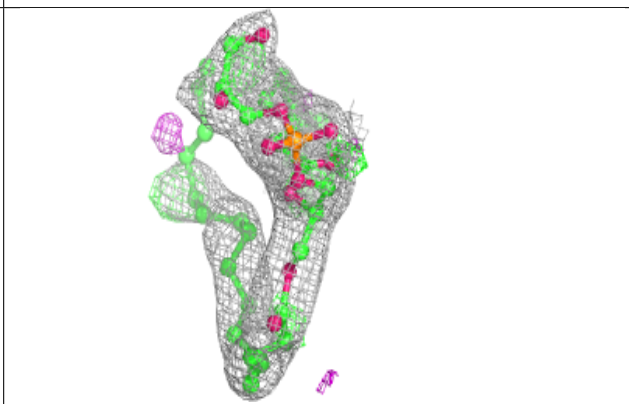
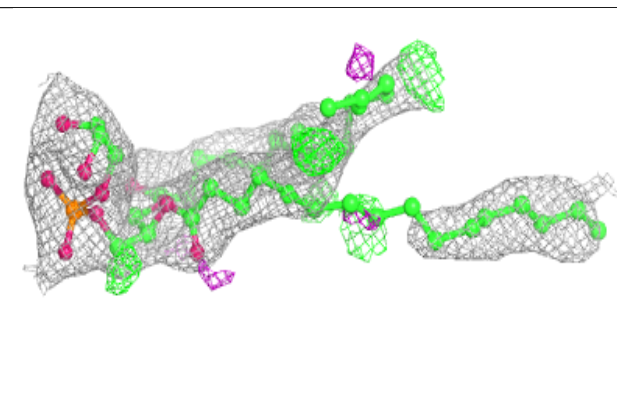
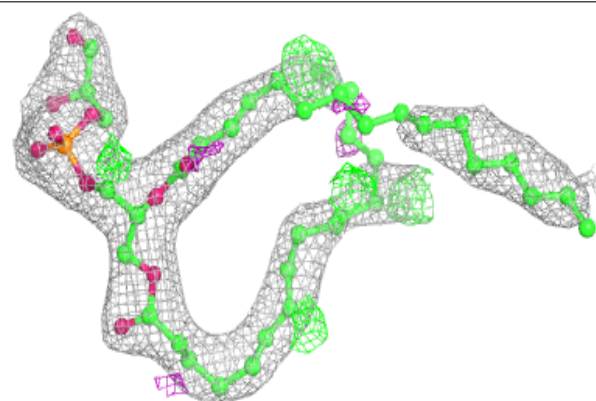


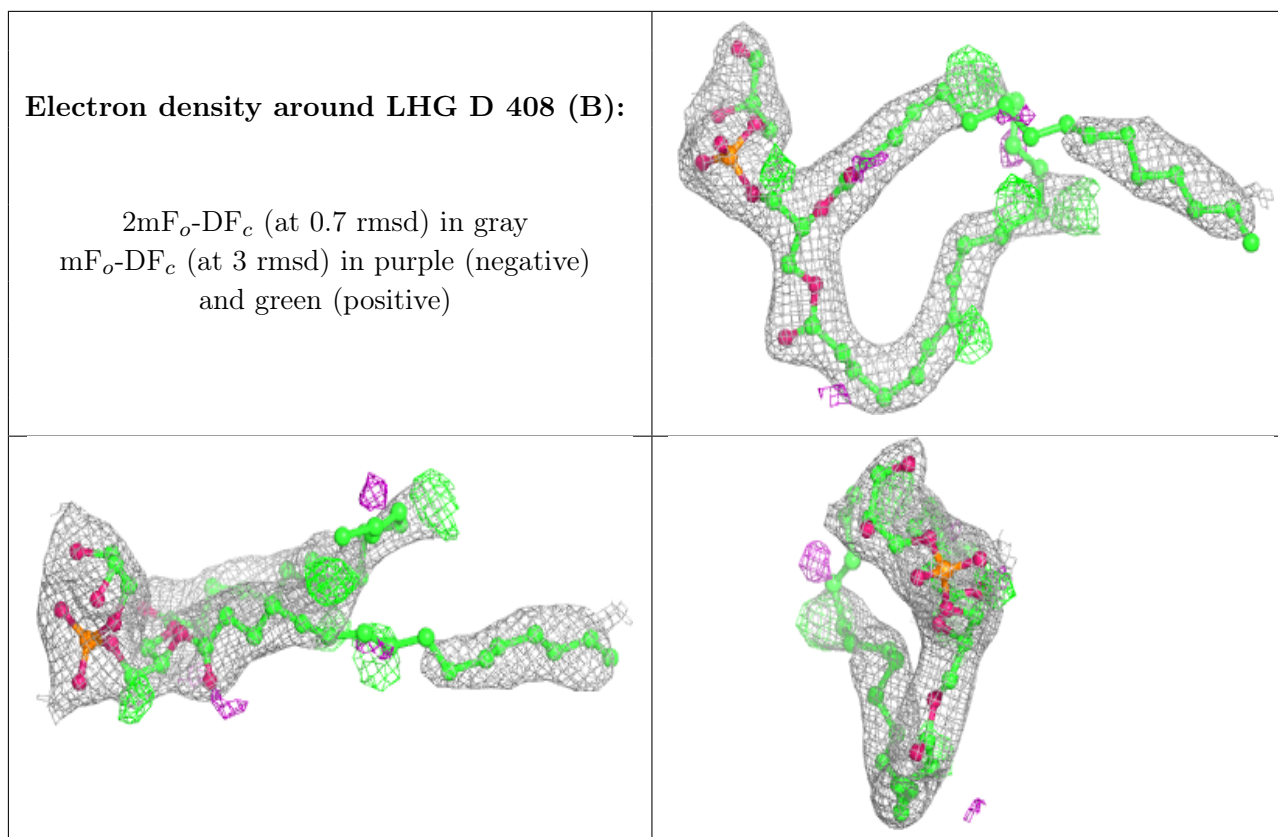
Electron density around LHG A 419 (B):

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

**Electron density around LHG D 408 (A):**

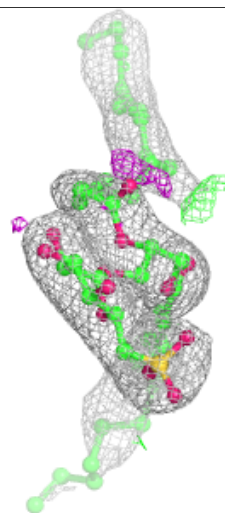
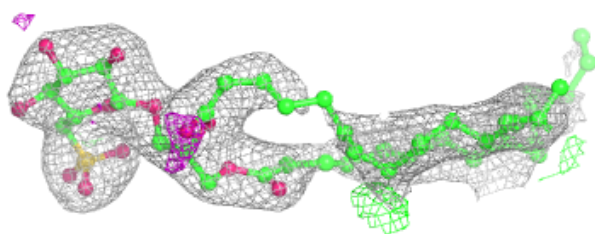
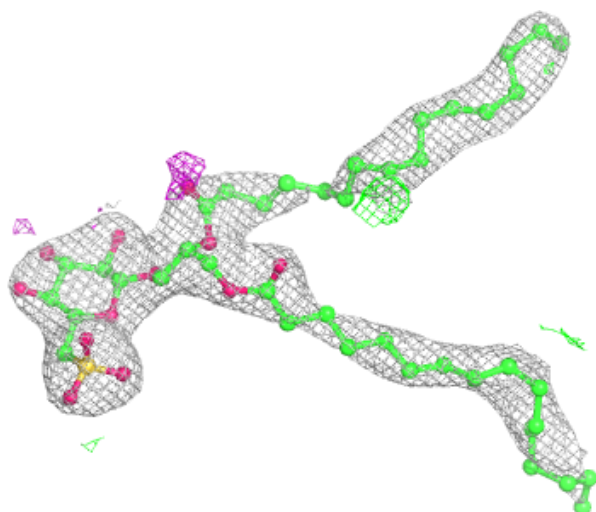
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





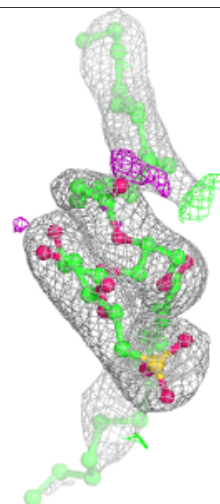
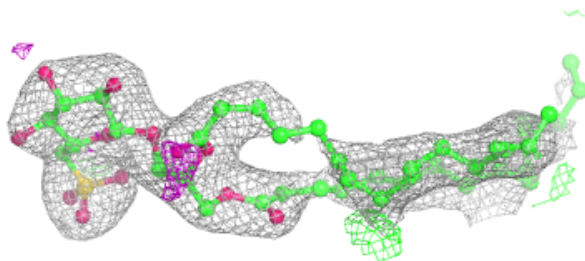
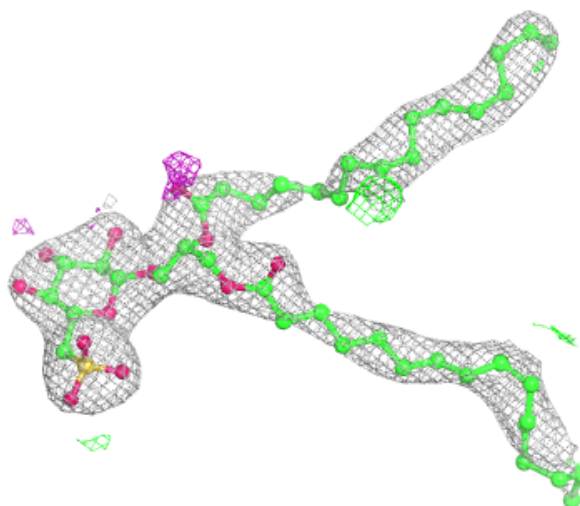
Electron density around SQD a 409 (A):

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



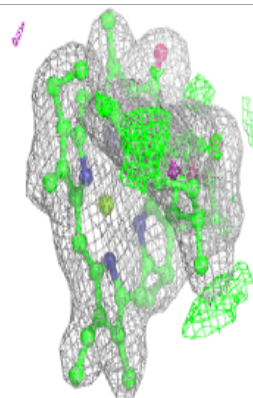
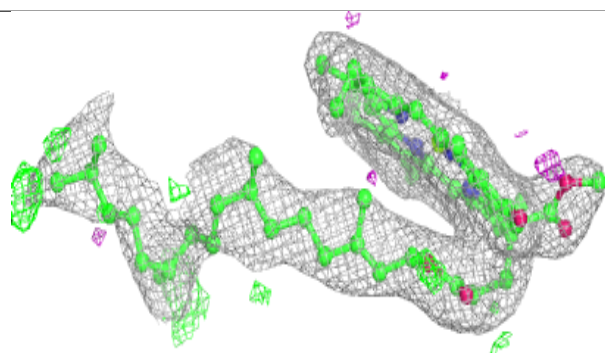
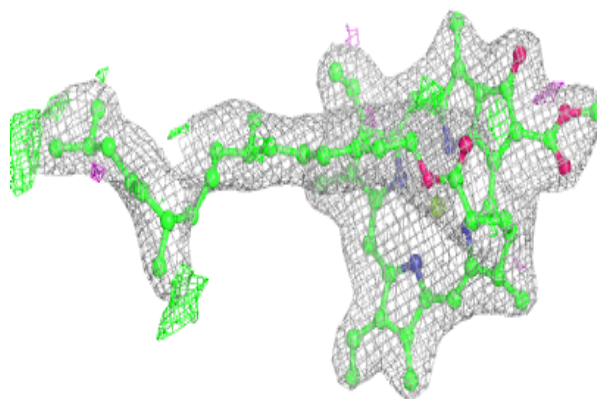
Electron density around SQD a 409 (B):

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

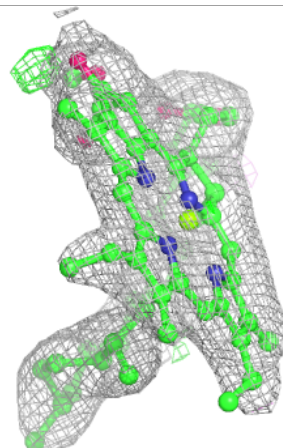
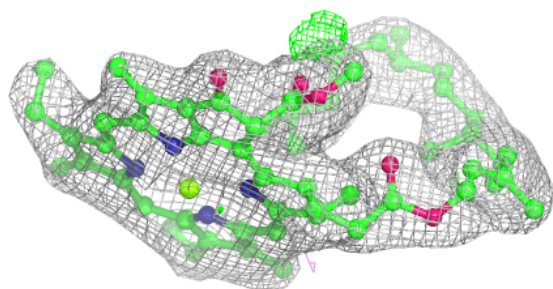
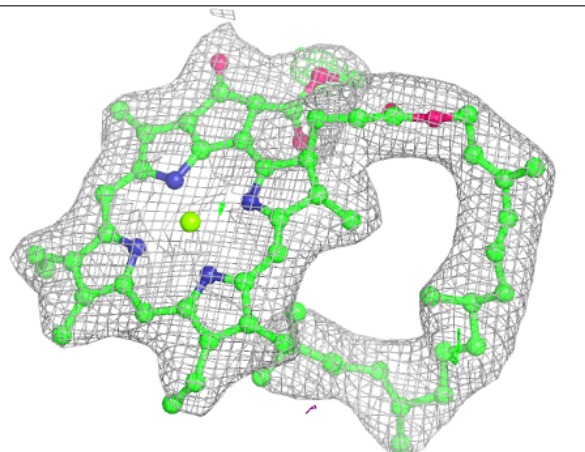


Electron density around CLA b 614:

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

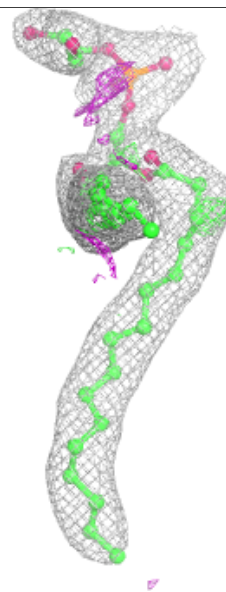
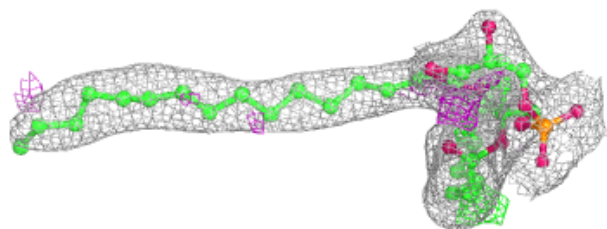
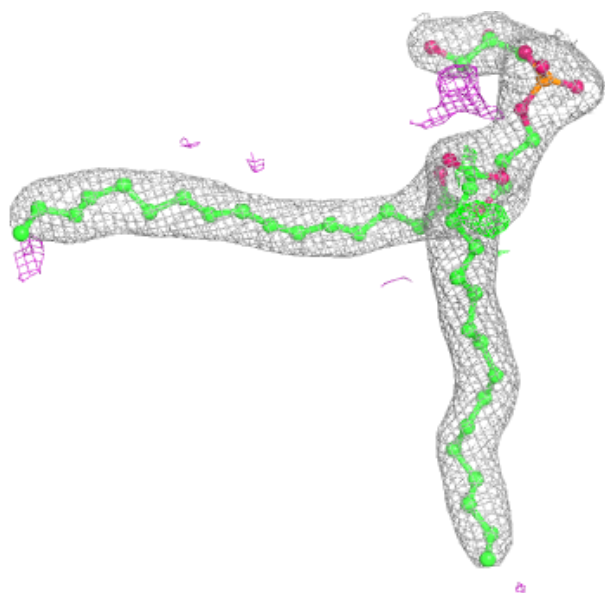
**Electron density around CLA b 615:**

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



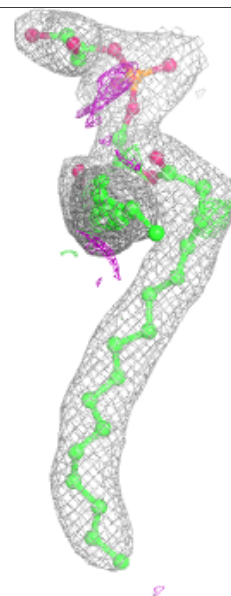
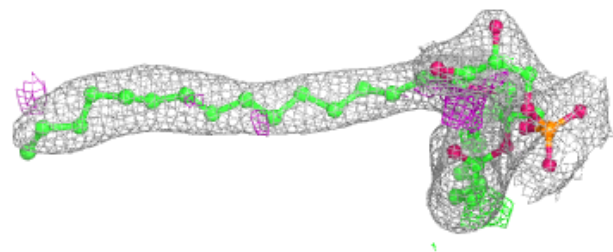
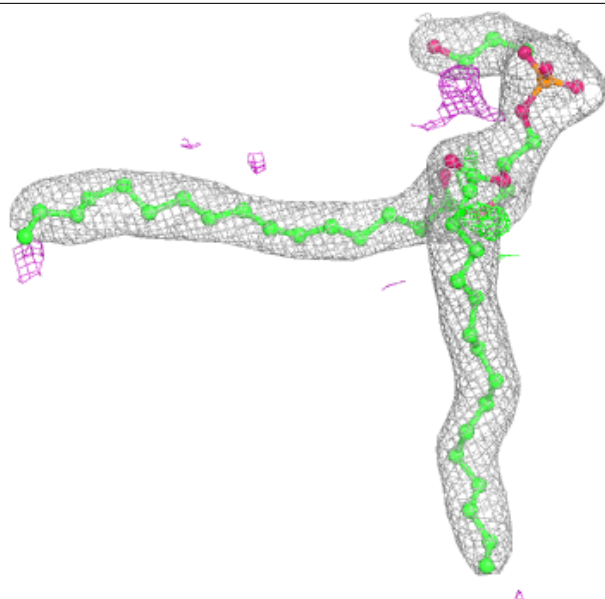
Electron density around LHG b 629 (A):

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



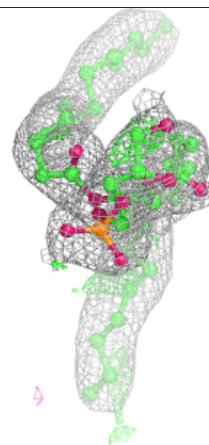
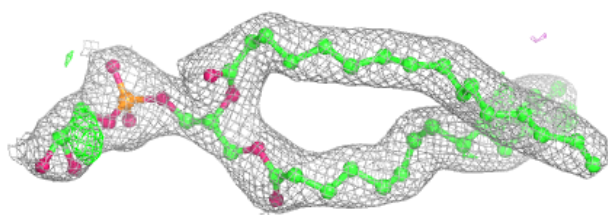
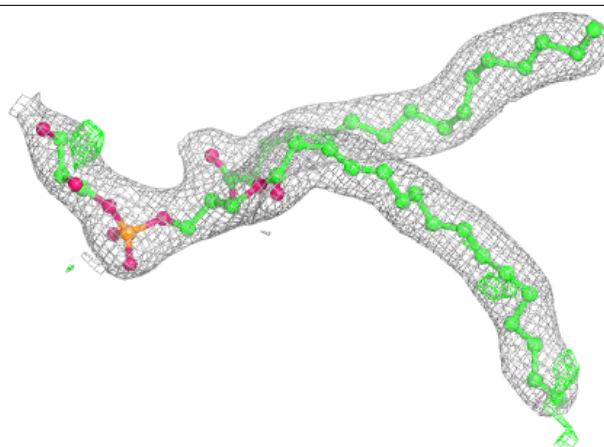
Electron density around LHG b 629 (B):

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



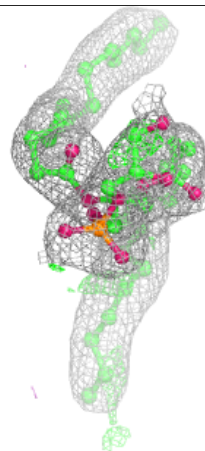
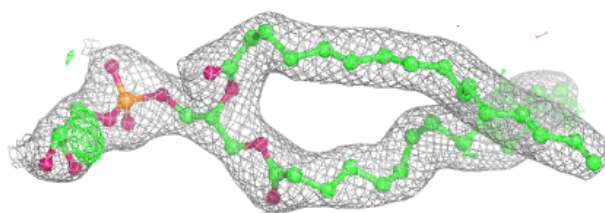
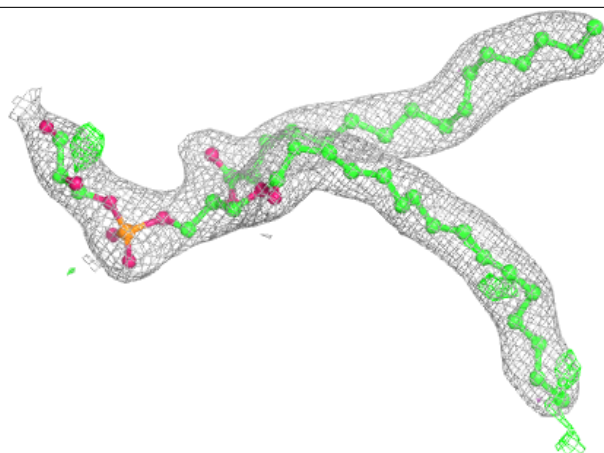
Electron density around LHG d 407 (A):

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

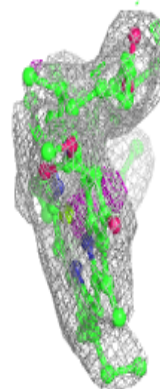
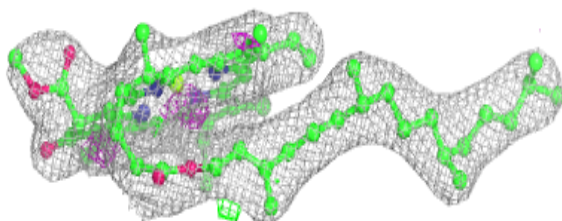
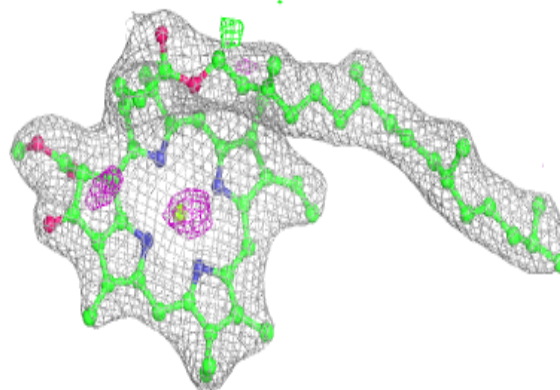


Electron density around LHG d 407 (B):

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

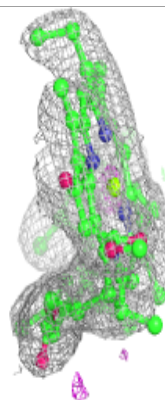
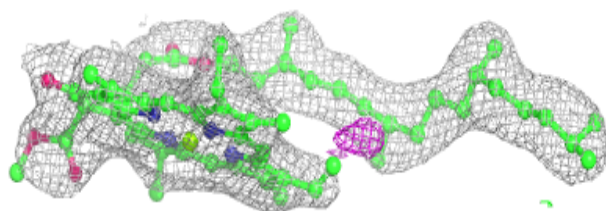
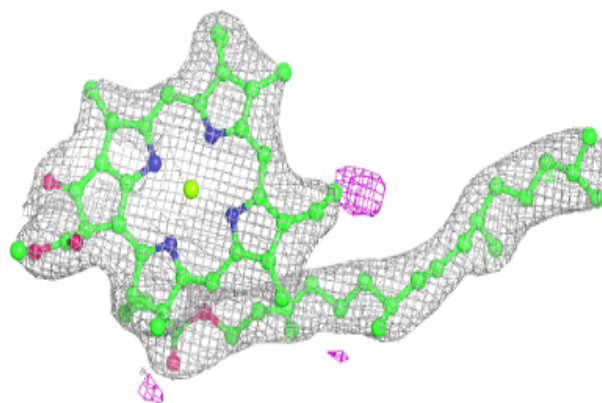
**Electron density around CLA C 501:**

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

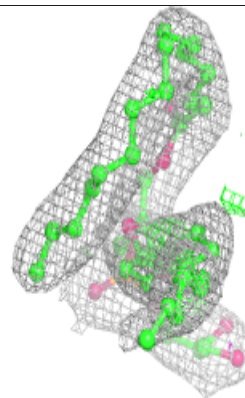
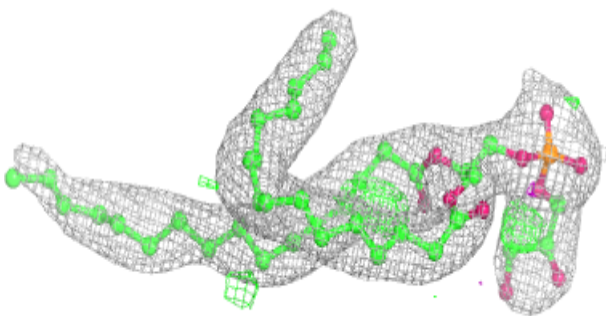
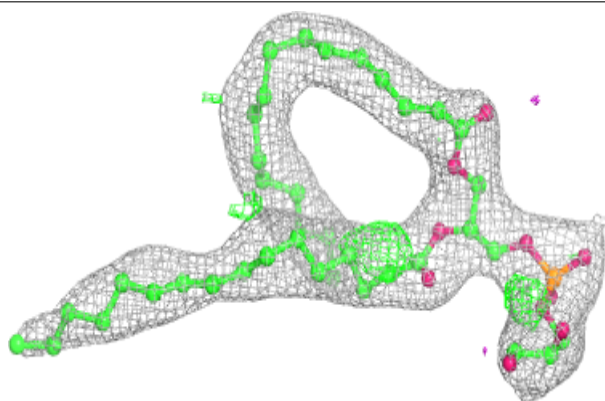


Electron density around CLA c 502:

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

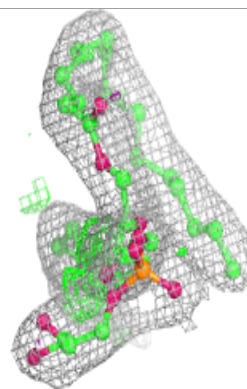
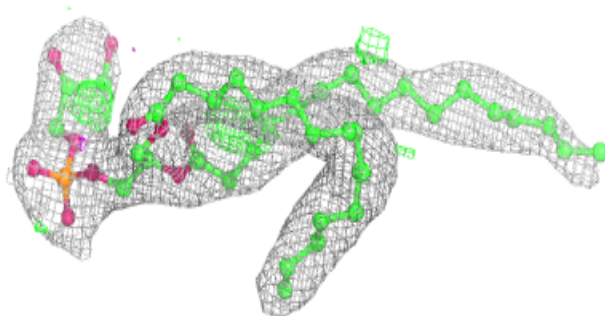
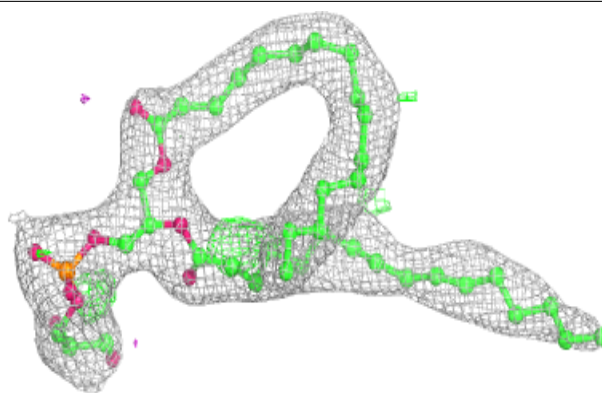
**Electron density around LHG d 414 (A):**

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

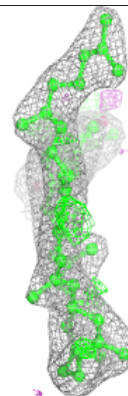
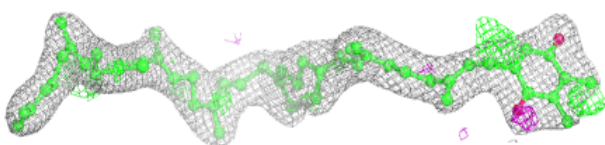
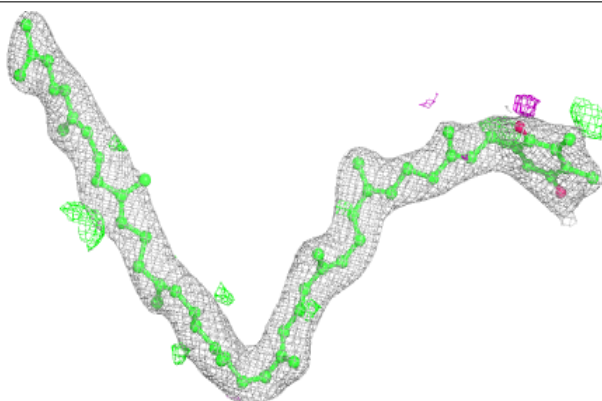


Electron density around LHG d 414 (B):

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

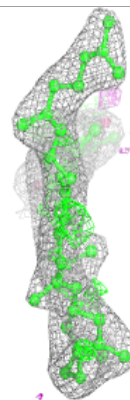
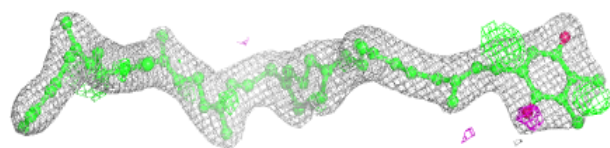
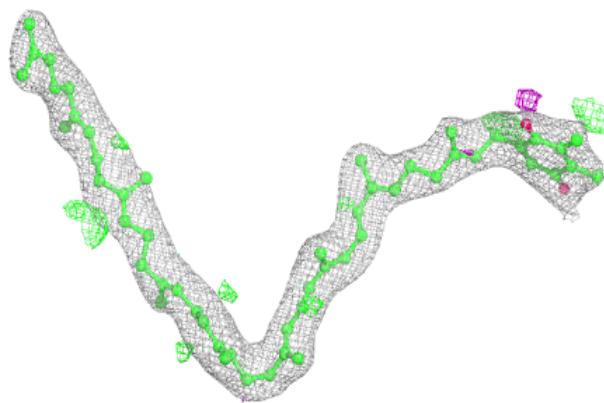
**Electron density around PL9 D 406 (A):**

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

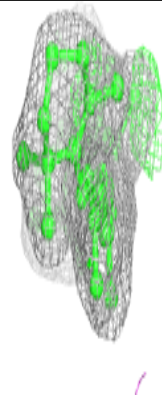
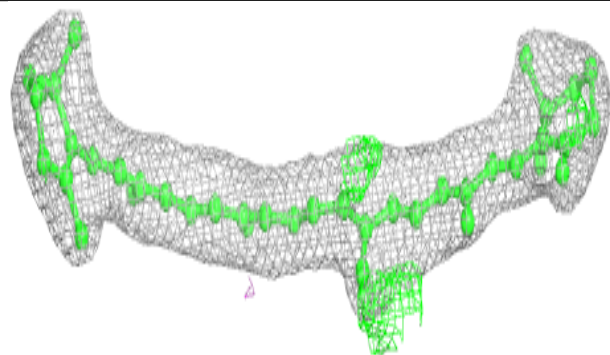
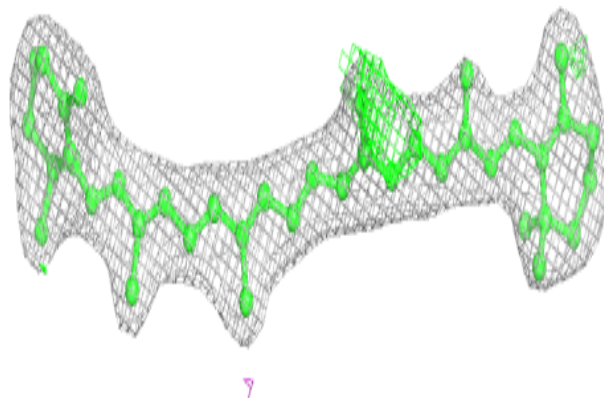


Electron density around PL9 D 406 (B):

