# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 10:56 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6W1O |
| Title | : | RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.08 Angstrom resolution |
| Authors | : | Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovski, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J. |
| Deposited on | : | 2020-03-04 |
| Resolution | : | 2.08 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

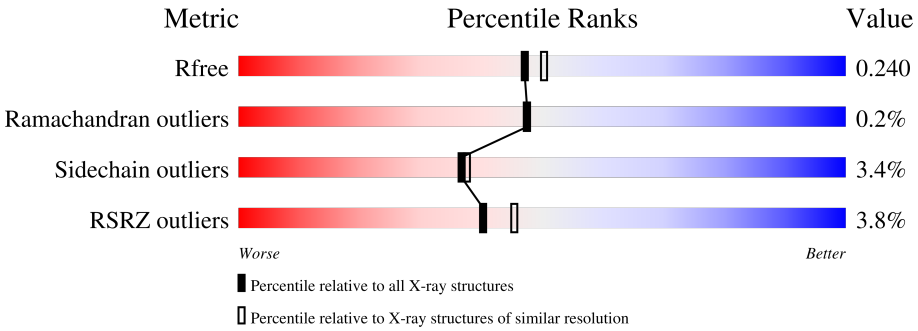
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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 | 6189 (2.10-2.06) |
| Ramachandran outliers | 138981 | 6663 (2.10-2.06) |
| Sidechain outliers | 138945 | 6664 (2.10-2.06) |
| RSRZ outliers | 127900 | 6057 (2.10-2.06) |

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 334 | % 99% . |
| 1 | a | 334 | 96% . |
| 2 | B | 506 | % 98% . |

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| | | |
|---|---|---|
| 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) | : | 2.35.1 |

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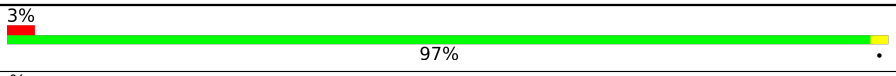
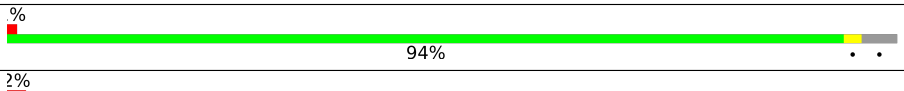
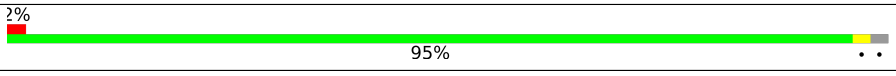
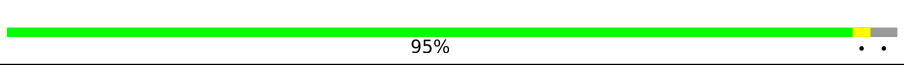
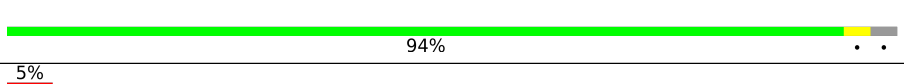
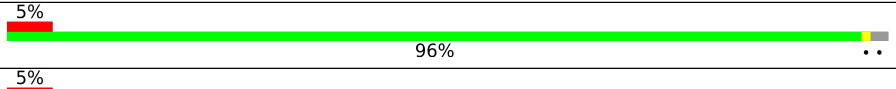
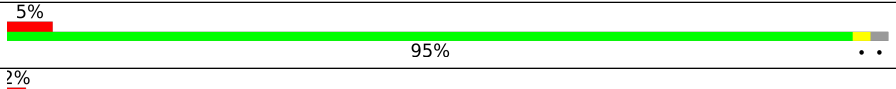
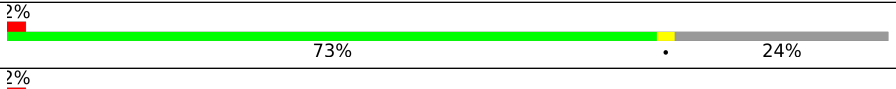
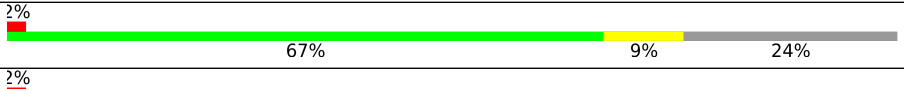
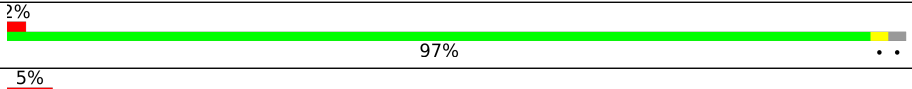
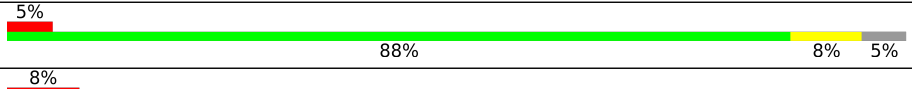
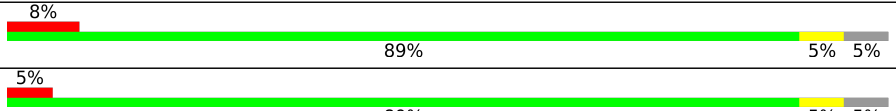
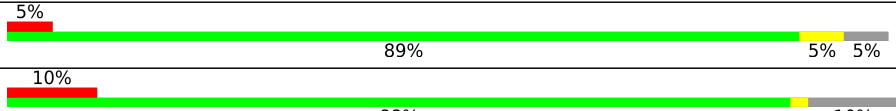
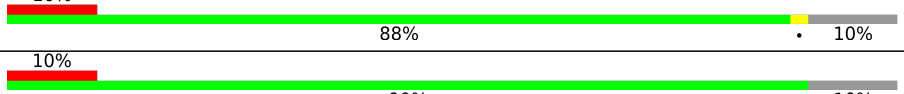
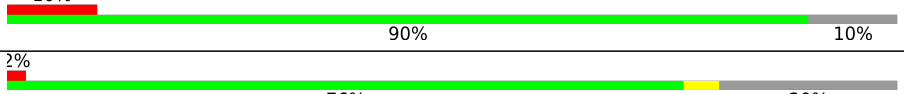
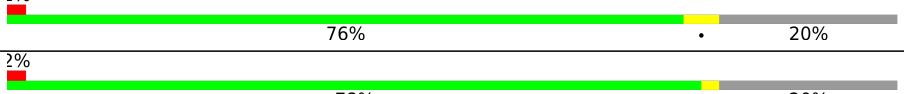
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | b | 506 |   |
| 3 | C | 461 |   |
| 3 | c | 461 |   |
| 4 | D | 352 |   |
| 4 | d | 352 |   |
| 5 | E | 84 |   |
| 5 | e | 84 |   |
| 6 | F | 45 |   |
| 6 | f | 45 |   |
| 7 | H | 66 |   |
| 7 | h | 66 |   |
| 8 | I | 38 |   |
| 8 | i | 38 |   |
| 9 | J | 40 |   |
| 9 | j | 40 |   |
| 10 | K | 46 |   |
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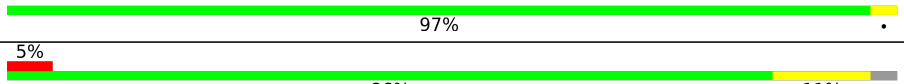
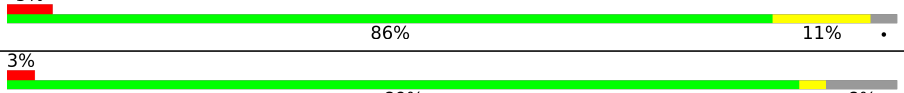
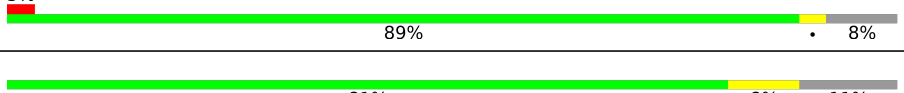
| 11 | L | 37 |   |
| 11 | l | 37 |   |
| 12 | M | 36 |   |
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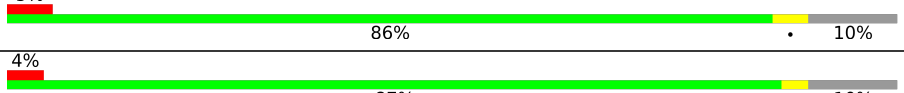
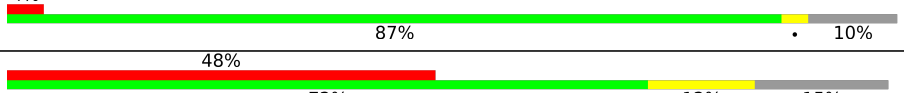
| 13 | O | 272 |   |
| 13 | o | 272 |   |
| 14 | R | 40 | |
| 14 | r | 40 | |

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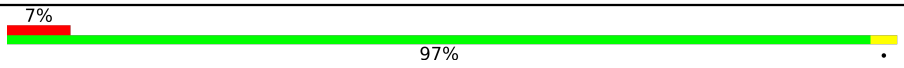
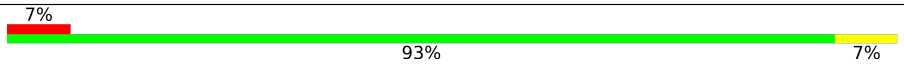
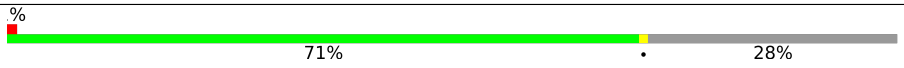
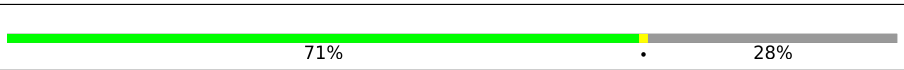
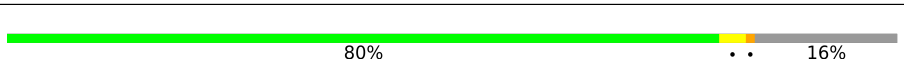
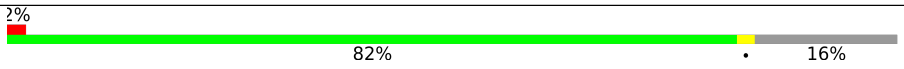
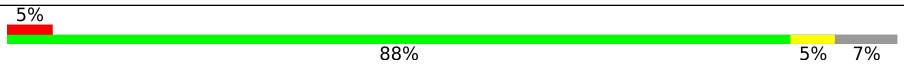
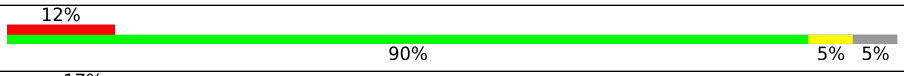
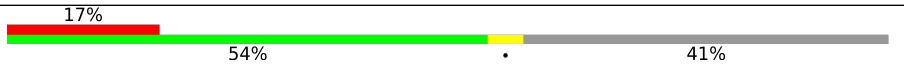
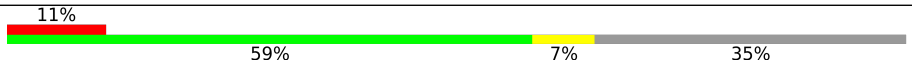
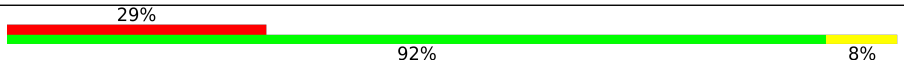
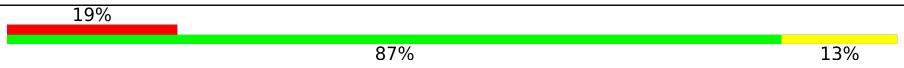
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | T | 30 |   |
| 15 | t | 30 |   |
| 16 | U | 134 |   |
| 16 | u | 134 |   |
| 17 | V | 163 |   |
| 17 | v | 163 |   |
| 18 | X | 41 |   |
| 18 | x | 41 |   |
| 19 | Y | 46 |   |
| 19 | y | 46 |   |
| 20 | Z | 62 |   |
| 20 | z | 62 |   |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 22 | CLA | A | 402 | X | - | - | - |
| 22 | CLA | A | 405 | X | - | - | - |
| 22 | CLA | B | 602 | X | - | - | - |
| 22 | CLA | B | 603 | X | - | - | - |
| 22 | CLA | B | 604 | X | - | - | - |
| 22 | CLA | B | 605 | X | - | - | - |
| 22 | CLA | B | 606 | X | - | - | - |
| 22 | CLA | B | 607 | X | - | - | - |
| 22 | CLA | B | 610 | X | - | - | - |
| 22 | CLA | B | 611 | X | - | - | - |
| 22 | CLA | B | 612 | X | - | - | - |
| 22 | CLA | B | 613 | X | - | - | - |
| 22 | CLA | B | 614 | X | - | - | - |
| 22 | CLA | B | 615 | X | - | - | - |
| 22 | CLA | B | 616 | X | - | - | - |
| 22 | CLA | C | 501 | X | - | - | - |
| 22 | CLA | C | 502 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 22 | CLA | C | 503 | X | - | - | - |
| 22 | CLA | C | 504 | X | - | - | - |
| 22 | CLA | C | 505 | X | - | - | - |
| 22 | CLA | C | 506 | X | - | - | - |
| 22 | CLA | C | 507 | X | - | - | - |
| 22 | CLA | C | 509 | X | - | - | - |
| 22 | CLA | C | 510 | X | - | - | - |
| 22 | CLA | C | 511 | X | - | - | - |
| 22 | CLA | C | 512 | X | - | - | - |
| 22 | CLA | C | 513 | X | - | - | - |
| 22 | CLA | D | 405 | X | - | - | - |
| 22 | CLA | H | 101 | X | - | - | - |
| 22 | CLA | a | 402 | X | - | - | - |
| 22 | CLA | a | 405 | X | - | - | - |
| 22 | CLA | b | 601 | X | - | - | - |
| 22 | CLA | b | 603 | X | - | - | - |
| 22 | CLA | b | 604 | X | - | - | - |
| 22 | CLA | b | 605 | X | - | - | - |
| 22 | CLA | b | 606 | X | - | - | - |
| 22 | CLA | b | 607 | X | - | - | - |
| 22 | CLA | b | 610 | X | - | - | - |
| 22 | CLA | b | 611 | X | - | - | - |
| 22 | CLA | b | 612 | X | - | - | - |
| 22 | CLA | b | 613 | X | - | - | - |
| 22 | CLA | b | 614 | X | - | - | - |
| 22 | CLA | b | 615 | X | - | - | - |
| 22 | CLA | b | 616 | X | - | - | - |
| 22 | CLA | c | 502 | X | - | - | - |
| 22 | CLA | c | 504 | X | - | - | - |
| 22 | CLA | c | 505 | X | - | - | - |
| 22 | CLA | c | 506 | X | - | - | - |
| 22 | CLA | c | 507 | X | - | - | - |
| 22 | CLA | c | 508 | X | - | - | - |
| 22 | CLA | c | 510 | X | - | - | - |
| 22 | CLA | c | 511 | X | - | - | - |
| 22 | CLA | c | 512 | X | - | - | - |
| 22 | CLA | c | 513 | X | - | - | - |
| 22 | CLA | c | 514 | X | - | - | - |
| 22 | CLA | d | 404 | X | - | - | - |
| 31 | STE | E | 102 | - | - | - | X |

# 2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 103895 atoms, of which 51610 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 334 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5130 | 1717 | 2508 | 431 | 459 | 15 | | | |
| 1 | a | 334 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5118 | 1714 | 2499 | 431 | 459 | 15 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 505 | Total | C | H | N | O | S | 0 | 5 | 0 |
| | | | 7864 | 2631 | 3859 | 666 | 695 | 13 | | | |
| 2 | b | 505 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 7800 | 2610 | 3822 | 665 | 690 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 442 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 6768 | 2249 | 3342 | 571 | 593 | 13 | | | |
| 3 | c | 451 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 6913 | 2290 | 3413 | 587 | 610 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 341 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5330 | 1800 | 2613 | 444 | 461 | 12 | | | |
| 4 | d | 341 | Total | C | H | N | O | S | 0 | 1 | 0 |
| | | | 5342 | 1804 | 2619 | 444 | 463 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 82 | Total | C | H | N | O | 0 | 1 | 0 |
| | | | 1316 | 436 | 650 | 107 | 123 | | | |
| 5 | e | 82 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1311 | 434 | 647 | 108 | 122 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 34 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 556 | 187 | 281 | 45 | 42 | 1 | | | |
| 6 | f | 34 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 556 | 187 | 281 | 45 | 42 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 7 | H | 65 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 1042 | 341 | 532 | 82 | 85 | 2 | | | |
| 7 | h | 63 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 1016 | 333 | 518 | 80 | 83 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 8 | I | 36 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 607 | 200 | 311 | 46 | 49 | 1 | | | |
| 8 | i | 36 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 607 | 200 | 311 | 46 | 49 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 36 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 525 | 174 | 268 | 40 | 42 | 1 | | | |
| 9 | j | 36 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 525 | 174 | 268 | 40 | 42 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 37 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 620 | 202 | 316 | 48 | 53 | 1 | | | |
| 11 | l | 36 | Total | C | H | N | O | | 0 | 0 | 0 |
| | | | 600 | 197 | 304 | 47 | 52 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 12 | M | 33 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 525 | 171 | 269 | 37 | 47 | 1 | | | |
| 12 | m | 32 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 518 | 168 | 267 | 36 | 46 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| M | 1 | FME | - | initiating methionine | UNP Q8DHA7 |
| m | 1 | FME | - | initiating methionine | UNP Q8DHA7 |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 244 | Total | C | H | N | O | S | 0 | 1 | 0 |
| | | | 3698 | 1168 | 1828 | 313 | 385 | 4 | | | |
| 13 | o | 244 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 3718 | 1170 | 1844 | 317 | 383 | 4 | | | |

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | U | 97 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1546 | 491 | 772 | 129 | 154 | | | |
| 16 | u | 97 | Total | C | H | N | O | 0 | 0 | 0 |
| | | | 1546 | 491 | 772 | 129 | 154 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 17 | V | 137 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2132 | 675 | 1068 | 177 | 208 | 4 | | | |
| 17 | v | 137 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2132 | 675 | 1068 | 177 | 208 | 4 | | | |

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

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

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

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

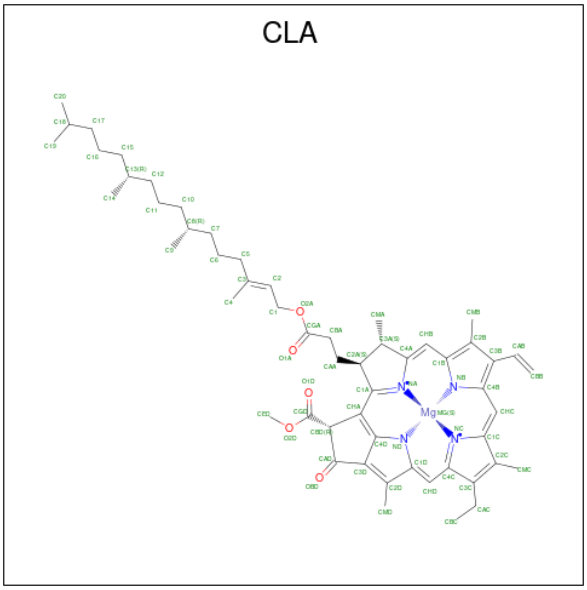
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




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

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 102 | 44 | 48 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | C | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 117 | 49 | 58 | 1 | 4 | 5 | | |

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

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

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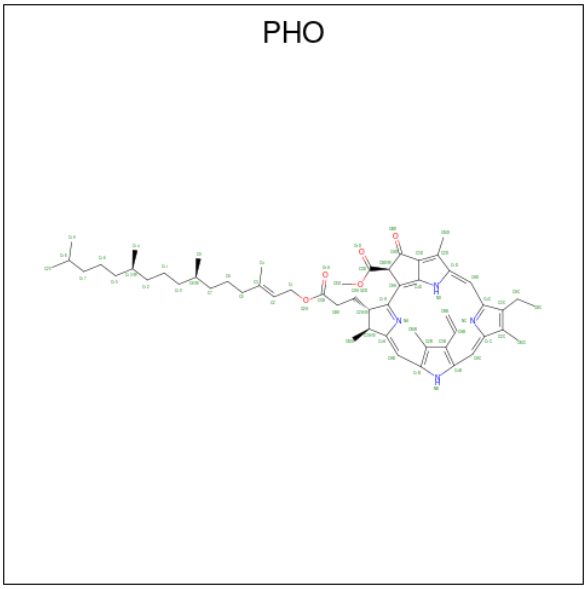
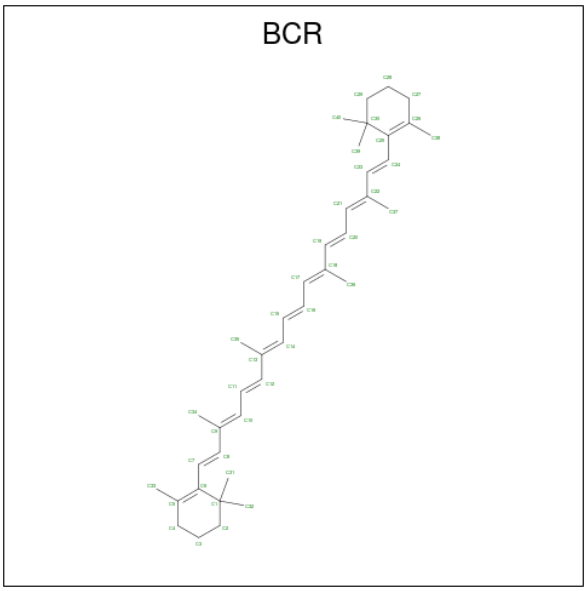
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | H | Mg | N | O | 0 | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | | |
| 22 |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

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




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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 24 | A | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | C | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | F | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | H | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | K | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | K | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | K | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | T | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | a | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | b | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | b | 1 | Total C H<br>96 40 56 | 0 | 0 |

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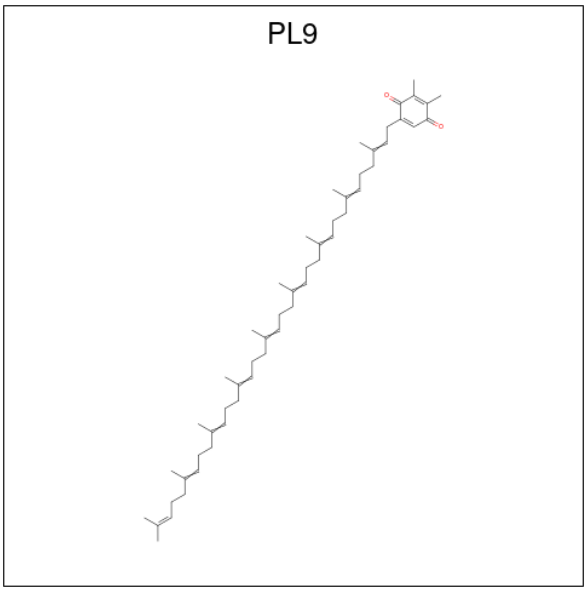
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 24 | b | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | c | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | c | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | d | 1 | Total C H<br>96 40 56 | 0 | 0 |
| 24 | h | 1 | Total C H<br>96 40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

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

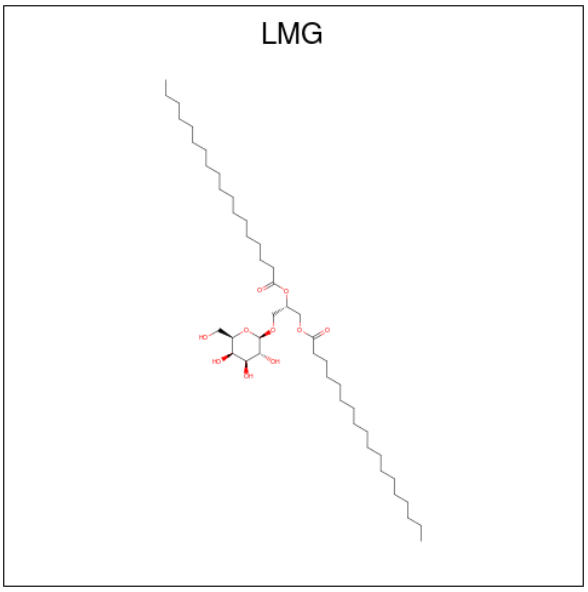
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 25 | A | 2 | Total Cl<br>2 2 | 0 | 0 |
| 25 | a | 2 | Total Cl<br>2 2 | 0 | 0 |

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



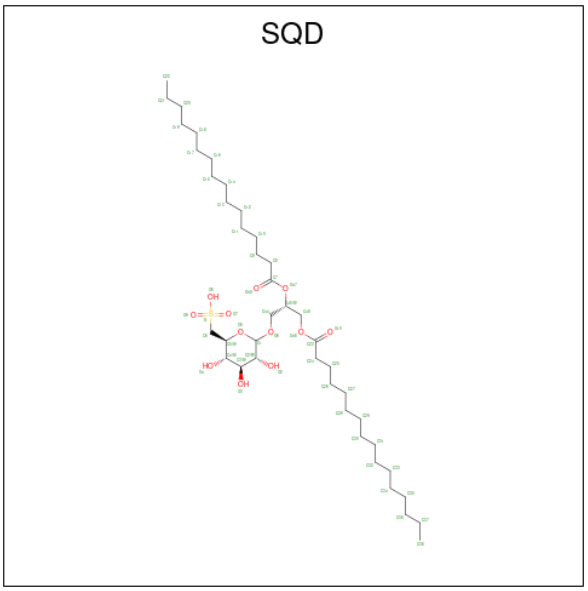

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 26 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 135 | 53 | 80 | 2 | | |
| 26 | a | 1 | Total | C | H | O | 0 | 0 |
| | | | 135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

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



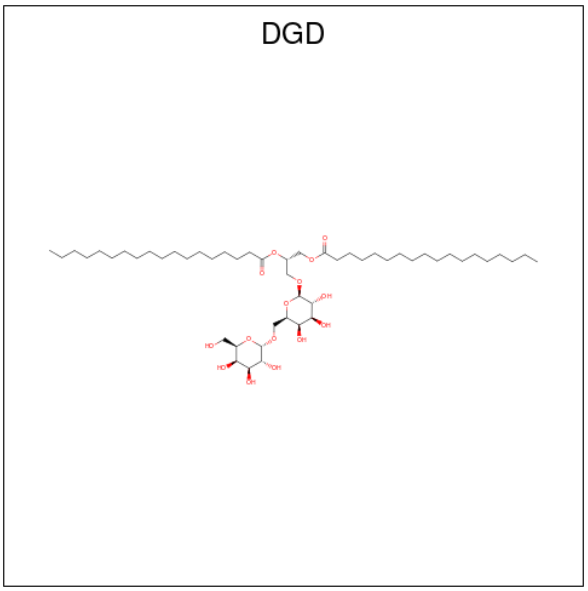
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 27 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 114 | 38 | 66 | 10 | | |
| 27 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 68 | 24 | 40 | 4 | | |
| 27 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 123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

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



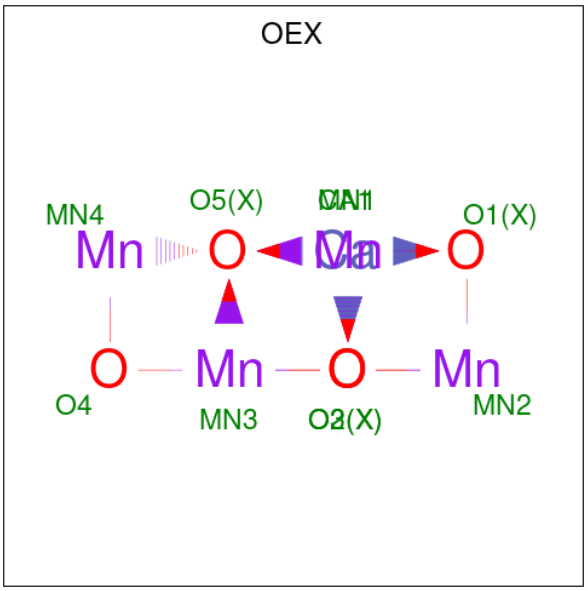

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 28 | A | 1 | Total C H O S<br>123 39 71 12 1 | 0 | 0 |
| 28 | A | 1 | Total C H O<br>104 35 65 4 | 0 | 0 |
| 28 | B | 1 | Total C H O S<br>132 41 78 12 1 | 0 | 0 |
| 28 | D | 1 | Total C H O S<br>82 25 46 10 1 | 0 | 0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

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



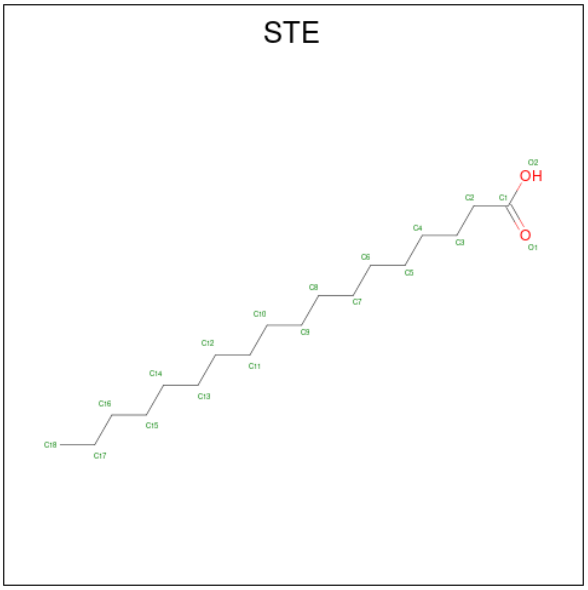

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 29 | A | 1 | Total | C | H | O | 0 | 0 |
| | | | 162 | 51 | 96 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | C | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | H | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 143 | 47 | 81 | 15 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | c | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |
| 29 | h | 1 | Total | C | H | O | 0 | 0 |
| | | | 144 | 47 | 82 | 15 | | |

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




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

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 28 | 10 | 16 | 2 | | |
| 31 | B | 1 | Total | C | H | O | 0 | 0 |
| | | | 43 | 15 | 26 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 31 | B | 1 | Total C H O<br>34 12 20 2 | 0 | 0 |
| 31 | B | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | B | 1 | Total C H O<br>46 16 28 2 | 0 | 0 |
| 31 | B | 1 | Total C H<br>47 16 31 | 0 | 0 |
| 31 | B | 1 | Total C H<br>41 15 26 | 0 | 0 |
| 31 | C | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | C | 1 | Total C H<br>47 16 31 | 0 | 0 |
| 31 | C | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | D | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |
| 31 | E | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | H | 1 | Total C H<br>53 18 35 | 0 | 0 |
| 31 | I | 1 | Total C H<br>41 15 26 | 0 | 0 |
| 31 | J | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | M | 1 | Total C H O<br>37 13 22 2 | 0 | 0 |
| 31 | M | 1 | Total C H<br>26 10 16 | 0 | 0 |
| 31 | T | 1 | Total C H<br>44 15 29 | 0 | 0 |
| 31 | Z | 1 | Total C H<br>20 8 12 | 0 | 0 |
| 31 | a | 1 | Total C H<br>26 10 16 | 0 | 0 |
| 31 | a | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | b | 1 | Total C H<br>47 16 31 | 0 | 0 |
| 31 | b | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |

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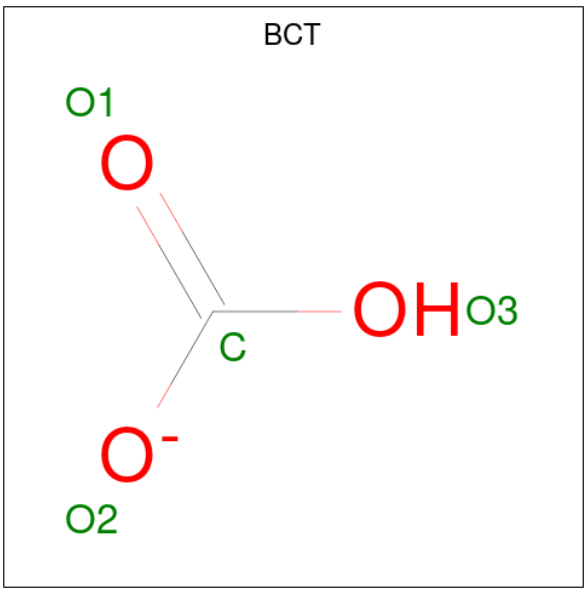
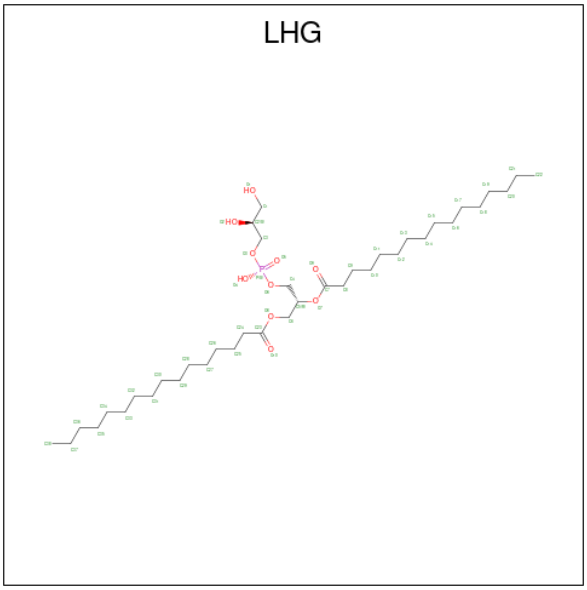
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 31 | b | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |
| 31 | b | 1 | Total C H<br>26 10 16 | 0 | 0 |
| 31 | b | 1 | Total C H<br>41 14 27 | 0 | 0 |
| 31 | b | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |
| 31 | c | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | c | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |
| 31 | d | 1 | Total C H O<br>40 14 24 2 | 0 | 0 |
| 31 | d | 1 | Total C H O<br>43 15 26 2 | 0 | 0 |
| 31 | d | 1 | Total C H O<br>55 18 35 2 | 0 | 0 |
| 31 | j | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |
| 31 | m | 1 | Total C H<br>53 18 35 | 0 | 0 |
| 31 | m | 1 | Total C H O<br>28 10 16 2 | 0 | 0 |

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: $CHO_3$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 32 | D | 1 | Total | C | H | O | 0 | 0 |
| | | | 5 | 1 | 1 | 3 | | |
| 32 | d | 1 | Total | C | H | O | 0 | 0 |
| | | | 5 | 1 | 1 | 3 | | |

- 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 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 114 | 36 | 67 | 10 | 1 | | |
| 33 | D | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | E | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | L | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |
| 33 | d | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 90 | 28 | 51 | 10 | 1 | | |
| 33 | e | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 99 | 31 | 57 | 10 | 1 | | |

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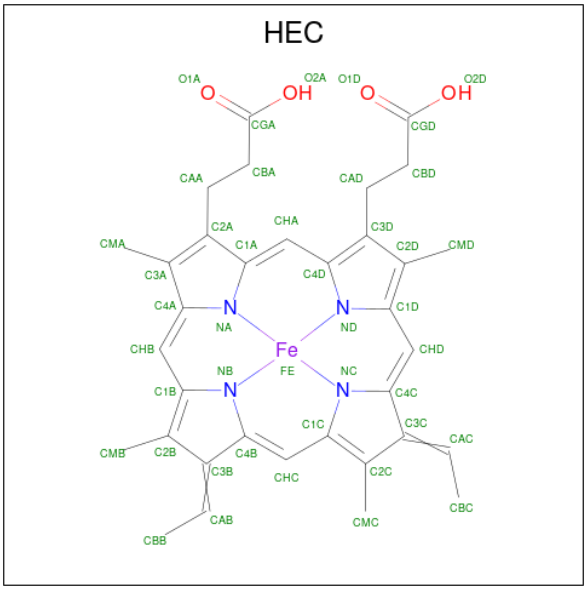
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 33 | l | 1 | Total | C | H | O | P | 0 | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | | |

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




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

- Molecule 35 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 35 | A | 142 | Total | O | 0 | 0 |
| | | | 142 | 142 | | |
| 35 | B | 212 | Total | O | 0 | 0 |
| | | | 212 | 212 | | |
| 35 | C | 184 | Total | O | 0 | 0 |
| | | | 184 | 184 | | |
| 35 | D | 138 | Total | O | 0 | 0 |
| | | | 138 | 138 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | E | 36 | Total O<br>36 36 | 0 | 0 |
| 35 | F | 8 | Total O<br>8 8 | 0 | 0 |
| 35 | H | 40 | Total O<br>40 40 | 0 | 0 |
| 35 | I | 24 | Total O<br>24 24 | 0 | 0 |
| 35 | J | 15 | Total O<br>15 15 | 0 | 0 |
| 35 | K | 7 | Total O<br>7 7 | 0 | 0 |
| 35 | L | 9 | Total O<br>9 9 | 0 | 0 |
| 35 | M | 11 | Total O<br>11 11 | 0 | 0 |
| 35 | O | 104 | Total O<br>104 104 | 0 | 0 |
| 35 | R | 4 | Total O<br>4 4 | 0 | 0 |
| 35 | T | 10 | Total O<br>10 10 | 0 | 0 |
| 35 | U | 52 | Total O<br>52 52 | 0 | 0 |
| 35 | V | 59 | Total O<br>59 59 | 0 | 0 |
| 35 | X | 15 | Total O<br>15 15 | 0 | 0 |
| 35 | Y | 5 | Total O<br>5 5 | 0 | 0 |
| 35 | Z | 6 | Total O<br>6 6 | 0 | 0 |
| 35 | a | 116 | Total O<br>116 116 | 0 | 0 |
| 35 | b | 201 | Total O<br>201 201 | 0 | 0 |
| 35 | c | 187 | Total O<br>187 187 | 0 | 0 |
| 35 | d | 115 | Total O<br>115 115 | 0 | 0 |
| 35 | e | 21 | Total O<br>21 21 | 0 | 0 |

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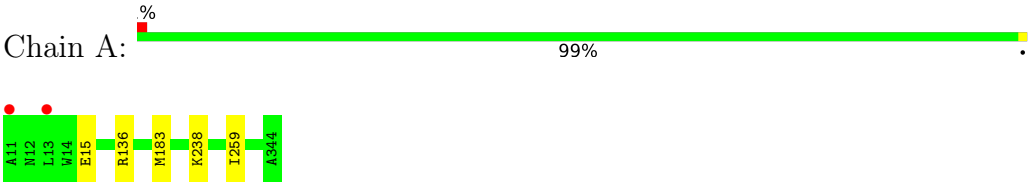
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | f | 6 | Total O<br>6 6 | 0 | 0 |
| 35 | h | 31 | Total O<br>31 31 | 0 | 0 |
| 35 | i | 12 | Total O<br>12 12 | 0 | 0 |
| 35 | j | 6 | Total O<br>6 6 | 0 | 0 |
| 35 | k | 7 | Total O<br>7 7 | 0 | 0 |
| 35 | l | 5 | Total O<br>5 5 | 0 | 0 |
| 35 | m | 10 | Total O<br>10 10 | 0 | 0 |
| 35 | o | 86 | Total O<br>86 86 | 0 | 0 |
| 35 | r | 6 | Total O<br>6 6 | 0 | 0 |
| 35 | t | 9 | Total O<br>9 9 | 0 | 0 |
| 35 | u | 53 | Total O<br>53 53 | 0 | 0 |
| 35 | v | 62 | Total O<br>62 62 | 0 | 0 |
| 35 | x | 8 | Total O<br>8 8 | 0 | 0 |
| 35 | y | 4 | Total O<br>4 4 | 0 | 0 |
| 35 | z | 11 | Total O<br>11 11 | 0 | 0 |

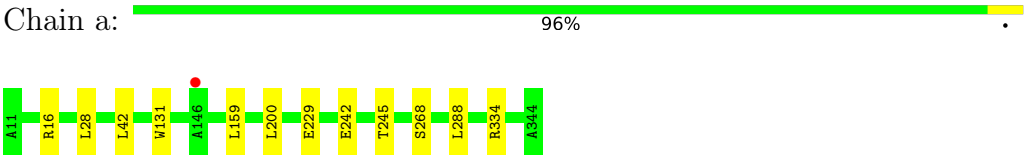
# 3 Residue-property plots (i)

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

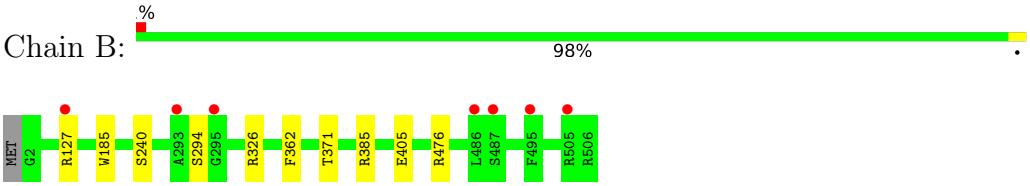
• Molecule 1: Photosystem II protein D1 1



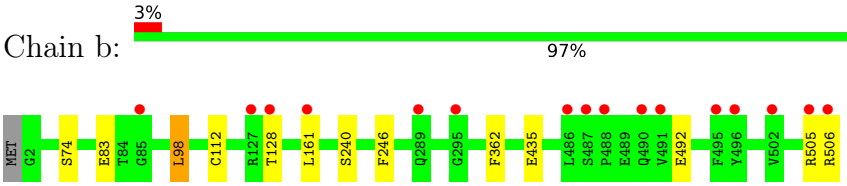

• Molecule 1: Photosystem II protein D1 1



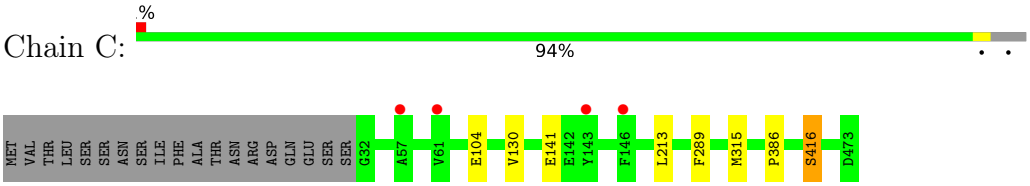

• Molecule 2: Photosystem II CP47 reaction center protein




• Molecule 2: Photosystem II CP47 reaction center protein

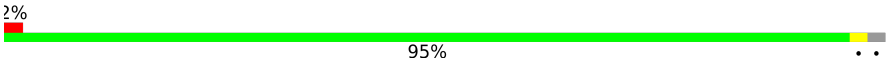


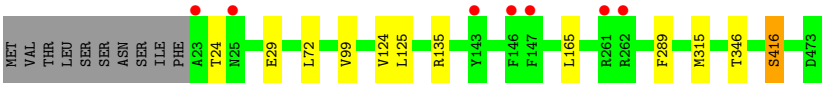

• Molecule 3: Photosystem II CP43 reaction center protein




• Molecule 3: Photosystem II CP43 reaction center protein

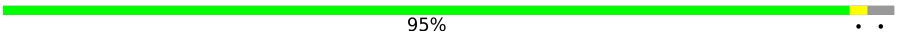
Chain c:



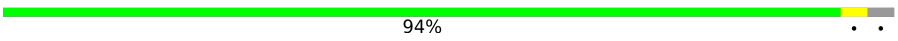

• Molecule 4: Photosystem II D2 protein

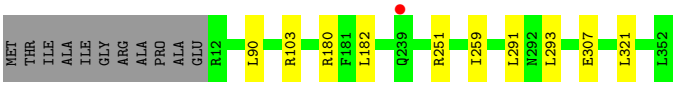
Chain D:



• Molecule 4: Photosystem II D2 protein

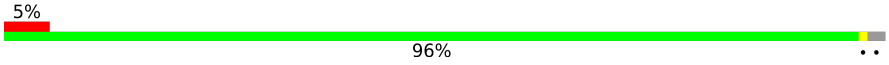
Chain d:

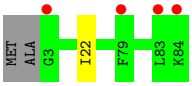



• Molecule 5: Cytochrome b559 subunit alpha

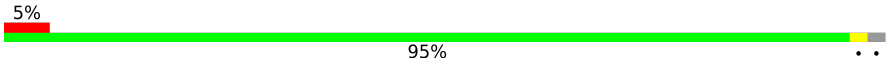
Chain E:

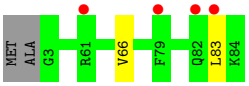



• Molecule 5: Cytochrome b559 subunit alpha

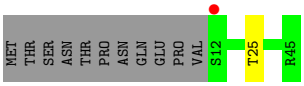
Chain e:



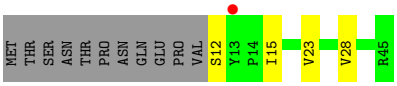

• Molecule 6: Cytochrome b559 subunit beta

Chain F:



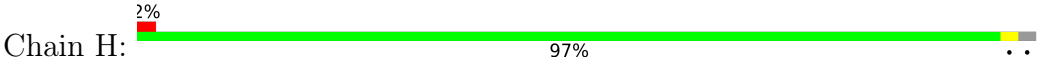

• Molecule 6: Cytochrome b559 subunit beta

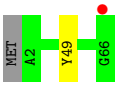
Chain f:



• Molecule 7: Photosystem II reaction center protein H

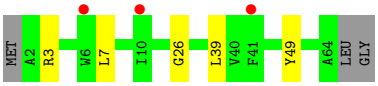
Chain H:



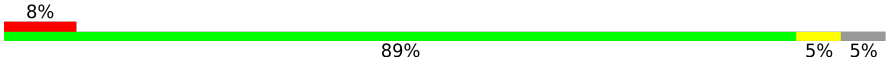

• Molecule 7: Photosystem II reaction center protein H

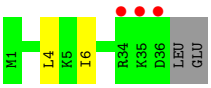
Chain h:




• Molecule 8: Photosystem II reaction center protein I

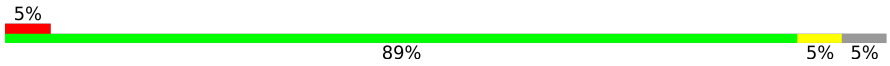
Chain I:

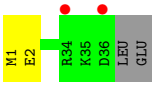



• Molecule 8: Photosystem II reaction center protein I

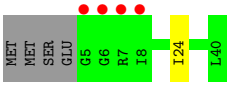
Chain i:



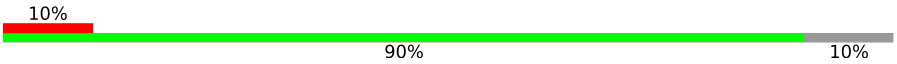

• Molecule 9: Photosystem II reaction center protein J

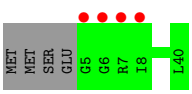
Chain J:




• Molecule 9: Photosystem II reaction center protein J

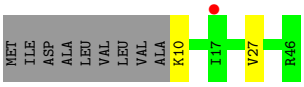
Chain j:



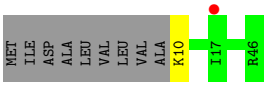

• Molecule 10: Photosystem II reaction center protein K

Chain K:



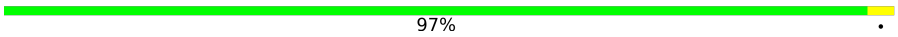

• Molecule 10: Photosystem II reaction center protein K

Chain k:




• Molecule 11: Photosystem II reaction center protein L

Chain L:

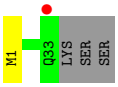


• Molecule 11: Photosystem II reaction center protein L

Chain l:

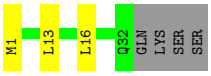
• Molecule 12: Photosystem II reaction center protein M

Chain M:



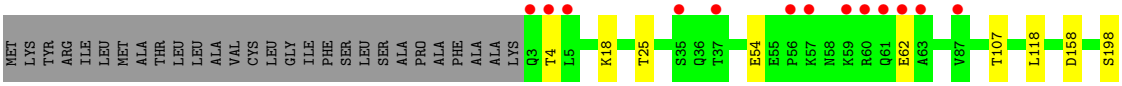

• Molecule 12: Photosystem II reaction center protein M

Chain m:



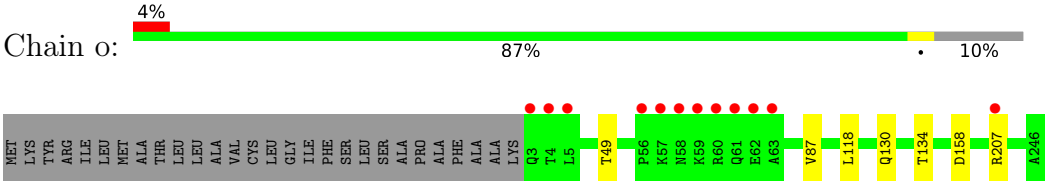

• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



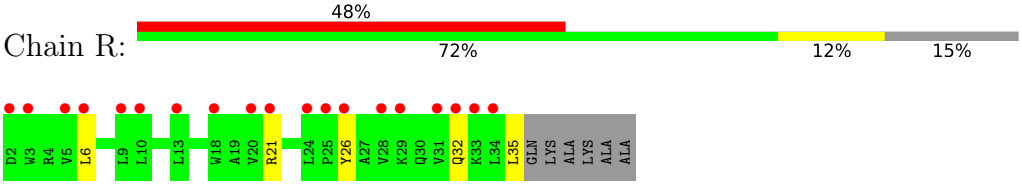
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



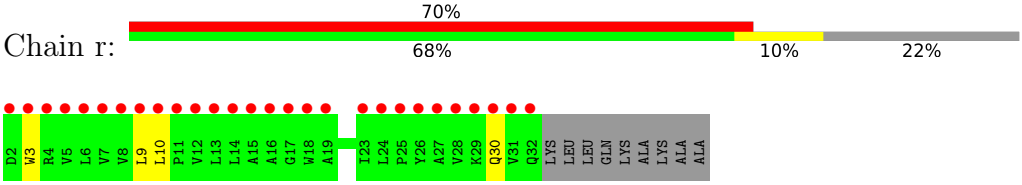

• Molecule 14: Photosystem II protein Y

Chain R:



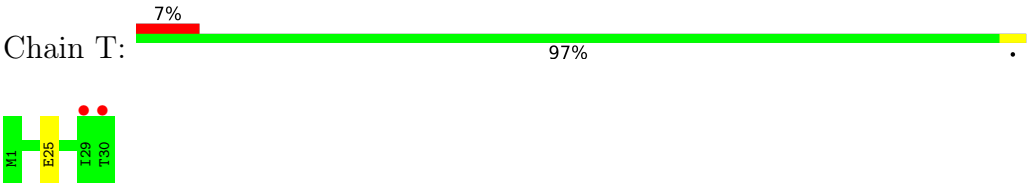

• Molecule 14: Photosystem II protein Y

Chain r:



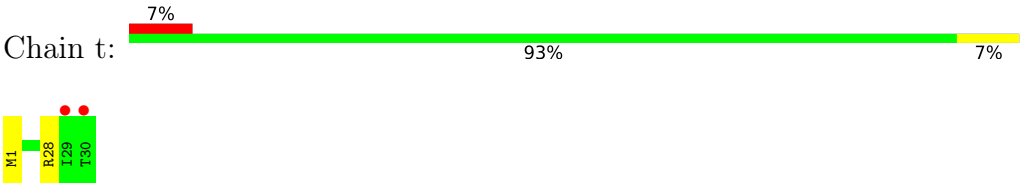

• Molecule 15: Photosystem II reaction center protein T

Chain T:



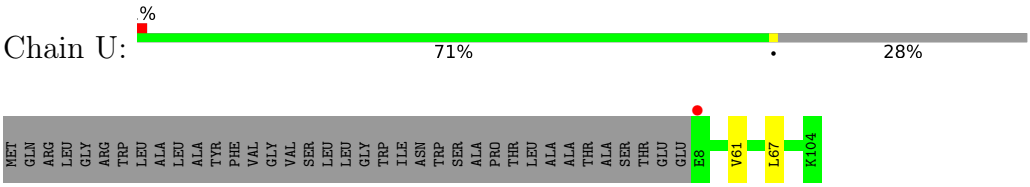

• Molecule 15: Photosystem II reaction center protein T

Chain t:




• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:




• Molecule 16: Photosystem II 12 kDa extrinsic protein

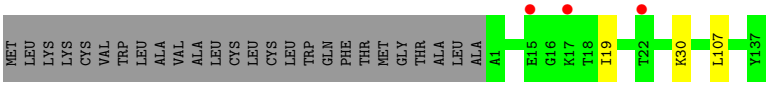
Chain u:

• Molecule 17: Cytochrome c-550

Chain V:

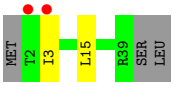
• Molecule 17: Cytochrome c-550

Chain v:



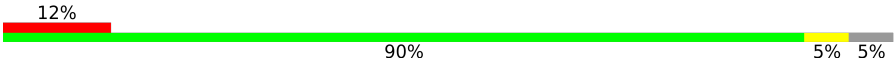

• Molecule 18: Photosystem II reaction center X protein

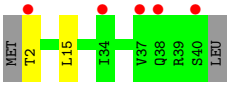
Chain X:




• Molecule 18: Photosystem II reaction center X protein

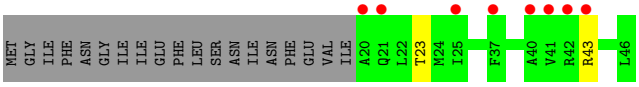
Chain x:



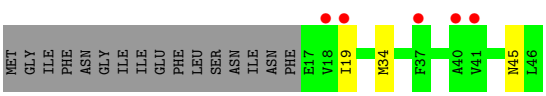

• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



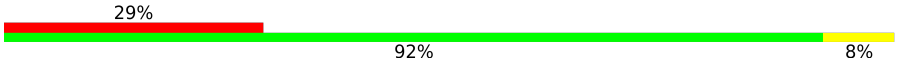

• Molecule 19: Photosystem II reaction center protein Ycf12

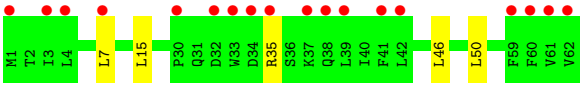
Chain y:




• Molecule 20: Photosystem II reaction center protein Z

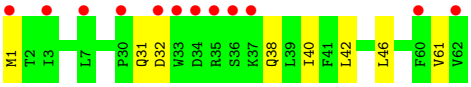
Chain Z:




• Molecule 20: Photosystem II reaction center protein Z

Chain z:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 116.92Å 221.63Å 307.83Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 33.64 – 2.08<br>33.64 – 2.08 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.6 (33.64-2.08)<br>85.1 (33.64-2.08) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.55 (at 2.08Å) | Xtriage |
| Refinement program | PHENIX 1.17.1_3660 | Depositor |
| R, $R_{free}$ | 0.181 , 0.240<br>0.181 , 0.240 | Depositor<br>DCC |
| $R_{free}$ test set | 4226 reflections (0.89%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 26.3 | Xtriage |
| Anisotropy | 0.197 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 63.8 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 103895 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 46.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.67 | 0/2707 | 0.70 | 2/3692 (0.1%) |
| 1 | a | 0.66 | 0/2704 | 0.71 | 2/3688 (0.1%) |
| 2 | B | 0.65 | 1/4161 (0.0%) | 0.68 | 1/5669 (0.0%) |
| 2 | b | 0.63 | 1/4118 (0.0%) | 0.68 | 1/5611 (0.0%) |
| 3 | C | 0.62 | 0/3547 | 0.68 | 0/4830 |
| 3 | c | 0.59 | 0/3619 | 0.66 | 0/4926 |
| 4 | D | 0.66 | 1/2812 (0.0%) | 0.69 | 1/3832 (0.0%) |
| 4 | d | 0.64 | 0/2821 | 0.69 | 1/3844 (0.0%) |
| 5 | E | 0.55 | 0/688 | 0.62 | 0/940 |
| 5 | e | 0.50 | 0/683 | 0.59 | 0/932 |
| 6 | F | 0.55 | 0/284 | 0.56 | 0/387 |
| 6 | f | 0.46 | 0/284 | 0.60 | 0/387 |
| 7 | H | 0.63 | 0/523 | 0.69 | 0/713 |
| 7 | h | 0.58 | 0/511 | 0.67 | 0/697 |
| 8 | I | 0.61 | 0/293 | 0.65 | 0/396 |
| 8 | i | 0.69 | 0/293 | 0.71 | 0/396 |
| 9 | J | 0.54 | 0/263 | 0.64 | 0/356 |
| 9 | j | 0.50 | 0/263 | 0.62 | 0/356 |
| 10 | K | 0.51 | 0/303 | 0.62 | 0/416 |
| 10 | k | 0.55 | 0/303 | 0.65 | 0/416 |
| 11 | L | 0.70 | 0/311 | 0.73 | 1/422 (0.2%) |
| 11 | l | 0.71 | 0/303 | 0.70 | 0/412 |
| 12 | M | 0.71 | 0/249 | 0.77 | 0/341 |
| 12 | m | 0.65 | 0/244 | 0.76 | 0/334 |
| 13 | O | 0.62 | 0/1904 | 0.73 | 1/2585 (0.0%) |
| 13 | o | 0.60 | 0/1905 | 0.75 | 1/2583 (0.0%) |
| 14 | R | 0.45 | 0/277 | 0.53 | 0/380 |
| 14 | r | 0.43 | 0/246 | 0.52 | 0/339 |
| 15 | T | 0.68 | 0/257 | 0.69 | 0/349 |
| 15 | t | 0.69 | 0/255 | 0.63 | 0/346 |
| 16 | U | 0.54 | 0/785 | 0.69 | 0/1064 |
| 16 | u | 0.64 | 0/785 | 0.74 | 0/1064 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | V | 0.60 | 0/1085 | 0.72 | 1/1473 (0.1%) |
| 17 | v | 0.55 | 0/1085 | 0.64 | 0/1473 |
| 18 | X | 0.51 | 0/284 | 0.63 | 0/384 |
| 18 | x | 0.39 | 0/289 | 0.55 | 0/391 |
| 19 | Y | 0.45 | 0/197 | 0.63 | 0/264 |
| 19 | y | 0.39 | 0/219 | 0.54 | 0/294 |
| 20 | Z | 0.46 | 0/490 | 0.55 | 0/669 |
| 20 | z | 0.45 | 0/488 | 0.55 | 0/666 |
| All | All | 0.62 | 3/42838 (0.0%) | 0.68 | 12/58317 (0.0%) |

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

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

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | D | 211 | CYS | CB-SG | -5.77 | 1.72 | 1.81 |
| 2 | B | 185 | TRP | CB-CG | -5.58 | 1.40 | 1.50 |
| 2 | b | 112 | CYS | CB-SG | -5.16 | 1.73 | 1.81 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | a | 334 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 17 | V | 63 | THR | C-N-CD | -6.82 | 105.61 | 120.60 |
| 13 | o | 158 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 2 | B | 326 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 4 | d | 251 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 2 | b | 98 | LEU | CA-CB-CG | 5.48 | 127.91 | 115.30 |
| 4 | D | 294 | ARG | NE-CZ-NH1 | -5.38 | 117.61 | 120.30 |
| 13 | O | 158 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | A | 183 | MET | CA-CB-CG | 5.26 | 122.25 | 113.30 |
| 1 | a | 131 | TRP | CA-CB-CG | -5.16 | 103.89 | 113.70 |
| 1 | A | 136 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 11 | L | 14 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 332/334 (99%) | 325 (98%) | 6 (2%) | 1 (0%) | 41 39 |
| 1 | a | 332/334 (99%) | 326 (98%) | 6 (2%) | 0 | 100 100 |
| 2 | B | 508/506 (100%) | 499 (98%) | 9 (2%) | 0 | 100 100 |
| 2 | b | 503/506 (99%) | 490 (97%) | 13 (3%) | 0 | 100 100 |
| 3 | C | 442/461 (96%) | 433 (98%) | 8 (2%) | 1 (0%) | 47 47 |
| 3 | c | 451/461 (98%) | 435 (96%) | 15 (3%) | 1 (0%) | 47 47 |
| 4 | D | 339/352 (96%) | 329 (97%) | 10 (3%) | 0 | 100 100 |
| 4 | d | 340/352 (97%) | 333 (98%) | 7 (2%) | 0 | 100 100 |
| 5 | E | 81/84 (96%) | 79 (98%) | 2 (2%) | 0 | 100 100 |
| 5 | e | 80/84 (95%) | 80 (100%) | 0 | 0 | 100 100 |
| 6 | F | 32/45 (71%) | 32 (100%) | 0 | 0 | 100 100 |
| 6 | f | 32/45 (71%) | 32 (100%) | 0 | 0 | 100 100 |
| 7 | H | 63/66 (96%) | 59 (94%) | 4 (6%) | 0 | 100 100 |
| 7 | h | 61/66 (92%) | 56 (92%) | 4 (7%) | 1 (2%) | 9 4 |
| 8 | I | 34/38 (90%) | 32 (94%) | 2 (6%) | 0 | 100 100 |
| 8 | i | 34/38 (90%) | 32 (94%) | 2 (6%) | 0 | 100 100 |
| 9 | J | 34/40 (85%) | 30 (88%) | 4 (12%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 9 | j | 34/40 (85%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 10 | K | 35/46 (76%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 10 | k | 35/46 (76%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 34/37 (92%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 31/36 (86%) | 31 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 30/36 (83%) | 28 (93%) | 2 (7%) | 0 | 100 | 100 |
| 13 | O | 243/272 (89%) | 224 (92%) | 18 (7%) | 1 (0%) | 34 | 31 |
| 13 | o | 242/272 (89%) | 230 (95%) | 12 (5%) | 0 | 100 | 100 |
| 14 | R | 32/40 (80%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 14 | r | 29/40 (72%) | 26 (90%) | 2 (7%) | 1 (3%) | 3 | 1 |
| 15 | T | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 15 | t | 28/30 (93%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 16 | U | 95/134 (71%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 16 | u | 95/134 (71%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | V | 135/163 (83%) | 129 (96%) | 5 (4%) | 1 (1%) | 22 | 17 |
| 17 | v | 135/163 (83%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 18 | X | 36/41 (88%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | x | 37/41 (90%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 19 | Y | 25/46 (54%) | 23 (92%) | 1 (4%) | 1 (4%) | 3 | 1 |
| 19 | y | 28/46 (61%) | 25 (89%) | 3 (11%) | 0 | 100 | 100 |
| 20 | Z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 20 | z | 60/62 (97%) | 54 (90%) | 5 (8%) | 1 (2%) | 9 | 4 |
| All | All | 5240/5666 (92%) | 5072 (97%) | 159 (3%) | 9 (0%) | 47 | 47 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 416 | SER |
| 17 | V | 64 | PRO |
| 3 | c | 416 | SER |
| 13 | O | 62 | GLU |
| 19 | Y | 43 | ARG |
| 14 | r | 30 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | z | 61 | VAL |
| 1 | A | 259 | ILE |
| 7 | h | 26 | GLY |

### 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 | 270/270 (100%) | 268 (99%) | 2 (1%) | 84 87 |
| 1 | a | 269/270 (100%) | 259 (96%) | 10 (4%) | 34 34 |
| 2 | B | 408/404 (101%) | 400 (98%) | 8 (2%) | 55 59 |
| 2 | b | 402/404 (100%) | 390 (97%) | 12 (3%) | 41 43 |
| 3 | C | 346/362 (96%) | 338 (98%) | 8 (2%) | 50 53 |
| 3 | c | 354/362 (98%) | 342 (97%) | 12 (3%) | 37 37 |
| 4 | D | 276/283 (98%) | 270 (98%) | 6 (2%) | 52 55 |
| 4 | d | 277/283 (98%) | 268 (97%) | 9 (3%) | 39 40 |
| 5 | E | 72/73 (99%) | 70 (97%) | 2 (3%) | 43 46 |
| 5 | e | 71/73 (97%) | 69 (97%) | 2 (3%) | 43 46 |
| 6 | F | 28/39 (72%) | 27 (96%) | 1 (4%) | 35 35 |
| 6 | f | 28/39 (72%) | 24 (86%) | 4 (14%) | 3 1 |
| 7 | H | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 61 |
| 7 | h | 53/55 (96%) | 49 (92%) | 4 (8%) | 13 9 |
| 8 | I | 32/34 (94%) | 30 (94%) | 2 (6%) | 18 14 |
| 8 | i | 32/34 (94%) | 31 (97%) | 1 (3%) | 40 41 |
| 9 | J | 24/28 (86%) | 23 (96%) | 1 (4%) | 30 29 |
| 9 | j | 24/28 (86%) | 24 (100%) | 0 | 100 100 |
| 10 | K | 30/37 (81%) | 28 (93%) | 2 (7%) | 16 12 |
| 10 | k | 30/37 (81%) | 29 (97%) | 1 (3%) | 38 39 |
| 11 | L | 35/35 (100%) | 35 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 11 | l | 34/35 (97%) | 30 (88%) | 4 (12%) | 5 2 |
| 12 | M | 28/32 (88%) | 28 (100%) | 0 | 100 100 |
| 12 | m | 28/32 (88%) | 26 (93%) | 2 (7%) | 14 11 |
| 13 | O | 206/228 (90%) | 198 (96%) | 8 (4%) | 32 32 |
| 13 | o | 207/228 (91%) | 201 (97%) | 6 (3%) | 42 44 |
| 14 | R | 28/32 (88%) | 23 (82%) | 5 (18%) | 2 1 |
| 14 | r | 23/32 (72%) | 20 (87%) | 3 (13%) | 4 2 |
| 15 | T | 26/26 (100%) | 25 (96%) | 1 (4%) | 33 33 |
| 15 | t | 25/26 (96%) | 24 (96%) | 1 (4%) | 31 31 |
| 16 | U | 84/112 (75%) | 82 (98%) | 2 (2%) | 49 52 |
| 16 | u | 84/112 (75%) | 82 (98%) | 2 (2%) | 49 52 |
| 17 | V | 117/138 (85%) | 113 (97%) | 4 (3%) | 37 37 |
| 17 | v | 117/138 (85%) | 114 (97%) | 3 (3%) | 46 49 |
| 18 | X | 31/34 (91%) | 29 (94%) | 2 (6%) | 17 13 |
| 18 | x | 31/34 (91%) | 29 (94%) | 2 (6%) | 17 13 |
| 19 | Y | 19/37 (51%) | 18 (95%) | 1 (5%) | 22 20 |
| 19 | y | 22/37 (60%) | 19 (86%) | 3 (14%) | 3 1 |
| 20 | Z | 52/52 (100%) | 47 (90%) | 5 (10%) | 8 5 |
| 20 | z | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 1 |
| All | All | 4328/4622 (94%) | 4179 (97%) | 149 (3%) | 37 37 |