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

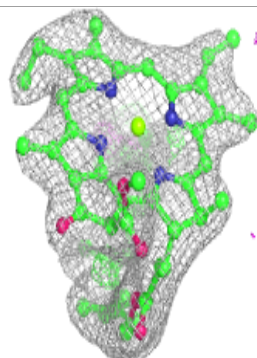
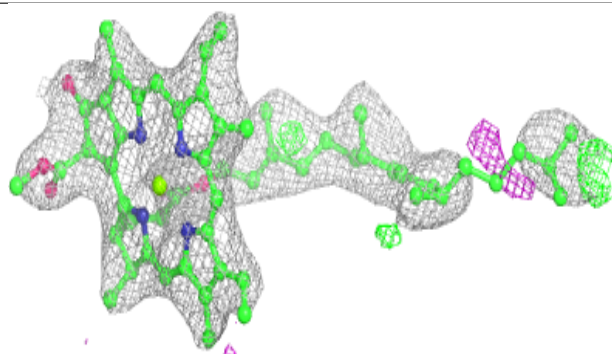
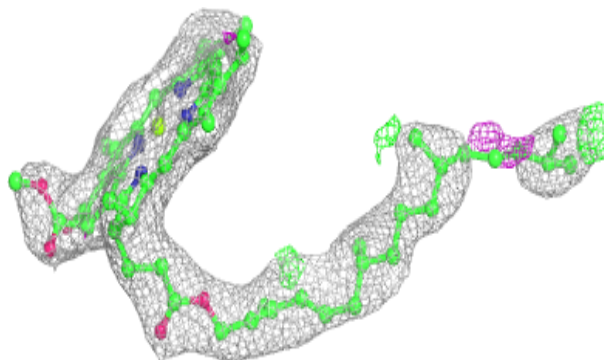
**Electron density around BCR T 101:**

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

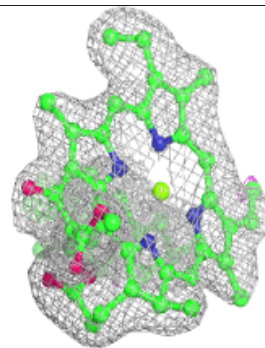
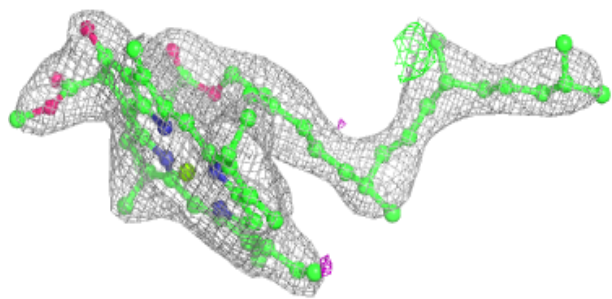
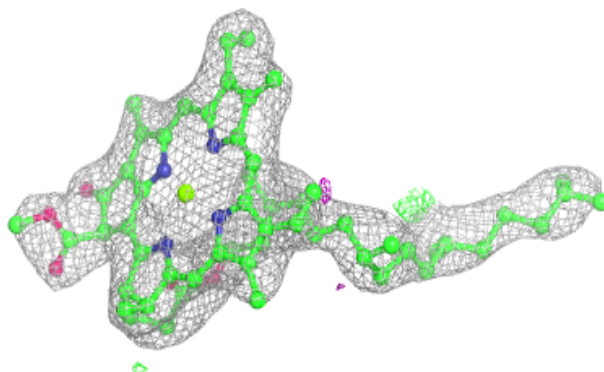


Electron density around CLA c 505:

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

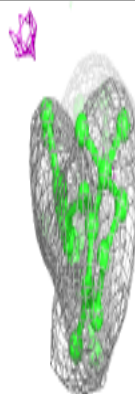
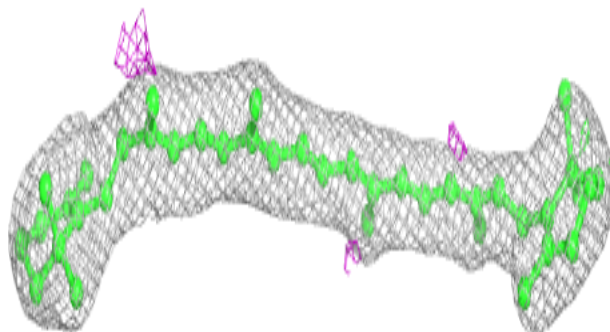
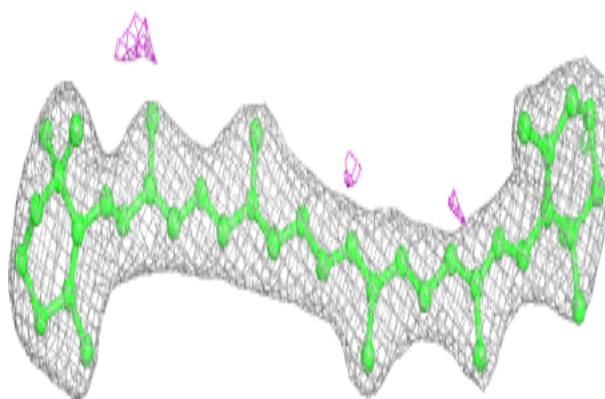
**Electron density around CLA c 506:**

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

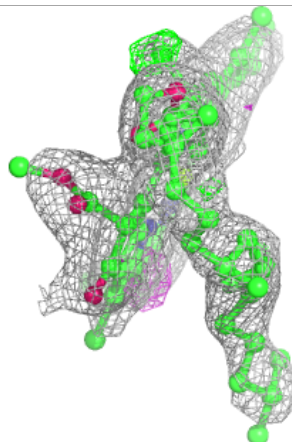
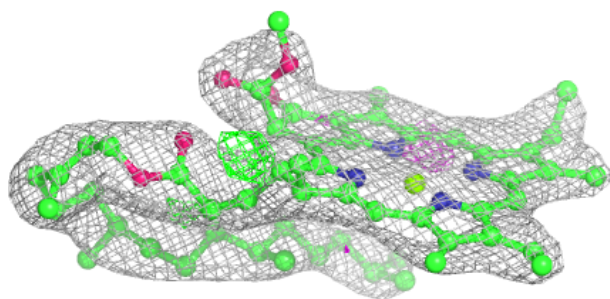
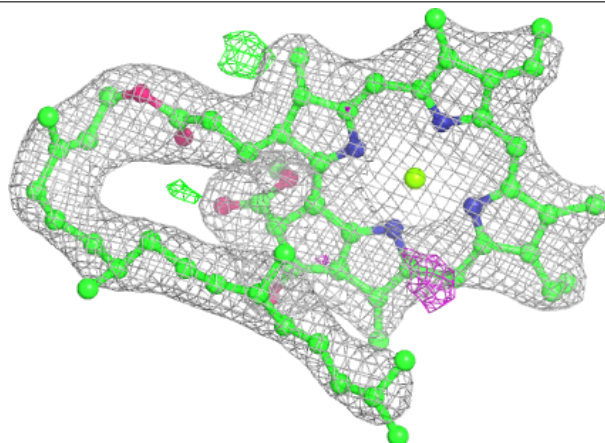


Electron density around BCR b 619:

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

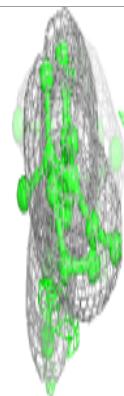
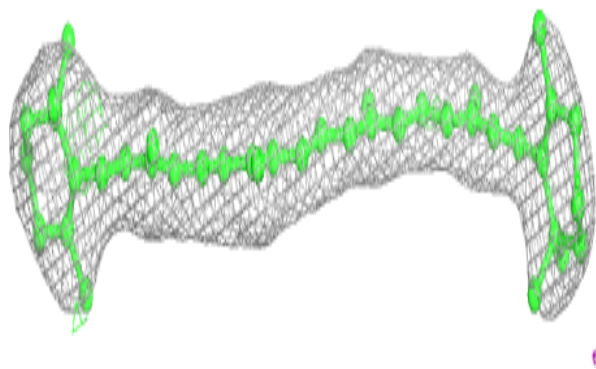
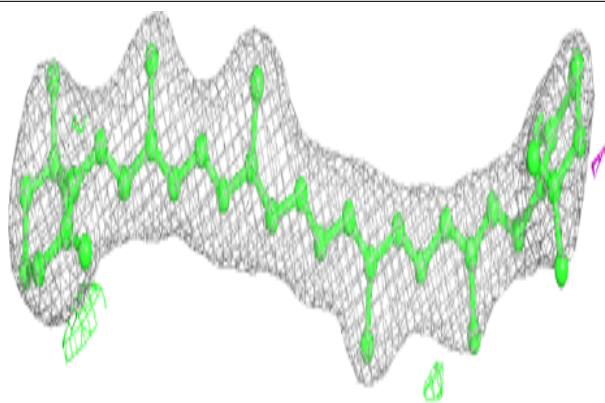
**Electron density around CLA C 509:**

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



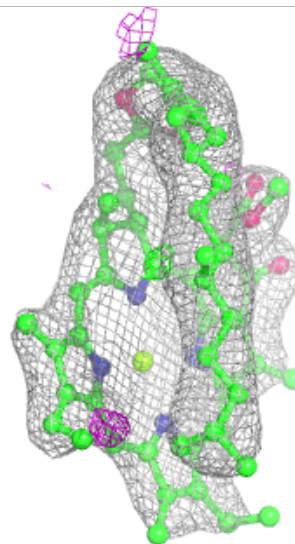
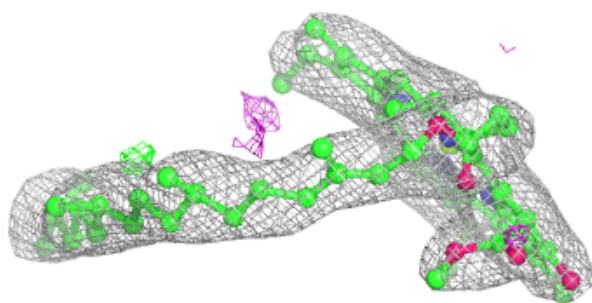
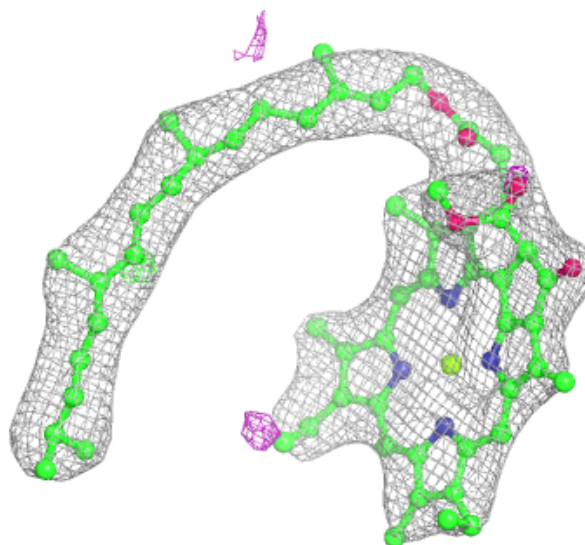
Electron density around BCR c 516:

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



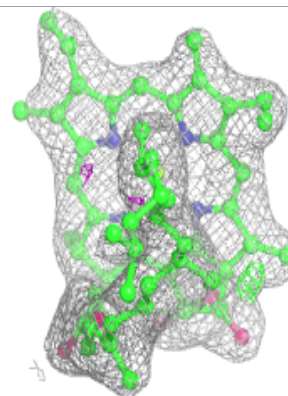
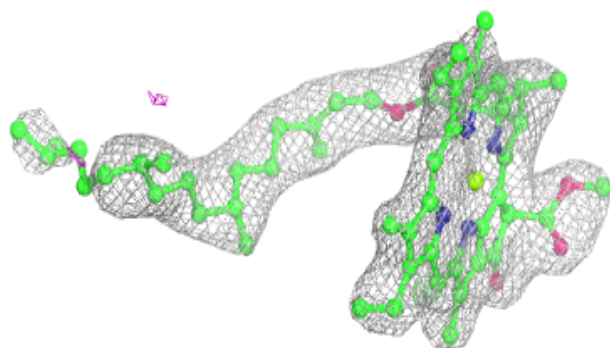
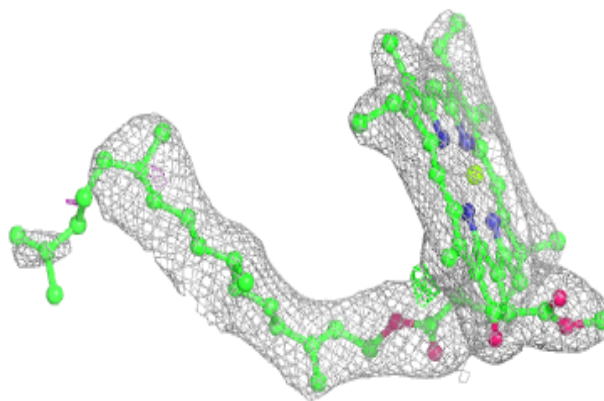
Electron density around CLA c 508:

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

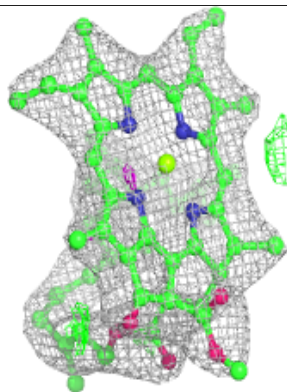
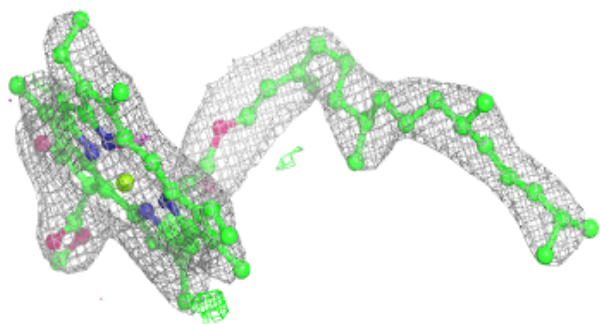
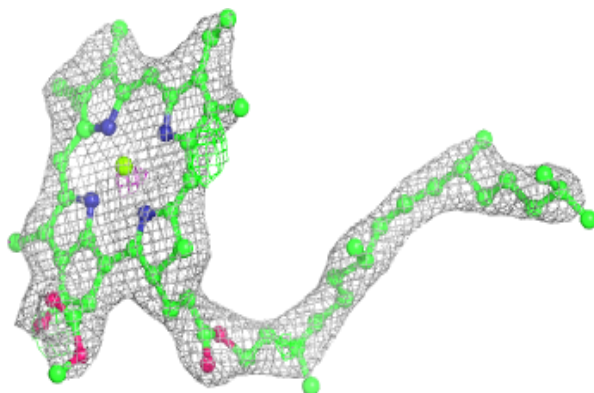


Electron density around CLA c 509:

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

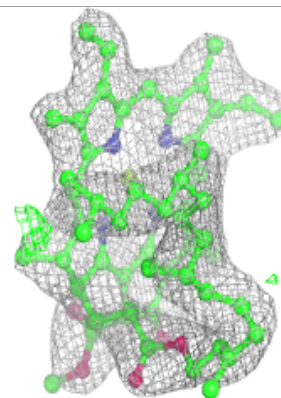
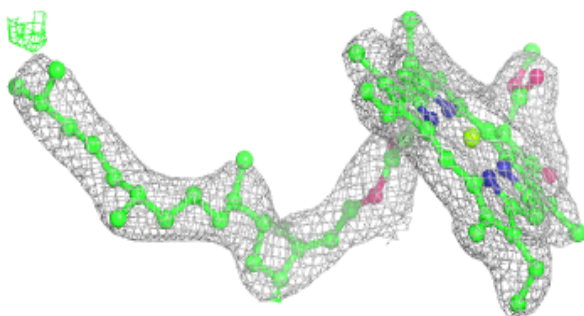
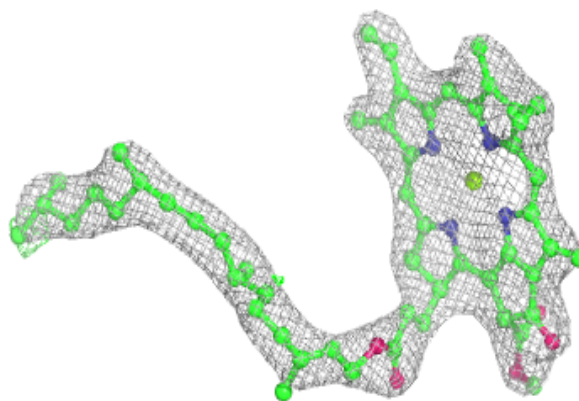
**Electron density around CLA c 512:**

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

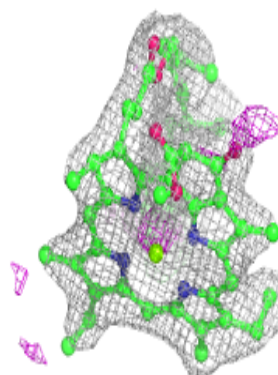
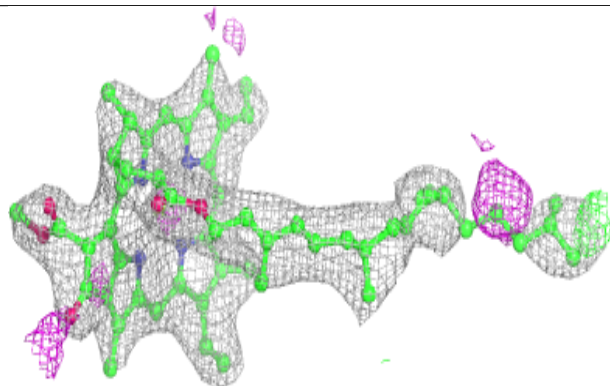
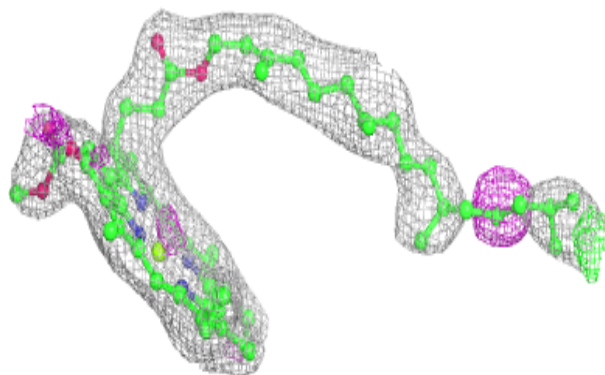


Electron density around CLA C 511:

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

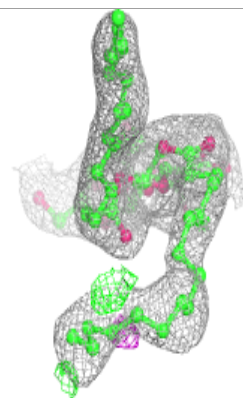
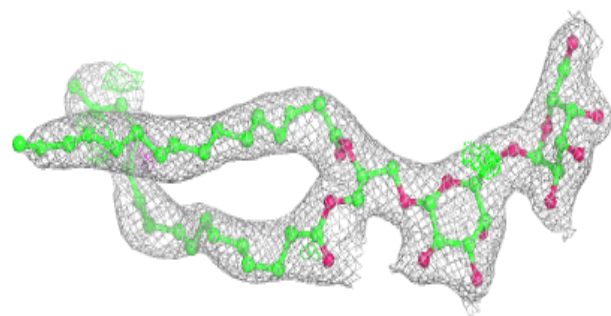
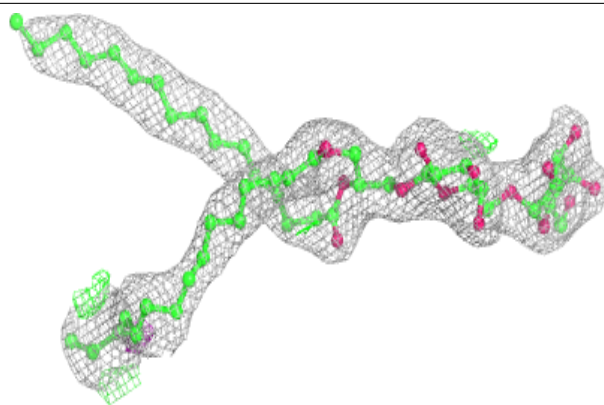
**Electron density around CLA C 504:**

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

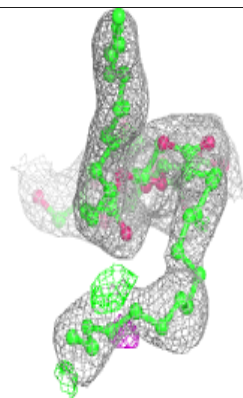
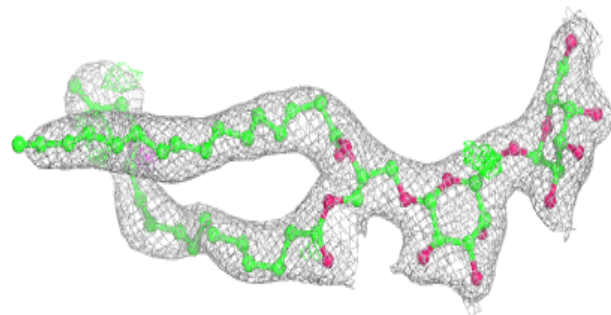
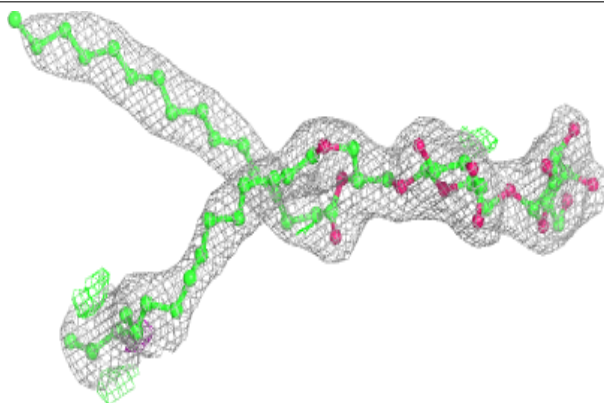


Electron density around DGD c 517 (A):

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

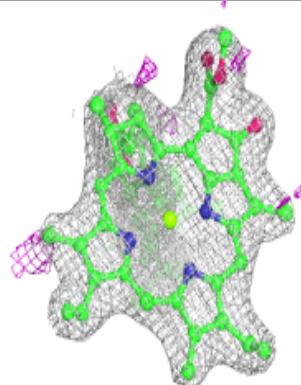
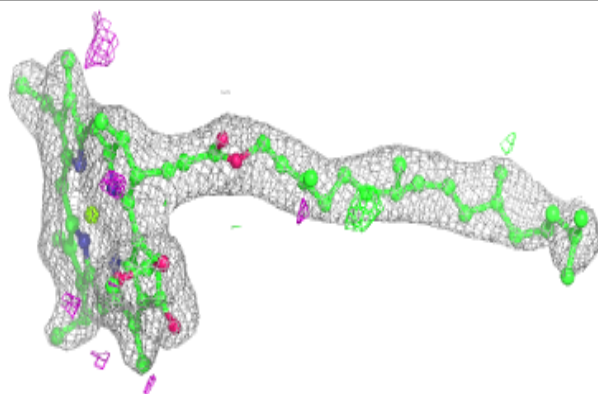
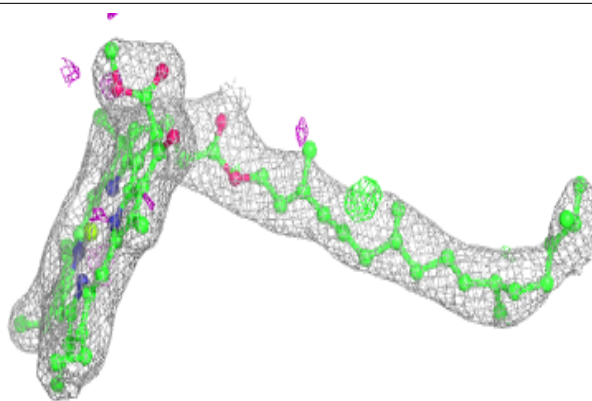
**Electron density around DGD c 517 (B):**

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

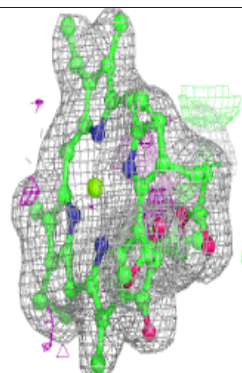
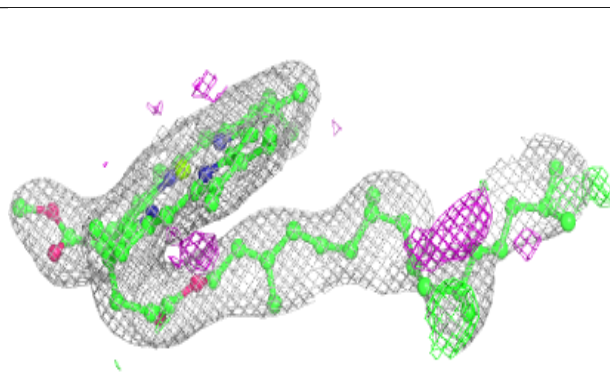
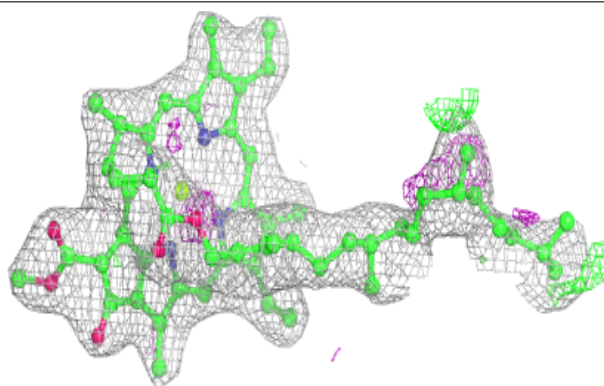


Electron density around CLA b 604:

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

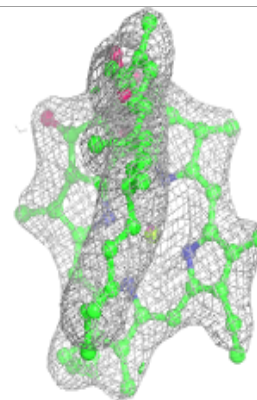
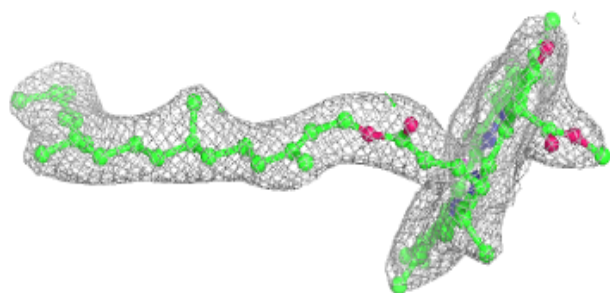
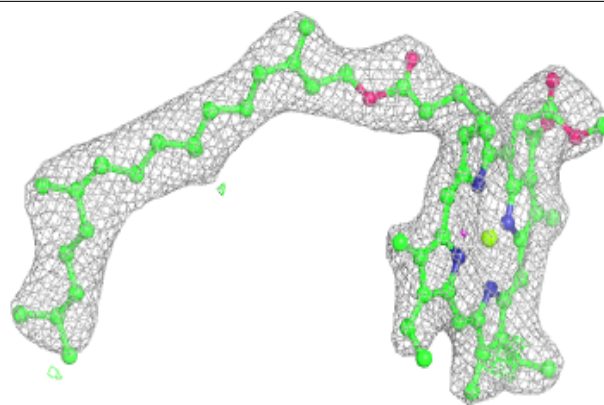
**Electron density around CLA B 614:**

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

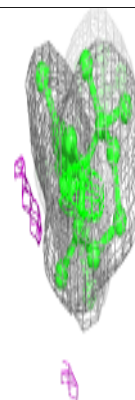
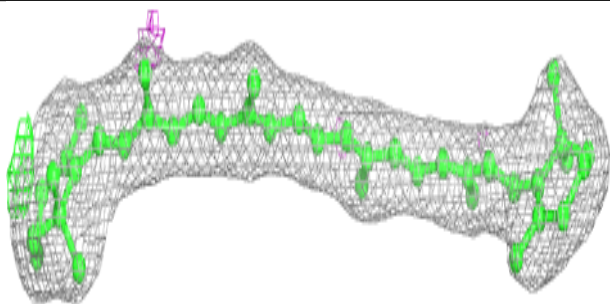
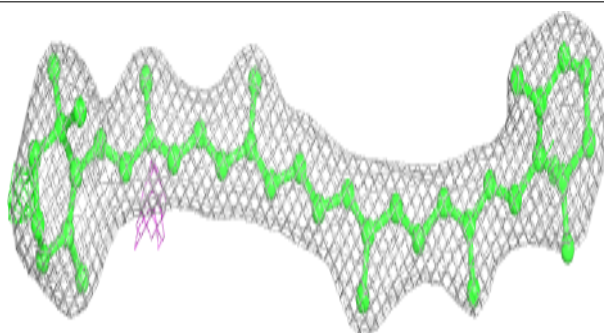


Electron density around CLA b 609:

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

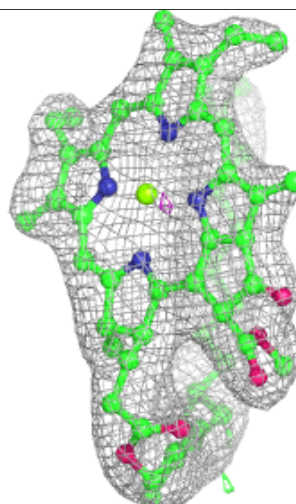
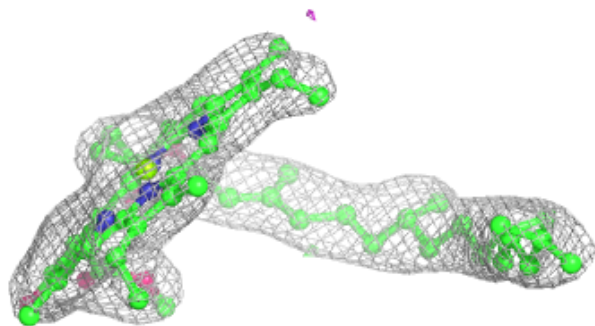
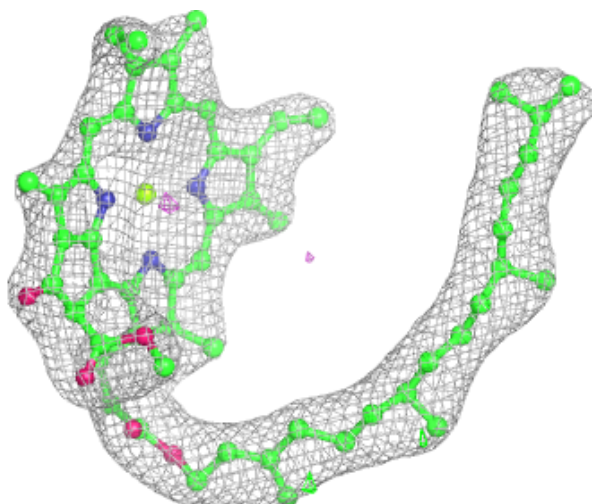
**Electron density around BCR B 619:**

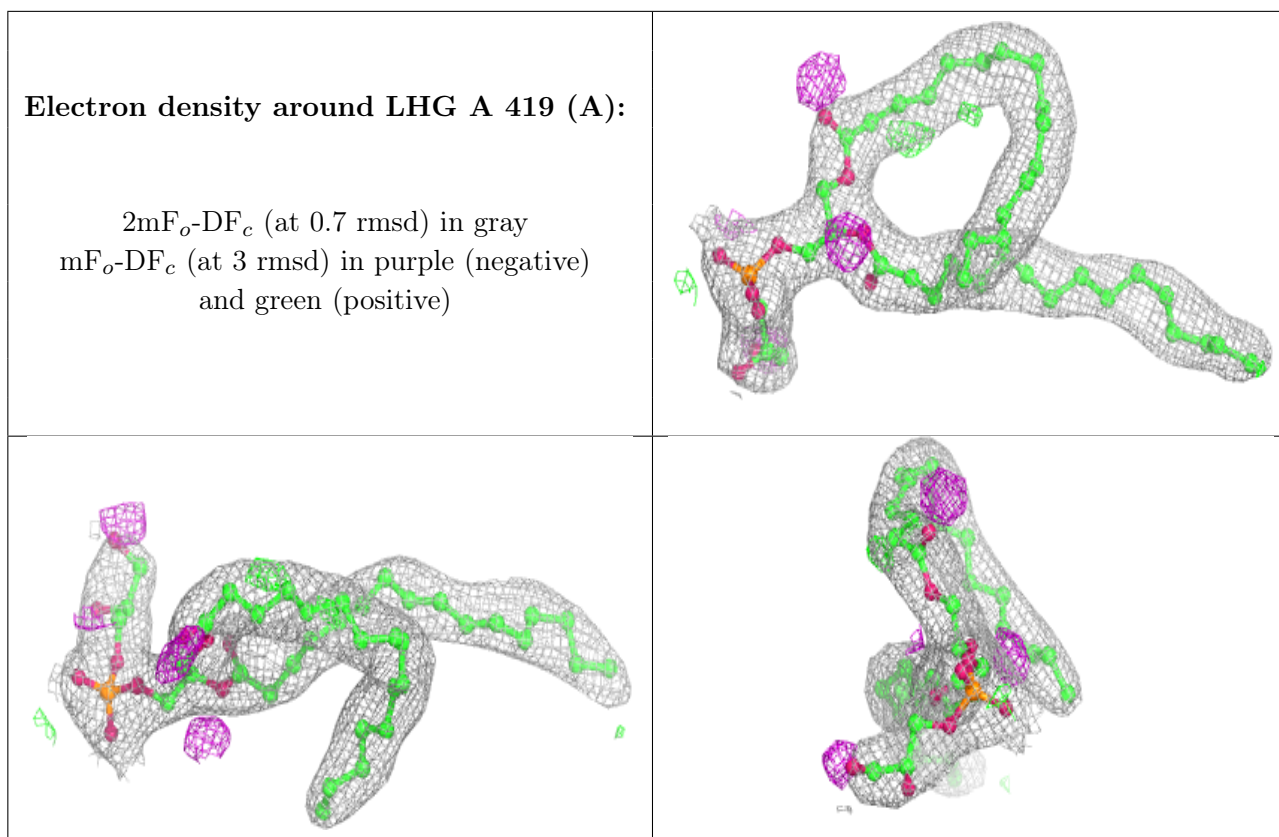
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 507:

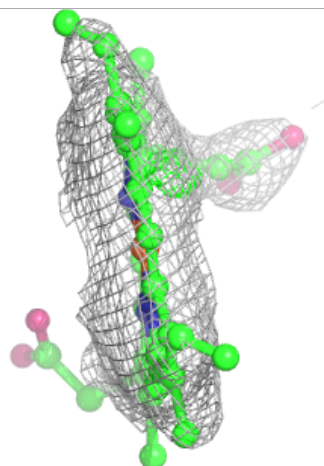
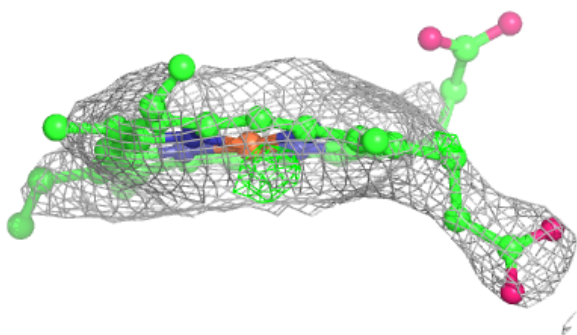
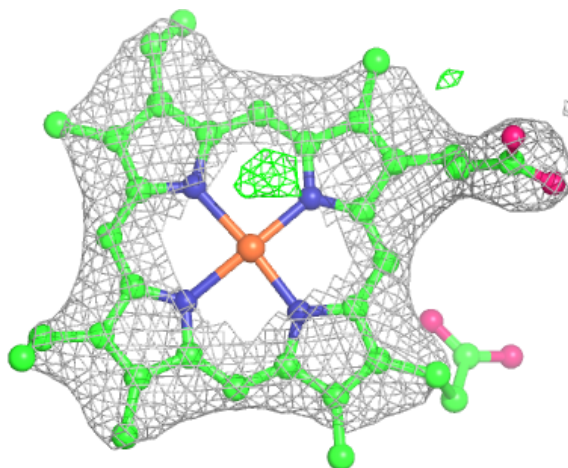
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





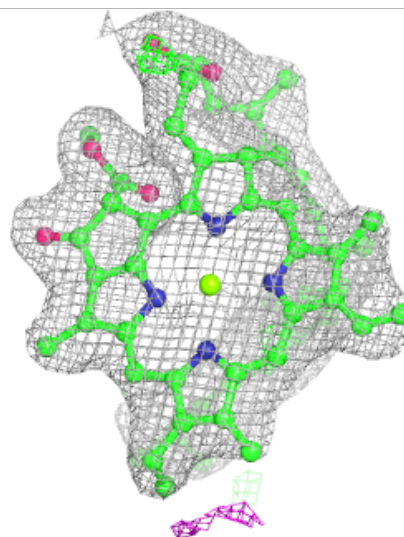
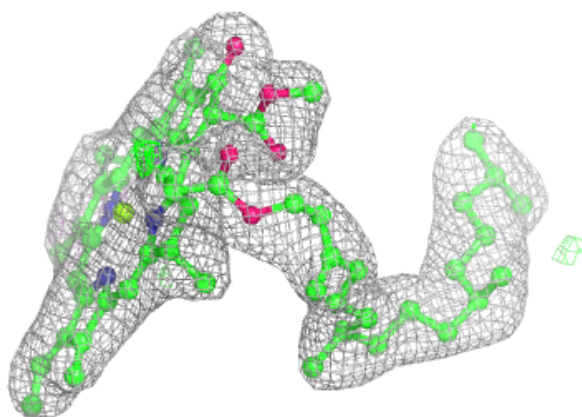
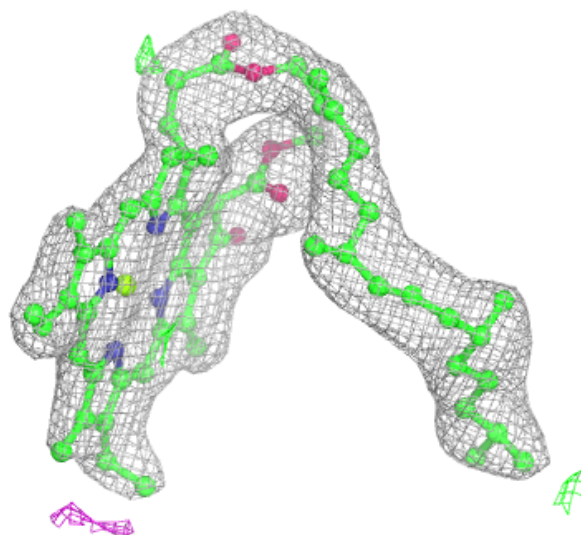
Electron density around HEM f 101:

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



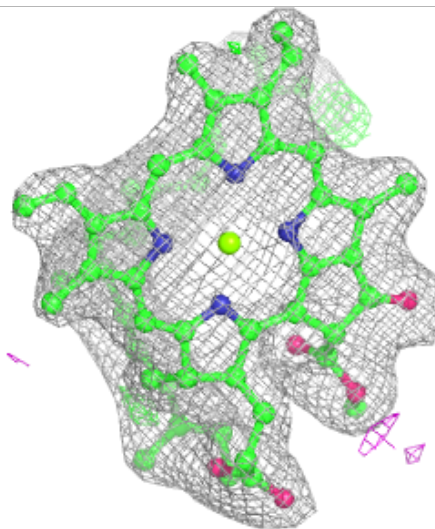
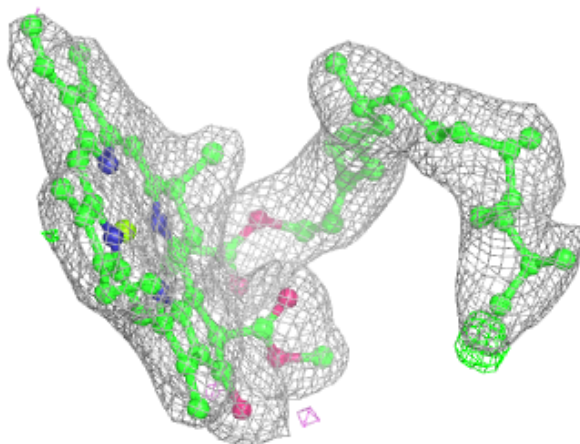
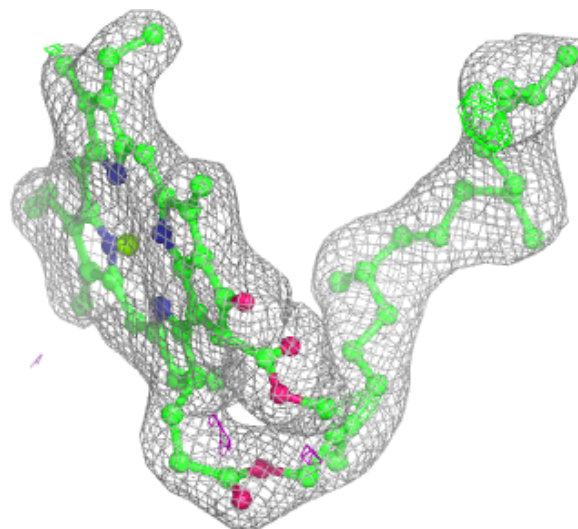
Electron density around CLA b 613:

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



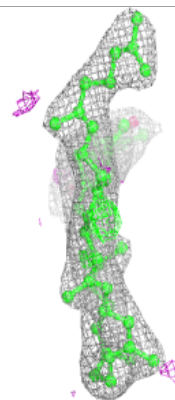
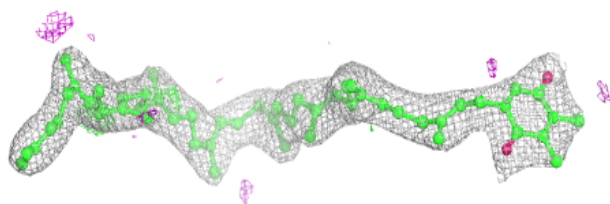
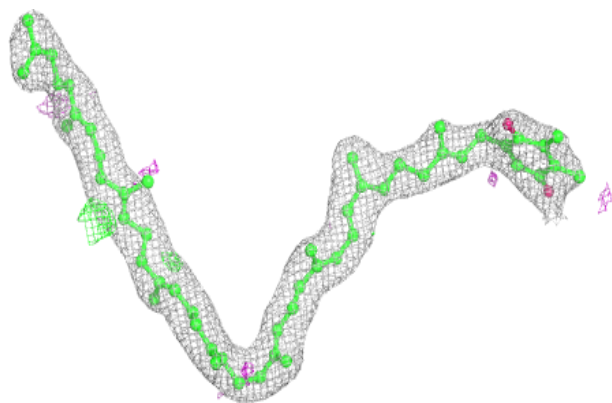
Electron density around CLA B 613:

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

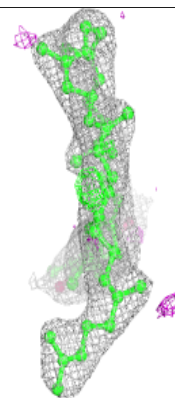
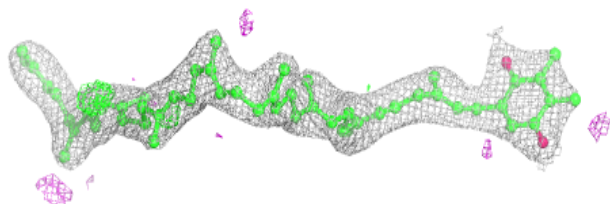
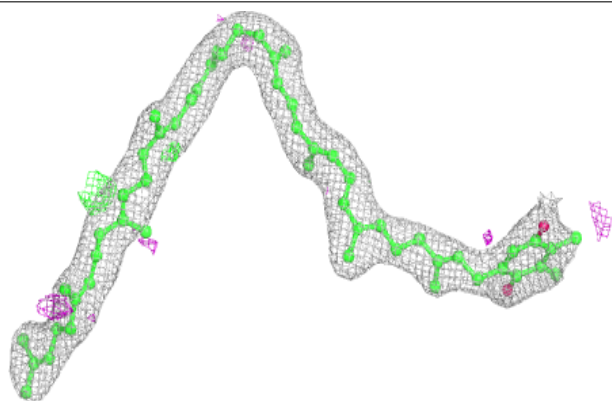


Electron density around PL9 d 406 (A):

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

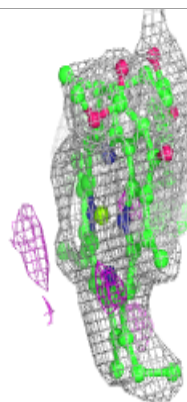
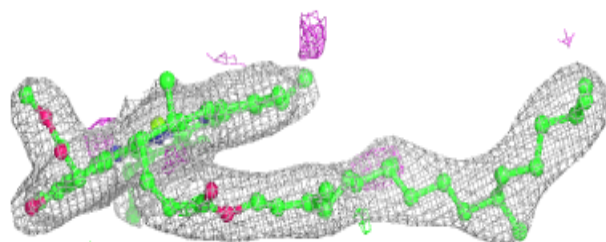
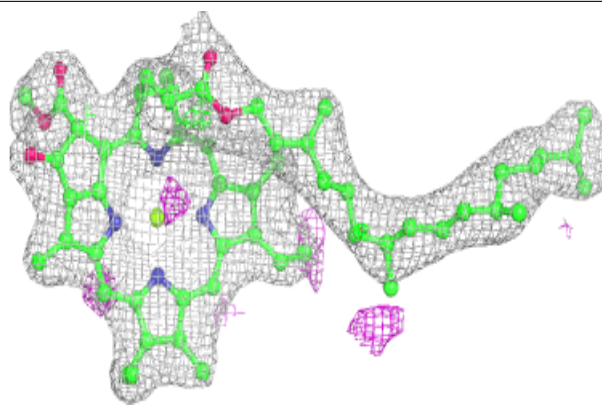
**Electron density around PL9 d 406 (B):**

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

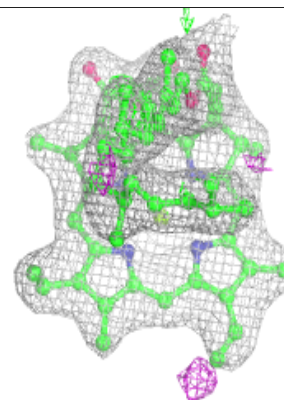
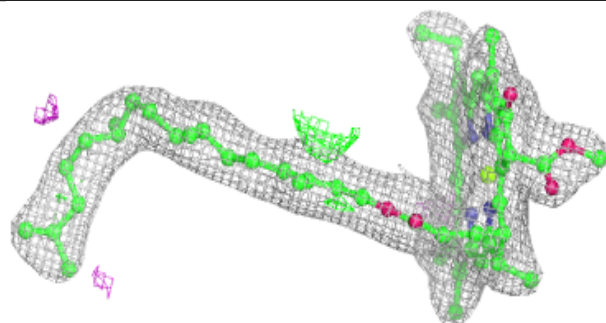
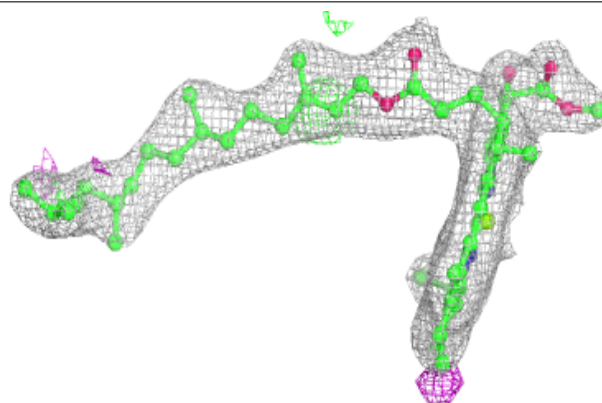


Electron density around CLA B 603:

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

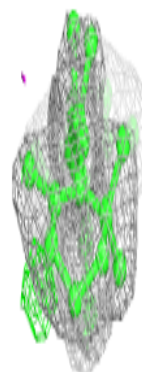
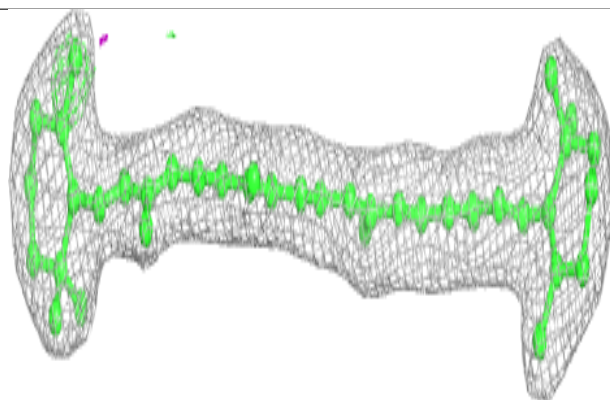
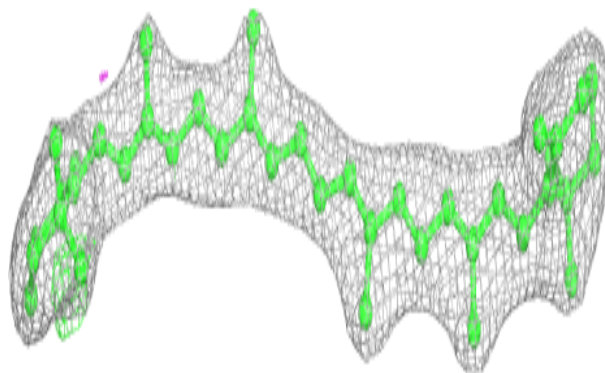
**Electron density around CLA B 605:**

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

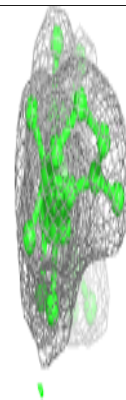
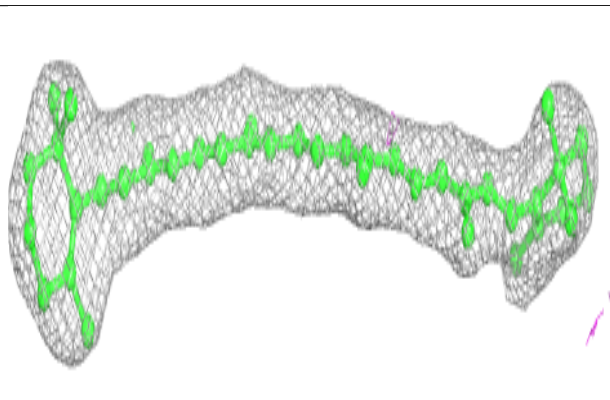
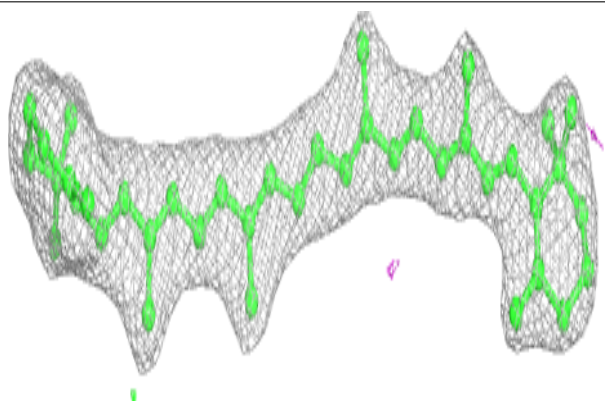


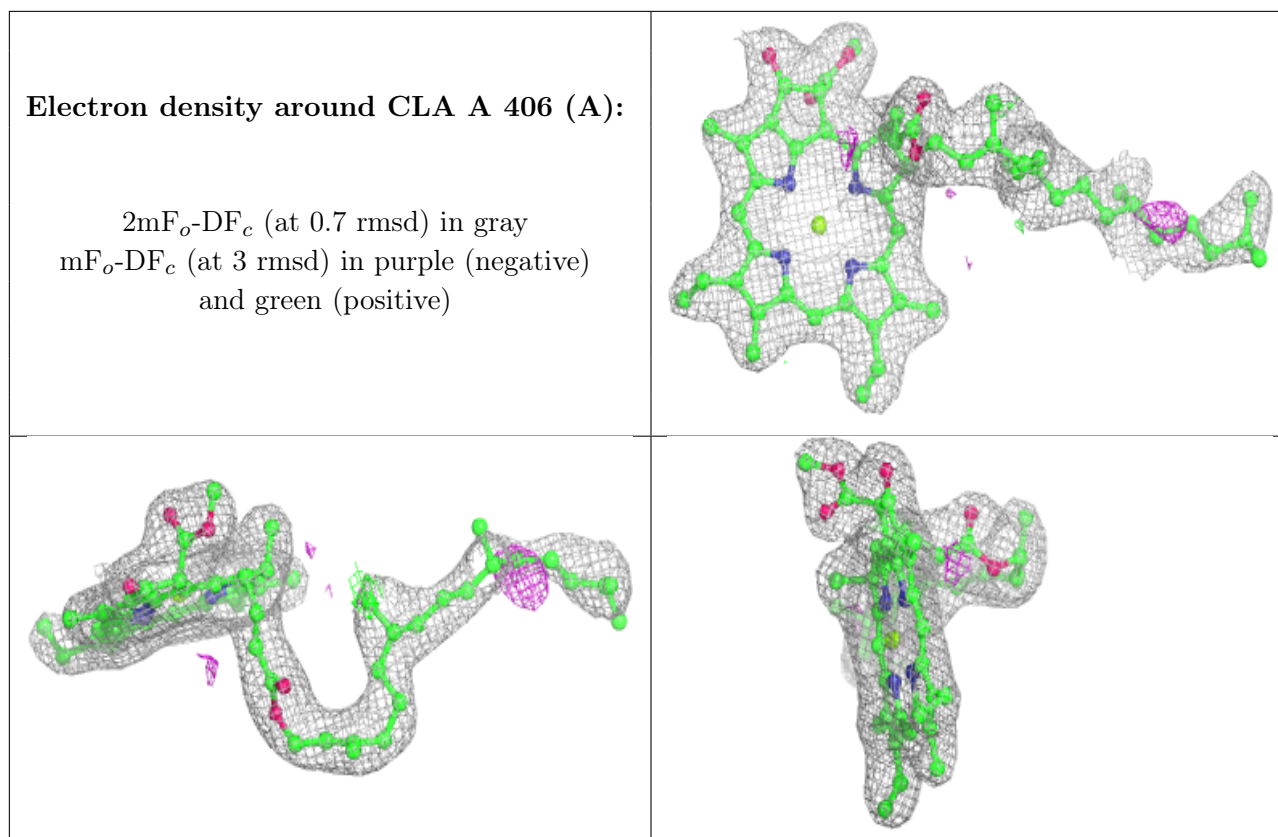
Electron density around BCR a 408:

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

**Electron density around BCR b 617:**

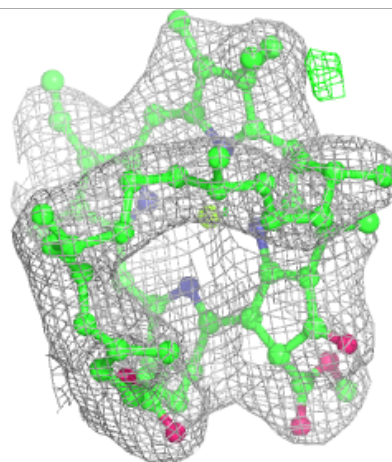
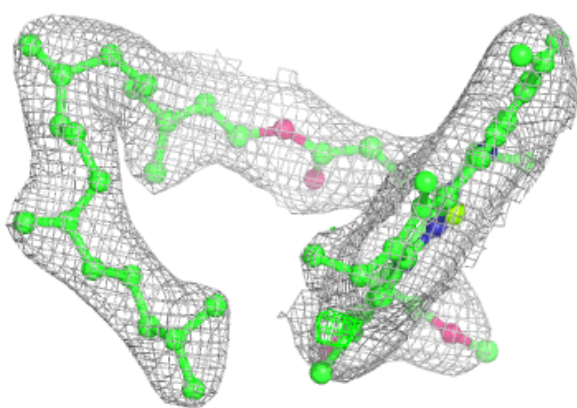
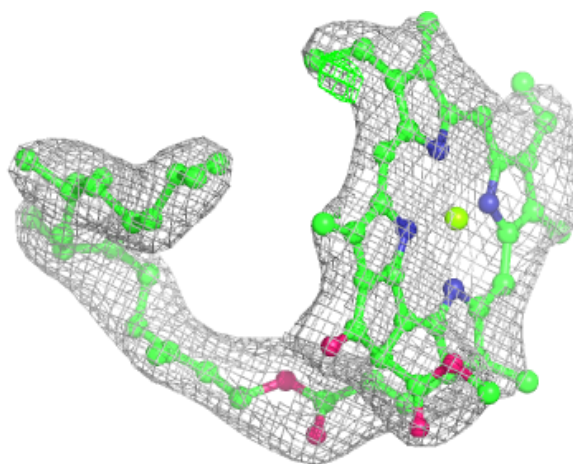
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





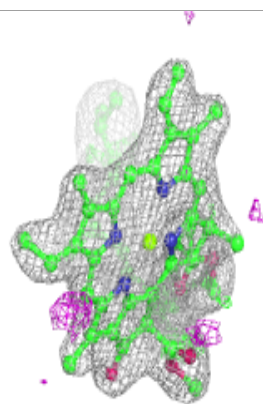
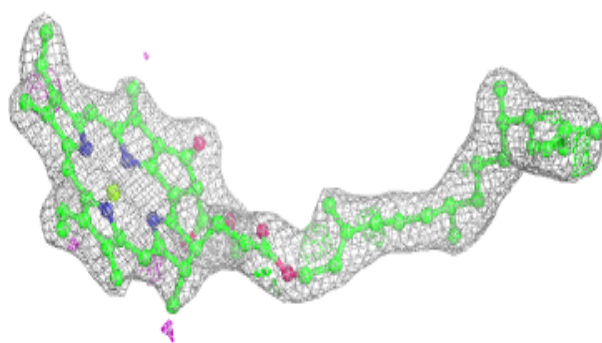
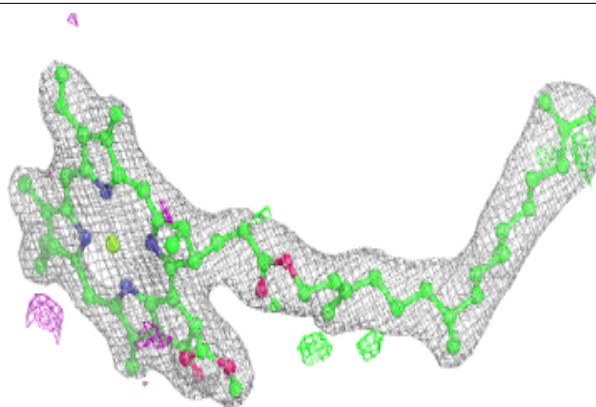
Electron density around CLA c 504:

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

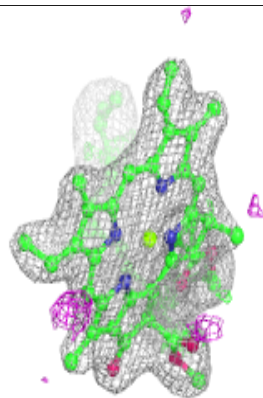
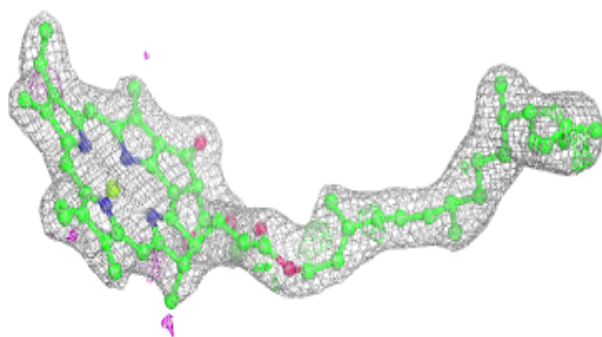
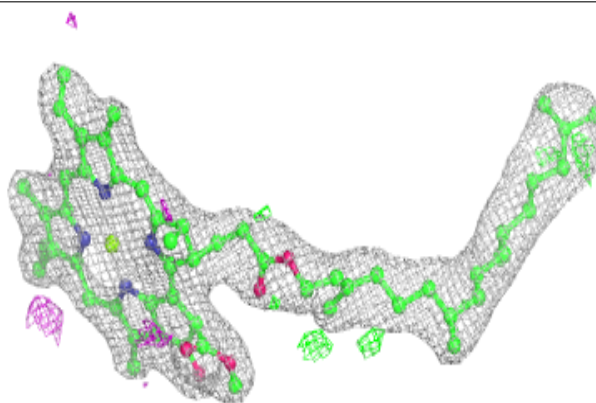


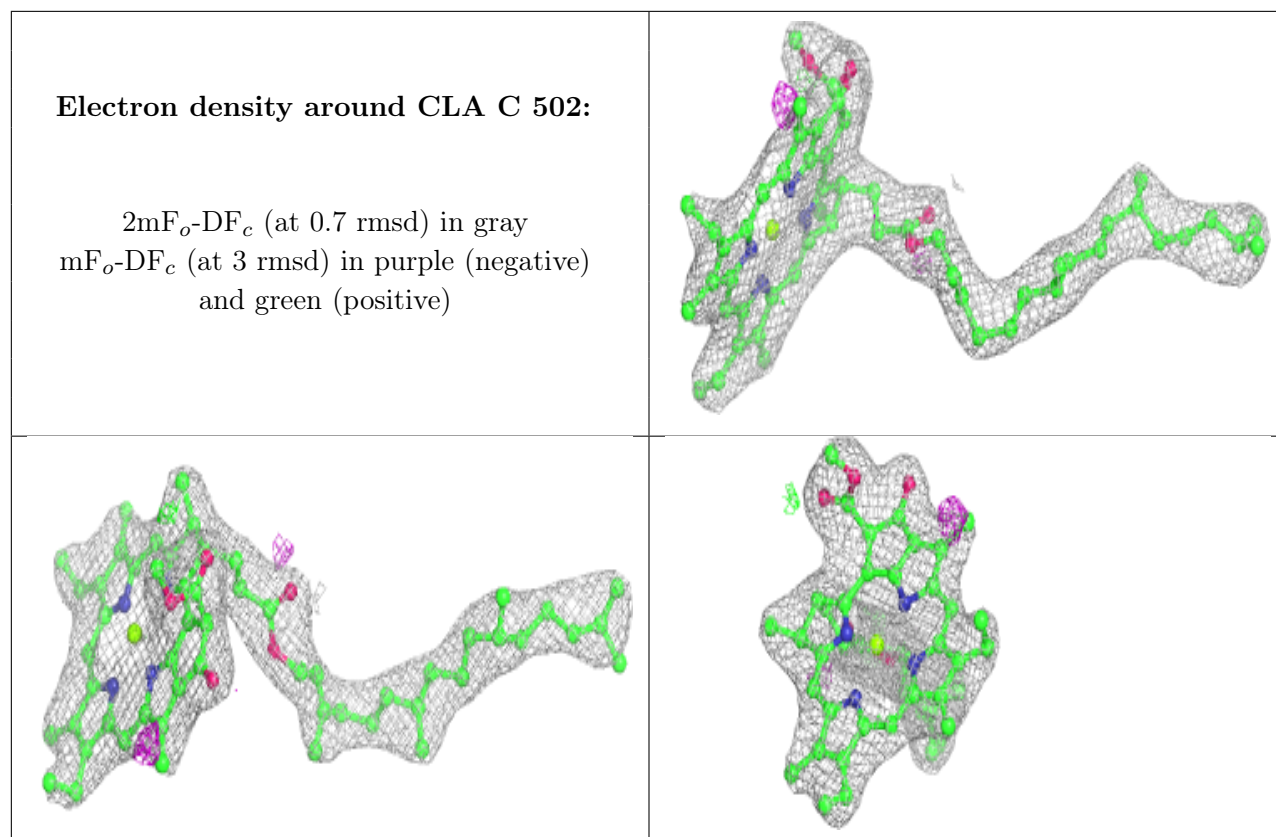
Electron density around CLA a 404 (A):

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

**Electron density around CLA a 404 (B):**

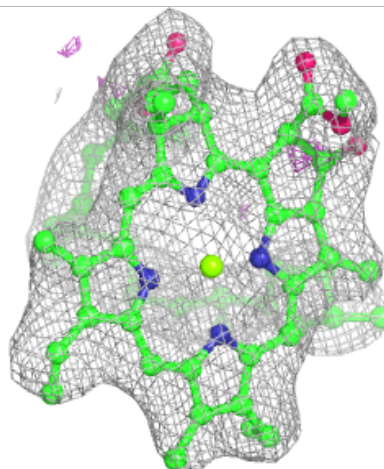
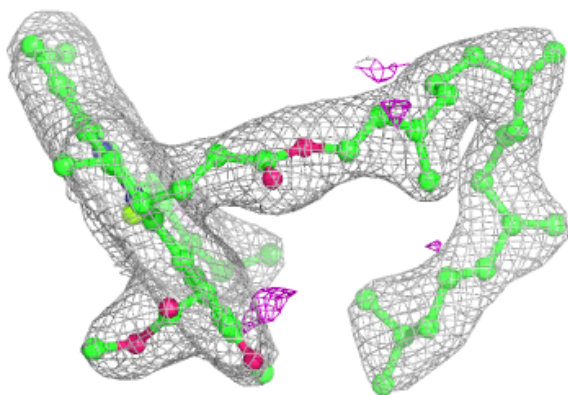
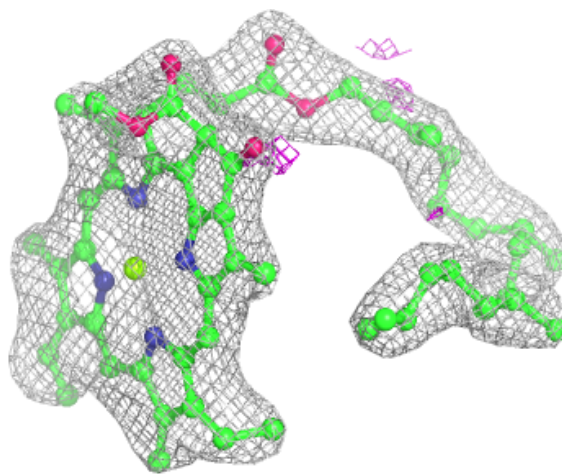
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





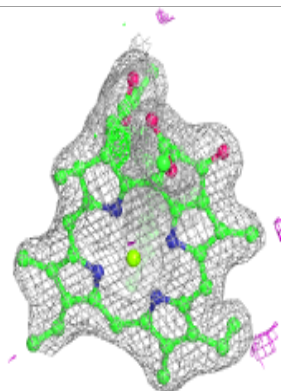
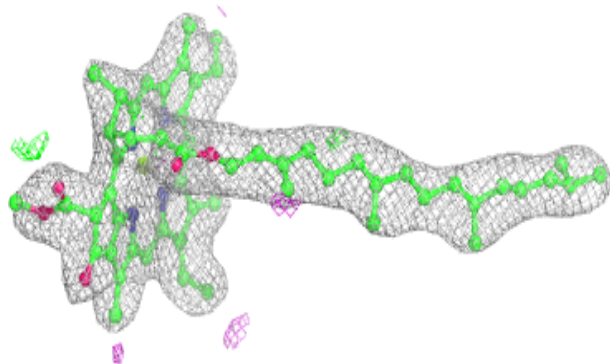
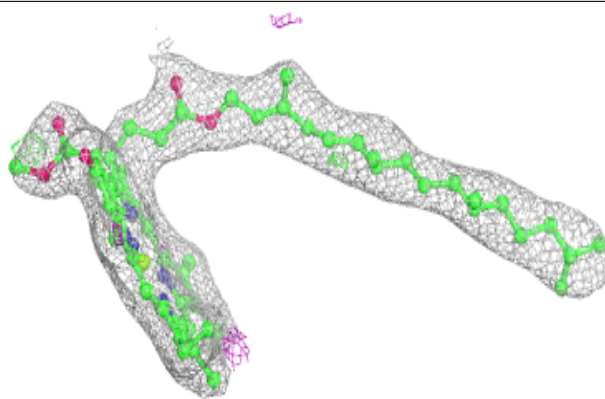
Electron density around CLA C 503:

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

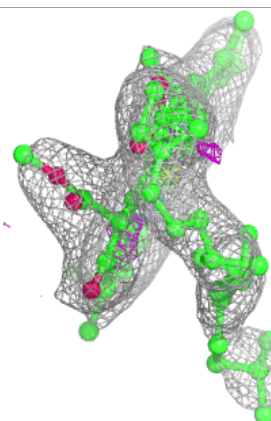
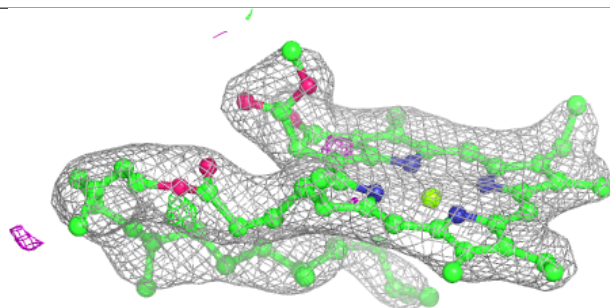
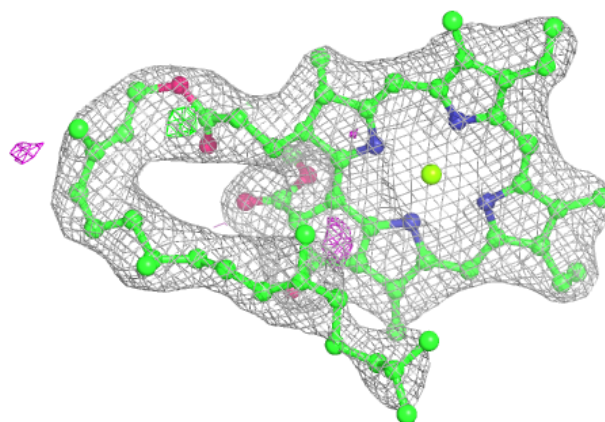


Electron density around CLA B 607:

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

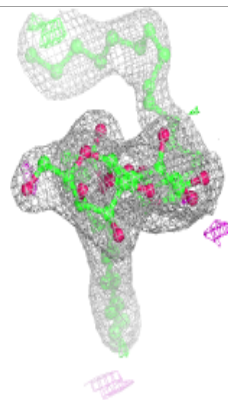
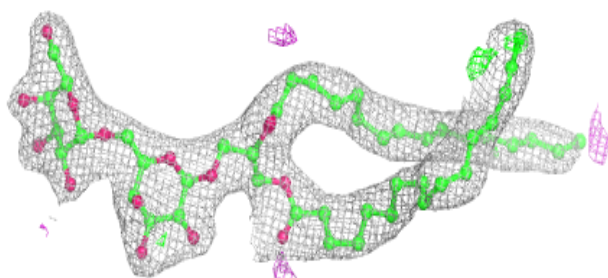
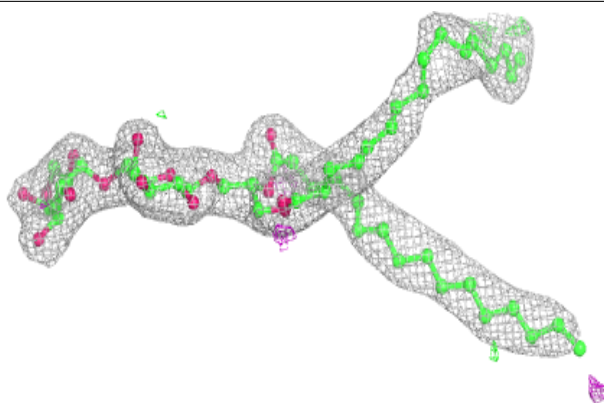
**Electron density around CLA c 510:**

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

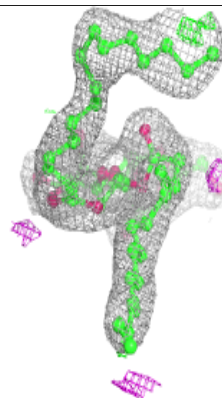
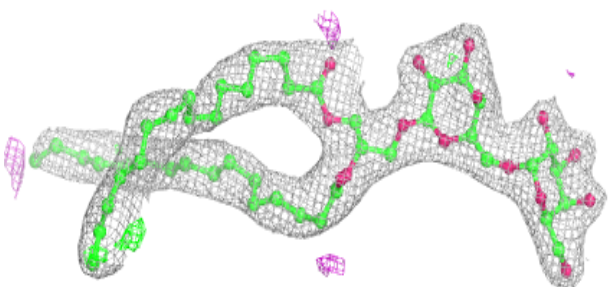
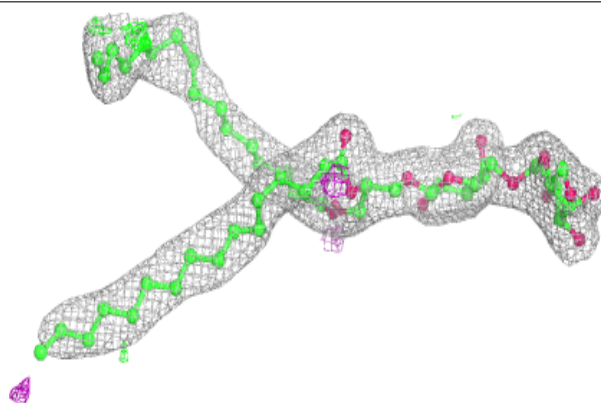


Electron density around DGD C 516 (A):

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

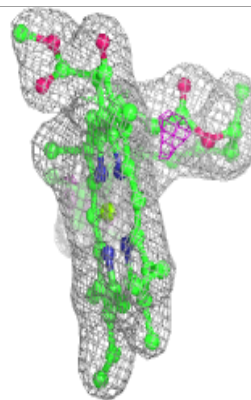
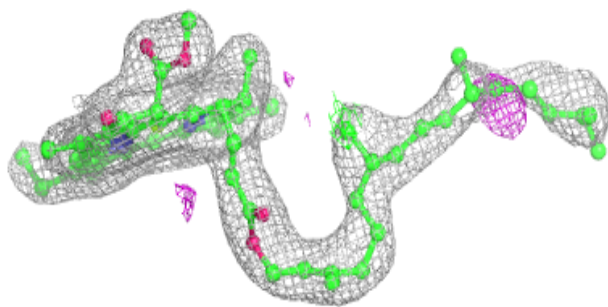
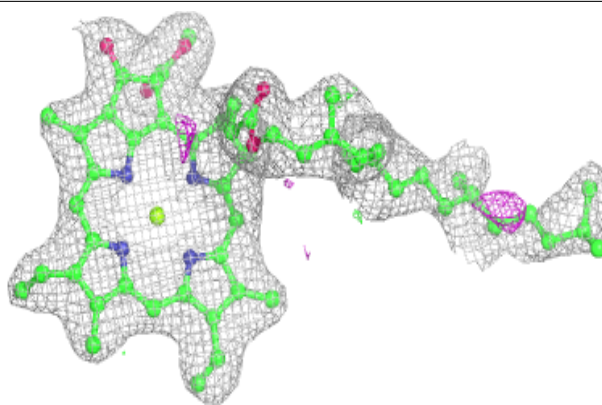
**Electron density around DGD C 516 (B):**

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

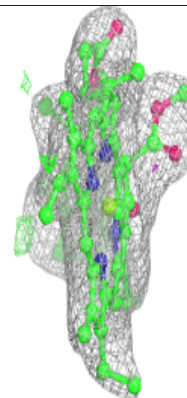
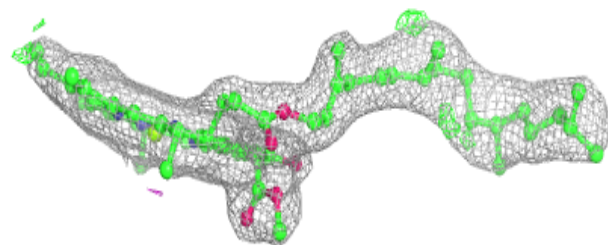
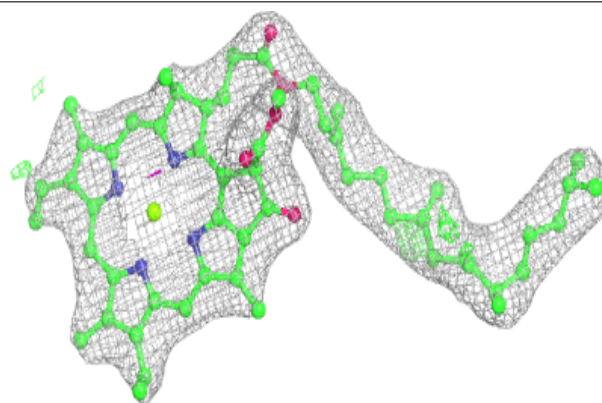


Electron density around CLA A 406 (B):

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

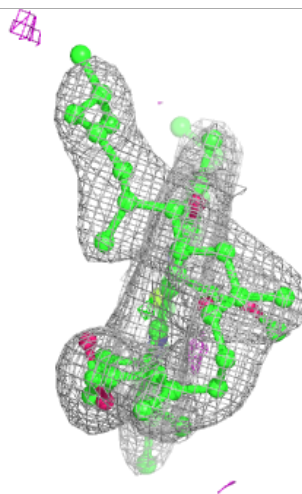
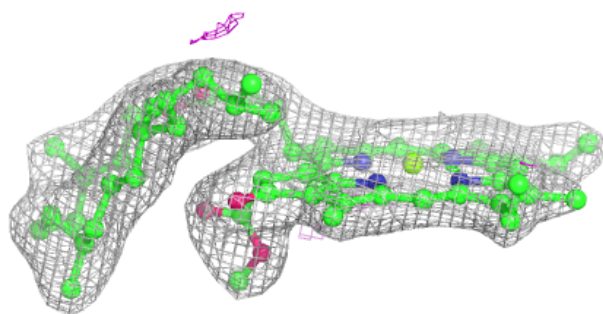
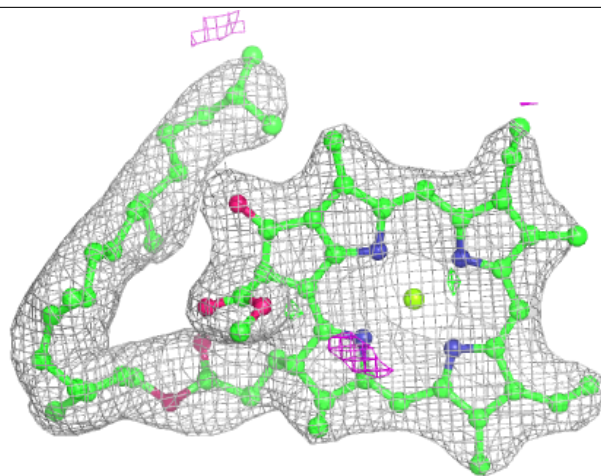
**Electron density around CLA b 602:**

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



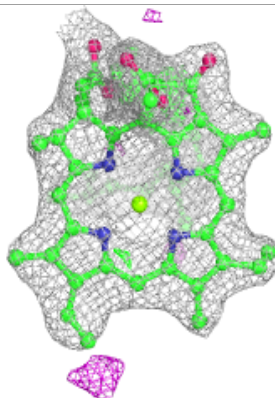
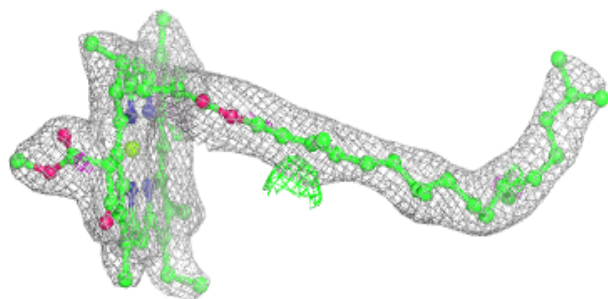
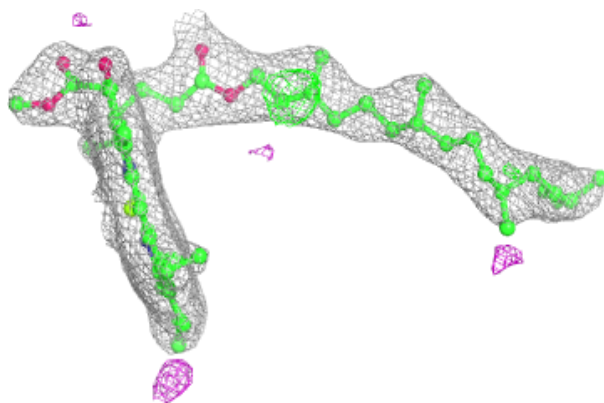
Electron density around CLA B 610:

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



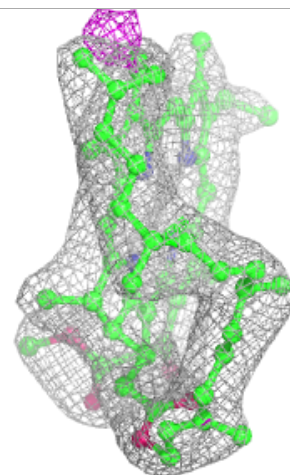
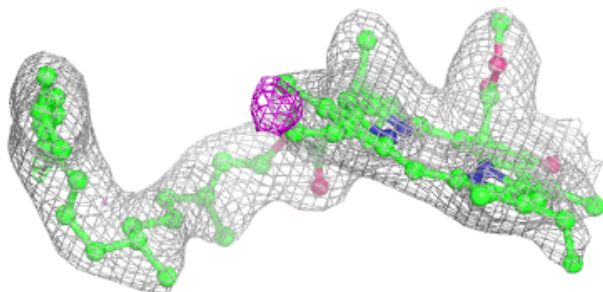
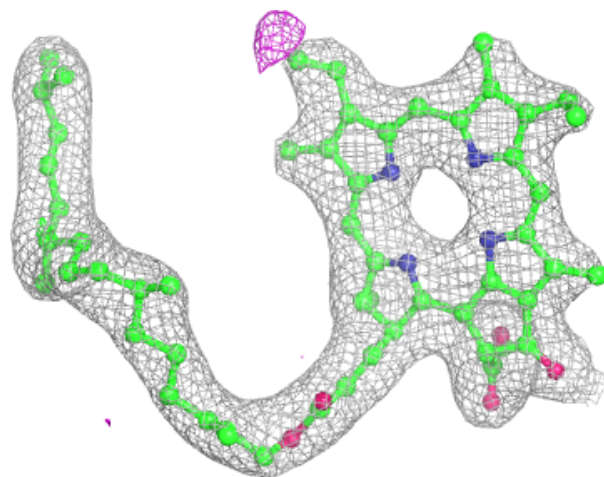
Electron density around CLA b 605:

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



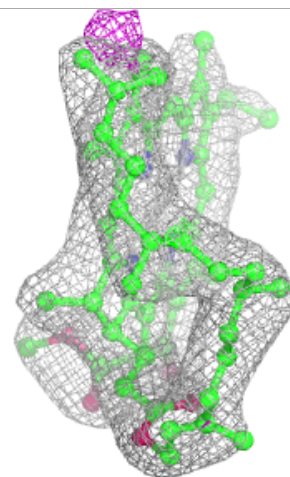
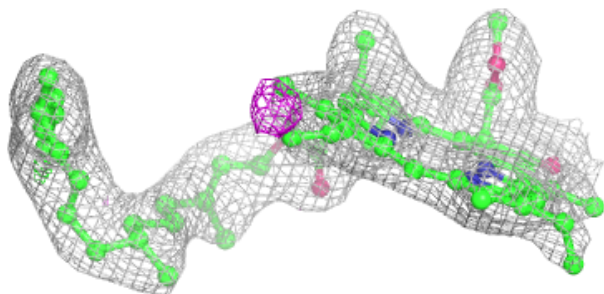
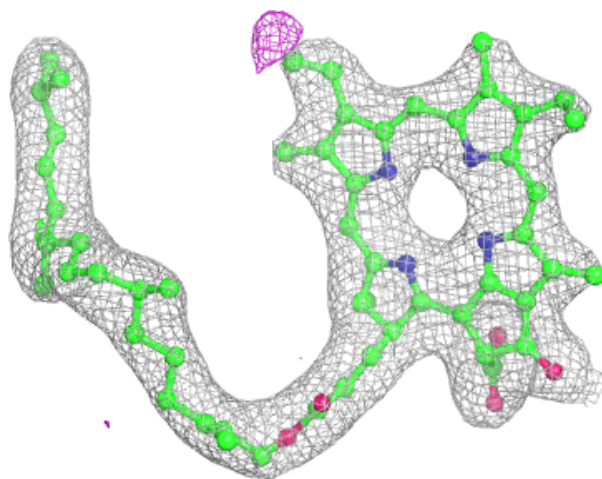
Electron density around PHO a 414 (A):

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



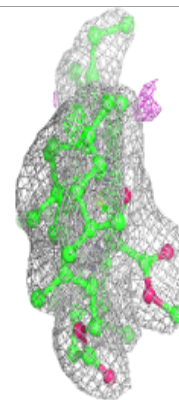
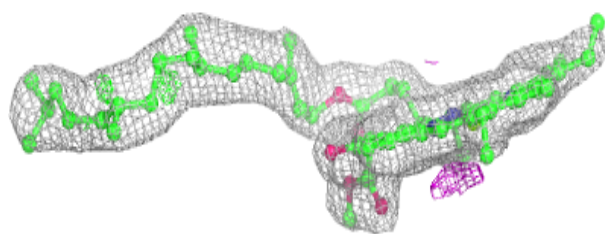
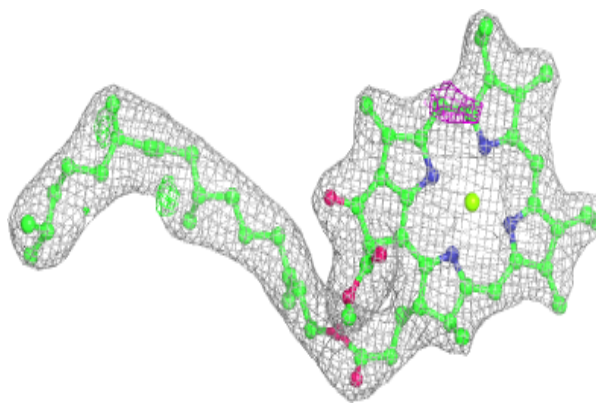
Electron density around PHO a 414 (B):

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

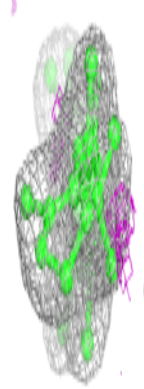
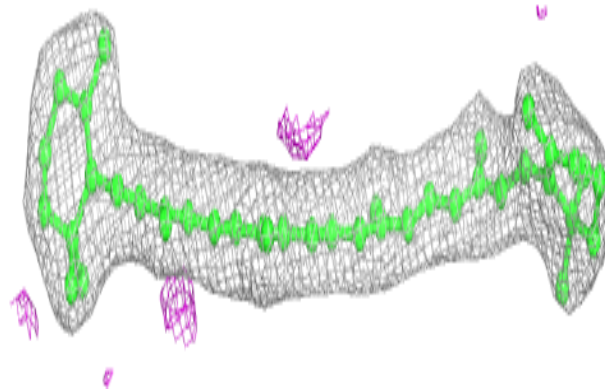
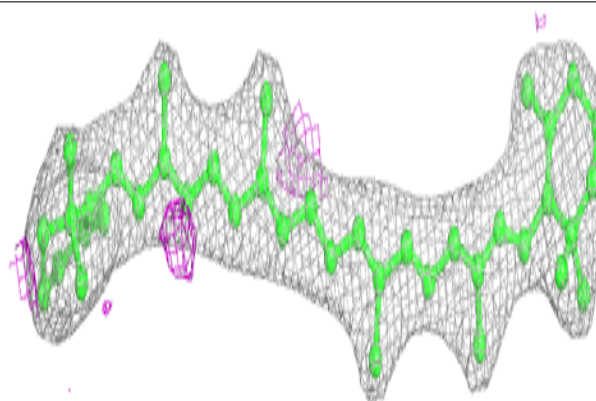


Electron density around CLA B 602:

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

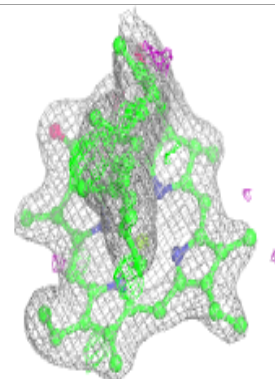
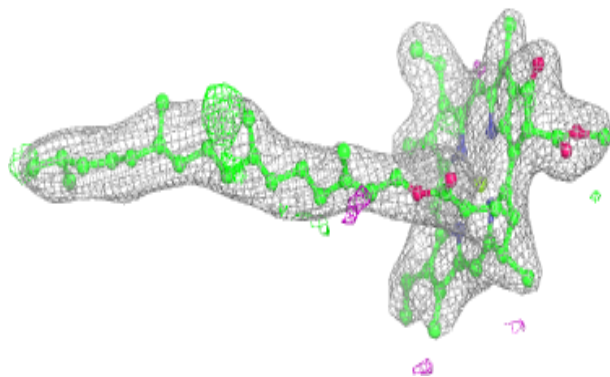
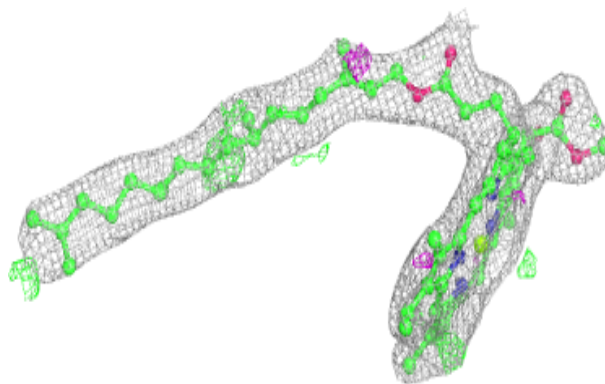
**Electron density around BCR B 617:**

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



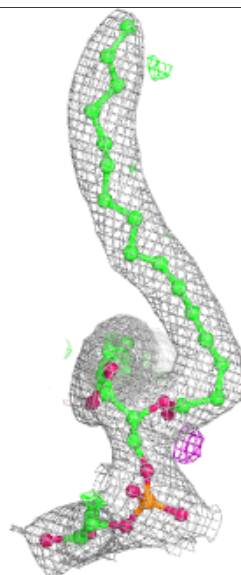
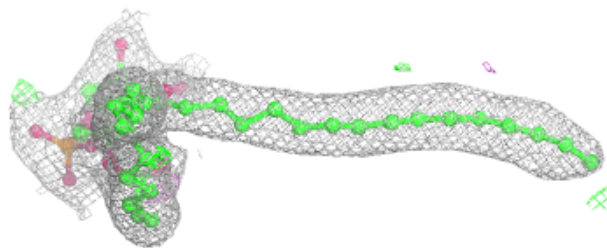
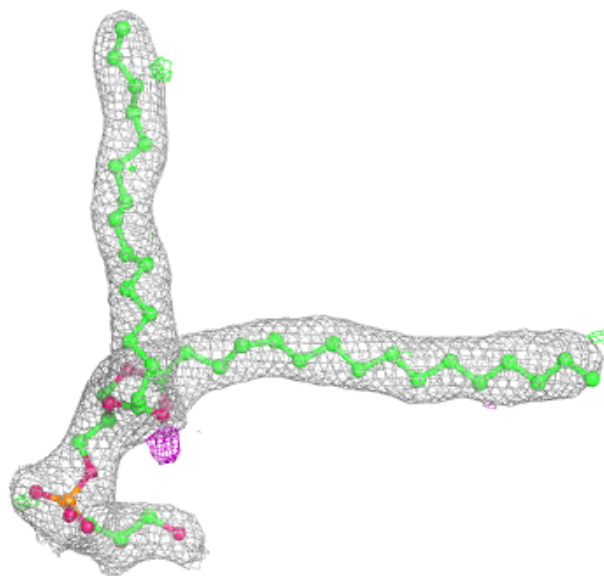
Electron density around CLA b 607:

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



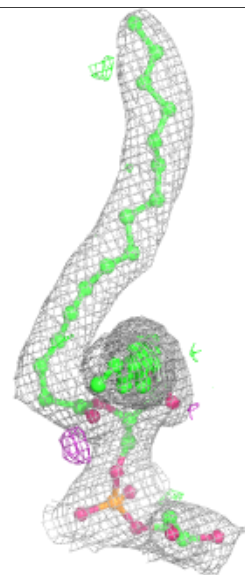
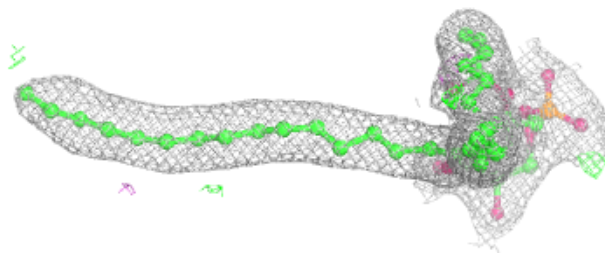
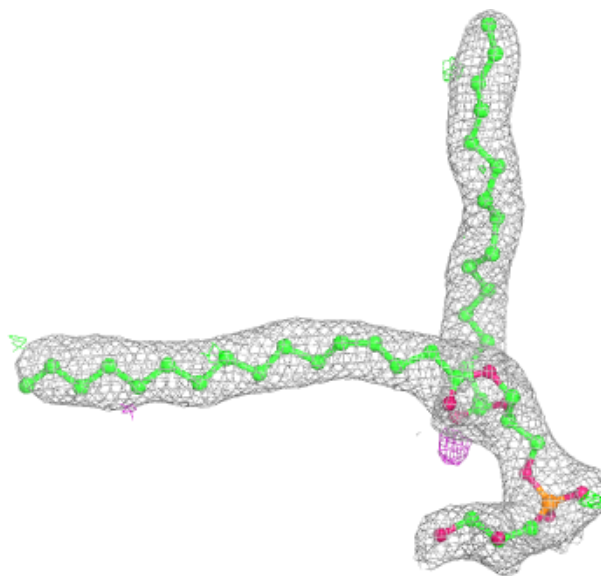
Electron density around LHG L 101 (A):

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



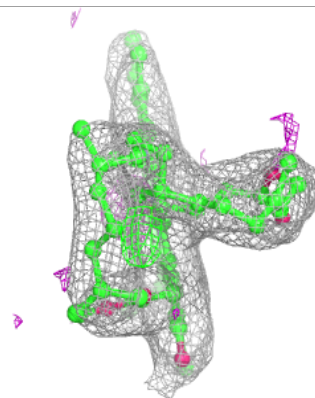
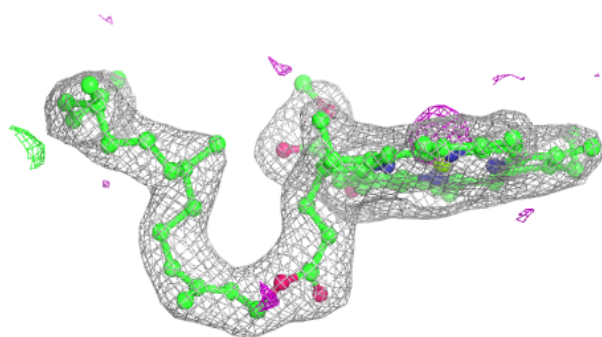
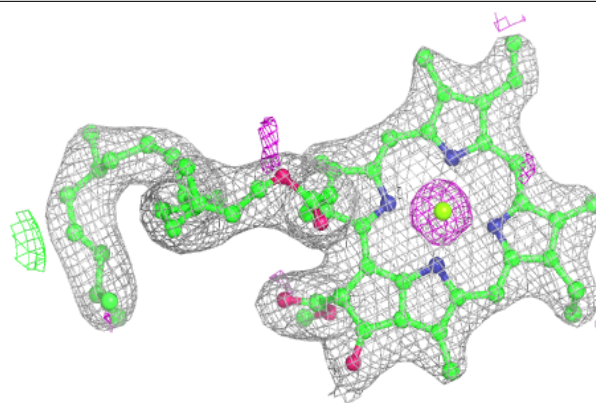
Electron density around LHG L 101 (B):

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

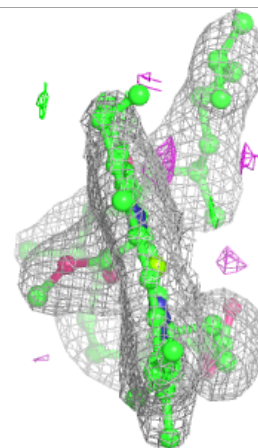
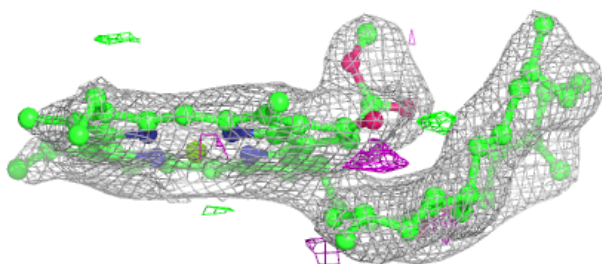
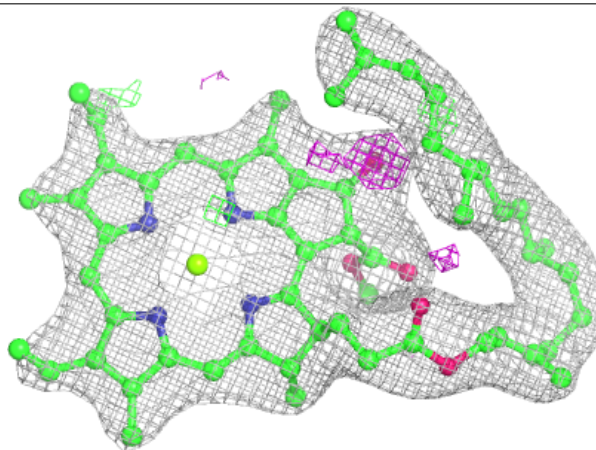


Electron density around CLA B 612:

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

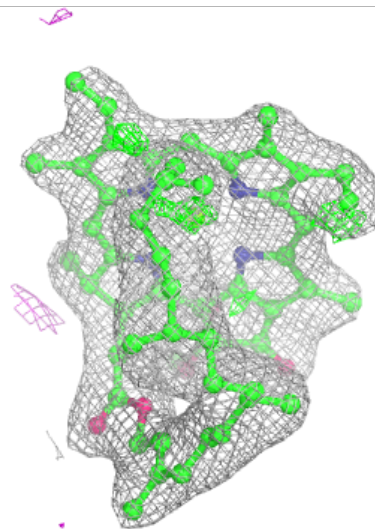
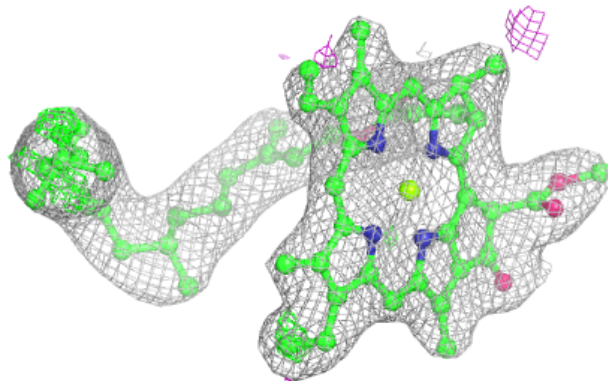
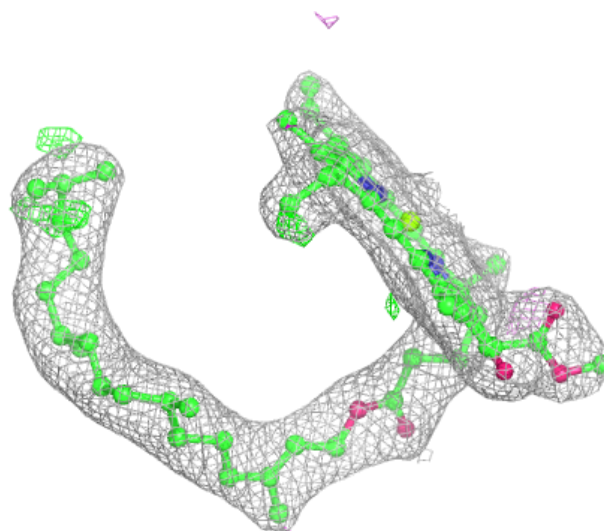
**Electron density around CLA b 610:**

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



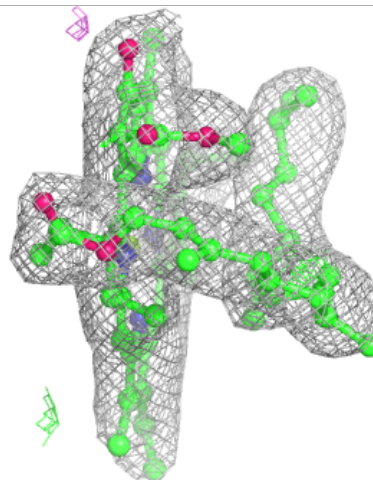
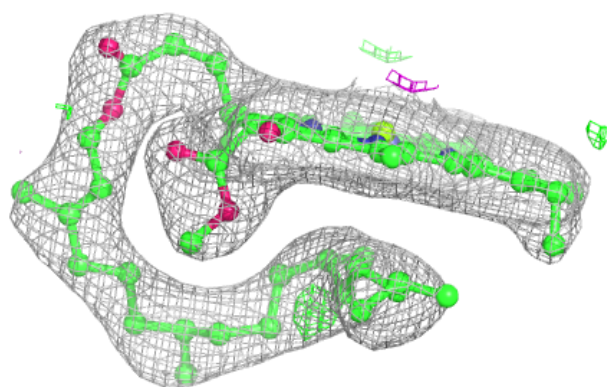
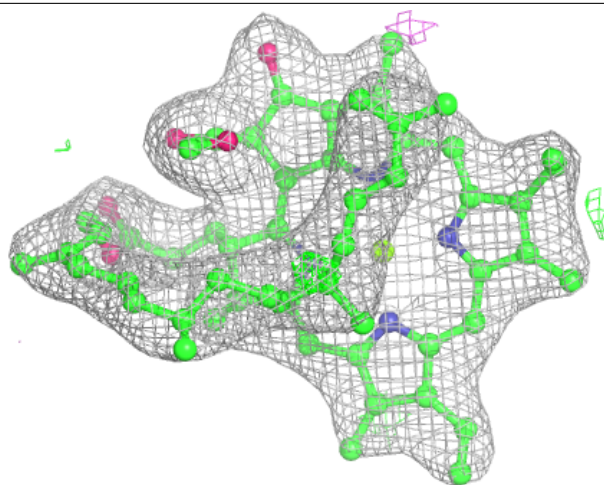
Electron density around CLA b 611:

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



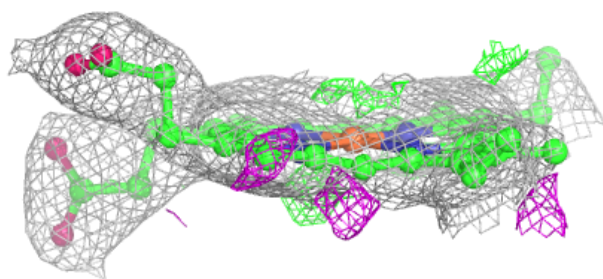
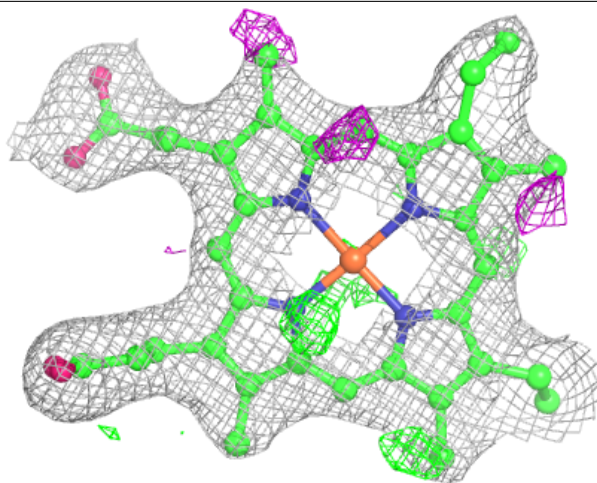
Electron density around CLA C 510:

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



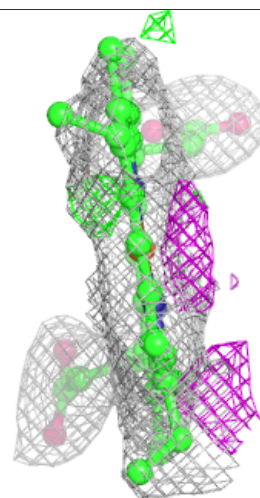
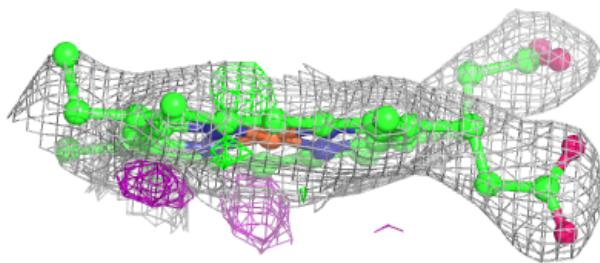
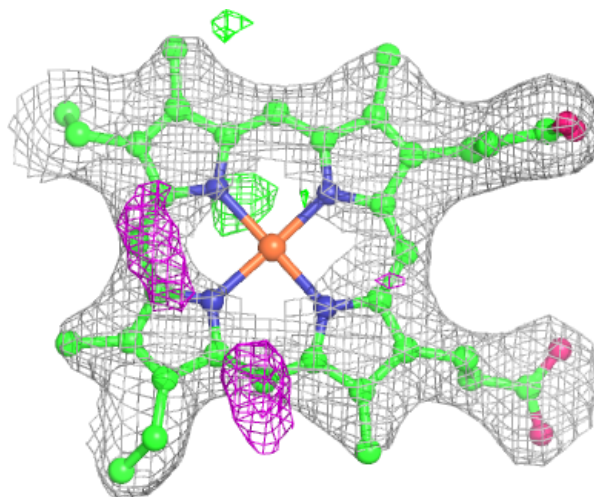
Electron density around HEC V 201:

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



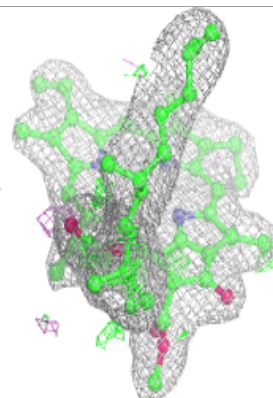
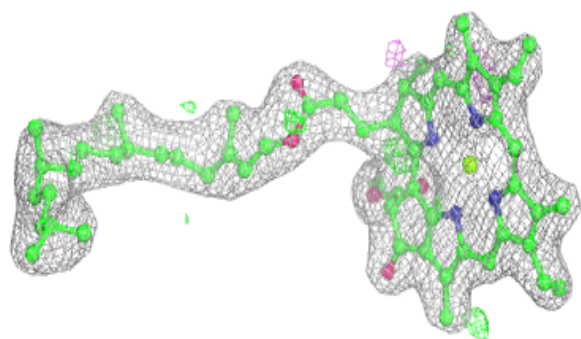
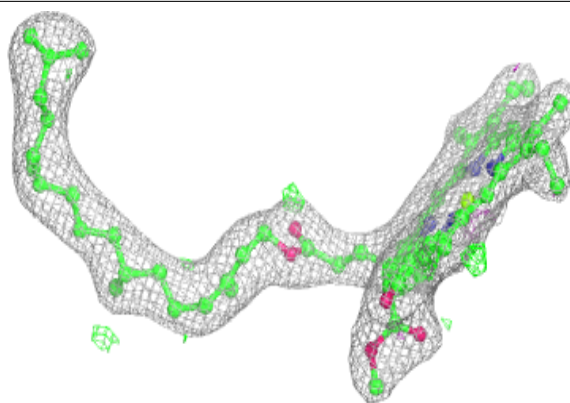
Electron density around HEC v 201:

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

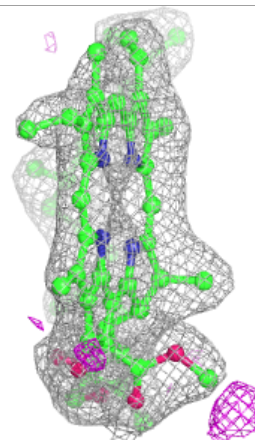
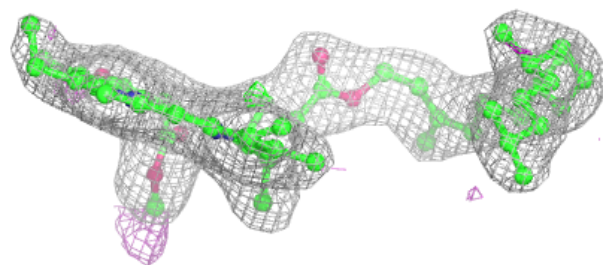
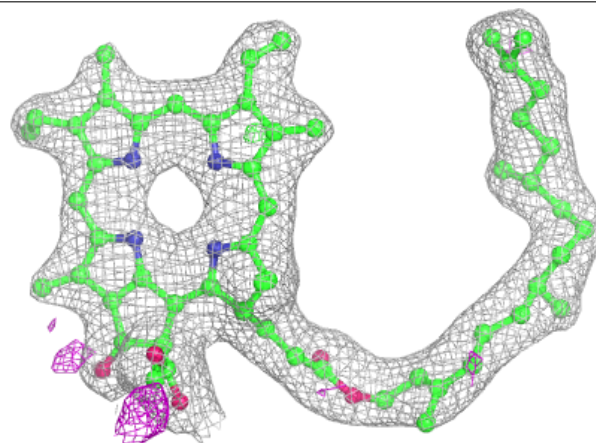


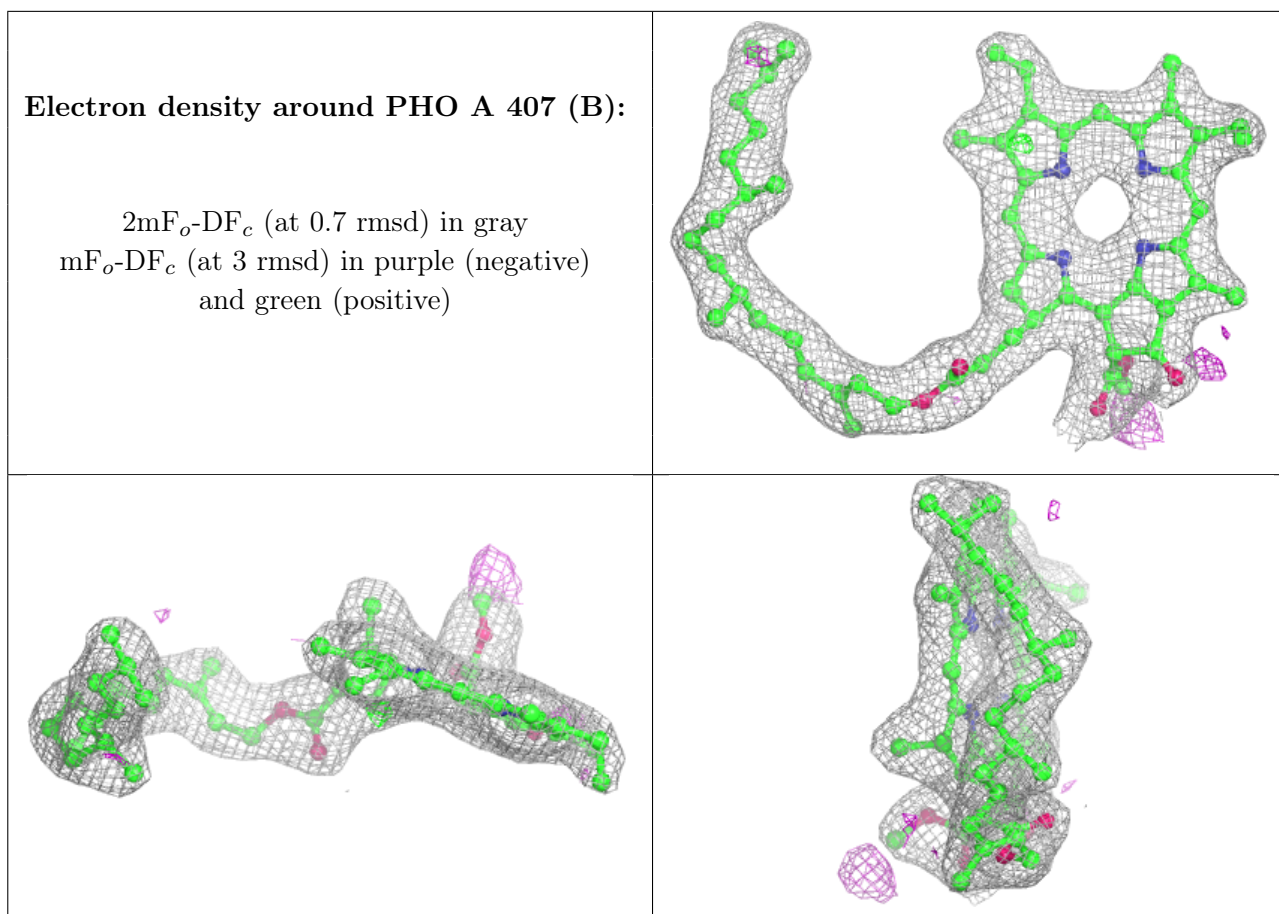
Electron density around CLA D 403 (A):

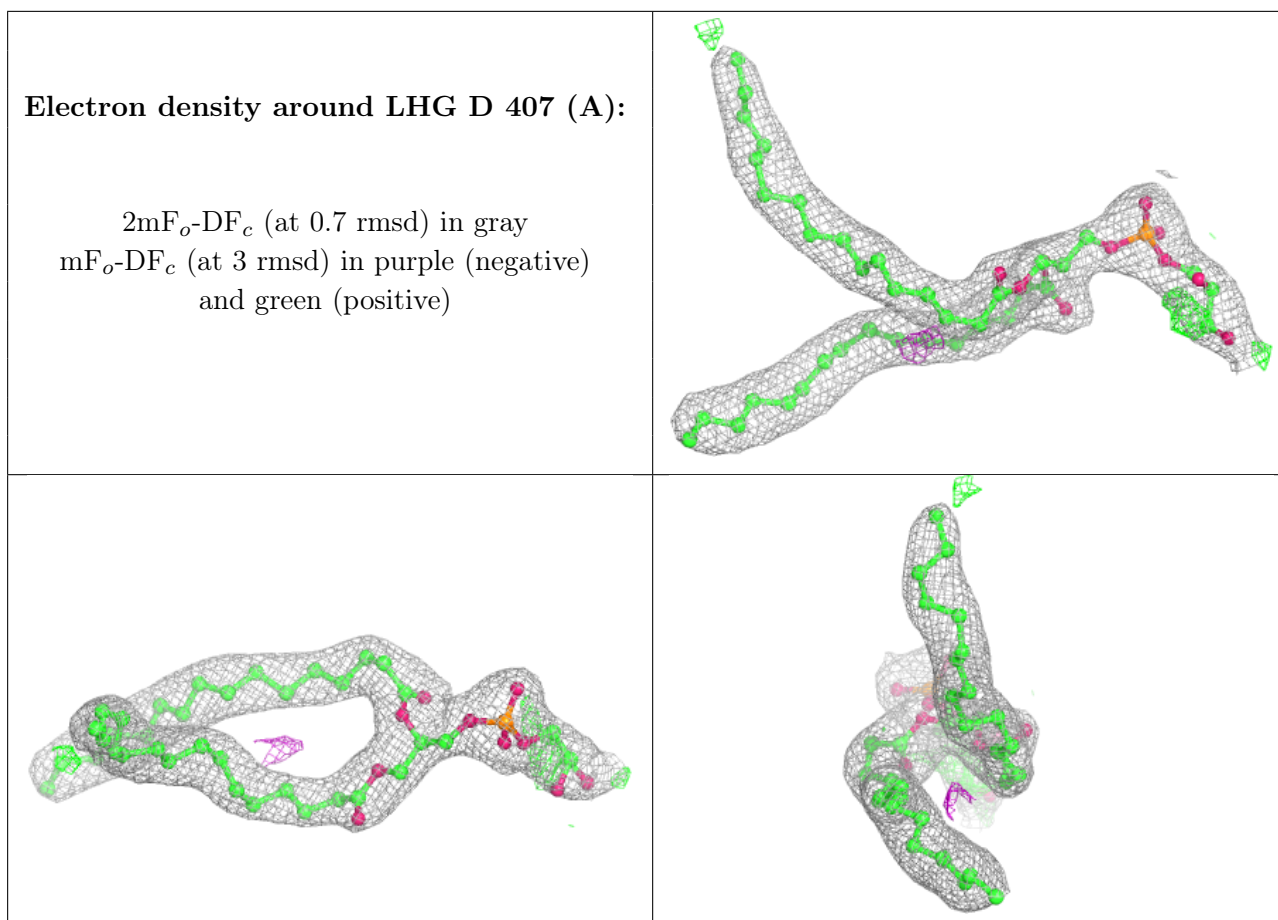
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PHO A 407 (A):**

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

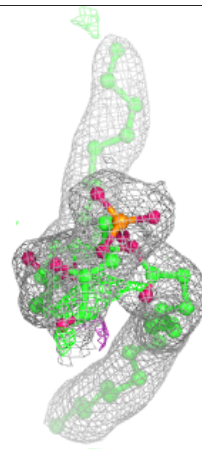
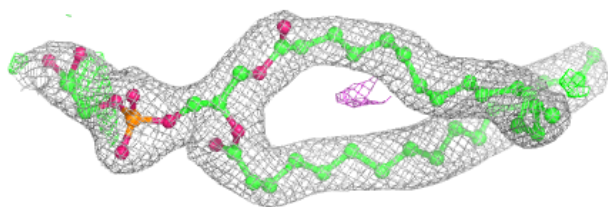
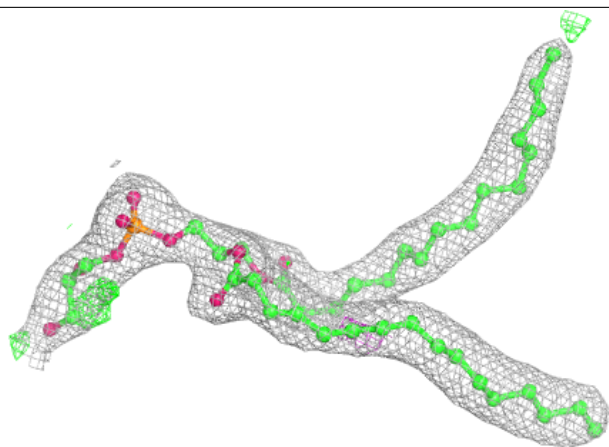


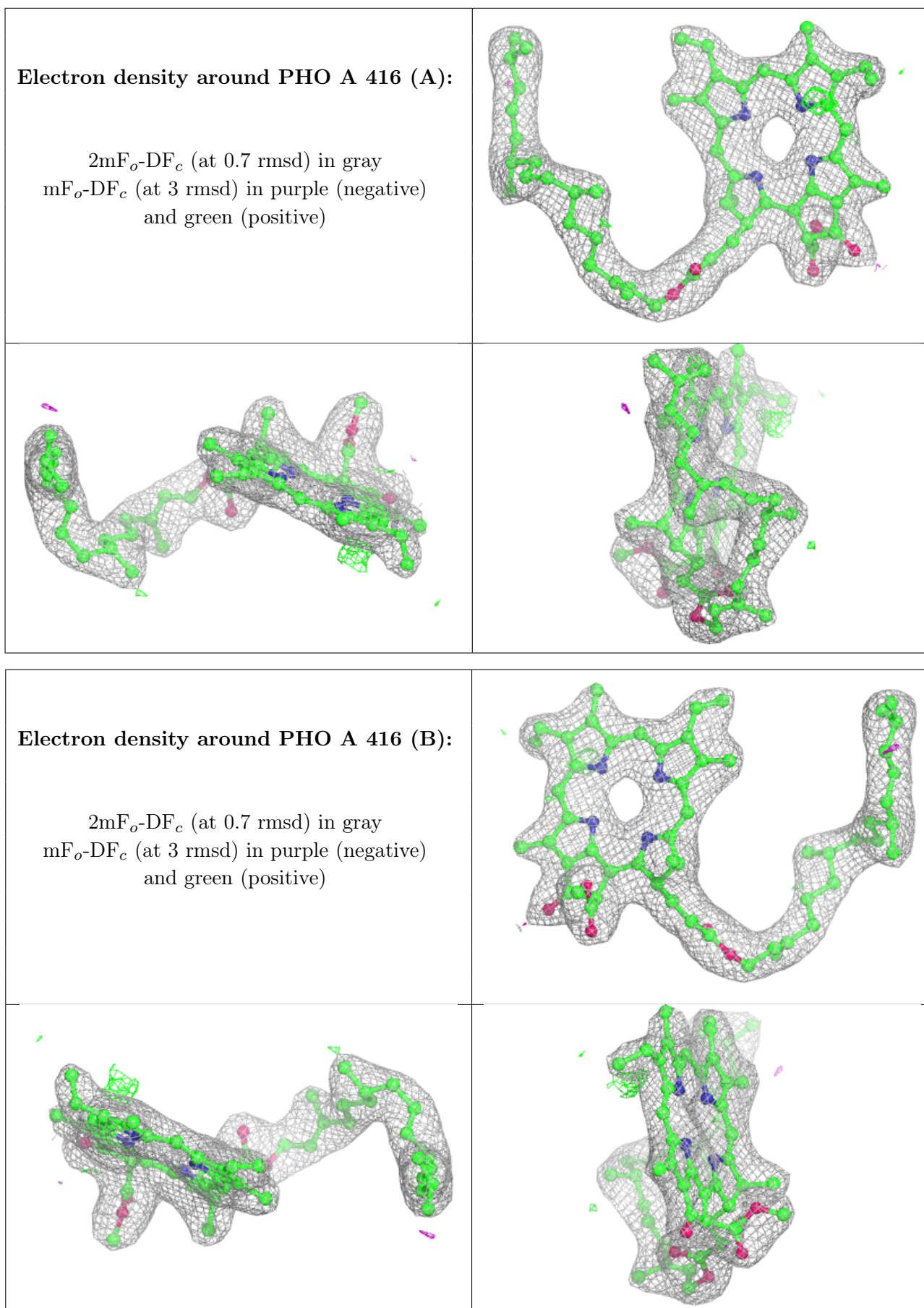




Electron density around LHG D 407 (B):

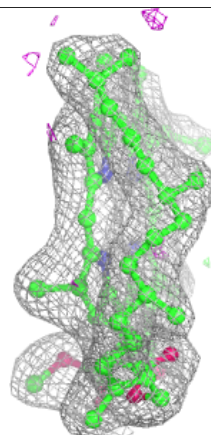
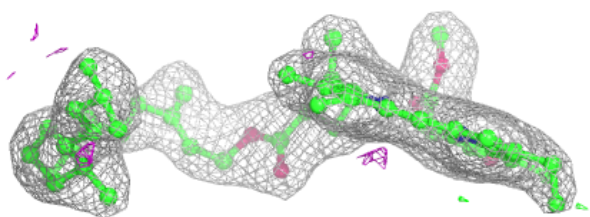
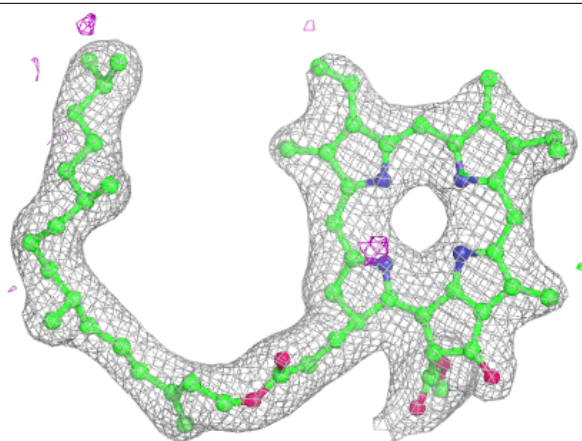
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





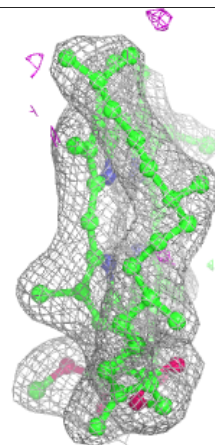
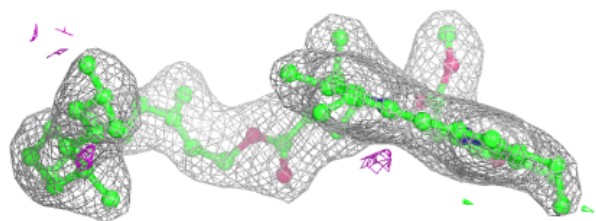
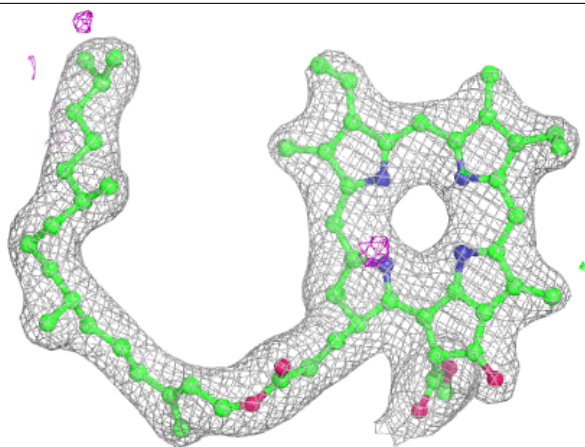
Electron density around PHO a 406 (A):

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

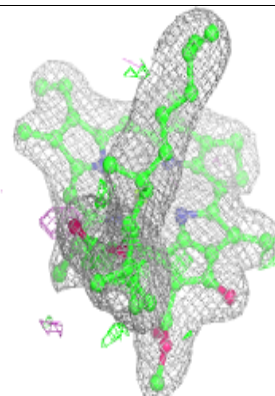
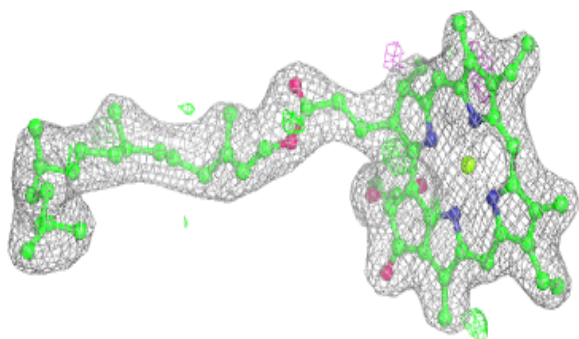
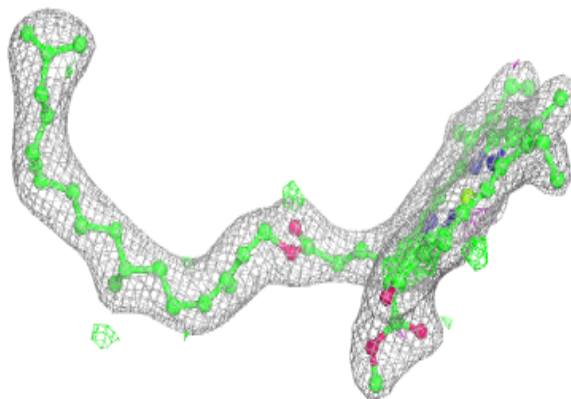


Electron density around PHO a 406 (B):

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

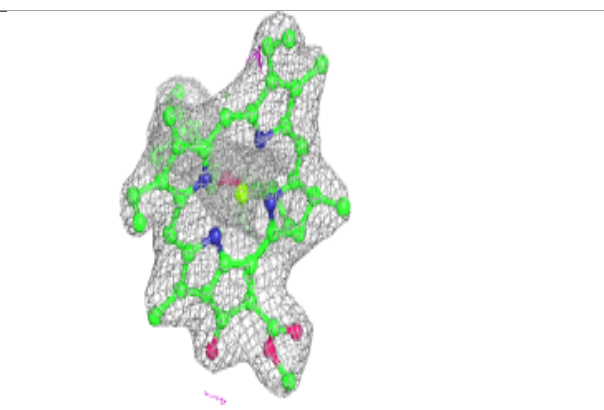
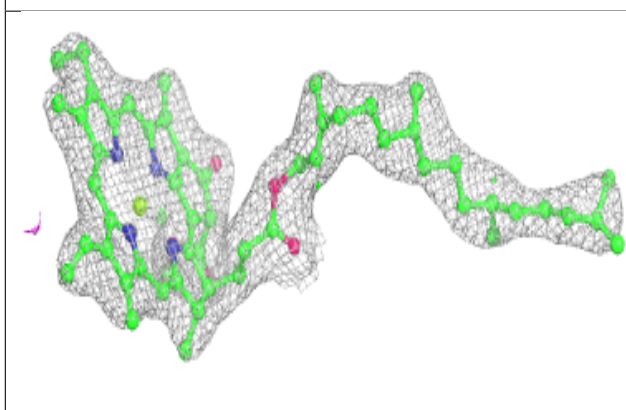
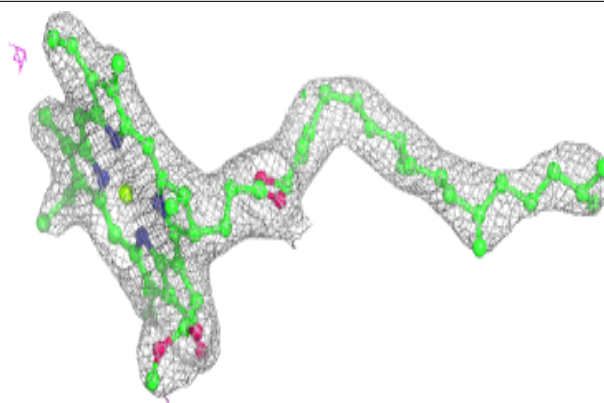
**Electron density around CLA D 403 (B):**