All (149) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 15 | GLU |
| 1 | A | 238 | LYS |
| 2 | B | 127 | ARG |
| 2 | B | 240 | SER |
| 2 | B | 294 | SER |
| 2 | B | 362 | PHE |
| 2 | B | 371 | THR |
| 2 | B | 385 | ARG |
| 2 | B | 405 | GLU |
| 2 | B | 476 | ARG |
| 3 | C | 104 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 130 | VAL |
| 3 | C | 141 | GLU |
| 3 | C | 213 | LEU |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 3 | C | 386 | PRO |
| 3 | C | 416 | SER |
| 4 | D | 26 | ARG |
| 4 | D | 43 | LEU |
| 4 | D | 171 | PRO |
| 4 | D | 180 | ARG |
| 4 | D | 264 | LYS |
| 4 | D | 295 | SER |
| 5 | E | 22[A] | ILE |
| 5 | E | 22[B] | ILE |
| 6 | F | 25 | THR |
| 7 | H | 49 | TYR |
| 8 | I | 4 | LEU |
| 8 | I | 6 | ILE |
| 9 | J | 24 | ILE |
| 10 | K | 10 | LYS |
| 10 | K | 27 | VAL |
| 13 | O | 4 | THR |
| 13 | O | 18 | LYS |
| 13 | O | 25 | THR |
| 13 | O | 54 | GLU |
| 13 | O | 107 | THR |
| 13 | O | 118 | LEU |
| 13 | O | 198 | SER |
| 13 | O | 214 | THR |
| 14 | R | 6 | LEU |
| 14 | R | 21 | ARG |
| 14 | R | 26 | TYR |
| 14 | R | 32 | GLN |
| 14 | R | 35 | LEU |
| 15 | T | 25 | GLU |
| 16 | U | 61 | VAL |
| 16 | U | 67 | LEU |
| 17 | V | 3 | LEU |
| 17 | V | 7 | VAL |
| 17 | V | 19 | ILE |
| 17 | V | 31 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | X | 3 | ILE |
| 18 | X | 15 | LEU |
| 19 | Y | 23 | THR |
| 20 | Z | 7 | LEU |
| 20 | Z | 15 | LEU |
| 20 | Z | 35 | ARG |
| 20 | Z | 46 | LEU |
| 20 | Z | 50 | LEU |
| 1 | a | 16 | ARG |
| 1 | a | 28 | LEU |
| 1 | a | 42 | LEU |
| 1 | a | 159 | LEU |
| 1 | a | 200 | LEU |
| 1 | a | 229 | GLU |
| 1 | a | 242 | GLU |
| 1 | a | 245 | THR |
| 1 | a | 268 | SER |
| 1 | a | 288 | LEU |
| 2 | b | 74 | SER |
| 2 | b | 83 | GLU |
| 2 | b | 98 | LEU |
| 2 | b | 128 | THR |
| 2 | b | 161 | LEU |
| 2 | b | 240 | SER |
| 2 | b | 246 | PHE |
| 2 | b | 362 | PHE |
| 2 | b | 435 | GLU |
| 2 | b | 492 | GLU |
| 2 | b | 505 | ARG |
| 2 | b | 506 | ARG |
| 3 | c | 24 | THR |
| 3 | c | 29 | GLU |
| 3 | c | 72 | LEU |
| 3 | c | 99 | VAL |
| 3 | c | 124 | VAL |
| 3 | c | 125 | LEU |
| 3 | c | 135 | ARG |
| 3 | c | 165 | LEU |
| 3 | c | 289 | PHE |
| 3 | c | 315 | MET |
| 3 | c | 346 | THR |
| 3 | c | 416 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | d | 90 | LEU |
| 4 | d | 103 | ARG |
| 4 | d | 180 | ARG |
| 4 | d | 182 | LEU |
| 4 | d | 259 | ILE |
| 4 | d | 291 | LEU |
| 4 | d | 293 | LEU |
| 4 | d | 307 | GLU |
| 4 | d | 321 | LEU |
| 5 | e | 66 | VAL |
| 5 | e | 83 | LEU |
| 6 | f | 12 | SER |
| 6 | f | 15 | ILE |
| 6 | f | 23 | VAL |
| 6 | f | 28 | VAL |
| 7 | h | 3 | ARG |
| 7 | h | 7 | LEU |
| 7 | h | 39 | LEU |
| 7 | h | 49 | TYR |
| 8 | i | 2 | GLU |
| 10 | k | 10 | LYS |
| 11 | l | 2 | GLU |
| 11 | l | 7 | ARG |
| 11 | l | 21 | LEU |
| 11 | l | 30 | LEU |
| 12 | m | 13 | LEU |
| 12 | m | 16 | LEU |
| 13 | o | 49 | THR |
| 13 | o | 87 | VAL |
| 13 | o | 118 | LEU |
| 13 | o | 130 | GLN |
| 13 | o | 134 | THR |
| 13 | o | 207 | ARG |
| 14 | r | 3 | TRP |
| 14 | r | 9 | LEU |
| 14 | r | 10 | LEU |
| 15 | t | 28 | ARG |
| 16 | u | 15 | GLU |
| 16 | u | 23 | GLU |
| 17 | v | 19 | ILE |
| 17 | v | 30 | LYS |
| 17 | v | 107 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | x | 2 | THR |
| 18 | x | 15 | LEU |
| 19 | y | 19 | ILE |
| 19 | y | 34 | MET |
| 19 | y | 45 | ASN |
| 20 | z | 1 | MET |
| 20 | z | 31 | GLN |
| 20 | z | 32 | ASP |
| 20 | z | 38 | GLN |
| 20 | z | 40 | ILE |
| 20 | z | 42 | LEU |
| 20 | z | 46 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 181 | ASN |
| 1 | A | 338 | ASN |
| 11 | L | 8 | GLN |
| 13 | O | 3 | GLN |
| 13 | O | 36 | GLN |
| 13 | O | 88 | ASN |
| 20 | Z | 6 | GLN |
| 20 | Z | 31 | GLN |
| 1 | a | 181 | ASN |
| 1 | a | 234 | ASN |
| 2 | b | 409 | GLN |
| 3 | c | 28 | GLN |
| 3 | c | 373 | ASN |
| 5 | e | 60 | GLN |
| 16 | u | 37 | 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 | $\#\|Z\| > 2$ |
| 8 | FME | I | 1 | 8 | 8,9,10 | 1.01 | 0 | 7,9,11 | 0.97 | 0 |
| 12 | FME | M | 1 | 12 | 8,9,10 | 1.07 | 1 (12%) | 7,9,11 | 0.79 | 0 |
| 15 | FME | T | 1 | 15 | 8,9,10 | 1.18 | 0 | 7,9,11 | 0.65 | 0 |
| 15 | FME | t | 1 | 15 | 8,9,10 | 1.06 | 0 | 7,9,11 | 1.26 | 1 (14%) |
| 8 | FME | i | 1 | 8 | 8,9,10 | 1.20 | 1 (12%) | 7,9,11 | 1.20 | 1 (14%) |
| 12 | FME | m | 1 | 12 | 8,9,10 | 1.12 | 1 (12%) | 7,9,11 | 0.44 | 0 |

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

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

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | i | 1 | FME | CA-N | -2.76 | 1.42 | 1.46 |
| 12 | m | 1 | FME | CA-N | -2.32 | 1.43 | 1.46 |
| 12 | M | 1 | FME | CA-N | -2.05 | 1.43 | 1.46 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | i | 1 | FME | CA-N-CN | -2.41 | 119.12 | 122.82 |
| 15 | t | 1 | FME | C-CA-N | 2.40 | 114.06 | 109.73 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 12 | M | 1 | FME | O-C-CA-CB |
| 15 | T | 1 | FME | O-C-CA-CB |
| 15 | t | 1 | FME | CB-CG-SD-CE |
| 15 | T | 1 | FME | CB-CG-SD-CE |
| 8 | I | 1 | FME | C-CA-CB-CG |
| 12 | M | 1 | FME | CB-CA-N-CN |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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 | $\#\|Z\| > 2$ |
| 31 | STE | B | 627 | - | 14,14,19 | 0.51 | 0 | 13,13,19 | 0.64 | 0 |
| 31 | STE | H | 104 | - | 17,17,19 | 0.40 | 0 | 16,16,19 | 0.88 | 0 |
| 22 | CLA | B | 613 | - | 65,73,73 | 1.85 | 12 (18%) | 76,113,113 | 1.45 | 10 (13%) |
| 26 | PL9 | a | 409 | - | 55,55,55 | 1.07 | 4 (7%) | 68,69,69 | 1.61 | 11 (16%) |
| 31 | STE | E | 102 | - | 11,11,19 | 0.96 | 1 (9%) | 11,11,19 | 0.99 | 1 (9%) |
| 31 | STE | C | 520 | - | 11,11,19 | 0.78 | 0 | 11,11,19 | 1.46 | 1 (9%) |
| 33 | LHG | d | 409 | - | 38,38,48 | 0.99 | 1 (2%) | 41,44,54 | 1.06 | 2 (4%) |
| 22 | CLA | C | 508 | - | 65,73,73 | 1.65 | 9 (13%) | 76,113,113 | 1.54 | 6 (7%) |
| 24 | BCR | b | 618 | - | 41,41,41 | 1.14 | 2 (4%) | 56,56,56 | 1.33 | 5 (8%) |
| 22 | CLA | b | 616 | - | 60,68,73 | 1.46 | 9 (15%) | 70,107,113 | 1.82 | 10 (14%) |
| 31 | STE | I | 101 | - | 14,14,19 | 0.53 | 0 | 13,13,19 | 0.45 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 22 | CLA | d | 403 | - | 65,73,73 | 1.48 | 8 (12%) | 76,113,113 | 1.36 | 10 (13%) |
| 22 | CLA | a | 410 | 35 | 65,73,73 | 1.60 | 8 (12%) | 76,113,113 | 1.48 | 11 (14%) |
| 27 | LMG | b | 623 | - | 55,55,55 | 0.87 | 3 (5%) | 63,63,63 | 1.60 | 11 (17%) |
| 22 | CLA | c | 502 | - | 65,73,73 | 1.60 | 10 (15%) | 76,113,113 | 1.59 | 7 (9%) |
| 29 | DGD | C | 516 | - | 63,63,67 | 1.20 | 9 (14%) | 77,77,81 | 1.40 | 11 (14%) |
| 22 | CLA | b | 605 | - | 65,73,73 | 1.42 | 6 (9%) | 76,113,113 | 1.63 | 17 (22%) |
| 31 | STE | j | 101 | - | 11,11,19 | 1.03 | 1 (9%) | 11,11,19 | 1.41 | 2 (18%) |
| 34 | HEC | V | 201 | 17 | 32,50,50 | 2.09 | 4 (12%) | 24,82,82 | 1.75 | 6 (25%) |
| 31 | STE | m | 102 | - | 11,11,19 | 0.74 | 0 | 11,11,19 | 1.31 | 2 (18%) |
| 27 | LMG | M | 101 | - | 51,51,55 | 1.13 | 3 (5%) | 59,59,63 | 1.48 | 10 (16%) |
| 27 | LMG | c | 523 | - | 49,49,55 | 1.04 | 5 (10%) | 57,57,63 | 1.30 | 5 (8%) |
| 33 | LHG | D | 412 | - | 48,48,48 | 0.76 | 1 (2%) | 51,54,54 | 1.32 | 5 (9%) |
| 24 | BCR | T | 101 | - | 41,41,41 | 1.18 | 4 (9%) | 56,56,56 | 1.19 | 4 (7%) |
| 22 | CLA | c | 509 | - | 64,72,73 | 1.52 | 10 (15%) | 74,111,113 | 1.48 | 11 (14%) |
| 22 | CLA | d | 404 | - | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.38 | 11 (14%) |
| 27 | LMG | a | 415 | - | 55,55,55 | 1.42 | 7 (12%) | 63,63,63 | 1.46 | 6 (9%) |
| 31 | STE | b | 626 | - | 13,13,19 | 0.40 | 0 | 12,12,19 | 0.77 | 0 |
| 28 | SQD | D | 408 | - | 35,36,54 | 0.94 | 2 (5%) | 42,45,65 | 1.87 | 9 (21%) |
| 28 | SQD | a | 412 | - | 35,35,54 | 1.19 | 2 (5%) | 37,37,65 | 1.46 | 4 (10%) |
| 33 | LHG | E | 101 | - | 48,48,48 | 0.86 | 3 (6%) | 51,54,54 | 1.20 | 6 (11%) |
| 22 | CLA | B | 602 | - | 65,73,73 | 1.64 | 7 (10%) | 76,113,113 | 1.49 | 11 (14%) |
| 22 | CLA | b | 611 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.83 | 11 (14%) |
| 22 | CLA | b | 608 | - | 65,73,73 | 1.63 | 9 (13%) | 76,113,113 | 1.40 | 10 (13%) |
| 31 | STE | b | 627 | - | 19,19,19 | 0.60 | 0 | 19,19,19 | 1.23 | 2 (10%) |
| 22 | CLA | b | 607 | 35 | 65,73,73 | 1.52 | 8 (12%) | 76,113,113 | 1.40 | 12 (15%) |
| 31 | STE | b | 622 | - | 19,19,19 | 0.70 | 0 | 19,19,19 | 0.91 | 0 |
| 34 | HEC | F | 102 | 6,5 | 32,50,50 | 2.37 | 5 (15%) | 24,82,82 | 2.11 | 6 (25%) |
| 23 | PHO | D | 401 | - | 51,69,69 | 1.10 | 4 (7%) | 47,99,99 | 1.13 | 3 (6%) |
| 29 | DGD | h | 102 | - | 63,63,67 | 1.16 | 10 (15%) | 77,77,81 | 1.38 | 10 (12%) |
| 33 | LHG | l | 101 | - | 48,48,48 | 0.60 | 0 | 51,54,54 | 1.14 | 4 (7%) |
| 29 | DGD | C | 515 | - | 63,63,67 | 1.44 | 11 (17%) | 77,77,81 | 1.46 | 12 (15%) |
| 22 | CLA | H | 101 | 35 | 65,73,73 | 1.77 | 12 (18%) | 76,113,113 | 1.56 | 10 (13%) |
| 22 | CLA | c | 511 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.53 | 10 (13%) |
| 24 | BCR | B | 618 | - | 41,41,41 | 0.97 | 1 (2%) | 56,56,56 | 1.40 | 9 (16%) |
| 27 | LMG | A | 410 | - | 48,48,55 | 0.99 | 2 (4%) | 56,56,63 | 1.43 | 7 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 31 | STE | B | 626 | - | 15,15,19 | 0.45 | 0 | 14,14,19 | 0.71 | 0 |
| 33 | LHG | d | 407 | - | 48,48,48 | 1.00 | 2 (4%) | 51,54,54 | 1.44 | 5 (9%) |
| 24 | BCR | c | 516 | - | 41,41,41 | 1.21 | 4 (9%) | 56,56,56 | 1.29 | 6 (10%) |
| 22 | CLA | B | 616 | - | 60,68,73 | 1.85 | 11 (18%) | 70,107,113 | 1.67 | 14 (20%) |
| 28 | SQD | A | 412 | - | 38,38,54 | 1.03 | 3 (7%) | 40,40,65 | 1.30 | 4 (10%) |
| 22 | CLA | C | 503 | - | 65,73,73 | 1.66 | 10 (15%) | 76,113,113 | 1.55 | 12 (15%) |
| 22 | CLA | A | 403 | 35 | 65,73,73 | 1.71 | 11 (16%) | 76,113,113 | 1.44 | 13 (17%) |
| 33 | LHG | e | 101 | - | 41,41,48 | 0.91 | 1 (2%) | 44,47,54 | 1.22 | 4 (9%) |
| 22 | CLA | c | 510 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.80 | 11 (14%) |
| 32 | BCT | d | 402 | 21 | 2,3,3 | 1.33 | 0 | 2,3,3 | 3.57 | 2 (100%) |
| 22 | CLA | B | 603 | - | 65,73,73 | 1.44 | 6 (9%) | 76,113,113 | 1.61 | 12 (15%) |
| 22 | CLA | c | 506 | - | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.43 | 10 (13%) |
| 22 | CLA | C | 511 | 3 | 65,73,73 | 1.52 | 8 (12%) | 76,113,113 | 1.29 | 4 (5%) |
| 22 | CLA | B | 612 | - | 65,73,73 | 1.35 | 6 (9%) | 76,113,113 | 1.57 | 12 (15%) |
| 29 | DGD | c | 517 | - | 63,63,67 | 1.37 | 7 (11%) | 77,77,81 | 1.34 | 8 (10%) |
| 22 | CLA | c | 507 | - | 65,73,73 | 1.53 | 7 (10%) | 76,113,113 | 1.40 | 12 (15%) |
| 22 | CLA | C | 506 | - | 65,73,73 | 2.03 | 9 (13%) | 76,113,113 | 1.32 | 8 (10%) |
| 22 | CLA | C | 513 | - | 65,73,73 | 1.51 | 11 (16%) | 76,113,113 | 1.58 | 12 (15%) |
| 24 | BCR | K | 101 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.44 | 9 (16%) |
| 22 | CLA | D | 403 | - | 65,73,73 | 1.49 | 7 (10%) | 76,113,113 | 1.53 | 12 (15%) |
| 24 | BCR | h | 101 | - | 41,41,41 | 1.00 | 2 (4%) | 56,56,56 | 1.38 | 9 (16%) |
| 23 | PHO | A | 404 | - | 51,69,69 | 1.28 | 8 (15%) | 47,99,99 | 1.21 | 4 (8%) |
| 31 | STE | B | 620 | - | 16,16,19 | 0.96 | 2 (12%) | 16,16,19 | 0.91 | 0 |
| 31 | STE | B | 624 | - | 11,11,19 | 0.94 | 0 | 11,11,19 | 1.06 | 0 |
| 24 | BCR | a | 406 | - | 41,41,41 | 1.22 | 3 (7%) | 56,56,56 | 1.22 | 6 (10%) |
| 31 | STE | B | 623 | - | 13,13,19 | 0.62 | 0 | 13,13,19 | 1.31 | 2 (15%) |
| 22 | CLA | B | 610 | 35 | 65,73,73 | 1.65 | 13 (20%) | 76,113,113 | 1.48 | 14 (18%) |
| 22 | CLA | b | 613 | - | 65,73,73 | 1.43 | 11 (16%) | 76,113,113 | 1.51 | 12 (15%) |
| 22 | CLA | B | 611 | - | 65,73,73 | 1.52 | 9 (13%) | 76,113,113 | 1.59 | 12 (15%) |
| 22 | CLA | a | 403 | 35 | 65,73,73 | 1.63 | 9 (13%) | 76,113,113 | 1.53 | 13 (17%) |
| 22 | CLA | b | 602 | - | 65,73,73 | 1.70 | 11 (16%) | 76,113,113 | 1.50 | 14 (18%) |
| 22 | CLA | C | 507 | 35 | 65,73,73 | 1.57 | 8 (12%) | 76,113,113 | 1.81 | 13 (17%) |
| 22 | CLA | b | 601 | 35 | 65,73,73 | 1.69 | 9 (13%) | 76,113,113 | 1.46 | 11 (14%) |
| 22 | CLA | C | 502 | - | 65,73,73 | 1.50 | 7 (10%) | 76,113,113 | 1.30 | 10 (13%) |
| 27 | LMG | b | 621 | - | 51,51,55 | 1.00 | 4 (7%) | 59,59,63 | 1.42 | 10 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 31 | STE | c | 521 | - | 19,19,19 | 0.73 | 1 (5%) | 19,19,19 | 0.92 | 1 (5%) |
| 34 | HEC | v | 201 | 17 | 32,50,50 | 2.16 | 4 (12%) | 24,82,82 | 1.87 | 4 (16%) |
| 22 | CLA | B | 614 | - | 65,73,73 | 1.62 | 10 (15%) | 76,113,113 | 1.33 | 11 (14%) |
| 22 | CLA | B | 605 | - | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.72 | 14 (18%) |
| 24 | BCR | b | 617 | - | 41,41,41 | 1.10 | 3 (7%) | 56,56,56 | 1.38 | 11 (19%) |
| 26 | PL9 | d | 406 | - | 55,55,55 | 1.54 | 10 (18%) | 68,69,69 | 1.84 | 16 (23%) |
| 24 | BCR | K | 103 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.32 | 8 (14%) |
| 22 | CLA | c | 512 | 3 | 65,73,73 | 1.76 | 9 (13%) | 76,113,113 | 1.47 | 6 (7%) |
| 22 | CLA | a | 402 | - | 65,73,73 | 1.63 | 6 (9%) | 76,113,113 | 1.51 | 12 (15%) |
| 26 | PL9 | A | 409 | - | 55,55,55 | 0.95 | 1 (1%) | 68,69,69 | 1.60 | 14 (20%) |
| 22 | CLA | A | 402 | - | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.43 | 8 (10%) |
| 27 | LMG | B | 621 | - | 26,26,55 | 0.65 | 0 | 26,26,63 | 1.28 | 3 (11%) |
| 22 | CLA | B | 615 | - | 65,73,73 | 1.64 | 11 (16%) | 76,113,113 | 1.38 | 8 (10%) |
| 28 | SQD | A | 411 | - | 51,52,54 | 1.11 | 5 (9%) | 60,63,65 | 1.70 | 11 (18%) |
| 31 | STE | J | 101 | - | 11,11,19 | 0.68 | 0 | 11,11,19 | 1.51 | 2 (18%) |
| 24 | BCR | F | 101 | - | 41,41,41 | 1.09 | 3 (7%) | 56,56,56 | 1.28 | 5 (8%) |
| 22 | CLA | C | 504 | 35 | 59,67,73 | 1.52 | 8 (13%) | 68,105,113 | 1.47 | 12 (17%) |
| 22 | CLA | c | 513 | - | 65,73,73 | 1.49 | 8 (12%) | 76,113,113 | 1.44 | 9 (11%) |
| 24 | BCR | H | 102 | - | 41,41,41 | 0.96 | 1 (2%) | 56,56,56 | 1.36 | 7 (12%) |
| 22 | CLA | C | 509 | - | 65,73,73 | 1.50 | 12 (18%) | 76,113,113 | 1.41 | 11 (14%) |
| 31 | STE | D | 413 | - | 19,19,19 | 0.69 | 0 | 19,19,19 | 0.99 | 0 |
| 22 | CLA | C | 510 | - | 65,73,73 | 1.39 | 10 (15%) | 76,113,113 | 1.34 | 10 (13%) |
| 31 | STE | b | 620 | - | 15,15,19 | 0.43 | 0 | 14,14,19 | 0.82 | 0 |
| 31 | STE | b | 624 | - | 19,19,19 | 0.67 | 0 | 19,19,19 | 1.34 | 3 (15%) |
| 22 | CLA | C | 512 | - | 65,73,73 | 1.59 | 8 (12%) | 76,113,113 | 1.37 | 13 (17%) |
| 29 | DGD | c | 518 | - | 63,63,67 | 1.15 | 6 (9%) | 77,77,81 | 1.41 | 11 (14%) |
| 24 | BCR | c | 515 | - | 41,41,41 | 1.08 | 2 (4%) | 56,56,56 | 1.17 | 2 (3%) |
| 27 | LMG | D | 411 | - | 31,31,55 | 1.11 | 3 (9%) | 33,33,63 | 1.15 | 2 (6%) |
| 31 | STE | m | 101 | - | 17,17,19 | 0.42 | 0 | 16,16,19 | 0.80 | 0 |
| 22 | CLA | B | 608 | - | 65,73,73 | 1.75 | 10 (15%) | 76,113,113 | 1.59 | 8 (10%) |
| 22 | CLA | B | 609 | - | 65,73,73 | 1.56 | 10 (15%) | 76,113,113 | 1.43 | 9 (11%) |
| 22 | CLA | c | 504 | - | 65,73,73 | 1.53 | 10 (15%) | 76,113,113 | 1.60 | 11 (14%) |
| 24 | BCR | A | 406 | - | 41,41,41 | 1.14 | 3 (7%) | 56,56,56 | 1.42 | 8 (14%) |
| 22 | CLA | B | 607 | 35 | 65,73,73 | 1.34 | 10 (15%) | 76,113,113 | 1.52 | 11 (14%) |
| 28 | SQD | a | 411 | - | 53,54,54 | 1.02 | 5 (9%) | 62,65,65 | 2.18 | 16 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | LMG | d | 410 | - | 44,44,55 | 1.15 | 4 (9%) | 52,52,63 | 1.31 | 5 (9%) |
| 24 | BCR | k | 102 | - | 41,41,41 | 0.94 | 2 (4%) | 56,56,56 | 1.20 | 5 (8%) |
| 22 | CLA | c | 514 | - | 65,73,73 | 1.74 | 10 (15%) | 76,113,113 | 1.32 | 10 (13%) |
| 28 | SQD | f | 102 | - | 40,41,54 | 1.11 | 4 (10%) | 49,52,65 | 1.91 | 10 (20%) |
| 31 | STE | c | 501 | - | 11,11,19 | 0.84 | 0 | 11,11,19 | 1.06 | 0 |
| 34 | HEC | f | 101 | 6,5 | 32,50,50 | 2.35 | 5 (15%) | 24,82,82 | 2.25 | 6 (25%) |
| 31 | STE | Z | 101 | - | 7,7,19 | 0.42 | 0 | 6,6,19 | 0.55 | 0 |
| 30 | OEX | A | 414 | 35,1,3 | 0,15,15 | - | - | - | | |
| 31 | STE | d | 413 | - | 19,19,19 | 0.68 | 0 | 19,19,19 | 0.95 | 1 (5%) |
| 31 | STE | a | 414 | - | 11,11,19 | 0.82 | 1 (9%) | 11,11,19 | 1.26 | 1 (9%) |
| 24 | BCR | B | 619 | - | 41,41,41 | 1.11 | 1 (2%) | 56,56,56 | 1.47 | 9 (16%) |
| 24 | BCR | C | 514 | - | 41,41,41 | 1.17 | 3 (7%) | 56,56,56 | 1.26 | 8 (14%) |
| 31 | STE | M | 103 | - | 9,9,19 | 0.47 | 0 | 8,8,19 | 0.72 | 0 |
| 29 | DGD | H | 103 | - | 63,63,67 | 1.32 | 8 (12%) | 77,77,81 | 1.53 | 14 (18%) |
| 31 | STE | d | 412 | - | 16,16,19 | 0.62 | 0 | 16,16,19 | 1.06 | 1 (6%) |
| 22 | CLA | b | 614 | - | 65,73,73 | 1.53 | 9 (13%) | 76,113,113 | 1.31 | 6 (7%) |
| 27 | LMG | c | 522 | - | 48,48,55 | 1.12 | 5 (10%) | 56,56,63 | 1.19 | 3 (5%) |
| 33 | LHG | d | 408 | - | 48,48,48 | 0.98 | 1 (2%) | 51,54,54 | 1.15 | 3 (5%) |
| 22 | CLA | c | 508 | 35 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.41 | 9 (11%) |
| 29 | DGD | c | 519 | - | 63,63,67 | 1.22 | 8 (12%) | 77,77,81 | 1.41 | 8 (10%) |
| 22 | CLA | c | 505 | 35 | 60,68,73 | 1.57 | 6 (10%) | 70,107,113 | 1.58 | 12 (17%) |
| 31 | STE | B | 601 | - | 11,11,19 | 0.60 | 0 | 11,11,19 | 1.30 | 1 (9%) |
| 22 | CLA | b | 604 | - | 65,73,73 | 1.88 | 9 (13%) | 76,113,113 | 1.73 | 8 (10%) |
| 31 | STE | M | 102 | - | 14,14,19 | 1.00 | 1 (7%) | 14,14,19 | 0.70 | 0 |
| 31 | STE | b | 625 | - | 9,9,19 | 0.50 | 0 | 8,8,19 | 0.54 | 0 |
| 31 | STE | a | 413 | - | 9,9,19 | 0.53 | 0 | 8,8,19 | 0.56 | 0 |
| 24 | BCR | K | 102 | - | 41,41,41 | 0.99 | 3 (7%) | 56,56,56 | 1.26 | 5 (8%) |
| 22 | CLA | a | 405 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.48 | 11 (14%) |
| 22 | CLA | A | 405 | - | 54,62,73 | 1.86 | 11 (20%) | 62,99,113 | 1.62 | 10 (16%) |
| 29 | DGD | C | 517 | - | 63,63,67 | 1.16 | 7 (11%) | 77,77,81 | 1.47 | 12 (15%) |
| 22 | CLA | b | 612 | - | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.57 | 14 (18%) |
| 22 | CLA | b | 606 | - | 65,73,73 | 1.74 | 11 (16%) | 76,113,113 | 1.54 | 7 (9%) |
| 29 | DGD | A | 413 | - | 67,67,67 | 1.31 | 10 (14%) | 81,81,81 | 1.53 | 13 (16%) |
| 22 | CLA | b | 603 | - | 65,73,73 | 1.49 | 9 (13%) | 76,113,113 | 1.62 | 12 (15%) |
| 22 | CLA | D | 405 | - | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.20 | 7 (9%) |
| 31 | STE | C | 519 | - | 15,15,19 | 0.56 | 0 | 14,14,19 | 0.50 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 22 | CLA | c | 503 | - | 65,73,73 | 1.38 | 9 (13%) | 76,113,113 | 1.45 | 8 (10%) |
| 28 | SQD | B | 622 | - | 53,54,54 | 1.00 | 3 (5%) | 62,65,65 | 1.87 | 13 (20%) |
| 24 | BCR | B | 617 | - | 41,41,41 | 1.07 | 2 (4%) | 56,56,56 | 1.27 | 5 (8%) |
| 27 | LMG | D | 407 | - | 51,51,55 | 0.91 | 2 (3%) | 59,59,63 | 1.37 | 8 (13%) |
| 31 | STE | B | 625 | - | 17,17,19 | 0.64 | 0 | 17,17,19 | 1.29 | 1 (5%) |
| 22 | CLA | B | 604 | - | 65,73,73 | 1.40 | 8 (12%) | 76,113,113 | 1.74 | 15 (19%) |
| 31 | STE | d | 411 | - | 15,15,19 | 0.88 | 1 (6%) | 15,15,19 | 0.96 | 2 (13%) |
| 32 | BCT | D | 402 | 21 | 2,3,3 | 1.19 | 0 | 2,3,3 | 2.94 | 1 (50%) |
| 31 | STE | T | 102 | - | 14,14,19 | 0.42 | 0 | 13,13,19 | 0.85 | 0 |
| 27 | LMG | Y | 101 | - | 48,48,55 | 0.96 | 2 (4%) | 56,56,63 | 1.35 | 6 (10%) |
| 24 | BCR | d | 405 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.25 | 5 (8%) |
| 24 | BCR | t | 101 | - | 41,41,41 | 0.97 | 1 (2%) | 56,56,56 | 1.47 | 12 (21%) |
| 33 | LHG | D | 409 | - | 48,48,48 | 0.92 | 2 (4%) | 51,54,54 | 1.28 | 6 (11%) |
| 22 | CLA | b | 610 | 35 | 65,73,73 | 1.47 | 11 (16%) | 76,113,113 | 1.54 | 17 (22%) |
| 27 | LMG | c | 520 | - | 37,37,55 | 1.17 | 4 (10%) | 45,45,63 | 1.27 | 5 (11%) |
| 22 | CLA | b | 615 | - | 65,73,73 | 2.00 | 9 (13%) | 76,113,113 | 1.47 | 10 (13%) |
| 23 | PHO | d | 401 | - | 51,69,69 | 1.01 | 3 (5%) | 47,99,99 | 1.48 | 7 (14%) |
| 26 | PL9 | D | 406 | - | 55,55,55 | 1.35 | 6 (10%) | 68,69,69 | 1.64 | 14 (20%) |
| 24 | BCR | k | 101 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.10 | 3 (5%) |
| 33 | LHG | D | 410 | - | 46,46,48 | 1.03 | 3 (6%) | 49,52,54 | 1.21 | 4 (8%) |
| 23 | PHO | a | 404 | - | 51,69,69 | 0.97 | 2 (3%) | 47,99,99 | 1.31 | 5 (10%) |
| 22 | CLA | B | 606 | - | 65,73,73 | 1.77 | 10 (15%) | 76,113,113 | 1.46 | 7 (9%) |
| 31 | STE | C | 518 | - | 11,11,19 | 0.77 | 0 | 11,11,19 | 0.96 | 0 |
| 30 | OEX | a | 416 | 35,1,3 | 0,15,15 | - | - | - | | |
| 22 | CLA | C | 501 | - | 65,73,73 | 1.76 | 11 (16%) | 76,113,113 | 1.55 | 13 (17%) |
| 22 | CLA | b | 609 | - | 65,73,73 | 1.74 | 10 (15%) | 76,113,113 | 1.37 | 12 (15%) |
| 28 | SQD | L | 101 | - | 48,49,54 | 0.94 | 2 (4%) | 57,60,65 | 2.40 | 16 (28%) |
| 22 | CLA | C | 505 | - | 65,73,73 | 1.64 | 8 (12%) | 76,113,113 | 1.46 | 10 (13%) |
| 33 | LHG | L | 102 | - | 48,48,48 | 0.79 | 2 (4%) | 51,54,54 | 1.18 | 3 (5%) |
| 24 | BCR | b | 619 | - | 41,41,41 | 1.08 | 2 (4%) | 56,56,56 | 1.28 | 10 (17%) |
| 22 | CLA | D | 404 | 35 | 65,73,73 | 1.69 | 9 (13%) | 76,113,113 | 1.33 | 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 |
|---|---|---|---|---|---|---|---|
| 31 | STE | B | 627 | - | - | 5/12/12/17 | - |
| 31 | STE | H | 104 | - | - | 9/15/15/17 | - |
| 22 | CLA | B | 613 | - | 1/1/20/20 | 13/37/115/115 | - |
| 26 | PL9 | a | 409 | - | - | 21/53/73/73 | 0/1/1/1 |
| 31 | STE | E | 102 | - | - | 4/9/9/17 | - |
| 31 | STE | C | 520 | - | - | 2/9/9/17 | - |
| 33 | LHG | d | 409 | - | - | 12/43/43/53 | - |
| 22 | CLA | C | 508 | - | - | 9/37/115/115 | - |
| 24 | BCR | b | 618 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | b | 616 | - | 1/1/19/20 | 10/31/109/115 | - |
| 31 | STE | I | 101 | - | - | 7/12/12/17 | - |
| 22 | CLA | d | 403 | - | - | 10/37/115/115 | - |
| 22 | CLA | a | 410 | 35 | - | 6/37/115/115 | - |
| 27 | LMG | b | 623 | - | - | 26/50/70/70 | 0/1/1/1 |
| 22 | CLA | c | 502 | - | 1/1/20/20 | 1/37/115/115 | - |
| 29 | DGD | C | 516 | - | - | 21/51/91/95 | 0/2/2/2 |
| 22 | CLA | b | 605 | - | 1/1/20/20 | 8/37/115/115 | - |
| 31 | STE | j | 101 | - | - | 4/9/9/17 | - |
| 34 | HEC | V | 201 | 17 | - | 2/10/54/54 | - |
| 31 | STE | m | 102 | - | - | 5/9/9/17 | - |
| 27 | LMG | M | 101 | - | - | 27/46/66/70 | 0/1/1/1 |
| 27 | LMG | c | 523 | - | - | 23/44/64/70 | 0/1/1/1 |
| 33 | LHG | D | 412 | - | - | 20/53/53/53 | - |
| 24 | BCR | T | 101 | - | - | 14/29/63/63 | 0/2/2/2 |
| 22 | CLA | d | 404 | - | 1/1/20/20 | 5/37/115/115 | - |
| 22 | CLA | c | 509 | - | - | 7/36/114/115 | - |
| 27 | LMG | a | 415 | - | - | 31/50/70/70 | 0/1/1/1 |
| 31 | STE | b | 626 | - | - | 5/11/11/17 | - |
| 28 | SQD | D | 408 | - | - | 13/28/48/69 | 0/1/1/1 |
| 28 | SQD | a | 412 | - | - | 15/37/37/69 | - |
| 33 | LHG | E | 101 | - | - | 31/53/53/53 | - |
| 22 | CLA | B | 602 | - | 1/1/20/20 | 8/37/115/115 | - |
| 22 | CLA | b | 611 | - | 1/1/20/20 | 7/37/115/115 | - |
| 22 | CLA | b | 608 | - | - | 5/37/115/115 | - |
| 31 | STE | b | 627 | - | - | 9/17/17/17 | - |

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*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 22 | CLA | b | 607 | 35 | 1/1/20/20 | 15/37/115/115 | - |
| 31 | STE | b | 622 | - | - | 8/17/17/17 | - |
| 34 | HEC | F | 102 | 6,5 | - | 2/10/54/54 | - |
| 23 | PHO | D | 401 | - | - | 1/37/103/103 | 0/5/6/6 |
| 29 | DGD | h | 102 | - | - | 18/51/91/95 | 0/2/2/2 |
| 33 | LHG | l | 101 | - | - | 17/53/53/53 | - |
| 29 | DGD | C | 515 | - | - | 22/51/91/95 | 0/2/2/2 |
| 22 | CLA | H | 101 | 35 | 1/1/20/20 | 20/37/115/115 | - |
| 22 | CLA | c | 511 | - | 1/1/20/20 | 7/37/115/115 | - |
| 24 | BCR | B | 618 | - | - | 9/29/63/63 | 0/2/2/2 |
| 27 | LMG | A | 410 | - | - | 18/43/63/70 | 0/1/1/1 |
| 31 | STE | B | 626 | - | - | 8/13/13/17 | - |
| 33 | LHG | d | 407 | - | - | 14/53/53/53 | - |
| 24 | BCR | c | 516 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 616 | - | 1/1/19/20 | 10/31/109/115 | - |
| 28 | SQD | A | 412 | - | - | 17/39/39/69 | - |
| 22 | CLA | C | 503 | - | 1/1/20/20 | 5/37/115/115 | - |
| 22 | CLA | A | 403 | 35 | - | 14/37/115/115 | - |
| 33 | LHG | e | 101 | - | - | 23/46/46/53 | - |
| 22 | CLA | c | 510 | - | 1/1/20/20 | 15/37/115/115 | - |
| 22 | CLA | B | 603 | - | 1/1/20/20 | 14/37/115/115 | - |
| 22 | CLA | c | 506 | - | 1/1/20/20 | 10/37/115/115 | - |
| 22 | CLA | C | 511 | 3 | 1/1/20/20 | 9/37/115/115 | - |
| 22 | CLA | B | 612 | - | 1/1/20/20 | 12/37/115/115 | - |
| 29 | DGD | c | 517 | - | - | 24/51/91/95 | 0/2/2/2 |
| 22 | CLA | c | 507 | - | 1/1/20/20 | 16/37/115/115 | - |
| 22 | CLA | C | 506 | - | 1/1/20/20 | 8/37/115/115 | - |
| 22 | CLA | C | 513 | - | 1/1/20/20 | 17/37/115/115 | - |
| 24 | BCR | K | 101 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | D | 403 | - | - | 5/37/115/115 | - |
| 24 | BCR | h | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 23 | PHO | A | 404 | - | - | 3/37/103/103 | 0/5/6/6 |
| 31 | STE | B | 620 | - | - | 9/14/14/17 | - |
| 31 | STE | B | 624 | - | - | 5/9/9/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | BCR | a | 406 | - | - | 3/29/63/63 | 0/2/2/2 |
| 31 | STE | B | 623 | - | - | 3/11/11/17 | - |
| 22 | CLA | B | 610 | 35 | 1/1/20/20 | 6/37/115/115 | - |
| 22 | CLA | b | 613 | - | 1/1/20/20 | 7/37/115/115 | - |
| 22 | CLA | B | 611 | - | 1/1/20/20 | 2/37/115/115 | - |
| 22 | CLA | a | 403 | 35 | - | 11/37/115/115 | - |
| 22 | CLA | b | 602 | - | - | 6/37/115/115 | - |
| 22 | CLA | C | 507 | 35 | 1/1/20/20 | 5/37/115/115 | - |
| 22 | CLA | b | 601 | 35 | 1/1/20/20 | 16/37/115/115 | - |
| 22 | CLA | C | 502 | - | 1/1/20/20 | 10/37/115/115 | - |
| 27 | LMG | b | 621 | - | - | 14/46/66/70 | 0/1/1/1 |
| 31 | STE | c | 521 | - | - | 11/17/17/17 | - |
| 34 | HEC | v | 201 | 17 | - | 2/10/54/54 | - |
| 22 | CLA | B | 614 | - | 1/1/20/20 | 10/37/115/115 | - |
| 22 | CLA | B | 605 | - | 1/1/20/20 | 9/37/115/115 | - |
| 24 | BCR | b | 617 | - | - | 8/29/63/63 | 0/2/2/2 |
| 26 | PL9 | d | 406 | - | - | 15/53/73/73 | 0/1/1/1 |
| 24 | BCR | K | 103 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 512 | 3 | 1/1/20/20 | 11/37/115/115 | - |
| 22 | CLA | a | 402 | - | 1/1/20/20 | 7/37/115/115 | - |
| 26 | PL9 | A | 409 | - | - | 22/53/73/73 | 0/1/1/1 |
| 22 | CLA | A | 402 | - | 1/1/20/20 | 5/37/115/115 | - |
| 27 | LMG | B | 621 | - | - | 11/22/22/70 | - |
| 22 | CLA | B | 615 | - | 1/1/20/20 | 9/37/115/115 | - |
| 28 | SQD | A | 411 | - | - | 9/47/67/69 | 0/1/1/1 |
| 31 | STE | J | 101 | - | - | 5/9/9/17 | - |
| 24 | BCR | F | 101 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 504 | 35 | 1/1/18/20 | 8/30/108/115 | - |
| 22 | CLA | c | 513 | - | 1/1/20/20 | 19/37/115/115 | - |
| 24 | BCR | H | 102 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 509 | - | 1/1/20/20 | 11/37/115/115 | - |
| 31 | STE | D | 413 | - | - | 9/17/17/17 | - |
| 22 | CLA | C | 510 | - | 1/1/20/20 | 8/37/115/115 | - |
| 31 | STE | b | 620 | - | - | 7/13/13/17 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | STE | b | 624 | - | - | 10/17/17/17 | - |
| 22 | CLA | C | 512 | - | 1/1/20/20 | 15/37/115/115 | - |
| 29 | DGD | c | 518 | - | - | 21/51/91/95 | 0/2/2/2 |
| 24 | BCR | c | 515 | - | - | 10/29/63/63 | 0/2/2/2 |
| 27 | LMG | D | 411 | - | - | 15/33/33/70 | - |
| 31 | STE | m | 101 | - | - | 7/15/15/17 | - |
| 22 | CLA | B | 608 | - | - | 4/37/115/115 | - |
| 22 | CLA | B | 609 | - | - | 8/37/115/115 | - |
| 22 | CLA | c | 504 | - | 1/1/20/20 | 11/37/115/115 | - |
| 24 | BCR | A | 406 | - | - | 11/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 607 | 35 | 1/1/20/20 | 7/37/115/115 | - |
| 28 | SQD | a | 411 | - | - | 23/49/69/69 | 0/1/1/1 |
| 27 | LMG | d | 410 | - | - | 11/39/59/70 | 0/1/1/1 |
| 24 | BCR | k | 102 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 514 | - | 1/1/20/20 | 10/37/115/115 | - |
| 28 | SQD | f | 102 | - | - | 15/36/56/69 | 0/1/1/1 |
| 31 | STE | c | 501 | - | - | 3/9/9/17 | - |
| 34 | HEC | f | 101 | 6,5 | - | 4/10/54/54 | - |
| 31 | STE | Z | 101 | - | - | 2/5/5/17 | - |
| 31 | STE | d | 413 | - | - | 11/17/17/17 | - |
| 31 | STE | a | 414 | - | - | 2/9/9/17 | - |
| 24 | BCR | B | 619 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | BCR | C | 514 | - | - | 6/29/63/63 | 0/2/2/2 |
| 31 | STE | M | 103 | - | - | 3/7/7/17 | - |
| 29 | DGD | H | 103 | - | - | 17/51/91/95 | 0/2/2/2 |
| 31 | STE | d | 412 | - | - | 7/14/14/17 | - |
| 22 | CLA | b | 614 | - | 1/1/20/20 | 16/37/115/115 | - |
| 27 | LMG | c | 522 | - | - | 24/43/63/70 | 0/1/1/1 |
| 33 | LHG | d | 408 | - | - | 20/53/53/53 | - |
| 22 | CLA | c | 508 | 35 | 1/1/20/20 | 8/37/115/115 | - |
| 29 | DGD | c | 519 | - | - | 18/51/91/95 | 0/2/2/2 |
| 22 | CLA | c | 505 | 35 | 1/1/19/20 | 7/31/109/115 | - |
| 31 | STE | B | 601 | - | - | 4/9/9/17 | - |
| 22 | CLA | b | 604 | - | 1/1/20/20 | 7/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | STE | M | 102 | - | - | 6/12/12/17 | - |
| 31 | STE | b | 625 | - | - | 6/7/7/17 | - |
| 31 | STE | a | 413 | - | - | 5/7/7/17 | - |
| 24 | BCR | K | 102 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | a | 405 | - | 1/1/20/20 | 7/37/115/115 | - |
| 22 | CLA | A | 405 | - | 1/1/17/20 | 3/24/102/115 | - |
| 29 | DGD | C | 517 | - | - | 14/51/91/95 | 0/2/2/2 |
| 22 | CLA | b | 612 | - | 1/1/20/20 | 8/37/115/115 | - |
| 22 | CLA | b | 606 | - | 1/1/20/20 | 7/37/115/115 | - |
| 29 | DGD | A | 413 | - | - | 30/55/95/95 | 0/2/2/2 |
| 22 | CLA | b | 603 | - | 1/1/20/20 | 10/37/115/115 | - |
| 22 | CLA | D | 405 | - | 1/1/20/20 | 7/37/115/115 | - |
| 31 | STE | C | 519 | - | - | 5/13/13/17 | - |
| 22 | CLA | c | 503 | - | - | 8/37/115/115 | - |
| 28 | SQD | B | 622 | - | - | 19/49/69/69 | 0/1/1/1 |
| 24 | BCR | B | 617 | - | - | 7/29/63/63 | 0/2/2/2 |
| 27 | LMG | D | 407 | - | - | 16/46/66/70 | 0/1/1/1 |
| 31 | STE | B | 625 | - | - | 15/15/15/17 | - |
| 22 | CLA | B | 604 | - | 1/1/20/20 | 12/37/115/115 | - |
| 31 | STE | d | 411 | - | - | 7/13/13/17 | - |
| 31 | STE | T | 102 | - | - | 7/12/12/17 | - |
| 27 | LMG | Y | 101 | - | - | 24/43/63/70 | 0/1/1/1 |
| 24 | BCR | d | 405 | - | - | 8/29/63/63 | 0/2/2/2 |
| 24 | BCR | t | 101 | - | - | 4/29/63/63 | 0/2/2/2 |
| 33 | LHG | D | 409 | - | - | 28/53/53/53 | - |
| 22 | CLA | b | 610 | 35 | 1/1/20/20 | 3/37/115/115 | - |
| 27 | LMG | c | 520 | - | - | 10/31/51/70 | 0/1/1/1 |
| 22 | CLA | b | 615 | - | 1/1/20/20 | 8/37/115/115 | - |
| 23 | PHO | d | 401 | - | - | 5/37/103/103 | 0/5/6/6 |
| 26 | PL9 | D | 406 | - | - | 12/53/73/73 | 0/1/1/1 |
| 24 | BCR | k | 101 | - | - | 10/29/63/63 | 0/2/2/2 |
| 33 | LHG | D | 410 | - | - | 22/51/51/53 | - |
| 23 | PHO | a | 404 | - | - | 6/37/103/103 | 0/5/6/6 |
| 22 | CLA | B | 606 | - | 1/1/20/20 | 13/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | STE | C | 518 | - | - | 6/9/9/17 | - |
| 22 | CLA | C | 501 | - | 1/1/20/20 | 3/37/115/115 | - |
| 22 | CLA | b | 609 | - | - | 8/37/115/115 | - |
| 28 | SQD | L | 101 | - | - | 22/44/64/69 | 0/1/1/1 |
| 22 | CLA | C | 505 | - | 1/1/20/20 | 12/37/115/115 | - |
| 33 | LHG | L | 102 | - | - | 20/53/53/53 | - |
| 24 | BCR | b | 619 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | CLA | D | 404 | 35 | - | 10/37/115/115 | - |