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

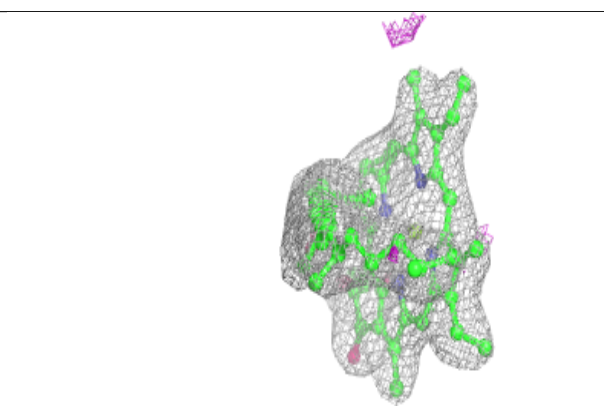
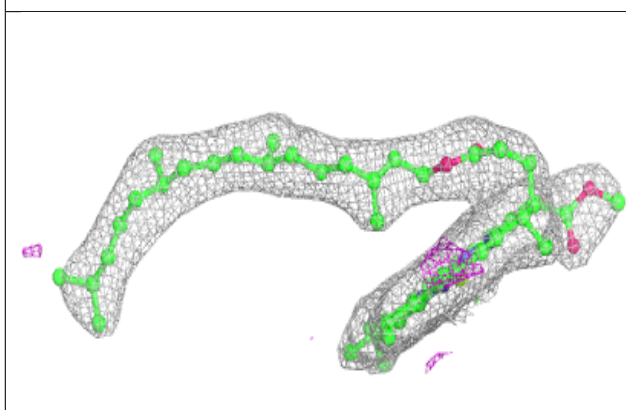
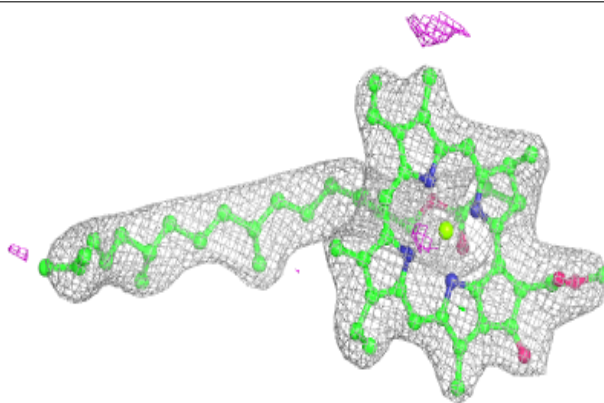


Electron density around CLA c 503:

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

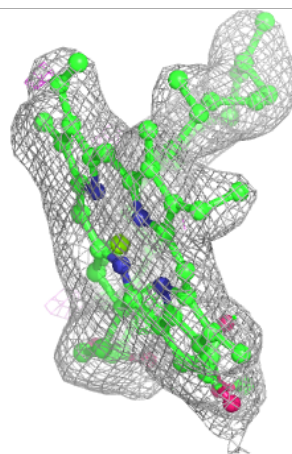
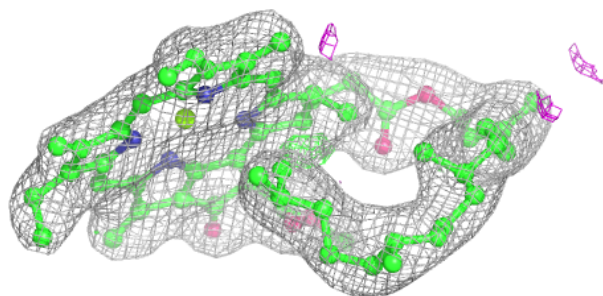
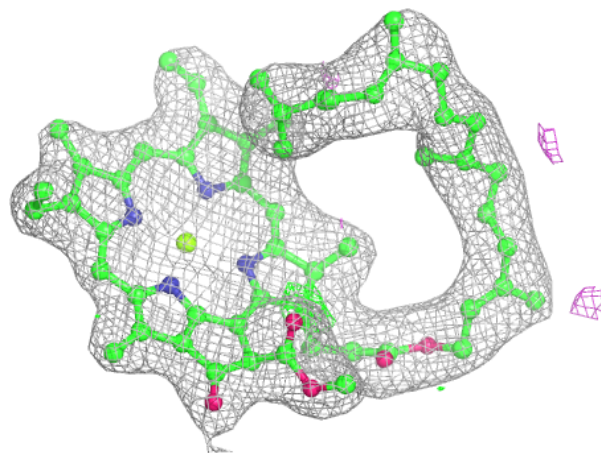
**Electron density around CLA B 608:**

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

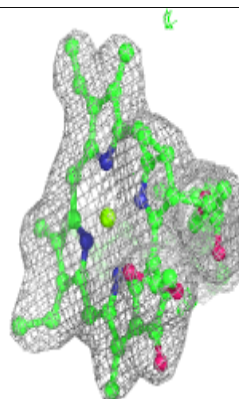
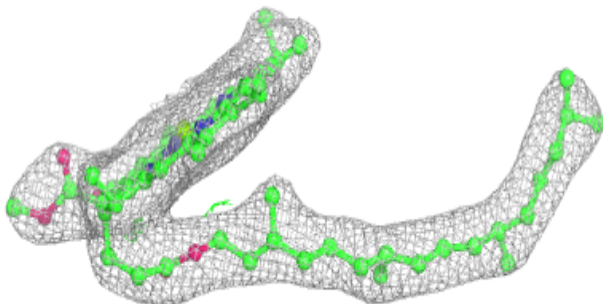
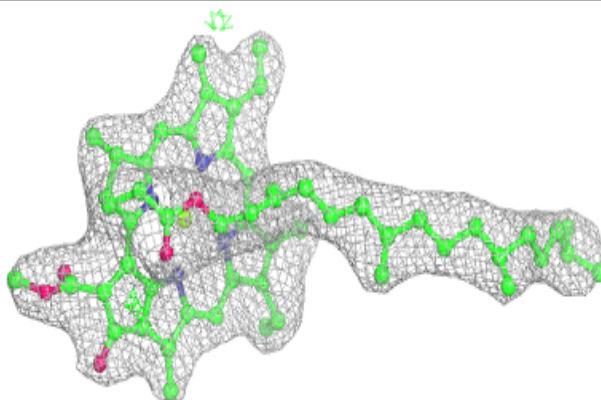


Electron density around CLA B 615:

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

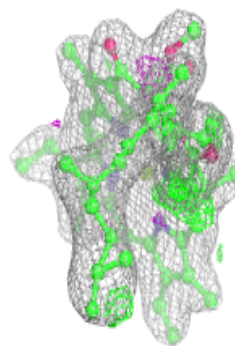
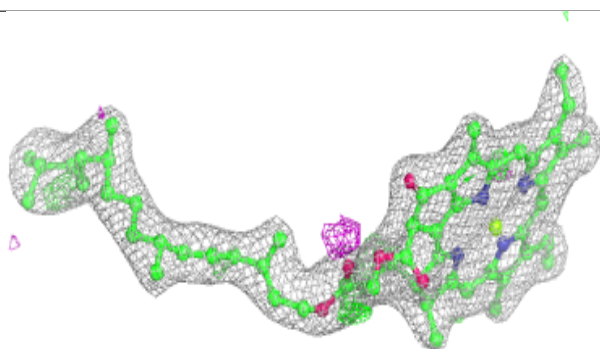
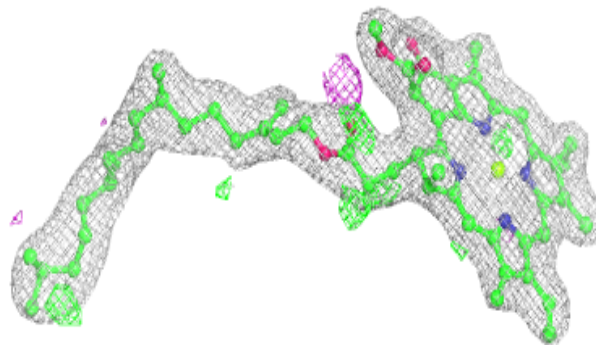
**Electron density around CLA b 608:**

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

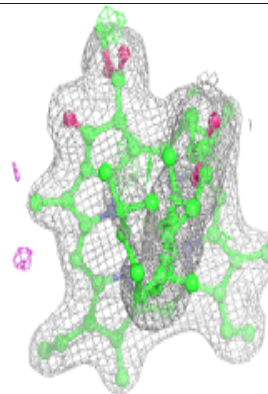
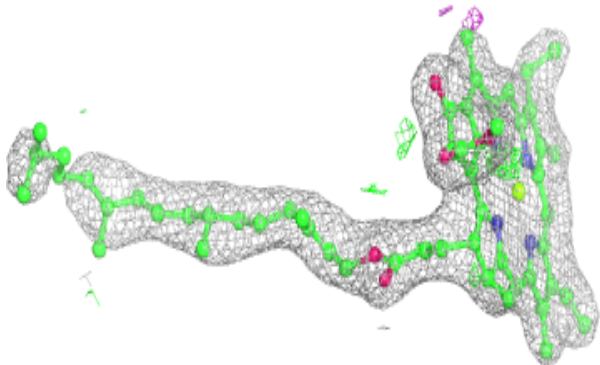
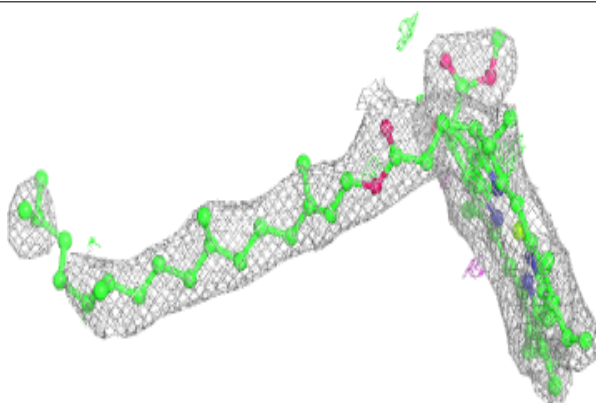


Electron density around CLA A 404 (B):

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

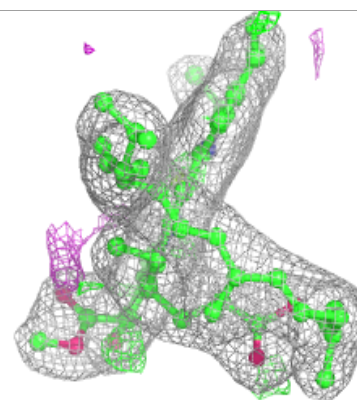
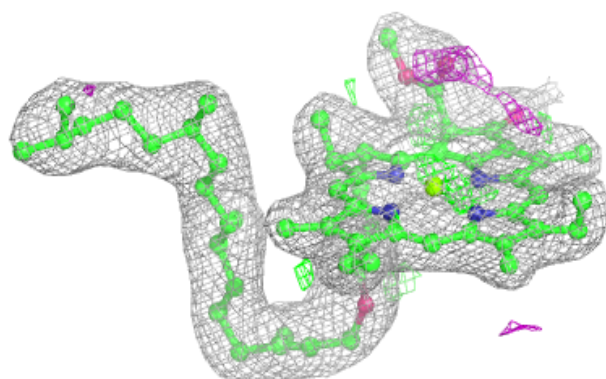
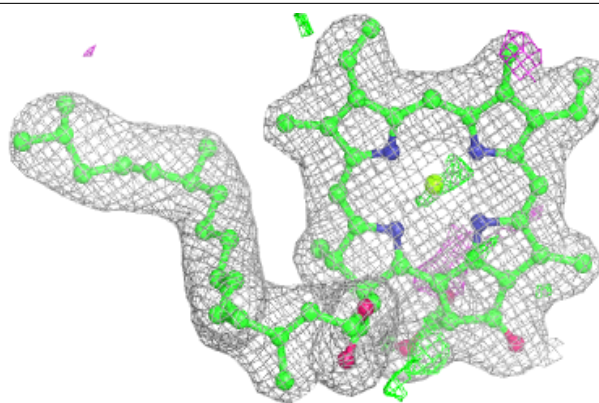
**Electron density around CLA B 604:**

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

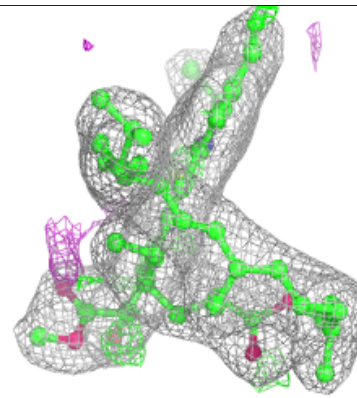
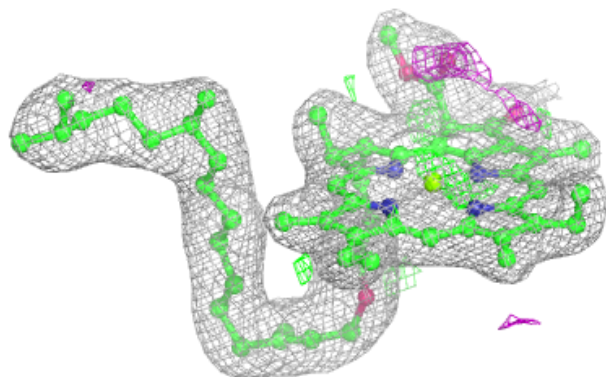
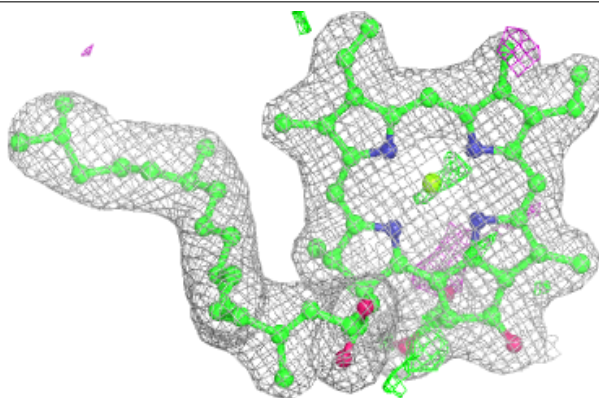


Electron density around CLA A 405 (A):

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

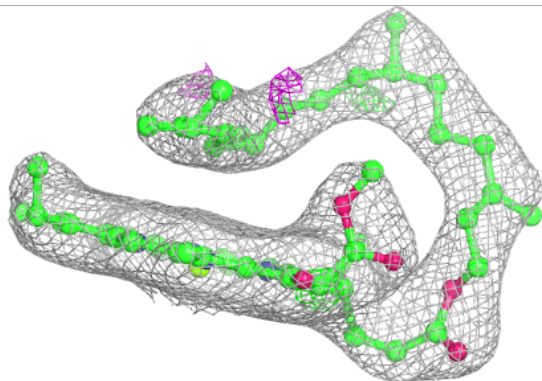
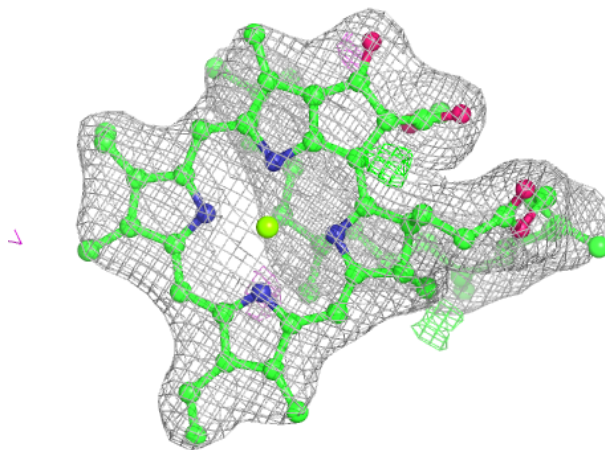
**Electron density around CLA A 405 (B):**

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



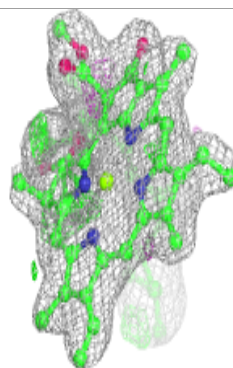
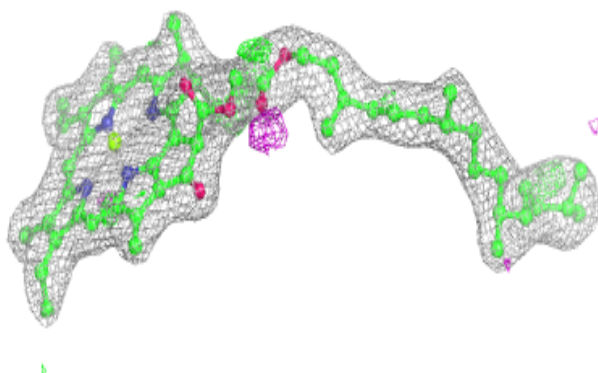
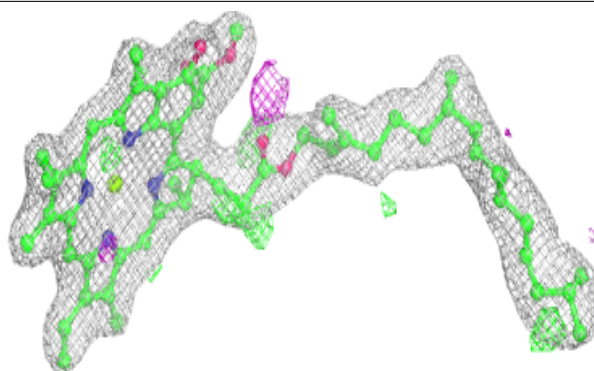
Electron density around CLA c 511:

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

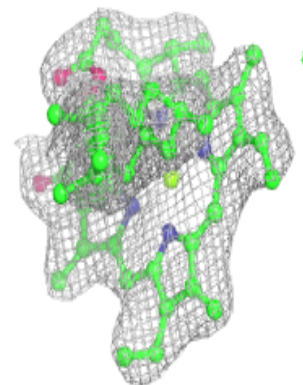
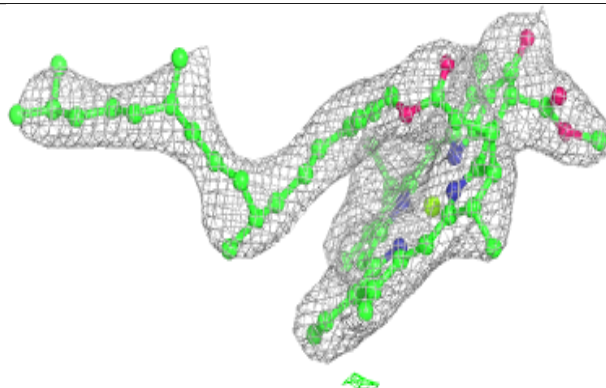
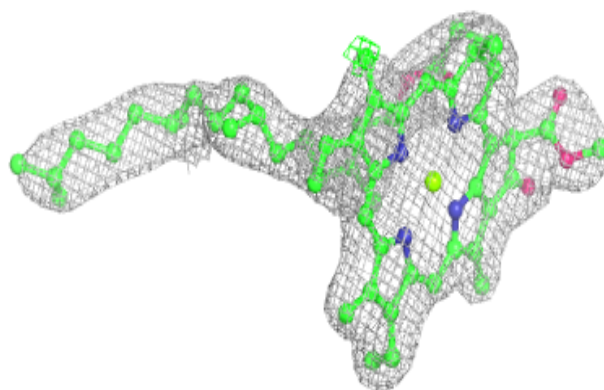


Electron density around CLA A 404 (A):

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

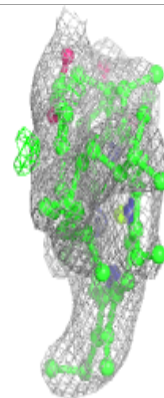
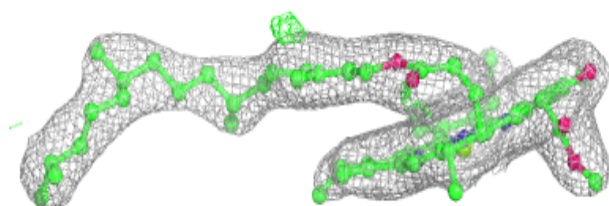
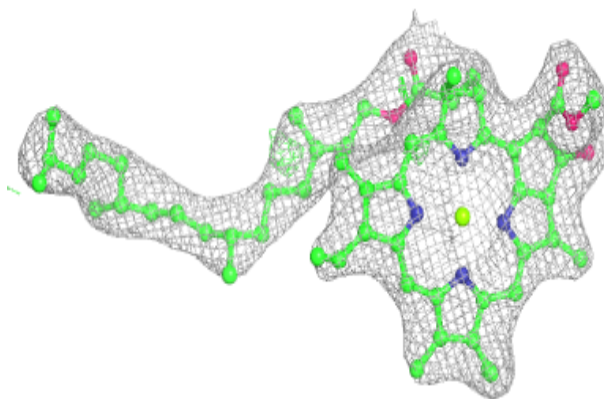
**Electron density around CLA C 505:**

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

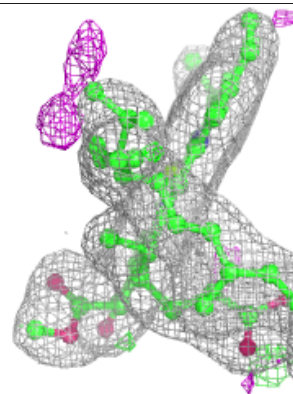
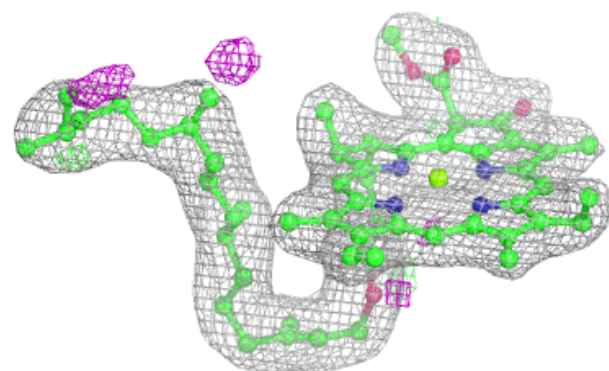
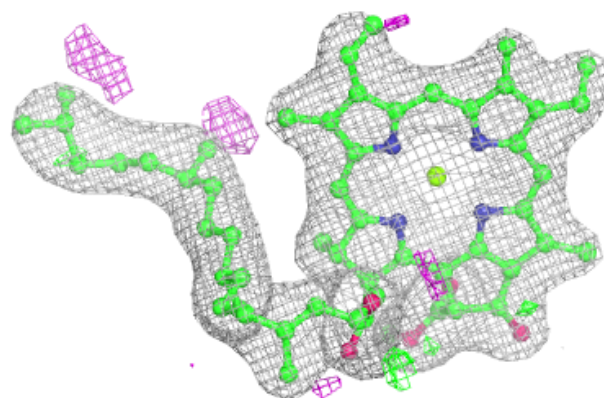


Electron density around CLA b 603:

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

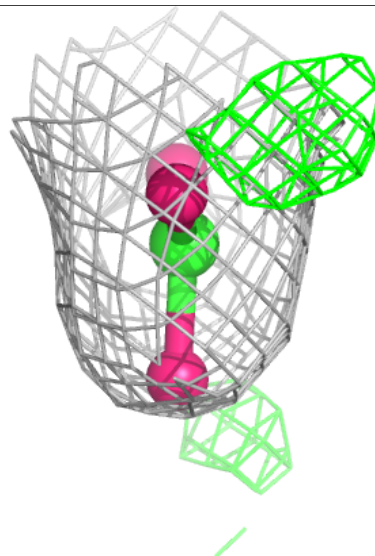
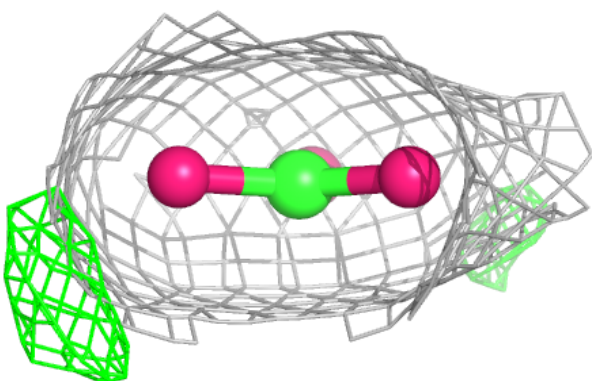
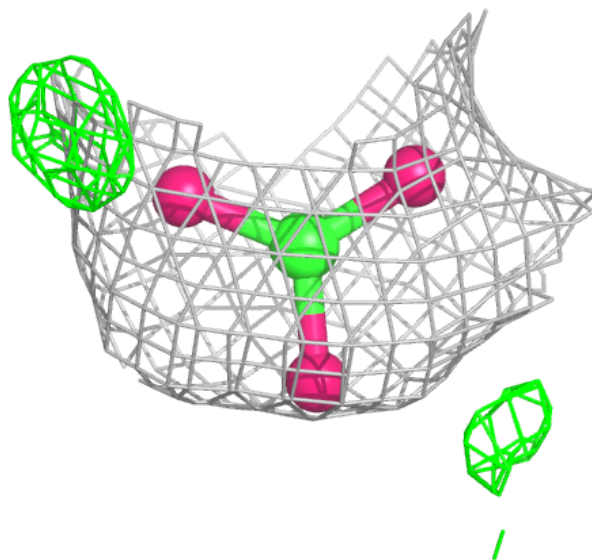
**Electron density around CLA d 402 (A):**

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



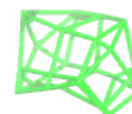
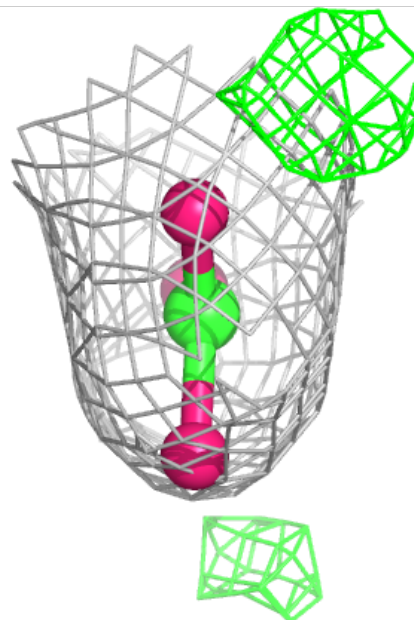
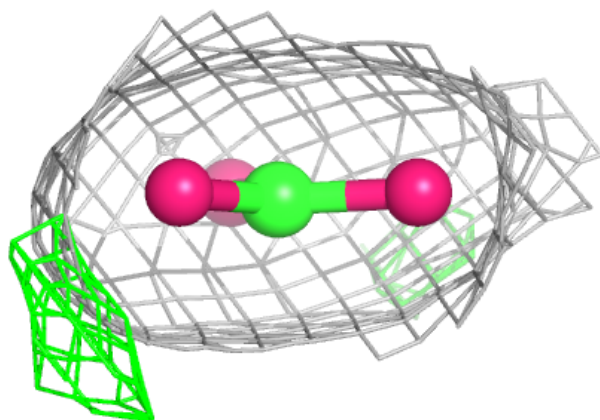
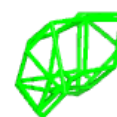
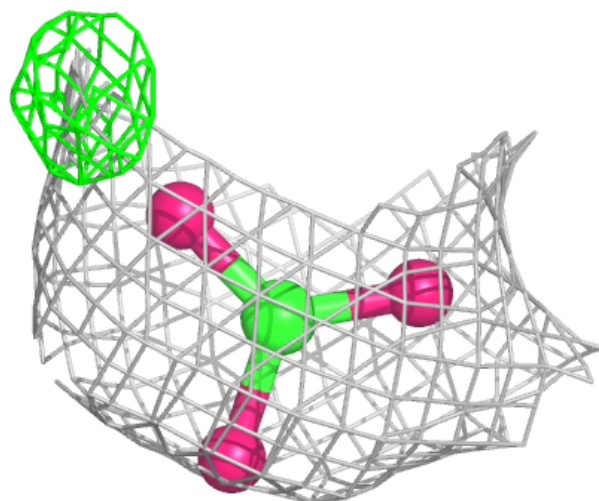
Electron density around BCT d 401 (A):

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



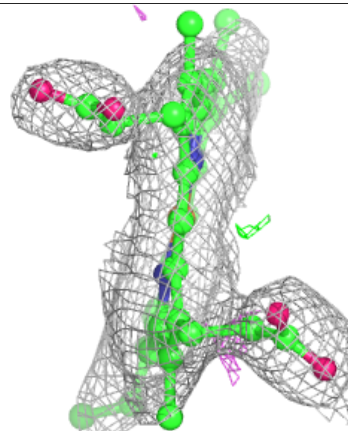
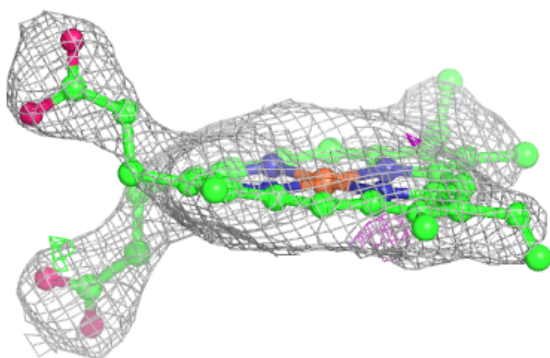
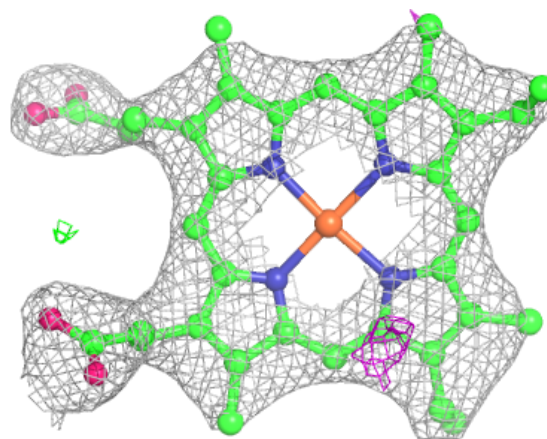
Electron density around BCT d 401 (B):

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

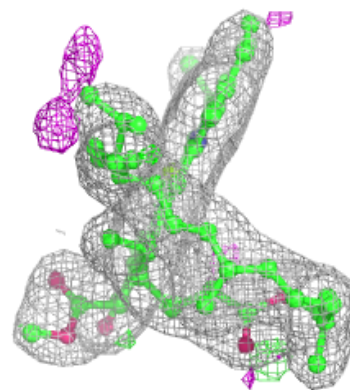
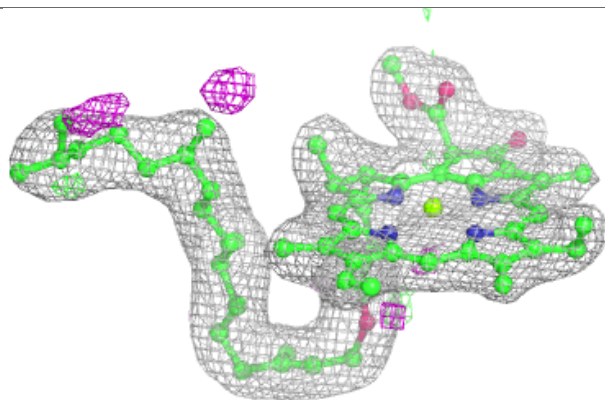
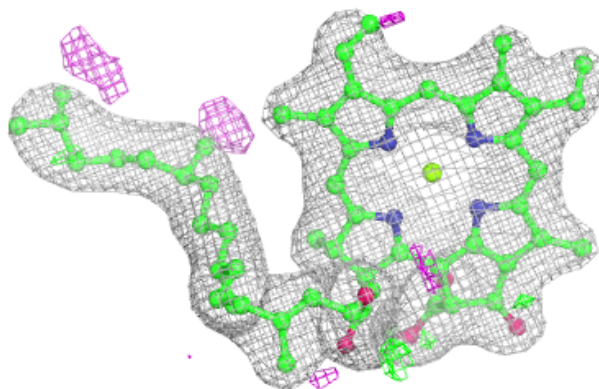


Electron density around HEM F 102:

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

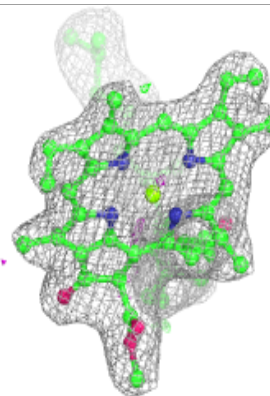
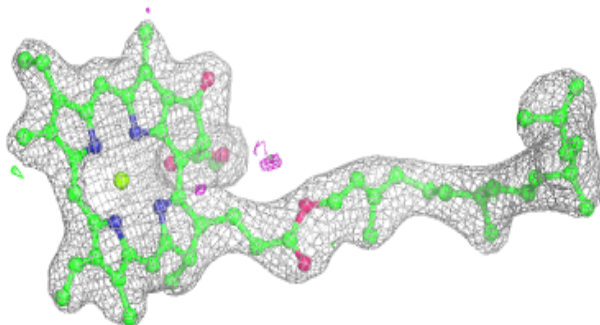
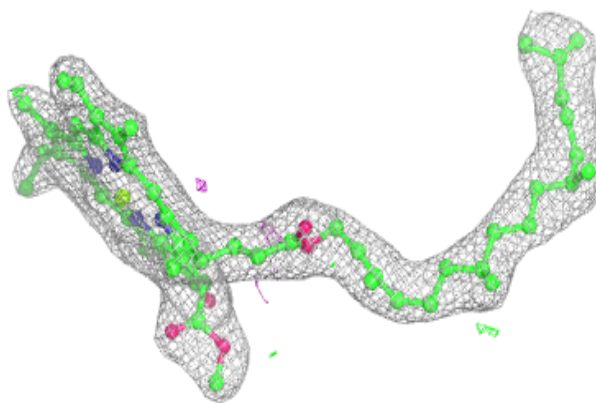
**Electron density around CLA d 402 (B):**