All (910) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | C | 506 | CLA | MG-ND | -9.62 | 1.86 | 2.05 |
| 22 | b | 604 | CLA | C4B-NB | 9.07 | 1.43 | 1.35 |
| 22 | b | 615 | CLA | MG-NA | 8.66 | 2.26 | 2.06 |
| 22 | b | 615 | CLA | C4B-NB | 8.52 | 1.42 | 1.35 |
| 22 | A | 405 | CLA | C4B-NB | 8.31 | 1.42 | 1.35 |
| 22 | c | 505 | CLA | C4B-NB | 8.28 | 1.42 | 1.35 |
| 34 | f | 101 | HEC | C2B-C3B | -8.12 | 1.32 | 1.40 |
| 22 | B | 613 | CLA | C4B-NB | 8.06 | 1.42 | 1.35 |
| 22 | B | 602 | CLA | C4B-NB | 7.98 | 1.42 | 1.35 |
| 22 | B | 616 | CLA | MG-NA | 7.90 | 2.25 | 2.06 |
| 22 | C | 505 | CLA | C4B-NB | 7.87 | 1.42 | 1.35 |
| 22 | C | 506 | CLA | C4B-NB | 7.85 | 1.42 | 1.35 |
| 22 | b | 606 | CLA | MG-NA | 7.76 | 2.24 | 2.06 |
| 22 | A | 403 | CLA | C4B-NB | 7.66 | 1.42 | 1.35 |
| 22 | H | 101 | CLA | C4B-NB | 7.64 | 1.42 | 1.35 |
| 22 | b | 604 | CLA | MG-NA | 7.64 | 2.24 | 2.06 |
| 22 | B | 608 | CLA | MG-NA | 7.61 | 2.24 | 2.06 |
| 22 | C | 501 | CLA | C4B-NB | 7.48 | 1.41 | 1.35 |
| 34 | F | 102 | HEC | C2B-C3B | -7.36 | 1.33 | 1.40 |
| 22 | c | 512 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 34 | v | 201 | HEC | C2B-C3B | -7.33 | 1.33 | 1.40 |
| 22 | C | 503 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 34 | V | 201 | HEC | C2B-C3B | -7.26 | 1.33 | 1.40 |
| 22 | b | 609 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 22 | a | 402 | CLA | C4B-NB | 7.21 | 1.41 | 1.35 |
| 22 | b | 601 | CLA | C4B-NB | 7.17 | 1.41 | 1.35 |
| 22 | B | 606 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 22 | a | 403 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | c | 507 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 22 | d | 403 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 22 | c | 514 | CLA | MG-NC | -7.03 | 1.89 | 2.06 |
| 22 | d | 404 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 22 | c | 512 | CLA | MG-NA | 7.01 | 2.22 | 2.06 |
| 34 | F | 102 | HEC | C3C-C2C | -6.99 | 1.33 | 1.40 |
| 22 | C | 511 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 22 | c | 502 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 22 | D | 403 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 22 | C | 502 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 22 | C | 508 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 22 | c | 513 | CLA | C4B-NB | 6.66 | 1.41 | 1.35 |
| 22 | b | 614 | CLA | C4B-NB | 6.53 | 1.41 | 1.35 |
| 22 | C | 504 | CLA | C4B-NB | 6.53 | 1.41 | 1.35 |
| 22 | C | 512 | CLA | C4B-NB | 6.50 | 1.41 | 1.35 |
| 22 | c | 504 | CLA | C4B-NB | 6.50 | 1.41 | 1.35 |
| 22 | b | 609 | CLA | MG-NA | 6.44 | 2.21 | 2.06 |
| 22 | b | 608 | CLA | MG-NA | 6.43 | 2.21 | 2.06 |
| 22 | D | 404 | CLA | C4B-NB | 6.41 | 1.40 | 1.35 |
| 22 | B | 613 | CLA | MG-ND | -6.40 | 1.93 | 2.05 |
| 22 | D | 404 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 22 | b | 605 | CLA | C4B-NB | 6.35 | 1.40 | 1.35 |
| 22 | B | 615 | CLA | C4B-NB | 6.33 | 1.40 | 1.35 |
| 22 | c | 514 | CLA | C4B-NB | 6.31 | 1.40 | 1.35 |
| 22 | b | 613 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 22 | b | 608 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 22 | C | 513 | CLA | C4B-NB | 6.27 | 1.40 | 1.35 |
| 22 | b | 601 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 22 | B | 608 | CLA | MG-NC | -6.25 | 1.91 | 2.06 |
| 22 | B | 614 | CLA | C4B-NB | 6.17 | 1.40 | 1.35 |
| 22 | C | 508 | CLA | MG-NA | 6.06 | 2.20 | 2.06 |
| 22 | b | 602 | CLA | MG-NA | 6.06 | 2.20 | 2.06 |
| 22 | a | 405 | CLA | C4B-NB | 6.05 | 1.40 | 1.35 |
| 22 | C | 509 | CLA | C4B-NB | 6.04 | 1.40 | 1.35 |
| 22 | a | 402 | CLA | MG-NA | 6.02 | 2.20 | 2.06 |
| 22 | C | 507 | CLA | MG-NA | 6.00 | 2.20 | 2.06 |
| 22 | B | 606 | CLA | MG-NC | 5.96 | 2.20 | 2.06 |
| 22 | b | 607 | CLA | C4B-NB | 5.96 | 1.40 | 1.35 |
| 22 | b | 612 | CLA | C4B-NB | 5.95 | 1.40 | 1.35 |
| 22 | c | 506 | CLA | C4B-NB | 5.93 | 1.40 | 1.35 |
| 22 | a | 410 | CLA | MG-NA | 5.92 | 2.20 | 2.06 |
| 22 | B | 611 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | c | 508 | CLA | C4B-NB | 5.91 | 1.40 | 1.35 |
| 22 | C | 503 | CLA | MG-NA | 5.87 | 2.20 | 2.06 |
| 22 | B | 603 | CLA | MG-ND | 5.83 | 2.17 | 2.05 |
| 22 | B | 616 | CLA | C4B-NB | 5.74 | 1.40 | 1.35 |
| 22 | H | 101 | CLA | MG-NA | 5.72 | 2.19 | 2.06 |
| 22 | C | 506 | CLA | MG-NA | 5.70 | 2.19 | 2.06 |
| 22 | B | 605 | CLA | C4B-NB | 5.69 | 1.40 | 1.35 |
| 22 | D | 405 | CLA | C4B-NB | 5.68 | 1.40 | 1.35 |
| 27 | a | 415 | LMG | C4-C5 | 5.67 | 1.65 | 1.53 |
| 22 | B | 609 | CLA | C4B-NB | 5.65 | 1.40 | 1.35 |
| 22 | c | 511 | CLA | C4B-NB | 5.64 | 1.40 | 1.35 |
| 22 | C | 507 | CLA | C4B-NB | 5.63 | 1.40 | 1.35 |
| 22 | b | 616 | CLA | C4B-NB | 5.62 | 1.40 | 1.35 |
| 22 | c | 510 | CLA | C4B-NB | 5.60 | 1.40 | 1.35 |
| 34 | v | 201 | HEC | C3C-C2C | -5.59 | 1.34 | 1.40 |
| 22 | B | 609 | CLA | MG-NA | 5.57 | 2.19 | 2.06 |
| 34 | f | 101 | HEC | C3C-C2C | -5.51 | 1.35 | 1.40 |
| 22 | A | 402 | CLA | C4B-NB | 5.49 | 1.40 | 1.35 |
| 34 | V | 201 | HEC | C3C-C2C | -5.48 | 1.35 | 1.40 |
| 22 | B | 610 | CLA | C4B-NB | 5.40 | 1.40 | 1.35 |
| 22 | b | 606 | CLA | C4B-NB | 5.40 | 1.40 | 1.35 |
| 22 | b | 603 | CLA | C4B-NB | 5.38 | 1.40 | 1.35 |
| 22 | C | 501 | CLA | MG-ND | -5.28 | 1.95 | 2.05 |
| 22 | b | 610 | CLA | C1D-ND | 5.26 | 1.44 | 1.37 |
| 22 | c | 514 | CLA | MG-NA | 5.13 | 2.18 | 2.06 |
| 22 | A | 403 | CLA | C4D-ND | -5.10 | 1.30 | 1.37 |
| 22 | B | 606 | CLA | MG-NA | 5.01 | 2.18 | 2.06 |
| 22 | b | 610 | CLA | C4B-NB | 5.01 | 1.39 | 1.35 |
| 22 | c | 503 | CLA | C4B-NB | 4.97 | 1.39 | 1.35 |
| 22 | B | 612 | CLA | C4B-NB | 4.93 | 1.39 | 1.35 |
| 22 | C | 512 | CLA | MG-ND | -4.92 | 1.96 | 2.05 |
| 22 | b | 602 | CLA | C4B-NB | 4.91 | 1.39 | 1.35 |
| 22 | c | 509 | CLA | C4B-NB | 4.87 | 1.39 | 1.35 |
| 22 | C | 510 | CLA | C4B-NB | 4.86 | 1.39 | 1.35 |
| 22 | B | 602 | CLA | C1D-ND | 4.85 | 1.43 | 1.37 |
| 22 | b | 602 | CLA | MG-NC | -4.82 | 1.94 | 2.06 |
| 22 | C | 512 | CLA | C4D-ND | -4.82 | 1.31 | 1.37 |
| 22 | b | 615 | CLA | MG-ND | -4.82 | 1.96 | 2.05 |
| 22 | B | 604 | CLA | MG-NA | 4.77 | 2.17 | 2.06 |
| 22 | b | 605 | CLA | C4D-ND | -4.77 | 1.31 | 1.37 |
| 22 | B | 610 | CLA | C1D-ND | 4.71 | 1.43 | 1.37 |
| 22 | b | 607 | CLA | MG-NA | 4.68 | 2.17 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | B | 608 | CLA | C4B-NB | 4.67 | 1.39 | 1.35 |
| 22 | a | 410 | CLA | C4B-NB | 4.65 | 1.39 | 1.35 |
| 29 | c | 517 | DGD | C3G-C2G | 4.64 | 1.64 | 1.50 |
| 22 | c | 504 | CLA | C4D-ND | -4.64 | 1.31 | 1.37 |
| 26 | d | 406 | PL9 | C6-C1 | -4.63 | 1.40 | 1.48 |
| 22 | b | 612 | CLA | C4D-ND | -4.62 | 1.31 | 1.37 |
| 22 | a | 403 | CLA | C4D-ND | -4.61 | 1.31 | 1.37 |
| 22 | B | 615 | CLA | MG-NC | 4.57 | 2.17 | 2.06 |
| 22 | B | 603 | CLA | C4B-NB | 4.54 | 1.39 | 1.35 |
| 22 | c | 509 | CLA | MG-NA | 4.54 | 2.17 | 2.06 |
| 22 | B | 612 | CLA | C4D-ND | -4.54 | 1.31 | 1.37 |
| 29 | H | 103 | DGD | C4E-C5E | 4.48 | 1.62 | 1.53 |
| 22 | c | 510 | CLA | C1D-ND | 4.48 | 1.43 | 1.37 |
| 26 | D | 406 | PL9 | C7-C3 | -4.45 | 1.46 | 1.51 |
| 27 | M | 101 | LMG | O7-C8 | -4.45 | 1.35 | 1.46 |
| 34 | f | 101 | HEC | CBB-CAB | -4.42 | 1.32 | 1.49 |
| 22 | B | 614 | CLA | MG-ND | -4.39 | 1.97 | 2.05 |
| 33 | d | 408 | LHG | O8-C6 | -4.39 | 1.35 | 1.45 |
| 22 | b | 612 | CLA | MG-ND | -4.35 | 1.97 | 2.05 |
| 34 | F | 102 | HEC | CBC-CAC | -4.35 | 1.33 | 1.49 |
| 22 | B | 616 | CLA | C1D-ND | 4.34 | 1.43 | 1.37 |
| 22 | c | 506 | CLA | MG-NA | 4.31 | 2.16 | 2.06 |
| 24 | C | 514 | BCR | C1-C6 | -4.30 | 1.47 | 1.53 |
| 22 | C | 505 | CLA | C4D-ND | -4.30 | 1.31 | 1.37 |
| 24 | b | 618 | BCR | C30-C25 | -4.30 | 1.47 | 1.53 |
| 22 | b | 611 | CLA | MG-ND | 4.30 | 2.14 | 2.05 |
| 22 | C | 501 | CLA | C1D-ND | 4.30 | 1.43 | 1.37 |
| 22 | D | 403 | CLA | C4D-ND | -4.27 | 1.31 | 1.37 |
| 22 | B | 604 | CLA | C4D-ND | -4.26 | 1.31 | 1.37 |
| 22 | C | 505 | CLA | CHC-C1C | 4.26 | 1.45 | 1.35 |
| 22 | B | 607 | CLA | C4B-NB | 4.26 | 1.39 | 1.35 |
| 24 | c | 516 | BCR | C1-C6 | -4.23 | 1.48 | 1.53 |
| 22 | B | 605 | CLA | C4D-ND | -4.22 | 1.31 | 1.37 |
| 22 | B | 614 | CLA | C4D-ND | -4.22 | 1.31 | 1.37 |
| 22 | c | 502 | CLA | C1D-ND | 4.19 | 1.42 | 1.37 |
| 29 | c | 517 | DGD | O3E-C3E | -4.18 | 1.33 | 1.43 |
| 22 | B | 605 | CLA | C1D-ND | 4.17 | 1.42 | 1.37 |
| 22 | b | 603 | CLA | MG-NA | 4.15 | 2.16 | 2.06 |
| 22 | B | 610 | CLA | MG-NC | -4.13 | 1.96 | 2.06 |
| 22 | c | 509 | CLA | CHC-C1C | 4.10 | 1.45 | 1.35 |
| 28 | a | 412 | SQD | O47-C7 | 4.10 | 1.45 | 1.34 |
| 22 | H | 101 | CLA | C1D-ND | 4.08 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | T | 101 | BCR | C1-C6 | -4.07 | 1.48 | 1.53 |
| 22 | B | 613 | CLA | MG-NA | 4.07 | 2.15 | 2.06 |
| 22 | d | 404 | CLA | C4D-ND | -4.07 | 1.32 | 1.37 |
| 22 | c | 506 | CLA | C4D-ND | -4.06 | 1.32 | 1.37 |
| 22 | b | 602 | CLA | C1D-ND | 4.05 | 1.42 | 1.37 |
| 22 | b | 614 | CLA | C4D-ND | -4.05 | 1.32 | 1.37 |
| 24 | a | 406 | BCR | C1-C6 | -4.05 | 1.48 | 1.53 |
| 22 | B | 609 | CLA | MG-ND | 4.04 | 2.13 | 2.05 |
| 29 | C | 515 | DGD | C6E-C5E | 4.04 | 1.65 | 1.51 |
| 28 | a | 411 | SQD | O48-C23 | 4.04 | 1.45 | 1.33 |
| 26 | D | 406 | PL9 | C52-C5 | -4.03 | 1.42 | 1.50 |
| 22 | D | 404 | CLA | C1D-ND | 4.03 | 1.42 | 1.37 |
| 34 | F | 102 | HEC | CBB-CAB | -4.03 | 1.34 | 1.49 |
| 22 | B | 611 | CLA | MG-NA | 4.03 | 2.15 | 2.06 |
| 34 | f | 101 | HEC | CBC-CAC | -4.03 | 1.34 | 1.49 |
| 22 | B | 604 | CLA | C4B-NB | 4.02 | 1.38 | 1.35 |
| 22 | C | 510 | CLA | C4D-ND | -4.01 | 1.32 | 1.37 |
| 22 | C | 511 | CLA | C4D-ND | -4.00 | 1.32 | 1.37 |
| 29 | C | 517 | DGD | O2G-C2G | -4.00 | 1.36 | 1.46 |
| 27 | d | 410 | LMG | C4-C5 | 3.97 | 1.61 | 1.53 |
| 26 | a | 409 | PL9 | C7-C3 | 3.97 | 1.55 | 1.51 |
| 29 | c | 518 | DGD | C4D-C3D | 3.97 | 1.62 | 1.52 |
| 22 | D | 403 | CLA | C1D-ND | 3.96 | 1.42 | 1.37 |
| 22 | c | 502 | CLA | C4D-ND | -3.96 | 1.32 | 1.37 |
| 22 | D | 404 | CLA | C4D-ND | -3.95 | 1.32 | 1.37 |
| 22 | C | 513 | CLA | C4D-ND | -3.93 | 1.32 | 1.37 |
| 22 | a | 410 | CLA | C1D-ND | 3.92 | 1.42 | 1.37 |
| 33 | D | 410 | LHG | P-O6 | 3.92 | 1.75 | 1.59 |
| 24 | d | 405 | BCR | C30-C25 | -3.90 | 1.48 | 1.53 |
| 29 | C | 515 | DGD | O2G-C2G | -3.89 | 1.36 | 1.46 |
| 22 | B | 610 | CLA | C3B-C2B | -3.88 | 1.35 | 1.40 |
| 22 | c | 511 | CLA | MG-NA | 3.87 | 2.15 | 2.06 |
| 22 | b | 611 | CLA | C4B-NB | 3.85 | 1.38 | 1.35 |
| 22 | c | 509 | CLA | C4D-ND | -3.85 | 1.32 | 1.37 |
| 34 | V | 201 | HEC | CBB-CAB | -3.85 | 1.35 | 1.49 |
| 27 | A | 410 | LMG | O1-C7 | -3.83 | 1.36 | 1.43 |
| 27 | D | 407 | LMG | C4-C5 | 3.82 | 1.61 | 1.53 |
| 22 | c | 512 | CLA | CHC-C1C | 3.82 | 1.44 | 1.35 |
| 22 | C | 502 | CLA | MG-NA | 3.82 | 2.15 | 2.06 |
| 22 | c | 503 | CLA | C4D-ND | -3.80 | 1.32 | 1.37 |
| 22 | c | 502 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 22 | c | 508 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | C | 511 | CLA | MG-NA | 3.77 | 2.15 | 2.06 |
| 22 | A | 405 | CLA | C4D-ND | -3.77 | 1.32 | 1.37 |
| 22 | D | 405 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 34 | v | 201 | HEC | CBC-CAC | -3.75 | 1.35 | 1.49 |
| 29 | c | 519 | DGD | O2E-C2E | -3.75 | 1.34 | 1.43 |
| 22 | B | 611 | CLA | C4D-ND | -3.74 | 1.32 | 1.37 |
| 22 | b | 603 | CLA | CMD-C2D | -3.72 | 1.42 | 1.50 |
| 22 | C | 507 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 29 | A | 413 | DGD | C3E-C2E | 3.71 | 1.61 | 1.52 |
| 22 | B | 610 | CLA | CMB-C2B | -3.70 | 1.43 | 1.51 |
| 28 | a | 412 | SQD | O48-C23 | 3.68 | 1.44 | 1.33 |
| 33 | D | 409 | LHG | O7-C5 | -3.68 | 1.37 | 1.46 |
| 22 | A | 402 | CLA | MG-ND | -3.68 | 1.98 | 2.05 |
| 22 | b | 609 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 22 | a | 402 | CLA | CHC-C1C | 3.65 | 1.44 | 1.35 |
| 29 | c | 517 | DGD | O2G-C2G | -3.65 | 1.37 | 1.46 |
| 22 | b | 608 | CLA | CHC-C1C | 3.65 | 1.44 | 1.35 |
| 22 | C | 501 | CLA | MG-NA | 3.64 | 2.14 | 2.06 |
| 22 | b | 606 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 27 | D | 411 | LMG | C9-C8 | 3.63 | 1.61 | 1.50 |
| 22 | b | 611 | CLA | MG-NA | 3.63 | 2.14 | 2.06 |
| 22 | D | 404 | CLA | CHC-C1C | 3.63 | 1.44 | 1.35 |
| 22 | a | 403 | CLA | CHC-C1C | 3.63 | 1.44 | 1.35 |
| 22 | B | 616 | CLA | C4D-ND | -3.63 | 1.32 | 1.37 |
| 22 | b | 611 | CLA | C4D-ND | -3.63 | 1.32 | 1.37 |
| 22 | b | 615 | CLA | CMD-C2D | -3.62 | 1.43 | 1.50 |
| 29 | c | 519 | DGD | O3D-C3D | -3.62 | 1.34 | 1.43 |
| 33 | d | 407 | LHG | C24-C23 | 3.61 | 1.61 | 1.50 |
| 22 | B | 607 | CLA | MG-ND | -3.60 | 1.98 | 2.05 |
| 22 | b | 602 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 22 | c | 507 | CLA | CHC-C1C | 3.59 | 1.44 | 1.35 |
| 22 | B | 610 | CLA | MG-ND | -3.59 | 1.98 | 2.05 |
| 22 | a | 410 | CLA | C4D-ND | -3.59 | 1.32 | 1.37 |
| 22 | d | 403 | CLA | MG-NA | 3.58 | 2.14 | 2.06 |
| 22 | C | 509 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 22 | b | 614 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 22 | b | 603 | CLA | C4D-ND | -3.57 | 1.32 | 1.37 |
| 22 | A | 405 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 22 | B | 606 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 22 | C | 513 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 24 | c | 515 | BCR | C1-C6 | -3.55 | 1.48 | 1.53 |
| 22 | B | 613 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | c | 502 | CLA | MG-NA | 3.53 | 2.14 | 2.06 |
| 29 | C | 515 | DGD | C4E-C3E | 3.52 | 1.61 | 1.52 |
| 22 | c | 506 | CLA | MG-NC | -3.52 | 1.97 | 2.06 |
| 24 | K | 102 | BCR | C30-C25 | -3.52 | 1.48 | 1.53 |
| 22 | B | 616 | CLA | MG-ND | 3.51 | 2.12 | 2.05 |
| 24 | F | 101 | BCR | C1-C6 | -3.51 | 1.48 | 1.53 |
| 22 | A | 405 | CLA | MG-NC | -3.51 | 1.97 | 2.06 |
| 22 | B | 602 | CLA | MG-ND | -3.51 | 1.98 | 2.05 |
| 22 | a | 410 | CLA | C3B-C2B | -3.51 | 1.35 | 1.40 |
| 27 | c | 522 | LMG | O1-C1 | 3.50 | 1.46 | 1.40 |
| 26 | d | 406 | PL9 | C46-C44 | -3.50 | 1.44 | 1.51 |
| 22 | c | 513 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 22 | C | 506 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 22 | c | 507 | CLA | MG-ND | -3.49 | 1.98 | 2.05 |
| 22 | b | 601 | CLA | CHC-C1C | 3.48 | 1.43 | 1.35 |
| 22 | C | 501 | CLA | C3B-C2B | -3.48 | 1.35 | 1.40 |
| 22 | B | 614 | CLA | MG-NA | 3.48 | 2.14 | 2.06 |
| 22 | B | 603 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 22 | a | 403 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 22 | C | 509 | CLA | MG-NA | 3.46 | 2.14 | 2.06 |
| 22 | a | 405 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 28 | B | 622 | SQD | O48-C23 | 3.45 | 1.43 | 1.33 |
| 22 | C | 501 | CLA | CHC-C1C | 3.44 | 1.43 | 1.35 |
| 24 | B | 619 | BCR | C1-C6 | -3.44 | 1.49 | 1.53 |
| 22 | c | 513 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |
| 22 | C | 505 | CLA | MG-NA | 3.43 | 2.14 | 2.06 |
| 22 | b | 611 | CLA | CHC-C1C | 3.43 | 1.43 | 1.35 |
| 23 | A | 404 | PHO | CBD-CGD | -3.43 | 1.47 | 1.52 |
| 22 | c | 505 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 22 | A | 405 | CLA | MG-NA | 3.42 | 2.14 | 2.06 |
| 22 | b | 616 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 22 | b | 616 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 22 | C | 502 | CLA | CHC-C1C | 3.40 | 1.43 | 1.35 |
| 24 | b | 619 | BCR | C30-C25 | -3.40 | 1.49 | 1.53 |
| 22 | C | 505 | CLA | MG-ND | 3.40 | 2.12 | 2.05 |
| 22 | A | 403 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 22 | c | 510 | CLA | CHC-C1C | 3.39 | 1.43 | 1.35 |
| 28 | B | 622 | SQD | O47-C7 | 3.38 | 1.43 | 1.34 |
| 24 | A | 406 | BCR | C1-C6 | -3.38 | 1.49 | 1.53 |
| 22 | b | 601 | CLA | C1D-ND | 3.38 | 1.41 | 1.37 |
| 28 | f | 102 | SQD | O48-C23 | 3.38 | 1.43 | 1.33 |
| 24 | K | 101 | BCR | C30-C25 | -3.38 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 28 | A | 412 | SQD | O48-C23 | 3.37 | 1.43 | 1.33 |
| 34 | V | 201 | HEC | CBC-CAC | -3.37 | 1.36 | 1.49 |
| 22 | c | 507 | CLA | C1D-ND | 3.37 | 1.41 | 1.37 |
| 26 | d | 406 | PL9 | C26-C24 | -3.36 | 1.44 | 1.51 |
| 22 | B | 607 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 22 | B | 613 | CLA | C1D-ND | 3.35 | 1.41 | 1.37 |
| 24 | d | 405 | BCR | C1-C6 | -3.35 | 1.49 | 1.53 |
| 22 | c | 514 | CLA | CHC-C1C | 3.35 | 1.43 | 1.35 |
| 34 | v | 201 | HEC | CBB-CAB | -3.35 | 1.36 | 1.49 |
| 22 | b | 604 | CLA | MG-ND | -3.34 | 1.99 | 2.05 |
| 22 | C | 503 | CLA | CHC-C1C | 3.34 | 1.43 | 1.35 |
| 22 | D | 405 | CLA | CMD-C2D | -3.33 | 1.43 | 1.50 |
| 22 | B | 615 | CLA | MG-NA | 3.33 | 2.14 | 2.06 |
| 22 | c | 514 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 22 | A | 402 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 22 | b | 606 | CLA | C3B-C2B | -3.30 | 1.35 | 1.40 |
| 24 | b | 617 | BCR | C30-C25 | -3.29 | 1.49 | 1.53 |
| 27 | c | 523 | LMG | C4-C5 | 3.29 | 1.60 | 1.53 |
| 27 | a | 415 | LMG | O8-C9 | -3.29 | 1.37 | 1.45 |
| 22 | C | 504 | CLA | CHC-C1C | 3.28 | 1.43 | 1.35 |
| 22 | d | 403 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 28 | A | 411 | SQD | O48-C23 | 3.28 | 1.42 | 1.33 |
| 27 | b | 621 | LMG | O7-C8 | -3.27 | 1.38 | 1.46 |
| 24 | h | 101 | BCR | C30-C25 | -3.27 | 1.49 | 1.53 |
| 22 | B | 609 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 22 | B | 613 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 22 | a | 403 | CLA | CMB-C2B | -3.25 | 1.44 | 1.51 |
| 22 | C | 511 | CLA | C1D-ND | 3.25 | 1.41 | 1.37 |
| 22 | B | 606 | CLA | CHC-C1C | 3.25 | 1.43 | 1.35 |
| 22 | H | 101 | CLA | C3B-C2B | -3.25 | 1.35 | 1.40 |
| 29 | A | 413 | DGD | C4D-C3D | 3.24 | 1.60 | 1.52 |
| 29 | H | 103 | DGD | C3E-C2E | 3.23 | 1.60 | 1.52 |
| 29 | A | 413 | DGD | C1E-C2E | 3.23 | 1.61 | 1.52 |
| 23 | A | 404 | PHO | CAC-C3C | -3.23 | 1.46 | 1.52 |
| 22 | a | 405 | CLA | C4B-CHC | -3.22 | 1.32 | 1.41 |
| 29 | H | 103 | DGD | C4D-C5D | 3.22 | 1.59 | 1.53 |
| 22 | c | 511 | CLA | CMB-C2B | -3.22 | 1.45 | 1.51 |
| 22 | a | 402 | CLA | CMB-C2B | -3.21 | 1.45 | 1.51 |
| 22 | C | 512 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 22 | c | 506 | CLA | CHC-C1C | 3.21 | 1.43 | 1.35 |
| 22 | b | 615 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 24 | B | 617 | BCR | C30-C25 | -3.20 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | a | 403 | CLA | C3B-C2B | -3.20 | 1.35 | 1.40 |
| 22 | b | 614 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 22 | H | 101 | CLA | MG-ND | -3.19 | 1.99 | 2.05 |
| 27 | d | 410 | LMG | O7-C8 | -3.19 | 1.38 | 1.46 |
| 24 | H | 102 | BCR | C30-C25 | -3.19 | 1.49 | 1.53 |
| 28 | L | 101 | SQD | O48-C23 | 3.19 | 1.42 | 1.33 |
| 22 | b | 610 | CLA | C3B-C2B | -3.18 | 1.36 | 1.40 |
| 22 | b | 606 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 24 | b | 619 | BCR | C1-C6 | -3.18 | 1.49 | 1.53 |
| 29 | A | 413 | DGD | C4E-C5E | 3.17 | 1.59 | 1.53 |
| 22 | C | 509 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 22 | c | 508 | CLA | MG-ND | 3.17 | 2.12 | 2.05 |
| 23 | D | 401 | PHO | CAC-C3C | -3.17 | 1.46 | 1.52 |
| 22 | c | 504 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 22 | A | 402 | CLA | MG-NA | 3.15 | 2.13 | 2.06 |
| 22 | c | 509 | CLA | C1D-ND | 3.14 | 1.41 | 1.37 |
| 22 | b | 613 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 24 | k | 101 | BCR | C1-C6 | -3.13 | 1.49 | 1.53 |
| 22 | B | 615 | CLA | CMD-C2D | -3.13 | 1.44 | 1.50 |
| 22 | a | 405 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 33 | d | 409 | LHG | P-O6 | 3.12 | 1.71 | 1.59 |
| 22 | b | 613 | CLA | CMB-C2B | -3.12 | 1.45 | 1.51 |
| 22 | c | 503 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 22 | B | 614 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 22 | A | 403 | CLA | C1B-NB | 3.11 | 1.38 | 1.35 |
| 29 | H | 103 | DGD | C1G-C2G | 3.10 | 1.60 | 1.50 |
| 22 | b | 609 | CLA | CMB-C2B | -3.10 | 1.45 | 1.51 |
| 22 | D | 403 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 27 | Y | 101 | LMG | O7-C8 | -3.09 | 1.38 | 1.46 |
| 22 | a | 403 | CLA | MG-NA | 3.09 | 2.13 | 2.06 |
| 22 | C | 508 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 22 | b | 607 | CLA | C3B-C2B | -3.09 | 1.36 | 1.40 |
| 26 | d | 406 | PL9 | C31-C29 | -3.09 | 1.44 | 1.51 |
| 22 | b | 602 | CLA | C3B-C2B | -3.09 | 1.36 | 1.40 |
| 22 | B | 615 | CLA | C1D-ND | 3.08 | 1.41 | 1.37 |
| 22 | c | 513 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 22 | b | 604 | CLA | C1B-NB | 3.08 | 1.38 | 1.35 |
| 22 | b | 602 | CLA | CMD-C2D | -3.07 | 1.44 | 1.50 |
| 28 | A | 412 | SQD | O47-C45 | -3.07 | 1.41 | 1.47 |
| 22 | C | 506 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 28 | f | 102 | SQD | O47-C7 | 3.07 | 1.43 | 1.34 |
| 22 | B | 608 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | b | 606 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 22 | C | 509 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 22 | a | 405 | CLA | CMC-C2C | -3.06 | 1.44 | 1.50 |
| 28 | D | 408 | SQD | O48-C23 | 3.05 | 1.42 | 1.33 |
| 26 | d | 406 | PL9 | C3-C4 | -3.05 | 1.44 | 1.49 |
| 22 | C | 502 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 22 | c | 512 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 22 | a | 410 | CLA | CMB-C2B | -3.04 | 1.45 | 1.51 |
| 22 | C | 513 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 22 | A | 403 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 22 | c | 507 | CLA | CMD-C2D | -3.04 | 1.44 | 1.50 |
| 29 | c | 519 | DGD | O4D-C4D | -3.03 | 1.35 | 1.43 |
| 22 | B | 611 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 22 | b | 611 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 22 | b | 604 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 22 | C | 511 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 22 | C | 513 | CLA | MG-NA | 3.01 | 2.13 | 2.06 |
| 23 | A | 404 | PHO | CMD-C2D | -3.00 | 1.44 | 1.51 |
| 22 | A | 403 | CLA | MG-ND | 3.00 | 2.11 | 2.05 |
| 28 | L | 101 | SQD | O47-C7 | 3.00 | 1.42 | 1.34 |
| 24 | a | 406 | BCR | C38-C26 | -3.00 | 1.46 | 1.50 |
| 22 | B | 611 | CLA | CMB-C2B | -3.00 | 1.45 | 1.51 |
| 22 | b | 605 | CLA | MG-ND | 3.00 | 2.11 | 2.05 |
| 26 | d | 406 | PL9 | C25-C24 | -2.99 | 1.43 | 1.50 |
| 22 | b | 606 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 28 | A | 412 | SQD | O47-C7 | 2.98 | 1.42 | 1.34 |
| 24 | K | 101 | BCR | C1-C6 | -2.98 | 1.49 | 1.53 |
| 22 | b | 607 | CLA | C1D-ND | 2.98 | 1.41 | 1.37 |
| 22 | b | 607 | CLA | MG-ND | -2.98 | 1.99 | 2.05 |
| 22 | c | 503 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 22 | B | 603 | CLA | CMB-C2B | -2.97 | 1.45 | 1.51 |
| 22 | C | 508 | CLA | MG-ND | 2.96 | 2.11 | 2.05 |
| 22 | B | 614 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 29 | A | 413 | DGD | O1G-C1G | -2.96 | 1.38 | 1.45 |
| 22 | b | 613 | CLA | MG-NA | 2.96 | 2.13 | 2.06 |
| 28 | A | 411 | SQD | O2-C2 | -2.96 | 1.36 | 1.43 |
| 22 | c | 507 | CLA | C4D-ND | -2.95 | 1.33 | 1.37 |
| 22 | B | 614 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 22 | b | 604 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 22 | B | 615 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 22 | b | 607 | CLA | CMB-C2B | -2.94 | 1.45 | 1.51 |
| 22 | B | 604 | CLA | C1D-ND | 2.93 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | H | 101 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 22 | b | 609 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 22 | b | 606 | CLA | C1B-NB | 2.93 | 1.37 | 1.35 |
| 22 | B | 611 | CLA | C1D-ND | 2.93 | 1.41 | 1.37 |
| 29 | C | 515 | DGD | O5D-C1E | 2.93 | 1.45 | 1.40 |
| 22 | C | 510 | CLA | MG-NC | 2.93 | 2.13 | 2.06 |
| 22 | b | 614 | CLA | C3B-CAB | -2.92 | 1.42 | 1.47 |
| 22 | b | 603 | CLA | CMC-C2C | -2.92 | 1.44 | 1.50 |
| 22 | B | 603 | CLA | CMD-C2D | -2.92 | 1.44 | 1.50 |
| 22 | B | 602 | CLA | CMB-C2B | -2.92 | 1.45 | 1.51 |
| 22 | B | 612 | CLA | C1C-NC | -2.91 | 1.33 | 1.37 |
| 22 | b | 605 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 22 | b | 608 | CLA | C1D-ND | 2.91 | 1.41 | 1.37 |
| 22 | B | 612 | CLA | CMC-C2C | -2.91 | 1.44 | 1.50 |
| 22 | B | 615 | CLA | C4D-ND | -2.90 | 1.33 | 1.37 |
| 24 | B | 618 | BCR | C30-C25 | -2.90 | 1.49 | 1.53 |
| 22 | c | 504 | CLA | C1D-ND | 2.90 | 1.41 | 1.37 |
| 24 | T | 101 | BCR | C30-C25 | -2.90 | 1.49 | 1.53 |
| 22 | C | 507 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 22 | B | 602 | CLA | MG-NA | 2.89 | 2.13 | 2.06 |
| 22 | B | 615 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 22 | b | 613 | CLA | MG-ND | -2.89 | 2.00 | 2.05 |
| 29 | A | 413 | DGD | O5D-C6D | -2.89 | 1.38 | 1.43 |
| 22 | b | 615 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 22 | B | 606 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 22 | C | 507 | CLA | MG-ND | 2.89 | 2.11 | 2.05 |
| 22 | B | 605 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 22 | A | 405 | CLA | MG-ND | -2.88 | 2.00 | 2.05 |
| 29 | c | 518 | DGD | C3E-C2E | 2.88 | 1.59 | 1.52 |
| 22 | B | 615 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 27 | c | 520 | LMG | O1-C1 | 2.87 | 1.45 | 1.40 |
| 22 | b | 610 | CLA | C4D-ND | -2.86 | 1.33 | 1.37 |
| 22 | C | 513 | CLA | CMB-C2B | -2.86 | 1.45 | 1.51 |
| 22 | c | 513 | CLA | MG-NA | 2.86 | 2.13 | 2.06 |
| 22 | b | 603 | CLA | C3B-C2B | -2.85 | 1.36 | 1.40 |
| 22 | b | 608 | CLA | C4D-ND | -2.85 | 1.33 | 1.37 |
| 27 | M | 101 | LMG | C4-C3 | 2.85 | 1.59 | 1.52 |
| 23 | d | 401 | PHO | CAC-C3C | -2.85 | 1.47 | 1.52 |
| 22 | c | 508 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 26 | D | 406 | PL9 | C31-C29 | -2.84 | 1.45 | 1.51 |
| 27 | b | 621 | LMG | C4-C3 | 2.84 | 1.59 | 1.52 |
| 22 | c | 512 | CLA | MG-ND | 2.84 | 2.11 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | c | 511 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 24 | b | 617 | BCR | C1-C6 | -2.84 | 1.49 | 1.53 |
| 22 | c | 511 | CLA | C4D-ND | -2.83 | 1.33 | 1.37 |
| 22 | D | 403 | CLA | CMB-C2B | -2.83 | 1.45 | 1.51 |
| 29 | C | 517 | DGD | C6E-C5E | 2.82 | 1.61 | 1.51 |
| 22 | D | 405 | CLA | MG-ND | -2.82 | 2.00 | 2.05 |
| 22 | a | 402 | CLA | C4D-ND | -2.82 | 1.33 | 1.37 |
| 24 | c | 515 | BCR | C30-C25 | -2.82 | 1.49 | 1.53 |
| 22 | C | 508 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 22 | c | 504 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 22 | B | 608 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 24 | B | 617 | BCR | C1-C6 | -2.81 | 1.49 | 1.53 |
| 22 | C | 504 | CLA | MG-NC | 2.81 | 2.12 | 2.06 |
| 22 | a | 402 | CLA | C1D-ND | 2.81 | 1.41 | 1.37 |
| 27 | c | 522 | LMG | C4-C3 | 2.81 | 1.59 | 1.52 |
| 33 | E | 101 | LHG | P-O6 | 2.81 | 1.70 | 1.59 |
| 27 | D | 411 | LMG | C7-C8 | 2.81 | 1.58 | 1.51 |
| 22 | c | 509 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 22 | b | 607 | CLA | CMD-C2D | -2.81 | 1.44 | 1.50 |
| 28 | A | 411 | SQD | O47-C7 | 2.80 | 1.42 | 1.34 |
| 22 | B | 607 | CLA | MG-NA | 2.80 | 2.12 | 2.06 |
| 22 | B | 614 | CLA | C3B-CAB | -2.80 | 1.42 | 1.47 |
| 22 | c | 508 | CLA | C4D-ND | -2.80 | 1.33 | 1.37 |
| 23 | D | 401 | PHO | CMB-C2B | -2.79 | 1.44 | 1.51 |
| 22 | B | 607 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 22 | B | 608 | CLA | C4D-ND | -2.79 | 1.33 | 1.37 |
| 22 | b | 613 | CLA | C4D-ND | -2.78 | 1.33 | 1.37 |
| 22 | C | 509 | CLA | MG-NC | -2.77 | 1.99 | 2.06 |
| 22 | B | 606 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 29 | A | 413 | DGD | O2G-C2G | -2.77 | 1.39 | 1.46 |
| 22 | b | 612 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 23 | a | 404 | PHO | CBD-CGD | -2.76 | 1.48 | 1.52 |
| 24 | T | 101 | BCR | C38-C26 | -2.76 | 1.46 | 1.50 |
| 23 | A | 404 | PHO | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 22 | C | 503 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 27 | c | 523 | LMG | O1-C7 | -2.75 | 1.38 | 1.43 |
| 22 | B | 610 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 22 | c | 502 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 22 | a | 405 | CLA | CMD-C2D | -2.73 | 1.45 | 1.50 |
| 27 | a | 415 | LMG | C3-C2 | 2.73 | 1.59 | 1.52 |
| 22 | c | 511 | CLA | C1D-ND | 2.73 | 1.41 | 1.37 |
| 22 | C | 512 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | c | 505 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 22 | C | 510 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 29 | c | 517 | DGD | O3D-C3D | -2.71 | 1.36 | 1.43 |
| 29 | C | 516 | DGD | C1E-C2E | 2.71 | 1.60 | 1.52 |
| 22 | b | 616 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 27 | c | 520 | LMG | C4-C3 | 2.70 | 1.59 | 1.52 |
| 22 | C | 501 | CLA | C4D-ND | -2.70 | 1.34 | 1.37 |
| 24 | K | 102 | BCR | C1-C6 | -2.70 | 1.50 | 1.53 |
| 29 | c | 517 | DGD | C4D-C3D | 2.70 | 1.59 | 1.52 |
| 24 | K | 103 | BCR | C1-C6 | -2.70 | 1.50 | 1.53 |
| 22 | b | 614 | CLA | CMC-C2C | -2.69 | 1.45 | 1.50 |
| 22 | A | 402 | CLA | CMB-C2B | -2.69 | 1.46 | 1.51 |
| 27 | c | 522 | LMG | C3-C2 | 2.69 | 1.59 | 1.52 |
| 22 | A | 402 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 22 | C | 507 | CLA | C4D-ND | -2.68 | 1.34 | 1.37 |
| 26 | a | 409 | PL9 | C53-C6 | -2.68 | 1.45 | 1.50 |
| 22 | C | 508 | CLA | C1B-NB | 2.68 | 1.37 | 1.35 |
| 22 | B | 615 | CLA | C3B-CAB | -2.68 | 1.42 | 1.47 |
| 29 | C | 517 | DGD | O3G-C1D | 2.67 | 1.44 | 1.40 |
| 22 | d | 403 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 22 | d | 403 | CLA | C3B-C2B | -2.66 | 1.36 | 1.40 |
| 22 | c | 505 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 22 | C | 511 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 22 | C | 502 | CLA | C1D-ND | 2.65 | 1.41 | 1.37 |
| 22 | b | 614 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 29 | A | 413 | DGD | C4D-C5D | 2.65 | 1.58 | 1.53 |
| 22 | B | 606 | CLA | C3B-CAB | -2.65 | 1.42 | 1.47 |
| 22 | C | 510 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 22 | b | 611 | CLA | MG-NC | 2.64 | 2.12 | 2.06 |
| 22 | A | 402 | CLA | C1D-ND | 2.64 | 1.41 | 1.37 |
| 29 | h | 102 | DGD | O3E-C3E | -2.64 | 1.36 | 1.43 |
| 27 | c | 522 | LMG | C1-C2 | 2.64 | 1.60 | 1.52 |
| 22 | B | 602 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 29 | c | 518 | DGD | O1G-C1G | -2.64 | 1.39 | 1.45 |
| 22 | c | 513 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 33 | D | 410 | LHG | O7-C5 | -2.63 | 1.40 | 1.46 |
| 22 | c | 508 | CLA | CMD-C2D | -2.63 | 1.45 | 1.50 |
| 22 | b | 612 | CLA | C1D-ND | 2.63 | 1.41 | 1.37 |
| 22 | C | 509 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 22 | C | 510 | CLA | CMD-C2D | -2.62 | 1.45 | 1.50 |
| 22 | b | 604 | CLA | C4D-ND | -2.62 | 1.34 | 1.37 |
| 22 | b | 609 | CLA | C3B-CAB | -2.62 | 1.42 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | k | 102 | BCR | C30-C25 | -2.62 | 1.50 | 1.53 |
| 22 | C | 504 | CLA | O2D-CGD | 2.61 | 1.39 | 1.33 |
| 22 | b | 603 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 22 | C | 503 | CLA | C3B-C2B | -2.61 | 1.36 | 1.40 |
| 22 | d | 403 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 22 | B | 607 | CLA | C1D-ND | 2.60 | 1.41 | 1.37 |
| 22 | B | 604 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 22 | c | 512 | CLA | MG-NC | 2.60 | 2.12 | 2.06 |
| 24 | F | 101 | BCR | C30-C25 | -2.60 | 1.50 | 1.53 |
| 29 | c | 518 | DGD | O3D-C3D | -2.60 | 1.36 | 1.43 |
| 22 | B | 610 | CLA | C4D-ND | -2.60 | 1.34 | 1.37 |
| 22 | b | 602 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 23 | A | 404 | PHO | CHA-CBD | -2.59 | 1.49 | 1.52 |
| 22 | A | 405 | CLA | CMD-C2D | -2.59 | 1.45 | 1.50 |
| 22 | B | 611 | CLA | MG-NC | -2.58 | 2.00 | 2.06 |
| 29 | h | 102 | DGD | O1G-C1G | -2.58 | 1.39 | 1.45 |
| 22 | B | 616 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 22 | b | 601 | CLA | O2A-CGA | 2.57 | 1.40 | 1.33 |
| 29 | H | 103 | DGD | C4E-C3E | 2.57 | 1.58 | 1.52 |
| 24 | k | 101 | BCR | C30-C25 | -2.56 | 1.50 | 1.53 |
| 22 | c | 510 | CLA | C4D-ND | -2.56 | 1.34 | 1.37 |
| 33 | L | 102 | LHG | O7-C5 | -2.56 | 1.40 | 1.46 |
| 22 | c | 510 | CLA | MG-ND | 2.56 | 2.10 | 2.05 |
| 22 | B | 611 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 22 | a | 410 | CLA | CHC-C1C | 2.56 | 1.41 | 1.35 |
| 29 | C | 516 | DGD | O2G-C2G | -2.56 | 1.40 | 1.46 |
| 24 | A | 406 | BCR | C33-C5 | -2.55 | 1.46 | 1.50 |
| 22 | b | 602 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 28 | A | 411 | SQD | O3-C3 | -2.55 | 1.37 | 1.43 |
| 29 | C | 515 | DGD | O1G-C1A | 2.54 | 1.40 | 1.33 |
| 29 | h | 102 | DGD | C4D-C3D | 2.54 | 1.58 | 1.52 |
| 22 | B | 616 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 22 | B | 609 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 33 | e | 101 | LHG | P-O6 | 2.53 | 1.69 | 1.59 |
| 33 | D | 412 | LHG | O7-C5 | -2.53 | 1.40 | 1.46 |
| 24 | A | 406 | BCR | C30-C25 | -2.53 | 1.50 | 1.53 |
| 22 | b | 606 | CLA | C4B-CHC | -2.53 | 1.34 | 1.41 |
| 22 | d | 403 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 24 | c | 516 | BCR | C30-C25 | -2.53 | 1.50 | 1.53 |
| 22 | c | 513 | CLA | CMD-C2D | -2.52 | 1.45 | 1.50 |
| 29 | c | 517 | DGD | C3D-C2D | 2.52 | 1.58 | 1.52 |
| 22 | C | 509 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | K | 103 | BCR | C30-C25 | -2.50 | 1.50 | 1.53 |
| 22 | d | 403 | CLA | C4B-CHC | -2.50 | 1.34 | 1.41 |
| 22 | B | 614 | CLA | CMC-C2C | -2.50 | 1.45 | 1.50 |
| 22 | C | 506 | CLA | CMC-C2C | -2.50 | 1.45 | 1.50 |
| 22 | c | 502 | CLA | CMD-C2D | -2.50 | 1.45 | 1.50 |
| 34 | F | 102 | HEC | CAD-C3D | 2.49 | 1.55 | 1.52 |
| 27 | d | 410 | LMG | O6-C5 | -2.49 | 1.38 | 1.44 |
| 22 | D | 405 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 22 | A | 403 | CLA | CMD-C2D | -2.49 | 1.45 | 1.50 |
| 22 | b | 613 | CLA | CMD-C2D | -2.49 | 1.45 | 1.50 |
| 22 | b | 614 | CLA | O2D-CGD | 2.49 | 1.39 | 1.33 |
| 29 | h | 102 | DGD | O2D-C2D | -2.49 | 1.37 | 1.43 |
| 22 | b | 608 | CLA | C1B-NB | 2.49 | 1.37 | 1.35 |
| 22 | D | 404 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 22 | b | 615 | CLA | C4D-ND | -2.48 | 1.34 | 1.37 |
| 33 | d | 407 | LHG | O7-C5 | -2.48 | 1.40 | 1.46 |
| 22 | c | 509 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 22 | b | 607 | CLA | C4D-ND | -2.48 | 1.34 | 1.37 |
| 22 | B | 609 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 23 | d | 401 | PHO | C3B-CAB | -2.48 | 1.42 | 1.47 |
| 22 | b | 609 | CLA | C4D-ND | -2.48 | 1.34 | 1.37 |
| 22 | b | 609 | CLA | C3B-C2B | -2.48 | 1.36 | 1.40 |
| 22 | b | 615 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 29 | C | 516 | DGD | C6E-C5E | 2.47 | 1.60 | 1.51 |
| 29 | H | 103 | DGD | O6D-C5D | -2.47 | 1.38 | 1.44 |
| 29 | C | 515 | DGD | C4D-C3D | 2.46 | 1.58 | 1.52 |
| 28 | B | 622 | SQD | O2-C2 | -2.46 | 1.37 | 1.43 |
| 22 | H | 101 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 22 | C | 504 | CLA | C1B-NB | -2.45 | 1.33 | 1.35 |
| 27 | c | 523 | LMG | C1-C2 | 2.45 | 1.59 | 1.52 |
| 22 | d | 404 | CLA | CHC-C1C | 2.45 | 1.41 | 1.35 |
| 22 | B | 615 | CLA | O2D-CGD | 2.44 | 1.39 | 1.33 |
| 22 | b | 616 | CLA | C3B-CAB | -2.44 | 1.43 | 1.47 |
| 22 | C | 504 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 22 | B | 610 | CLA | MG-NA | 2.43 | 2.12 | 2.06 |
| 22 | B | 612 | CLA | CHC-C1C | 2.43 | 1.41 | 1.35 |
| 22 | c | 505 | CLA | CMD-C2D | -2.43 | 1.45 | 1.50 |
| 22 | c | 503 | CLA | MG-NA | 2.43 | 2.12 | 2.06 |
| 22 | b | 602 | CLA | C4B-CHC | -2.43 | 1.34 | 1.41 |
| 22 | b | 612 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 22 | c | 514 | CLA | C1D-ND | 2.42 | 1.40 | 1.37 |
| 33 | E | 101 | LHG | C24-C23 | 2.42 | 1.57 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | C | 504 | CLA | C1D-ND | 2.42 | 1.40 | 1.37 |
| 22 | b | 610 | CLA | MG-NC | 2.42 | 2.12 | 2.06 |
| 22 | B | 614 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 24 | C | 514 | BCR | C30-C25 | -2.41 | 1.50 | 1.53 |
| 22 | A | 405 | CLA | C4B-CHC | -2.41 | 1.34 | 1.41 |
| 27 | b | 621 | LMG | C1-C2 | 2.41 | 1.59 | 1.52 |
| 22 | C | 503 | CLA | C4D-ND | -2.41 | 1.34 | 1.37 |
| 27 | b | 621 | LMG | C4-C5 | 2.41 | 1.58 | 1.53 |
| 22 | c | 506 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 28 | f | 102 | SQD | O3-C3 | -2.40 | 1.37 | 1.43 |
| 22 | d | 404 | CLA | C1D-ND | 2.40 | 1.40 | 1.37 |
| 24 | b | 618 | BCR | C1-C6 | -2.40 | 1.50 | 1.53 |
| 22 | C | 507 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 22 | c | 512 | CLA | C1D-ND | 2.40 | 1.40 | 1.37 |
| 29 | C | 516 | DGD | O3D-C3D | -2.40 | 1.37 | 1.43 |
| 22 | C | 513 | CLA | MG-ND | 2.40 | 2.10 | 2.05 |
| 22 | c | 510 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 29 | h | 102 | DGD | C4E-C5E | 2.39 | 1.58 | 1.53 |
| 33 | D | 410 | LHG | O3-C3 | -2.39 | 1.35 | 1.44 |
| 22 | c | 503 | CLA | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 22 | c | 503 | CLA | CMD-C2D | -2.38 | 1.45 | 1.50 |
| 22 | C | 513 | CLA | CMC-C2C | -2.38 | 1.45 | 1.50 |
| 22 | A | 403 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 26 | d | 406 | PL9 | C53-C6 | -2.37 | 1.45 | 1.50 |
| 22 | C | 503 | CLA | C4B-CHC | -2.37 | 1.34 | 1.41 |
| 23 | A | 404 | PHO | C3B-CAB | -2.37 | 1.43 | 1.47 |
| 22 | C | 512 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 22 | C | 501 | CLA | C1D-C2D | 2.36 | 1.50 | 1.45 |
| 31 | j | 101 | STE | C2-C1 | 2.36 | 1.56 | 1.50 |
| 22 | c | 509 | CLA | MG-NC | -2.36 | 2.00 | 2.06 |
| 22 | a | 403 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 24 | c | 516 | BCR | C33-C5 | -2.36 | 1.47 | 1.50 |
| 22 | D | 405 | CLA | C4B-CHC | -2.35 | 1.34 | 1.41 |
| 22 | c | 504 | CLA | C5-C3 | -2.35 | 1.46 | 1.51 |
| 22 | C | 504 | CLA | C4D-ND | -2.35 | 1.34 | 1.37 |
| 27 | c | 520 | LMG | O2-C2 | -2.35 | 1.37 | 1.43 |
| 24 | a | 406 | BCR | C30-C25 | -2.35 | 1.50 | 1.53 |
| 27 | b | 623 | LMG | C4-C5 | 2.35 | 1.58 | 1.53 |
| 27 | a | 415 | LMG | C4-C3 | 2.35 | 1.58 | 1.52 |
| 22 | B | 606 | CLA | CMC-C2C | -2.35 | 1.45 | 1.50 |
| 22 | B | 616 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 22 | d | 404 | CLA | MG-ND | -2.34 | 2.01 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | b | 609 | CLA | O2D-CGD | 2.34 | 1.38 | 1.33 |
| 26 | d | 406 | PL9 | C30-C29 | -2.34 | 1.44 | 1.50 |
| 22 | B | 616 | CLA | CAC-C3C | -2.33 | 1.45 | 1.51 |
| 22 | b | 616 | CLA | MG-NC | -2.33 | 2.00 | 2.06 |
| 27 | c | 523 | LMG | O8-C9 | -2.33 | 1.39 | 1.45 |
| 22 | b | 613 | CLA | CAA-C2A | -2.33 | 1.49 | 1.54 |
| 22 | c | 504 | CLA | MG-NC | 2.33 | 2.11 | 2.06 |
| 29 | c | 519 | DGD | O3G-C3G | -2.33 | 1.39 | 1.43 |
| 29 | C | 516 | DGD | C4E-C3E | 2.33 | 1.58 | 1.52 |
| 24 | b | 617 | BCR | C33-C5 | -2.33 | 1.47 | 1.50 |
| 22 | B | 605 | CLA | C3B-C2B | -2.32 | 1.37 | 1.40 |
| 22 | B | 605 | CLA | CMC-C2C | -2.32 | 1.45 | 1.50 |
| 22 | c | 509 | CLA | C3B-C2B | -2.32 | 1.37 | 1.40 |
| 22 | A | 402 | CLA | C5-C3 | -2.32 | 1.46 | 1.51 |
| 22 | B | 609 | CLA | C1D-ND | 2.32 | 1.40 | 1.37 |
| 29 | c | 519 | DGD | C2A-C1A | -2.32 | 1.43 | 1.50 |
| 22 | B | 610 | CLA | C3D-C4D | 2.32 | 1.49 | 1.44 |
| 27 | Y | 101 | LMG | C3-C2 | 2.32 | 1.58 | 1.52 |
| 22 | b | 606 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 22 | b | 605 | CLA | C4B-CHC | -2.32 | 1.34 | 1.41 |
| 22 | b | 616 | CLA | CMC-C2C | -2.32 | 1.45 | 1.50 |
| 22 | B | 609 | CLA | C3B-CAB | -2.31 | 1.43 | 1.47 |
| 23 | D | 401 | PHO | O2D-CGD | 2.31 | 1.38 | 1.33 |
| 24 | t | 101 | BCR | C30-C25 | -2.31 | 1.50 | 1.53 |
| 22 | d | 404 | CLA | C4B-CHC | -2.31 | 1.34 | 1.41 |
| 28 | a | 411 | SQD | O3-C3 | -2.31 | 1.37 | 1.43 |
| 22 | C | 508 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 22 | A | 405 | CLA | CHC-C1C | 2.30 | 1.40 | 1.35 |
| 29 | c | 517 | DGD | C4E-C3E | 2.30 | 1.58 | 1.52 |
| 22 | b | 610 | CLA | C3B-CAB | -2.30 | 1.43 | 1.47 |
| 22 | C | 510 | CLA | MG-NA | 2.30 | 2.11 | 2.06 |
| 23 | d | 401 | PHO | CMC-C2C | -2.30 | 1.46 | 1.51 |
| 22 | C | 508 | CLA | C1D-ND | 2.30 | 1.40 | 1.37 |
| 22 | b | 614 | CLA | C1A-CHA | -2.30 | 1.33 | 1.43 |
| 22 | b | 611 | CLA | CMB-C2B | -2.30 | 1.46 | 1.51 |
| 22 | B | 616 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 29 | C | 517 | DGD | C4E-C3E | 2.30 | 1.58 | 1.52 |
| 29 | A | 413 | DGD | C3G-C2G | 2.29 | 1.57 | 1.50 |
| 22 | H | 101 | CLA | CMC-C2C | -2.29 | 1.45 | 1.50 |
| 29 | c | 519 | DGD | O4E-C4E | -2.29 | 1.37 | 1.43 |
| 22 | c | 508 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 31 | B | 620 | STE | C2-C1 | 2.29 | 1.55 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | C | 503 | CLA | C3B-CAB | -2.29 | 1.43 | 1.47 |
| 22 | b | 601 | CLA | C1B-NB | 2.29 | 1.37 | 1.35 |
| 27 | a | 415 | LMG | C14-C13 | 2.28 | 1.64 | 1.51 |
| 22 | B | 610 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 22 | c | 502 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 22 | b | 615 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 22 | c | 505 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 22 | b | 612 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 22 | b | 616 | CLA | CHC-C1C | 2.27 | 1.40 | 1.35 |
| 22 | C | 506 | CLA | C4D-ND | -2.27 | 1.34 | 1.37 |
| 22 | a | 405 | CLA | CHC-C1C | 2.27 | 1.40 | 1.35 |
| 22 | a | 403 | CLA | MG-NC | 2.27 | 2.11 | 2.06 |
| 29 | c | 519 | DGD | C1D-C2D | 2.27 | 1.59 | 1.52 |
| 22 | B | 607 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 28 | a | 411 | SQD | O47-C7 | 2.27 | 1.40 | 1.34 |
| 22 | B | 613 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 22 | B | 613 | CLA | MG-NC | 2.26 | 2.11 | 2.06 |
| 22 | B | 613 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 27 | c | 523 | LMG | O7-C8 | -2.26 | 1.40 | 1.46 |
| 27 | b | 623 | LMG | C4-C3 | 2.26 | 1.58 | 1.52 |
| 22 | b | 613 | CLA | CHC-C1C | 2.25 | 1.40 | 1.35 |
| 22 | b | 601 | CLA | C1D-C2D | 2.25 | 1.49 | 1.45 |
| 22 | B | 602 | CLA | C4D-ND | -2.25 | 1.34 | 1.37 |
| 22 | C | 511 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 22 | C | 501 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 29 | C | 517 | DGD | C3D-C2D | 2.24 | 1.58 | 1.52 |
| 28 | f | 102 | SQD | O2-C2 | -2.24 | 1.37 | 1.43 |
| 24 | C | 514 | BCR | C33-C5 | -2.24 | 1.47 | 1.50 |
| 22 | a | 410 | CLA | MG-NC | -2.23 | 2.01 | 2.06 |
| 22 | C | 512 | CLA | MG-NA | 2.23 | 2.11 | 2.06 |
| 22 | H | 101 | CLA | C1D-C2D | 2.23 | 1.49 | 1.45 |
| 24 | T | 101 | BCR | C27-C26 | -2.23 | 1.46 | 1.51 |
| 22 | D | 405 | CLA | C4D-ND | -2.23 | 1.34 | 1.37 |
| 22 | d | 404 | CLA | CMB-C2B | -2.22 | 1.47 | 1.51 |
| 22 | C | 506 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 22 | b | 604 | CLA | C3D-C4D | 2.22 | 1.49 | 1.44 |
| 22 | b | 601 | CLA | C4D-ND | -2.22 | 1.34 | 1.37 |
| 22 | c | 503 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 22 | b | 605 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 22 | B | 608 | CLA | C1D-C2D | 2.22 | 1.49 | 1.45 |
| 22 | B | 612 | CLA | MG-NC | 2.22 | 2.11 | 2.06 |
| 22 | H | 101 | CLA | C4B-CHC | -2.22 | 1.34 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | D | 404 | CLA | O2D-CGD | 2.22 | 1.38 | 1.33 |
| 22 | b | 608 | CLA | CMB-C2B | -2.21 | 1.47 | 1.51 |
| 31 | M | 102 | STE | O1-C1 | 2.21 | 1.29 | 1.22 |
| 29 | c | 518 | DGD | O2E-C2E | -2.21 | 1.37 | 1.43 |
| 22 | H | 101 | CLA | C4D-ND | -2.21 | 1.34 | 1.37 |
| 24 | c | 516 | BCR | C36-C18 | -2.21 | 1.46 | 1.50 |
| 22 | B | 605 | CLA | C5-C3 | -2.21 | 1.46 | 1.51 |
| 27 | a | 415 | LMG | O7-C10 | 2.21 | 1.40 | 1.34 |
| 22 | b | 602 | CLA | CAC-C3C | -2.21 | 1.45 | 1.51 |
| 26 | d | 406 | PL9 | C45-C44 | -2.21 | 1.45 | 1.50 |
| 22 | b | 610 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 23 | A | 404 | PHO | CMC-C2C | -2.20 | 1.46 | 1.51 |
| 22 | a | 405 | CLA | CMB-C2B | -2.20 | 1.47 | 1.51 |
| 29 | C | 517 | DGD | O6D-C5D | -2.20 | 1.39 | 1.44 |
| 22 | B | 616 | CLA | C4B-CHC | -2.20 | 1.34 | 1.41 |
| 22 | B | 607 | CLA | CMB-C2B | -2.20 | 1.47 | 1.51 |
| 22 | B | 603 | CLA | CHC-C1C | 2.20 | 1.40 | 1.35 |
| 22 | B | 608 | CLA | C4B-CHC | -2.20 | 1.34 | 1.41 |
| 22 | C | 501 | CLA | CMB-C2B | -2.20 | 1.47 | 1.51 |
| 22 | C | 508 | CLA | C1D-C2D | 2.20 | 1.49 | 1.45 |
| 22 | D | 404 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 22 | C | 502 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 22 | c | 504 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 22 | c | 504 | CLA | C3D-C4D | 2.19 | 1.49 | 1.44 |
| 23 | A | 404 | PHO | CMB-C2B | -2.19 | 1.46 | 1.51 |
| 29 | c | 518 | DGD | C6D-C5D | 2.19 | 1.58 | 1.51 |
| 22 | C | 510 | CLA | O2A-CGA | 2.19 | 1.39 | 1.33 |
| 29 | h | 102 | DGD | C4E-C3E | 2.18 | 1.57 | 1.52 |
| 26 | A | 409 | PL9 | C31-C29 | -2.18 | 1.46 | 1.51 |
| 22 | B | 606 | CLA | C4D-ND | -2.18 | 1.34 | 1.37 |
| 22 | C | 510 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 28 | A | 411 | SQD | O47-C45 | -2.18 | 1.41 | 1.46 |
| 22 | b | 601 | CLA | C3B-CAB | -2.18 | 1.43 | 1.47 |
| 22 | B | 613 | CLA | O2D-CED | -2.18 | 1.40 | 1.45 |
| 22 | c | 514 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 29 | C | 516 | DGD | O4E-C4E | -2.18 | 1.37 | 1.43 |
| 22 | b | 610 | CLA | C4B-CHC | -2.18 | 1.34 | 1.41 |
| 29 | H | 103 | DGD | O2D-C2D | -2.18 | 1.37 | 1.43 |
| 22 | b | 616 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 22 | B | 613 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 29 | h | 102 | DGD | O2E-C2E | -2.17 | 1.37 | 1.43 |
| 26 | a | 409 | PL9 | C18-C19 | 2.17 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | C | 512 | CLA | CMB-C2B | -2.17 | 1.47 | 1.51 |
| 22 | C | 502 | CLA | C1B-NB | 2.17 | 1.37 | 1.35 |
| 22 | c | 507 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 22 | A | 402 | CLA | C4B-CHC | -2.17 | 1.35 | 1.41 |
| 22 | C | 503 | CLA | C1D-ND | 2.16 | 1.40 | 1.37 |
| 27 | c | 520 | LMG | C7-C8 | 2.16 | 1.57 | 1.50 |
| 22 | C | 501 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 22 | b | 610 | CLA | CMB-C2B | -2.16 | 1.47 | 1.51 |
| 22 | c | 508 | CLA | CMB-C2B | -2.16 | 1.47 | 1.51 |
| 33 | D | 409 | LHG | C3-C2 | 2.16 | 1.58 | 1.51 |
| 27 | M | 101 | LMG | C9-C8 | 2.16 | 1.57 | 1.50 |
| 22 | C | 509 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 31 | d | 411 | STE | C2-C1 | 2.16 | 1.55 | 1.50 |
| 29 | C | 515 | DGD | C3E-C2E | 2.15 | 1.57 | 1.52 |
| 22 | c | 512 | CLA | CMB-C2B | -2.15 | 1.47 | 1.51 |
| 29 | h | 102 | DGD | C1E-C2E | 2.14 | 1.58 | 1.52 |
| 26 | a | 409 | PL9 | C3-C4 | 2.14 | 1.53 | 1.49 |
| 29 | H | 103 | DGD | C1E-C2E | 2.14 | 1.58 | 1.52 |
| 28 | a | 411 | SQD | O2-C2 | -2.14 | 1.37 | 1.43 |
| 28 | D | 408 | SQD | O4-C4 | -2.14 | 1.37 | 1.43 |
| 26 | D | 406 | PL9 | C26-C24 | -2.14 | 1.46 | 1.51 |
| 22 | c | 514 | CLA | CMB-C2B | -2.14 | 1.47 | 1.51 |
| 29 | h | 102 | DGD | O3D-C3D | -2.13 | 1.37 | 1.43 |
| 22 | B | 604 | CLA | CMB-C2B | -2.13 | 1.47 | 1.51 |
| 23 | D | 401 | PHO | CMD-C2D | -2.13 | 1.46 | 1.51 |
| 33 | L | 102 | LHG | O8-C23 | 2.12 | 1.39 | 1.33 |
| 23 | a | 404 | PHO | CAC-C3C | -2.12 | 1.48 | 1.52 |
| 22 | b | 610 | CLA | C3D-C4D | 2.12 | 1.49 | 1.44 |
| 22 | b | 610 | CLA | CHC-C1C | 2.12 | 1.40 | 1.35 |
| 22 | D | 403 | CLA | C4B-CHC | -2.12 | 1.35 | 1.41 |
| 22 | B | 608 | CLA | C3C-C2C | 2.12 | 1.41 | 1.36 |
| 22 | B | 611 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 22 | B | 604 | CLA | O2A-CGA | 2.12 | 1.39 | 1.33 |
| 29 | A | 413 | DGD | O3G-C1D | 2.11 | 1.43 | 1.40 |
| 22 | c | 514 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 22 | B | 609 | CLA | O2D-CGD | 2.11 | 1.38 | 1.33 |
| 22 | C | 509 | CLA | O2D-CGD | 2.11 | 1.38 | 1.33 |
| 22 | b | 604 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 26 | D | 406 | PL9 | C36-C34 | 2.11 | 1.55 | 1.51 |
| 22 | B | 609 | CLA | CHC-C1C | 2.11 | 1.40 | 1.35 |
| 26 | d | 406 | PL9 | C21-C19 | -2.11 | 1.46 | 1.51 |
| 22 | C | 505 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | A | 403 | CLA | C3C-C2C | 2.11 | 1.41 | 1.36 |
| 22 | A | 403 | CLA | CAA-C2A | -2.11 | 1.50 | 1.54 |
| 31 | a | 414 | STE | O1-C1 | 2.11 | 1.29 | 1.22 |
| 22 | B | 613 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 22 | C | 505 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 22 | b | 608 | CLA | C3D-C4D | 2.10 | 1.48 | 1.44 |
| 29 | C | 517 | DGD | O2E-C2E | -2.10 | 1.38 | 1.43 |
| 22 | c | 510 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 31 | c | 521 | STE | C2-C1 | 2.10 | 1.55 | 1.50 |
| 29 | C | 515 | DGD | O1G-C1G | -2.10 | 1.40 | 1.45 |
| 26 | D | 406 | PL9 | C27-C28 | -2.10 | 1.43 | 1.50 |
| 29 | C | 516 | DGD | C1G-C2G | 2.10 | 1.57 | 1.50 |
| 22 | A | 405 | CLA | CAC-C3C | -2.09 | 1.45 | 1.51 |
| 29 | C | 516 | DGD | C4D-C3D | 2.09 | 1.57 | 1.52 |
| 22 | c | 508 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 22 | B | 607 | CLA | CAC-C3C | -2.09 | 1.45 | 1.51 |
| 22 | c | 503 | CLA | O2D-CGD | 2.09 | 1.38 | 1.33 |
| 22 | D | 405 | CLA | CHC-C1C | 2.08 | 1.40 | 1.35 |
| 29 | C | 516 | DGD | O3G-C3G | -2.08 | 1.39 | 1.43 |
| 22 | b | 606 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 22 | c | 514 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 24 | F | 101 | BCR | C27-C26 | -2.07 | 1.46 | 1.51 |
| 22 | C | 513 | CLA | C4B-CHC | -2.07 | 1.35 | 1.41 |
| 22 | D | 403 | CLA | C3D-C4D | 2.07 | 1.48 | 1.44 |
| 27 | A | 410 | LMG | C3-C2 | 2.07 | 1.57 | 1.52 |
| 22 | d | 404 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 22 | b | 603 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 22 | H | 101 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 22 | b | 613 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 27 | c | 522 | LMG | O7-C8 | -2.06 | 1.41 | 1.46 |
| 29 | c | 519 | DGD | O6D-C5D | -2.06 | 1.39 | 1.44 |
| 22 | c | 511 | CLA | C5-C3 | -2.06 | 1.47 | 1.51 |
| 22 | C | 511 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 22 | b | 609 | CLA | C3D-C4D | 2.06 | 1.48 | 1.44 |
| 24 | h | 101 | BCR | C1-C6 | -2.05 | 1.50 | 1.53 |
| 22 | c | 511 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 22 | D | 405 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 22 | C | 513 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 22 | B | 610 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 22 | B | 608 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 33 | E | 101 | LHG | O8-C23 | 2.05 | 1.39 | 1.33 |
| 22 | c | 510 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | D | 407 | LMG | O6-C5 | -2.04 | 1.39 | 1.44 |
| 22 | c | 502 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 31 | B | 620 | STE | O1-C1 | 2.04 | 1.28 | 1.22 |
| 24 | k | 102 | BCR | C1-C6 | -2.04 | 1.51 | 1.53 |
| 29 | h | 102 | DGD | O2G-C1B | 2.04 | 1.40 | 1.34 |
| 22 | c | 509 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 29 | C | 515 | DGD | O3G-C1D | -2.04 | 1.36 | 1.40 |
| 22 | b | 608 | CLA | CMA-C3A | -2.04 | 1.48 | 1.53 |
| 27 | D | 411 | LMG | O8-C28 | 2.03 | 1.39 | 1.33 |
| 22 | A | 405 | CLA | CMB-C2B | -2.03 | 1.47 | 1.51 |
| 31 | E | 102 | STE | C2-C1 | 2.03 | 1.55 | 1.50 |
| 34 | f | 101 | HEC | C4B-C3B | 2.03 | 1.46 | 1.43 |
| 22 | C | 513 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 28 | a | 411 | SQD | O4-C4 | -2.03 | 1.38 | 1.43 |
| 22 | c | 513 | CLA | MG-NC | 2.03 | 2.11 | 2.06 |
| 22 | C | 510 | CLA | CMB-C2B | -2.03 | 1.47 | 1.51 |
| 22 | C | 505 | CLA | CMB-C2B | -2.03 | 1.47 | 1.51 |
| 22 | D | 404 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 22 | c | 502 | CLA | CMB-C2B | -2.03 | 1.47 | 1.51 |
| 27 | a | 415 | LMG | C7-C8 | 2.03 | 1.56 | 1.50 |
| 22 | B | 604 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 22 | B | 605 | CLA | MG-NA | 2.02 | 2.11 | 2.06 |
| 22 | C | 503 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 22 | b | 603 | CLA | CHC-C1C | 2.02 | 1.40 | 1.35 |
| 22 | b | 613 | CLA | C4B-CHC | -2.02 | 1.35 | 1.41 |
| 22 | C | 507 | CLA | C3C-C2C | 2.02 | 1.41 | 1.36 |
| 22 | c | 506 | CLA | MG-ND | 2.01 | 2.09 | 2.05 |
| 22 | C | 509 | CLA | O2A-CGA | 2.01 | 1.39 | 1.33 |
| 27 | b | 623 | LMG | C3-C2 | 2.01 | 1.57 | 1.52 |
| 22 | A | 403 | CLA | C5-C3 | -2.01 | 1.47 | 1.51 |
| 22 | C | 509 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 29 | C | 515 | DGD | O6D-C5D | -2.01 | 1.39 | 1.44 |
| 22 | B | 610 | CLA | CMA-C3A | -2.01 | 1.48 | 1.53 |
| 22 | c | 512 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | d | 404 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 22 | B | 607 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 27 | d | 410 | LMG | O1-C7 | -2.00 | 1.40 | 1.43 |
| 22 | B | 605 | CLA | CMD-C2D | -2.00 | 1.46 | 1.50 |
| 29 | C | 515 | DGD | C1G-C2G | 2.00 | 1.56 | 1.50 |
| 22 | C | 506 | CLA | C3D-C4D | 2.00 | 1.48 | 1.44 |
| 24 | K | 102 | BCR | C38-C26 | -2.00 | 1.47 | 1.50 |
| 22 | c | 504 | CLA | MG-NA | 2.00 | 2.11 | 2.06 |