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

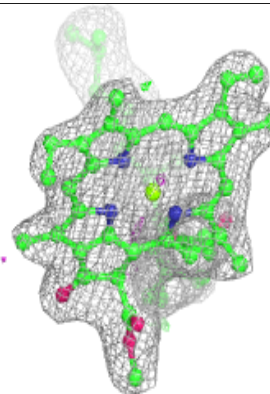
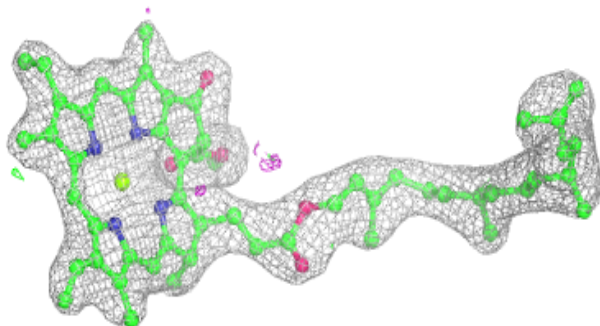
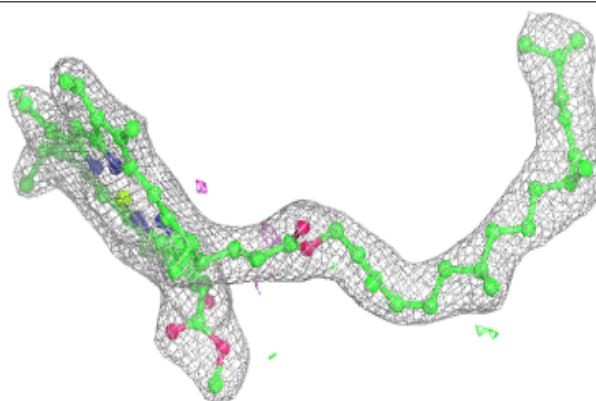


Electron density around CLA d 403 (A):

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

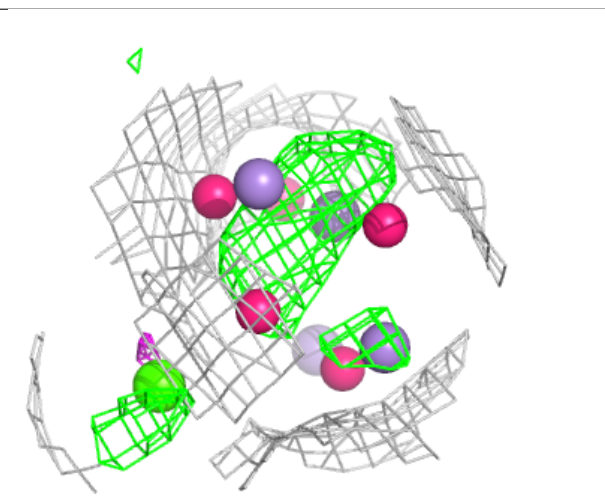
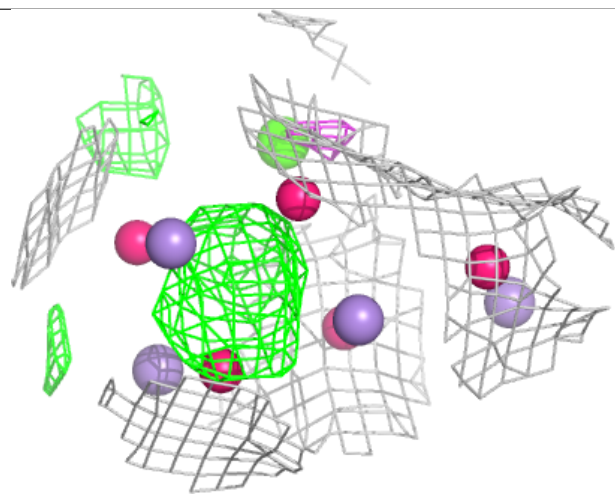
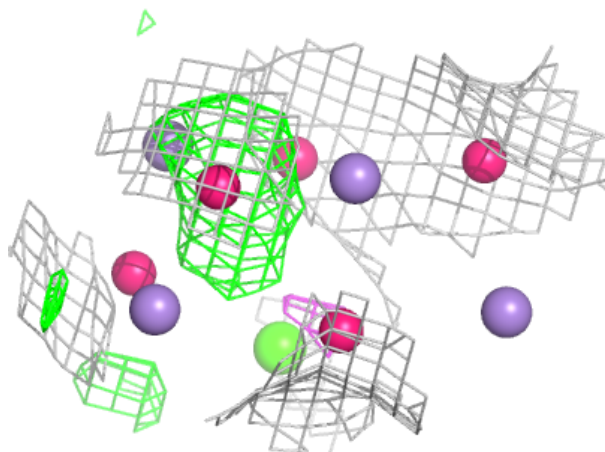
**Electron density around CLA d 403 (B):**

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



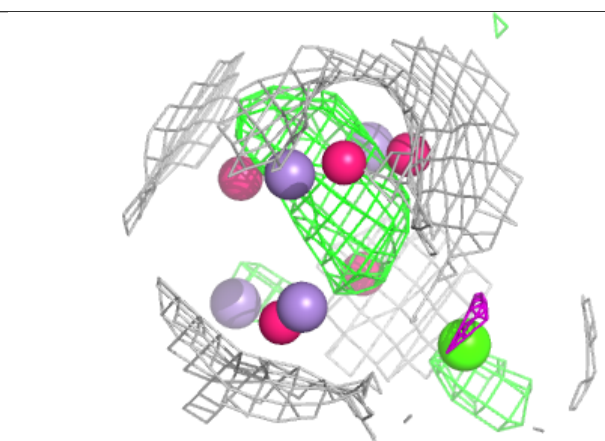
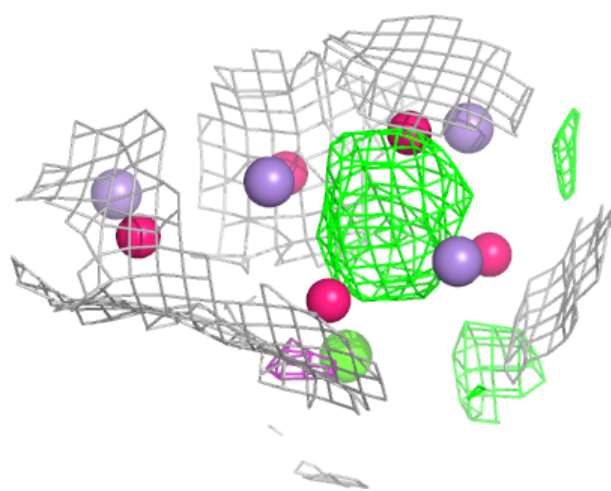
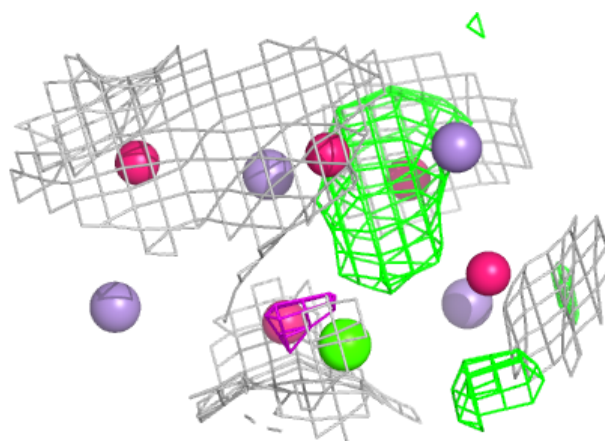
Electron density around OEX a 411 (A):

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



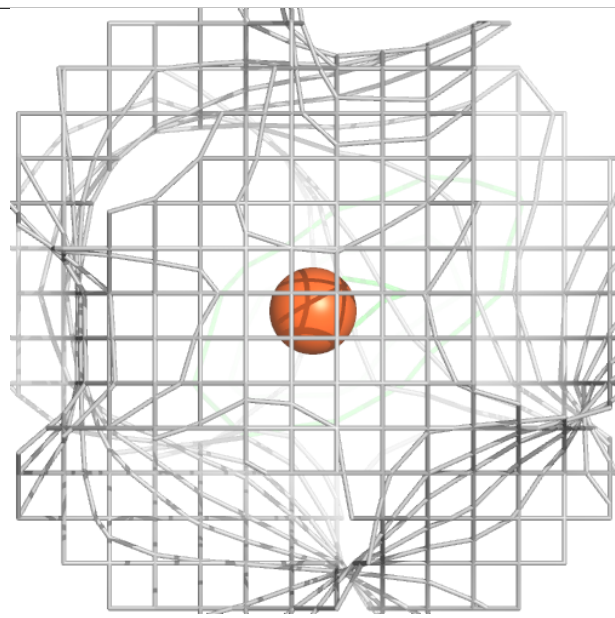
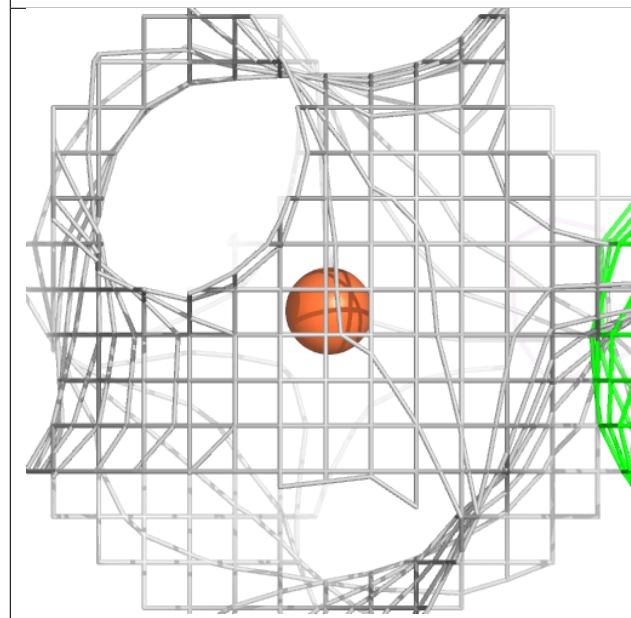
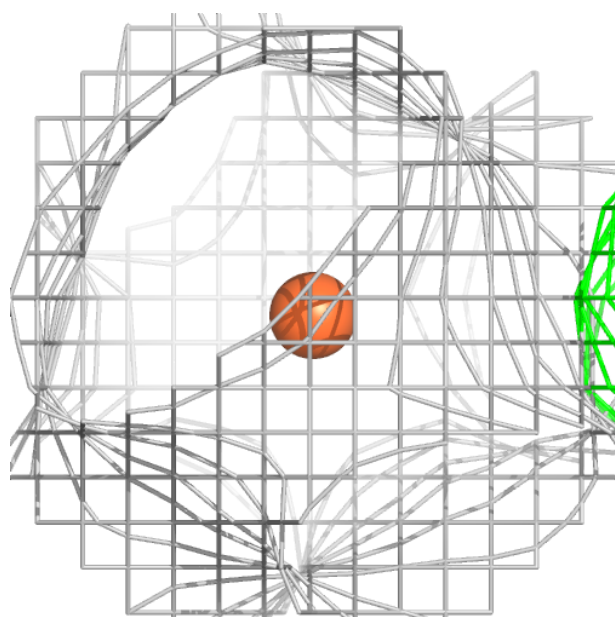
Electron density around OEX a 411 (B):

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



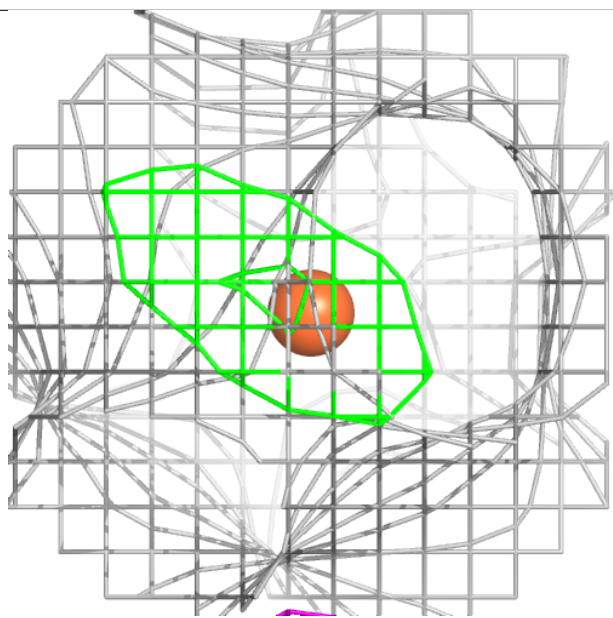
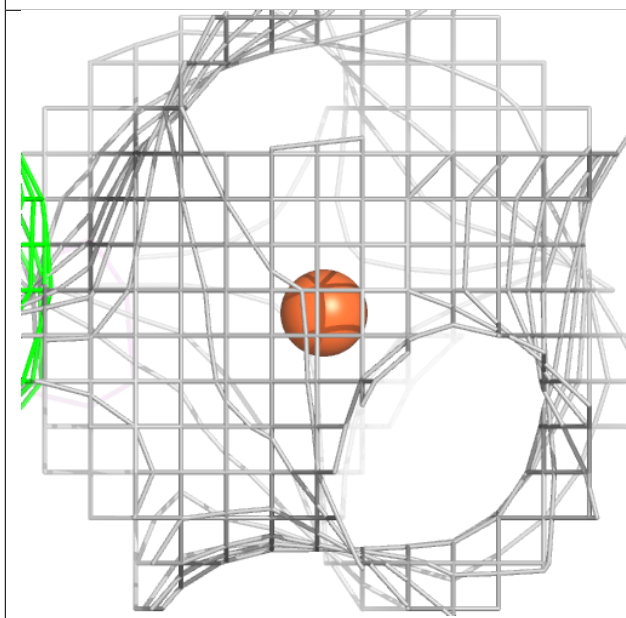
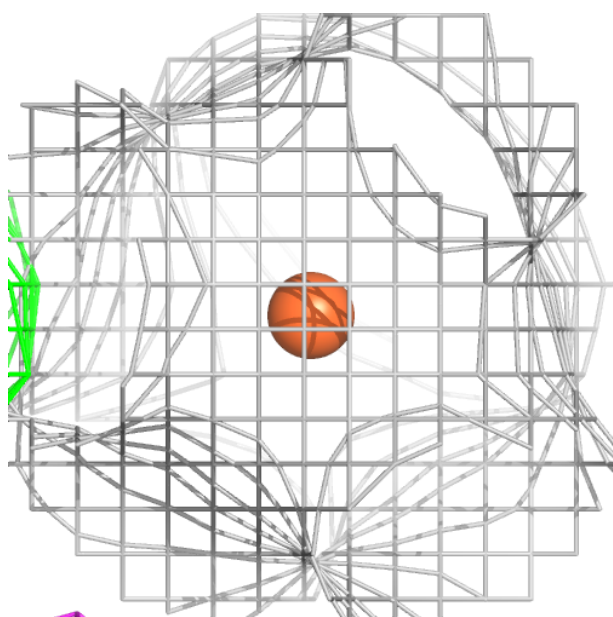
Electron density around FE2 A 401 (A):

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



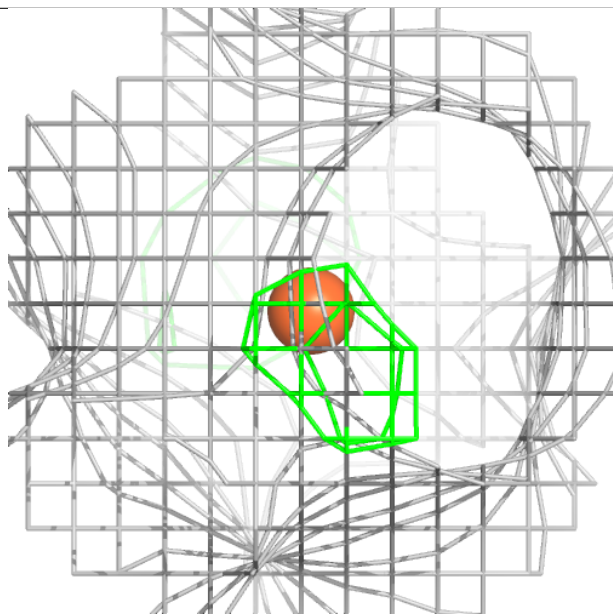
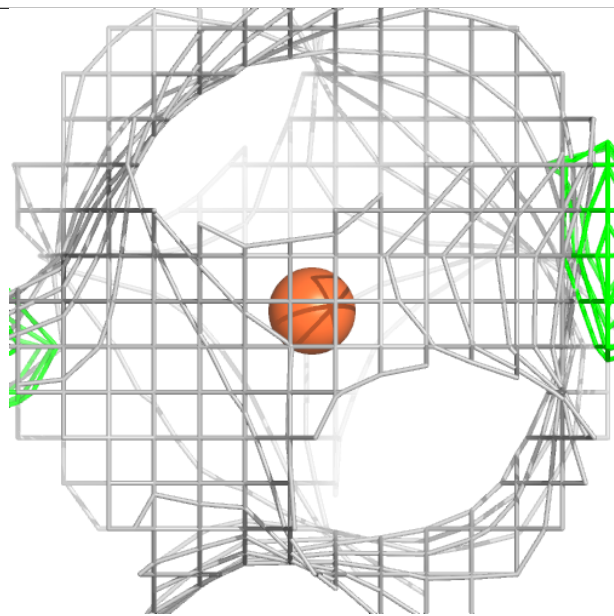
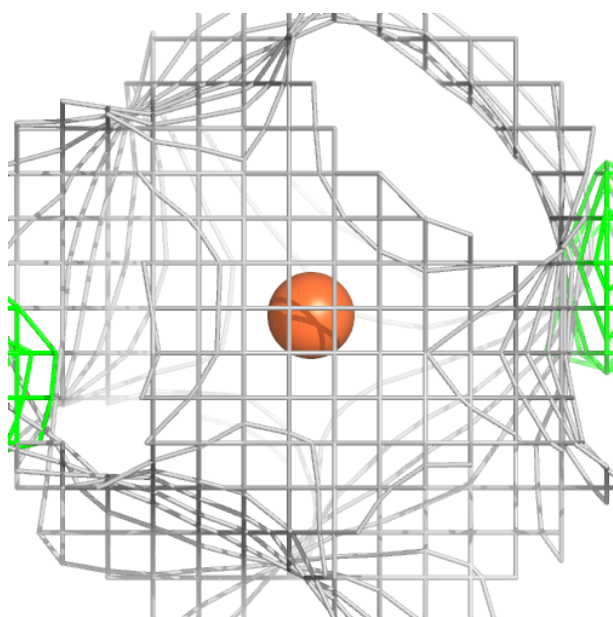
Electron density around FE2 A 401 (B):

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



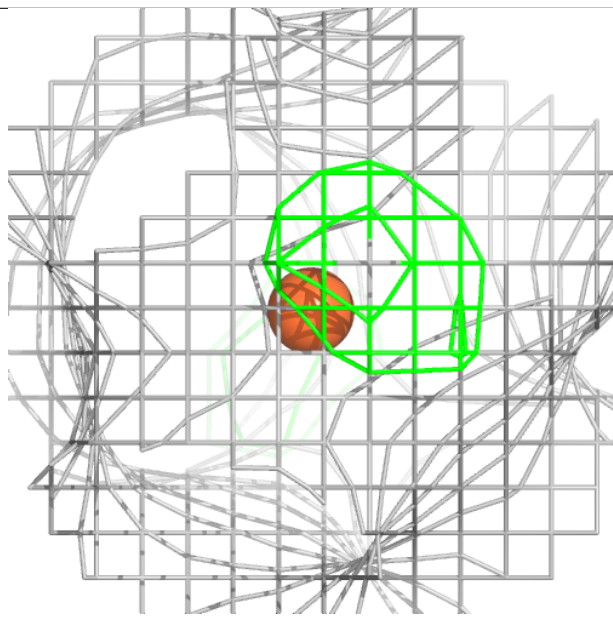
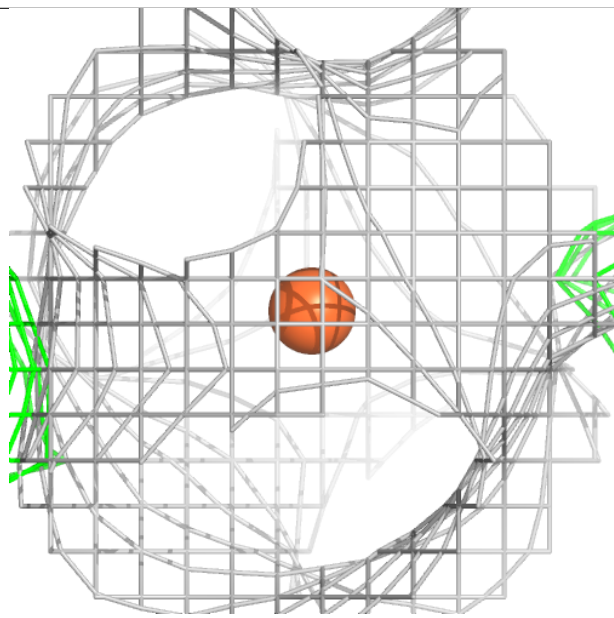
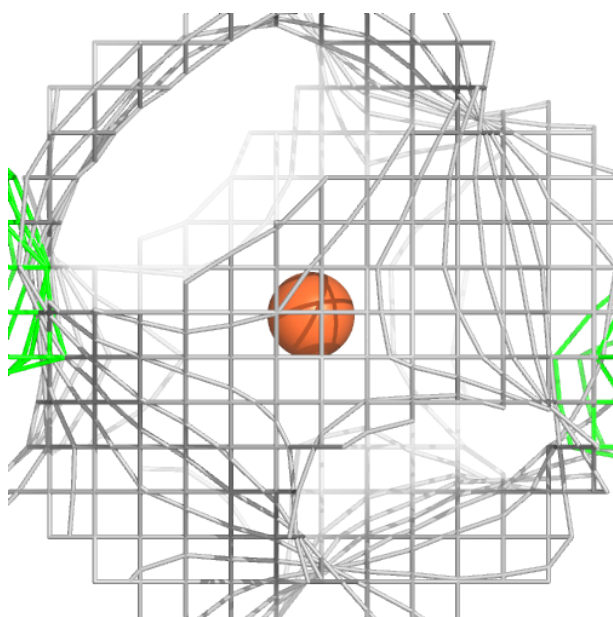
Electron density around FE2 a 401 (A):

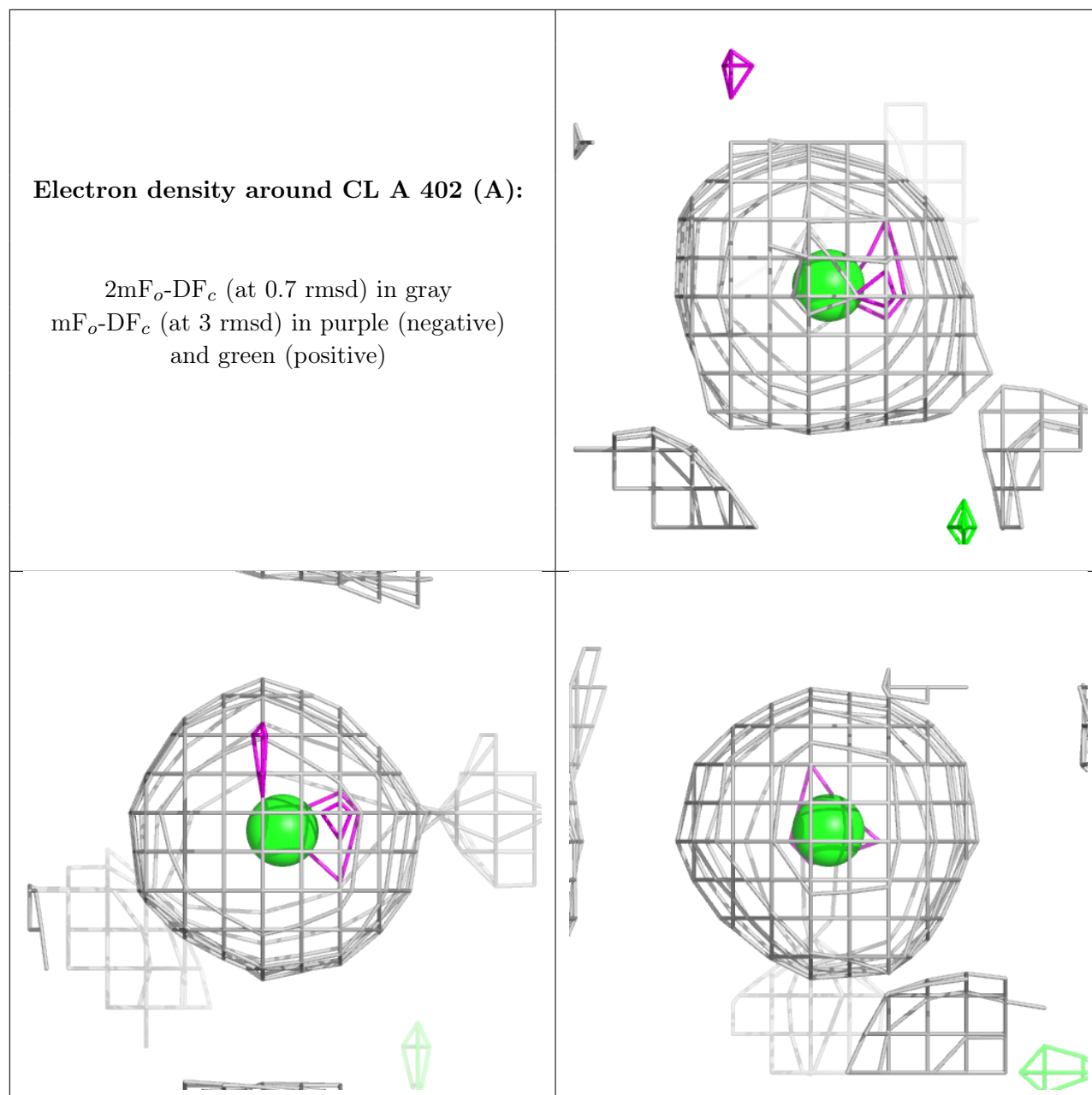
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

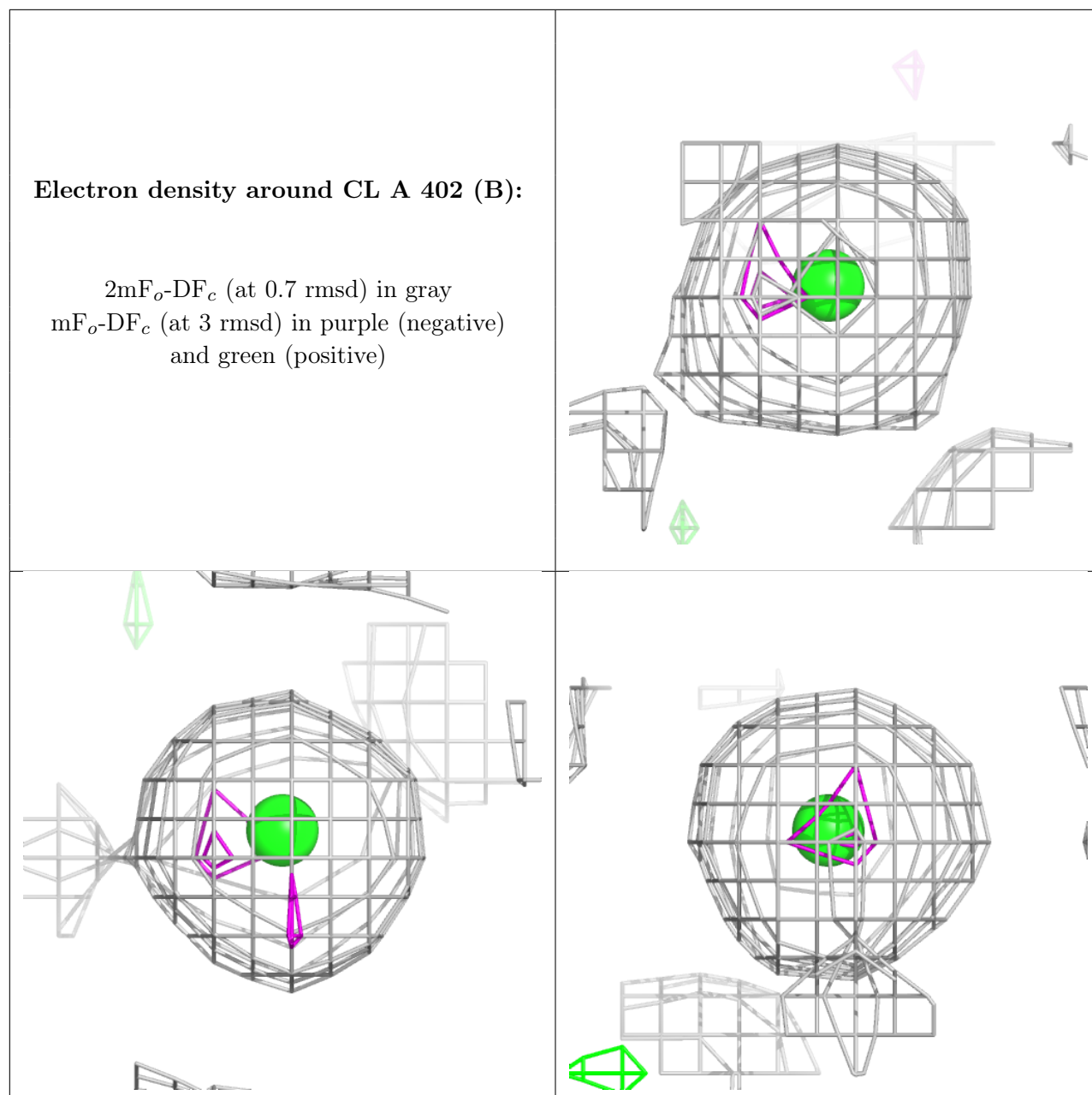


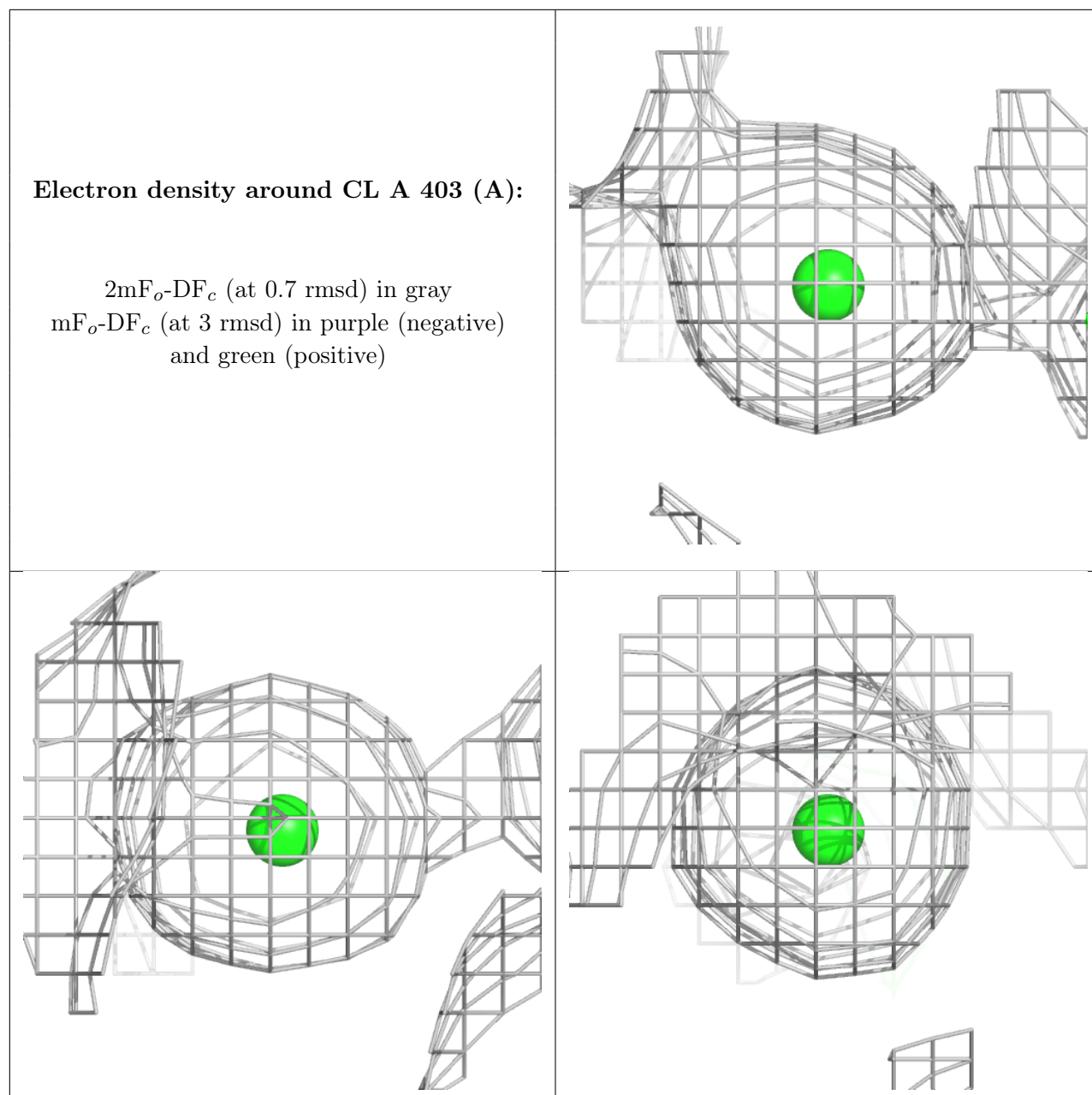
Electron density around FE2 a 401 (B):