All (1322) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | L | 101 | SQD | O6-C1-C2 | 10.32 | 124.41 | 108.30 |
| 28 | a | 411 | SQD | O6-C1-C2 | 9.80 | 123.61 | 108.30 |
| 22 | b | 604 | CLA | C4A-NA-C1A | 9.48 | 110.97 | 106.71 |
| 22 | b | 611 | CLA | C4A-NA-C1A | 9.46 | 110.96 | 106.71 |
| 22 | c | 510 | CLA | C4A-NA-C1A | 9.26 | 110.87 | 106.71 |
| 22 | C | 507 | CLA | C4A-NA-C1A | 8.60 | 110.57 | 106.71 |
| 22 | c | 512 | CLA | C4A-NA-C1A | 8.30 | 110.44 | 106.71 |
| 22 | B | 604 | CLA | C4A-NA-C1A | 8.26 | 110.42 | 106.71 |
| 22 | c | 504 | CLA | C4A-NA-C1A | 8.14 | 110.37 | 106.71 |
| 28 | f | 102 | SQD | O9-S-C6 | 7.89 | 116.32 | 106.94 |
| 22 | b | 606 | CLA | C4A-NA-C1A | 7.86 | 110.24 | 106.71 |
| 22 | B | 616 | CLA | C4A-NA-C1A | 7.85 | 110.23 | 106.71 |
| 34 | f | 101 | HEC | CBD-CAD-C3D | -7.82 | 99.27 | 112.62 |
| 22 | C | 508 | CLA | C4A-NA-C1A | 7.73 | 110.18 | 106.71 |
| 22 | H | 101 | CLA | C4A-NA-C1A | 7.72 | 110.18 | 106.71 |
| 22 | B | 605 | CLA | C4A-NA-C1A | 7.56 | 110.10 | 106.71 |
| 22 | C | 511 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 22 | C | 513 | CLA | C4A-NA-C1A | 7.40 | 110.03 | 106.71 |
| 22 | c | 502 | CLA | C4A-NA-C1A | 7.34 | 110.00 | 106.71 |
| 28 | L | 101 | SQD | O7-S-C6 | 7.16 | 115.45 | 106.94 |
| 22 | c | 511 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 22 | c | 503 | CLA | C4A-NA-C1A | 6.86 | 109.79 | 106.71 |
| 22 | B | 606 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 28 | A | 411 | SQD | O6-C1-C2 | 6.71 | 118.78 | 108.30 |
| 26 | a | 409 | PL9 | C7-C3-C4 | 6.66 | 122.29 | 116.88 |
| 22 | B | 609 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 22 | D | 404 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 26 | d | 406 | PL9 | C7-C3-C4 | 6.62 | 122.26 | 116.88 |
| 22 | a | 410 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 22 | a | 403 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 28 | D | 408 | SQD | O9-S-C6 | 6.51 | 114.67 | 106.94 |
| 22 | C | 503 | CLA | C4A-NA-C1A | 6.50 | 109.63 | 106.71 |
| 22 | C | 501 | CLA | C4A-NA-C1A | 6.21 | 109.50 | 106.71 |
| 28 | a | 411 | SQD | O9-S-C6 | 6.12 | 114.22 | 106.94 |
| 28 | B | 622 | SQD | O6-C1-C2 | 6.05 | 117.75 | 108.30 |
| 22 | b | 601 | CLA | C4A-NA-C1A | 6.03 | 109.42 | 106.71 |
| 22 | c | 505 | CLA | CMB-C2B-C1B | -6.02 | 119.22 | 128.46 |
| 22 | B | 607 | CLA | C4A-NA-C1A | 5.98 | 109.39 | 106.71 |
| 22 | C | 505 | CLA | C4A-NA-C1A | 5.90 | 109.36 | 106.71 |
| 22 | b | 615 | CLA | C4A-NA-C1A | 5.90 | 109.36 | 106.71 |
| 22 | a | 402 | CLA | C4A-NA-C1A | 5.85 | 109.34 | 106.71 |
| 22 | c | 513 | CLA | C4A-NA-C1A | 5.82 | 109.32 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 402 | CLA | C4A-NA-C1A | 5.75 | 109.29 | 106.71 |
| 22 | D | 403 | CLA | C4A-NA-C1A | 5.55 | 109.20 | 106.71 |
| 22 | b | 616 | CLA | O2D-CGD-O1D | -5.55 | 112.99 | 123.84 |
| 22 | c | 502 | CLA | O2D-CGD-O1D | -5.54 | 113.01 | 123.84 |
| 22 | B | 603 | CLA | CMB-C2B-C1B | -5.38 | 120.19 | 128.46 |
| 22 | B | 615 | CLA | C4A-NA-C1A | 5.38 | 109.12 | 106.71 |
| 22 | b | 616 | CLA | C4A-NA-C1A | 5.37 | 109.12 | 106.71 |
| 27 | a | 415 | LMG | C1-C2-C3 | -5.36 | 98.83 | 110.00 |
| 28 | a | 412 | SQD | O47-C7-C8 | 5.35 | 123.03 | 111.50 |
| 27 | b | 623 | LMG | O1-C1-C2 | -5.33 | 99.98 | 108.30 |
| 22 | B | 608 | CLA | CMB-C2B-C1B | -5.29 | 120.33 | 128.46 |
| 22 | B | 602 | CLA | C4A-NA-C1A | 5.19 | 109.04 | 106.71 |
| 22 | b | 616 | CLA | CMB-C2B-C1B | -5.17 | 120.51 | 128.46 |
| 22 | b | 604 | CLA | CMB-C2B-C1B | -5.15 | 120.55 | 128.46 |
| 34 | F | 102 | HEC | CBD-CAD-C3D | -5.15 | 103.84 | 112.62 |
| 22 | a | 402 | CLA | CMB-C2B-C1B | -5.14 | 120.56 | 128.46 |
| 22 | b | 616 | CLA | CMB-C2B-C3B | 5.14 | 134.29 | 124.68 |
| 22 | B | 608 | CLA | C4A-NA-C1A | 5.12 | 109.01 | 106.71 |
| 22 | A | 405 | CLA | C4A-NA-C1A | 5.08 | 108.99 | 106.71 |
| 22 | b | 605 | CLA | C4A-NA-C1A | 5.05 | 108.98 | 106.71 |
| 29 | H | 103 | DGD | O3G-C3G-C2G | -5.03 | 98.76 | 110.90 |
| 22 | b | 603 | CLA | C4A-NA-C1A | 5.00 | 108.95 | 106.71 |
| 22 | c | 508 | CLA | C4A-NA-C1A | 4.99 | 108.95 | 106.71 |
| 22 | B | 612 | CLA | CMB-C2B-C1B | -4.98 | 120.82 | 128.46 |
| 22 | a | 405 | CLA | C4A-NA-C1A | 4.98 | 108.94 | 106.71 |
| 22 | b | 613 | CLA | C4A-NA-C1A | 4.96 | 108.94 | 106.71 |
| 26 | A | 409 | PL9 | C7-C3-C4 | 4.88 | 120.84 | 116.88 |
| 22 | B | 608 | CLA | CMB-C2B-C3B | 4.76 | 133.59 | 124.68 |
| 28 | D | 408 | SQD | O6-C1-C2 | 4.74 | 115.71 | 108.30 |
| 22 | b | 615 | CLA | CMB-C2B-C1B | -4.74 | 121.18 | 128.46 |
| 22 | b | 613 | CLA | CMB-C2B-C1B | -4.73 | 121.19 | 128.46 |
| 22 | c | 509 | CLA | C4A-NA-C1A | 4.68 | 108.81 | 106.71 |
| 22 | c | 502 | CLA | O2D-CGD-CBD | 4.67 | 119.56 | 111.27 |
| 28 | L | 101 | SQD | C1-C2-C3 | -4.65 | 100.31 | 110.00 |
| 22 | b | 602 | CLA | C4A-NA-C1A | 4.65 | 108.80 | 106.71 |
| 26 | D | 406 | PL9 | C7-C3-C4 | 4.64 | 120.64 | 116.88 |
| 28 | B | 622 | SQD | O7-S-C6 | 4.63 | 112.44 | 106.94 |
| 34 | F | 102 | HEC | CBA-CAA-C2A | -4.63 | 104.80 | 112.60 |
| 34 | v | 201 | HEC | CBD-CAD-C3D | -4.62 | 104.73 | 112.62 |
| 23 | d | 401 | PHO | O1D-CGD-CBD | 4.60 | 132.41 | 124.74 |
| 22 | B | 602 | CLA | CMB-C2B-C1B | -4.57 | 121.44 | 128.46 |
| 29 | C | 517 | DGD | O3G-C3G-C2G | -4.56 | 99.89 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | b | 608 | CLA | C4A-NA-C1A | 4.56 | 108.75 | 106.71 |
| 22 | B | 612 | CLA | CMB-C2B-C3B | 4.54 | 133.18 | 124.68 |
| 22 | b | 612 | CLA | CMB-C2B-C1B | -4.54 | 121.49 | 128.46 |
| 22 | C | 507 | CLA | CMB-C2B-C1B | -4.53 | 121.50 | 128.46 |
| 22 | c | 505 | CLA | C4A-NA-C1A | 4.53 | 108.74 | 106.71 |
| 22 | B | 604 | CLA | CMB-C2B-C1B | -4.50 | 121.54 | 128.46 |
| 22 | c | 505 | CLA | CMB-C2B-C3B | 4.48 | 133.05 | 124.68 |
| 22 | B | 613 | CLA | C4A-NA-C1A | 4.47 | 108.71 | 106.71 |
| 22 | C | 502 | CLA | C4A-NA-C1A | 4.46 | 108.71 | 106.71 |
| 29 | C | 516 | DGD | O3G-C3G-C2G | -4.44 | 100.19 | 110.90 |
| 22 | B | 603 | CLA | CMB-C2B-C3B | 4.42 | 132.95 | 124.68 |
| 22 | C | 506 | CLA | C4A-NA-C1A | 4.42 | 108.69 | 106.71 |
| 22 | b | 604 | CLA | CMB-C2B-C3B | 4.37 | 132.85 | 124.68 |
| 22 | B | 611 | CLA | O2D-CGD-O1D | -4.36 | 115.31 | 123.84 |
| 22 | b | 614 | CLA | CHD-C1D-ND | -4.35 | 120.46 | 124.45 |
| 22 | c | 507 | CLA | CMB-C2B-C1B | -4.34 | 121.79 | 128.46 |
| 22 | b | 611 | CLA | O2D-CGD-O1D | -4.34 | 115.35 | 123.84 |
| 23 | a | 404 | PHO | CMB-C2B-C3B | 4.33 | 132.79 | 124.68 |
| 22 | C | 510 | CLA | C4A-NA-C1A | 4.32 | 108.65 | 106.71 |
| 22 | c | 514 | CLA | CMB-C2B-C1B | -4.31 | 121.83 | 128.46 |
| 22 | B | 613 | CLA | C1-C2-C3 | -4.31 | 118.59 | 126.04 |
| 28 | f | 102 | SQD | O6-C1-C2 | 4.31 | 115.03 | 108.30 |
| 22 | b | 616 | CLA | O1D-CGD-CBD | 4.30 | 133.28 | 124.48 |
| 28 | B | 622 | SQD | O47-C7-C8 | 4.28 | 120.73 | 111.50 |
| 22 | C | 506 | CLA | CMB-C2B-C1B | -4.26 | 121.91 | 128.46 |
| 22 | c | 506 | CLA | O2D-CGD-O1D | -4.26 | 115.51 | 123.84 |
| 22 | A | 405 | CLA | CMB-C2B-C1B | -4.25 | 121.94 | 128.46 |
| 22 | b | 603 | CLA | O2D-CGD-O1D | -4.24 | 115.54 | 123.84 |
| 33 | E | 101 | LHG | O4-P-O5 | 4.24 | 133.19 | 112.24 |
| 22 | B | 605 | CLA | O2D-CGD-O1D | -4.24 | 115.55 | 123.84 |
| 28 | A | 411 | SQD | C1-C2-C3 | -4.22 | 101.21 | 110.00 |
| 22 | B | 608 | CLA | CHD-C1D-ND | -4.22 | 120.58 | 124.45 |
| 29 | A | 413 | DGD | O3G-C3G-C2G | -4.19 | 100.79 | 110.90 |
| 22 | B | 610 | CLA | C4A-NA-C1A | 4.16 | 108.58 | 106.71 |
| 22 | c | 509 | CLA | CHD-C1D-ND | -4.16 | 120.63 | 124.45 |
| 22 | B | 611 | CLA | O2D-CGD-CBD | 4.16 | 118.66 | 111.27 |
| 22 | B | 602 | CLA | O2D-CGD-CBD | 4.16 | 118.66 | 111.27 |
| 33 | D | 410 | LHG | O4-P-O5 | 4.16 | 132.79 | 112.24 |
| 32 | d | 402 | BCT | O2-C-O1 | 4.15 | 130.32 | 119.55 |
| 22 | C | 509 | CLA | CMB-C2B-C1B | -4.15 | 122.09 | 128.46 |
| 22 | B | 612 | CLA | C11-C12-C13 | -4.12 | 102.61 | 115.92 |
| 24 | T | 101 | BCR | C7-C8-C9 | -4.12 | 120.02 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | b | 623 | LMG | C1-O6-C5 | -4.11 | 105.62 | 113.69 |
| 22 | d | 403 | CLA | CMB-C2B-C1B | -4.10 | 122.16 | 128.46 |
| 22 | A | 403 | CLA | O2D-CGD-O1D | -4.10 | 115.83 | 123.84 |
| 22 | C | 510 | CLA | CMB-C2B-C3B | 4.10 | 132.34 | 124.68 |
| 29 | c | 519 | DGD | O3G-C3G-C2G | -4.09 | 101.03 | 110.90 |
| 33 | e | 101 | LHG | O4-P-O5 | 4.08 | 132.42 | 112.24 |
| 28 | D | 408 | SQD | O8-S-C6 | 4.08 | 112.24 | 105.74 |
| 28 | f | 102 | SQD | O9-S-O7 | -4.08 | 99.84 | 113.95 |
| 33 | L | 102 | LHG | O4-P-O5 | 4.08 | 132.40 | 112.24 |
| 22 | c | 506 | CLA | C4A-NA-C1A | 4.07 | 108.54 | 106.71 |
| 22 | b | 605 | CLA | O2D-CGD-O1D | -4.07 | 115.88 | 123.84 |
| 22 | A | 402 | CLA | CHB-C4A-NA | 4.06 | 130.13 | 124.51 |
| 33 | d | 407 | LHG | O4-P-O5 | 4.06 | 132.30 | 112.24 |
| 22 | C | 508 | CLA | CMB-C2B-C1B | -4.05 | 122.23 | 128.46 |
| 22 | b | 603 | CLA | CMB-C2B-C1B | -4.04 | 122.26 | 128.46 |
| 22 | A | 405 | CLA | O2D-CGD-O1D | -4.03 | 115.96 | 123.84 |
| 22 | C | 507 | CLA | CMB-C2B-C3B | 4.03 | 132.21 | 124.68 |
| 22 | b | 609 | CLA | CMB-C2B-C1B | -4.01 | 122.29 | 128.46 |
| 22 | b | 611 | CLA | CMB-C2B-C1B | -4.01 | 122.30 | 128.46 |
| 29 | C | 515 | DGD | O6D-C1D-O3G | -4.00 | 100.50 | 109.97 |
| 28 | A | 412 | SQD | O47-C7-C8 | 4.00 | 120.11 | 111.50 |
| 22 | D | 403 | CLA | CMB-C2B-C1B | -3.97 | 122.37 | 128.46 |
| 22 | b | 601 | CLA | CHD-C1D-ND | -3.96 | 120.81 | 124.45 |
| 34 | v | 201 | HEC | CBA-CAA-C2A | -3.96 | 105.92 | 112.60 |
| 22 | B | 610 | CLA | O2D-CGD-O1D | -3.96 | 116.10 | 123.84 |
| 22 | d | 403 | CLA | C2D-C1D-ND | -3.96 | 107.19 | 110.10 |
| 22 | b | 612 | CLA | C1B-CHB-C4A | -3.94 | 122.31 | 130.12 |
| 26 | D | 406 | PL9 | C36-C34-C33 | -3.93 | 113.17 | 121.12 |
| 33 | d | 408 | LHG | O4-P-O5 | 3.93 | 131.66 | 112.24 |
| 22 | H | 101 | CLA | CAA-CBA-CGA | -3.93 | 101.78 | 113.25 |
| 28 | B | 622 | SQD | O8-S-C6 | 3.92 | 111.98 | 105.74 |
| 28 | B | 622 | SQD | C1-O5-C5 | -3.92 | 106.00 | 113.69 |
| 28 | a | 412 | SQD | O48-C23-C24 | 3.91 | 124.18 | 111.91 |
| 22 | B | 603 | CLA | C2D-C1D-ND | -3.91 | 107.22 | 110.10 |
| 22 | C | 510 | CLA | CMB-C2B-C1B | -3.90 | 122.47 | 128.46 |
| 22 | b | 611 | CLA | C2D-C1D-ND | -3.89 | 107.23 | 110.10 |
| 22 | C | 503 | CLA | O2A-C1-C2 | -3.89 | 98.41 | 108.64 |
| 22 | C | 505 | CLA | CMB-C2B-C1B | -3.89 | 122.49 | 128.46 |
| 28 | B | 622 | SQD | O5-C5-C4 | 3.88 | 116.75 | 109.69 |
| 31 | B | 625 | STE | C3-C2-C1 | -3.88 | 104.68 | 114.47 |
| 29 | C | 515 | DGD | O3G-C3G-C2G | -3.88 | 101.54 | 110.90 |
| 22 | b | 607 | CLA | CMB-C2B-C1B | -3.86 | 122.54 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | c | 508 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 28 | a | 411 | SQD | C1-O5-C5 | -3.84 | 106.14 | 113.69 |
| 22 | b | 602 | CLA | O2D-CGD-CBD | 3.84 | 118.10 | 111.27 |
| 26 | d | 406 | PL9 | C41-C39-C38 | -3.84 | 113.34 | 121.12 |
| 22 | B | 608 | CLA | O2D-CGD-O1D | -3.84 | 116.33 | 123.84 |
| 24 | B | 619 | BCR | C2-C1-C6 | 3.84 | 116.39 | 110.48 |
| 22 | C | 507 | CLA | CHD-C1D-ND | -3.84 | 120.93 | 124.45 |
| 33 | d | 407 | LHG | O8-C23-C24 | 3.83 | 123.94 | 111.91 |
| 22 | c | 510 | CLA | CHB-C4A-NA | 3.83 | 129.81 | 124.51 |
| 22 | d | 404 | CLA | CMB-C2B-C1B | -3.83 | 122.58 | 128.46 |
| 22 | C | 504 | CLA | CMB-C2B-C1B | -3.82 | 122.60 | 128.46 |
| 33 | d | 409 | LHG | O4-P-O5 | 3.81 | 131.08 | 112.24 |
| 26 | a | 409 | PL9 | C7-C3-C2 | -3.81 | 118.29 | 123.30 |
| 22 | c | 511 | CLA | CMB-C2B-C1B | -3.81 | 122.61 | 128.46 |
| 22 | b | 603 | CLA | CHD-C1D-ND | -3.80 | 120.96 | 124.45 |
| 26 | d | 406 | PL9 | C22-C23-C24 | -3.80 | 118.51 | 127.66 |
| 29 | c | 517 | DGD | O3G-C3G-C2G | -3.78 | 101.77 | 110.90 |
| 24 | b | 618 | BCR | C35-C13-C14 | -3.78 | 117.62 | 122.92 |
| 28 | L | 101 | SQD | O2-C2-C1 | 3.78 | 119.22 | 110.05 |
| 34 | V | 201 | HEC | CBD-CAD-C3D | -3.77 | 106.18 | 112.62 |
| 28 | A | 411 | SQD | O8-S-C6 | 3.77 | 111.75 | 105.74 |
| 33 | l | 101 | LHG | O4-P-O5 | 3.76 | 130.85 | 112.24 |
| 22 | B | 612 | CLA | C4A-NA-C1A | 3.76 | 108.40 | 106.71 |
| 22 | c | 510 | CLA | CHD-C1D-ND | -3.76 | 121.00 | 124.45 |
| 22 | b | 605 | CLA | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 22 | b | 612 | CLA | CMB-C2B-C3B | 3.76 | 131.71 | 124.68 |
| 22 | c | 503 | CLA | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 22 | C | 508 | CLA | CHD-C1D-ND | -3.75 | 121.01 | 124.45 |
| 33 | D | 409 | LHG | O4-P-O5 | 3.75 | 130.76 | 112.24 |
| 28 | f | 102 | SQD | O5-C5-C4 | 3.74 | 116.48 | 109.69 |
| 24 | K | 101 | BCR | C15-C16-C17 | -3.73 | 115.83 | 123.47 |
| 28 | a | 411 | SQD | O9-S-O7 | -3.73 | 101.05 | 113.95 |
| 22 | B | 605 | CLA | CHD-C1D-ND | -3.73 | 121.03 | 124.45 |
| 23 | d | 401 | PHO | CMC-C2C-C3C | 3.72 | 131.96 | 124.94 |
| 33 | d | 407 | LHG | O8-C23-O10 | -3.72 | 114.19 | 123.59 |
| 26 | d | 406 | PL9 | C7-C3-C2 | -3.72 | 118.41 | 123.30 |
| 22 | C | 512 | CLA | CHB-C4A-NA | 3.72 | 129.66 | 124.51 |
| 22 | c | 508 | CLA | CMB-C2B-C3B | 3.72 | 131.64 | 124.68 |
| 33 | D | 412 | LHG | O4-P-O5 | 3.72 | 130.63 | 112.24 |
| 22 | D | 404 | CLA | CHB-C4A-NA | 3.71 | 129.65 | 124.51 |
| 22 | a | 405 | CLA | CMB-C2B-C1B | -3.71 | 122.76 | 128.46 |
| 22 | b | 614 | CLA | CMB-C2B-C3B | 3.71 | 131.62 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 606 | CLA | CMB-C2B-C1B | -3.71 | 122.77 | 128.46 |
| 24 | b | 617 | BCR | C2-C1-C6 | 3.70 | 116.17 | 110.48 |
| 27 | a | 415 | LMG | O6-C1-C2 | -3.69 | 102.55 | 110.35 |
| 22 | c | 506 | CLA | CMB-C2B-C1B | -3.68 | 122.81 | 128.46 |
| 22 | C | 501 | CLA | O2D-CGD-O1D | -3.68 | 116.65 | 123.84 |
| 22 | d | 404 | CLA | CMB-C2B-C3B | 3.67 | 131.55 | 124.68 |
| 22 | b | 603 | CLA | C1B-CHB-C4A | -3.67 | 122.85 | 130.12 |
| 32 | D | 402 | BCT | O2-C-O1 | 3.66 | 129.05 | 119.55 |
| 22 | c | 514 | CLA | CMB-C2B-C3B | 3.66 | 131.52 | 124.68 |
| 22 | c | 507 | CLA | CMB-C2B-C3B | 3.66 | 131.52 | 124.68 |
| 22 | B | 610 | CLA | C1B-CHB-C4A | -3.65 | 122.88 | 130.12 |
| 28 | a | 411 | SQD | C1-C2-C3 | -3.65 | 102.39 | 110.00 |
| 23 | d | 401 | PHO | O2D-CGD-O1D | -3.65 | 116.69 | 123.84 |
| 22 | B | 607 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 22 | C | 503 | CLA | C7-C6-C5 | -3.65 | 103.45 | 113.36 |
| 22 | b | 607 | CLA | C4A-NA-C1A | 3.64 | 108.34 | 106.71 |
| 31 | b | 624 | STE | C3-C2-C1 | -3.64 | 105.30 | 114.47 |
| 29 | c | 518 | DGD | O3G-C3G-C2G | -3.64 | 102.12 | 110.90 |
| 22 | a | 402 | CLA | CMB-C2B-C3B | 3.63 | 131.47 | 124.68 |
| 28 | L | 101 | SQD | O48-C23-C24 | 3.62 | 123.26 | 111.91 |
| 22 | b | 614 | CLA | CMB-C2B-C1B | -3.61 | 122.92 | 128.46 |
| 28 | a | 411 | SQD | O47-C7-O49 | -3.61 | 114.99 | 123.70 |
| 22 | B | 604 | CLA | CMB-C2B-C3B | 3.60 | 131.41 | 124.68 |
| 24 | b | 618 | BCR | C36-C18-C17 | -3.59 | 117.89 | 122.92 |
| 22 | B | 613 | CLA | C4-C3-C5 | 3.59 | 121.31 | 115.27 |
| 22 | C | 513 | CLA | O2D-CGD-O1D | -3.58 | 116.84 | 123.84 |
| 34 | F | 102 | HEC | C1D-C2D-C3D | 3.58 | 109.49 | 107.00 |
| 23 | A | 404 | PHO | CMB-C2B-C3B | 3.58 | 131.38 | 124.68 |
| 28 | a | 411 | SQD | O7-S-C6 | 3.58 | 111.19 | 106.94 |
| 22 | b | 613 | CLA | CMB-C2B-C3B | 3.58 | 131.37 | 124.68 |
| 28 | B | 622 | SQD | C3-C4-C5 | 3.58 | 116.62 | 110.24 |
| 22 | C | 509 | CLA | CMB-C2B-C3B | 3.57 | 131.37 | 124.68 |
| 22 | A | 403 | CLA | CMB-C2B-C1B | -3.57 | 122.97 | 128.46 |
| 22 | b | 608 | CLA | CMB-C2B-C1B | -3.56 | 122.99 | 128.46 |
| 22 | c | 509 | CLA | CHB-C4A-NA | 3.56 | 129.44 | 124.51 |
| 22 | A | 405 | CLA | CMB-C2B-C3B | 3.55 | 131.32 | 124.68 |
| 22 | b | 601 | CLA | O2D-CGD-O1D | -3.55 | 116.90 | 123.84 |
| 22 | c | 510 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 22 | B | 602 | CLA | CHB-C4A-NA | 3.54 | 129.41 | 124.51 |
| 22 | b | 606 | CLA | O2D-CGD-CBD | 3.53 | 117.55 | 111.27 |
| 22 | B | 611 | CLA | CHD-C1D-ND | -3.53 | 121.21 | 124.45 |
| 24 | A | 406 | BCR | C27-C26-C25 | 3.52 | 127.84 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | b | 605 | CLA | C1-C2-C3 | -3.52 | 119.96 | 126.04 |
| 22 | b | 607 | CLA | C4-C3-C5 | 3.52 | 121.19 | 115.27 |
| 22 | C | 504 | CLA | C4A-NA-C1A | 3.51 | 108.29 | 106.71 |
| 22 | b | 614 | CLA | C1B-CHB-C4A | -3.50 | 123.18 | 130.12 |
| 22 | c | 502 | CLA | CMB-C2B-C1B | -3.50 | 123.08 | 128.46 |
| 22 | A | 403 | CLA | CHD-C1D-ND | -3.50 | 121.24 | 124.45 |
| 22 | C | 509 | CLA | C4A-NA-C1A | 3.50 | 108.28 | 106.71 |
| 22 | C | 512 | CLA | CMB-C2B-C1B | -3.50 | 123.09 | 128.46 |
| 22 | H | 101 | CLA | O2D-CGD-O1D | -3.49 | 117.02 | 123.84 |
| 24 | K | 101 | BCR | C2-C1-C6 | 3.49 | 115.85 | 110.48 |
| 34 | f | 101 | HEC | CBA-CAA-C2A | -3.49 | 106.73 | 112.60 |
| 22 | b | 603 | CLA | O2D-CGD-CBD | 3.48 | 117.46 | 111.27 |
| 22 | a | 410 | CLA | CHD-C1D-ND | -3.48 | 121.25 | 124.45 |
| 28 | A | 411 | SQD | C1-O5-C5 | -3.48 | 106.85 | 113.69 |
| 22 | C | 507 | CLA | O2D-CGD-O1D | -3.48 | 117.03 | 123.84 |
| 22 | c | 510 | CLA | O2A-CGA-O1A | -3.48 | 114.81 | 123.59 |
| 22 | B | 610 | CLA | CHD-C1D-ND | -3.47 | 121.26 | 124.45 |
| 22 | c | 514 | CLA | CHD-C1D-ND | -3.47 | 121.26 | 124.45 |
| 34 | V | 201 | HEC | CMC-C2C-C1C | -3.46 | 123.14 | 128.46 |
| 22 | B | 608 | CLA | O2D-CGD-CBD | 3.46 | 117.41 | 111.27 |
| 22 | b | 607 | CLA | C6-C7-C8 | -3.45 | 104.75 | 115.92 |
| 26 | A | 409 | PL9 | C35-C34-C36 | 3.45 | 121.07 | 115.27 |
| 22 | b | 616 | CLA | CHD-C1D-ND | -3.45 | 121.29 | 124.45 |
| 22 | c | 513 | CLA | CMB-C2B-C1B | -3.45 | 123.17 | 128.46 |
| 28 | L | 101 | SQD | O9-S-O7 | -3.44 | 102.03 | 113.95 |
| 22 | C | 501 | CLA | O2D-CGD-CBD | 3.44 | 117.38 | 111.27 |
| 26 | D | 406 | PL9 | C50-C49-C48 | -3.44 | 112.71 | 122.65 |
| 22 | C | 513 | CLA | CMB-C2B-C1B | -3.44 | 123.18 | 128.46 |
| 24 | K | 101 | BCR | C11-C10-C9 | -3.44 | 122.41 | 127.31 |
| 31 | C | 520 | STE | C3-C2-C1 | -3.44 | 105.81 | 114.47 |
| 22 | B | 614 | CLA | CMB-C2B-C1B | -3.43 | 123.19 | 128.46 |
| 22 | b | 616 | CLA | CHB-C4A-NA | 3.43 | 129.26 | 124.51 |
| 28 | A | 411 | SQD | O47-C7-C8 | 3.43 | 118.90 | 111.50 |
| 22 | b | 610 | CLA | O2D-CGD-O1D | -3.43 | 117.13 | 123.84 |
| 22 | c | 510 | CLA | O2D-CGD-O1D | -3.43 | 117.13 | 123.84 |
| 22 | C | 513 | CLA | CHD-C1D-ND | -3.43 | 121.30 | 124.45 |
| 22 | B | 603 | CLA | CHD-C1D-ND | -3.43 | 121.31 | 124.45 |
| 22 | c | 511 | CLA | O2D-CGD-O1D | -3.42 | 117.14 | 123.84 |
| 24 | F | 101 | BCR | C28-C27-C26 | -3.42 | 107.97 | 114.08 |
| 22 | B | 613 | CLA | CMB-C2B-C1B | -3.42 | 123.20 | 128.46 |
| 22 | b | 612 | CLA | C11-C12-C13 | -3.42 | 104.87 | 115.92 |
| 26 | d | 406 | PL9 | C36-C34-C33 | -3.42 | 114.20 | 121.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | b | 611 | CLA | O2D-CGD-CBD | 3.42 | 117.34 | 111.27 |
| 22 | B | 606 | CLA | O2A-CGA-O1A | -3.41 | 114.98 | 123.59 |
| 22 | b | 611 | CLA | C1D-ND-C4D | 3.41 | 108.75 | 106.33 |
| 29 | C | 516 | DGD | O2D-C2D-C1D | -3.40 | 101.78 | 110.05 |
| 22 | b | 610 | CLA | C4A-NA-C1A | 3.40 | 108.23 | 106.71 |
| 22 | c | 514 | CLA | O2D-CGD-O1D | -3.39 | 117.20 | 123.84 |
| 22 | a | 410 | CLA | CHB-C4A-NA | 3.38 | 129.19 | 124.51 |
| 26 | d | 406 | PL9 | C35-C34-C36 | 3.38 | 120.96 | 115.27 |
| 22 | B | 602 | CLA | CMB-C2B-C3B | 3.37 | 130.98 | 124.68 |
| 22 | B | 614 | CLA | O2D-CGD-O1D | -3.37 | 117.25 | 123.84 |
| 22 | B | 615 | CLA | O2D-CGD-CBD | 3.37 | 117.25 | 111.27 |
| 24 | t | 101 | BCR | C7-C8-C9 | -3.36 | 121.15 | 126.23 |
| 22 | d | 404 | CLA | CHD-C1D-ND | -3.36 | 121.36 | 124.45 |
| 22 | C | 508 | CLA | CMB-C2B-C3B | 3.36 | 130.97 | 124.68 |
| 24 | b | 619 | BCR | C29-C30-C25 | 3.36 | 115.66 | 110.48 |
| 22 | C | 512 | CLA | C4A-NA-C1A | 3.36 | 108.22 | 106.71 |
| 22 | D | 403 | CLA | C6-C5-C3 | 3.36 | 122.27 | 113.45 |
| 22 | D | 405 | CLA | O2D-CGD-O1D | -3.36 | 117.27 | 123.84 |
| 22 | c | 508 | CLA | CHD-C1D-ND | -3.35 | 121.37 | 124.45 |
| 22 | c | 510 | CLA | CMB-C2B-C3B | 3.35 | 130.95 | 124.68 |
| 22 | b | 603 | CLA | CMB-C2B-C3B | 3.34 | 130.93 | 124.68 |
| 22 | b | 615 | CLA | CMB-C2B-C3B | 3.34 | 130.92 | 124.68 |
| 22 | d | 403 | CLA | CMB-C2B-C3B | 3.34 | 130.92 | 124.68 |
| 29 | H | 103 | DGD | O2D-C2D-C1D | -3.33 | 101.97 | 110.05 |
| 24 | K | 101 | BCR | C33-C5-C6 | -3.32 | 120.80 | 124.53 |
| 22 | c | 503 | CLA | CMB-C2B-C3B | 3.32 | 130.89 | 124.68 |
| 26 | D | 406 | PL9 | C22-C23-C24 | -3.32 | 119.67 | 127.66 |
| 22 | C | 501 | CLA | CHD-C1D-ND | -3.32 | 121.41 | 124.45 |
| 24 | B | 617 | BCR | C2-C1-C6 | 3.31 | 115.58 | 110.48 |
| 23 | a | 404 | PHO | C1-C2-C3 | -3.31 | 120.32 | 126.04 |
| 22 | B | 615 | CLA | C2D-C1D-ND | -3.31 | 107.67 | 110.10 |
| 27 | b | 621 | LMG | O3-C3-C2 | -3.31 | 102.71 | 110.35 |
| 22 | H | 101 | CLA | O2D-CGD-CBD | 3.30 | 117.14 | 111.27 |
| 22 | B | 606 | CLA | C1B-CHB-C4A | -3.30 | 123.58 | 130.12 |
| 22 | C | 507 | CLA | O2D-CGD-CBD | 3.30 | 117.13 | 111.27 |
| 22 | b | 616 | CLA | C1B-CHB-C4A | -3.28 | 123.61 | 130.12 |
| 24 | B | 618 | BCR | C29-C30-C25 | 3.28 | 115.53 | 110.48 |
| 22 | B | 615 | CLA | CHB-C4A-NA | 3.28 | 129.04 | 124.51 |
| 22 | b | 606 | CLA | CMB-C2B-C1B | -3.27 | 123.43 | 128.46 |
| 22 | C | 506 | CLA | O2D-CGD-O1D | -3.26 | 117.45 | 123.84 |
| 22 | c | 513 | CLA | O2D-CGD-O1D | -3.26 | 117.46 | 123.84 |
| 22 | C | 506 | CLA | CMB-C2B-C3B | 3.25 | 130.76 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 611 | CLA | C14-C13-C15 | -3.25 | 99.53 | 111.29 |
| 22 | D | 403 | CLA | C1B-CHB-C4A | -3.23 | 123.72 | 130.12 |
| 28 | L | 101 | SQD | O9-S-C6 | 3.23 | 110.77 | 106.94 |
| 22 | D | 403 | CLA | CHB-C4A-NA | 3.23 | 128.97 | 124.51 |
| 22 | A | 405 | CLA | C4-C3-C5 | 3.22 | 120.68 | 115.27 |
| 22 | a | 405 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 29 | c | 517 | DGD | C3D-C4D-C5D | -3.20 | 104.52 | 110.24 |
| 29 | C | 516 | DGD | O5D-C6D-C5D | -3.20 | 103.12 | 109.05 |
| 22 | c | 508 | CLA | C1B-CHB-C4A | -3.20 | 123.78 | 130.12 |
| 26 | A | 409 | PL9 | C36-C34-C33 | -3.19 | 114.65 | 121.12 |
| 27 | M | 101 | LMG | O6-C1-O1 | -3.19 | 102.41 | 109.97 |
| 22 | c | 509 | CLA | O2D-CGD-O1D | -3.19 | 117.60 | 123.84 |
| 22 | B | 614 | CLA | C1B-CHB-C4A | -3.18 | 123.83 | 130.12 |
| 22 | b | 605 | CLA | CHD-C1D-ND | -3.17 | 121.54 | 124.45 |
| 22 | a | 410 | CLA | CMB-C2B-C1B | -3.17 | 123.59 | 128.46 |
| 22 | D | 403 | CLA | CMB-C2B-C3B | 3.17 | 130.61 | 124.68 |
| 33 | D | 412 | LHG | O8-C23-O10 | -3.17 | 115.59 | 123.59 |
| 22 | a | 405 | CLA | CHB-C4A-NA | 3.17 | 128.89 | 124.51 |
| 31 | j | 101 | STE | O2-C1-O1 | -3.17 | 115.41 | 123.30 |
| 22 | b | 612 | CLA | CHB-C4A-NA | 3.16 | 128.89 | 124.51 |
| 29 | C | 517 | DGD | O3E-C3E-C2E | -3.16 | 103.04 | 110.35 |
| 22 | D | 405 | CLA | C4A-NA-C1A | 3.16 | 108.13 | 106.71 |
| 22 | b | 601 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 22 | C | 505 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 22 | A | 405 | CLA | C1B-CHB-C4A | -3.15 | 123.87 | 130.12 |
| 29 | C | 517 | DGD | O6D-C1D-O3G | -3.15 | 102.52 | 109.97 |
| 24 | h | 101 | BCR | C27-C26-C25 | 3.14 | 127.30 | 122.73 |
| 22 | B | 610 | CLA | CHB-C4A-NA | 3.14 | 128.86 | 124.51 |
| 22 | B | 604 | CLA | C1-C2-C3 | -3.14 | 120.61 | 126.04 |
| 26 | A | 409 | PL9 | C7-C3-C2 | -3.14 | 119.17 | 123.30 |
| 22 | a | 405 | CLA | O2D-CGD-O1D | -3.14 | 117.70 | 123.84 |
| 22 | C | 505 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 29 | h | 102 | DGD | C3D-C4D-C5D | -3.14 | 104.65 | 110.24 |
| 22 | C | 506 | CLA | O1D-CGD-CBD | 3.14 | 130.90 | 124.48 |
| 29 | A | 413 | DGD | C4E-C3E-C2E | -3.13 | 105.35 | 110.82 |
| 29 | h | 102 | DGD | O3G-C3G-C2G | -3.13 | 103.35 | 110.90 |
| 22 | B | 616 | CLA | CMB-C2B-C1B | -3.12 | 123.66 | 128.46 |
| 22 | c | 504 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 22 | b | 606 | CLA | O2D-CGD-O1D | -3.12 | 117.74 | 123.84 |
| 28 | B | 622 | SQD | O48-C23-C24 | 3.12 | 121.69 | 111.91 |
| 22 | b | 608 | CLA | CMB-C2B-C3B | 3.12 | 130.51 | 124.68 |
| 31 | a | 414 | STE | C3-C2-C1 | -3.11 | 106.62 | 114.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 602 | CLA | O2D-CGD-O1D | -3.11 | 117.75 | 123.84 |
| 22 | D | 403 | CLA | C4-C3-C5 | 3.10 | 120.48 | 115.27 |
| 33 | D | 412 | LHG | O8-C23-C24 | 3.10 | 121.63 | 111.91 |
| 22 | A | 402 | CLA | CAA-CBA-CGA | -3.10 | 104.20 | 113.25 |
| 34 | v | 201 | HEC | CMC-C2C-C1C | -3.10 | 123.70 | 128.46 |
| 22 | b | 615 | CLA | C1-C2-C3 | 3.09 | 131.40 | 126.04 |
| 22 | B | 605 | CLA | CMB-C2B-C1B | -3.09 | 123.71 | 128.46 |
| 22 | B | 607 | CLA | CMB-C2B-C3B | 3.09 | 130.47 | 124.68 |
| 26 | d | 406 | PL9 | C30-C29-C31 | -3.09 | 110.07 | 115.27 |
| 23 | D | 401 | PHO | CMB-C2B-C3B | 3.09 | 130.46 | 124.68 |
| 29 | A | 413 | DGD | O5E-C6E-C5E | -3.09 | 100.69 | 111.29 |
| 28 | L | 101 | SQD | O47-C7-C8 | 3.09 | 118.16 | 111.50 |
| 22 | b | 612 | CLA | CHD-C1D-ND | -3.08 | 121.62 | 124.45 |
| 24 | c | 516 | BCR | C27-C26-C25 | 3.08 | 127.20 | 122.73 |
| 22 | b | 602 | CLA | CMB-C2B-C1B | -3.08 | 123.73 | 128.46 |
| 26 | D | 406 | PL9 | C37-C38-C39 | -3.08 | 120.25 | 127.66 |
| 22 | c | 513 | CLA | CHB-C4A-NA | 3.08 | 128.77 | 124.51 |
| 24 | B | 619 | BCR | C36-C18-C17 | -3.08 | 118.61 | 122.92 |
| 29 | c | 519 | DGD | C3G-C2G-C1G | -3.07 | 104.52 | 111.79 |
| 29 | A | 413 | DGD | O5D-C6D-C5D | -3.07 | 103.36 | 109.05 |
| 27 | b | 623 | LMG | O2-C2-C1 | -3.07 | 102.58 | 110.05 |
| 26 | D | 406 | PL9 | C35-C34-C36 | 3.07 | 120.44 | 115.27 |
| 27 | D | 407 | LMG | O6-C1-O1 | -3.07 | 102.70 | 109.97 |
| 22 | c | 513 | CLA | CMB-C2B-C3B | 3.07 | 130.42 | 124.68 |
| 22 | C | 503 | CLA | CHD-C1D-ND | -3.06 | 121.64 | 124.45 |
| 22 | c | 504 | CLA | C7-C6-C5 | -3.06 | 105.06 | 113.36 |
| 22 | A | 403 | CLA | CMB-C2B-C3B | 3.06 | 130.40 | 124.68 |
| 22 | b | 605 | CLA | CMB-C2B-C3B | 3.06 | 130.39 | 124.68 |
| 22 | C | 502 | CLA | CMB-C2B-C1B | -3.05 | 123.77 | 128.46 |
| 22 | C | 508 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 22 | C | 512 | CLA | CMB-C2B-C3B | 3.05 | 130.38 | 124.68 |
| 22 | c | 511 | CLA | C6-C5-C3 | -3.05 | 105.46 | 113.45 |
| 29 | C | 515 | DGD | O5D-C6D-C5D | -3.05 | 103.40 | 109.05 |
| 29 | C | 516 | DGD | O6E-C1E-O5D | -3.05 | 102.76 | 109.97 |
| 24 | d | 405 | BCR | C38-C26-C25 | -3.05 | 121.11 | 124.53 |
| 22 | b | 614 | CLA | O2A-CGA-O1A | -3.05 | 115.91 | 123.59 |
| 22 | C | 509 | CLA | C1B-CHB-C4A | -3.04 | 124.09 | 130.12 |
| 31 | J | 101 | STE | C3-C2-C1 | -3.04 | 106.81 | 114.47 |
| 26 | a | 409 | PL9 | C35-C34-C36 | 3.04 | 120.38 | 115.27 |
| 22 | B | 604 | CLA | CHB-C4A-NA | 3.04 | 128.71 | 124.51 |
| 24 | k | 102 | BCR | C2-C1-C6 | 3.04 | 115.15 | 110.48 |
| 22 | a | 403 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | a | 405 | CLA | O2D-CGD-CBD | 3.03 | 116.66 | 111.27 |
| 24 | F | 101 | BCR | C7-C8-C9 | -3.02 | 121.67 | 126.23 |
| 22 | C | 513 | CLA | CMB-C2B-C3B | 3.02 | 130.33 | 124.68 |
| 22 | B | 614 | CLA | CMB-C2B-C3B | 3.02 | 130.33 | 124.68 |
| 22 | c | 504 | CLA | C5-C3-C2 | -3.02 | 115.01 | 121.12 |
| 22 | C | 509 | CLA | C1-C2-C3 | -3.02 | 120.83 | 126.04 |
| 22 | b | 611 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |
| 29 | C | 517 | DGD | O6D-C5D-C6D | -3.02 | 100.58 | 106.67 |
| 22 | b | 602 | CLA | C1B-CHB-C4A | -3.01 | 124.16 | 130.12 |
| 22 | C | 504 | CLA | O2A-CGA-O1A | -3.00 | 116.01 | 123.59 |
| 24 | T | 101 | BCR | C27-C26-C25 | 3.00 | 127.09 | 122.73 |
| 22 | B | 612 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 27 | d | 410 | LMG | O6-C1-O1 | -3.00 | 102.87 | 109.97 |
| 22 | B | 604 | CLA | C11-C10-C8 | -3.00 | 106.23 | 115.92 |
| 29 | c | 519 | DGD | C3D-C4D-C5D | -2.99 | 104.90 | 110.24 |
| 27 | a | 415 | LMG | C9-C8-C7 | -2.99 | 104.72 | 111.79 |
| 22 | b | 602 | CLA | C2D-C1D-ND | -2.99 | 107.90 | 110.10 |
| 22 | b | 606 | CLA | CHB-C4A-NA | 2.99 | 128.64 | 124.51 |
| 22 | C | 504 | CLA | CHD-C1D-ND | -2.99 | 121.71 | 124.45 |
| 22 | b | 603 | CLA | C4D-CHA-C1A | 2.99 | 124.88 | 121.25 |
| 22 | c | 511 | CLA | CHB-C4A-NA | 2.98 | 128.64 | 124.51 |
| 27 | c | 523 | LMG | O6-C1-O1 | -2.98 | 102.91 | 109.97 |
| 22 | b | 609 | CLA | CMB-C2B-C3B | 2.98 | 130.26 | 124.68 |
| 22 | D | 404 | CLA | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 28 | a | 411 | SQD | O5-C1-C2 | -2.97 | 104.06 | 110.35 |
| 27 | Y | 101 | LMG | O1-C1-C2 | -2.97 | 103.67 | 108.30 |
| 22 | C | 512 | CLA | O2D-CGD-CBD | 2.97 | 116.54 | 111.27 |
| 29 | h | 102 | DGD | O6E-C5E-C4E | 2.97 | 115.08 | 109.69 |
| 22 | c | 506 | CLA | C6-C7-C8 | -2.96 | 106.35 | 115.92 |
| 27 | a | 415 | LMG | O6-C5-C4 | 2.96 | 115.06 | 109.69 |
| 22 | B | 607 | CLA | CED-O2D-CGD | 2.96 | 122.62 | 115.94 |
| 22 | b | 613 | CLA | CAC-C3C-C4C | 2.95 | 128.64 | 124.81 |
| 22 | b | 605 | CLA | C4-C3-C5 | 2.95 | 120.24 | 115.27 |
| 24 | B | 617 | BCR | C3-C4-C5 | -2.95 | 108.81 | 114.08 |
| 24 | c | 515 | BCR | C24-C23-C22 | -2.95 | 121.78 | 126.23 |
| 27 | b | 623 | LMG | C8-O7-C10 | 2.95 | 125.04 | 117.79 |
| 24 | b | 617 | BCR | C29-C30-C25 | 2.95 | 115.02 | 110.48 |
| 22 | B | 605 | CLA | O1D-CGD-CBD | 2.94 | 130.50 | 124.48 |
| 22 | c | 506 | CLA | CMB-C2B-C3B | 2.94 | 130.18 | 124.68 |
| 22 | B | 602 | CLA | C1B-CHB-C4A | -2.94 | 124.29 | 130.12 |
| 24 | F | 101 | BCR | C24-C23-C22 | -2.94 | 121.79 | 126.23 |
| 22 | b | 610 | CLA | C1B-CHB-C4A | -2.94 | 124.29 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | L | 101 | SQD | O5-C1-C2 | -2.94 | 104.13 | 110.35 |
| 27 | c | 520 | LMG | O3-C3-C2 | -2.94 | 103.56 | 110.35 |
| 27 | b | 621 | LMG | O1-C1-C2 | -2.93 | 103.72 | 108.30 |
| 22 | C | 504 | CLA | O2D-CGD-O1D | -2.93 | 118.11 | 123.84 |
| 22 | B | 613 | CLA | CHA-C1A-NA | -2.93 | 119.69 | 126.40 |
| 26 | D | 406 | PL9 | C31-C32-C33 | -2.93 | 102.25 | 111.88 |
| 29 | A | 413 | DGD | O6E-C5E-C4E | 2.93 | 115.02 | 109.69 |
| 26 | A | 409 | PL9 | C22-C23-C24 | -2.93 | 120.61 | 127.66 |
| 27 | M | 101 | LMG | C1-O6-C5 | -2.92 | 107.96 | 113.69 |
| 22 | A | 403 | CLA | C1B-CHB-C4A | -2.92 | 124.33 | 130.12 |
| 22 | b | 609 | CLA | C4A-NA-C1A | 2.92 | 108.02 | 106.71 |
| 22 | d | 404 | CLA | C1B-CHB-C4A | -2.92 | 124.34 | 130.12 |
| 22 | B | 611 | CLA | C1C-C2C-C3C | -2.91 | 103.89 | 106.96 |
| 22 | b | 602 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 22 | C | 501 | CLA | O2A-CGA-O1A | -2.91 | 116.26 | 123.59 |
| 29 | c | 517 | DGD | CBB-CAB-C9B | -2.90 | 99.68 | 114.42 |
| 28 | f | 102 | SQD | O47-C7-C8 | 2.90 | 118.90 | 110.80 |
| 22 | C | 507 | CLA | C4-C3-C5 | 2.90 | 120.15 | 115.27 |
| 22 | B | 613 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 28 | L | 101 | SQD | C3-C4-C5 | 2.90 | 115.41 | 110.24 |
| 28 | A | 412 | SQD | O48-C23-C24 | 2.90 | 121.00 | 111.91 |
| 23 | D | 401 | PHO | C1-C2-C3 | -2.90 | 121.03 | 126.04 |
| 22 | B | 611 | CLA | CMB-C2B-C1B | -2.89 | 124.02 | 128.46 |
| 22 | b | 601 | CLA | CMB-C2B-C3B | 2.89 | 130.09 | 124.68 |
| 22 | B | 612 | CLA | C16-C15-C13 | -2.89 | 106.57 | 115.92 |
| 22 | B | 606 | CLA | CGD-CBD-CAD | -2.89 | 101.37 | 110.73 |
| 22 | b | 610 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 24 | A | 406 | BCR | C37-C22-C21 | -2.89 | 118.88 | 122.92 |
| 22 | b | 614 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 28 | a | 411 | SQD | O48-C23-C24 | 2.88 | 120.96 | 111.91 |
| 28 | a | 411 | SQD | O2-C2-C1 | 2.88 | 117.05 | 110.05 |
| 22 | b | 611 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 22 | B | 608 | CLA | C6-C7-C8 | -2.88 | 106.61 | 115.92 |
| 31 | B | 623 | STE | C3-C2-C1 | -2.88 | 107.21 | 114.47 |
| 22 | c | 503 | CLA | CHD-C1D-ND | -2.87 | 121.81 | 124.45 |
| 22 | C | 513 | CLA | O2A-CGA-O1A | -2.87 | 116.34 | 123.59 |
| 34 | F | 102 | HEC | CMD-C2D-C1D | -2.87 | 124.05 | 128.46 |
| 27 | Y | 101 | LMG | O2-C2-C1 | -2.87 | 103.07 | 110.05 |
| 22 | b | 610 | CLA | CAC-C3C-C4C | 2.87 | 128.54 | 124.81 |
| 22 | b | 605 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 27 | A | 410 | LMG | O6-C1-O1 | -2.87 | 103.18 | 109.97 |
| 24 | a | 406 | BCR | C27-C26-C25 | 2.87 | 126.89 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | b | 621 | LMG | O6-C1-O1 | -2.87 | 103.18 | 109.97 |
| 22 | b | 602 | CLA | CHD-C1D-ND | -2.87 | 121.82 | 124.45 |
| 24 | h | 101 | BCR | C35-C13-C14 | -2.87 | 118.91 | 122.92 |
| 27 | A | 410 | LMG | C9-C8-C7 | -2.86 | 105.01 | 111.79 |
| 22 | B | 612 | CLA | CHD-C1D-ND | -2.86 | 121.82 | 124.45 |
| 28 | A | 411 | SQD | O47-C7-O49 | -2.86 | 116.78 | 123.70 |
| 24 | b | 619 | BCR | C16-C15-C14 | -2.86 | 117.61 | 123.47 |
| 32 | d | 402 | BCT | O3-C-O1 | -2.86 | 112.12 | 119.55 |
| 24 | F | 101 | BCR | C2-C1-C6 | 2.86 | 114.89 | 110.48 |
| 31 | j | 101 | STE | O2-C1-C2 | 2.86 | 123.22 | 114.03 |
| 22 | b | 607 | CLA | CMB-C2B-C3B | 2.86 | 130.03 | 124.68 |
| 28 | a | 411 | SQD | O47-C7-C8 | 2.85 | 117.65 | 111.50 |
| 22 | B | 603 | CLA | CHD-C1D-C2D | 2.85 | 131.47 | 125.48 |
| 24 | H | 102 | BCR | C2-C1-C6 | 2.85 | 114.88 | 110.48 |
| 27 | b | 623 | LMG | C3-C4-C5 | -2.85 | 105.15 | 110.24 |
| 22 | B | 609 | CLA | C2C-C1C-NC | 2.85 | 112.64 | 109.97 |
| 24 | B | 618 | BCR | C37-C22-C21 | -2.85 | 118.93 | 122.92 |
| 22 | a | 403 | CLA | CMB-C2B-C1B | -2.85 | 124.08 | 128.46 |
| 22 | c | 507 | CLA | C4-C3-C2 | -2.85 | 116.37 | 123.68 |
| 22 | b | 613 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 22 | d | 403 | CLA | O1D-CGD-CBD | 2.84 | 130.30 | 124.48 |
| 24 | K | 103 | BCR | C15-C16-C17 | -2.84 | 117.66 | 123.47 |
| 29 | c | 519 | DGD | O6D-C1D-O3G | -2.84 | 103.26 | 109.97 |
| 22 | B | 602 | CLA | C1-C2-C3 | -2.83 | 121.14 | 126.04 |
| 22 | c | 503 | CLA | C1-C2-C3 | -2.83 | 121.14 | 126.04 |
| 26 | d | 406 | PL9 | C37-C38-C39 | -2.83 | 120.84 | 127.66 |
| 22 | C | 502 | CLA | CMB-C2B-C3B | 2.83 | 129.98 | 124.68 |
| 22 | c | 502 | CLA | CMB-C2B-C3B | 2.83 | 129.97 | 124.68 |
| 22 | c | 510 | CLA | C1B-CHB-C4A | -2.83 | 124.52 | 130.12 |
| 27 | d | 410 | LMG | O2-C2-C1 | -2.82 | 103.19 | 110.05 |
| 22 | c | 511 | CLA | C4-C3-C5 | 2.82 | 120.02 | 115.27 |
| 22 | c | 512 | CLA | CHD-C1D-ND | -2.82 | 121.87 | 124.45 |
| 22 | B | 603 | CLA | O2D-CGD-O1D | -2.81 | 118.33 | 123.84 |
| 24 | H | 102 | BCR | C38-C26-C25 | -2.81 | 121.37 | 124.53 |
| 29 | H | 103 | DGD | C1D-C2D-C3D | -2.81 | 104.14 | 110.00 |
| 22 | C | 504 | CLA | CMB-C2B-C3B | 2.81 | 129.94 | 124.68 |
| 22 | B | 611 | CLA | CHD-C4C-NC | 2.81 | 128.63 | 124.20 |
| 22 | B | 613 | CLA | CAC-C3C-C4C | 2.81 | 128.46 | 124.81 |
| 31 | m | 102 | STE | O2-C1-C2 | 2.81 | 123.05 | 114.03 |
| 22 | A | 402 | CLA | C6-C5-C3 | 2.81 | 120.82 | 113.45 |
| 24 | H | 102 | BCR | C35-C13-C14 | -2.81 | 118.99 | 122.92 |
| 29 | H | 103 | DGD | C6D-C5D-C4D | 2.80 | 117.95 | 112.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 605 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 26 | a | 409 | PL9 | O2-C1-C2 | -2.80 | 115.36 | 121.78 |
| 22 | c | 507 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 28 | f | 102 | SQD | C1-C2-C3 | -2.80 | 104.16 | 110.00 |
| 22 | C | 501 | CLA | C2D-C1D-ND | -2.80 | 108.04 | 110.10 |
| 24 | t | 101 | BCR | C3-C4-C5 | -2.80 | 109.09 | 114.08 |
| 22 | C | 504 | CLA | C4-C3-C5 | 2.79 | 119.96 | 115.27 |
| 22 | B | 613 | CLA | C2A-C1A-CHA | 2.79 | 128.73 | 123.86 |
| 22 | c | 505 | CLA | O2D-CGD-CBD | 2.79 | 116.22 | 111.27 |
| 28 | D | 408 | SQD | O9-S-O7 | -2.79 | 104.31 | 113.95 |
| 22 | b | 609 | CLA | CHA-C1A-NA | -2.79 | 120.02 | 126.40 |
| 22 | c | 504 | CLA | CMB-C2B-C1B | -2.78 | 124.19 | 128.46 |
| 22 | B | 614 | CLA | C4A-NA-C1A | 2.78 | 107.95 | 106.71 |
| 22 | c | 509 | CLA | O2A-CGA-O1A | -2.77 | 116.59 | 123.59 |
| 22 | b | 610 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 22 | b | 601 | CLA | O2D-CGD-CBD | 2.77 | 116.19 | 111.27 |
| 34 | V | 201 | HEC | CMB-C2B-C1B | -2.77 | 124.21 | 128.46 |
| 22 | B | 605 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 26 | a | 409 | PL9 | C22-C23-C24 | -2.77 | 120.99 | 127.66 |
| 28 | a | 412 | SQD | O48-C23-O10 | -2.77 | 116.61 | 123.59 |
| 22 | b | 602 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 27 | d | 410 | LMG | O1-C1-C2 | -2.76 | 103.99 | 108.30 |
| 28 | L | 101 | SQD | C45-O47-C7 | 2.76 | 124.58 | 117.79 |
| 22 | a | 405 | CLA | C4-C3-C5 | 2.76 | 119.91 | 115.27 |
| 22 | B | 616 | CLA | CMB-C2B-C3B | 2.76 | 129.83 | 124.68 |
| 22 | C | 511 | CLA | CHB-C4A-NA | 2.76 | 128.32 | 124.51 |
| 22 | A | 405 | CLA | O2D-CGD-CBD | 2.75 | 116.15 | 111.27 |
| 22 | B | 610 | CLA | O2D-CGD-CBD | 2.75 | 116.15 | 111.27 |
| 22 | a | 410 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 22 | B | 605 | CLA | C16-C15-C13 | -2.74 | 107.05 | 115.92 |
| 24 | B | 618 | BCR | C2-C1-C6 | 2.74 | 114.70 | 110.48 |
| 22 | B | 609 | CLA | CMC-C2C-C1C | 2.74 | 129.21 | 125.04 |
| 22 | c | 512 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 22 | b | 601 | CLA | CMB-C2B-C1B | -2.74 | 124.26 | 128.46 |
| 22 | b | 616 | CLA | C4-C3-C5 | 2.74 | 119.87 | 115.27 |
| 24 | k | 102 | BCR | C27-C26-C25 | 2.74 | 126.70 | 122.73 |
| 24 | t | 101 | BCR | C2-C1-C6 | 2.73 | 114.68 | 110.48 |
| 22 | D | 403 | CLA | CED-O2D-CGD | 2.72 | 122.10 | 115.94 |
| 22 | a | 403 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 22 | B | 607 | CLA | O2A-CGA-O1A | -2.72 | 116.72 | 123.59 |
| 24 | K | 103 | BCR | C3-C4-C5 | -2.72 | 109.22 | 114.08 |
| 24 | B | 619 | BCR | C29-C30-C25 | 2.72 | 114.67 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | C | 505 | CLA | C1-C2-C3 | -2.72 | 121.34 | 126.04 |
| 27 | M | 101 | LMG | C38-C37-C36 | -2.72 | 100.64 | 114.42 |
| 24 | h | 101 | BCR | C38-C26-C25 | -2.71 | 121.48 | 124.53 |
| 22 | b | 610 | CLA | C6-C5-C3 | 2.71 | 120.56 | 113.45 |
| 26 | D | 406 | PL9 | C7-C3-C2 | -2.71 | 119.74 | 123.30 |
| 22 | D | 404 | CLA | C1B-CHB-C4A | -2.71 | 124.76 | 130.12 |
| 29 | c | 519 | DGD | C1D-C2D-C3D | -2.71 | 104.36 | 110.00 |
| 22 | C | 511 | CLA | CMB-C2B-C1B | -2.71 | 124.31 | 128.46 |
| 22 | a | 403 | CLA | C2D-C1D-ND | -2.70 | 108.11 | 110.10 |
| 28 | L | 101 | SQD | O5-C5-C4 | 2.70 | 114.60 | 109.69 |
| 24 | h | 101 | BCR | C2-C1-C6 | 2.70 | 114.63 | 110.48 |
| 22 | C | 504 | CLA | CED-O2D-CGD | 2.70 | 122.03 | 115.94 |
| 22 | B | 605 | CLA | C4D-CHA-C1A | 2.69 | 124.52 | 121.25 |
| 22 | c | 508 | CLA | C4-C3-C5 | 2.69 | 119.80 | 115.27 |
| 29 | C | 515 | DGD | C2G-O2G-C1B | 2.69 | 124.41 | 117.79 |
| 24 | A | 406 | BCR | C2-C1-C6 | 2.69 | 114.62 | 110.48 |
| 22 | A | 402 | CLA | CHD-C1D-ND | -2.69 | 121.98 | 124.45 |
| 31 | b | 624 | STE | O2-C1-C2 | 2.69 | 122.66 | 114.03 |
| 22 | C | 504 | CLA | O2D-CGD-CBD | 2.68 | 116.04 | 111.27 |
| 22 | a | 403 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 22 | b | 601 | CLA | C1B-CHB-C4A | -2.68 | 124.80 | 130.12 |
| 22 | b | 603 | CLA | CMA-C3A-C4A | 2.68 | 118.98 | 111.77 |
| 26 | d | 406 | PL9 | C20-C19-C21 | 2.68 | 119.78 | 115.27 |
| 22 | b | 609 | CLA | CHD-C1D-ND | -2.68 | 121.99 | 124.45 |
| 29 | c | 517 | DGD | O6D-C1D-O3G | -2.68 | 103.63 | 109.97 |
| 22 | B | 612 | CLA | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 27 | c | 522 | LMG | O7-C10-O9 | -2.68 | 117.23 | 123.70 |
| 22 | a | 410 | CLA | C1B-CHB-C4A | -2.68 | 124.82 | 130.12 |
| 29 | H | 103 | DGD | C3E-C4E-C5E | -2.67 | 105.47 | 110.24 |
| 29 | A | 413 | DGD | C1D-C2D-C3D | -2.67 | 104.43 | 110.00 |
| 29 | H | 103 | DGD | C3D-C4D-C5D | -2.67 | 105.47 | 110.24 |
| 22 | B | 609 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 22 | b | 610 | CLA | O2A-CGA-O1A | -2.67 | 116.85 | 123.59 |
| 22 | B | 605 | CLA | C7-C6-C5 | -2.67 | 106.11 | 113.36 |
| 22 | B | 609 | CLA | CMB-C2B-C3B | 2.66 | 129.66 | 124.68 |
| 22 | b | 609 | CLA | C3C-C4C-NC | -2.66 | 107.59 | 110.57 |
| 22 | B | 611 | CLA | C11-C12-C13 | -2.66 | 107.33 | 115.92 |
| 29 | A | 413 | DGD | C3G-C2G-C1G | -2.66 | 105.50 | 111.79 |
| 24 | A | 406 | BCR | C36-C18-C17 | -2.66 | 119.20 | 122.92 |
| 27 | c | 522 | LMG | O3-C3-C2 | -2.65 | 104.21 | 110.35 |
| 22 | a | 402 | CLA | O2D-CGD-O1D | -2.65 | 118.65 | 123.84 |
| 22 | B | 607 | CLA | CHD-C1D-ND | -2.65 | 122.02 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | H | 102 | BCR | C29-C30-C25 | 2.65 | 114.56 | 110.48 |
| 22 | D | 405 | CLA | C1B-CHB-C4A | -2.65 | 124.87 | 130.12 |
| 24 | a | 406 | BCR | C2-C1-C6 | 2.65 | 114.56 | 110.48 |
| 33 | D | 409 | LHG | O8-C23-O10 | -2.65 | 116.91 | 123.59 |
| 33 | D | 409 | LHG | C18-C17-C16 | -2.65 | 100.99 | 114.42 |
| 22 | b | 607 | CLA | CHD-C1D-ND | -2.65 | 122.02 | 124.45 |
| 24 | t | 101 | BCR | C15-C16-C17 | -2.65 | 118.05 | 123.47 |
| 28 | L | 101 | SQD | O48-C23-O10 | -2.65 | 116.91 | 123.59 |
| 22 | B | 609 | CLA | CMB-C2B-C1B | -2.65 | 124.40 | 128.46 |
| 23 | d | 401 | PHO | C1B-NB-C4B | 2.64 | 112.52 | 107.09 |
| 22 | c | 504 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 29 | c | 518 | DGD | O2G-C1B-O1B | -2.64 | 117.32 | 123.70 |
| 22 | b | 608 | CLA | CHA-C1A-NA | -2.64 | 120.35 | 126.40 |
| 22 | b | 613 | CLA | C7-C6-C5 | -2.64 | 106.19 | 113.36 |
| 24 | B | 618 | BCR | C35-C13-C14 | -2.64 | 119.22 | 122.92 |
| 27 | b | 623 | LMG | C4-C3-C2 | -2.64 | 106.21 | 110.82 |
| 26 | d | 406 | PL9 | C40-C39-C41 | 2.64 | 119.71 | 115.27 |
| 22 | c | 507 | CLA | CHD-C1D-ND | -2.64 | 122.03 | 124.45 |
| 22 | A | 403 | CLA | C4A-NA-C1A | 2.64 | 107.89 | 106.71 |
| 22 | c | 505 | CLA | O2A-CGA-O1A | -2.63 | 116.94 | 123.59 |
| 22 | A | 403 | CLA | O2D-CGD-CBD | 2.63 | 115.95 | 111.27 |
| 27 | Y | 101 | LMG | O1-C7-C8 | -2.63 | 104.54 | 110.90 |
| 26 | D | 406 | PL9 | C30-C29-C31 | -2.63 | 110.85 | 115.27 |
| 28 | A | 412 | SQD | C45-O47-C7 | 2.63 | 121.25 | 117.88 |
| 23 | A | 404 | PHO | C5-C3-C2 | 2.62 | 126.43 | 121.12 |
| 22 | b | 602 | CLA | CED-O2D-CGD | 2.62 | 121.87 | 115.94 |
| 23 | A | 404 | PHO | C1-O2A-CGA | 2.62 | 123.32 | 116.44 |
| 22 | b | 602 | CLA | CHC-C1C-NC | 2.62 | 128.18 | 124.20 |
| 22 | B | 610 | CLA | O2A-CGA-O1A | -2.62 | 116.98 | 123.59 |
| 29 | A | 413 | DGD | O2D-C2D-C1D | -2.62 | 103.69 | 110.05 |
| 26 | d | 406 | PL9 | C40-C39-C38 | -2.62 | 116.97 | 123.68 |
| 22 | c | 505 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 22 | D | 405 | CLA | CAC-C3C-C4C | 2.61 | 128.20 | 124.81 |
| 22 | a | 403 | CLA | O2D-CGD-CBD | 2.61 | 115.91 | 111.27 |
| 27 | b | 623 | LMG | O8-C28-O10 | -2.61 | 117.00 | 123.59 |
| 22 | B | 603 | CLA | C4-C3-C5 | 2.61 | 119.66 | 115.27 |
| 29 | c | 518 | DGD | C3G-O3G-C1D | 2.61 | 118.84 | 113.74 |
| 22 | B | 606 | CLA | CMB-C2B-C3B | 2.61 | 129.56 | 124.68 |
| 29 | C | 517 | DGD | O1G-C1A-C2A | -2.61 | 103.72 | 111.91 |
| 27 | c | 522 | LMG | O6-C1-O1 | -2.60 | 103.81 | 109.97 |
| 24 | C | 514 | BCR | C35-C13-C14 | -2.60 | 119.28 | 122.92 |
| 22 | b | 604 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 603 | CLA | CHD-C4C-NC | 2.60 | 128.30 | 124.20 |
| 31 | d | 413 | STE | C3-C2-C1 | -2.60 | 107.92 | 114.47 |
| 22 | b | 603 | CLA | O2A-CGA-O1A | -2.60 | 117.03 | 123.59 |
| 27 | b | 623 | LMG | O7-C10-O9 | -2.60 | 117.42 | 123.70 |
| 22 | c | 506 | CLA | C11-C10-C8 | -2.60 | 107.53 | 115.92 |
| 22 | c | 511 | CLA | CMB-C2B-C3B | 2.59 | 129.53 | 124.68 |
| 26 | A | 409 | PL9 | C31-C32-C33 | -2.59 | 103.35 | 111.88 |
| 22 | B | 609 | CLA | CHD-C1D-ND | -2.59 | 122.07 | 124.45 |
| 22 | B | 610 | CLA | CHC-C1C-NC | 2.59 | 128.13 | 124.20 |
| 27 | b | 621 | LMG | C38-C37-C36 | -2.59 | 101.29 | 114.42 |
| 24 | b | 618 | BCR | C15-C14-C13 | -2.58 | 123.62 | 127.31 |
| 33 | l | 101 | LHG | O8-C23-C24 | 2.58 | 120.01 | 111.91 |
| 22 | c | 503 | CLA | O2A-CGA-O1A | -2.58 | 117.08 | 123.59 |
| 33 | d | 409 | LHG | C26-C25-C24 | 2.58 | 122.46 | 113.19 |
| 22 | d | 404 | CLA | O2A-CGA-O1A | -2.58 | 117.09 | 123.59 |
| 26 | D | 406 | PL9 | C7-C8-C9 | -2.58 | 122.50 | 126.79 |
| 22 | a | 402 | CLA | C3A-C2A-C1A | 2.58 | 105.20 | 101.34 |
| 24 | t | 101 | BCR | C34-C9-C10 | -2.57 | 119.32 | 122.92 |
| 27 | A | 410 | LMG | C1-O6-C5 | -2.57 | 108.63 | 113.69 |
| 34 | F | 102 | HEC | O2D-CGD-CBD | 2.57 | 122.29 | 114.03 |
| 28 | D | 408 | SQD | O48-C23-O10 | -2.57 | 117.11 | 123.59 |
| 22 | B | 611 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 28 | a | 411 | SQD | O10-C23-C24 | -2.57 | 113.72 | 123.73 |
| 23 | D | 401 | PHO | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 27 | c | 523 | LMG | O8-C28-O10 | -2.57 | 117.11 | 123.59 |
| 24 | T | 101 | BCR | C38-C26-C27 | -2.57 | 108.69 | 113.62 |
| 28 | A | 411 | SQD | O5-C1-O6 | 2.56 | 116.05 | 109.97 |
| 24 | a | 406 | BCR | C8-C7-C6 | -2.56 | 120.01 | 127.20 |
| 22 | C | 507 | CLA | C1B-CHB-C4A | -2.56 | 125.05 | 130.12 |
| 27 | b | 621 | LMG | O7-C10-O9 | -2.56 | 117.52 | 123.70 |
| 24 | H | 102 | BCR | C16-C15-C14 | -2.56 | 118.23 | 123.47 |
| 22 | B | 616 | CLA | CHA-C1A-NA | -2.56 | 120.55 | 126.40 |
| 22 | a | 403 | CLA | O2A-CGA-O1A | -2.55 | 117.14 | 123.59 |
| 24 | K | 103 | BCR | C16-C15-C14 | -2.55 | 118.24 | 123.47 |
| 22 | C | 512 | CLA | CHD-C1D-ND | -2.55 | 122.11 | 124.45 |
| 22 | B | 614 | CLA | O2A-CGA-O1A | -2.55 | 117.16 | 123.59 |
| 24 | B | 619 | BCR | C38-C26-C25 | -2.55 | 121.67 | 124.53 |
| 26 | A | 409 | PL9 | O2-C1-C2 | -2.55 | 115.94 | 121.78 |
| 29 | c | 518 | DGD | C3D-C4D-C5D | -2.55 | 105.70 | 110.24 |
| 22 | b | 613 | CLA | C1-C2-C3 | -2.54 | 121.64 | 126.04 |
| 22 | B | 616 | CLA | C1-O2A-CGA | 2.54 | 123.11 | 116.44 |
| 22 | C | 512 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 618 | BCR | C38-C26-C25 | -2.54 | 121.68 | 124.53 |
| 22 | C | 509 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 24 | d | 405 | BCR | C27-C26-C25 | 2.54 | 126.41 | 122.73 |
| 24 | b | 617 | BCR | C37-C22-C21 | -2.53 | 119.37 | 122.92 |
| 24 | K | 101 | BCR | C7-C8-C9 | -2.53 | 122.41 | 126.23 |
| 22 | b | 611 | CLA | CHD-C1D-ND | -2.53 | 122.13 | 124.45 |
| 33 | D | 409 | LHG | O8-C23-C24 | 2.53 | 119.85 | 111.91 |
| 26 | d | 406 | PL9 | C31-C32-C33 | -2.53 | 103.57 | 111.88 |
| 22 | c | 509 | CLA | CHC-C1C-NC | 2.53 | 128.04 | 124.20 |
| 24 | A | 406 | BCR | C15-C16-C17 | -2.53 | 118.30 | 123.47 |
| 22 | b | 612 | CLA | CBC-CAC-C3C | 2.53 | 119.39 | 112.43 |
| 34 | v | 201 | HEC | CMD-C2D-C1D | -2.53 | 124.58 | 128.46 |
| 27 | Y | 101 | LMG | O6-C1-O1 | -2.53 | 103.99 | 109.97 |
| 22 | B | 607 | CLA | C2C-C1C-NC | 2.52 | 112.33 | 109.97 |
| 22 | C | 513 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 22 | B | 614 | CLA | CBC-CAC-C3C | -2.52 | 105.49 | 112.43 |
| 26 | A | 409 | PL9 | O1-C4-C3 | -2.52 | 117.95 | 120.72 |
| 29 | c | 518 | DGD | O2D-C2D-C1D | -2.51 | 103.94 | 110.05 |
| 22 | B | 603 | CLA | C1D-ND-C4D | 2.51 | 108.12 | 106.33 |
| 22 | c | 506 | CLA | O2D-CGD-CBD | 2.51 | 115.73 | 111.27 |
| 22 | a | 403 | CLA | CHC-C1C-NC | 2.51 | 128.01 | 124.20 |
| 22 | c | 510 | CLA | CHC-C1C-NC | 2.51 | 128.01 | 124.20 |
| 22 | C | 509 | CLA | CHA-C4D-ND | 2.51 | 137.75 | 132.50 |
| 24 | B | 619 | BCR | C15-C16-C17 | -2.51 | 118.33 | 123.47 |
| 24 | b | 617 | BCR | C3-C4-C5 | -2.51 | 109.60 | 114.08 |
| 24 | H | 102 | BCR | C27-C26-C25 | 2.51 | 126.37 | 122.73 |
| 27 | D | 407 | LMG | C9-C8-C7 | -2.51 | 105.86 | 111.79 |
| 22 | C | 512 | CLA | O2A-CGA-O1A | -2.50 | 117.28 | 123.59 |
| 31 | d | 412 | STE | O2-C1-C2 | 2.49 | 122.05 | 114.03 |
| 22 | A | 403 | CLA | C2D-C1D-ND | -2.49 | 108.27 | 110.10 |
| 33 | e | 101 | LHG | O8-C23-C24 | 2.49 | 119.73 | 111.91 |
| 22 | c | 512 | CLA | O2D-CGD-CBD | 2.49 | 115.69 | 111.27 |
| 27 | D | 407 | LMG | C31-C30-C29 | -2.49 | 104.25 | 113.19 |
| 22 | a | 410 | CLA | CMB-C2B-C3B | 2.48 | 129.32 | 124.68 |
| 24 | d | 405 | BCR | C2-C1-C6 | 2.48 | 114.30 | 110.48 |
| 24 | C | 514 | BCR | C34-C9-C10 | -2.48 | 119.45 | 122.92 |
| 31 | b | 624 | STE | O1-C1-C2 | -2.48 | 115.11 | 123.08 |
| 22 | B | 616 | CLA | O1D-CGD-CBD | 2.48 | 129.55 | 124.48 |
| 24 | c | 516 | BCR | C2-C1-C6 | 2.47 | 114.29 | 110.48 |
| 24 | k | 101 | BCR | C27-C26-C25 | 2.47 | 126.32 | 122.73 |
| 22 | B | 615 | CLA | C1-O2A-CGA | 2.47 | 122.94 | 116.44 |
| 22 | B | 610 | CLA | C1-C2-C3 | -2.47 | 121.77 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | b | 610 | CLA | C1-C2-C3 | -2.47 | 121.77 | 126.04 |
| 28 | A | 411 | SQD | O7-S-C6 | 2.47 | 109.88 | 106.94 |
| 27 | Y | 101 | LMG | C40-C39-C38 | -2.47 | 101.88 | 114.42 |
| 22 | c | 509 | CLA | C11-C10-C8 | -2.47 | 107.93 | 115.92 |
| 24 | b | 617 | BCR | C36-C18-C17 | -2.47 | 119.46 | 122.92 |
| 27 | M | 101 | LMG | C1-C2-C3 | -2.47 | 104.86 | 110.00 |
| 22 | C | 512 | CLA | C6-C5-C3 | -2.47 | 106.99 | 113.45 |
| 24 | K | 102 | BCR | C36-C18-C17 | -2.46 | 119.47 | 122.92 |
| 33 | d | 407 | LHG | C11-C10-C9 | -2.46 | 101.93 | 114.42 |
| 28 | a | 411 | SQD | O8-S-C6 | 2.46 | 109.66 | 105.74 |
| 24 | k | 102 | BCR | C40-C30-C25 | 2.46 | 114.29 | 110.30 |
| 24 | b | 619 | BCR | C11-C10-C9 | -2.46 | 123.80 | 127.31 |
| 22 | b | 613 | CLA | CHA-C1A-NA | -2.46 | 120.76 | 126.40 |
| 23 | a | 404 | PHO | OBD-CAD-CBD | -2.46 | 122.22 | 125.82 |
| 27 | A | 410 | LMG | C40-C39-C38 | -2.46 | 101.95 | 114.42 |
| 22 | b | 610 | CLA | CAA-CBA-CGA | -2.46 | 106.07 | 113.25 |
| 24 | K | 101 | BCR | C27-C26-C25 | 2.46 | 126.30 | 122.73 |
| 22 | d | 403 | CLA | C1D-ND-C4D | 2.45 | 108.08 | 106.33 |
| 27 | B | 621 | LMG | O7-C10-O9 | -2.45 | 117.18 | 123.30 |
| 22 | c | 512 | CLA | CMB-C2B-C1B | -2.45 | 124.69 | 128.46 |
| 22 | b | 605 | CLA | CHC-C1C-NC | 2.45 | 127.92 | 124.20 |
| 22 | C | 510 | CLA | C11-C10-C8 | -2.45 | 108.00 | 115.92 |
| 27 | D | 411 | LMG | O8-C28-O10 | -2.45 | 117.41 | 123.59 |
| 26 | A | 409 | PL9 | C20-C19-C21 | 2.45 | 119.39 | 115.27 |
| 22 | a | 402 | CLA | C7-C6-C5 | -2.45 | 106.71 | 113.36 |
| 22 | B | 612 | CLA | CHB-C4A-NA | 2.45 | 127.89 | 124.51 |
| 27 | c | 520 | LMG | O2-C2-C3 | -2.45 | 104.69 | 110.35 |
| 22 | B | 616 | CLA | O2D-CGD-O1D | -2.44 | 119.06 | 123.84 |
| 22 | b | 607 | CLA | CHA-C1A-NA | -2.44 | 120.81 | 126.40 |
| 24 | B | 619 | BCR | C37-C22-C21 | -2.44 | 119.51 | 122.92 |
| 22 | B | 605 | CLA | C11-C10-C8 | -2.43 | 108.05 | 115.92 |
| 23 | d | 401 | PHO | CMB-C2B-C3B | 2.43 | 129.23 | 124.68 |
| 29 | c | 517 | DGD | C2G-O2G-C1B | 2.43 | 123.78 | 117.79 |
| 26 | a | 409 | PL9 | C36-C34-C33 | -2.43 | 116.20 | 121.12 |
| 22 | C | 512 | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 24 | K | 102 | BCR | C27-C26-C25 | 2.43 | 126.26 | 122.73 |
| 22 | b | 611 | CLA | CHD-C1D-C2D | 2.43 | 130.57 | 125.48 |
| 29 | A | 413 | DGD | O3G-C1D-C2D | -2.43 | 104.51 | 108.30 |
| 34 | f | 101 | HEC | O2D-CGD-CBD | 2.43 | 121.83 | 114.03 |
| 24 | a | 406 | BCR | C30-C25-C26 | -2.43 | 119.20 | 122.61 |
| 22 | b | 607 | CLA | C2C-C1C-NC | 2.43 | 112.25 | 109.97 |
| 22 | d | 403 | CLA | C1B-CHB-C4A | -2.43 | 125.31 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | A | 409 | PL9 | C40-C39-C41 | 2.42 | 119.35 | 115.27 |
| 22 | c | 504 | CLA | C11-C12-C13 | -2.42 | 108.09 | 115.92 |
| 22 | b | 610 | CLA | C3A-C2A-C1A | 2.42 | 104.96 | 101.34 |
| 22 | b | 610 | CLA | C4-C3-C5 | 2.42 | 119.34 | 115.27 |
| 22 | C | 507 | CLA | O2A-CGA-O1A | -2.42 | 117.49 | 123.59 |
| 22 | C | 503 | CLA | C6-C7-C8 | -2.42 | 108.11 | 115.92 |
| 28 | B | 622 | SQD | O47-C45-C46 | 2.42 | 117.15 | 108.40 |
| 22 | b | 608 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 22 | B | 614 | CLA | C4-C3-C5 | 2.41 | 119.33 | 115.27 |
| 31 | d | 411 | STE | O2-C1-O1 | -2.41 | 117.28 | 123.30 |
| 22 | C | 501 | CLA | CHD-C1D-C2D | 2.41 | 130.54 | 125.48 |
| 28 | D | 408 | SQD | C1-C2-C3 | -2.41 | 104.98 | 110.00 |
| 22 | c | 511 | CLA | O2A-C1-C2 | -2.41 | 102.30 | 108.64 |
| 29 | C | 517 | DGD | O3D-C3D-C4D | -2.41 | 104.78 | 110.35 |
| 29 | C | 516 | DGD | C1D-C2D-C3D | -2.41 | 104.98 | 110.00 |
| 26 | d | 406 | PL9 | C7-C8-C9 | -2.41 | 122.78 | 126.79 |
| 22 | c | 505 | CLA | C7-C6-C5 | -2.41 | 106.82 | 113.36 |
| 34 | f | 101 | HEC | CMC-C2C-C1C | -2.41 | 124.76 | 128.46 |
| 29 | C | 515 | DGD | O2G-C1B-C2B | -2.40 | 106.32 | 111.50 |
| 27 | b | 623 | LMG | O6-C5-C6 | 2.40 | 112.41 | 106.44 |
| 24 | F | 101 | BCR | C8-C7-C6 | -2.40 | 120.45 | 127.20 |
| 22 | b | 603 | CLA | C7-C6-C5 | -2.40 | 106.83 | 113.36 |
| 22 | c | 507 | CLA | CED-O2D-CGD | 2.40 | 121.37 | 115.94 |
| 22 | b | 612 | CLA | CMD-C2D-C3D | 2.40 | 133.14 | 127.61 |
| 27 | M | 101 | LMG | C17-C16-C15 | -2.40 | 102.23 | 114.42 |
| 22 | B | 607 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 22 | a | 410 | CLA | C1-O2A-CGA | 2.40 | 122.74 | 116.44 |
| 24 | B | 618 | BCR | C15-C16-C17 | -2.40 | 118.56 | 123.47 |
| 29 | c | 517 | DGD | C4A-C3A-C2A | -2.40 | 104.57 | 113.19 |
| 22 | c | 511 | CLA | CHD-C1D-ND | -2.40 | 122.25 | 124.45 |
| 29 | C | 517 | DGD | O2D-C2D-C1D | -2.40 | 104.22 | 110.05 |
| 24 | K | 103 | BCR | C11-C10-C9 | -2.40 | 123.89 | 127.31 |
| 22 | a | 403 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 28 | D | 408 | SQD | O5-C5-C4 | 2.40 | 114.05 | 109.69 |
| 22 | C | 501 | CLA | CMB-C2B-C1B | -2.39 | 124.78 | 128.46 |
| 27 | A | 410 | LMG | C38-C37-C36 | -2.39 | 102.27 | 114.42 |
| 27 | c | 520 | LMG | C1-O6-C5 | -2.39 | 109.00 | 113.69 |
| 22 | c | 505 | CLA | CHD-C1D-ND | -2.39 | 122.26 | 124.45 |
| 22 | a | 403 | CLA | C4D-CHA-C1A | 2.39 | 124.15 | 121.25 |
| 27 | d | 410 | LMG | C3-C4-C5 | -2.39 | 105.98 | 110.24 |
| 29 | h | 102 | DGD | O5E-C6E-C5E | -2.39 | 103.11 | 111.29 |
| 29 | C | 516 | DGD | O6D-C1D-O3G | -2.38 | 104.33 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 403 | CLA | CHD-C1D-C2D | 2.38 | 130.48 | 125.48 |
| 29 | C | 515 | DGD | O1G-C1A-C2A | -2.38 | 104.43 | 111.91 |
| 22 | B | 604 | CLA | C6-C5-C3 | -2.38 | 107.21 | 113.45 |
| 24 | b | 619 | BCR | C2-C1-C6 | 2.38 | 114.15 | 110.48 |
| 29 | c | 518 | DGD | O4D-C4D-C3D | 2.38 | 115.85 | 110.35 |
| 27 | M | 101 | LMG | O2-C2-C1 | -2.38 | 104.27 | 110.05 |
| 22 | d | 403 | CLA | C6-C5-C3 | 2.38 | 119.69 | 113.45 |
| 24 | b | 617 | BCR | C38-C26-C25 | -2.38 | 121.86 | 124.53 |
| 29 | C | 517 | DGD | CAB-C9B-C8B | -2.38 | 102.36 | 114.42 |
| 24 | A | 406 | BCR | C1-C6-C5 | -2.38 | 119.27 | 122.61 |
| 24 | K | 103 | BCR | C27-C26-C25 | 2.38 | 126.18 | 122.73 |
| 22 | b | 612 | CLA | CAC-C3C-C4C | 2.38 | 127.89 | 124.81 |
| 22 | c | 509 | CLA | CMB-C2B-C1B | -2.38 | 124.81 | 128.46 |
| 27 | b | 621 | LMG | C20-C19-C18 | -2.37 | 102.37 | 114.42 |
| 28 | a | 412 | SQD | O49-C7-C8 | -2.37 | 114.47 | 123.73 |
| 28 | A | 411 | SQD | O9-S-O7 | -2.37 | 105.74 | 113.95 |
| 28 | D | 408 | SQD | O48-C23-C24 | 2.37 | 119.35 | 111.91 |
| 33 | D | 410 | LHG | O8-C23-O10 | -2.37 | 117.61 | 123.59 |
| 22 | D | 404 | CLA | CMB-C2B-C1B | -2.37 | 124.83 | 128.46 |
| 22 | c | 514 | CLA | CHB-C4A-NA | 2.37 | 127.78 | 124.51 |
| 23 | d | 401 | PHO | C1-C2-C3 | -2.37 | 121.95 | 126.04 |
| 31 | b | 627 | STE | C3-C2-C1 | -2.37 | 108.51 | 114.47 |
| 22 | c | 503 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 22 | c | 504 | CLA | C4-C3-C5 | 2.36 | 119.25 | 115.27 |
| 22 | C | 501 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 22 | D | 405 | CLA | O2D-CGD-CBD | 2.36 | 115.46 | 111.27 |
| 22 | b | 615 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 22 | C | 507 | CLA | CAA-CBA-CGA | -2.36 | 106.36 | 113.25 |
| 24 | h | 101 | BCR | C36-C18-C17 | -2.36 | 119.62 | 122.92 |
| 22 | B | 616 | CLA | CBC-CAC-C3C | -2.36 | 105.94 | 112.43 |
| 24 | b | 619 | BCR | C28-C27-C26 | -2.35 | 109.87 | 114.08 |
| 33 | D | 412 | LHG | C20-C19-C18 | -2.35 | 102.48 | 114.42 |
| 24 | C | 514 | BCR | C15-C16-C17 | -2.35 | 118.65 | 123.47 |
| 27 | D | 407 | LMG | O2-C2-C1 | -2.35 | 104.33 | 110.05 |
| 22 | B | 608 | CLA | CHD-C4C-NC | 2.35 | 127.91 | 124.20 |
| 22 | B | 607 | CLA | C3A-C2A-C1A | 2.35 | 104.86 | 101.34 |
| 22 | b | 610 | CLA | C2C-C1C-NC | 2.35 | 112.17 | 109.97 |
| 22 | B | 604 | CLA | CHA-C1A-NA | -2.35 | 121.02 | 126.40 |
| 22 | B | 615 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 22 | c | 504 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 29 | c | 519 | DGD | O3D-C3D-C4D | -2.34 | 104.94 | 110.35 |
| 29 | A | 413 | DGD | O1G-C1A-O1A | -2.34 | 117.69 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | a | 406 | BCR | C38-C26-C27 | -2.34 | 109.12 | 113.62 |
| 22 | A | 405 | CLA | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 24 | k | 101 | BCR | C38-C26-C25 | -2.34 | 121.90 | 124.53 |
| 29 | C | 517 | DGD | CBB-CAB-C9B | -2.34 | 102.56 | 114.42 |
| 22 | a | 410 | CLA | O2D-CGD-CBD | 2.34 | 115.42 | 111.27 |
| 22 | B | 604 | CLA | CGD-CBD-CAD | -2.33 | 103.17 | 110.73 |
| 22 | H | 101 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 22 | b | 606 | CLA | C4-C3-C5 | 2.33 | 119.20 | 115.27 |
| 26 | D | 406 | PL9 | O2-C1-C2 | -2.33 | 116.44 | 121.78 |
| 22 | C | 505 | CLA | C16-C15-C13 | -2.33 | 108.38 | 115.92 |
| 22 | c | 503 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 22 | D | 403 | CLA | CMD-C2D-C3D | 2.33 | 132.98 | 127.61 |
| 22 | c | 510 | CLA | CAC-C3C-C4C | 2.33 | 127.83 | 124.81 |
| 22 | b | 605 | CLA | C16-C15-C13 | -2.33 | 108.39 | 115.92 |
| 29 | c | 518 | DGD | O3G-C1D-C2D | -2.33 | 104.67 | 108.30 |
| 27 | D | 407 | LMG | O8-C28-O10 | -2.33 | 117.71 | 123.59 |
| 22 | C | 507 | CLA | CHB-C4A-NA | 2.33 | 127.73 | 124.51 |
| 22 | B | 607 | CLA | C1C-C2C-C3C | -2.33 | 104.51 | 106.96 |
| 22 | c | 514 | CLA | C4A-NA-C1A | 2.33 | 107.75 | 106.71 |
| 22 | A | 402 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 22 | B | 602 | CLA | C11-C12-C13 | -2.33 | 108.40 | 115.92 |
| 22 | c | 502 | CLA | CED-O2D-CGD | -2.32 | 110.68 | 115.94 |
| 22 | B | 611 | CLA | C3C-C4C-NC | -2.32 | 107.97 | 110.57 |
| 22 | b | 608 | CLA | O2A-CGA-O1A | -2.32 | 117.73 | 123.59 |
| 22 | C | 502 | CLA | CHA-C1A-NA | -2.32 | 121.08 | 126.40 |
| 22 | C | 502 | CLA | C4D-CHA-C1A | 2.32 | 124.08 | 121.25 |
| 22 | C | 509 | CLA | CED-O2D-CGD | 2.32 | 121.19 | 115.94 |
| 29 | h | 102 | DGD | O3E-C3E-C2E | -2.32 | 104.98 | 110.35 |
| 26 | D | 406 | PL9 | C42-C43-C44 | -2.32 | 122.07 | 127.66 |
| 22 | b | 615 | CLA | C3B-C4B-NB | -2.32 | 106.21 | 109.21 |
| 22 | c | 507 | CLA | C4-C3-C5 | 2.32 | 119.17 | 115.27 |
| 22 | b | 603 | CLA | CHD-C1D-C2D | 2.32 | 130.34 | 125.48 |
| 29 | H | 103 | DGD | C7B-C6B-C5B | -2.32 | 102.66 | 114.42 |
| 26 | a | 409 | PL9 | O2-C1-C6 | 2.32 | 124.60 | 120.59 |
| 24 | K | 103 | BCR | C37-C22-C21 | -2.32 | 119.68 | 122.92 |
| 22 | b | 608 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 24 | C | 514 | BCR | C33-C5-C6 | -2.32 | 121.93 | 124.53 |
| 22 | c | 509 | CLA | C1B-CHB-C4A | -2.31 | 125.53 | 130.12 |
| 28 | B | 622 | SQD | C46-C45-C44 | -2.31 | 106.32 | 111.79 |
| 31 | J | 101 | STE | O2-C1-C2 | 2.31 | 121.46 | 114.03 |
| 22 | C | 510 | CLA | C2D-C1D-ND | -2.31 | 108.40 | 110.10 |
| 22 | d | 404 | CLA | C1-C2-C3 | -2.31 | 122.04 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | C | 515 | DGD | C3D-C4D-C5D | -2.31 | 106.12 | 110.24 |
| 24 | d | 405 | BCR | C24-C23-C22 | -2.31 | 122.75 | 126.23 |
| 22 | B | 614 | CLA | CHA-C1A-NA | -2.31 | 121.12 | 126.40 |
| 24 | d | 405 | BCR | C16-C15-C14 | -2.31 | 118.75 | 123.47 |
| 27 | M | 101 | LMG | O7-C10-C11 | -2.30 | 106.53 | 111.50 |
| 29 | h | 102 | DGD | C7B-C6B-C5B | -2.30 | 102.74 | 114.42 |
| 22 | b | 607 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 22 | C | 501 | CLA | C9-C8-C10 | -2.30 | 102.97 | 111.29 |
| 22 | C | 502 | CLA | CAA-C2A-C3A | -2.30 | 106.48 | 112.78 |
| 22 | b | 612 | CLA | O2D-CGD-O1D | -2.30 | 119.34 | 123.84 |
| 23 | a | 404 | PHO | CMC-C2C-C3C | 2.30 | 129.28 | 124.94 |
| 22 | C | 505 | CLA | CAA-CBA-CGA | -2.30 | 106.54 | 113.25 |
| 33 | e | 101 | LHG | C11-C10-C9 | -2.30 | 102.76 | 114.42 |
| 27 | b | 621 | LMG | O8-C28-O10 | -2.30 | 117.80 | 123.59 |
| 22 | C | 505 | CLA | O2A-CGA-O1A | -2.30 | 117.80 | 123.59 |
| 24 | K | 101 | BCR | C36-C18-C17 | -2.30 | 119.71 | 122.92 |
| 22 | B | 603 | CLA | O2A-CGA-O1A | -2.30 | 117.80 | 123.59 |
| 24 | t | 101 | BCR | C27-C26-C25 | 2.29 | 126.06 | 122.73 |
| 22 | b | 605 | CLA | O1D-CGD-CBD | 2.29 | 129.18 | 124.48 |
| 29 | C | 517 | DGD | C8B-C7B-C6B | -2.29 | 102.78 | 114.42 |
| 29 | C | 515 | DGD | C3B-C2B-C1B | -2.29 | 105.29 | 113.62 |
| 22 | B | 616 | CLA | C2A-C1A-CHA | 2.29 | 127.87 | 123.86 |
| 24 | b | 617 | BCR | C8-C7-C6 | -2.29 | 120.77 | 127.20 |
| 22 | B | 610 | CLA | O1A-CGA-CBA | 2.29 | 132.67 | 123.73 |
| 29 | c | 518 | DGD | C6D-O5D-C1E | 2.29 | 118.21 | 113.74 |
| 22 | C | 505 | CLA | O2A-C1-C2 | -2.29 | 102.62 | 108.64 |
| 29 | C | 517 | DGD | C1D-C2D-C3D | -2.29 | 105.23 | 110.00 |
| 24 | t | 101 | BCR | C38-C26-C27 | -2.29 | 109.22 | 113.62 |
| 22 | C | 503 | CLA | CAA-CBA-CGA | -2.29 | 106.57 | 113.25 |
| 31 | B | 623 | STE | O2-C1-C2 | 2.29 | 121.37 | 114.03 |
| 22 | b | 602 | CLA | CHD-C1D-C2D | 2.28 | 130.27 | 125.48 |
| 24 | B | 619 | BCR | C28-C27-C26 | -2.28 | 110.00 | 114.08 |
| 22 | B | 612 | CLA | O2A-CGA-O1A | -2.28 | 117.83 | 123.59 |
| 22 | a | 402 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 24 | b | 619 | BCR | C8-C7-C6 | -2.28 | 120.80 | 127.20 |
| 22 | B | 604 | CLA | C1-O2A-CGA | -2.28 | 110.47 | 116.44 |
| 29 | h | 102 | DGD | C1D-O6D-C5D | -2.28 | 109.22 | 113.69 |
| 22 | a | 402 | CLA | C4-C3-C5 | 2.28 | 119.10 | 115.27 |
| 26 | a | 409 | PL9 | C12-C13-C14 | -2.28 | 122.18 | 127.66 |
| 24 | c | 515 | BCR | C15-C14-C13 | -2.28 | 124.06 | 127.31 |
| 27 | c | 523 | LMG | C1-O6-C5 | -2.27 | 109.22 | 113.69 |
| 29 | H | 103 | DGD | C1D-O6D-C5D | -2.27 | 109.22 | 113.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | c | 508 | CLA | O2A-CGA-O1A | -2.27 | 117.86 | 123.59 |
| 24 | b | 617 | BCR | C27-C26-C25 | 2.27 | 126.03 | 122.73 |
| 22 | C | 507 | CLA | C4D-CHA-C1A | 2.27 | 124.01 | 121.25 |
| 22 | C | 509 | CLA | O2D-CGD-O1D | -2.27 | 119.40 | 123.84 |
| 33 | L | 102 | LHG | C12-C11-C10 | -2.27 | 102.90 | 114.42 |
| 22 | B | 602 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 24 | B | 617 | BCR | C7-C8-C9 | -2.27 | 122.81 | 126.23 |
| 28 | A | 411 | SQD | O48-C23-C24 | 2.27 | 119.03 | 111.91 |
| 27 | c | 520 | LMG | C40-C39-C38 | -2.27 | 102.91 | 114.42 |
| 22 | A | 403 | CLA | CHB-C4A-NA | 2.27 | 127.65 | 124.51 |
| 22 | B | 605 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 22 | d | 404 | CLA | CHB-C4A-NA | 2.27 | 127.65 | 124.51 |
| 29 | H | 103 | DGD | C4D-C3D-C2D | -2.27 | 106.87 | 110.82 |
| 22 | c | 512 | CLA | C4D-CHA-C1A | 2.27 | 124.01 | 121.25 |
| 22 | c | 514 | CLA | C1B-CHB-C4A | -2.26 | 125.63 | 130.12 |
| 33 | D | 412 | LHG | C11-C10-C9 | -2.26 | 102.94 | 114.42 |
| 24 | C | 514 | BCR | C2-C1-C6 | 2.26 | 113.96 | 110.48 |
| 22 | b | 613 | CLA | C16-C15-C13 | -2.26 | 108.61 | 115.92 |
| 26 | A | 409 | PL9 | C7-C8-C9 | -2.26 | 123.03 | 126.79 |
| 22 | C | 512 | CLA | CAA-CBA-CGA | -2.26 | 106.66 | 113.25 |
| 22 | b | 606 | CLA | CMB-C2B-C3B | 2.26 | 128.90 | 124.68 |
| 23 | a | 404 | PHO | O2A-CGA-O1A | -2.25 | 117.90 | 123.59 |
| 22 | b | 604 | CLA | O2A-CGA-O1A | -2.25 | 117.91 | 123.59 |
| 22 | b | 605 | CLA | C2D-C1D-ND | -2.25 | 108.44 | 110.10 |
| 22 | b | 609 | CLA | C2D-C1D-ND | -2.25 | 108.44 | 110.10 |
| 22 | b | 602 | CLA | CHA-C4D-ND | 2.25 | 137.21 | 132.50 |
| 22 | C | 502 | CLA | CHD-C1D-ND | -2.25 | 122.39 | 124.45 |
| 22 | A | 402 | CLA | CMB-C2B-C1B | -2.25 | 125.01 | 128.46 |
| 31 | B | 601 | STE | O2-C1-C2 | 2.25 | 121.25 | 114.03 |
| 29 | H | 103 | DGD | CAB-C9B-C8B | -2.25 | 103.02 | 114.42 |
| 28 | B | 622 | SQD | O8-S-O7 | -2.25 | 105.79 | 111.27 |
| 29 | A | 413 | DGD | CDB-CCB-CBB | -2.24 | 103.03 | 114.42 |
| 22 | b | 608 | CLA | CHD-C1D-ND | -2.24 | 122.40 | 124.45 |
| 34 | F | 102 | HEC | CMC-C2C-C1C | -2.24 | 125.02 | 128.46 |
| 24 | t | 101 | BCR | C11-C10-C9 | -2.24 | 124.12 | 127.31 |
| 33 | E | 101 | LHG | O8-C23-C24 | 2.24 | 118.93 | 111.91 |
| 22 | B | 615 | CLA | C1C-C2C-C3C | -2.24 | 104.61 | 106.96 |
| 22 | C | 503 | CLA | C1B-CHB-C4A | -2.24 | 125.69 | 130.12 |
| 22 | B | 610 | CLA | CHC-C1C-C2C | -2.24 | 120.54 | 126.72 |
| 29 | c | 517 | DGD | O3D-C3D-C4D | -2.23 | 105.18 | 110.35 |
| 24 | B | 619 | BCR | C40-C30-C29 | -2.23 | 99.97 | 108.91 |
| 22 | C | 504 | CLA | CHC-C1C-NC | 2.23 | 127.59 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 609 | CLA | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 24 | h | 101 | BCR | C35-C13-C12 | 2.23 | 121.59 | 118.08 |
| 24 | K | 101 | BCR | C24-C23-C22 | -2.23 | 122.87 | 126.23 |
| 26 | A | 409 | PL9 | C27-C28-C29 | -2.23 | 122.30 | 127.66 |
| 27 | A | 410 | LMG | C3-C4-C5 | -2.22 | 106.27 | 110.24 |
| 22 | D | 403 | CLA | C1-C2-C3 | -2.22 | 122.20 | 126.04 |
| 22 | C | 506 | CLA | O2A-CGA-O1A | -2.22 | 117.98 | 123.59 |
| 24 | b | 617 | BCR | C11-C10-C9 | -2.22 | 124.14 | 127.31 |
| 22 | c | 505 | CLA | O2A-C1-C2 | -2.22 | 102.80 | 108.64 |
| 22 | c | 507 | CLA | C4A-NA-C1A | 2.22 | 107.70 | 106.71 |
| 22 | B | 612 | CLA | C1-C2-C3 | -2.22 | 122.20 | 126.04 |
| 26 | A | 409 | PL9 | C30-C29-C31 | -2.22 | 111.54 | 115.27 |
| 22 | b | 611 | CLA | C2A-C3A-C4A | 2.22 | 105.45 | 101.87 |
| 33 | d | 408 | LHG | C20-C19-C18 | -2.22 | 103.17 | 114.42 |
| 22 | a | 402 | CLA | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 34 | V | 201 | HEC | CMD-C2D-C1D | -2.22 | 125.06 | 128.46 |
| 22 | c | 505 | CLA | C1B-CHB-C4A | -2.22 | 125.73 | 130.12 |
| 22 | b | 602 | CLA | O2D-CGD-O1D | -2.22 | 119.51 | 123.84 |
| 33 | D | 409 | LHG | C27-C26-C25 | -2.21 | 103.19 | 114.42 |
| 22 | b | 609 | CLA | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 22 | H | 101 | CLA | CAA-C2A-C1A | -2.21 | 104.72 | 111.97 |
| 22 | b | 609 | CLA | CED-O2D-CGD | 2.21 | 120.94 | 115.94 |
| 29 | c | 518 | DGD | O6D-C1D-O3G | -2.21 | 104.73 | 109.97 |
| 27 | M | 101 | LMG | C23-C22-C21 | -2.21 | 103.20 | 114.42 |
| 22 | b | 605 | CLA | C1D-ND-C4D | 2.21 | 107.91 | 106.33 |
| 22 | C | 509 | CLA | CAA-C2A-C3A | -2.21 | 106.73 | 112.78 |
| 27 | b | 621 | LMG | C22-C21-C20 | -2.21 | 103.21 | 114.42 |
| 29 | h | 102 | DGD | C1D-C2D-C3D | -2.21 | 105.39 | 110.00 |
| 24 | B | 618 | BCR | C38-C26-C25 | -2.21 | 122.05 | 124.53 |
| 29 | C | 515 | DGD | C1D-C2D-C3D | -2.21 | 105.40 | 110.00 |
| 24 | B | 619 | BCR | C11-C10-C9 | -2.21 | 124.16 | 127.31 |
| 34 | f | 101 | HEC | C4C-C3C-C2C | 2.21 | 108.73 | 106.35 |
| 22 | a | 402 | CLA | O2A-CGA-O1A | -2.21 | 118.03 | 123.59 |
| 26 | a | 409 | PL9 | C31-C32-C33 | -2.20 | 104.64 | 111.88 |
| 22 | b | 602 | CLA | CHC-C1C-C2C | -2.20 | 120.63 | 126.72 |
| 29 | h | 102 | DGD | O2D-C2D-C1D | -2.20 | 104.70 | 110.05 |
| 24 | b | 617 | BCR | C15-C16-C17 | -2.20 | 118.97 | 123.47 |
| 22 | c | 507 | CLA | O2D-CGD-O1D | -2.20 | 119.54 | 123.84 |
| 22 | B | 613 | CLA | CHB-C4A-NA | 2.20 | 127.55 | 124.51 |
| 22 | D | 403 | CLA | O2D-CGD-O1D | -2.20 | 119.54 | 123.84 |
| 22 | C | 510 | CLA | CHB-C4A-NA | 2.20 | 127.55 | 124.51 |
| 28 | A | 412 | SQD | O47-C45-C46 | 2.20 | 111.22 | 106.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | A | 409 | PL9 | C36-C37-C38 | -2.20 | 104.67 | 111.88 |
| 27 | Y | 101 | LMG | C3-C4-C5 | -2.19 | 106.32 | 110.24 |
| 23 | A | 404 | PHO | OBD-CAD-CBD | -2.19 | 122.60 | 125.82 |
| 22 | B | 604 | CLA | C2A-C3A-C4A | 2.19 | 105.41 | 101.87 |
| 27 | c | 523 | LMG | C4-C3-C2 | -2.19 | 107.00 | 110.82 |
| 22 | H | 101 | CLA | CHD-C1D-ND | -2.19 | 122.44 | 124.45 |
| 22 | c | 514 | CLA | O2A-CGA-O1A | -2.19 | 118.06 | 123.59 |
| 27 | b | 623 | LMG | C40-C39-C38 | -2.19 | 103.30 | 114.42 |
| 22 | b | 609 | CLA | C7-C6-C5 | -2.19 | 107.41 | 113.36 |
| 33 | d | 408 | LHG | O8-C23-C24 | 2.19 | 118.78 | 111.91 |
| 33 | E | 101 | LHG | C26-C25-C24 | 2.19 | 121.06 | 113.19 |
| 31 | b | 627 | STE | O2-C1-C2 | 2.19 | 121.06 | 114.03 |
| 24 | H | 102 | BCR | C1-C6-C5 | -2.19 | 119.53 | 122.61 |
| 28 | a | 411 | SQD | O4-C4-C3 | -2.19 | 105.29 | 110.35 |
| 22 | B | 616 | CLA | C5-C3-C2 | 2.18 | 125.54 | 121.12 |
| 26 | d | 406 | PL9 | O2-C1-C2 | -2.18 | 116.78 | 121.78 |
| 27 | b | 621 | LMG | O1-C7-C8 | -2.18 | 105.63 | 110.90 |
| 22 | C | 503 | CLA | O1D-CGD-CBD | 2.18 | 128.95 | 124.48 |
| 24 | c | 516 | BCR | C7-C8-C9 | -2.18 | 122.94 | 126.23 |
| 22 | B | 609 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 22 | C | 511 | CLA | O2D-CGD-O1D | -2.18 | 119.57 | 123.84 |
| 29 | C | 516 | DGD | C1D-O6D-C5D | -2.18 | 109.41 | 113.69 |
| 22 | B | 616 | CLA | C2C-C1C-NC | 2.18 | 112.01 | 109.97 |
| 29 | H | 103 | DGD | C9A-C8A-C7A | -2.18 | 103.36 | 114.42 |
| 22 | C | 513 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 22 | C | 513 | CLA | C4-C3-C5 | 2.18 | 118.94 | 115.27 |
| 24 | t | 101 | BCR | C36-C18-C19 | 2.18 | 121.50 | 118.08 |
| 29 | C | 515 | DGD | C5B-C4B-C3B | -2.18 | 103.38 | 114.42 |
| 24 | K | 102 | BCR | C33-C5-C6 | -2.17 | 122.09 | 124.53 |
| 22 | B | 604 | CLA | C2A-C1A-CHA | 2.17 | 127.66 | 123.86 |
| 29 | H | 103 | DGD | C7A-C6A-C5A | -2.17 | 103.40 | 114.42 |
| 22 | b | 607 | CLA | O2A-CGA-O1A | -2.17 | 118.11 | 123.59 |
| 22 | A | 403 | CLA | C1-C2-C3 | -2.17 | 122.29 | 126.04 |
| 22 | c | 509 | CLA | CHD-C1D-C2D | 2.17 | 130.03 | 125.48 |
| 33 | l | 101 | LHG | C11-C10-C9 | -2.17 | 103.41 | 114.42 |
| 22 | c | 507 | CLA | C2D-C1D-ND | -2.17 | 108.51 | 110.10 |
| 22 | C | 513 | CLA | C3A-C2A-C1A | 2.17 | 104.58 | 101.34 |
| 22 | b | 612 | CLA | C1D-ND-C4D | -2.17 | 104.80 | 106.33 |
| 24 | K | 103 | BCR | C7-C8-C9 | -2.16 | 122.96 | 126.23 |
| 22 | H | 101 | CLA | C2D-C1D-ND | -2.16 | 108.51 | 110.10 |
| 22 | b | 605 | CLA | CHD-C1D-C2D | 2.16 | 130.01 | 125.48 |
| 22 | D | 405 | CLA | O2A-C1-C2 | -2.16 | 102.96 | 108.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | c | 508 | CLA | CED-O2D-CGD | 2.16 | 120.82 | 115.94 |
| 22 | a | 402 | CLA | C17-C16-C15 | -2.16 | 103.32 | 113.24 |
| 22 | B | 603 | CLA | CMA-C3A-C4A | 2.16 | 117.57 | 111.77 |
| 22 | C | 509 | CLA | CHD-C1D-ND | -2.16 | 122.47 | 124.45 |
| 22 | C | 506 | CLA | CHA-C1A-NA | -2.16 | 121.46 | 126.40 |
| 22 | c | 504 | CLA | O1D-CGD-CBD | 2.16 | 128.90 | 124.48 |
| 24 | b | 617 | BCR | C35-C13-C14 | -2.16 | 119.90 | 122.92 |
| 27 | c | 523 | LMG | O5-C6-C5 | -2.16 | 103.90 | 111.29 |
| 22 | A | 405 | CLA | O2A-CGA-O1A | -2.15 | 118.15 | 123.59 |
| 22 | a | 402 | CLA | C2A-C1A-CHA | 2.15 | 127.63 | 123.86 |
| 22 | c | 513 | CLA | O2A-CGA-O1A | -2.15 | 118.16 | 123.59 |
| 22 | D | 405 | CLA | CHB-C4A-NA | 2.15 | 127.49 | 124.51 |
| 24 | B | 618 | BCR | C15-C14-C13 | -2.15 | 124.24 | 127.31 |
| 29 | H | 103 | DGD | O6D-C1D-O3G | -2.15 | 104.89 | 109.97 |
| 26 | D | 406 | PL9 | C21-C19-C18 | -2.15 | 116.77 | 121.12 |
| 28 | L | 101 | SQD | O8-S-C6 | 2.15 | 109.16 | 105.74 |
| 22 | c | 506 | CLA | CMD-C2D-C3D | 2.15 | 132.56 | 127.61 |
| 27 | b | 623 | LMG | C1-C2-C3 | -2.15 | 105.53 | 110.00 |
| 29 | c | 518 | DGD | CDB-CCB-CBB | -2.15 | 103.53 | 114.42 |
| 22 | c | 507 | CLA | CHD-C4C-NC | 2.15 | 127.58 | 124.20 |
| 22 | H | 101 | CLA | C4-C3-C5 | 2.14 | 118.88 | 115.27 |
| 22 | C | 512 | CLA | C1B-CHB-C4A | -2.14 | 125.87 | 130.12 |
| 28 | L | 101 | SQD | O47-C45-C46 | 2.14 | 116.16 | 108.40 |
| 22 | B | 610 | CLA | C1D-CHD-C4C | -2.14 | 121.44 | 126.06 |
| 22 | b | 601 | CLA | C11-C12-C13 | -2.14 | 108.99 | 115.92 |
| 22 | c | 504 | CLA | CHD-C1D-ND | -2.14 | 122.48 | 124.45 |
| 22 | b | 612 | CLA | O2D-CGD-CBD | 2.14 | 115.07 | 111.27 |
| 27 | M | 101 | LMG | O3-C3-C2 | -2.14 | 105.40 | 110.35 |
| 22 | B | 613 | CLA | CED-O2D-CGD | 2.14 | 120.78 | 115.94 |
| 29 | h | 102 | DGD | C1E-O6E-C5E | 2.14 | 117.89 | 113.69 |
| 24 | h | 101 | BCR | C16-C15-C14 | -2.14 | 119.09 | 123.47 |
| 34 | V | 201 | HEC | O2D-CGD-CBD | 2.14 | 120.90 | 114.03 |
| 22 | a | 403 | CLA | C1D-ND-C4D | 2.14 | 107.85 | 106.33 |
| 33 | D | 410 | LHG | O8-C6-C5 | -2.14 | 102.22 | 108.43 |
| 24 | k | 102 | BCR | C35-C13-C14 | -2.14 | 119.93 | 122.92 |
| 22 | b | 604 | CLA | CHB-C4A-NA | 2.14 | 127.47 | 124.51 |
| 22 | C | 505 | CLA | C4-C3-C2 | -2.13 | 118.20 | 123.68 |
| 22 | b | 615 | CLA | CHB-C4A-NA | 2.13 | 127.46 | 124.51 |
| 24 | C | 514 | BCR | C1-C6-C5 | -2.13 | 119.61 | 122.61 |
| 22 | b | 610 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 22 | d | 403 | CLA | CHA-C4D-ND | 2.13 | 136.96 | 132.50 |
| 24 | K | 103 | BCR | C2-C1-C6 | 2.13 | 113.76 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | c | 513 | CLA | C1-C2-C3 | -2.13 | 122.36 | 126.04 |
| 22 | A | 405 | CLA | C5-C3-C2 | -2.13 | 116.81 | 121.12 |
| 22 | d | 403 | CLA | O2D-CGD-O1D | -2.13 | 119.68 | 123.84 |
| 22 | a | 405 | CLA | CHC-C1C-NC | 2.13 | 127.43 | 124.20 |
| 22 | B | 604 | CLA | O2D-CGD-O1D | -2.13 | 119.68 | 123.84 |
| 22 | B | 616 | CLA | C1D-ND-C4D | 2.13 | 107.84 | 106.33 |
| 22 | b | 605 | CLA | CHC-C1C-C2C | -2.12 | 120.84 | 126.72 |
| 33 | E | 101 | LHG | C11-C10-C9 | -2.12 | 103.64 | 114.42 |
| 22 | a | 405 | CLA | CHD-C4C-NC | 2.12 | 127.55 | 124.20 |
| 22 | B | 616 | CLA | CHD-C1D-ND | -2.12 | 122.50 | 124.45 |
| 22 | d | 404 | CLA | O1D-CGD-CBD | 2.12 | 128.83 | 124.48 |
| 24 | k | 101 | BCR | C1-C6-C5 | -2.12 | 119.62 | 122.61 |
| 22 | C | 501 | CLA | C2C-C1C-NC | -2.12 | 107.98 | 109.97 |
| 29 | c | 519 | DGD | CAB-C9B-C8B | -2.12 | 103.65 | 114.42 |
| 26 | a | 409 | PL9 | C40-C39-C41 | 2.12 | 118.84 | 115.27 |
| 33 | d | 407 | LHG | C25-C24-C23 | 2.12 | 121.34 | 113.62 |
| 27 | d | 410 | LMG | O7-C10-O9 | -2.12 | 118.58 | 123.70 |
| 24 | c | 516 | BCR | C36-C18-C17 | -2.12 | 119.95 | 122.92 |
| 24 | K | 101 | BCR | C31-C1-C6 | 2.12 | 113.74 | 110.30 |
| 22 | b | 609 | CLA | C1-C2-C3 | -2.12 | 122.38 | 126.04 |
| 22 | b | 604 | CLA | C1B-CHB-C4A | -2.12 | 125.92 | 130.12 |
| 28 | f | 102 | SQD | O7-S-C6 | 2.12 | 109.46 | 106.94 |
| 28 | f | 102 | SQD | O5-C1-O6 | 2.12 | 114.99 | 109.97 |
| 24 | k | 102 | BCR | C16-C15-C14 | -2.12 | 119.14 | 123.47 |
| 22 | d | 404 | CLA | CBC-CAC-C3C | -2.12 | 106.59 | 112.43 |
| 22 | B | 614 | CLA | O1D-CGD-CBD | 2.12 | 128.82 | 124.48 |
| 33 | e | 101 | LHG | C20-C19-C18 | -2.12 | 103.68 | 114.42 |
| 29 | C | 515 | DGD | CCB-CBB-CAB | -2.12 | 103.68 | 114.42 |
| 22 | B | 602 | CLA | C2A-C1A-CHA | 2.11 | 127.56 | 123.86 |
| 31 | E | 102 | STE | O2-C1-C2 | 2.11 | 120.82 | 114.03 |
| 22 | B | 603 | CLA | C5-C3-C2 | -2.11 | 116.84 | 121.12 |
| 24 | B | 618 | BCR | C3-C4-C5 | -2.11 | 110.31 | 114.08 |
| 22 | b | 608 | CLA | C1B-CHB-C4A | -2.11 | 125.94 | 130.12 |
| 33 | E | 101 | LHG | C20-C19-C18 | -2.11 | 103.72 | 114.42 |
| 24 | T | 101 | BCR | C30-C25-C26 | -2.11 | 119.64 | 122.61 |
| 33 | E | 101 | LHG | C18-C17-C16 | -2.11 | 103.73 | 114.42 |
| 22 | c | 505 | CLA | CMC-C2C-C1C | 2.11 | 128.25 | 125.04 |
| 22 | C | 510 | CLA | C1B-CHB-C4A | -2.11 | 125.95 | 130.12 |
| 22 | C | 502 | CLA | C2A-C1A-CHA | 2.11 | 127.54 | 123.86 |
| 24 | K | 102 | BCR | C16-C15-C14 | -2.10 | 119.16 | 123.47 |
| 22 | C | 510 | CLA | CHA-C1A-NA | -2.10 | 121.58 | 126.40 |
| 24 | t | 101 | BCR | C2-C3-C4 | -2.10 | 106.67 | 111.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | f | 102 | SQD | O47-C7-O49 | -2.10 | 118.62 | 123.70 |
| 22 | a | 410 | CLA | C3C-C4C-NC | -2.10 | 108.22 | 110.57 |
| 22 | c | 505 | CLA | CHB-C4A-NA | 2.10 | 127.42 | 124.51 |
| 22 | b | 610 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 24 | b | 619 | BCR | C30-C25-C26 | -2.10 | 119.66 | 122.61 |
| 24 | b | 618 | BCR | C27-C26-C25 | 2.10 | 125.78 | 122.73 |
| 22 | C | 512 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 27 | D | 407 | LMG | O3-C3-C2 | -2.10 | 105.50 | 110.35 |
| 27 | A | 410 | LMG | C1-C2-C3 | -2.10 | 105.63 | 110.00 |
| 23 | d | 401 | PHO | CAA-CBA-CGA | -2.10 | 107.13 | 113.25 |
| 22 | c | 502 | CLA | CHB-C4A-NA | 2.09 | 127.41 | 124.51 |
| 24 | c | 516 | BCR | C15-C16-C17 | -2.09 | 119.18 | 123.47 |
| 22 | C | 503 | CLA | C1-C2-C3 | 2.09 | 129.66 | 126.04 |
| 22 | A | 403 | CLA | C1D-ND-C4D | 2.09 | 107.82 | 106.33 |
| 29 | c | 519 | DGD | CDB-CCB-CBB | -2.09 | 103.80 | 114.42 |
| 22 | B | 610 | CLA | C4D-CHA-C1A | 2.09 | 123.80 | 121.25 |
| 22 | C | 510 | CLA | O2A-CGA-O1A | -2.09 | 118.31 | 123.59 |
| 27 | a | 415 | LMG | C1-O6-C5 | -2.09 | 109.58 | 113.69 |
| 22 | B | 605 | CLA | CHD-C1D-C2D | 2.09 | 129.86 | 125.48 |
| 22 | B | 611 | CLA | C1-C2-C3 | -2.09 | 122.43 | 126.04 |
| 22 | b | 612 | CLA | C2D-C1D-ND | 2.09 | 111.64 | 110.10 |
| 22 | H | 101 | CLA | CHA-C4D-ND | 2.09 | 136.87 | 132.50 |
| 33 | D | 409 | LHG | C20-C19-C18 | -2.09 | 103.83 | 114.42 |
| 26 | D | 406 | PL9 | C20-C19-C21 | 2.09 | 118.78 | 115.27 |
| 22 | b | 613 | CLA | C2A-C1A-CHA | 2.09 | 127.51 | 123.86 |
| 22 | c | 506 | CLA | O1D-CGD-CBD | 2.08 | 128.75 | 124.48 |
| 22 | b | 601 | CLA | CBA-CAA-C2A | 2.08 | 120.02 | 113.86 |
| 29 | C | 517 | DGD | CDB-CCB-CBB | -2.08 | 103.84 | 114.42 |
| 27 | B | 621 | LMG | O9-C10-C11 | 2.08 | 129.78 | 123.08 |
| 28 | B | 622 | SQD | C1-C2-C3 | -2.08 | 105.66 | 110.00 |
| 22 | b | 608 | CLA | C2A-C3A-C4A | 2.08 | 105.23 | 101.87 |
| 22 | C | 502 | CLA | O2D-CGD-O1D | -2.08 | 119.76 | 123.84 |
| 29 | C | 516 | DGD | C4E-C3E-C2E | -2.08 | 107.19 | 110.82 |
| 29 | A | 413 | DGD | C5B-C4B-C3B | -2.08 | 103.85 | 114.42 |
| 22 | C | 513 | CLA | CHC-C1C-NC | 2.08 | 127.36 | 124.20 |
| 22 | b | 615 | CLA | CHA-C4D-ND | 2.08 | 136.85 | 132.50 |
| 22 | b | 615 | CLA | C1B-CHB-C4A | -2.08 | 126.00 | 130.12 |
| 26 | d | 406 | PL9 | O1-C4-C3 | -2.07 | 118.44 | 120.72 |
| 27 | b | 621 | LMG | C1-O6-C5 | -2.07 | 109.62 | 113.69 |
| 24 | c | 516 | BCR | C1-C6-C5 | -2.07 | 119.70 | 122.61 |
| 24 | b | 619 | BCR | C38-C26-C25 | -2.07 | 122.20 | 124.53 |
| 24 | h | 101 | BCR | C1-C6-C5 | -2.07 | 119.70 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | C | 516 | DGD | C8B-C7B-C6B | -2.07 | 103.93 | 114.42 |
| 22 | b | 616 | CLA | O2A-CGA-O1A | -2.07 | 118.38 | 123.59 |
| 24 | h | 101 | BCR | C16-C17-C18 | -2.07 | 124.36 | 127.31 |
| 24 | a | 406 | BCR | C24-C23-C22 | -2.07 | 123.11 | 126.23 |
| 29 | c | 517 | DGD | O3E-C3E-C2E | -2.06 | 105.58 | 110.35 |
| 29 | C | 515 | DGD | C9B-C8B-C7B | -2.06 | 103.95 | 114.42 |
| 29 | A | 413 | DGD | O5D-C1E-C2E | 2.06 | 111.52 | 108.30 |
| 22 | a | 410 | CLA | C2A-C1A-CHA | 2.06 | 127.46 | 123.86 |
| 22 | C | 503 | CLA | C3A-C2A-C1A | 2.06 | 104.42 | 101.34 |
| 33 | l | 101 | LHG | C20-C19-C18 | -2.06 | 103.98 | 114.42 |
| 22 | b | 605 | CLA | O1A-CGA-CBA | 2.06 | 131.75 | 123.73 |
| 22 | b | 609 | CLA | CHA-C4D-ND | 2.06 | 136.80 | 132.50 |
| 22 | B | 606 | CLA | O2D-CGD-O1D | -2.06 | 119.82 | 123.84 |
| 31 | m | 102 | STE | O2-C1-O1 | -2.05 | 118.18 | 123.30 |
| 22 | c | 513 | CLA | C1B-CHB-C4A | -2.05 | 126.05 | 130.12 |
| 22 | d | 403 | CLA | C2C-C1C-NC | 2.05 | 111.89 | 109.97 |
| 31 | d | 411 | STE | O2-C1-C2 | 2.05 | 120.62 | 114.03 |
| 31 | c | 521 | STE | O2-C1-C2 | 2.05 | 120.62 | 114.03 |
| 22 | b | 613 | CLA | C1B-CHB-C4A | -2.05 | 126.05 | 130.12 |
| 22 | C | 503 | CLA | C5-C3-C2 | -2.05 | 116.97 | 121.12 |
| 22 | C | 513 | CLA | O1D-CGD-CBD | 2.05 | 128.68 | 124.48 |
| 22 | B | 607 | CLA | CHC-C1C-C2C | -2.05 | 121.06 | 126.72 |
| 22 | D | 403 | CLA | C1D-ND-C4D | -2.05 | 104.88 | 106.33 |
| 22 | C | 508 | CLA | CHB-C4A-NA | 2.05 | 127.34 | 124.51 |
| 22 | B | 605 | CLA | C1B-CHB-C4A | -2.05 | 126.06 | 130.12 |
| 22 | B | 615 | CLA | C3B-C4B-NB | -2.05 | 106.56 | 109.21 |
| 26 | d | 406 | PL9 | C46-C47-C48 | -2.05 | 105.16 | 111.88 |
| 22 | c | 506 | CLA | CHD-C1D-ND | -2.05 | 122.57 | 124.45 |
| 28 | f | 102 | SQD | C45-O47-C7 | 2.05 | 122.83 | 117.79 |
| 29 | c | 518 | DGD | C8B-C7B-C6B | -2.04 | 104.05 | 114.42 |
| 24 | t | 101 | BCR | C1-C6-C5 | -2.04 | 119.74 | 122.61 |
| 33 | L | 102 | LHG | O6-P-O5 | -2.04 | 101.09 | 109.07 |
| 28 | a | 411 | SQD | O5-C5-C4 | 2.04 | 113.40 | 109.69 |
| 22 | a | 405 | CLA | O2A-CGA-O1A | -2.04 | 118.44 | 123.59 |
| 22 | A | 402 | CLA | C1D-ND-C4D | -2.04 | 104.89 | 106.33 |
| 22 | c | 513 | CLA | CHC-C1C-NC | 2.04 | 127.30 | 124.20 |
| 22 | c | 514 | CLA | CHD-C4C-NC | 2.04 | 127.42 | 124.20 |
| 22 | c | 511 | CLA | O2D-CGD-CBD | 2.04 | 114.89 | 111.27 |
| 24 | C | 514 | BCR | C15-C14-C13 | -2.04 | 124.40 | 127.31 |
| 29 | H | 103 | DGD | C8B-C7B-C6B | -2.04 | 104.08 | 114.42 |
| 27 | D | 407 | LMG | C38-C37-C36 | -2.04 | 104.09 | 114.42 |
| 22 | B | 612 | CLA | C4C-C3C-C2C | -2.04 | 103.93 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | c | 520 | LMG | O6-C1-O1 | -2.04 | 105.15 | 109.97 |
| 27 | a | 415 | LMG | O1-C1-C2 | 2.04 | 111.48 | 108.30 |
| 22 | b | 607 | CLA | O2A-C1-C2 | -2.03 | 103.29 | 108.64 |
| 22 | B | 614 | CLA | CHD-C1D-ND | -2.03 | 122.58 | 124.45 |
| 24 | B | 617 | BCR | C37-C22-C23 | 2.03 | 121.28 | 118.08 |
| 22 | c | 507 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 34 | V | 201 | HEC | CAD-CBD-CGD | -2.03 | 108.06 | 113.76 |
| 28 | D | 408 | SQD | C44-O6-C1 | 2.03 | 117.21 | 113.84 |
| 22 | C | 503 | CLA | C4D-CHA-C1A | 2.03 | 123.72 | 121.25 |
| 22 | c | 508 | CLA | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 22 | b | 607 | CLA | C4D-CHA-C1A | 2.03 | 123.72 | 121.25 |
| 22 | d | 404 | CLA | CHD-C1D-C2D | 2.03 | 129.74 | 125.48 |
| 22 | b | 605 | CLA | O2D-CGD-CBD | 2.03 | 114.88 | 111.27 |
| 26 | a | 409 | PL9 | C27-C28-C29 | -2.03 | 122.77 | 127.66 |
| 22 | a | 403 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 22 | b | 613 | CLA | O2A-CGA-O1A | -2.03 | 118.47 | 123.59 |
| 22 | B | 616 | CLA | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 22 | d | 404 | CLA | O2D-CGD-O1D | -2.03 | 119.87 | 123.84 |
| 22 | b | 610 | CLA | CMB-C2B-C1B | -2.03 | 125.35 | 128.46 |
| 27 | D | 411 | LMG | O7-C10-O9 | -2.03 | 118.80 | 123.70 |
| 22 | C | 504 | CLA | CHC-C1C-C2C | -2.03 | 121.11 | 126.72 |
| 22 | b | 612 | CLA | C1-C2-C3 | -2.03 | 122.54 | 126.04 |
| 22 | C | 504 | CLA | CHA-C1A-NA | -2.03 | 121.76 | 126.40 |
| 24 | t | 101 | BCR | C16-C15-C14 | -2.02 | 119.33 | 123.47 |
| 22 | B | 604 | CLA | C11-C12-C13 | -2.02 | 109.38 | 115.92 |
| 27 | D | 407 | LMG | O1-C1-C2 | -2.02 | 105.15 | 108.30 |
| 29 | C | 516 | DGD | O3G-C1D-C2D | -2.02 | 105.15 | 108.30 |
| 22 | b | 604 | CLA | C2A-C1A-CHA | 2.02 | 127.39 | 123.86 |
| 22 | C | 506 | CLA | C1B-CHB-C4A | -2.02 | 126.12 | 130.12 |
| 22 | C | 501 | CLA | C3D-C4D-ND | 2.02 | 113.50 | 110.24 |
| 22 | B | 610 | CLA | CMA-C3A-C4A | -2.02 | 106.35 | 111.77 |
| 22 | c | 510 | CLA | O2D-CGD-CBD | 2.02 | 114.86 | 111.27 |
| 22 | c | 509 | CLA | CMB-C2B-C3B | 2.02 | 128.45 | 124.68 |
| 28 | A | 411 | SQD | O5-C5-C4 | 2.02 | 113.36 | 109.69 |
| 22 | C | 501 | CLA | OBD-CAD-C3D | 2.02 | 133.38 | 128.52 |
| 22 | A | 403 | CLA | O2A-CGA-O1A | -2.02 | 118.50 | 123.59 |
| 22 | c | 514 | CLA | O1D-CGD-CBD | 2.02 | 128.61 | 124.48 |
| 29 | C | 516 | DGD | O3D-C3D-C4D | -2.02 | 105.69 | 110.35 |
| 28 | a | 411 | SQD | O8-S-O9 | -2.01 | 106.35 | 111.27 |
| 28 | B | 622 | SQD | O3-C3-C2 | -2.01 | 105.69 | 110.35 |
| 24 | b | 619 | BCR | C15-C16-C17 | -2.01 | 119.35 | 123.47 |
| 28 | L | 101 | SQD | O3-C3-C4 | 2.01 | 115.00 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | M | 101 | LMG | C32-C31-C30 | -2.01 | 104.21 | 114.42 |
| 22 | C | 510 | CLA | O2D-CGD-O1D | -2.01 | 119.90 | 123.84 |
| 22 | C | 507 | CLA | CHA-C4D-ND | 2.01 | 136.71 | 132.50 |
| 22 | C | 502 | CLA | CED-O2D-CGD | 2.01 | 120.49 | 115.94 |
| 24 | C | 514 | BCR | C29-C30-C25 | 2.01 | 113.58 | 110.48 |
| 22 | B | 604 | CLA | C6-C7-C8 | -2.01 | 109.42 | 115.92 |
| 24 | A | 406 | BCR | C38-C26-C27 | -2.01 | 109.75 | 113.62 |
| 24 | B | 618 | BCR | C40-C30-C25 | 2.01 | 113.56 | 110.30 |
| 27 | B | 621 | LMG | C30-C29-C28 | -2.01 | 109.41 | 114.47 |
| 22 | b | 610 | CLA | O2D-CGD-CBD | 2.01 | 114.84 | 111.27 |
| 33 | D | 410 | LHG | C6-C5-C4 | 2.01 | 116.53 | 111.79 |
| 24 | K | 102 | BCR | C38-C26-C25 | -2.00 | 122.28 | 124.53 |
| 22 | a | 405 | CLA | C1B-CHB-C4A | -2.00 | 126.15 | 130.12 |
| 22 | b | 615 | CLA | C5-C3-C2 | -2.00 | 117.06 | 121.12 |
| 34 | f | 101 | HEC | O1A-CGA-CBA | -2.00 | 116.65 | 123.08 |
| 24 | B | 617 | BCR | C15-C16-C17 | -2.00 | 119.37 | 123.47 |
| 22 | b | 601 | CLA | CHD-C1D-C2D | 2.00 | 129.68 | 125.48 |
| 22 | B | 611 | CLA | C4A-NA-C1A | 2.00 | 107.61 | 106.71 |
| 24 | A | 406 | BCR | C4-C5-C6 | 2.00 | 125.64 | 122.73 |
| 24 | b | 619 | BCR | C36-C18-C17 | -2.00 | 120.12 | 122.92 |