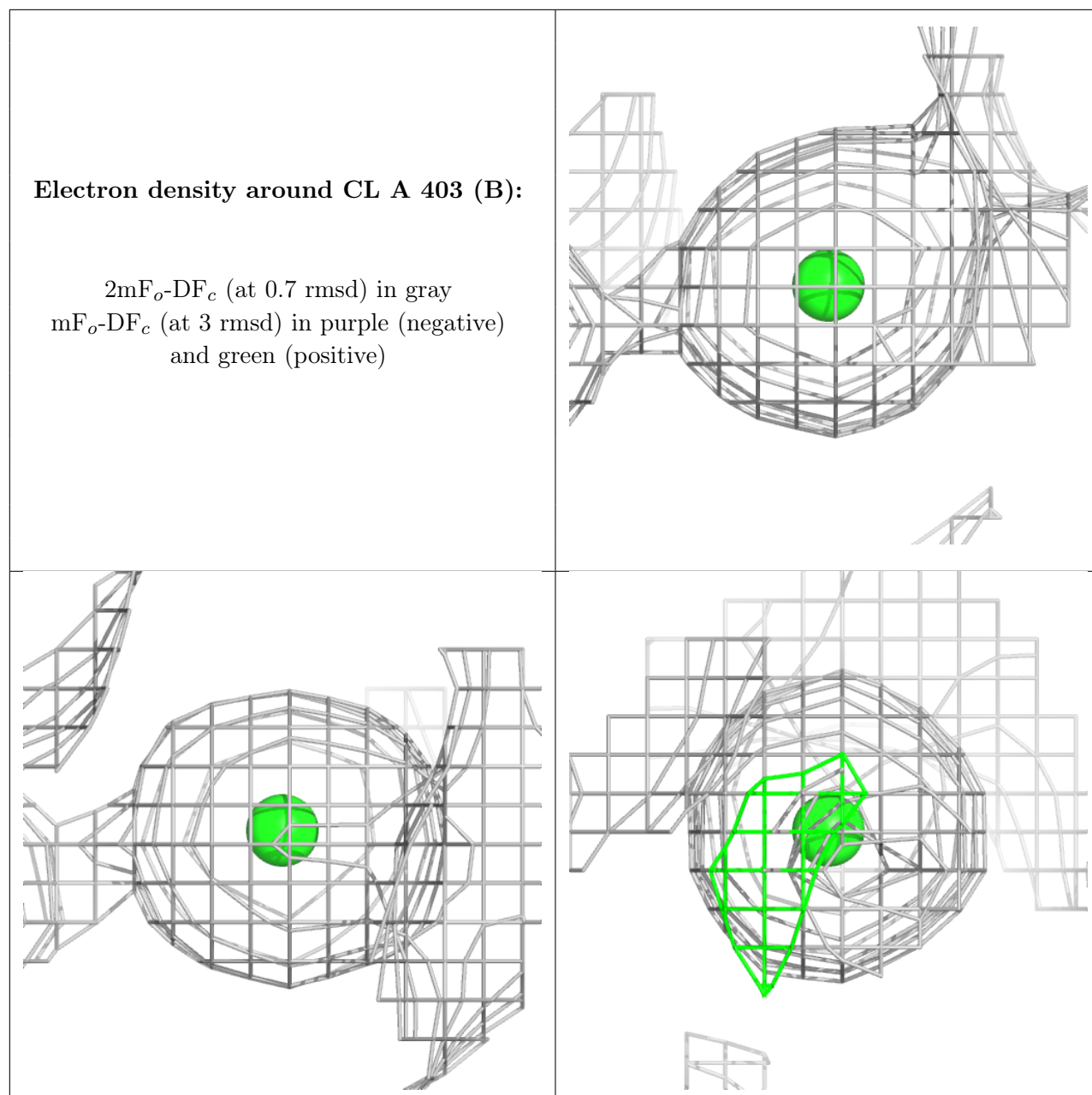
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

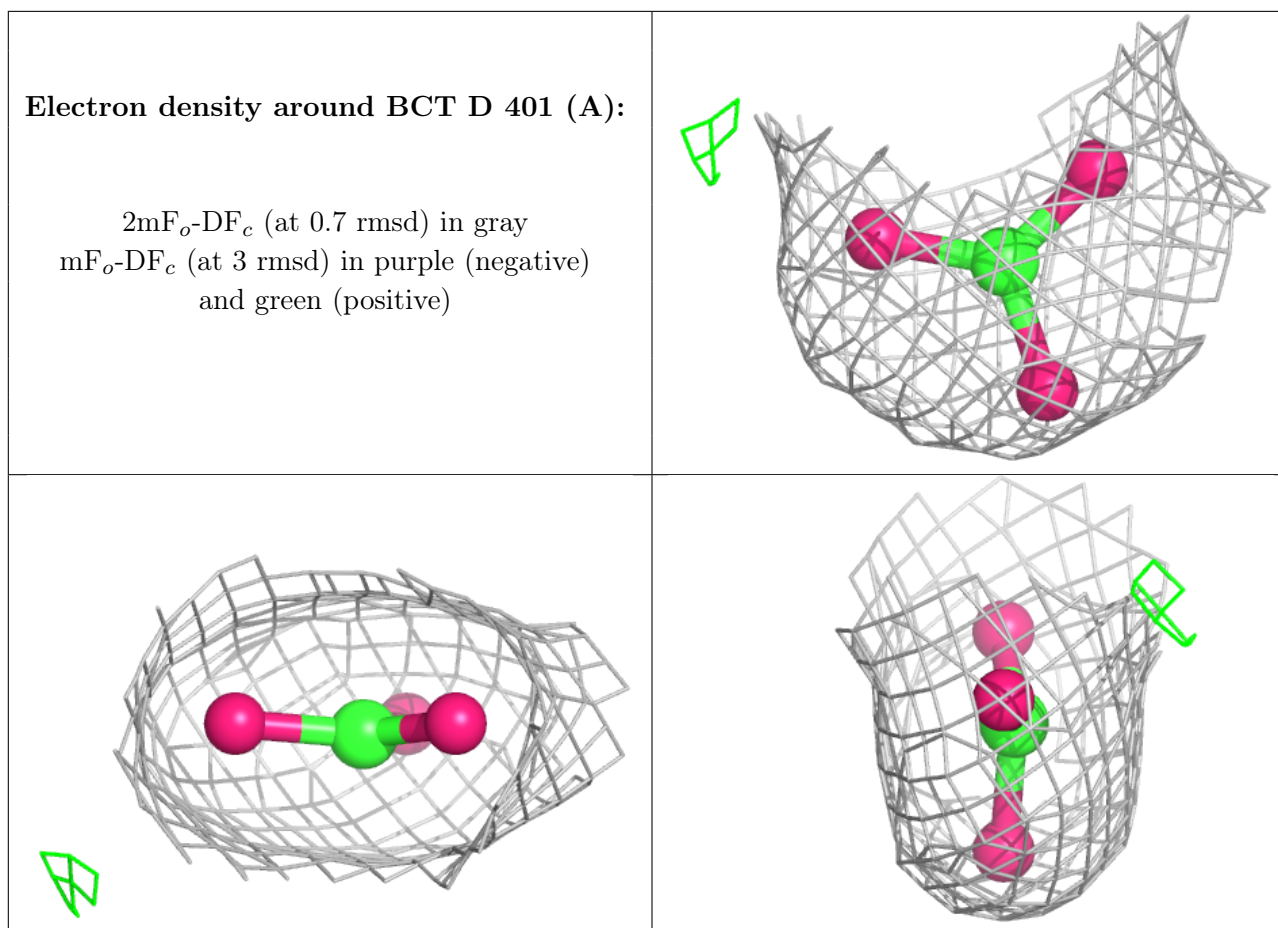






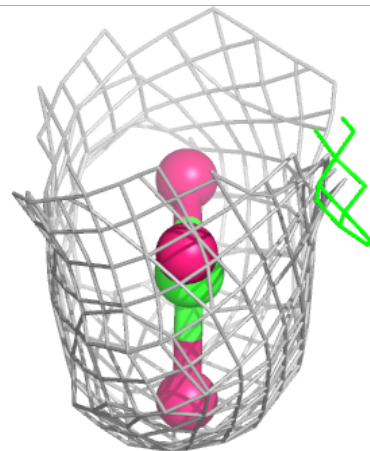
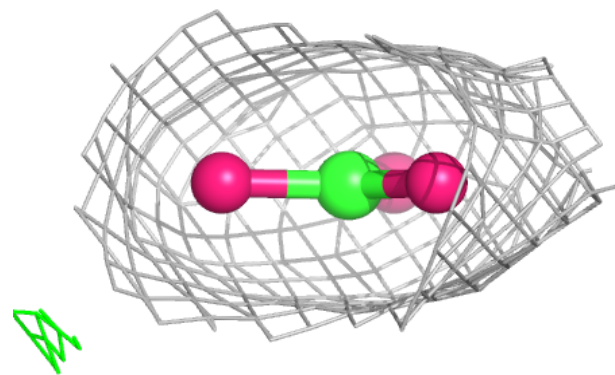
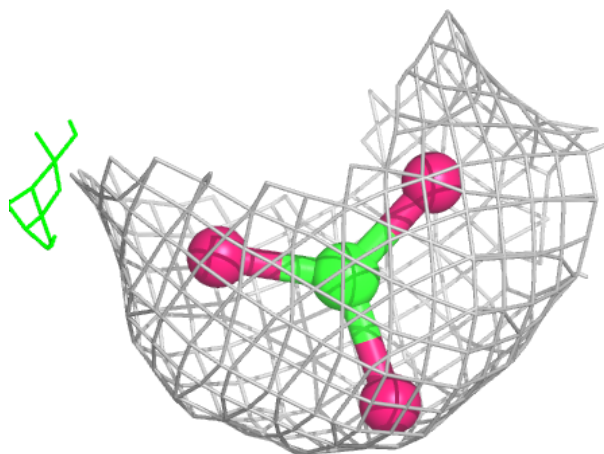


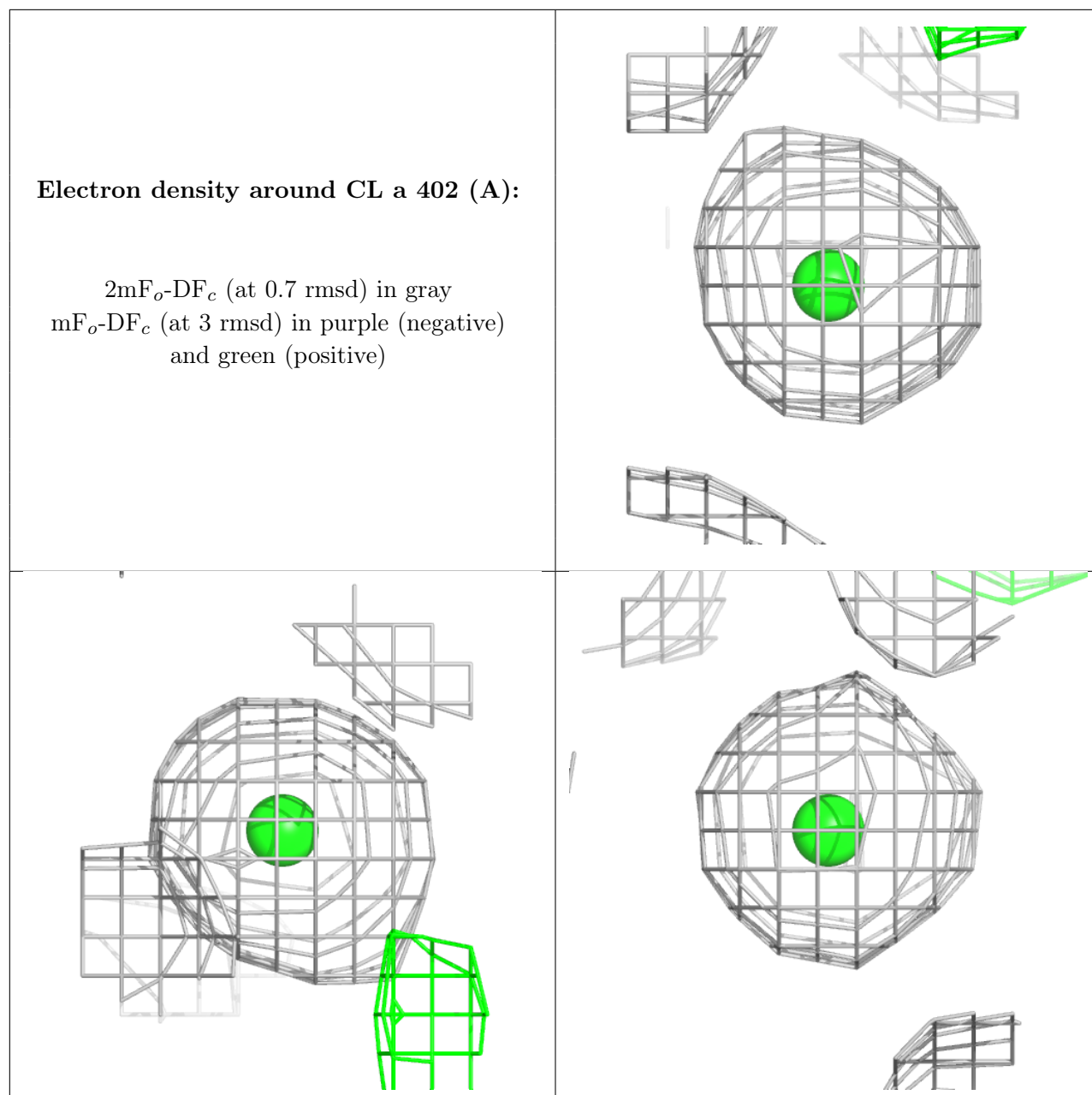




Electron density around BCT D 401 (B):

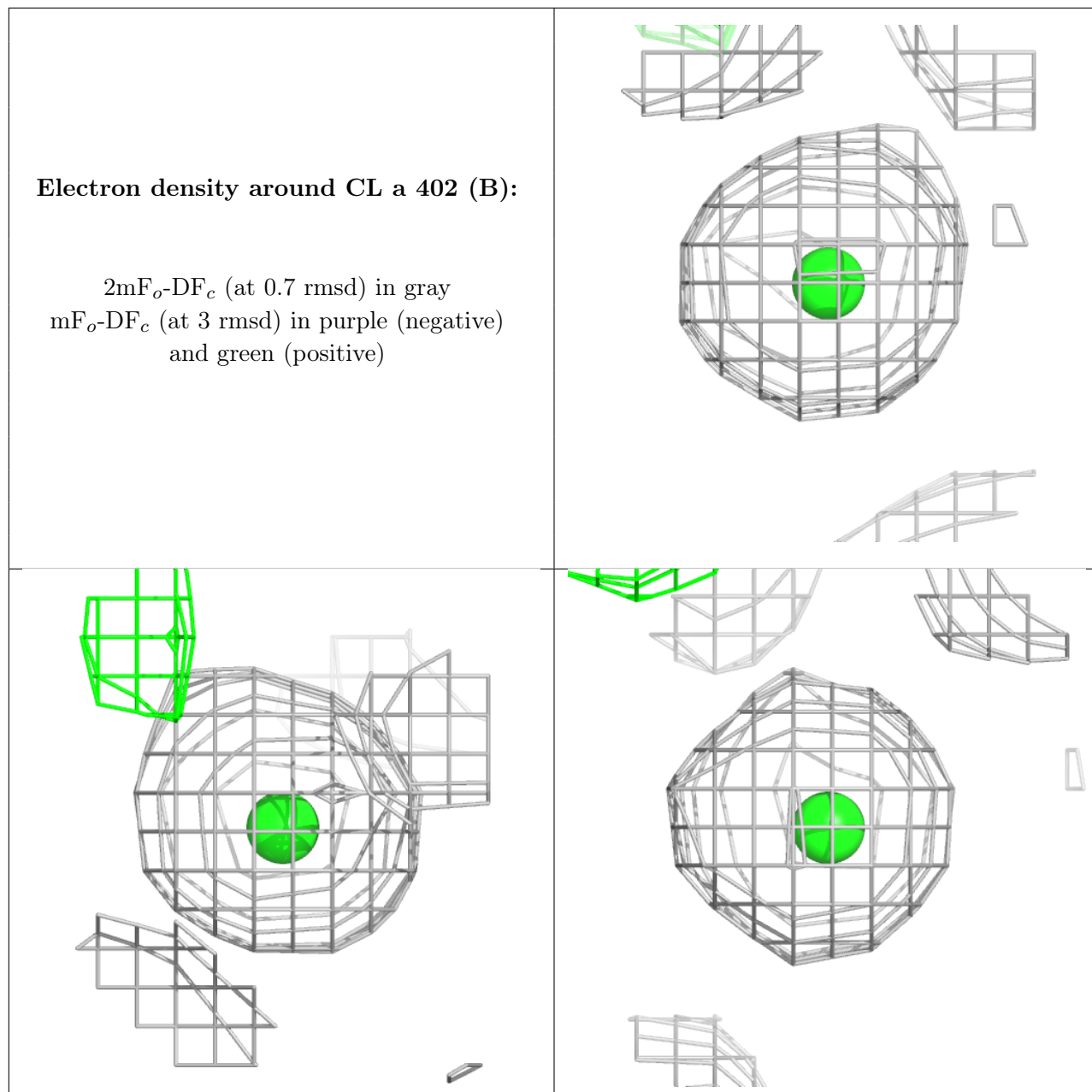
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

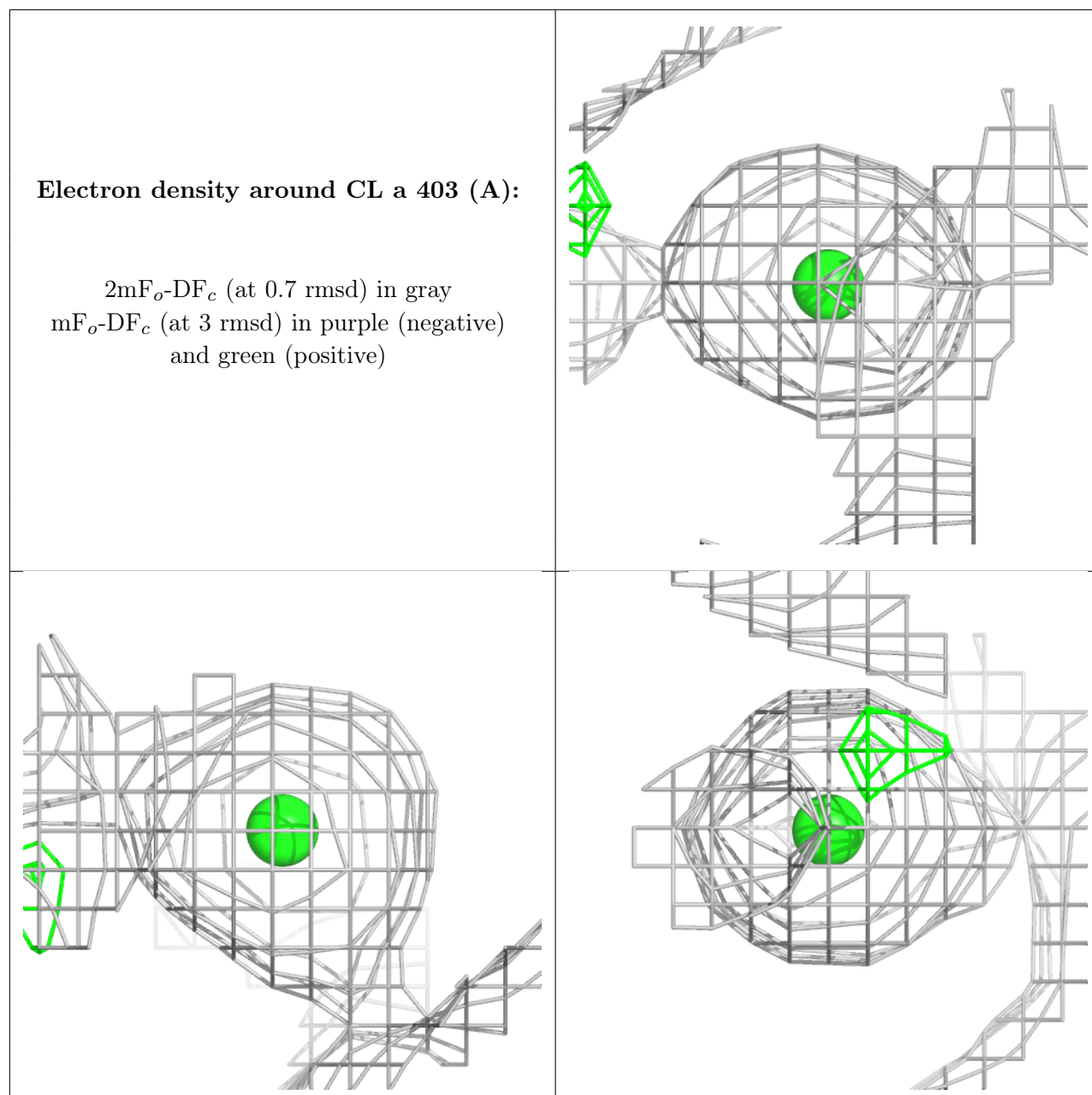




Electron density around CL a 402 (B):

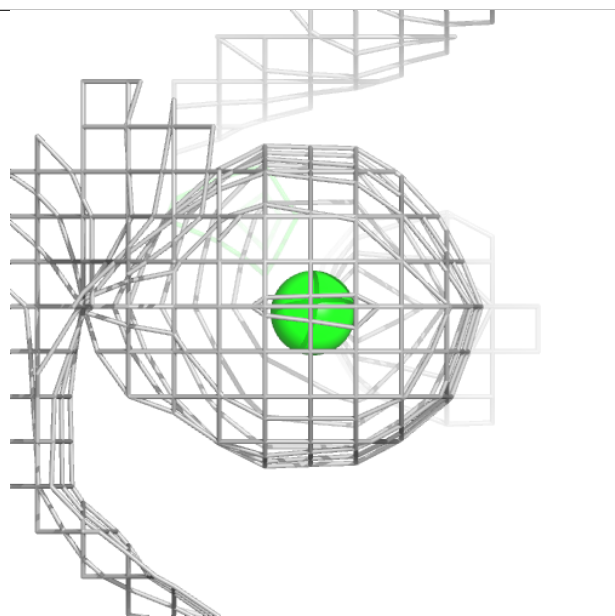
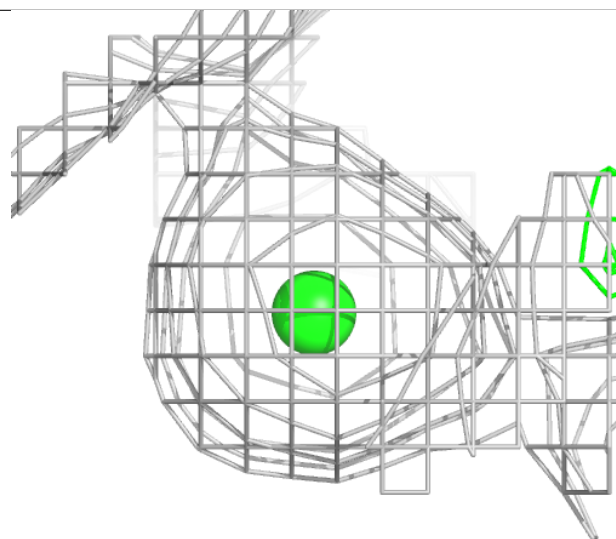
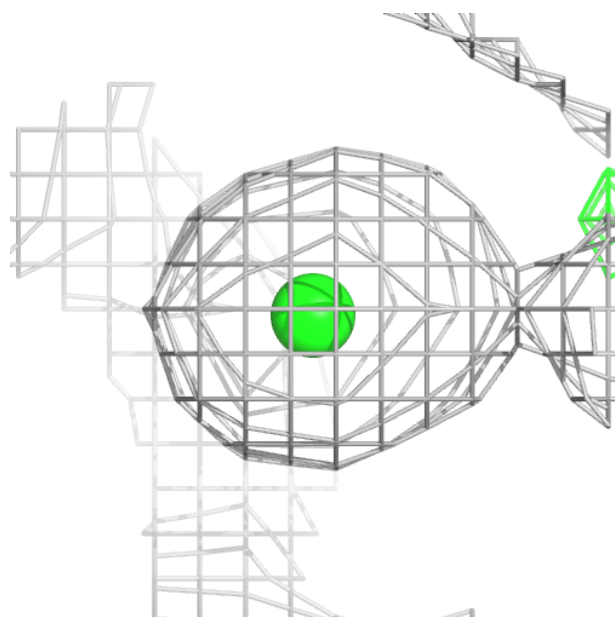
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





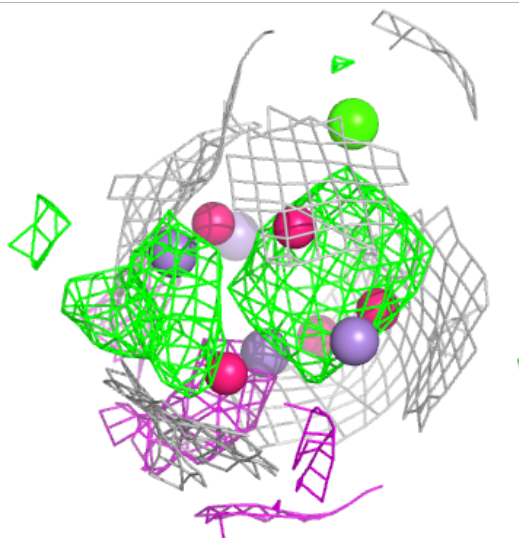
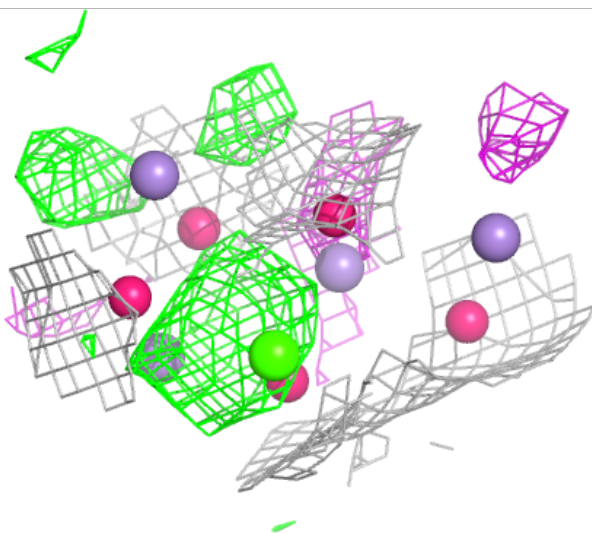
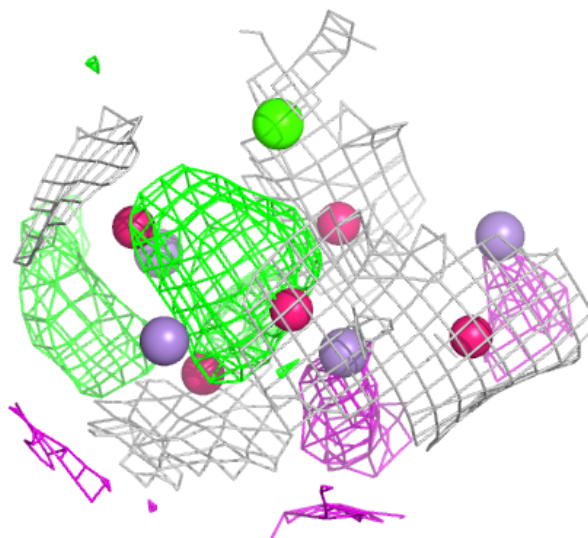
Electron density around CL a 403 (B):

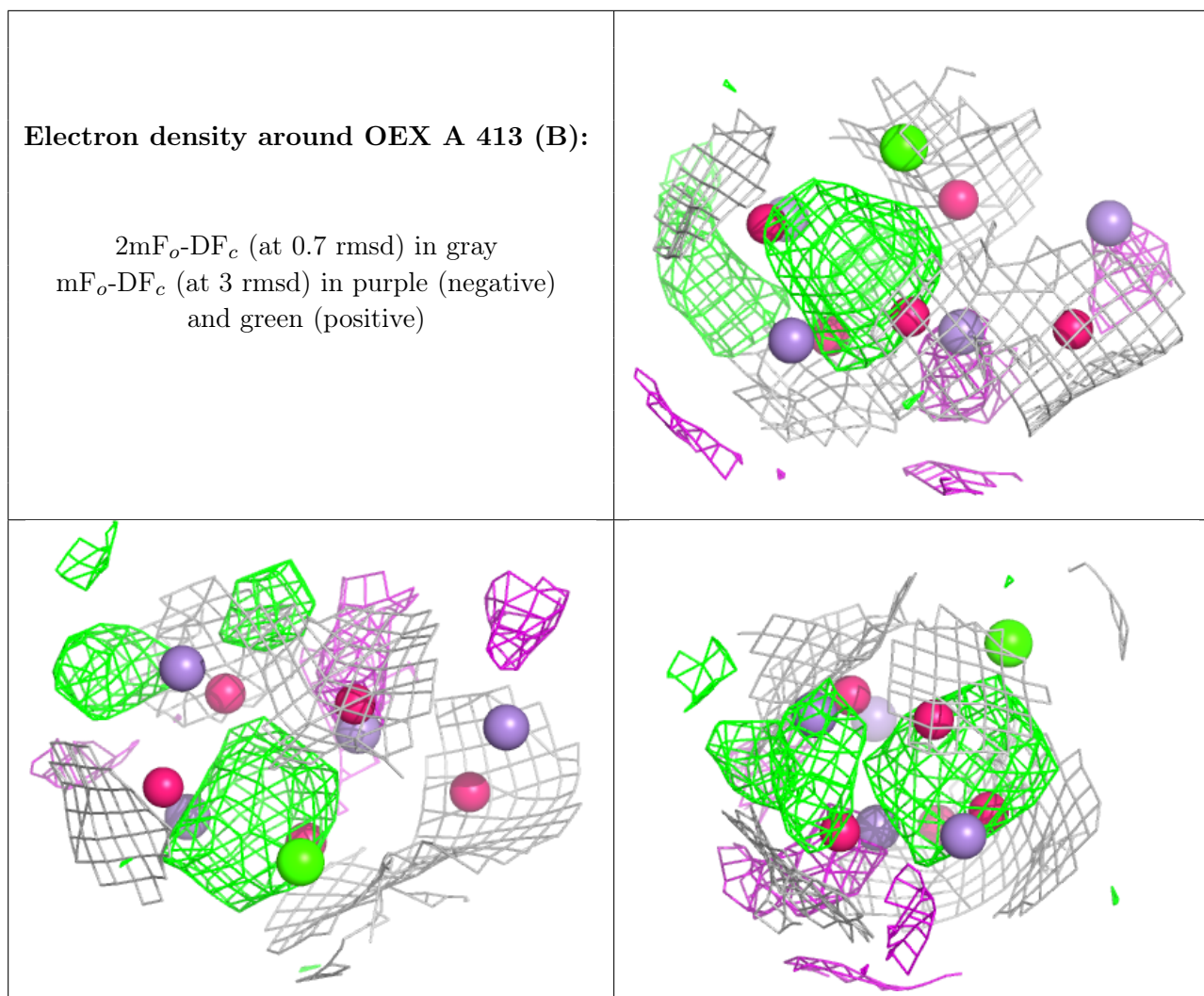
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX A 413 (A):

$2mF_o-DF_c$ (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.