All (56) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 22 | A | 402 | CLA | ND |
| 22 | A | 405 | CLA | ND |
| 22 | B | 602 | CLA | ND |
| 22 | B | 603 | CLA | ND |
| 22 | B | 604 | CLA | ND |
| 22 | B | 605 | CLA | ND |
| 22 | B | 606 | CLA | ND |
| 22 | B | 607 | CLA | ND |
| 22 | B | 610 | CLA | ND |
| 22 | B | 611 | CLA | ND |
| 22 | B | 612 | CLA | ND |
| 22 | B | 613 | CLA | ND |
| 22 | B | 614 | CLA | ND |
| 22 | B | 615 | CLA | ND |
| 22 | B | 616 | CLA | ND |
| 22 | C | 501 | CLA | ND |
| 22 | C | 502 | CLA | ND |
| 22 | C | 503 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 22 | C | 504 | CLA | ND |
| 22 | C | 505 | CLA | ND |
| 22 | C | 506 | CLA | ND |
| 22 | C | 507 | CLA | ND |
| 22 | C | 509 | CLA | ND |
| 22 | C | 510 | CLA | ND |
| 22 | C | 511 | CLA | ND |
| 22 | C | 512 | CLA | ND |
| 22 | C | 513 | CLA | ND |
| 22 | D | 405 | CLA | ND |
| 22 | H | 101 | CLA | ND |
| 22 | a | 402 | CLA | ND |
| 22 | a | 405 | CLA | ND |
| 22 | b | 601 | CLA | ND |
| 22 | b | 603 | CLA | ND |
| 22 | b | 604 | CLA | ND |
| 22 | b | 605 | CLA | ND |
| 22 | b | 606 | CLA | ND |
| 22 | b | 607 | CLA | ND |
| 22 | b | 610 | CLA | ND |
| 22 | b | 611 | CLA | ND |
| 22 | b | 612 | CLA | ND |
| 22 | b | 613 | CLA | ND |
| 22 | b | 614 | CLA | ND |
| 22 | b | 615 | CLA | ND |
| 22 | b | 616 | CLA | ND |
| 22 | c | 502 | CLA | ND |
| 22 | c | 504 | CLA | ND |
| 22 | c | 505 | CLA | ND |
| 22 | c | 506 | CLA | ND |
| 22 | c | 507 | CLA | ND |
| 22 | c | 508 | CLA | ND |
| 22 | c | 510 | CLA | ND |
| 22 | c | 511 | CLA | ND |
| 22 | c | 512 | CLA | ND |
| 22 | c | 513 | CLA | ND |
| 22 | c | 514 | CLA | ND |
| 22 | d | 404 | CLA | ND |

All (1888) torsion outliers are listed below:

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | A | 405 | CLA | C2-C3-C5-C6 |
| 22 | A | 405 | CLA | C4-C3-C5-C6 |
| 22 | B | 606 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 606 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 614 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 614 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 614 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 614 | CLA | C4-C3-C5-C6 |
| 22 | C | 502 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 509 | CLA | C11-C10-C8-C9 |
| 22 | C | 512 | CLA | C11-C10-C8-C9 |
| 22 | D | 404 | CLA | CHA-CBD-CGD-O2D |
| 22 | a | 403 | CLA | CHA-CBD-CGD-O1D |
| 22 | a | 403 | CLA | CHA-CBD-CGD-O2D |
| 22 | a | 410 | CLA | CHA-CBD-CGD-O1D |
| 22 | a | 410 | CLA | CHA-CBD-CGD-O2D |
| 22 | b | 601 | CLA | C1A-C2A-CAA-CBA |
| 22 | b | 606 | CLA | CHA-CBD-CGD-O1D |
| 22 | b | 606 | CLA | CHA-CBD-CGD-O2D |
| 22 | b | 607 | CLA | C2-C3-C5-C6 |
| 22 | b | 607 | CLA | C4-C3-C5-C6 |
| 22 | b | 614 | CLA | CAD-CBD-CGD-O1D |
| 22 | b | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 507 | CLA | C12-C13-C15-C16 |
| 22 | c | 508 | CLA | C2-C3-C5-C6 |
| 22 | c | 508 | CLA | C4-C3-C5-C6 |
| 22 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 22 | c | 513 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 513 | CLA | C2A-CAA-CBA-CGA |
| 22 | c | 514 | CLA | CBD-CGD-O2D-CED |
| 24 | A | 406 | BCR | C7-C8-C9-C34 |
| 24 | A | 406 | BCR | C11-C12-C13-C14 |
| 24 | A | 406 | BCR | C20-C21-C22-C37 |
| 24 | A | 406 | BCR | C37-C22-C23-C24 |
| 24 | B | 617 | BCR | C1-C6-C7-C8 |
| 24 | B | 617 | BCR | C7-C8-C9-C34 |
| 24 | B | 617 | BCR | C35-C13-C14-C15 |
| 24 | B | 618 | BCR | C20-C21-C22-C37 |
| 24 | B | 618 | BCR | C37-C22-C23-C24 |
| 24 | B | 618 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | C | 514 | BCR | C16-C17-C18-C19 |
| 24 | C | 514 | BCR | C36-C18-C19-C20 |
| 24 | F | 101 | BCR | C23-C24-C25-C26 |
| 24 | F | 101 | BCR | C23-C24-C25-C30 |
| 24 | H | 102 | BCR | C11-C12-C13-C14 |
| 24 | H | 102 | BCR | C11-C12-C13-C35 |
| 24 | K | 101 | BCR | C16-C17-C18-C19 |
| 24 | K | 101 | BCR | C16-C17-C18-C36 |
| 24 | K | 102 | BCR | C1-C6-C7-C8 |
| 24 | K | 102 | BCR | C5-C6-C7-C8 |
| 24 | K | 102 | BCR | C21-C22-C23-C24 |
| 24 | K | 102 | BCR | C37-C22-C23-C24 |
| 24 | K | 103 | BCR | C7-C8-C9-C34 |
| 24 | T | 101 | BCR | C7-C8-C9-C10 |
| 24 | T | 101 | BCR | C11-C12-C13-C35 |
| 24 | T | 101 | BCR | C12-C13-C14-C15 |
| 24 | T | 101 | BCR | C16-C17-C18-C36 |
| 24 | T | 101 | BCR | C17-C18-C19-C20 |
| 24 | T | 101 | BCR | C36-C18-C19-C20 |
| 24 | T | 101 | BCR | C20-C21-C22-C37 |
| 24 | a | 406 | BCR | C36-C18-C19-C20 |
| 24 | a | 406 | BCR | C37-C22-C23-C24 |
| 24 | b | 617 | BCR | C36-C18-C19-C20 |
| 24 | b | 617 | BCR | C20-C21-C22-C37 |
| 24 | b | 618 | BCR | C23-C24-C25-C30 |
| 24 | b | 619 | BCR | C11-C12-C13-C35 |
| 24 | b | 619 | BCR | C16-C17-C18-C36 |
| 24 | b | 619 | BCR | C20-C21-C22-C37 |
| 24 | c | 515 | BCR | C11-C12-C13-C35 |
| 24 | c | 515 | BCR | C22-C23-C24-C25 |
| 24 | c | 516 | BCR | C36-C18-C19-C20 |
| 24 | k | 101 | BCR | C7-C8-C9-C34 |
| 24 | k | 101 | BCR | C35-C13-C14-C15 |
| 24 | k | 101 | BCR | C17-C18-C19-C20 |
| 24 | k | 101 | BCR | C36-C18-C19-C20 |
| 24 | k | 101 | BCR | C37-C22-C23-C24 |
| 24 | k | 102 | BCR | C35-C13-C14-C15 |
| 26 | A | 409 | PL9 | C23-C24-C26-C27 |
| 26 | A | 409 | PL9 | C32-C33-C34-C35 |
| 26 | A | 409 | PL9 | C32-C33-C34-C36 |
| 26 | A | 409 | PL9 | C37-C38-C39-C40 |
| 26 | A | 409 | PL9 | C37-C38-C39-C41 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | D | 406 | PL9 | C32-C33-C34-C36 |
| 26 | a | 409 | PL9 | C12-C13-C14-C16 |
| 26 | a | 409 | PL9 | C22-C23-C24-C25 |
| 26 | a | 409 | PL9 | C22-C23-C24-C26 |
| 26 | a | 409 | PL9 | C32-C33-C34-C36 |
| 26 | a | 409 | PL9 | C42-C43-C44-C45 |
| 26 | a | 409 | PL9 | C44-C46-C47-C48 |
| 26 | a | 409 | PL9 | C47-C48-C49-C50 |
| 26 | d | 406 | PL9 | C32-C33-C34-C36 |
| 26 | d | 406 | PL9 | C37-C38-C39-C41 |
| 26 | d | 406 | PL9 | C42-C43-C44-C45 |
| 26 | d | 406 | PL9 | C42-C43-C44-C46 |
| 26 | d | 406 | PL9 | C47-C48-C49-C51 |
| 27 | A | 410 | LMG | O9-C10-O7-C8 |
| 27 | b | 623 | LMG | C2-C1-O1-C7 |
| 27 | b | 623 | LMG | O6-C1-O1-C7 |
| 27 | c | 522 | LMG | O6-C1-O1-C7 |
| 27 | c | 523 | LMG | O6-C1-O1-C7 |
| 28 | B | 622 | SQD | C2-C1-O6-C44 |
| 28 | B | 622 | SQD | O5-C1-O6-C44 |
| 28 | B | 622 | SQD | O6-C44-C45-O47 |
| 28 | B | 622 | SQD | O49-C7-O47-C45 |
| 28 | B | 622 | SQD | C8-C7-O47-C45 |
| 28 | D | 408 | SQD | C45-C44-O6-C1 |
| 28 | D | 408 | SQD | C5-C6-S-O8 |
| 28 | L | 101 | SQD | C8-C7-O47-C45 |
| 28 | L | 101 | SQD | O10-C23-O48-C46 |
| 28 | L | 101 | SQD | C24-C23-O48-C46 |
| 28 | a | 412 | SQD | C8-C7-O47-C45 |
| 28 | a | 412 | SQD | O10-C23-O48-C46 |
| 28 | a | 412 | SQD | C24-C23-O48-C46 |
| 28 | f | 102 | SQD | O5-C1-O6-C44 |
| 28 | f | 102 | SQD | O49-C7-O47-C45 |
| 29 | A | 413 | DGD | C2B-C1B-O2G-C2G |
| 29 | A | 413 | DGD | O1B-C1B-O2G-C2G |
| 33 | D | 409 | LHG | O2-C2-C3-O3 |
| 33 | D | 409 | LHG | C3-O3-P-O4 |
| 33 | D | 409 | LHG | C4-O6-P-O4 |
| 33 | D | 410 | LHG | C1-C2-C3-O3 |
| 33 | D | 410 | LHG | C3-O3-P-O4 |
| 33 | D | 412 | LHG | O1-C1-C2-C3 |
| 33 | E | 101 | LHG | O1-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | E | 101 | LHG | O1-C1-C2-C3 |
| 33 | E | 101 | LHG | C4-O6-P-O4 |
| 33 | L | 102 | LHG | C3-O3-P-O4 |
| 33 | L | 102 | LHG | C4-O6-P-O4 |
| 33 | d | 408 | LHG | O1-C1-C2-C3 |
| 33 | d | 408 | LHG | C4-O6-P-O4 |
| 33 | d | 408 | LHG | C4-O6-P-O5 |
| 33 | e | 101 | LHG | O1-C1-C2-C3 |
| 33 | e | 101 | LHG | C1-C2-C3-O3 |
| 33 | e | 101 | LHG | C3-O3-P-O5 |
| 33 | l | 101 | LHG | C4-O6-P-O3 |
| 33 | l | 101 | LHG | C4-O6-P-O4 |
| 33 | l | 101 | LHG | C4-O6-P-O5 |
| 22 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 22 | b | 601 | CLA | CBD-CGD-O2D-CED |
| 22 | c | 512 | CLA | CBD-CGD-O2D-CED |
| 23 | d | 401 | PHO | CBD-CGD-O2D-CED |
| 27 | M | 101 | LMG | O10-C28-O8-C9 |
| 27 | c | 523 | LMG | O10-C28-O8-C9 |
| 28 | f | 102 | SQD | O10-C23-O48-C46 |
| 33 | e | 101 | LHG | O10-C23-O8-C6 |
| 22 | b | 601 | CLA | O1D-CGD-O2D-CED |
| 22 | d | 403 | CLA | C3-C5-C6-C7 |
| 28 | D | 408 | SQD | C24-C23-O48-C46 |
| 26 | a | 409 | PL9 | C47-C48-C49-C51 |
| 22 | b | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | d | 403 | CLA | CBD-CGD-O2D-CED |
| 28 | D | 408 | SQD | O10-C23-O48-C46 |
| 27 | D | 411 | LMG | O9-C10-O7-C8 |
| 28 | a | 412 | SQD | O49-C7-O47-C45 |
| 27 | c | 520 | LMG | C11-C10-O7-C8 |
| 22 | b | 614 | CLA | C3-C5-C6-C7 |
| 27 | M | 101 | LMG | C29-C28-O8-C9 |
| 27 | c | 523 | LMG | C29-C28-O8-C9 |
| 33 | e | 101 | LHG | C24-C23-O8-C6 |
| 27 | A | 410 | LMG | C11-C10-O7-C8 |
| 28 | f | 102 | SQD | C8-C7-O47-C45 |
| 22 | c | 514 | CLA | O1D-CGD-O2D-CED |
| 22 | C | 513 | CLA | C4-C3-C5-C6 |
| 26 | A | 409 | PL9 | C35-C34-C36-C37 |
| 22 | B | 614 | CLA | C2-C3-C5-C6 |
| 26 | d | 406 | PL9 | C38-C39-C41-C42 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | C | 511 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 403 | CLA | C3-C5-C6-C7 |
| 22 | C | 513 | CLA | CBA-CGA-O2A-C1 |
| 27 | a | 415 | LMG | C29-C28-O8-C9 |
| 29 | h | 102 | DGD | O6E-C5E-C6E-O5E |
| 22 | c | 512 | CLA | O1D-CGD-O2D-CED |
| 26 | d | 406 | PL9 | C47-C48-C49-C50 |
| 26 | A | 409 | PL9 | C12-C13-C14-C15 |
| 22 | c | 507 | CLA | CBD-CGD-O2D-CED |
| 23 | d | 401 | PHO | O1D-CGD-O2D-CED |
| 26 | A | 409 | PL9 | C22-C23-C24-C26 |
| 27 | c | 522 | LMG | O10-C28-O8-C9 |
| 27 | c | 520 | LMG | O9-C10-O7-C8 |
| 22 | B | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 501 | CLA | CBD-CGD-O2D-CED |
| 22 | b | 616 | CLA | CBD-CGD-O2D-CED |
| 33 | D | 410 | LHG | O2-C2-C3-O3 |
| 33 | E | 101 | LHG | O2-C2-C3-O3 |
| 33 | e | 101 | LHG | O2-C2-C3-O3 |
| 22 | C | 513 | CLA | C3-C5-C6-C7 |
| 27 | Y | 101 | LMG | C29-C28-O8-C9 |
| 29 | A | 413 | DGD | C2A-C1A-O1G-C1G |
| 26 | A | 409 | PL9 | C47-C48-C49-C50 |
| 22 | c | 503 | CLA | CBD-CGD-O2D-CED |
| 27 | c | 522 | LMG | O6-C5-C6-O5 |
| 29 | C | 515 | DGD | O6E-C5E-C6E-O5E |
| 33 | E | 101 | LHG | C24-C25-C26-C27 |
| 29 | H | 103 | DGD | C4E-C5E-C6E-O5E |
| 33 | D | 409 | LHG | C23-C24-C25-C26 |
| 33 | l | 101 | LHG | C7-C8-C9-C10 |
| 28 | f | 102 | SQD | C24-C23-O48-C46 |
| 27 | M | 101 | LMG | O6-C5-C6-O5 |
| 29 | A | 413 | DGD | O6E-C5E-C6E-O5E |
| 27 | b | 621 | LMG | O9-C10-O7-C8 |
| 28 | L | 101 | SQD | O49-C7-O47-C45 |
| 29 | h | 102 | DGD | C4E-C5E-C6E-O5E |
| 22 | C | 513 | CLA | O1A-CGA-O2A-C1 |
| 27 | a | 415 | LMG | O10-C28-O8-C9 |
| 26 | A | 409 | PL9 | C47-C48-C49-C51 |
| 26 | D | 406 | PL9 | C47-C48-C49-C51 |
| 26 | a | 409 | PL9 | C33-C34-C36-C37 |
| 26 | A | 409 | PL9 | C9-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | A | 409 | PL9 | C14-C16-C17-C18 |
| 26 | a | 409 | PL9 | C19-C21-C22-C23 |
| 26 | a | 409 | PL9 | C24-C26-C27-C28 |
| 26 | a | 409 | PL9 | C34-C36-C37-C38 |
| 26 | d | 406 | PL9 | C34-C36-C37-C38 |
| 27 | c | 522 | LMG | C29-C28-O8-C9 |
| 28 | B | 622 | SQD | C24-C23-O48-C46 |
| 27 | M | 101 | LMG | C4-C5-C6-O5 |
| 27 | a | 415 | LMG | C4-C5-C6-O5 |
| 31 | B | 627 | STE | C5-C6-C7-C8 |
| 27 | Y | 101 | LMG | C11-C10-O7-C8 |
| 31 | B | 626 | STE | C11-C12-C13-C14 |
| 26 | A | 409 | PL9 | C22-C23-C24-C25 |
| 26 | a | 409 | PL9 | C42-C43-C44-C46 |
| 22 | A | 405 | CLA | C3-C5-C6-C7 |
| 22 | b | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | c | 507 | CLA | CBA-CGA-O2A-C1 |
| 29 | c | 519 | DGD | C2A-C1A-O1G-C1G |
| 27 | A | 410 | LMG | O6-C5-C6-O5 |
| 29 | A | 413 | DGD | C4E-C5E-C6E-O5E |
| 22 | C | 509 | CLA | C13-C15-C16-C17 |
| 22 | a | 405 | CLA | C10-C11-C12-C13 |
| 22 | b | 611 | CLA | C13-C15-C16-C17 |
| 22 | c | 512 | CLA | C15-C16-C17-C18 |
| 27 | A | 410 | LMG | C28-C29-C30-C31 |
| 27 | c | 523 | LMG | C2-C1-O1-C7 |
| 28 | f | 102 | SQD | C2-C1-O6-C44 |
| 28 | a | 411 | SQD | O6-C44-C45-O47 |
| 29 | c | 519 | DGD | O1A-C1A-O1G-C1G |
| 22 | C | 507 | CLA | C4-C3-C5-C6 |
| 22 | b | 616 | CLA | C4-C3-C5-C6 |
| 22 | C | 513 | CLA | C2-C3-C5-C6 |
| 22 | A | 403 | CLA | C14-C13-C15-C16 |
| 22 | B | 606 | CLA | C11-C10-C8-C9 |
| 22 | C | 506 | CLA | C6-C7-C8-C9 |
| 22 | C | 513 | CLA | C6-C7-C8-C9 |
| 22 | H | 101 | CLA | C11-C12-C13-C14 |
| 22 | b | 605 | CLA | C11-C10-C8-C9 |
| 22 | c | 510 | CLA | C6-C7-C8-C9 |
| 22 | c | 510 | CLA | C11-C12-C13-C14 |
| 22 | c | 511 | CLA | C11-C10-C8-C9 |
| 23 | A | 404 | PHO | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 22 | b | 604 | CLA | C10-C11-C12-C13 |
| 24 | F | 101 | BCR | C37-C22-C23-C24 |
| 24 | b | 619 | BCR | C7-C8-C9-C34 |
| 24 | d | 405 | BCR | C37-C22-C23-C24 |
| 24 | c | 515 | BCR | C11-C12-C13-C14 |
| 24 | d | 405 | BCR | C21-C22-C23-C24 |
| 27 | b | 623 | LMG | O9-C10-O7-C8 |
| 31 | C | 520 | STE | C4-C5-C6-C7 |
| 33 | d | 409 | LHG | C24-C25-C26-C27 |
| 27 | A | 410 | LMG | C4-C5-C6-O5 |
| 27 | M | 101 | LMG | C10-C11-C12-C13 |
| 31 | B | 601 | STE | C1-C2-C3-C4 |
| 33 | e | 101 | LHG | C23-C24-C25-C26 |
| 27 | b | 623 | LMG | O10-C28-O8-C9 |
| 22 | A | 402 | CLA | C15-C16-C17-C18 |
| 22 | b | 601 | CLA | C3-C5-C6-C7 |
| 34 | f | 101 | HEC | C2A-CAA-CBA-CGA |
| 22 | B | 609 | CLA | C13-C15-C16-C17 |
| 22 | C | 504 | CLA | C8-C10-C11-C12 |
| 22 | D | 403 | CLA | C15-C16-C17-C18 |
| 22 | b | 603 | CLA | C5-C6-C7-C8 |
| 22 | b | 608 | CLA | C13-C15-C16-C17 |
| 28 | A | 411 | SQD | C7-C8-C9-C10 |
| 28 | B | 622 | SQD | C23-C24-C25-C26 |
| 29 | c | 517 | DGD | C1B-C2B-C3B-C4B |
| 22 | c | 504 | CLA | CBD-CGD-O2D-CED |
| 29 | H | 103 | DGD | O6E-C5E-C6E-O5E |
| 22 | B | 603 | CLA | C8-C10-C11-C12 |
| 22 | B | 606 | CLA | C15-C16-C17-C18 |
| 22 | B | 615 | CLA | C5-C6-C7-C8 |
| 22 | C | 505 | CLA | C5-C6-C7-C8 |
| 22 | C | 513 | CLA | C15-C16-C17-C18 |
| 22 | D | 404 | CLA | C13-C15-C16-C17 |
| 22 | D | 405 | CLA | C13-C15-C16-C17 |
| 22 | a | 403 | CLA | C8-C10-C11-C12 |
| 22 | b | 606 | CLA | C15-C16-C17-C18 |
| 22 | b | 607 | CLA | C10-C11-C12-C13 |
| 22 | b | 611 | CLA | C8-C10-C11-C12 |
| 22 | b | 616 | CLA | C10-C11-C12-C13 |
| 22 | c | 504 | CLA | C8-C10-C11-C12 |
| 22 | c | 506 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 510 | CLA | C10-C11-C12-C13 |
| 22 | d | 403 | CLA | O1D-CGD-O2D-CED |
| 26 | a | 409 | PL9 | C12-C13-C14-C15 |
| 27 | D | 411 | LMG | C10-C11-C12-C13 |
| 27 | d | 410 | LMG | C28-C29-C30-C31 |
| 28 | L | 101 | SQD | C23-C24-C25-C26 |
| 31 | C | 518 | STE | C1-C2-C3-C4 |
| 22 | d | 404 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 403 | CLA | C13-C15-C16-C17 |
| 22 | B | 605 | CLA | C15-C16-C17-C18 |
| 22 | B | 612 | CLA | C13-C15-C16-C17 |
| 22 | c | 506 | CLA | C15-C16-C17-C18 |
| 22 | B | 614 | CLA | C13-C15-C16-C17 |
| 22 | C | 505 | CLA | C10-C11-C12-C13 |
| 22 | C | 512 | CLA | C10-C11-C12-C13 |
| 22 | C | 513 | CLA | C5-C6-C7-C8 |
| 22 | b | 606 | CLA | C10-C11-C12-C13 |
| 27 | D | 407 | LMG | C10-C11-C12-C13 |
| 22 | B | 607 | CLA | C15-C16-C17-C18 |
| 22 | b | 605 | CLA | C5-C6-C7-C8 |
| 22 | C | 508 | CLA | C12-C13-C15-C16 |
| 22 | a | 402 | CLA | C12-C13-C15-C16 |
| 22 | b | 614 | CLA | C11-C12-C13-C15 |
| 22 | c | 507 | CLA | O1A-CGA-O2A-C1 |
| 33 | E | 101 | LHG | C27-C28-C29-C30 |
| 22 | B | 616 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 606 | CLA | C13-C15-C16-C17 |
| 22 | B | 607 | CLA | C13-C15-C16-C17 |
| 22 | C | 511 | CLA | C8-C10-C11-C12 |
| 22 | a | 405 | CLA | C15-C16-C17-C18 |
| 22 | b | 605 | CLA | C15-C16-C17-C18 |
| 22 | b | 614 | CLA | C5-C6-C7-C8 |
| 29 | C | 515 | DGD | C4E-C5E-C6E-O5E |
| 28 | A | 412 | SQD | C44-C45-O47-C7 |
| 28 | A | 412 | SQD | C46-C45-O47-C7 |
| 22 | C | 513 | CLA | CBD-CGD-O2D-CED |
| 29 | C | 516 | DGD | O6E-C1E-O5D-C6D |
| 22 | c | 512 | CLA | C13-C15-C16-C17 |
| 26 | A | 409 | PL9 | C19-C21-C22-C23 |
| 26 | A | 409 | PL9 | C24-C26-C27-C28 |
| 26 | A | 409 | PL9 | C34-C36-C37-C38 |
| 26 | A | 409 | PL9 | C44-C46-C47-C48 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | c | 522 | LMG | C10-C11-C12-C13 |
| 29 | c | 518 | DGD | C1A-C2A-C3A-C4A |
| 31 | j | 101 | STE | C1-C2-C3-C4 |
| 24 | B | 618 | BCR | C18-C19-C20-C21 |
| 24 | K | 101 | BCR | C18-C19-C20-C21 |
| 24 | K | 102 | BCR | C10-C11-C12-C13 |
| 24 | c | 515 | BCR | C18-C19-C20-C21 |
| 24 | d | 405 | BCR | C10-C11-C12-C13 |
| 33 | d | 407 | LHG | O2-C2-C3-O3 |
| 22 | B | 603 | CLA | C13-C15-C16-C17 |
| 22 | C | 506 | CLA | C8-C10-C11-C12 |
| 22 | C | 506 | CLA | C13-C15-C16-C17 |
| 22 | b | 616 | CLA | C8-C10-C11-C12 |
| 22 | B | 606 | CLA | C8-C10-C11-C12 |
| 22 | C | 502 | CLA | C13-C15-C16-C17 |
| 22 | a | 405 | CLA | C5-C6-C7-C8 |
| 22 | b | 615 | CLA | C5-C6-C7-C8 |
| 27 | a | 415 | LMG | C12-C13-C14-C15 |
| 33 | D | 409 | LHG | C3-O3-P-O6 |
| 33 | D | 410 | LHG | C3-O3-P-O6 |
| 33 | d | 408 | LHG | C4-O6-P-O3 |
| 33 | e | 101 | LHG | C3-O3-P-O6 |
| 29 | C | 515 | DGD | C1B-C2B-C3B-C4B |
| 22 | B | 608 | CLA | C3-C5-C6-C7 |
| 22 | b | 602 | CLA | C15-C16-C17-C18 |
| 22 | b | 605 | CLA | C10-C11-C12-C13 |
| 33 | D | 409 | LHG | C1-C2-C3-O3 |
| 33 | E | 101 | LHG | C1-C2-C3-O3 |
| 33 | d | 407 | LHG | C1-C2-C3-O3 |
| 22 | c | 513 | CLA | C13-C15-C16-C17 |
| 22 | B | 606 | CLA | C2A-CAA-CBA-CGA |
| 22 | b | 606 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 615 | CLA | C16-C17-C18-C20 |
| 22 | C | 502 | CLA | C16-C17-C18-C20 |
| 22 | b | 615 | CLA | C16-C17-C18-C19 |
| 22 | D | 403 | CLA | C3-C5-C6-C7 |
| 27 | c | 522 | LMG | C4-C5-C6-O5 |
| 27 | c | 520 | LMG | C36-C37-C38-C39 |
| 29 | C | 515 | DGD | C3B-C4B-C5B-C6B |
| 29 | C | 517 | DGD | C8A-C9A-CAA-CBA |
| 29 | c | 519 | DGD | C5B-C6B-C7B-C8B |
| 29 | h | 102 | DGD | C6B-C7B-C8B-C9B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | c | 521 | STE | C9-C10-C11-C12 |
| 24 | A | 406 | BCR | C11-C10-C9-C34 |
| 24 | A | 406 | BCR | C35-C13-C14-C15 |
| 24 | B | 618 | BCR | C35-C13-C14-C15 |
| 24 | B | 619 | BCR | C11-C10-C9-C34 |
| 24 | B | 619 | BCR | C20-C21-C22-C37 |
| 24 | C | 514 | BCR | C16-C17-C18-C36 |
| 24 | F | 101 | BCR | C35-C13-C14-C15 |
| 24 | F | 101 | BCR | C20-C21-C22-C37 |
| 24 | K | 103 | BCR | C11-C10-C9-C34 |
| 24 | K | 103 | BCR | C35-C13-C14-C15 |
| 24 | T | 101 | BCR | C35-C13-C14-C15 |
| 24 | b | 617 | BCR | C35-C13-C14-C15 |
| 24 | b | 618 | BCR | C35-C13-C14-C15 |
| 24 | b | 618 | BCR | C16-C17-C18-C36 |
| 24 | b | 619 | BCR | C35-C13-C14-C15 |
| 24 | c | 515 | BCR | C35-C13-C14-C15 |
| 24 | c | 516 | BCR | C16-C17-C18-C36 |
| 24 | c | 516 | BCR | C20-C21-C22-C37 |
| 24 | d | 405 | BCR | C35-C13-C14-C15 |
| 24 | t | 101 | BCR | C11-C10-C9-C34 |
| 24 | t | 101 | BCR | C35-C13-C14-C15 |
| 24 | t | 101 | BCR | C16-C17-C18-C36 |
| 27 | b | 621 | LMG | C16-C17-C18-C19 |
| 27 | b | 623 | LMG | C32-C33-C34-C35 |
| 27 | c | 523 | LMG | C15-C16-C17-C18 |
| 28 | a | 411 | SQD | C18-C19-C20-C21 |
| 29 | C | 515 | DGD | C5B-C6B-C7B-C8B |
| 29 | c | 517 | DGD | C4A-C5A-C6A-C7A |
| 29 | h | 102 | DGD | C6A-C7A-C8A-C9A |
| 31 | B | 625 | STE | C11-C12-C13-C14 |
| 31 | C | 518 | STE | C4-C5-C6-C7 |
| 31 | c | 521 | STE | C7-C8-C9-C10 |
| 33 | E | 101 | LHG | C18-C19-C20-C21 |
| 33 | E | 101 | LHG | C32-C33-C34-C35 |
| 33 | d | 407 | LHG | C17-C18-C19-C20 |
| 33 | d | 407 | LHG | C28-C29-C30-C31 |
| 33 | d | 408 | LHG | C13-C14-C15-C16 |
| 33 | l | 101 | LHG | C17-C18-C19-C20 |
| 22 | c | 507 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 616 | CLA | C11-C12-C13-C15 |
| 22 | c | 504 | CLA | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 604 | CLA | CBA-CGA-O2A-C1 |
| 28 | L | 101 | SQD | C26-C27-C28-C29 |
| 29 | C | 516 | DGD | C7A-C8A-C9A-CAA |
| 29 | c | 519 | DGD | C4A-C5A-C6A-C7A |
| 27 | b | 623 | LMG | C9-C8-O7-C10 |
| 28 | L | 101 | SQD | C46-C45-O47-C7 |
| 31 | B | 624 | STE | C1-C2-C3-C4 |
| 27 | A | 410 | LMG | C31-C32-C33-C34 |
| 28 | a | 411 | SQD | C9-C10-C11-C12 |
| 29 | c | 517 | DGD | C6B-C7B-C8B-C9B |
| 29 | c | 519 | DGD | CCB-CDB-CEB-CFB |
| 31 | Z | 101 | STE | C11-C12-C13-C14 |
| 31 | d | 412 | STE | C5-C6-C7-C8 |
| 33 | D | 410 | LHG | C29-C30-C31-C32 |
| 33 | d | 408 | LHG | C26-C27-C28-C29 |
| 22 | B | 613 | CLA | O1D-CGD-O2D-CED |
| 27 | a | 415 | LMG | O6-C5-C6-O5 |
| 27 | M | 101 | LMG | C37-C38-C39-C40 |
| 27 | a | 415 | LMG | C36-C37-C38-C39 |
| 31 | B | 623 | STE | C11-C10-C9-C8 |
| 31 | B | 627 | STE | C9-C10-C11-C12 |
| 31 | E | 102 | STE | C6-C7-C8-C9 |
| 33 | E | 101 | LHG | C12-C13-C14-C15 |
| 22 | c | 503 | CLA | O1D-CGD-O2D-CED |
| 28 | A | 411 | SQD | C10-C11-C12-C13 |
| 28 | a | 412 | SQD | C14-C15-C16-C17 |
| 31 | H | 104 | STE | C4-C5-C6-C7 |
| 31 | b | 622 | STE | C6-C7-C8-C9 |
| 31 | m | 101 | STE | C9-C10-C11-C12 |
| 31 | m | 101 | STE | C10-C11-C12-C13 |
| 33 | D | 410 | LHG | C25-C26-C27-C28 |
| 33 | L | 102 | LHG | C14-C15-C16-C17 |
| 27 | M | 101 | LMG | C28-C29-C30-C31 |
| 33 | d | 407 | LHG | C23-C24-C25-C26 |
| 22 | C | 511 | CLA | O1D-CGD-O2D-CED |
| 22 | b | 616 | CLA | O1D-CGD-O2D-CED |
| 24 | B | 617 | BCR | C11-C10-C9-C8 |
| 24 | B | 617 | BCR | C12-C13-C14-C15 |
| 24 | B | 619 | BCR | C12-C13-C14-C15 |
| 24 | C | 514 | BCR | C12-C13-C14-C15 |
| 24 | K | 101 | BCR | C11-C10-C9-C8 |
| 24 | T | 101 | BCR | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | b | 617 | BCR | C20-C21-C22-C23 |
| 24 | h | 101 | BCR | C11-C10-C9-C8 |
| 24 | k | 101 | BCR | C12-C13-C14-C15 |
| 28 | D | 408 | SQD | C2-C1-O6-C44 |
| 29 | C | 516 | DGD | C2E-C1E-O5D-C6D |
| 29 | c | 518 | DGD | C2E-C1E-O5D-C6D |
| 27 | D | 407 | LMG | C15-C16-C17-C18 |
| 27 | M | 101 | LMG | C32-C33-C34-C35 |
| 27 | a | 415 | LMG | C14-C15-C16-C17 |
| 27 | b | 621 | LMG | C33-C34-C35-C36 |
| 28 | A | 412 | SQD | C15-C16-C17-C18 |
| 28 | a | 411 | SQD | C34-C35-C36-C37 |
| 28 | f | 102 | SQD | C33-C34-C35-C36 |
| 29 | C | 516 | DGD | C3A-C4A-C5A-C6A |
| 31 | B | 624 | STE | C6-C7-C8-C9 |
| 31 | I | 101 | STE | C7-C8-C9-C10 |
| 33 | d | 408 | LHG | C29-C30-C31-C32 |
| 22 | B | 609 | CLA | C16-C17-C18-C19 |
| 22 | a | 402 | CLA | C16-C17-C18-C20 |
| 22 | c | 513 | CLA | C16-C17-C18-C20 |
| 22 | C | 510 | CLA | C4-C3-C5-C6 |
| 22 | b | 609 | CLA | C4-C3-C5-C6 |
| 26 | D | 406 | PL9 | C30-C29-C31-C32 |
| 26 | a | 409 | PL9 | C15-C14-C16-C17 |
| 27 | A | 410 | LMG | C16-C17-C18-C19 |
| 27 | c | 522 | LMG | C31-C32-C33-C34 |
| 29 | A | 413 | DGD | C5B-C6B-C7B-C8B |
| 29 | c | 518 | DGD | C2A-C3A-C4A-C5A |
| 31 | b | 620 | STE | C6-C7-C8-C9 |
| 31 | d | 412 | STE | C3-C4-C5-C6 |
| 31 | d | 412 | STE | C11-C12-C13-C14 |
| 33 | d | 408 | LHG | C28-C29-C30-C31 |
| 22 | C | 510 | CLA | C2-C3-C5-C6 |
| 22 | b | 616 | CLA | C2-C3-C5-C6 |
| 22 | B | 604 | CLA | C11-C10-C8-C9 |
| 22 | C | 508 | CLA | C11-C10-C8-C9 |
| 22 | C | 511 | CLA | C6-C7-C8-C9 |
| 22 | C | 512 | CLA | C11-C12-C13-C14 |
| 22 | a | 402 | CLA | C14-C13-C15-C16 |
| 22 | b | 601 | CLA | C11-C12-C13-C14 |
| 22 | b | 607 | CLA | C11-C10-C8-C9 |
| 22 | b | 616 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 503 | CLA | C11-C12-C13-C14 |
| 22 | c | 507 | CLA | C14-C13-C15-C16 |
| 22 | c | 513 | CLA | C14-C13-C15-C16 |
| 27 | b | 623 | LMG | C28-C29-C30-C31 |
| 27 | c | 522 | LMG | C30-C31-C32-C33 |
| 28 | B | 622 | SQD | C33-C34-C35-C36 |
| 28 | L | 101 | SQD | C24-C25-C26-C27 |
| 29 | c | 517 | DGD | C4B-C5B-C6B-C7B |
| 29 | h | 102 | DGD | C2B-C3B-C4B-C5B |
| 31 | B | 626 | STE | C4-C5-C6-C7 |
| 31 | T | 102 | STE | C10-C11-C12-C13 |
| 31 | d | 413 | STE | C9-C10-C11-C12 |
| 31 | d | 413 | STE | C10-C11-C12-C13 |
| 33 | D | 409 | LHG | C31-C32-C33-C34 |
| 33 | E | 101 | LHG | C30-C31-C32-C33 |
| 33 | d | 407 | LHG | C16-C17-C18-C19 |
| 22 | C | 512 | CLA | C13-C15-C16-C17 |
| 22 | b | 603 | CLA | C8-C10-C11-C12 |
| 22 | b | 615 | CLA | C15-C16-C17-C18 |
| 22 | c | 507 | CLA | C13-C15-C16-C17 |
| 27 | A | 410 | LMG | C12-C13-C14-C15 |
| 27 | D | 411 | LMG | C34-C35-C36-C37 |
| 27 | Y | 101 | LMG | C36-C37-C38-C39 |
| 27 | a | 415 | LMG | C13-C14-C15-C16 |
| 27 | b | 623 | LMG | C19-C20-C21-C22 |
| 27 | c | 520 | LMG | C39-C40-C41-C42 |
| 29 | C | 517 | DGD | C9A-CAA-CBA-CCA |
| 29 | h | 102 | DGD | C5B-C6B-C7B-C8B |
| 31 | B | 626 | STE | C5-C6-C7-C8 |
| 31 | c | 521 | STE | C6-C7-C8-C9 |
| 33 | l | 101 | LHG | C29-C30-C31-C32 |
| 33 | d | 407 | LHG | O1-C1-C2-C3 |
| 33 | d | 409 | LHG | O1-C1-C2-C3 |
| 22 | b | 602 | CLA | C3-C5-C6-C7 |
| 27 | D | 407 | LMG | C17-C18-C19-C20 |
| 27 | d | 410 | LMG | C38-C39-C40-C41 |
| 28 | B | 622 | SQD | C11-C12-C13-C14 |
| 33 | D | 410 | LHG | C34-C35-C36-C37 |
| 33 | L | 102 | LHG | C30-C31-C32-C33 |
| 27 | D | 407 | LMG | C12-C13-C14-C15 |
| 27 | D | 407 | LMG | C30-C31-C32-C33 |
| 27 | M | 101 | LMG | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | c | 523 | LMG | C17-C18-C19-C20 |
| 27 | c | 523 | LMG | C31-C32-C33-C34 |
| 28 | a | 412 | SQD | C11-C12-C13-C14 |
| 28 | f | 102 | SQD | C24-C25-C26-C27 |
| 29 | A | 413 | DGD | C4B-C5B-C6B-C7B |
| 29 | C | 516 | DGD | C4A-C5A-C6A-C7A |
| 29 | C | 516 | DGD | C6A-C7A-C8A-C9A |
| 29 | C | 517 | DGD | CBA-CCA-CDA-CEA |
| 29 | h | 102 | DGD | C3A-C4A-C5A-C6A |
| 31 | B | 620 | STE | C10-C11-C12-C13 |
| 31 | B | 625 | STE | C2-C3-C4-C5 |
| 31 | H | 104 | STE | C6-C7-C8-C9 |
| 31 | M | 102 | STE | C7-C8-C9-C10 |
| 31 | M | 102 | STE | C11-C10-C9-C8 |
| 31 | b | 624 | STE | C3-C4-C5-C6 |
| 31 | b | 627 | STE | C10-C11-C12-C13 |
| 31 | d | 411 | STE | C2-C3-C4-C5 |
| 31 | m | 102 | STE | C3-C4-C5-C6 |
| 33 | d | 408 | LHG | C34-C35-C36-C37 |
| 33 | e | 101 | LHG | C16-C17-C18-C19 |
| 33 | l | 101 | LHG | C32-C33-C34-C35 |
| 22 | B | 609 | CLA | C16-C17-C18-C20 |
| 22 | c | 513 | CLA | C16-C17-C18-C19 |
| 29 | c | 518 | DGD | O6E-C1E-O5D-C6D |
| 27 | Y | 101 | LMG | C13-C14-C15-C16 |
| 27 | b | 621 | LMG | C37-C38-C39-C40 |
| 27 | b | 623 | LMG | C18-C19-C20-C21 |
| 29 | c | 519 | DGD | C9A-CAA-CBA-CCA |
| 33 | D | 409 | LHG | C29-C30-C31-C32 |
| 33 | D | 409 | LHG | C34-C35-C36-C37 |
| 33 | D | 410 | LHG | C13-C14-C15-C16 |
| 33 | L | 102 | LHG | C12-C13-C14-C15 |
| 33 | d | 408 | LHG | C11-C12-C13-C14 |
| 22 | d | 404 | CLA | O1D-CGD-O2D-CED |
| 27 | d | 410 | LMG | C36-C37-C38-C39 |
| 29 | A | 413 | DGD | C8B-C9B-CAB-CBB |
| 29 | H | 103 | DGD | C7B-C8B-C9B-CAB |
| 29 | c | 517 | DGD | C3B-C4B-C5B-C6B |
| 29 | c | 518 | DGD | C8B-C9B-CAB-CBB |
| 31 | B | 601 | STE | C5-C6-C7-C8 |
| 33 | E | 101 | LHG | C13-C14-C15-C16 |
| 33 | L | 102 | LHG | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | f | 102 | SQD | C23-C24-C25-C26 |
| 22 | B | 602 | CLA | C13-C15-C16-C17 |
| 28 | D | 408 | SQD | C27-C28-C29-C30 |
| 31 | b | 622 | STE | C5-C6-C7-C8 |
| 28 | a | 411 | SQD | C24-C23-O48-C46 |
| 27 | a | 415 | LMG | C38-C39-C40-C41 |
| 28 | a | 411 | SQD | C15-C16-C17-C18 |
| 29 | C | 515 | DGD | C4B-C5B-C6B-C7B |
| 31 | D | 413 | STE | C4-C5-C6-C7 |
| 31 | M | 102 | STE | C6-C7-C8-C9 |
| 31 | d | 411 | STE | C4-C5-C6-C7 |
| 33 | d | 409 | LHG | C26-C27-C28-C29 |
| 22 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 22 | H | 101 | CLA | C3A-C2A-CAA-CBA |
| 22 | b | 601 | CLA | C3A-C2A-CAA-CBA |
| 22 | c | 513 | CLA | C3A-C2A-CAA-CBA |
| 22 | b | 612 | CLA | C13-C15-C16-C17 |
| 22 | b | 615 | CLA | C8-C10-C11-C12 |
| 27 | A | 410 | LMG | C35-C36-C37-C38 |
| 28 | a | 412 | SQD | C15-C16-C17-C18 |
| 29 | H | 103 | DGD | C7A-C8A-C9A-CAA |
| 31 | c | 521 | STE | C11-C12-C13-C14 |
| 33 | D | 410 | LHG | C9-C10-C11-C12 |
| 22 | a | 402 | CLA | C16-C17-C18-C19 |
| 27 | M | 101 | LMG | C35-C36-C37-C38 |
| 27 | c | 522 | LMG | C14-C15-C16-C17 |
| 27 | c | 522 | LMG | C39-C40-C41-C42 |
| 29 | H | 103 | DGD | C6B-C7B-C8B-C9B |
| 31 | T | 102 | STE | C7-C8-C9-C10 |
| 31 | b | 620 | STE | C9-C10-C11-C12 |
| 33 | e | 101 | LHG | C27-C28-C29-C30 |
| 28 | f | 102 | SQD | C28-C29-C30-C31 |
| 29 | C | 516 | DGD | C5A-C6A-C7A-C8A |
| 31 | D | 413 | STE | C9-C10-C11-C12 |
| 31 | d | 411 | STE | C6-C7-C8-C9 |
| 27 | b | 623 | LMG | C38-C39-C40-C41 |
| 27 | c | 522 | LMG | C38-C39-C40-C41 |
| 28 | L | 101 | SQD | C13-C14-C15-C16 |
| 31 | b | 622 | STE | C12-C13-C14-C15 |
| 31 | c | 521 | STE | C3-C4-C5-C6 |
| 31 | d | 413 | STE | C12-C13-C14-C15 |
| 22 | B | 613 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | C | 507 | CLA | C2-C3-C5-C6 |
| 27 | D | 411 | LMG | C11-C10-O7-C8 |
| 29 | C | 516 | DGD | CCA-CDA-CEA-CFA |
| 29 | c | 517 | DGD | CBB-CCB-CDB-CEB |
| 31 | b | 622 | STE | C14-C15-C16-C17 |
| 27 | Y | 101 | LMG | O6-C5-C6-O5 |
| 33 | D | 412 | LHG | O1-C1-C2-O2 |
| 33 | e | 101 | LHG | O1-C1-C2-O2 |
| 28 | B | 622 | SQD | C17-C18-C19-C20 |
| 29 | C | 517 | DGD | C5A-C6A-C7A-C8A |
| 29 | c | 518 | DGD | CAA-CBA-CCA-CDA |
| 31 | C | 519 | STE | C4-C5-C6-C7 |
| 31 | b | 622 | STE | C13-C14-C15-C16 |
| 33 | D | 412 | LHG | C32-C33-C34-C35 |
| 31 | a | 414 | STE | C4-C5-C6-C7 |
| 29 | A | 413 | DGD | CBB-CCB-CDB-CEB |
| 22 | H | 101 | CLA | CBA-CGA-O2A-C1 |
| 28 | A | 411 | SQD | C26-C27-C28-C29 |
| 31 | H | 104 | STE | C2-C3-C4-C5 |
| 22 | C | 512 | CLA | CBD-CGD-O2D-CED |
| 27 | Y | 101 | LMG | C35-C36-C37-C38 |
| 27 | c | 520 | LMG | C33-C34-C35-C36 |
| 28 | A | 411 | SQD | C24-C25-C26-C27 |
| 28 | D | 408 | SQD | C25-C26-C27-C28 |
| 33 | d | 407 | LHG | C11-C10-C9-C8 |
| 27 | Y | 101 | LMG | O9-C10-O7-C8 |
| 27 | D | 407 | LMG | C35-C36-C37-C38 |
| 27 | M | 101 | LMG | C34-C35-C36-C37 |
| 27 | c | 523 | LMG | C32-C33-C34-C35 |
| 28 | a | 412 | SQD | C24-C25-C26-C27 |
| 29 | A | 413 | DGD | CAA-CBA-CCA-CDA |
| 29 | C | 516 | DGD | C8B-C9B-CAB-CBB |
| 31 | b | 627 | STE | C13-C14-C15-C16 |
| 33 | D | 409 | LHG | C14-C15-C16-C17 |
| 22 | b | 602 | CLA | C8-C10-C11-C12 |
| 27 | Y | 101 | LMG | C37-C38-C39-C40 |
| 29 | C | 517 | DGD | C4A-C5A-C6A-C7A |
| 33 | E | 101 | LHG | C28-C29-C30-C31 |
| 33 | d | 409 | LHG | C27-C28-C29-C30 |
| 33 | l | 101 | LHG | C34-C35-C36-C37 |
| 24 | A | 406 | BCR | C23-C24-C25-C26 |
| 24 | A | 406 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 617 | BCR | C5-C6-C7-C8 |
| 24 | H | 102 | BCR | C23-C24-C25-C26 |
| 24 | H | 102 | BCR | C23-C24-C25-C30 |
| 24 | T | 101 | BCR | C1-C6-C7-C8 |
| 24 | T | 101 | BCR | C5-C6-C7-C8 |
| 24 | b | 618 | BCR | C23-C24-C25-C26 |
| 24 | c | 515 | BCR | C1-C6-C7-C8 |
| 24 | c | 515 | BCR | C5-C6-C7-C8 |
| 24 | k | 101 | BCR | C1-C6-C7-C8 |
| 24 | k | 101 | BCR | C5-C6-C7-C8 |
| 28 | D | 408 | SQD | C32-C33-C34-C35 |
| 29 | c | 519 | DGD | CBA-CCA-CDA-CEA |
| 31 | B | 625 | STE | C7-C8-C9-C10 |
| 31 | I | 101 | STE | C10-C11-C12-C13 |
| 33 | D | 412 | LHG | C29-C30-C31-C32 |
| 27 | b | 621 | LMG | C11-C10-O7-C8 |
| 27 | Y | 101 | LMG | C17-C18-C19-C20 |
| 27 | a | 415 | LMG | C41-C42-C43-C44 |
| 29 | C | 517 | DGD | C6B-C7B-C8B-C9B |
| 31 | b | 627 | STE | C5-C6-C7-C8 |
| 31 | d | 413 | STE | C4-C5-C6-C7 |
| 31 | m | 101 | STE | C4-C5-C6-C7 |
| 33 | D | 409 | LHG | C28-C29-C30-C31 |
| 33 | D | 412 | LHG | C28-C29-C30-C31 |
| 28 | B | 622 | SQD | O10-C23-O48-C46 |
| 22 | c | 511 | CLA | CBD-CGD-O2D-CED |
| 31 | c | 521 | STE | C1-C2-C3-C4 |
| 29 | c | 519 | DGD | CCA-CDA-CEA-CFA |
| 27 | A | 410 | LMG | C33-C34-C35-C36 |
| 22 | A | 403 | CLA | C11-C12-C13-C15 |
| 22 | B | 602 | CLA | C11-C12-C13-C15 |
| 22 | B | 604 | CLA | C11-C12-C13-C15 |
| 22 | C | 508 | CLA | C11-C10-C8-C7 |
| 22 | C | 512 | CLA | C11-C12-C13-C15 |
| 22 | C | 513 | CLA | C11-C10-C8-C7 |
| 22 | b | 604 | CLA | C12-C13-C15-C16 |
| 22 | b | 609 | CLA | C2-C3-C5-C6 |
| 22 | b | 612 | CLA | C12-C13-C15-C16 |
| 22 | b | 616 | CLA | C11-C10-C8-C7 |
| 22 | c | 503 | CLA | C11-C12-C13-C15 |
| 22 | c | 506 | CLA | C6-C7-C8-C10 |
| 22 | c | 507 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 513 | CLA | C12-C13-C15-C16 |
| 26 | D | 406 | PL9 | C13-C14-C16-C17 |
| 26 | d | 406 | PL9 | C43-C44-C46-C47 |
| 22 | B | 604 | CLA | O1A-CGA-O2A-C1 |
| 27 | Y | 101 | LMG | O10-C28-O8-C9 |
| 33 | L | 102 | LHG | O10-C23-O8-C6 |
| 22 | C | 503 | CLA | C5-C6-C7-C8 |
| 22 | d | 403 | CLA | C16-C17-C18-C19 |
| 22 | C | 501 | CLA | O1D-CGD-O2D-CED |
| 27 | c | 522 | LMG | O9-C10-O7-C8 |
| 31 | J | 101 | STE | C1-C2-C3-C4 |
| 31 | d | 413 | STE | C1-C2-C3-C4 |
| 31 | B | 620 | STE | C11-C12-C13-C14 |
| 33 | L | 102 | LHG | C13-C14-C15-C16 |
| 22 | B | 613 | CLA | C5-C6-C7-C8 |
| 27 | a | 415 | LMG | C39-C40-C41-C42 |
| 28 | B | 622 | SQD | C9-C10-C11-C12 |
| 31 | E | 102 | STE | C5-C6-C7-C8 |
| 28 | a | 411 | SQD | C12-C13-C14-C15 |
| 29 | c | 518 | DGD | C7A-C8A-C9A-CAA |
| 29 | H | 103 | DGD | C1A-C2A-C3A-C4A |
| 33 | E | 101 | LHG | C16-C17-C18-C19 |
| 33 | e | 101 | LHG | C11-C10-C9-C8 |
| 26 | D | 406 | PL9 | C32-C33-C34-C35 |
| 26 | d | 406 | PL9 | C32-C33-C34-C35 |
| 22 | c | 504 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 402 | CLA | C2C-C3C-CAC-CBC |
| 27 | B | 621 | LMG | C16-C17-C18-C19 |
| 27 | Y | 101 | LMG | C15-C16-C17-C18 |
| 29 | C | 515 | DGD | C6A-C7A-C8A-C9A |
| 33 | D | 412 | LHG | C11-C12-C13-C14 |
| 33 | l | 101 | LHG | C13-C14-C15-C16 |
| 24 | B | 617 | BCR | C6-C7-C8-C9 |
| 24 | d | 405 | BCR | C22-C23-C24-C25 |
| 22 | B | 612 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 614 | CLA | CBD-CGD-O2D-CED |
| 27 | b | 621 | LMG | C29-C28-O8-C9 |
| 28 | L | 101 | SQD | O5-C1-O6-C44 |
| 26 | d | 406 | PL9 | C44-C46-C47-C48 |
| 27 | c | 520 | LMG | C34-C35-C36-C37 |
| 27 | c | 520 | LMG | C38-C39-C40-C41 |
| 28 | a | 411 | SQD | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | C | 515 | DGD | CCB-CDB-CEB-CFB |
| 31 | b | 626 | STE | C6-C7-C8-C9 |
| 33 | E | 101 | LHG | C23-C24-C25-C26 |
| 27 | M | 101 | LMG | C11-C10-O7-C8 |
| 27 | b | 623 | LMG | C11-C10-O7-C8 |
| 33 | D | 409 | LHG | C8-C7-O7-C5 |
| 28 | A | 412 | SQD | C13-C14-C15-C16 |
| 29 | H | 103 | DGD | CCA-CDA-CEA-CFA |
| 29 | c | 518 | DGD | CBB-CCB-CDB-CEB |
| 31 | M | 102 | STE | C9-C10-C11-C12 |
| 33 | D | 412 | LHG | C27-C28-C29-C30 |
| 22 | H | 101 | CLA | C5-C6-C7-C8 |
| 22 | b | 603 | CLA | CBD-CGD-O2D-CED |
| 31 | b | 620 | STE | C11-C10-C9-C8 |
| 27 | c | 523 | LMG | C38-C39-C40-C41 |
| 29 | h | 102 | DGD | C3B-C4B-C5B-C6B |
| 31 | B | 625 | STE | C11-C10-C9-C8 |
| 27 | a | 415 | LMG | O7-C8-C9-O8 |
| 29 | A | 413 | DGD | O2G-C2G-C3G-O3G |
| 22 | c | 513 | CLA | CBA-CGA-O2A-C1 |
| 33 | d | 409 | LHG | C34-C35-C36-C37 |
| 22 | C | 513 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 615 | CLA | C16-C17-C18-C19 |
| 22 | D | 404 | CLA | C16-C17-C18-C20 |
| 22 | H | 101 | CLA | C16-C17-C18-C20 |
| 22 | b | 615 | CLA | C16-C17-C18-C20 |
| 33 | L | 102 | LHG | C32-C33-C34-C35 |
| 22 | C | 505 | CLA | C2-C3-C5-C6 |
| 27 | M | 101 | LMG | C12-C13-C14-C15 |
| 29 | A | 413 | DGD | C2B-C3B-C4B-C5B |
| 29 | H | 103 | DGD | CBB-CCB-CDB-CEB |
| 22 | A | 403 | CLA | C11-C12-C13-C14 |
| 22 | B | 602 | CLA | C11-C12-C13-C14 |
| 22 | B | 604 | CLA | C11-C12-C13-C14 |
| 22 | C | 513 | CLA | C11-C10-C8-C9 |
| 22 | D | 404 | CLA | C11-C12-C13-C14 |
| 22 | b | 601 | CLA | C11-C10-C8-C9 |
| 22 | b | 604 | CLA | C14-C13-C15-C16 |
| 22 | b | 612 | CLA | C14-C13-C15-C16 |
| 22 | c | 507 | CLA | C11-C10-C8-C9 |
| 22 | c | 513 | CLA | C6-C7-C8-C9 |
| 31 | d | 413 | STE | C3-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 31 | d | 413 | STE | C11-C12-C13-C14 |
| 33 | D | 410 | LHG | C32-C33-C34-C35 |
| 29 | h | 102 | DGD | C2A-C3A-C4A-C5A |
| 24 | h | 101 | BCR | C11-C12-C13-C14 |
| 22 | H | 101 | CLA | O1A-CGA-O2A-C1 |
| 22 | C | 503 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 513 | CLA | C1A-C2A-CAA-CBA |
| 22 | H | 101 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 509 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 512 | CLA | C1A-C2A-CAA-CBA |
| 22 | c | 514 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 616 | CLA | C11-C12-C13-C14 |
| 22 | b | 611 | CLA | C16-C17-C18-C19 |
| 22 | c | 504 | CLA | C16-C17-C18-C19 |
| 27 | c | 523 | LMG | O9-C10-O7-C8 |
| 27 | c | 522 | LMG | C15-C16-C17-C18 |
| 27 | d | 410 | LMG | C30-C31-C32-C33 |
| 28 | A | 411 | SQD | C16-C17-C18-C19 |
| 29 | C | 517 | DGD | C4B-C5B-C6B-C7B |
| 29 | H | 103 | DGD | C3A-C4A-C5A-C6A |
| 31 | T | 102 | STE | C11-C10-C9-C8 |
| 31 | j | 101 | STE | C3-C4-C5-C6 |
| 33 | L | 102 | LHG | C17-C18-C19-C20 |
| 33 | D | 409 | LHG | C4-O6-P-O3 |
| 33 | e | 101 | LHG | C4-O6-P-O3 |
| 28 | f | 102 | SQD | C32-C33-C34-C35 |
| 29 | A | 413 | DGD | C4A-C5A-C6A-C7A |
| 29 | c | 518 | DGD | C7B-C8B-C9B-CAB |
| 31 | T | 102 | STE | C12-C13-C14-C15 |
| 33 | d | 409 | LHG | C23-C24-C25-C26 |
| 22 | B | 607 | CLA | C3-C5-C6-C7 |
| 29 | C | 516 | DGD | CCB-CDB-CEB-CFB |
| 31 | T | 102 | STE | C9-C10-C11-C12 |
| 22 | C | 509 | CLA | C5-C6-C7-C8 |
| 22 | b | 607 | CLA | C8-C10-C11-C12 |
| 22 | c | 504 | CLA | C5-C6-C7-C8 |
| 29 | c | 517 | DGD | O6E-C5E-C6E-O5E |
| 27 | B | 621 | LMG | C29-C30-C31-C32 |
| 27 | D | 407 | LMG | C38-C39-C40-C41 |
| 27 | b | 623 | LMG | C40-C41-C42-C43 |
| 29 | c | 519 | DGD | C3A-C4A-C5A-C6A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | A | 413 | DGD | CDB-CEB-CFB-CGB |
| 33 | D | 410 | LHG | C16-C17-C18-C19 |
| 31 | b | 626 | STE | C10-C11-C12-C13 |
| 33 | E | 101 | LHG | C29-C30-C31-C32 |
| 33 | l | 101 | LHG | C14-C15-C16-C17 |
| 31 | D | 413 | STE | C5-C6-C7-C8 |
| 33 | d | 407 | LHG | C29-C30-C31-C32 |
| 33 | e | 101 | LHG | C12-C13-C14-C15 |
| 23 | a | 404 | PHO | C4-C3-C5-C6 |
| 27 | b | 623 | LMG | C15-C16-C17-C18 |
| 31 | H | 104 | STE | C11-C10-C9-C8 |
| 31 | b | 620 | STE | C5-C6-C7-C8 |
| 31 | b | 627 | STE | C2-C3-C4-C5 |
| 22 | C | 512 | CLA | C8-C10-C11-C12 |
| 22 | b | 613 | CLA | C10-C11-C12-C13 |
| 22 | C | 502 | CLA | CBD-CGD-O2D-CED |
| 28 | a | 412 | SQD | C17-C18-C19-C20 |
| 31 | C | 518 | STE | C2-C3-C4-C5 |
| 31 | M | 102 | STE | C1-C2-C3-C4 |
| 22 | c | 513 | CLA | O1A-CGA-O2A-C1 |
| 27 | M | 101 | LMG | C16-C17-C18-C19 |
| 27 | c | 522 | LMG | C40-C41-C42-C43 |
| 29 | c | 517 | DGD | C9B-CAB-CBB-CCB |
| 33 | e | 101 | LHG | C11-C12-C13-C14 |
| 33 | l | 101 | LHG | C27-C28-C29-C30 |
| 22 | b | 611 | CLA | C16-C17-C18-C20 |
| 22 | d | 403 | CLA | C16-C17-C18-C20 |
| 27 | D | 407 | LMG | O6-C5-C6-O5 |
| 27 | M | 101 | LMG | C7-C8-C9-O8 |
| 27 | c | 523 | LMG | O1-C7-C8-C9 |
| 28 | B | 622 | SQD | O6-C44-C45-C46 |
| 28 | a | 411 | SQD | O6-C44-C45-C46 |
| 29 | A | 413 | DGD | C1G-C2G-C3G-O3G |
| 33 | e | 101 | LHG | C4-C5-C6-O8 |
| 27 | b | 623 | LMG | O6-C5-C6-O5 |
| 22 | b | 616 | CLA | C5-C6-C7-C8 |
| 28 | L | 101 | SQD | C10-C11-C12-C13 |
| 31 | H | 104 | STE | C14-C15-C16-C17 |
| 33 | d | 408 | LHG | C19-C20-C21-C22 |
| 27 | a | 415 | LMG | C8-C7-O1-C1 |
| 29 | C | 516 | DGD | C2G-C3G-O3G-C1D |
| 29 | c | 518 | DGD | C5D-C6D-O5D-C1E |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | h | 102 | DGD | CDB-CEB-CFB-CGB |
| 31 | B | 625 | STE | C13-C14-C15-C16 |
| 33 | d | 409 | LHG | C35-C36-C37-C38 |
| 27 | d | 410 | LMG | C40-C41-C42-C43 |
| 28 | a | 412 | SQD | C31-C32-C33-C34 |
| 33 | L | 102 | LHG | C11-C12-C13-C14 |
| 33 | D | 409 | LHG | C7-C8-C9-C10 |
| 22 | b | 610 | CLA | C2C-C3C-CAC-CBC |
| 22 | d | 403 | CLA | C2C-C3C-CAC-CBC |
| 33 | d | 407 | LHG | O1-C1-C2-O2 |
| 31 | m | 101 | STE | C14-C15-C16-C17 |
| 33 | d | 409 | LHG | C33-C34-C35-C36 |
| 27 | c | 520 | LMG | O6-C5-C6-O5 |
| 28 | B | 622 | SQD | C13-C14-C15-C16 |
| 28 | L | 101 | SQD | C27-C28-C29-C30 |
| 33 | D | 409 | LHG | C17-C18-C19-C20 |
| 27 | c | 523 | LMG | C11-C10-O7-C8 |
| 31 | I | 101 | STE | C4-C5-C6-C7 |
| 31 | b | 626 | STE | C5-C6-C7-C8 |
| 22 | C | 507 | CLA | C5-C6-C7-C8 |
| 22 | C | 505 | CLA | C4-C3-C5-C6 |
| 26 | d | 406 | PL9 | C45-C44-C46-C47 |
| 27 | D | 411 | LMG | C11-C12-C13-C14 |
| 27 | D | 411 | LMG | C36-C37-C38-C39 |
| 28 | L | 101 | SQD | C19-C20-C21-C22 |
| 31 | b | 626 | STE | C11-C10-C9-C8 |
| 33 | L | 102 | LHG | C18-C19-C20-C21 |
| 27 | D | 411 | LMG | C29-C28-O8-C9 |
| 31 | b | 625 | STE | C7-C8-C9-C10 |
| 22 | b | 601 | CLA | C10-C11-C12-C13 |
| 28 | A | 411 | SQD | C11-C10-C9-C8 |
| 31 | T | 102 | STE | C4-C5-C6-C7 |
| 33 | e | 101 | LHG | C28-C29-C30-C31 |
| 27 | d | 410 | LMG | O6-C5-C6-O5 |
| 22 | B | 616 | CLA | C2-C1-O2A-CGA |
| 29 | h | 102 | DGD | C4A-C5A-C6A-C7A |
| 31 | m | 102 | STE | C5-C6-C7-C8 |
| 27 | c | 523 | LMG | C18-C19-C20-C21 |
| 31 | B | 626 | STE | C6-C7-C8-C9 |
| 22 | c | 510 | CLA | C5-C6-C7-C8 |
| 31 | B | 620 | STE | C9-C10-C11-C12 |
| 29 | h | 102 | DGD | O2G-C1B-C2B-C3B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | a | 411 | SQD | C29-C30-C31-C32 |
| 22 | C | 513 | CLA | C8-C10-C11-C12 |
| 31 | b | 627 | STE | C6-C7-C8-C9 |
| 27 | c | 523 | LMG | C33-C34-C35-C36 |
| 28 | L | 101 | SQD | C16-C17-C18-C19 |
| 29 | C | 516 | DGD | CDB-CEB-CFB-CGB |
| 24 | H | 102 | BCR | C11-C10-C9-C8 |
| 24 | b | 617 | BCR | C11-C10-C9-C8 |
| 27 | M | 101 | LMG | C40-C41-C42-C43 |
| 31 | d | 413 | STE | C2-C3-C4-C5 |
| 29 | H | 103 | DGD | O2G-C1B-C2B-C3B |
| 28 | L | 101 | SQD | O6-C44-C45-O47 |
| 29 | c | 518 | DGD | C5B-C6B-C7B-C8B |
| 31 | B | 601 | STE | C4-C5-C6-C7 |
| 31 | M | 103 | STE | C1-C2-C3-C4 |
| 29 | A | 413 | DGD | O6D-C5D-C6D-O5D |
| 22 | H | 101 | CLA | C16-C17-C18-C19 |
| 27 | b | 623 | LMG | C12-C13-C14-C15 |
| 27 | b | 623 | LMG | C35-C36-C37-C38 |
| 27 | c | 522 | LMG | C33-C34-C35-C36 |
| 28 | f | 102 | SQD | C26-C27-C28-C29 |
| 29 | c | 519 | DGD | CBB-CCB-CDB-CEB |
| 31 | d | 411 | STE | C11-C10-C9-C8 |
| 27 | b | 621 | LMG | C32-C33-C34-C35 |
| 29 | c | 518 | DGD | C9B-CAB-CBB-CCB |
| 22 | A | 403 | CLA | C12-C13-C15-C16 |
| 22 | B | 611 | CLA | C11-C10-C8-C7 |
| 22 | B | 613 | CLA | C12-C13-C15-C16 |
| 22 | C | 505 | CLA | C12-C13-C15-C16 |
| 22 | C | 509 | CLA | C11-C10-C8-C7 |
| 22 | C | 511 | CLA | C6-C7-C8-C10 |
| 22 | C | 512 | CLA | C11-C10-C8-C7 |
| 22 | C | 513 | CLA | C6-C7-C8-C10 |
| 22 | D | 404 | CLA | C11-C12-C13-C15 |
| 22 | b | 607 | CLA | C6-C7-C8-C10 |
| 22 | b | 607 | CLA | C11-C10-C8-C7 |
| 22 | c | 506 | CLA | C11-C10-C8-C7 |
| 22 | c | 507 | CLA | C6-C7-C8-C10 |
| 22 | c | 509 | CLA | C12-C13-C15-C16 |
| 22 | d | 403 | CLA | C6-C7-C8-C10 |
| 33 | e | 101 | LHG | C14-C15-C16-C17 |
| 22 | B | 613 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 615 | CLA | C11-C12-C13-C14 |
| 22 | C | 505 | CLA | C14-C13-C15-C16 |
| 22 | C | 508 | CLA | C14-C13-C15-C16 |
| 22 | C | 510 | CLA | C11-C10-C8-C9 |
| 22 | D | 403 | CLA | C11-C10-C8-C9 |
| 22 | H | 101 | CLA | C11-C10-C8-C9 |
| 22 | a | 403 | CLA | C6-C7-C8-C9 |
| 22 | a | 403 | CLA | C11-C10-C8-C9 |
| 22 | b | 609 | CLA | C14-C13-C15-C16 |
| 22 | b | 613 | CLA | C6-C7-C8-C9 |
| 22 | b | 614 | CLA | C6-C7-C8-C9 |
| 22 | b | 615 | CLA | C14-C13-C15-C16 |
| 22 | c | 506 | CLA | C6-C7-C8-C9 |
| 22 | c | 506 | CLA | C11-C10-C8-C9 |
| 22 | c | 508 | CLA | C11-C12-C13-C14 |
| 22 | c | 508 | CLA | C14-C13-C15-C16 |
| 22 | c | 509 | CLA | C14-C13-C15-C16 |
| 24 | C | 514 | BCR | C13-C14-C15-C16 |
| 22 | D | 405 | CLA | CBD-CGD-O2D-CED |
| 24 | K | 101 | BCR | C14-C15-C16-C17 |
| 29 | C | 516 | DGD | CDA-CEA-CFA-CGA |
| 22 | H | 101 | CLA | C8-C10-C11-C12 |
| 22 | b | 609 | CLA | C15-C16-C17-C18 |
| 24 | B | 618 | BCR | C7-C8-C9-C34 |
| 24 | b | 617 | BCR | C11-C12-C13-C35 |
| 22 | A | 403 | CLA | C16-C17-C18-C20 |
| 22 | b | 607 | CLA | C16-C17-C18-C19 |
| 27 | b | 621 | LMG | C30-C31-C32-C33 |
| 29 | C | 517 | DGD | CAB-CBB-CCB-CDB |
| 29 | c | 517 | DGD | CAA-CBA-CCA-CDA |
| 33 | D | 412 | LHG | C9-C10-C11-C12 |
| 27 | a | 415 | LMG | C18-C19-C20-C21 |
| 29 | c | 517 | DGD | CAB-CBB-CCB-CDB |
| 29 | C | 515 | DGD | O6D-C5D-C6D-O5D |
| 22 | B | 612 | CLA | C10-C11-C12-C13 |
| 29 | C | 516 | DGD | CBB-CCB-CDB-CEB |
| 31 | I | 101 | STE | C12-C13-C14-C15 |
| 31 | b | 624 | STE | C9-C10-C11-C12 |
| 33 | D | 412 | LHG | C24-C25-C26-C27 |
| 27 | a | 415 | LMG | C42-C43-C44-C45 |
| 27 | c | 523 | LMG | C12-C13-C14-C15 |
| 29 | c | 519 | DGD | CDA-CEA-CFA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | D | 410 | LHG | C30-C31-C32-C33 |
| 22 | b | 604 | CLA | C15-C16-C17-C18 |
| 22 | b | 614 | CLA | C8-C10-C11-C12 |
| 27 | Y | 101 | LMG | C18-C19-C20-C21 |
| 27 | c | 523 | LMG | C29-C30-C31-C32 |
| 31 | H | 104 | STE | C9-C10-C11-C12 |
| 31 | d | 412 | STE | C2-C3-C4-C5 |
| 27 | D | 407 | LMG | C36-C37-C38-C39 |
| 28 | A | 412 | SQD | C18-C19-C20-C21 |
| 31 | I | 101 | STE | C2-C3-C4-C5 |
| 22 | B | 605 | CLA | C10-C11-C12-C13 |
| 27 | Y | 101 | LMG | C29-C30-C31-C32 |
| 31 | j | 101 | STE | C2-C3-C4-C5 |
| 33 | d | 408 | LHG | C12-C13-C14-C15 |
| 28 | A | 412 | SQD | C16-C17-C18-C19 |
| 22 | b | 613 | CLA | C13-C15-C16-C17 |
| 22 | c | 508 | CLA | C10-C11-C12-C13 |
| 33 | d | 407 | LHG | C7-C8-C9-C10 |
| 27 | Y | 101 | LMG | C32-C33-C34-C35 |
| 31 | m | 102 | STE | C6-C7-C8-C9 |
| 29 | A | 413 | DGD | O1A-C1A-O1G-C1G |
| 22 | C | 512 | CLA | O1D-CGD-O2D-CED |
| 22 | b | 601 | CLA | C16-C17-C18-C20 |
| 22 | b | 607 | CLA | C16-C17-C18-C20 |
| 27 | a | 415 | LMG | C16-C17-C18-C19 |
| 27 | a | 415 | LMG | C29-C30-C31-C32 |
| 28 | a | 411 | SQD | C16-C17-C18-C19 |
| 29 | H | 103 | DGD | CBA-CCA-CDA-CEA |
| 29 | H | 103 | DGD | C3B-C4B-C5B-C6B |
| 29 | c | 518 | DGD | C4A-C5A-C6A-C7A |
| 22 | a | 405 | CLA | CBA-CGA-O2A-C1 |
| 29 | c | 517 | DGD | O6D-C5D-C6D-O5D |
| 29 | H | 103 | DGD | CCB-CDB-CEB-CFB |
| 31 | b | 624 | STE | C12-C13-C14-C15 |
| 27 | B | 621 | LMG | C30-C31-C32-C33 |
| 31 | C | 519 | STE | C5-C6-C7-C8 |
| 33 | E | 101 | LHG | C11-C10-C9-C8 |
| 24 | K | 101 | BCR | C15-C16-C17-C18 |
| 27 | a | 415 | LMG | C21-C22-C23-C24 |
| 28 | B | 622 | SQD | C16-C17-C18-C19 |
| 31 | c | 501 | STE | C2-C3-C4-C5 |
| 31 | c | 501 | STE | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | D | 410 | LHG | C27-C28-C29-C30 |
| 27 | D | 407 | LMG | C19-C20-C21-C22 |
| 27 | a | 415 | LMG | C37-C38-C39-C40 |
| 28 | a | 411 | SQD | C30-C31-C32-C33 |
| 27 | b | 623 | LMG | C29-C28-O8-C9 |
| 22 | B | 616 | CLA | C5-C6-C7-C8 |
| 27 | Y | 101 | LMG | O1-C7-C8-C9 |
| 27 | b | 623 | LMG | O1-C7-C8-C9 |
| 28 | a | 412 | SQD | C44-C45-C46-O48 |
| 33 | e | 101 | LHG | O9-C7-O7-C5 |
| 27 | D | 407 | LMG | C20-C21-C22-C23 |
| 27 | b | 623 | LMG | C29-C30-C31-C32 |
| 31 | B | 620 | STE | C3-C4-C5-C6 |
| 31 | b | 627 | STE | C14-C15-C16-C17 |
| 29 | h | 102 | DGD | O1A-C1A-O1G-C1G |
| 27 | D | 407 | LMG | C37-C38-C39-C40 |
| 29 | C | 515 | DGD | CDA-CEA-CFA-CGA |
| 22 | c | 504 | CLA | C15-C16-C17-C18 |
| 28 | A | 412 | SQD | C32-C33-C34-C35 |
| 29 | H | 103 | DGD | CDB-CEB-CFB-CGB |
| 31 | b | 620 | STE | C12-C13-C14-C15 |
| 22 | B | 616 | CLA | O1D-CGD-O2D-CED |
| 27 | D | 411 | LMG | C28-C29-C30-C31 |
| 31 | b | 625 | STE | C4-C5-C6-C7 |
| 31 | c | 501 | STE | C5-C6-C7-C8 |
| 33 | l | 101 | LHG | C25-C26-C27-C28 |
| 22 | C | 502 | CLA | C16-C17-C18-C19 |
| 26 | d | 406 | PL9 | C33-C34-C36-C37 |
| 27 | Y | 101 | LMG | C14-C15-C16-C17 |
| 29 | c | 518 | DGD | CDB-CEB-CFB-CGB |
| 31 | a | 413 | STE | C2-C3-C4-C5 |
| 33 | D | 412 | LHG | C25-C26-C27-C28 |
| 22 | c | 511 | CLA | O1D-CGD-O2D-CED |
| 33 | L | 102 | LHG | C4-O6-P-O3 |
| 27 | c | 522 | LMG | C17-C18-C19-C20 |
| 31 | d | 413 | STE | C6-C7-C8-C9 |
| 33 | D | 409 | LHG | O1-C1-C2-O2 |
| 33 | d | 408 | LHG | O1-C1-C2-O2 |
| 31 | D | 413 | STE | C10-C11-C12-C13 |
| 27 | a | 415 | LMG | C30-C31-C32-C33 |
| 22 | D | 404 | CLA | C16-C17-C18-C19 |
| 29 | c | 519 | DGD | C8B-C9B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | D | 409 | LHG | C24-C25-C26-C27 |
| 33 | D | 409 | LHG | C35-C36-C37-C38 |
| 22 | c | 513 | CLA | C8-C10-C11-C12 |
| 29 | A | 413 | DGD | C8A-C9A-CAA-CBA |
| 29 | h | 102 | DGD | CAB-CBB-CCB-CDB |
| 28 | A | 412 | SQD | O47-C45-C46-O48 |
| 27 | c | 523 | LMG | O1-C7-C8-O7 |
| 28 | a | 411 | SQD | O47-C45-C46-O48 |
| 22 | c | 510 | CLA | C8-C10-C11-C12 |
| 28 | A | 412 | SQD | C9-C10-C11-C12 |
| 33 | L | 102 | LHG | C31-C32-C33-C34 |
| 22 | b | 601 | CLA | C16-C17-C18-C19 |
| 31 | b | 620 | STE | C15-C16-C17-C18 |
| 27 | d | 410 | LMG | O9-C10-O7-C8 |
| 22 | B | 613 | CLA | C2-C1-O2A-CGA |
| 22 | C | 506 | CLA | C2-C1-O2A-CGA |
| 27 | Y | 101 | LMG | C33-C34-C35-C36 |
| 31 | a | 413 | STE | C1-C2-C3-C4 |
| 22 | A | 403 | CLA | C11-C10-C8-C9 |
| 22 | B | 613 | CLA | C11-C12-C13-C14 |
| 22 | C | 504 | CLA | C11-C10-C8-C9 |
| 22 | b | 601 | CLA | C6-C7-C8-C9 |
| 22 | b | 608 | CLA | C11-C12-C13-C14 |
| 22 | c | 505 | CLA | C11-C10-C8-C9 |
| 22 | c | 508 | CLA | C6-C7-C8-C9 |
| 22 | c | 512 | CLA | C14-C13-C15-C16 |
| 22 | c | 514 | CLA | C11-C12-C13-C14 |
| 22 | d | 403 | CLA | C6-C7-C8-C9 |
| 27 | M | 101 | LMG | C31-C32-C33-C34 |
| 28 | L | 101 | SQD | C29-C30-C31-C32 |
| 33 | D | 409 | LHG | C30-C31-C32-C33 |
| 27 | a | 415 | LMG | C32-C33-C34-C35 |
| 29 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 33 | D | 412 | LHG | C15-C16-C17-C18 |
| 33 | d | 408 | LHG | C25-C26-C27-C28 |
| 22 | b | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 602 | CLA | C16-C17-C18-C20 |
| 22 | C | 508 | CLA | C16-C17-C18-C19 |
| 24 | k | 102 | BCR | C5-C6-C7-C8 |
| 24 | c | 516 | BCR | C37-C22-C23-C24 |
| 31 | C | 519 | STE | C9-C10-C11-C12 |
| 24 | K | 103 | BCR | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | b | 617 | BCR | C21-C22-C23-C24 |
| 29 | A | 413 | DGD | CEA-CFA-CGA-CHA |
| 27 | B | 621 | LMG | C28-C29-C30-C31 |
| 24 | c | 515 | BCR | C14-C15-C16-C17 |
| 24 | k | 101 | BCR | C14-C15-C16-C17 |
| 27 | c | 522 | LMG | C29-C30-C31-C32 |
| 31 | J | 101 | STE | C2-C3-C4-C5 |
| 29 | C | 515 | DGD | C4D-C5D-C6D-O5D |
| 22 | B | 604 | CLA | C13-C15-C16-C17 |
| 27 | b | 623 | LMG | C30-C31-C32-C33 |
| 27 | c | 523 | LMG | C20-C21-C22-C23 |
| 27 | d | 410 | LMG | C14-C15-C16-C17 |
| 33 | l | 101 | LHG | O6-C4-C5-C6 |
| 27 | D | 411 | LMG | C16-C17-C18-C19 |
| 27 | D | 411 | LMG | C32-C33-C34-C35 |
| 28 | a | 411 | SQD | C17-C18-C19-C20 |
| 29 | A | 413 | DGD | C7A-C8A-C9A-CAA |
| 29 | c | 517 | DGD | C7B-C8B-C9B-CAB |
| 31 | d | 412 | STE | C10-C11-C12-C13 |
| 22 | A | 403 | CLA | C11-C10-C8-C7 |
| 22 | B | 604 | CLA | C11-C10-C8-C7 |
| 22 | B | 606 | CLA | C11-C12-C13-C15 |
| 22 | B | 615 | CLA | C11-C12-C13-C15 |
| 22 | C | 504 | CLA | C11-C10-C8-C7 |
| 22 | C | 510 | CLA | C11-C10-C8-C7 |
| 22 | C | 512 | CLA | C12-C13-C15-C16 |
| 22 | H | 101 | CLA | C11-C10-C8-C7 |
| 22 | a | 403 | CLA | C6-C7-C8-C10 |
| 22 | a | 403 | CLA | C11-C10-C8-C7 |
| 22 | a | 405 | CLA | C11-C10-C8-C7 |
| 22 | b | 601 | CLA | C6-C7-C8-C10 |
| 22 | b | 605 | CLA | C11-C10-C8-C7 |
| 22 | b | 608 | CLA | C11-C12-C13-C15 |
| 22 | b | 609 | CLA | C12-C13-C15-C16 |
| 22 | b | 615 | CLA | C12-C13-C15-C16 |
| 22 | c | 505 | CLA | C11-C10-C8-C7 |
| 22 | c | 508 | CLA | C11-C12-C13-C15 |
| 22 | c | 510 | CLA | C6-C7-C8-C10 |
| 22 | c | 512 | CLA | C12-C13-C15-C16 |
| 22 | c | 513 | CLA | C6-C7-C8-C10 |
| 22 | c | 514 | CLA | C11-C12-C13-C15 |
| 23 | a | 404 | PHO | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | a | 404 | PHO | C6-C7-C8-C10 |
| 27 | a | 415 | LMG | C34-C35-C36-C37 |
| 27 | a | 415 | LMG | C23-C24-C25-C26 |
| 27 | c | 523 | LMG | C11-C12-C13-C14 |
| 22 | B | 614 | CLA | C8-C10-C11-C12 |
| 29 | A | 413 | DGD | C2A-C3A-C4A-C5A |
| 24 | K | 101 | BCR | C11-C10-C9-C34 |
| 24 | K | 102 | BCR | C35-C13-C14-C15 |
| 24 | c | 515 | BCR | C20-C21-C22-C37 |
| 24 | h | 101 | BCR | C20-C21-C22-C37 |
| 24 | k | 102 | BCR | C20-C21-C22-C37 |
| 31 | m | 101 | STE | C2-C3-C4-C5 |
| 22 | C | 512 | CLA | C3-C5-C6-C7 |
| 27 | M | 101 | LMG | C29-C30-C31-C32 |
| 31 | b | 626 | STE | C11-C12-C13-C14 |
| 33 | d | 409 | LHG | C32-C33-C34-C35 |
| 22 | B | 602 | CLA | C16-C17-C18-C19 |
| 27 | c | 523 | LMG | C37-C38-C39-C40 |
| 31 | m | 101 | STE | C12-C13-C14-C15 |
| 33 | D | 412 | LHG | C14-C15-C16-C17 |
| 27 | M | 101 | LMG | C18-C19-C20-C21 |
| 28 | f | 102 | SQD | C29-C30-C31-C32 |
| 29 | A | 413 | DGD | C6B-C7B-C8B-C9B |
| 31 | B | 626 | STE | C11-C10-C9-C8 |
| 29 | C | 515 | DGD | C9B-CAB-CBB-CCB |
| 22 | B | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 501 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 503 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 505 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 513 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 613 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 616 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 504 | CLA | CAD-CBD-CGD-O2D |
| 27 | a | 415 | LMG | C9-C8-O7-C10 |
| 27 | c | 523 | LMG | C9-C8-O7-C10 |
| 28 | L | 101 | SQD | C18-C19-C20-C21 |
| 28 | a | 412 | SQD | C29-C30-C31-C32 |
| 33 | d | 408 | LHG | C9-C10-C11-C12 |
| 22 | C | 509 | CLA | C10-C11-C12-C13 |
| 27 | D | 411 | LMG | C14-C15-C16-C17 |
| 29 | C | 516 | DGD | CBA-CCA-CDA-CEA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | a | 413 | STE | C4-C5-C6-C7 |
| 22 | c | 512 | CLA | CBA-CGA-O2A-C1 |
| 22 | c | 510 | CLA | C16-C17-C18-C19 |
| 27 | c | 522 | LMG | C11-C12-C13-C14 |
| 31 | b | 620 | STE | C10-C11-C12-C13 |
| 26 | a | 409 | PL9 | C13-C14-C16-C17 |
| 28 | A | 412 | SQD | C35-C36-C37-C38 |
| 28 | L | 101 | SQD | C12-C13-C14-C15 |
| 23 | A | 404 | PHO | C2C-C3C-CAC-CBC |
| 23 | d | 401 | PHO | C2C-C3C-CAC-CBC |
| 33 | D | 409 | LHG | C4-C5-C6-O8 |
| 33 | E | 101 | LHG | C4-C5-C6-O8 |
| 33 | d | 409 | LHG | C2-C3-O3-P |
| 22 | B | 607 | CLA | CBD-CGD-O2D-CED |
| 33 | D | 409 | LHG | O10-C23-O8-C6 |
| 31 | T | 102 | STE | C11-C12-C13-C14 |
| 22 | A | 403 | CLA | C16-C17-C18-C19 |
| 22 | c | 510 | CLA | C16-C17-C18-C20 |
| 22 | a | 410 | CLA | C4C-C3C-CAC-CBC |
| 29 | c | 517 | DGD | O1B-C1B-O2G-C2G |
| 22 | C | 502 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 508 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 512 | CLA | CHA-CBD-CGD-O1D |
| 22 | H | 101 | CLA | CHA-CBD-CGD-O1D |
| 22 | b | 603 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 503 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 503 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 505 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 509 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 509 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 510 | CLA | CHA-CBD-CGD-O1D |
| 22 | c | 510 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 612 | CLA | C3-C5-C6-C7 |
| 22 | a | 405 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 607 | CLA | O1D-CGD-O2D-CED |
| 24 | t | 101 | BCR | C16-C17-C18-C19 |
| 28 | A | 411 | SQD | O6-C44-C45-O47 |
| 29 | C | 515 | DGD | O1G-C1G-C2G-O2G |
| 29 | c | 517 | DGD | O1G-C1G-C2G-O2G |
| 33 | D | 409 | LHG | O7-C5-C6-O8 |
| 33 | E | 101 | LHG | O7-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 603 | CLA | CBD-CGD-O2D-CED |
| 29 | c | 519 | DGD | C9B-CAB-CBB-CCB |
| 31 | Z | 101 | STE | C13-C14-C15-C16 |
| 29 | c | 517 | DGD | C4D-C5D-C6D-O5D |
| 33 | d | 409 | LHG | O1-C1-C2-O2 |
| 27 | B | 621 | LMG | C12-C13-C14-C15 |
| 29 | A | 413 | DGD | C6A-C7A-C8A-C9A |
| 22 | H | 101 | CLA | C4-C3-C5-C6 |
| 27 | d | 410 | LMG | C32-C33-C34-C35 |
| 22 | B | 604 | CLA | C14-C13-C15-C16 |
| 22 | C | 509 | CLA | C14-C13-C15-C16 |
| 22 | C | 511 | CLA | C11-C12-C13-C14 |
| 22 | a | 403 | CLA | C14-C13-C15-C16 |
| 22 | a | 405 | CLA | C11-C10-C8-C9 |
| 22 | b | 608 | CLA | C11-C10-C8-C9 |
| 22 | c | 507 | CLA | C11-C12-C13-C14 |
| 28 | B | 622 | SQD | C45-C46-O48-C23 |
| 27 | c | 522 | LMG | C34-C35-C36-C37 |
| 27 | B | 621 | LMG | C33-C34-C35-C36 |
| 28 | f | 102 | SQD | C25-C26-C27-C28 |
| 29 | c | 517 | DGD | C5A-C6A-C7A-C8A |
| 22 | B | 605 | CLA | C3-C5-C6-C7 |
| 27 | D | 407 | LMG | C39-C40-C41-C42 |
| 24 | B | 618 | BCR | C36-C18-C19-C20 |
| 31 | B | 620 | STE | C12-C13-C14-C15 |
| 33 | D | 409 | LHG | C12-C13-C14-C15 |
| 33 | d | 407 | LHG | C10-C11-C12-C13 |
| 31 | D | 413 | STE | C2-C3-C4-C5 |
| 22 | B | 610 | CLA | C16-C17-C18-C19 |
| 28 | a | 411 | SQD | C25-C26-C27-C28 |
| 28 | D | 408 | SQD | O6-C44-C45-C46 |
| 27 | A | 410 | LMG | C19-C20-C21-C22 |
| 27 | D | 411 | LMG | C37-C38-C39-C40 |
| 33 | L | 102 | LHG | C33-C34-C35-C36 |
| 24 | C | 514 | BCR | C15-C16-C17-C18 |
| 24 | T | 101 | BCR | C13-C14-C15-C16 |
| 33 | d | 408 | LHG | C3-O3-P-O6 |
| 33 | D | 410 | LHG | C14-C15-C16-C17 |
| 31 | b | 627 | STE | C12-C13-C14-C15 |
| 22 | B | 603 | CLA | C2-C3-C5-C6 |
| 26 | A | 409 | PL9 | C33-C34-C36-C37 |
| 26 | A | 409 | PL9 | C43-C44-C46-C47 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | D | 410 | LHG | C3-O3-P-O5 |
| 33 | E | 101 | LHG | C3-O3-P-O4 |
| 33 | d | 408 | LHG | C3-O3-P-O4 |
| 33 | e | 101 | LHG | C4-O6-P-O4 |
| 22 | d | 404 | CLA | C16-C17-C18-C19 |
| 27 | b | 621 | LMG | C38-C39-C40-C41 |
| 28 | a | 411 | SQD | C11-C12-C13-C14 |
| 33 | D | 410 | LHG | C11-C12-C13-C14 |
| 27 | Y | 101 | LMG | O6-C1-O1-C7 |
| 33 | d | 408 | LHG | C10-C11-C12-C13 |
| 22 | C | 502 | CLA | O1D-CGD-O2D-CED |
| 33 | E | 101 | LHG | C7-C8-C9-C10 |
| 22 | B | 616 | CLA | C3-C5-C6-C7 |
| 22 | a | 410 | CLA | C2C-C3C-CAC-CBC |
| 22 | D | 404 | CLA | C15-C16-C17-C18 |
| 33 | D | 410 | LHG | C11-C10-C9-C8 |
| 22 | B | 603 | CLA | C16-C17-C18-C20 |
| 22 | C | 508 | CLA | C16-C17-C18-C20 |
| 22 | b | 614 | CLA | C16-C17-C18-C19 |
| 22 | C | 502 | CLA | CAD-CBD-CGD-O1D |
| 22 | c | 503 | CLA | CAD-CBD-CGD-O1D |
| 22 | c | 507 | CLA | CAD-CBD-CGD-O1D |
| 28 | D | 408 | SQD | C5-C6-S-O7 |
| 29 | A | 413 | DGD | C4D-C5D-C6D-O5D |
| 28 | A | 411 | SQD | C32-C33-C34-C35 |
| 33 | D | 412 | LHG | C26-C27-C28-C29 |
| 22 | C | 509 | CLA | C3-C5-C6-C7 |
| 31 | I | 101 | STE | C1-C2-C3-C4 |
| 31 | B | 625 | STE | C4-C5-C6-C7 |
| 33 | D | 412 | LHG | C33-C34-C35-C36 |
| 22 | c | 504 | CLA | CBA-CGA-O2A-C1 |
| 22 | D | 405 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 604 | CLA | C12-C13-C15-C16 |
| 22 | B | 605 | CLA | C11-C10-C8-C7 |
| 22 | B | 609 | CLA | C11-C12-C13-C15 |
| 22 | B | 616 | CLA | C6-C7-C8-C10 |
| 22 | C | 505 | CLA | C6-C7-C8-C10 |
| 22 | C | 509 | CLA | C12-C13-C15-C16 |
| 22 | H | 101 | CLA | C12-C13-C15-C16 |
| 22 | a | 403 | CLA | C12-C13-C15-C16 |
| 22 | b | 601 | CLA | C11-C12-C13-C15 |
| 22 | b | 607 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | b | 608 | CLA | C11-C10-C8-C7 |
| 22 | b | 614 | CLA | C12-C13-C15-C16 |
| 22 | c | 506 | CLA | C12-C13-C15-C16 |
| 22 | c | 511 | CLA | C11-C10-C8-C7 |
| 22 | c | 514 | CLA | C11-C10-C8-C7 |
| 27 | M | 101 | LMG | C22-C23-C24-C25 |
| 31 | d | 411 | STE | C7-C8-C9-C10 |
| 22 | B | 609 | CLA | O1A-CGA-O2A-C1 |
| 31 | c | 521 | STE | C15-C16-C17-C18 |
| 22 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 29 | c | 518 | DGD | C5A-C6A-C7A-C8A |
| 22 | a | 402 | CLA | C2C-C3C-CAC-CBC |
| 27 | D | 411 | LMG | C12-C13-C14-C15 |
| 31 | b | 624 | STE | C7-C8-C9-C10 |
| 29 | C | 517 | DGD | O1A-C1A-O1G-C1G |
| 31 | B | 627 | STE | C7-C8-C9-C10 |
| 22 | C | 505 | CLA | CBD-CGD-O2D-CED |
| 26 | a | 409 | PL9 | C32-C33-C34-C35 |
| 29 | c | 519 | DGD | C3B-C4B-C5B-C6B |
| 28 | a | 411 | SQD | C7-C8-C9-C10 |
| 29 | c | 518 | DGD | C4E-C5E-C6E-O5E |
| 22 | b | 609 | CLA | O1D-CGD-O2D-CED |
| 27 | a | 415 | LMG | C7-C8-C9-O8 |
| 29 | C | 515 | DGD | C1G-C2G-C3G-O3G |
| 27 | Y | 101 | LMG | O1-C7-C8-O7 |
| 27 | b | 623 | LMG | O1-C7-C8-O7 |
| 33 | e | 101 | LHG | O7-C5-C6-O8 |
| 27 | d | 410 | LMG | C15-C16-C17-C18 |
| 31 | b | 625 | STE | C2-C3-C4-C5 |
| 29 | C | 516 | DGD | C5D-C6D-O5D-C1E |
| 29 | c | 518 | DGD | C2G-C3G-O3G-C1D |
| 29 | C | 515 | DGD | O1G-C1A-C2A-C3A |
| 26 | D | 406 | PL9 | C15-C14-C16-C17 |
| 26 | d | 406 | PL9 | C15-C14-C16-C17 |
| 22 | A | 402 | CLA | C4C-C3C-CAC-CBC |
| 27 | D | 407 | LMG | C21-C22-C23-C24 |
| 33 | D | 412 | LHG | C18-C19-C20-C21 |
| 33 | E | 101 | LHG | C10-C11-C12-C13 |
| 26 | d | 406 | PL9 | C28-C29-C31-C32 |
| 22 | C | 512 | CLA | C14-C13-C15-C16 |
| 22 | H | 101 | CLA | C14-C13-C15-C16 |
| 22 | b | 614 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 507 | CLA | C6-C7-C8-C9 |
| 22 | c | 511 | CLA | C11-C12-C13-C14 |
| 23 | a | 404 | PHO | C6-C7-C8-C9 |
| 27 | c | 522 | LMG | C36-C37-C38-C39 |
| 31 | m | 101 | STE | C13-C14-C15-C16 |
| 31 | B | 626 | STE | C7-C8-C9-C10 |
| 22 | b | 606 | CLA | O1A-CGA-O2A-C1 |
| 28 | B | 622 | SQD | C34-C35-C36-C37 |
| 24 | B | 619 | BCR | C11-C12-C13-C35 |
| 29 | A | 413 | DGD | CBA-CCA-CDA-CEA |
| 33 | D | 412 | LHG | C7-C8-C9-C10 |
| 31 | B | 625 | STE | C12-C13-C14-C15 |
| 29 | c | 517 | DGD | O1G-C1A-C2A-C3A |
| 33 | D | 412 | LHG | O9-C7-O7-C5 |
| 31 | b | 627 | STE | C15-C16-C17-C18 |
| 22 | B | 604 | CLA | C15-C16-C17-C18 |
| 33 | d | 409 | LHG | C9-C10-C11-C12 |
| 22 | H | 101 | CLA | C2-C3-C5-C6 |
| 31 | M | 103 | STE | C3-C4-C5-C6 |
| 28 | A | 412 | SQD | C19-C20-C21-C22 |
| 31 | C | 518 | STE | C7-C8-C9-C10 |
| 27 | A | 410 | LMG | C38-C39-C40-C41 |
| 29 | c | 517 | DGD | CCB-CDB-CEB-CFB |
| 31 | D | 413 | STE | C6-C7-C8-C9 |
| 28 | D | 408 | SQD | C28-C29-C30-C31 |
| 22 | B | 603 | CLA | C10-C11-C12-C13 |
| 27 | D | 411 | LMG | C9-C8-O7-C10 |
| 22 | b | 610 | CLA | C2A-CAA-CBA-CGA |
| 33 | L | 102 | LHG | C27-C28-C29-C30 |
| 22 | b | 606 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 612 | CLA | C2-C1-O2A-CGA |
| 22 | c | 513 | CLA | C2-C1-O2A-CGA |
| 22 | d | 403 | CLA | C2-C1-O2A-CGA |
| 33 | D | 412 | LHG | C19-C20-C21-C22 |
| 22 | B | 603 | CLA | C16-C17-C18-C19 |
| 31 | a | 413 | STE | C7-C8-C9-C10 |
| 33 | E | 101 | LHG | C2-C3-O3-P |
| 31 | D | 413 | STE | C12-C13-C14-C15 |
| 33 | l | 101 | LHG | C15-C16-C17-C18 |
| 22 | B | 609 | CLA | CBA-CGA-O2A-C1 |
| 33 | l | 101 | LHG | O6-C4-C5-O7 |
| 22 | b | 612 | CLA | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | c | 505 | CLA | C4-C3-C5-C6 |
| 26 | A | 409 | PL9 | C20-C19-C21-C22 |
| 29 | h | 102 | DGD | CBA-CCA-CDA-CEA |
| 24 | B | 618 | BCR | C23-C24-C25-C26 |
| 22 | B | 610 | CLA | O1D-CGD-O2D-CED |
| 27 | a | 415 | LMG | C31-C32-C33-C34 |
| 31 | E | 102 | STE | C7-C8-C9-C10 |
| 31 | c | 521 | STE | C11-C10-C9-C8 |
| 28 | D | 408 | SQD | O5-C1-O6-C44 |
| 24 | c | 516 | BCR | C20-C21-C22-C23 |
| 29 | c | 517 | DGD | C7A-C8A-C9A-CAA |
| 22 | c | 512 | CLA | O1A-CGA-O2A-C1 |
| 27 | M | 101 | LMG | O7-C8-C9-O8 |
| 27 | c | 522 | LMG | O1-C7-C8-O7 |
| 28 | a | 412 | SQD | O47-C45-C46-O48 |
| 29 | A | 413 | DGD | C5A-C6A-C7A-C8A |
| 31 | b | 624 | STE | C15-C16-C17-C18 |
| 22 | b | 609 | CLA | CBD-CGD-O2D-CED |
| 33 | E | 101 | LHG | C3-O3-P-O6 |
| 31 | b | 624 | STE | C2-C3-C4-C5 |
| 29 | c | 519 | DGD | O6D-C5D-C6D-O5D |
| 27 | D | 407 | LMG | C16-C17-C18-C19 |
| 28 | A | 412 | SQD | C11-C10-C9-C8 |
| 22 | B | 612 | CLA | O1D-CGD-O2D-CED |
| 28 | a | 411 | SQD | C14-C15-C16-C17 |
| 29 | c | 517 | DGD | O1G-C1G-C2G-C3G |
| 27 | a | 415 | LMG | C35-C36-C37-C38 |
| 22 | B | 604 | CLA | C10-C11-C12-C13 |
| 22 | B | 606 | CLA | C6-C7-C8-C10 |
| 22 | C | 506 | CLA | C12-C13-C15-C16 |
| 22 | C | 511 | CLA | C11-C12-C13-C15 |
| 22 | b | 614 | CLA | C6-C7-C8-C10 |
| 22 | c | 507 | CLA | C11-C12-C13-C15 |
| 26 | D | 406 | PL9 | C28-C29-C31-C32 |
| 27 | a | 415 | LMG | O8-C28-C29-C30 |
| 22 | d | 403 | CLA | C4C-C3C-CAC-CBC |
| 28 | a | 411 | SQD | C11-C10-C9-C8 |
| 31 | H | 104 | STE | C10-C11-C12-C13 |
| 22 | B | 605 | CLA | C11-C10-C8-C9 |
| 22 | B | 606 | CLA | C11-C12-C13-C14 |
| 22 | B | 614 | CLA | C14-C13-C15-C16 |
| 22 | B | 616 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | f | 102 | SQD | O47-C7-C8-C9 |
| 24 | B | 618 | BCR | C15-C16-C17-C18 |
| 24 | c | 515 | BCR | C9-C10-C11-C12 |
| 24 | k | 101 | BCR | C19-C20-C21-C22 |
| 22 | C | 510 | CLA | C16-C17-C18-C20 |
| 22 | b | 614 | CLA | C16-C17-C18-C20 |
| 27 | c | 520 | LMG | C32-C33-C34-C35 |
| 31 | b | 624 | STE | C1-C2-C3-C4 |
| 22 | A | 403 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 613 | CLA | C15-C16-C17-C18 |
| 22 | c | 504 | CLA | C10-C11-C12-C13 |
| 31 | B | 626 | STE | C3-C4-C5-C6 |
| 31 | b | 625 | STE | C1-C2-C3-C4 |
| 31 | a | 413 | STE | C6-C7-C8-C9 |
| 24 | K | 103 | BCR | C11-C12-C13-C35 |
| 24 | b | 618 | BCR | C37-C22-C23-C24 |
| 27 | Y | 101 | LMG | C31-C32-C33-C34 |
| 33 | E | 101 | LHG | C31-C32-C33-C34 |
| 33 | l | 101 | LHG | C11-C12-C13-C14 |
| 27 | A | 410 | LMG | C13-C14-C15-C16 |
| 22 | B | 603 | CLA | C4-C3-C5-C6 |
| 22 | C | 504 | CLA | C4-C3-C5-C6 |
| 33 | D | 412 | LHG | C24-C23-O8-C6 |
| 22 | B | 611 | CLA | C13-C15-C16-C17 |
| 22 | B | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 29 | C | 515 | DGD | O6E-C1E-O5D-C6D |
| 33 | E | 101 | LHG | O6-C4-C5-C6 |
| 33 | d | 408 | LHG | O6-C4-C5-C6 |
| 29 | A | 413 | DGD | CAB-CBB-CCB-CDB |
| 31 | d | 412 | STE | O1-C1-C2-C3 |
| 27 | c | 523 | LMG | C35-C36-C37-C38 |
| 22 | b | 614 | CLA | C4-C3-C5-C6 |
| 26 | D | 406 | PL9 | C45-C44-C46-C47 |
| 31 | B | 624 | STE | O1-C1-C2-C3 |
| 27 | B | 621 | LMG | C36-C37-C38-C39 |
| 28 | a | 411 | SQD | C33-C34-C35-C36 |
| 29 | C | 517 | DGD | C7A-C8A-C9A-CAA |
| 22 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 22 | c | 504 | CLA | O1A-CGA-O2A-C1 |
| 28 | B | 622 | SQD | C11-C10-C9-C8 |
| 29 | C | 517 | DGD | CDA-CEA-CFA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | B | 627 | STE | C11-C12-C13-C14 |
| 31 | C | 520 | STE | C5-C6-C7-C8 |
| 29 | C | 517 | DGD | C8B-C9B-CAB-CBB |
| 22 | D | 403 | CLA | C2-C1-O2A-CGA |
| 27 | A | 410 | LMG | C15-C16-C17-C18 |
| 34 | f | 101 | HEC | CAA-CBA-CGA-O1A |
| 22 | c | 502 | CLA | C2A-CAA-CBA-CGA |
| 27 | c | 520 | LMG | C30-C31-C32-C33 |
| 31 | B | 625 | STE | C10-C11-C12-C13 |
| 27 | B | 621 | LMG | O10-C28-C29-C30 |
| 29 | c | 518 | DGD | CCB-CDB-CEB-CFB |
| 27 | a | 415 | LMG | C11-C12-C13-C14 |
| 27 | Y | 101 | LMG | C4-C5-C6-O5 |
| 26 | A | 409 | PL9 | C4-C3-C7-C8 |
| 26 | a | 409 | PL9 | C4-C3-C7-C8 |
| 22 | B | 605 | CLA | C6-C7-C8-C9 |
| 22 | B | 610 | CLA | C14-C13-C15-C16 |
| 22 | B | 612 | CLA | C11-C10-C8-C9 |
| 22 | C | 503 | CLA | C11-C10-C8-C9 |
| 22 | a | 410 | CLA | C14-C13-C15-C16 |
| 23 | D | 401 | PHO | C6-C7-C8-C9 |
| 31 | B | 624 | STE | O2-C1-C2-C3 |
| 29 | c | 519 | DGD | C2B-C3B-C4B-C5B |
| 27 | b | 623 | LMG | C31-C32-C33-C34 |
| 28 | a | 412 | SQD | C30-C31-C32-C33 |
| 24 | K | 101 | BCR | C35-C13-C14-C15 |
| 24 | b | 617 | BCR | C16-C17-C18-C36 |
| 33 | d | 407 | LHG | C31-C32-C33-C34 |
| 22 | b | 601 | CLA | O2A-C1-C2-C3 |
| 23 | a | 404 | PHO | O2A-C1-C2-C3 |
| 29 | C | 516 | DGD | O6D-C1D-O3G-C3G |
| 27 | b | 621 | LMG | C18-C19-C20-C21 |
| 24 | K | 103 | BCR | C37-C22-C23-C24 |
| 34 | F | 102 | HEC | CAD-CBD-CGD-O1D |
| 22 | c | 508 | CLA | C5-C6-C7-C8 |
| 29 | C | 515 | DGD | C2A-C3A-C4A-C5A |
| 29 | C | 515 | DGD | CBA-CCA-CDA-CEA |
| 34 | V | 201 | HEC | CAD-CBD-CGD-O1D |
| 27 | M | 101 | LMG | C9-C8-O7-C10 |
| 22 | B | 606 | CLA | C10-C11-C12-C13 |
| 29 | C | 517 | DGD | O6D-C5D-C6D-O5D |
| 31 | E | 102 | STE | C4-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | a | 414 | STE | C5-C6-C7-C8 |
| 22 | B | 605 | CLA | C12-C13-C15-C16 |
| 22 | B | 612 | CLA | C11-C10-C8-C7 |
| 22 | B | 615 | CLA | C6-C7-C8-C10 |
| 22 | b | 602 | CLA | C11-C12-C13-C15 |
| 22 | c | 510 | CLA | C11-C12-C13-C15 |
| 22 | b | 611 | CLA | C15-C16-C17-C18 |
| 28 | a | 411 | SQD | C32-C33-C34-C35 |
| 27 | D | 411 | LMG | O10-C28-O8-C9 |
| 27 | B | 621 | LMG | O8-C28-C29-C30 |
| 22 | b | 614 | CLA | C13-C15-C16-C17 |
| 33 | D | 410 | LHG | O6-C4-C5-C6 |
| 34 | f | 101 | HEC | CAA-CBA-CGA-O2A |
| 22 | c | 513 | CLA | C4-C3-C5-C6 |
| 22 | c | 511 | CLA | C15-C16-C17-C18 |
| 31 | B | 625 | STE | C5-C6-C7-C8 |
| 31 | d | 412 | STE | O2-C1-C2-C3 |
| 22 | C | 510 | CLA | C13-C15-C16-C17 |
| 29 | C | 516 | DGD | O1A-C1A-O1G-C1G |
| 22 | B | 610 | CLA | C16-C17-C18-C20 |
| 27 | Y | 101 | LMG | C2-C1-O1-C7 |
| 31 | B | 620 | STE | O2-C1-C2-C3 |
| 31 | B | 625 | STE | O2-C1-C2-C3 |
| 31 | b | 624 | STE | O2-C1-C2-C3 |
| 31 | c | 521 | STE | O2-C1-C2-C3 |
| 31 | j | 101 | STE | C7-C8-C9-C10 |
| 27 | M | 101 | LMG | C36-C37-C38-C39 |
| 27 | b | 621 | LMG | C39-C40-C41-C42 |
| 22 | C | 509 | CLA | C16-C17-C18-C19 |
| 33 | E | 101 | LHG | C34-C35-C36-C37 |
| 29 | A | 413 | DGD | O6D-C1D-O3G-C3G |
| 22 | b | 612 | CLA | C10-C11-C12-C13 |
| 28 | L | 101 | SQD | C14-C15-C16-C17 |
| 22 | b | 604 | CLA | C3-C5-C6-C7 |
| 22 | a | 402 | CLA | C2-C1-O2A-CGA |
| 33 | L | 102 | LHG | C29-C30-C31-C32 |
| 31 | B | 620 | STE | O1-C1-C2-C3 |
| 31 | b | 624 | STE | O1-C1-C2-C3 |
| 31 | c | 521 | STE | O1-C1-C2-C3 |
| 33 | D | 410 | LHG | C17-C18-C19-C20 |
| 22 | A | 402 | CLA | C14-C13-C15-C16 |
| 28 | A | 412 | SQD | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | A | 403 | CLA | O1A-CGA-O2A-C1 |
| 27 | c | 522 | LMG | C35-C36-C37-C38 |
| 28 | B | 622 | SQD | C35-C36-C37-C38 |
| 26 | D | 406 | PL9 | C16-C17-C18-C19 |
| 29 | H | 103 | DGD | C9B-CAB-CBB-CCB |
| 24 | A | 406 | BCR | C1-C6-C7-C8 |
| 24 | A | 406 | BCR | C5-C6-C7-C8 |
| 24 | K | 103 | BCR | C23-C24-C25-C30 |
| 24 | d | 405 | BCR | C23-C24-C25-C30 |
| 24 | h | 101 | BCR | C23-C24-C25-C30 |
| 24 | k | 102 | BCR | C1-C6-C7-C8 |
| 24 | k | 102 | BCR | C23-C24-C25-C26 |
| 24 | k | 102 | BCR | C23-C24-C25-C30 |
| 29 | c | 518 | DGD | C9A-CAA-CBA-CCA |
| 29 | c | 518 | DGD | CAB-CBB-CCB-CDB |
| 33 | D | 409 | LHG | O1-C1-C2-C3 |
| 31 | b | 627 | STE | C4-C5-C6-C7 |
| 24 | T | 101 | BCR | C9-C10-C11-C12 |
| 24 | b | 619 | BCR | C9-C10-C11-C12 |
| 26 | A | 409 | PL9 | C40-C39-C41-C42 |
| 27 | a | 415 | LMG | C33-C34-C35-C36 |
| 31 | c | 521 | STE | C10-C11-C12-C13 |
| 26 | D | 406 | PL9 | C33-C34-C36-C37 |
| 34 | V | 201 | HEC | CAD-CBD-CGD-O2D |
| 31 | B | 625 | STE | C9-C10-C11-C12 |
| 27 | M | 101 | LMG | C8-C7-O1-C1 |
| 33 | D | 410 | LHG | O6-C4-C5-O7 |
| 34 | F | 102 | HEC | CAD-CBD-CGD-O2D |
| 31 | B | 624 | STE | C4-C5-C6-C7 |
| 27 | b | 623 | LMG | C17-C18-C19-C20 |
| 31 | B | 623 | STE | C3-C4-C5-C6 |
| 31 | B | 625 | STE | O1-C1-C2-C3 |
| 31 | b | 622 | STE | O2-C1-C2-C3 |
| 22 | b | 603 | CLA | C4-C3-C5-C6 |
| 22 | B | 608 | CLA | C6-C7-C8-C10 |
| 22 | B | 612 | CLA | C6-C7-C8-C10 |
| 22 | C | 510 | CLA | C6-C7-C8-C10 |
| 22 | b | 611 | CLA | C6-C7-C8-C10 |
| 26 | a | 409 | PL9 | C28-C29-C31-C32 |
| 31 | C | 519 | STE | C14-C15-C16-C17 |
| 31 | b | 625 | STE | C5-C6-C7-C8 |
| 33 | E | 101 | LHG | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | B | 623 | STE | C9-C10-C11-C12 |
| 31 | B | 625 | STE | C6-C7-C8-C9 |
| 27 | A | 410 | LMG | O7-C8-C9-O8 |
| 28 | L | 101 | SQD | O47-C45-C46-O48 |
| 29 | C | 515 | DGD | O1A-C1A-O1G-C1G |
| 29 | H | 103 | DGD | CAB-CBB-CCB-CDB |
| 22 | D | 405 | CLA | C3-C5-C6-C7 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O2A |
| 27 | d | 410 | LMG | O7-C10-C11-C12 |
| 24 | d | 405 | BCR | C16-C17-C18-C36 |
| 29 | C | 516 | DGD | C5B-C6B-C7B-C8B |
| 26 | a | 409 | PL9 | C35-C34-C36-C37 |
| 22 | B | 616 | CLA | C10-C11-C12-C13 |
| 27 | c | 523 | LMG | C36-C37-C38-C39 |
| 29 | c | 517 | DGD | C5B-C6B-C7B-C8B |
| 31 | m | 102 | STE | C4-C5-C6-C7 |
| 22 | C | 504 | CLA | C2-C3-C5-C6 |
| 22 | b | 614 | CLA | C2-C3-C5-C6 |
| 22 | c | 505 | CLA | C2-C3-C5-C6 |
| 22 | c | 513 | CLA | C2-C3-C5-C6 |
| 28 | a | 411 | SQD | O47-C7-C8-C9 |
| 22 | B | 609 | CLA | C14-C13-C15-C16 |
| 22 | C | 505 | CLA | C6-C7-C8-C9 |
| 22 | b | 604 | CLA | C6-C7-C8-C9 |
| 22 | b | 607 | CLA | C6-C7-C8-C9 |
| 22 | b | 607 | CLA | C11-C12-C13-C14 |
| 22 | b | 611 | CLA | C6-C7-C8-C9 |
| 22 | b | 614 | CLA | C14-C13-C15-C16 |
| 22 | c | 506 | CLA | C14-C13-C15-C16 |
| 22 | c | 512 | CLA | C6-C7-C8-C9 |
| 22 | c | 514 | CLA | C11-C10-C8-C9 |
| 22 | A | 403 | CLA | C3A-C2A-CAA-CBA |
| 27 | M | 101 | LMG | C21-C22-C23-C24 |
| 31 | J | 101 | STE | O2-C1-C2-C3 |
| 31 | b | 622 | STE | O1-C1-C2-C3 |
| 22 | B | 604 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 605 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 609 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 506 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 508 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 512 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | b | 604 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 605 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | b | 612 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 511 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 513 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 514 | CLA | CAD-CBD-CGD-O2D |
| 22 | d | 404 | CLA | CAD-CBD-CGD-O2D |
| 22 | c | 514 | CLA | C13-C15-C16-C17 |
| 22 | c | 514 | CLA | C2-C1-O2A-CGA |
| 24 | b | 619 | BCR | C6-C7-C8-C9 |
| 22 | a | 402 | CLA | C4C-C3C-CAC-CBC |
| 22 | c | 506 | CLA | C2-C3-C5-C6 |
| 26 | D | 406 | PL9 | C43-C44-C46-C47 |
| 28 | a | 412 | SQD | C16-C17-C18-C19 |
| 24 | T | 101 | BCR | C11-C12-C13-C14 |
| 24 | a | 406 | BCR | C21-C22-C23-C24 |
| 31 | m | 102 | STE | C1-C2-C3-C4 |
| 27 | A | 410 | LMG | C7-C8-C9-O8 |
| 27 | M | 101 | LMG | O1-C7-C8-C9 |
| 29 | C | 515 | DGD | O1G-C1G-C2G-C3G |
| 34 | v | 201 | HEC | CAD-CBD-CGD-O2D |
| 31 | J | 101 | STE | C4-C5-C6-C7 |
| 26 | a | 409 | PL9 | C11-C12-C13-C14 |
| 24 | A | 406 | BCR | C18-C19-C20-C21 |
| 24 | B | 619 | BCR | C10-C11-C12-C13 |
| 31 | B | 625 | STE | C3-C4-C5-C6 |
| 22 | C | 509 | CLA | O2A-C1-C2-C3 |
| 22 | C | 512 | CLA | O2A-C1-C2-C3 |
| 22 | D | 405 | CLA | O2A-C1-C2-C3 |
| 22 | d | 404 | CLA | O2A-C1-C2-C3 |
| 29 | C | 516 | DGD | C2B-C3B-C4B-C5B |
| 33 | D | 410 | LHG | C24-C25-C26-C27 |
| 22 | B | 603 | CLA | C2A-CAA-CBA-CGA |
| 27 | b | 623 | LMG | O7-C10-C11-C12 |
| 28 | A | 412 | SQD | O48-C23-C24-C25 |
| 31 | B | 620 | STE | C7-C8-C9-C10 |
| 31 | b | 624 | STE | C14-C15-C16-C17 |
| 22 | B | 602 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 607 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 504 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | C | 505 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 507 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 507 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 508 | CLA | CHA-CBD-CGD-O2D |
| 22 | D | 404 | CLA | CHA-CBD-CGD-O1D |
| 22 | H | 101 | CLA | CHA-CBD-CGD-O2D |
| 22 | b | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | b | 607 | CLA | CHA-CBD-CGD-O1D |
| 22 | b | 607 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 505 | CLA | CHA-CBD-CGD-O2D |
| 22 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 24 | K | 101 | BCR | C9-C10-C11-C12 |
| 34 | v | 201 | HEC | CAD-CBD-CGD-O1D |
| 27 | c | 522 | LMG | C42-C43-C44-C45 |
| 29 | C | 516 | DGD | C8A-C9A-CAA-CBA |
| 33 | D | 409 | LHG | C18-C19-C20-C21 |
| 27 | A | 410 | LMG | O1-C7-C8-O7 |
| 29 | C | 515 | DGD | O2G-C2G-C3G-O3G |
| 28 | L | 101 | SQD | C11-C10-C9-C8 |
| 22 | D | 405 | CLA | C10-C11-C12-C13 |
| 31 | J | 101 | STE | O1-C1-C2-C3 |
| 28 | A | 411 | SQD | O47-C7-C8-C9 |
| 27 | M | 101 | LMG | C30-C31-C32-C33 |
| 31 | b | 625 | STE | C3-C4-C5-C6 |
| 23 | d | 401 | PHO | CHA-CBD-CGD-O1D |
| 23 | d | 401 | PHO | CHA-CBD-CGD-O2D |
| 29 | h | 102 | DGD | O1B-C1B-C2B-C3B |
| 27 | a | 415 | LMG | C11-C10-O7-C8 |
| 29 | C | 515 | DGD | O2G-C1B-C2B-C3B |
| 22 | B | 606 | CLA | C11-C10-C8-C7 |
| 22 | B | 615 | CLA | C12-C13-C15-C16 |
| 22 | C | 502 | CLA | C12-C13-C15-C16 |
| 22 | C | 506 | CLA | C6-C7-C8-C10 |
| 22 | b | 603 | CLA | C6-C7-C8-C10 |
| 22 | c | 509 | CLA | O1D-CGD-O2D-CED |
| 28 | A | 412 | SQD | O49-C7-O47-C45 |
| 22 | B | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 613 | CLA | C6-C7-C8-C9 |
| 22 | B | 615 | CLA | C6-C7-C8-C9 |
| 22 | C | 502 | CLA | C14-C13-C15-C16 |
| 22 | C | 506 | CLA | C14-C13-C15-C16 |
| 22 | C | 510 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | D | 405 | CLA | C6-C7-C8-C9 |
| 31 | d | 411 | STE | C1-C2-C3-C4 |
| 26 | D | 406 | PL9 | C34-C36-C37-C38 |
| 31 | B | 625 | STE | C1-C2-C3-C4 |
| 22 | H | 101 | CLA | C15-C16-C17-C18 |
| 31 | B | 620 | STE | C4-C5-C6-C7 |
| 33 | l | 101 | LHG | O7-C7-C8-C9 |
| 22 | B | 603 | CLA | O1D-CGD-O2D-CED |
| 33 | d | 408 | LHG | C30-C31-C32-C33 |
| 31 | C | 518 | STE | O1-C1-C2-C3 |
| 29 | c | 518 | DGD | O1A-C1A-C2A-C3A |
| 22 | b | 613 | CLA | C16-C17-C18-C19 |
| 31 | B | 627 | STE | C12-C13-C14-C15 |
| 22 | a | 403 | CLA | CBD-CGD-O2D-CED |
| 24 | b | 619 | BCR | C7-C8-C9-C10 |
| 22 | D | 404 | CLA | C2C-C3C-CAC-CBC |
| 22 | A | 403 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 602 | CLA | C1A-C2A-CAA-CBA |
| 28 | A | 412 | SQD | C31-C32-C33-C34 |
| 22 | C | 509 | CLA | C16-C17-C18-C20 |
| 31 | b | 622 | STE | C11-C10-C9-C8 |
| 33 | E | 101 | LHG | C15-C16-C17-C18 |
| 23 | A | 404 | PHO | C10-C11-C12-C13 |
| 27 | b | 623 | LMG | O10-C28-C29-C30 |
| 31 | B | 601 | STE | C3-C4-C5-C6 |
| 31 | B | 626 | STE | C10-C11-C12-C13 |
| 28 | L | 101 | SQD | O6-C44-C45-C46 |
| 29 | h | 102 | DGD | C1G-C2G-C3G-O3G |
| 33 | E | 101 | LHG | C4-O6-P-O3 |
| 22 | b | 603 | CLA | C13-C15-C16-C17 |
| 27 | b | 621 | LMG | C36-C37-C38-C39 |
| 27 | b | 623 | LMG | C16-C17-C18-C19 |
| 22 | c | 506 | CLA | C4-C3-C5-C6 |
| 27 | D | 407 | LMG | C18-C19-C20-C21 |
| 31 | M | 103 | STE | C7-C8-C9-C10 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O1A |
| 31 | d | 413 | STE | O2-C1-C2-C3 |
| 33 | D | 409 | LHG | C4-O6-P-O5 |
| 33 | D | 410 | LHG | C4-O6-P-O4 |
| 33 | E | 101 | LHG | C3-O3-P-O5 |
| 33 | L | 102 | LHG | C4-O6-P-O5 |
| 33 | e | 101 | LHG | C3-O3-P-O4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | e | 101 | LHG | C4-O6-P-O5 |
| 29 | c | 519 | DGD | O6D-C1D-O3G-C3G |
| 24 | h | 101 | BCR | C11-C10-C9-C34 |
| 31 | C | 519 | STE | C11-C10-C9-C8 |
| 33 | D | 409 | LHG | C19-C20-C21-C22 |
| 31 | C | 518 | STE | O2-C1-C2-C3 |
| 31 | D | 413 | STE | O2-C1-C2-C3 |
| 24 | h | 101 | BCR | C23-C24-C25-C26 |
| 22 | D | 404 | CLA | C4C-C3C-CAC-CBC |
| 33 | L | 102 | LHG | C28-C29-C30-C31 |
| 22 | B | 603 | CLA | C15-C16-C17-C18 |
| 24 | d | 405 | BCR | C18-C19-C20-C21 |
| 33 | D | 409 | LHG | O10-C23-C24-C25 |
| 22 | B | 608 | CLA | C13-C15-C16-C17 |
| 22 | a | 410 | CLA | C15-C16-C17-C18 |
| 27 | b | 621 | LMG | C40-C41-C42-C43 |
| 29 | H | 103 | DGD | C4A-C5A-C6A-C7A |
| 31 | H | 104 | STE | C3-C4-C5-C6 |
| 23 | a | 404 | PHO | C8-C10-C11-C12 |
| 22 | c | 509 | CLA | C4-C3-C5-C6 |
| 33 | D | 412 | LHG | C16-C17-C18-C19 |
| 22 | B | 608 | CLA | C16-C17-C18-C19 |
| 29 | c | 519 | DGD | C2A-C3A-C4A-C5A |
| 31 | d | 413 | STE | O1-C1-C2-C3 |
| 22 | B | 607 | CLA | CAD-CBD-CGD-O1D |
| 22 | C | 504 | CLA | CAD-CBD-CGD-O1D |
| 22 | H | 101 | CLA | CAD-CBD-CGD-O1D |
| 22 | b | 607 | CLA | CAD-CBD-CGD-O1D |
| 22 | b | 609 | CLA | CAD-CBD-CGD-O1D |
| 22 | c | 505 | CLA | CAD-CBD-CGD-O1D |
| 28 | D | 408 | SQD | C5-C6-S-O9 |
| 27 | Y | 101 | LMG | C34-C35-C36-C37 |
| 27 | c | 522 | LMG | C32-C33-C34-C35 |
| 22 | B | 606 | CLA | C5-C6-C7-C8 |
| 22 | B | 603 | CLA | C14-C13-C15-C16 |
| 22 | B | 605 | CLA | C14-C13-C15-C16 |
| 22 | B | 615 | CLA | C14-C13-C15-C16 |
| 22 | b | 603 | CLA | C6-C7-C8-C9 |
| 22 | b | 605 | CLA | C11-C12-C13-C14 |
| 22 | b | 612 | CLA | C11-C10-C8-C9 |
| 22 | c | 510 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 517 | DGD | O2G-C1B-C2B-C3B |

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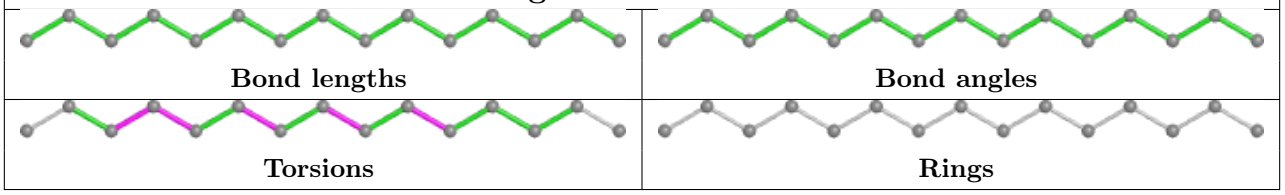
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | A | 410 | LMG | C14-C15-C16-C17 |
| 29 | A | 413 | DGD | O2G-C1B-C2B-C3B |
| 31 | M | 102 | STE | O2-C1-C2-C3 |
| 22 | c | 503 | CLA | C2C-C3C-CAC-CBC |
| 22 | b | 605 | CLA | C4-C3-C5-C6 |
| 27 | B | 621 | LMG | C14-C15-C16-C17 |
| 22 | A | 402 | CLA | C12-C13-C15-C16 |
| 22 | B | 603 | CLA | C12-C13-C15-C16 |
| 22 | B | 613 | CLA | C6-C7-C8-C10 |
| 22 | C | 505 | CLA | C11-C12-C13-C15 |
| 22 | H | 101 | CLA | C11-C12-C13-C15 |
| 22 | b | 602 | CLA | C12-C13-C15-C16 |
| 22 | b | 603 | CLA | C2-C3-C5-C6 |
| 22 | c | 512 | CLA | C6-C7-C8-C10 |
| 28 | A | 412 | SQD | O10-C23-C24-C25 |
| 34 | f | 101 | HEC | CAD-CBD-CGD-O1D |
| 22 | b | 601 | CLA | CAA-CBA-CGA-O2A |
| 27 | b | 621 | LMG | O8-C28-C29-C30 |
| 33 | d | 407 | LHG | O8-C23-C24-C25 |
| 22 | D | 403 | CLA | C10-C11-C12-C13 |
| 24 | H | 102 | BCR | C7-C8-C9-C10 |
| 24 | c | 516 | BCR | C17-C18-C19-C20 |
| 31 | D | 413 | STE | O1-C1-C2-C3 |
| 31 | I | 101 | STE | C6-C7-C8-C9 |
| 27 | Y | 101 | LMG | O8-C28-C29-C30 |
| 29 | A | 413 | DGD | O6E-C1E-O5D-C6D |
| 29 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 22 | C | 503 | CLA | C8-C10-C11-C12 |
| 22 | B | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 613 | CLA | CAA-CBA-CGA-O1A |
| 28 | a | 411 | SQD | O10-C23-C24-C25 |
| 22 | b | 615 | CLA | C13-C15-C16-C17 |
| 31 | H | 104 | STE | C11-C12-C13-C14 |
| 33 | L | 102 | LHG | O7-C7-C8-C9 |
| 27 | B | 621 | LMG | C32-C33-C34-C35 |
| 22 | C | 513 | CLA | C13-C15-C16-C17 |
| 29 | c | 517 | DGD | O1B-C1B-C2B-C3B |
| 22 | a | 403 | CLA | C16-C17-C18-C20 |
| 31 | d | 411 | STE | C3-C4-C5-C6 |
| 22 | C | 504 | CLA | C11-C12-C13-C14 |
| 22 | b | 612 | CLA | CAA-CBA-CGA-O2A |

There are no ring outliers.

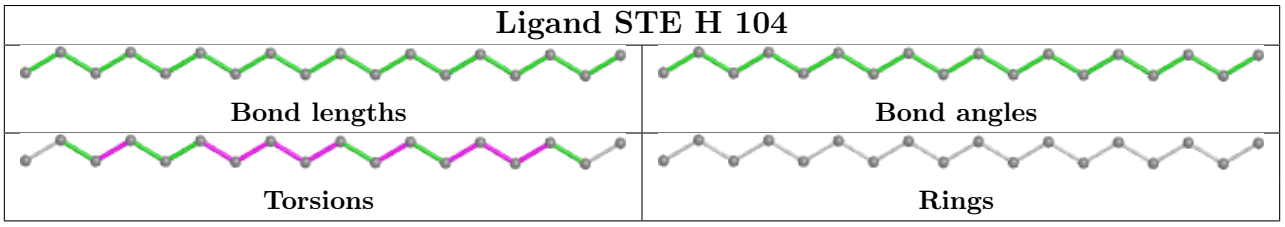
No monomer is involved in short contacts.

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

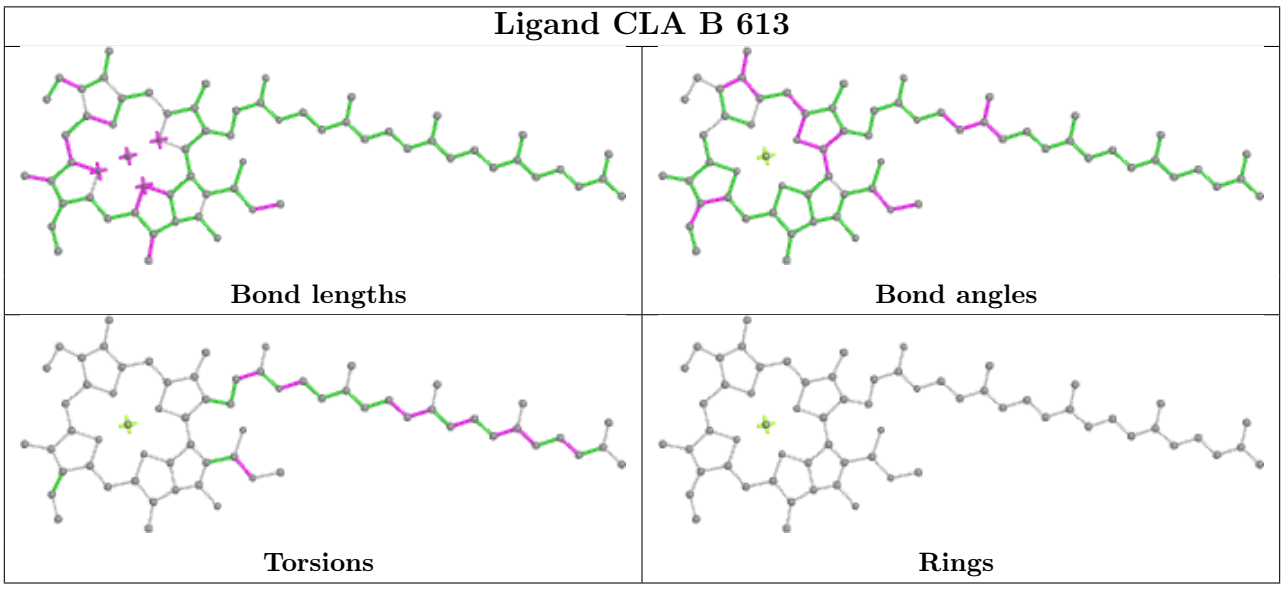
**Ligand STE B 627**



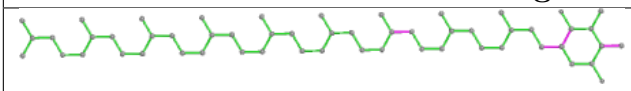

**Ligand STE H 104**

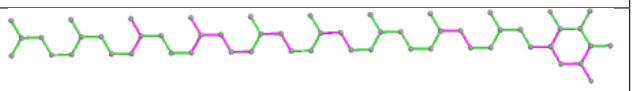


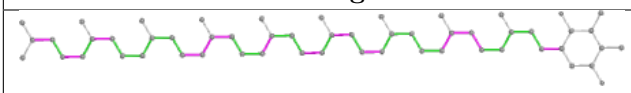

**Ligand CLA B 613**

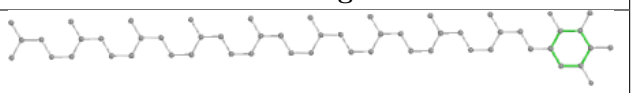


### Ligand PL9 a 409

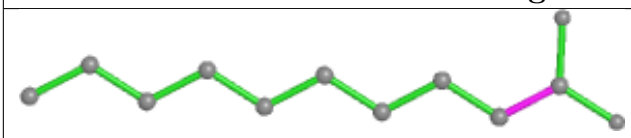

Bond lengths

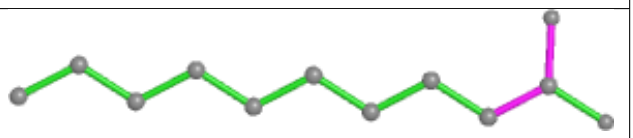

Bond angles

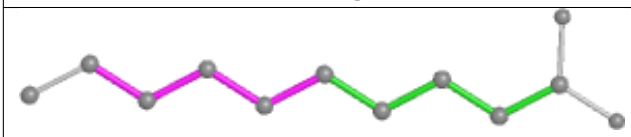

Torsions

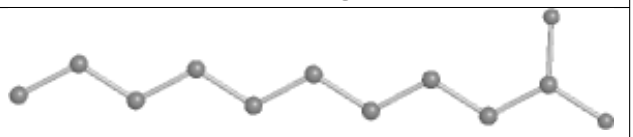

Rings

### Ligand STE E 102

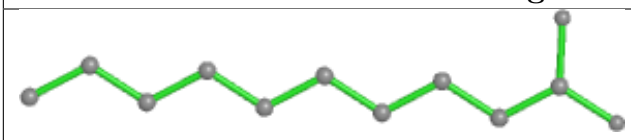

Bond lengths

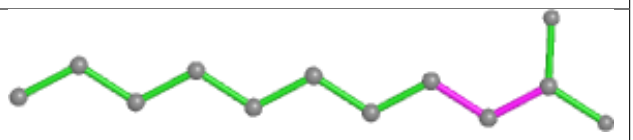

Bond angles

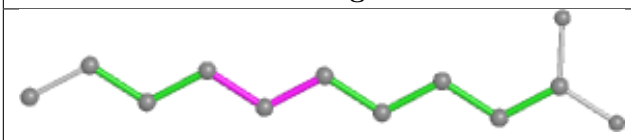

Torsions

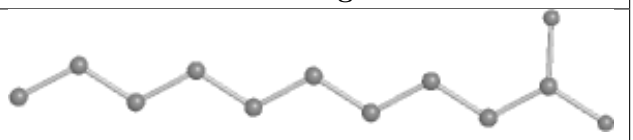

Rings

### Ligand STE C 520

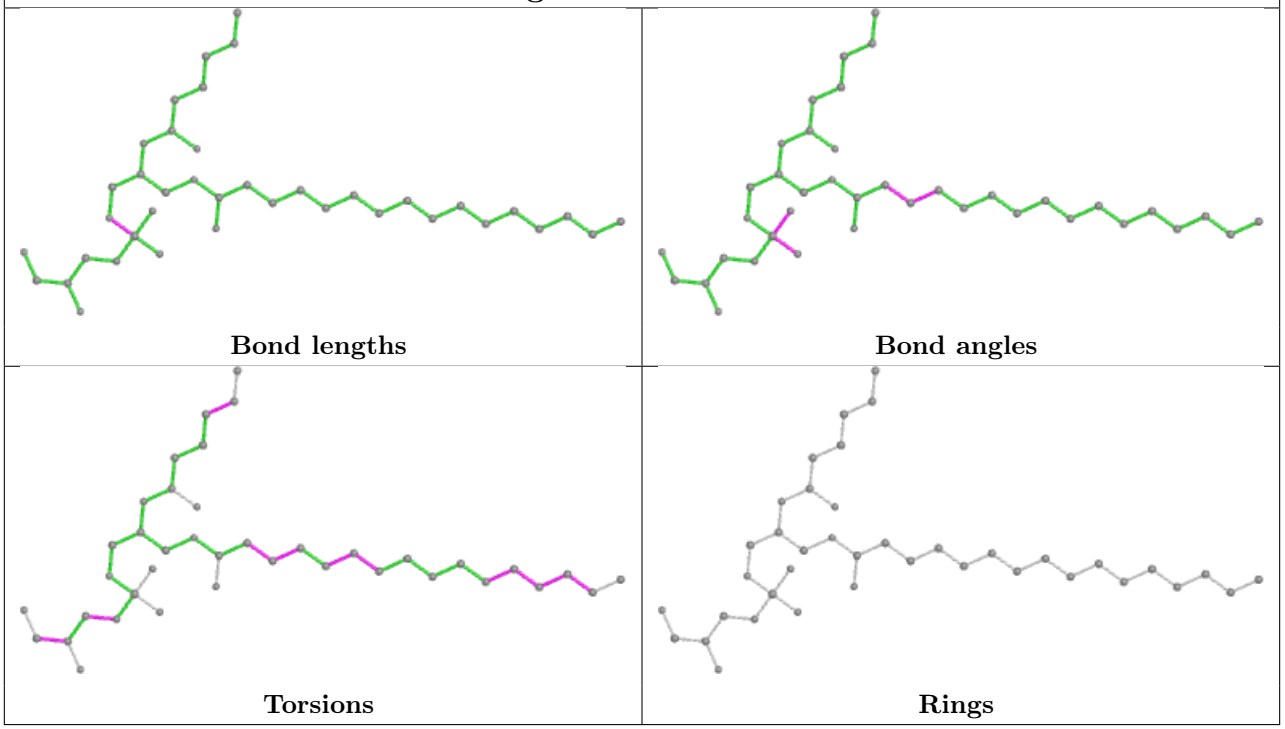

Bond lengths


Bond angles

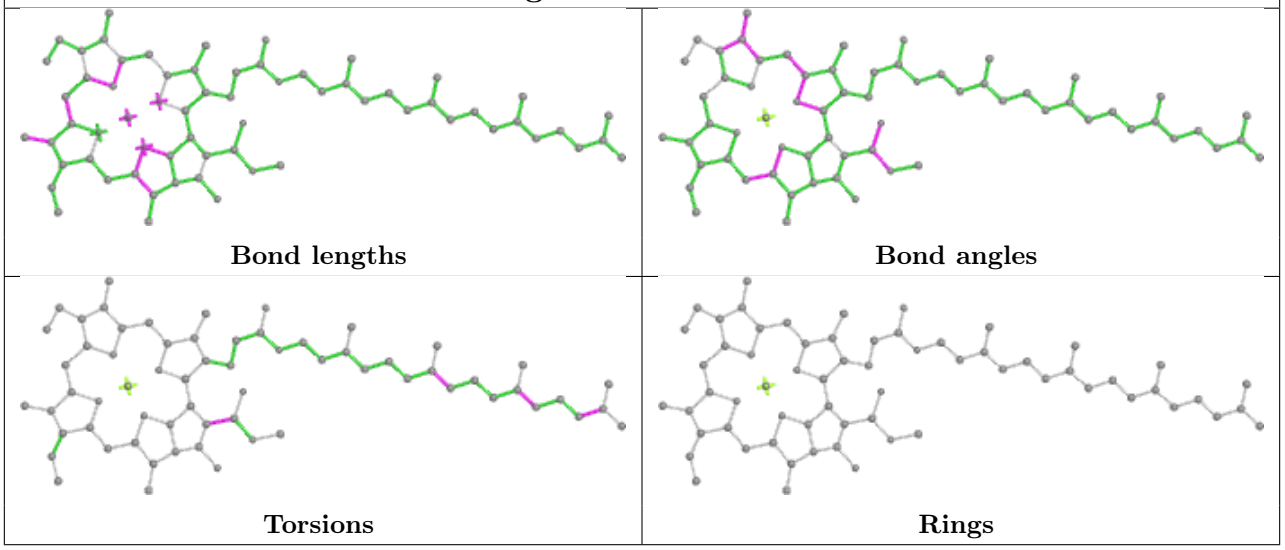

Torsions


Rings

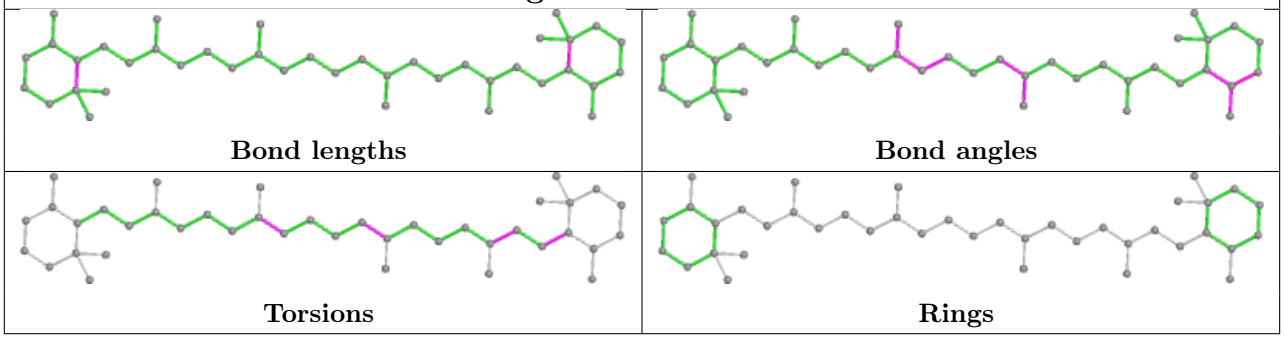
### Ligand LHG d 409



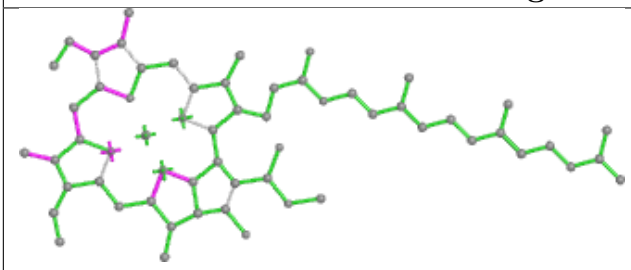

### Ligand CLA C 508



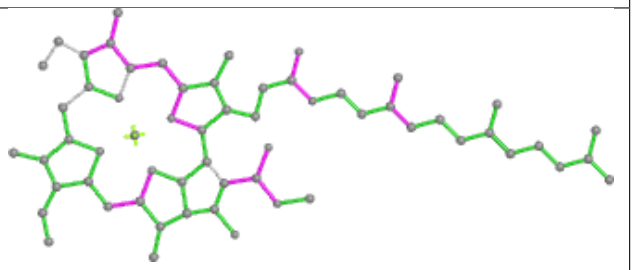

### Ligand BCR b 618



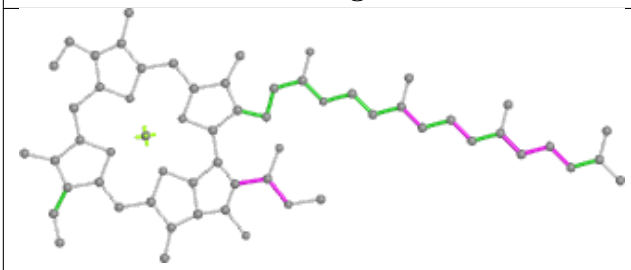
### Ligand CLA b 616



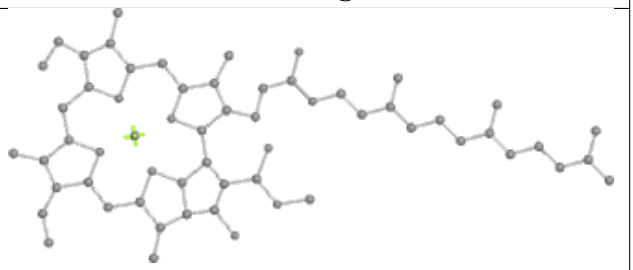
Bond lengths



Bond angles

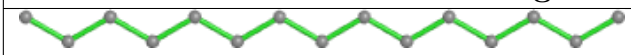


Torsions



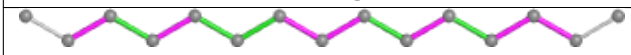
Rings

### Ligand STE I 101



Bond lengths

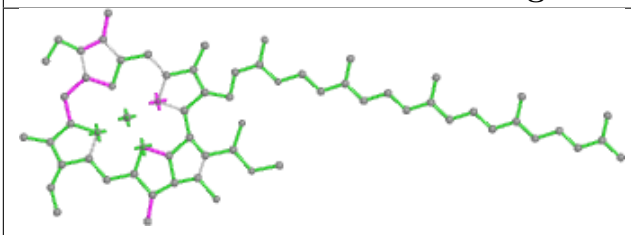
Bond angles



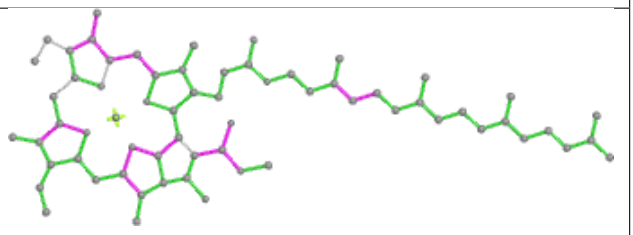
Torsions

Rings

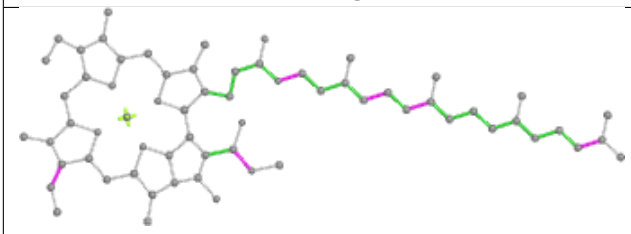
### Ligand CLA d 403



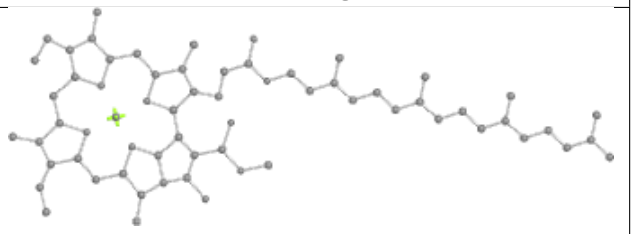
Bond lengths



Bond angles

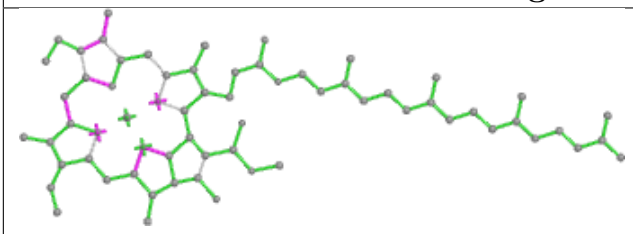


Torsions

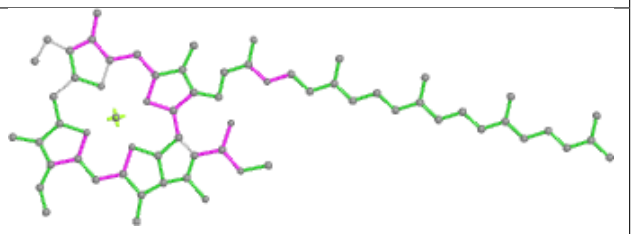


Rings

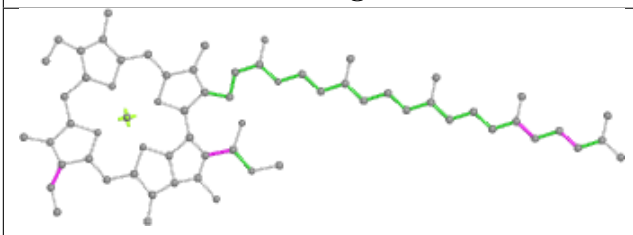
### Ligand CLA a 410



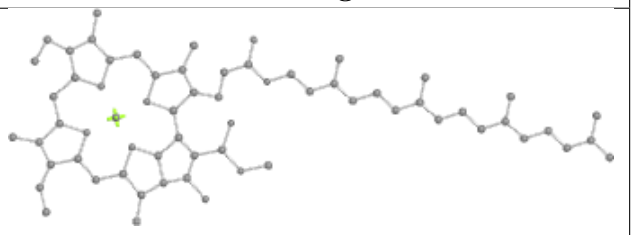
Bond lengths



Bond angles

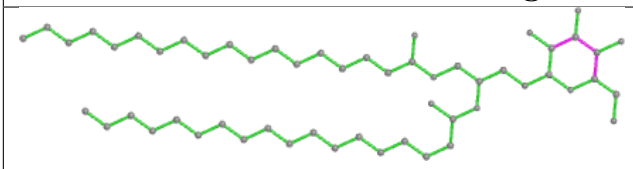


Torsions

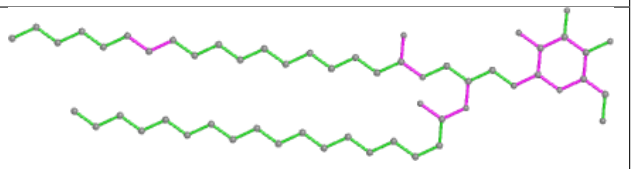


Rings

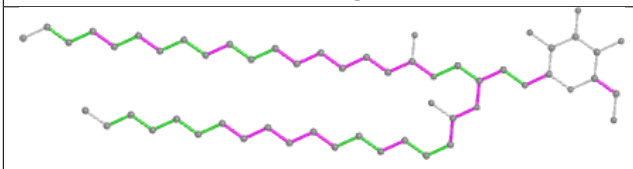
### Ligand LMG b 623



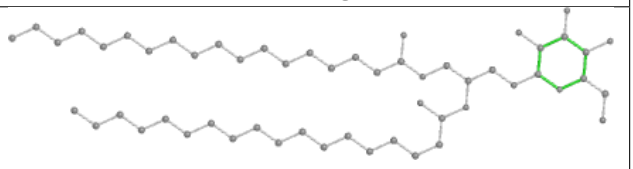
Bond lengths



Bond angles

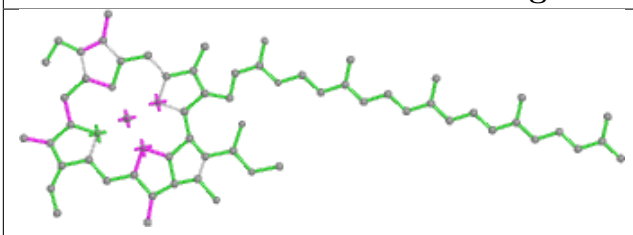


Torsions

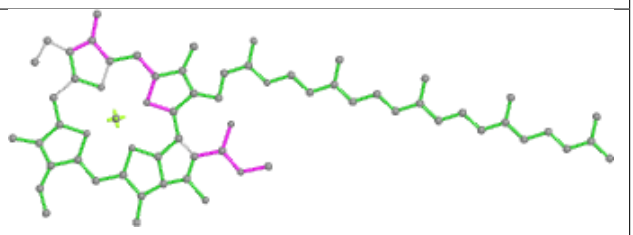


Rings

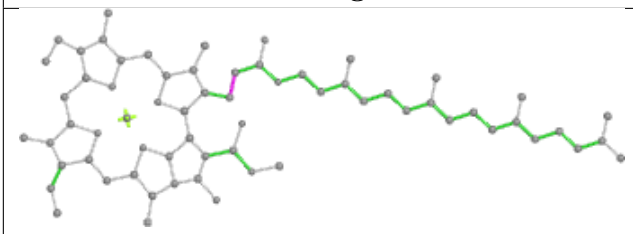
### Ligand CLA c 502



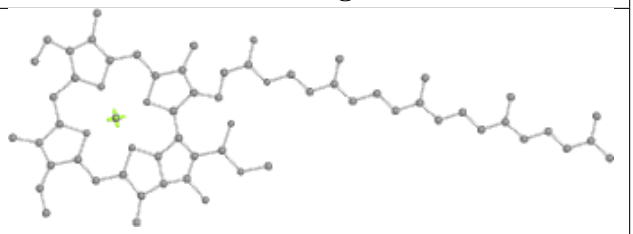
Bond lengths



Bond angles

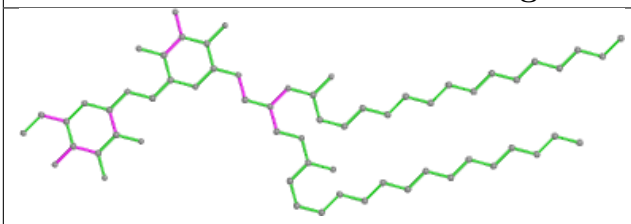


Torsions

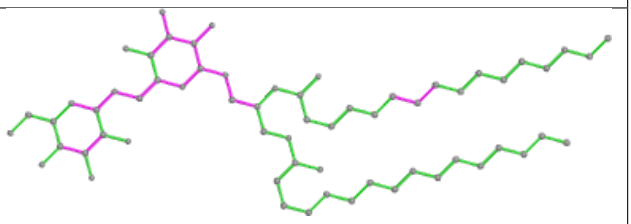


Rings

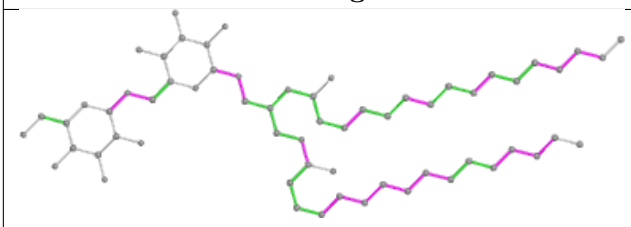
### Ligand DGD C 516



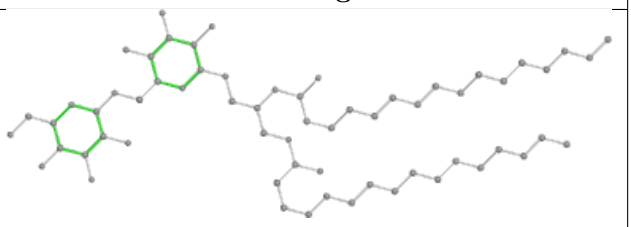
Bond lengths



Bond angles

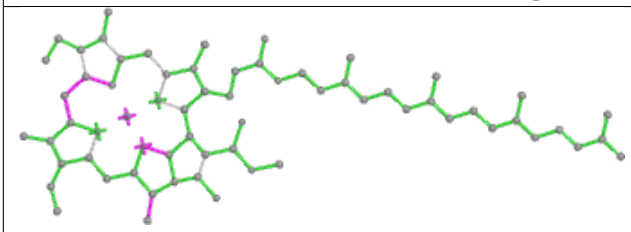


Torsions

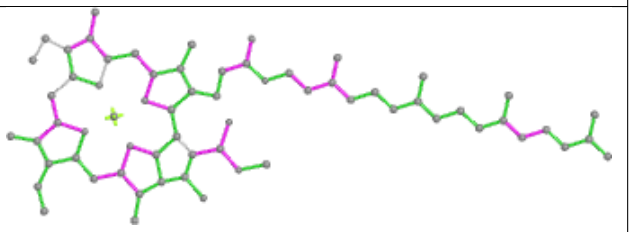


Rings

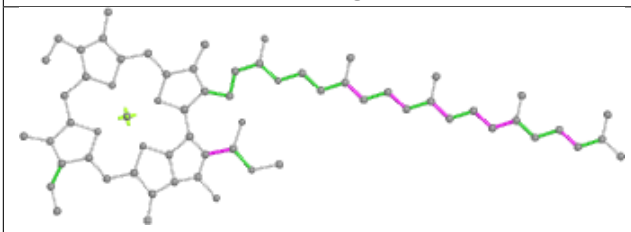
### Ligand CLA b 605



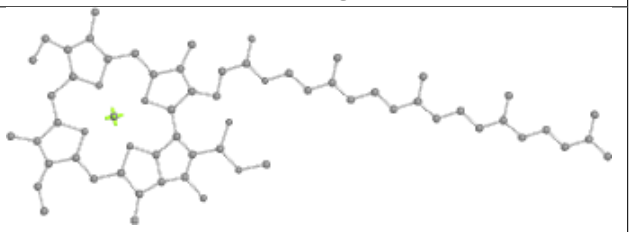
Bond lengths



Bond angles

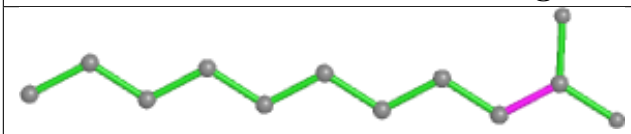


Torsions

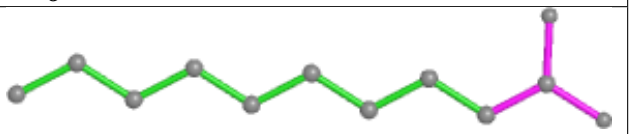


Rings

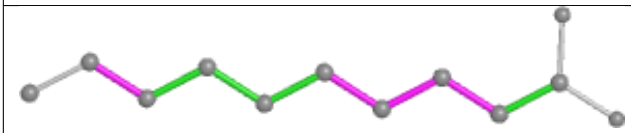
### Ligand STE j 101



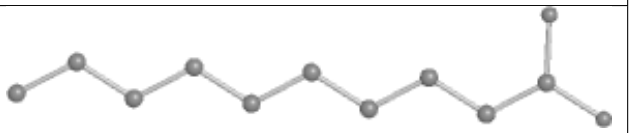
Bond lengths



Bond angles

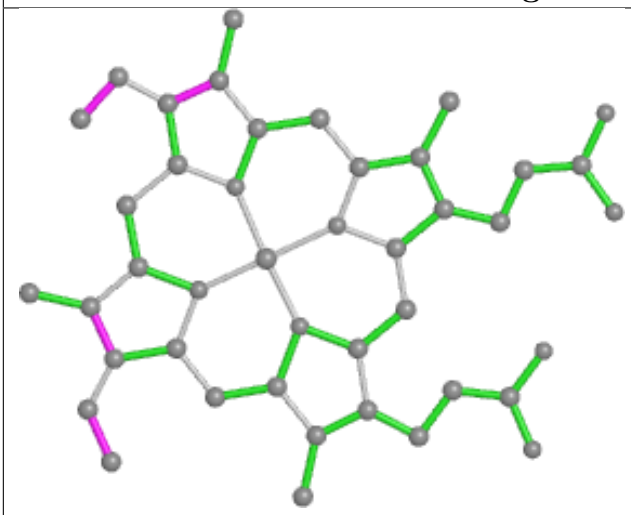


Torsions

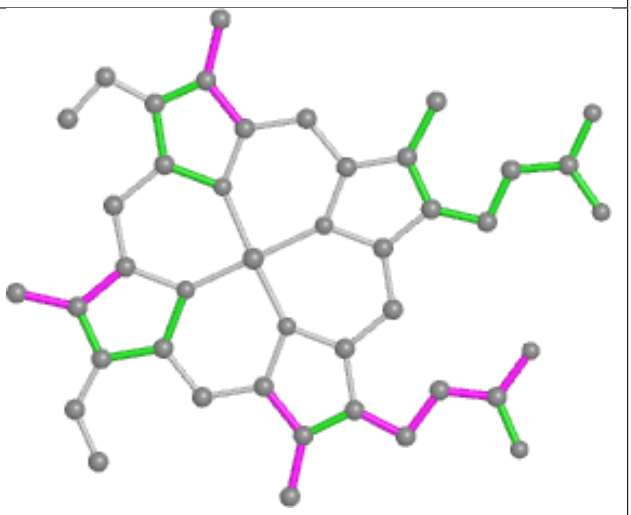


Rings

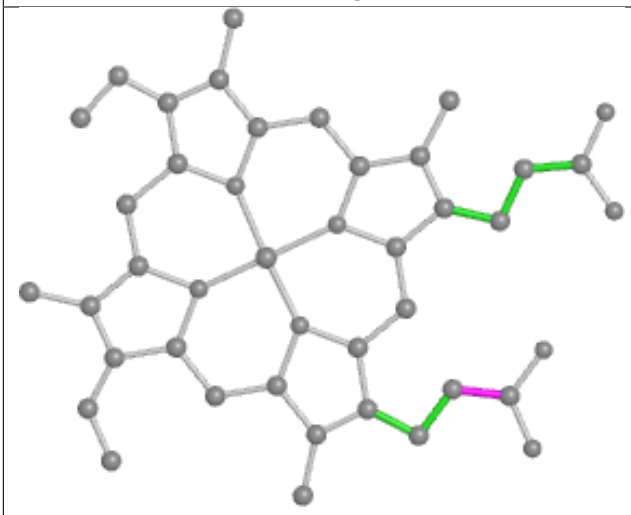
**Ligand HEC V 201**



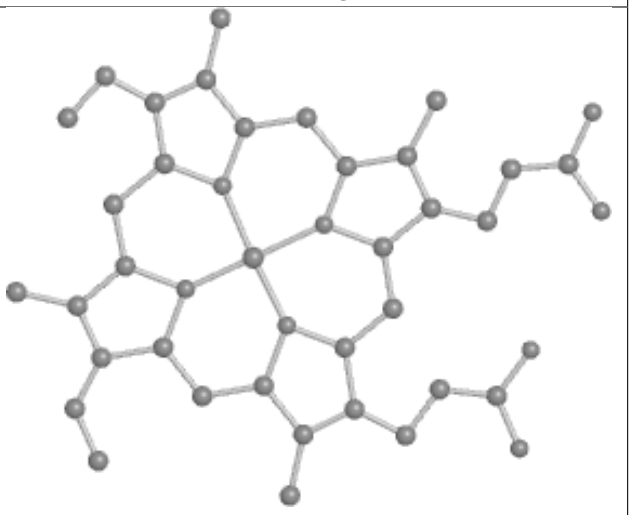
Bond lengths



Bond angles

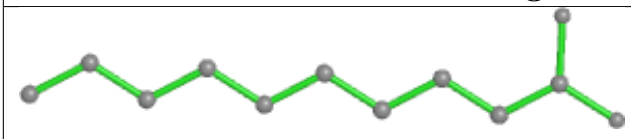


Torsions

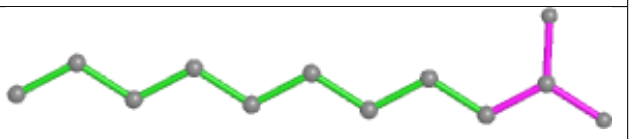


Rings

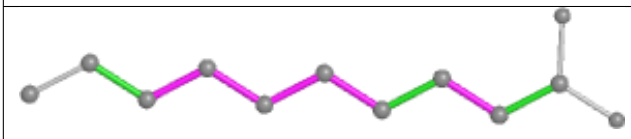
**Ligand STE m 102**



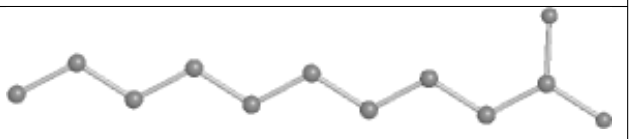
Bond lengths



Bond angles

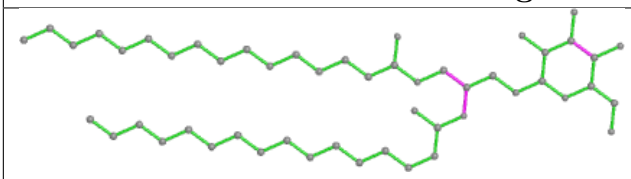


Torsions

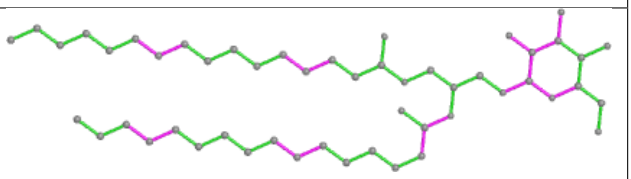


Rings

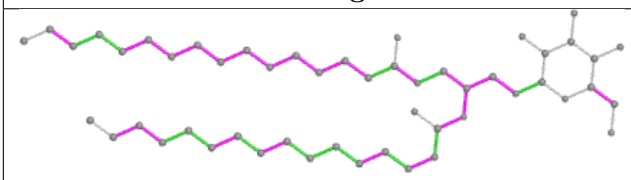
### Ligand LMG M 101



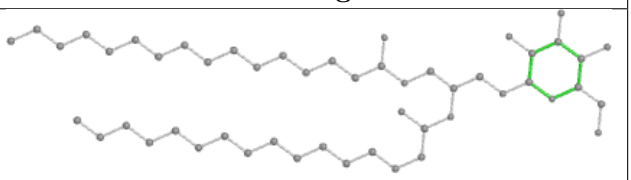
Bond lengths



Bond angles

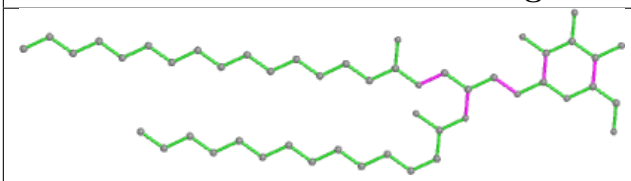


Torsions

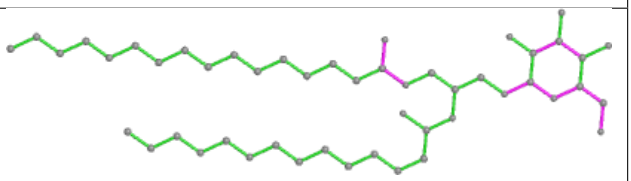


Rings

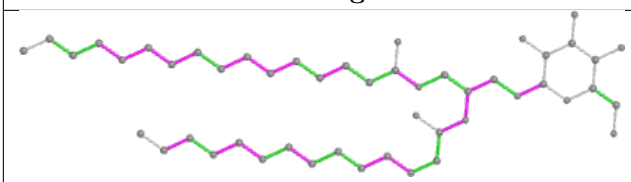
### Ligand LMG c 523



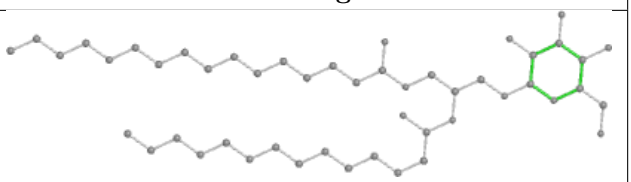
Bond lengths



Bond angles

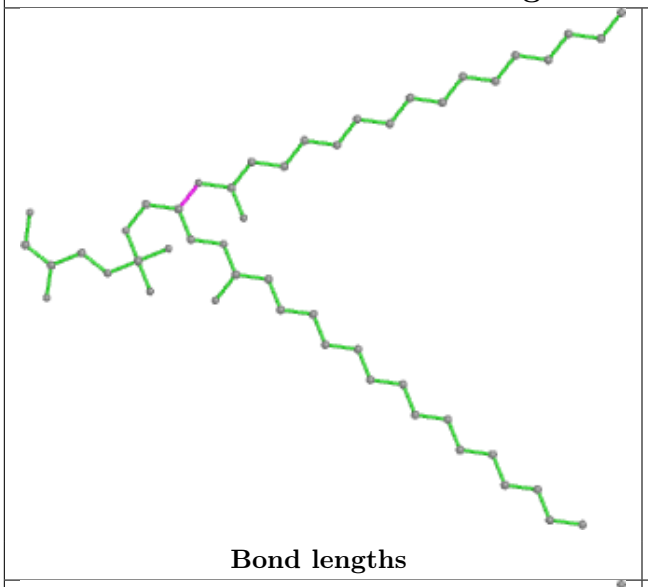


Torsions

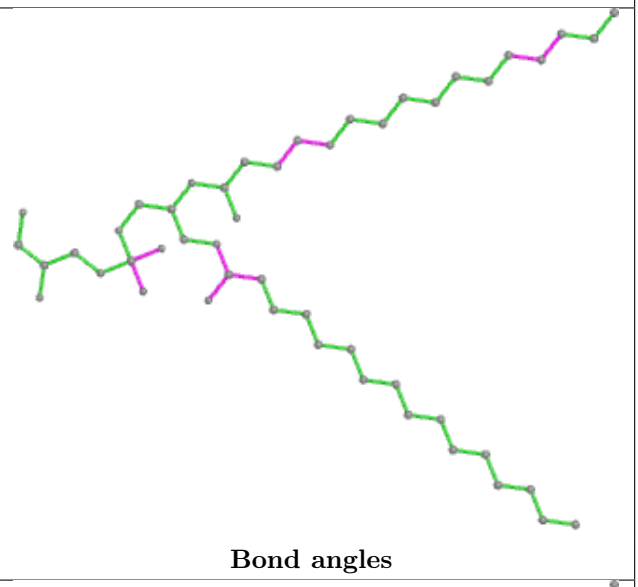


Rings

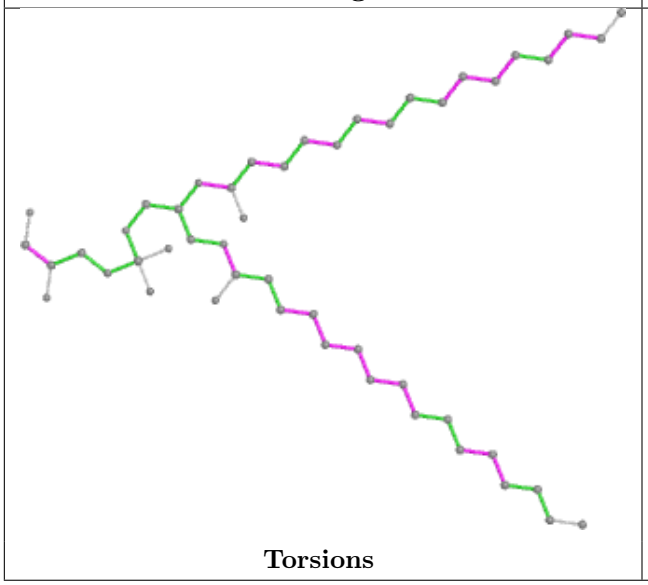
## Ligand LHG D 412



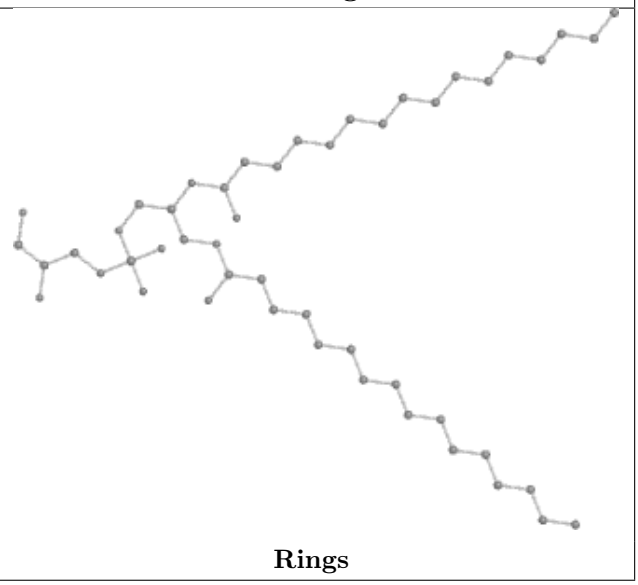
Bond lengths



Bond angles

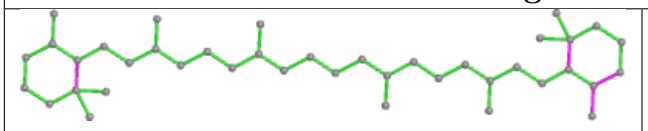


Torsions



Rings

## Ligand BCR T 101



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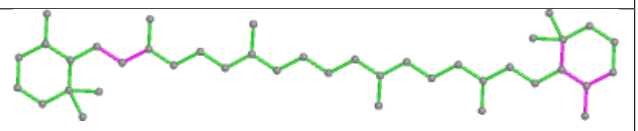
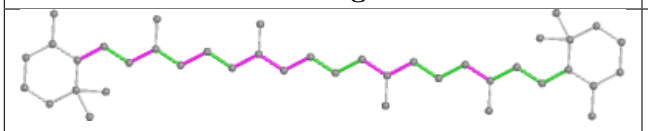
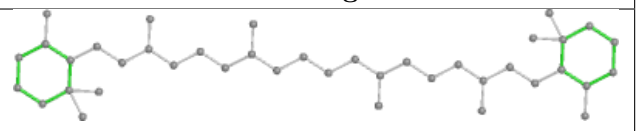


Bond angles

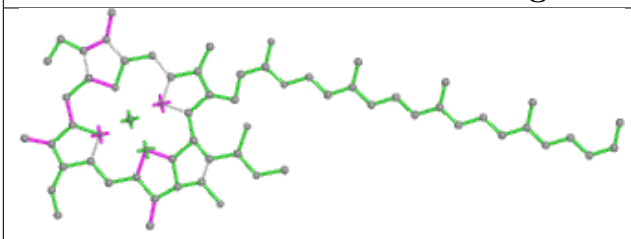


Torsions

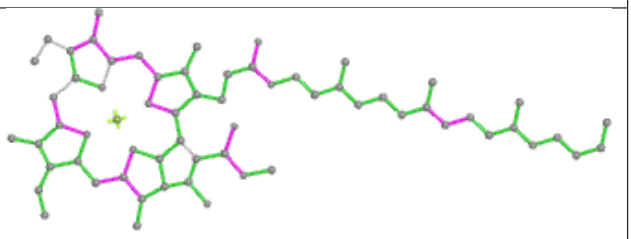


Rings

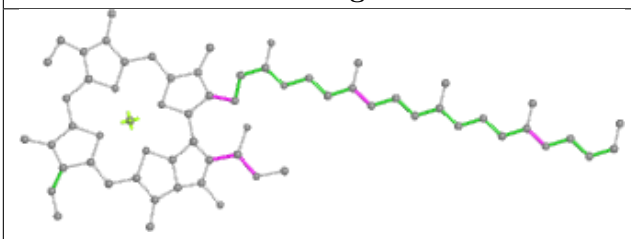
### Ligand CLA c 509



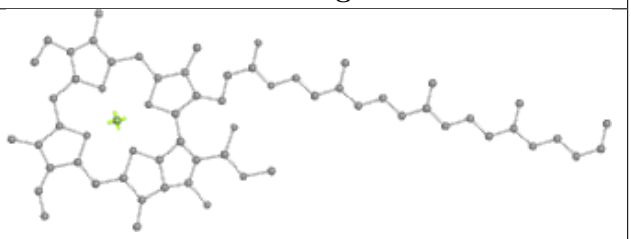
Bond lengths



Bond angles

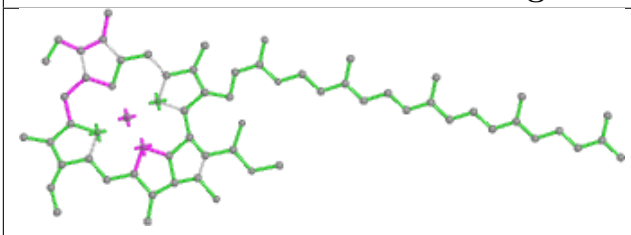


Torsions

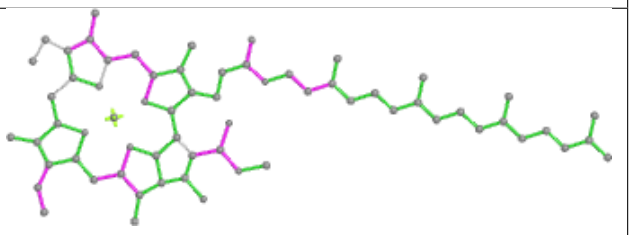


Rings

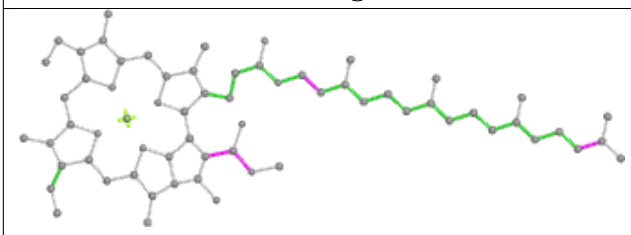
### Ligand CLA d 404



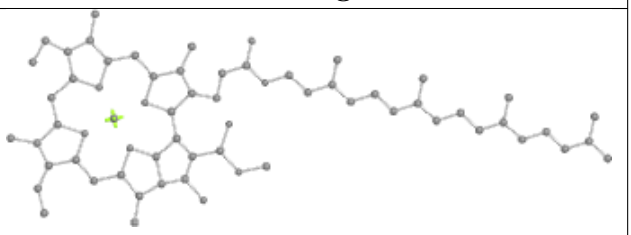
Bond lengths



Bond angles

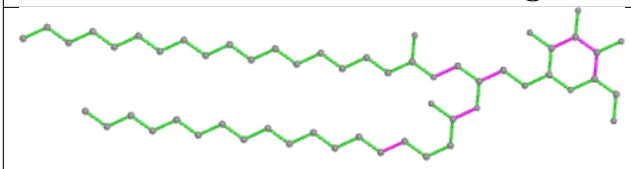


Torsions

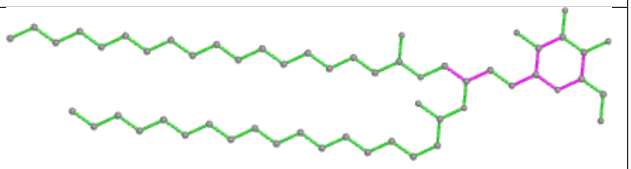


Rings

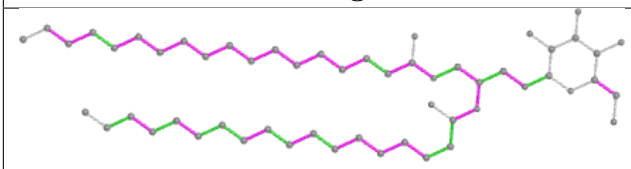
### Ligand LMG a 415



Bond lengths



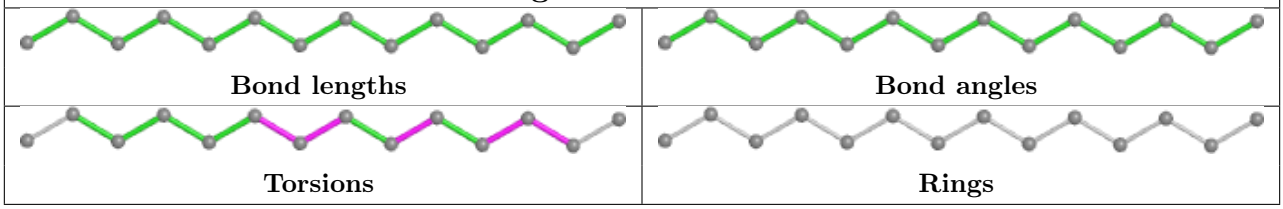
Bond angles



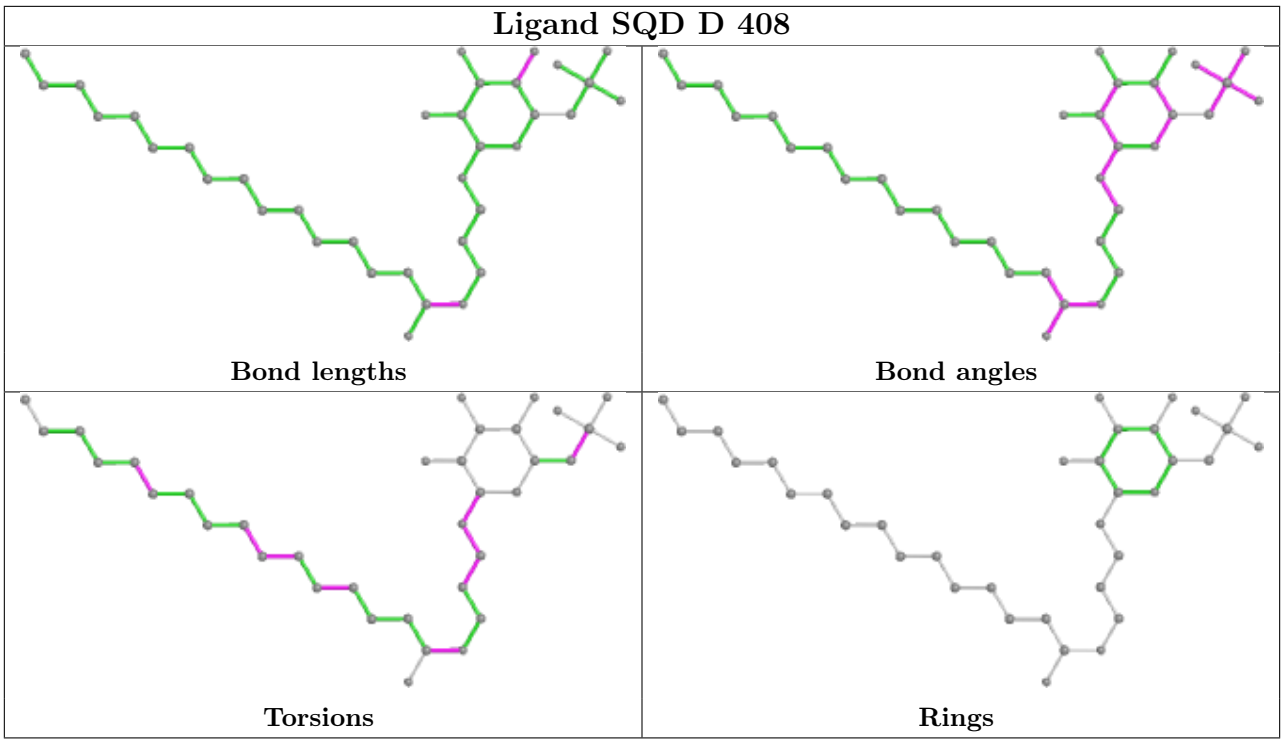
Torsions

Rings

### Ligand STE b 626




### Ligand SQD D 408

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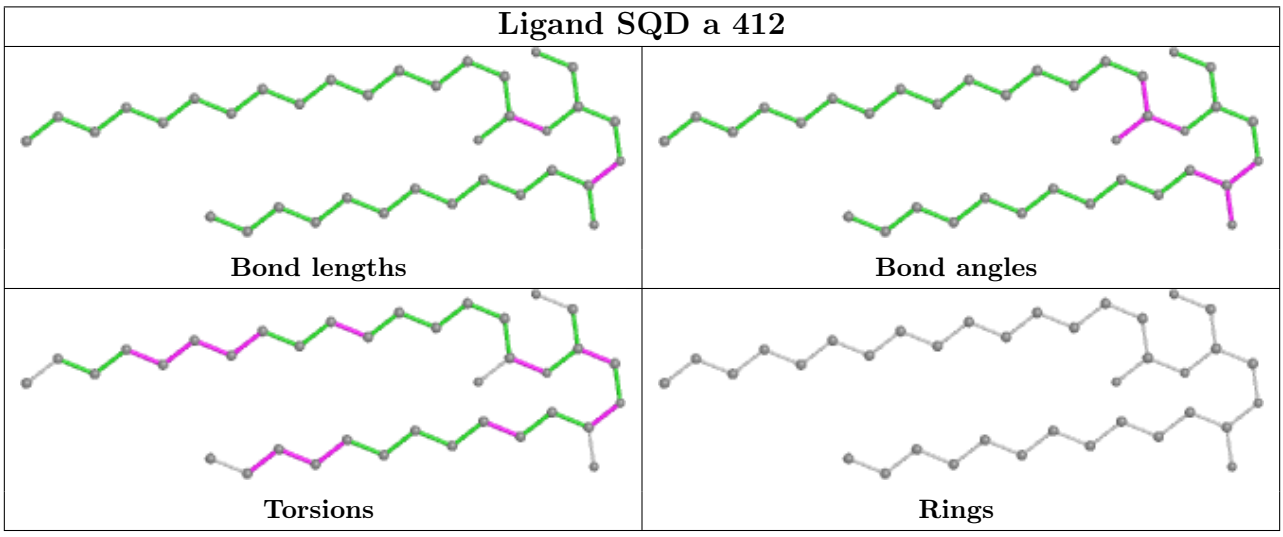
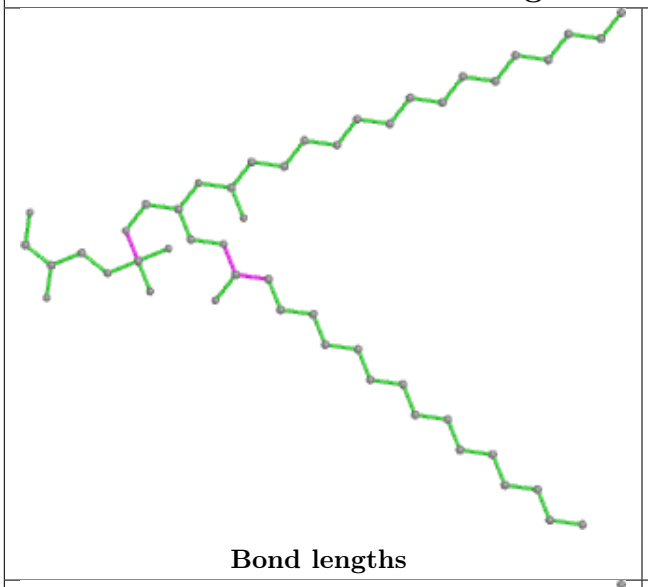
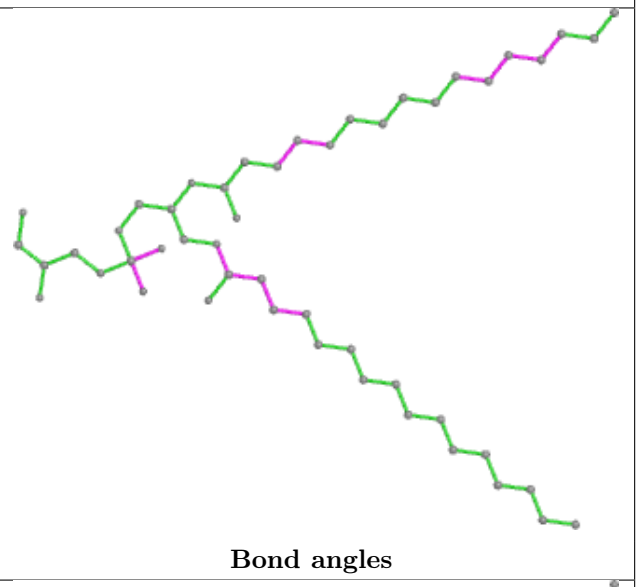


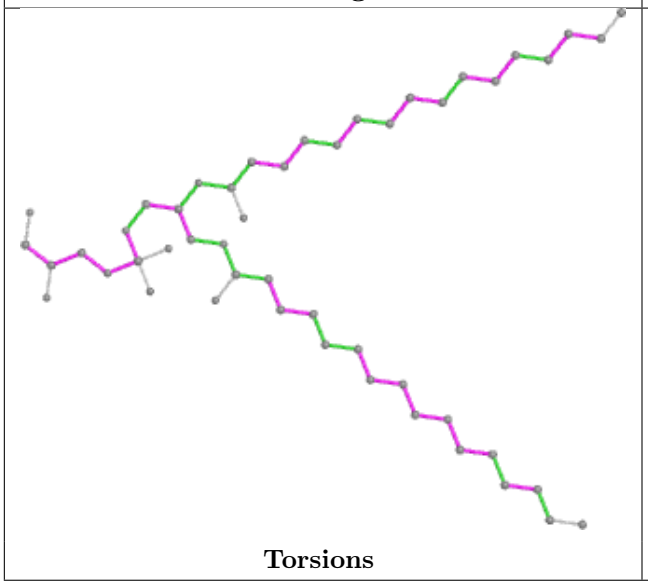
## Ligand LHG E 101



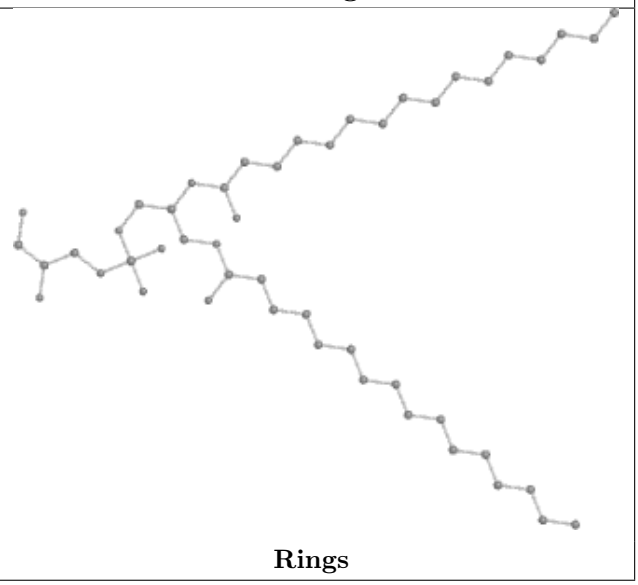
Bond lengths



Bond angles

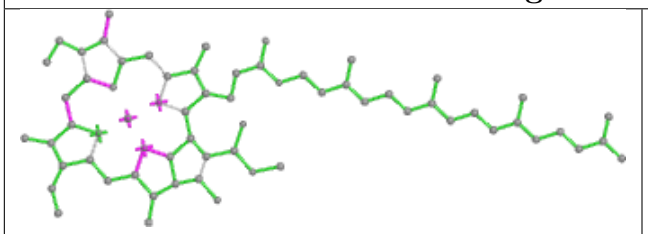


Torsions

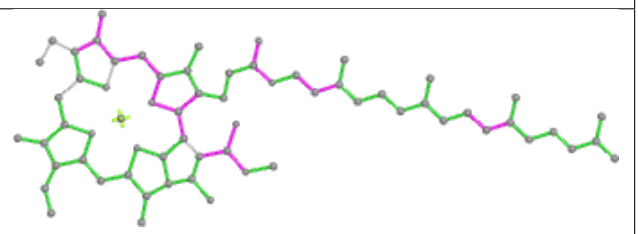


Rings

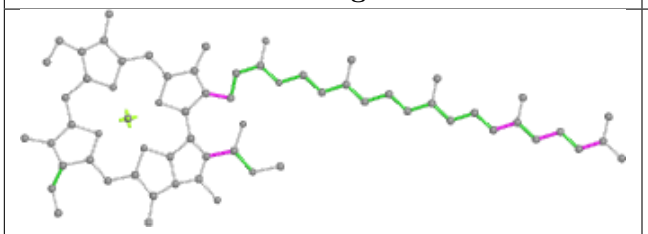
## Ligand CLA B 602



Bond lengths



Bond angles



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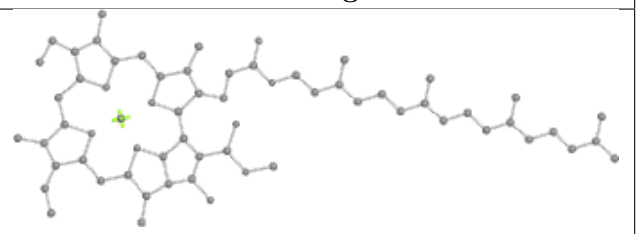
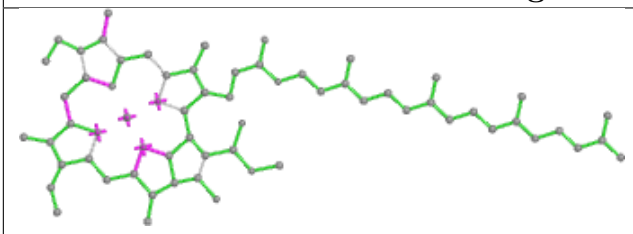


Rings

### Ligand CLA b 611



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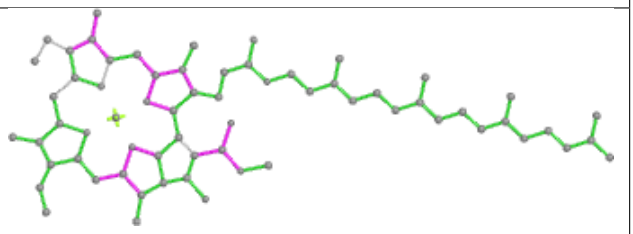
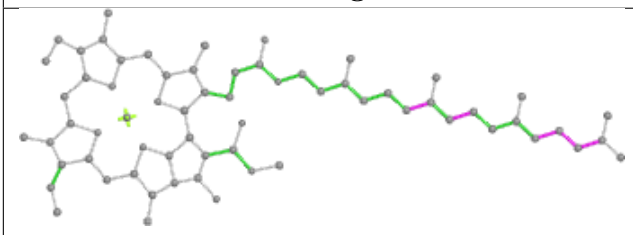
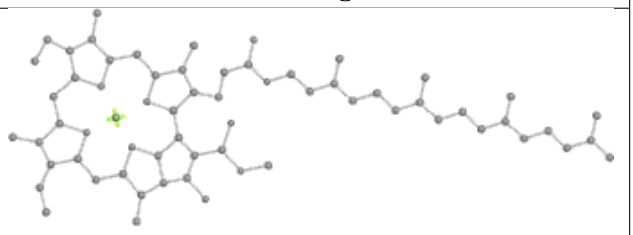


Bond angles

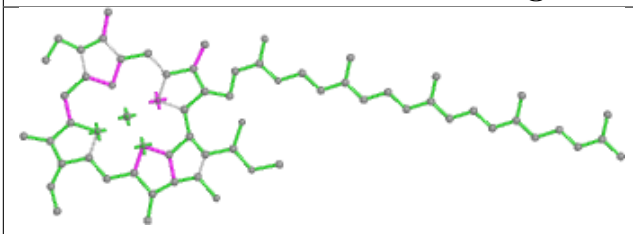


Torsions

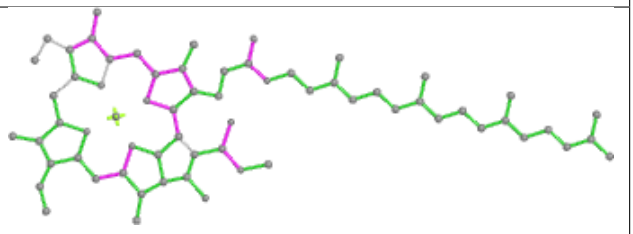


Rings

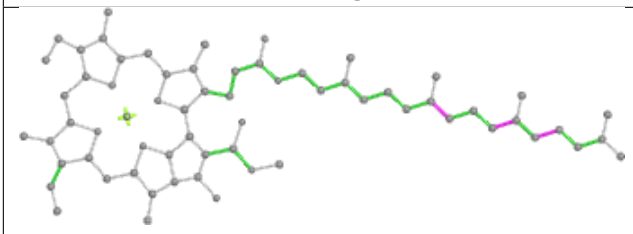
### Ligand CLA b 608



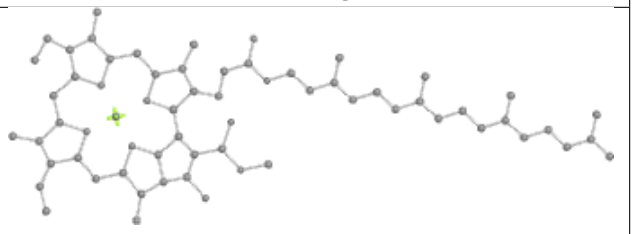
Bond lengths



Bond angles

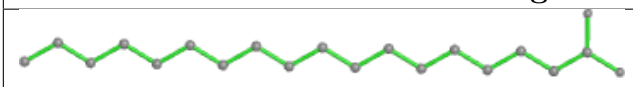


Torsions

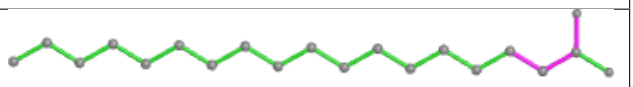


Rings

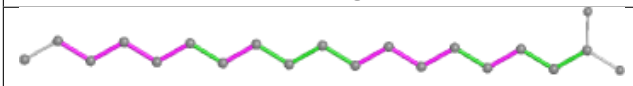
### Ligand STE b 627



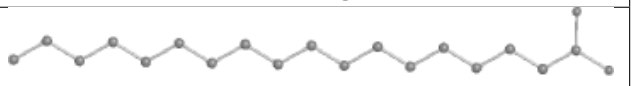
Bond lengths



Bond angles

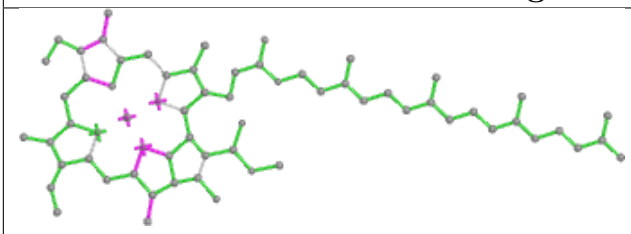


Torsions

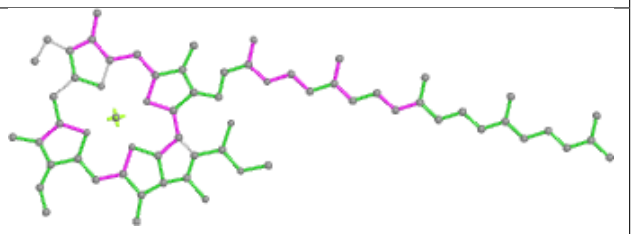


Rings

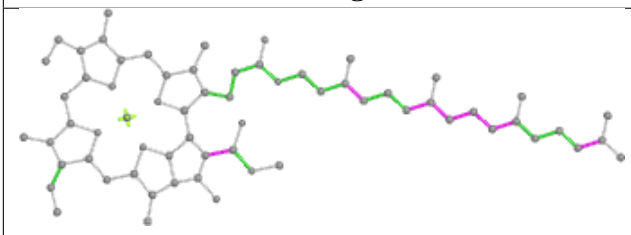
**Ligand CLA b 607**



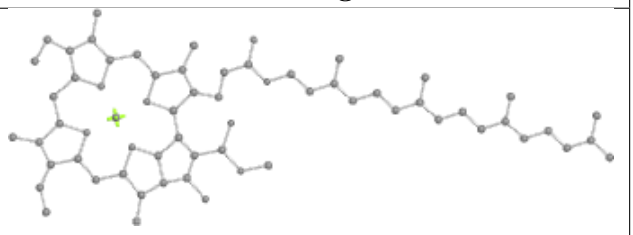
Bond lengths



Bond angles

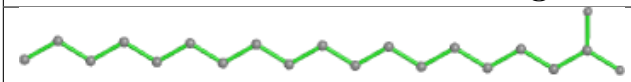


Torsions

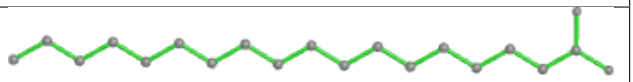


Rings

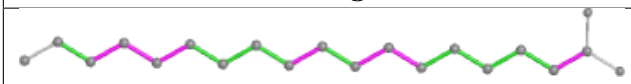
**Ligand STE b 622**



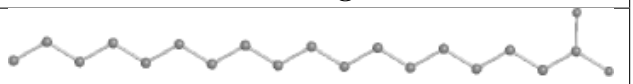
Bond lengths



Bond angles

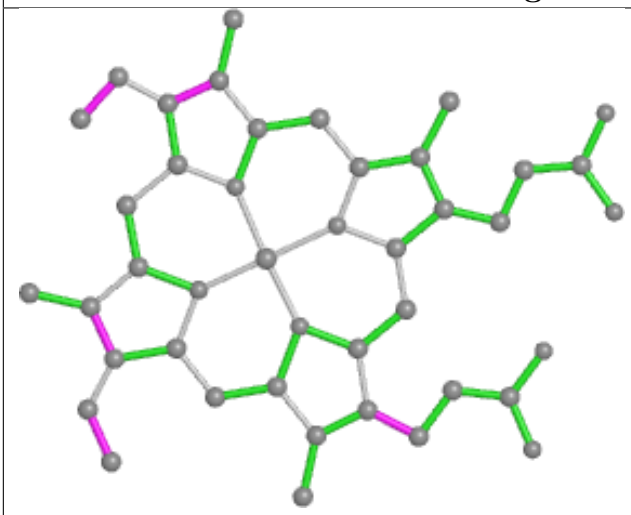


Torsions

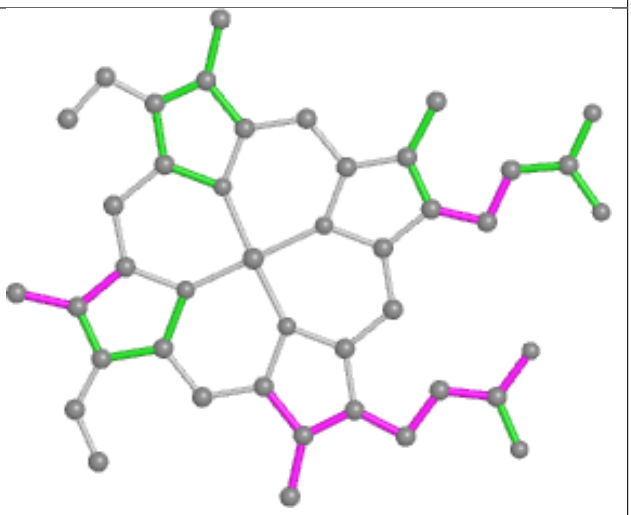


Rings

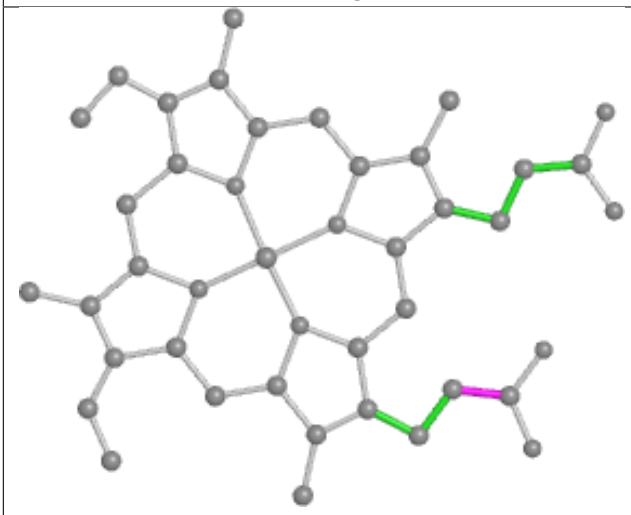
## Ligand HEC F 102



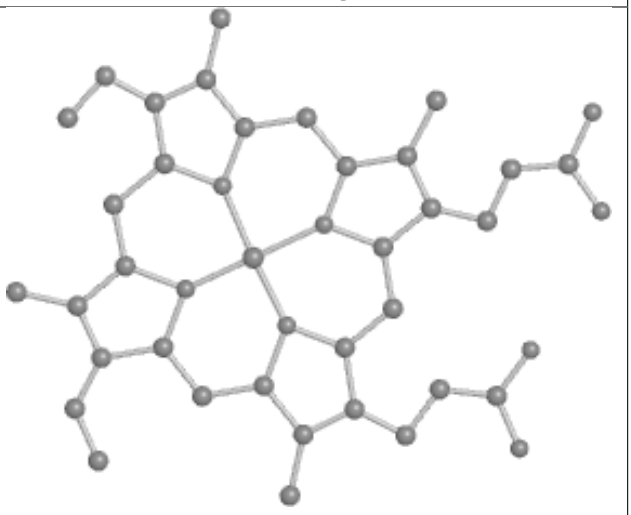
Bond lengths



Bond angles

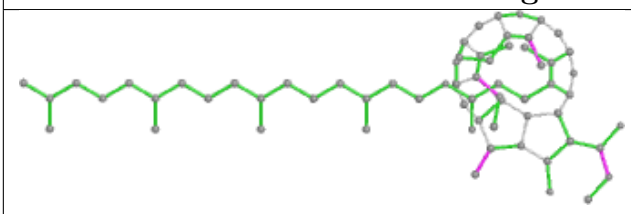


Torsions

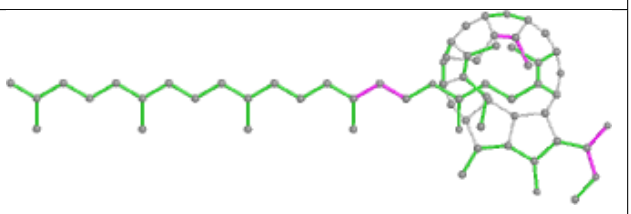


Rings

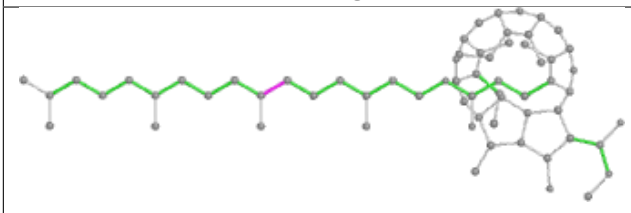
## Ligand PHO D 401



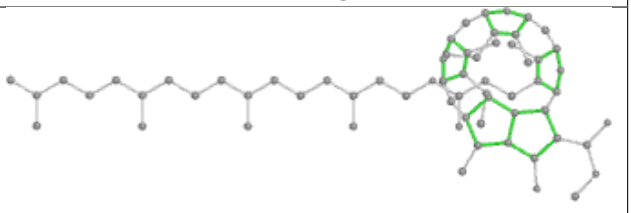
Bond lengths



Bond angles

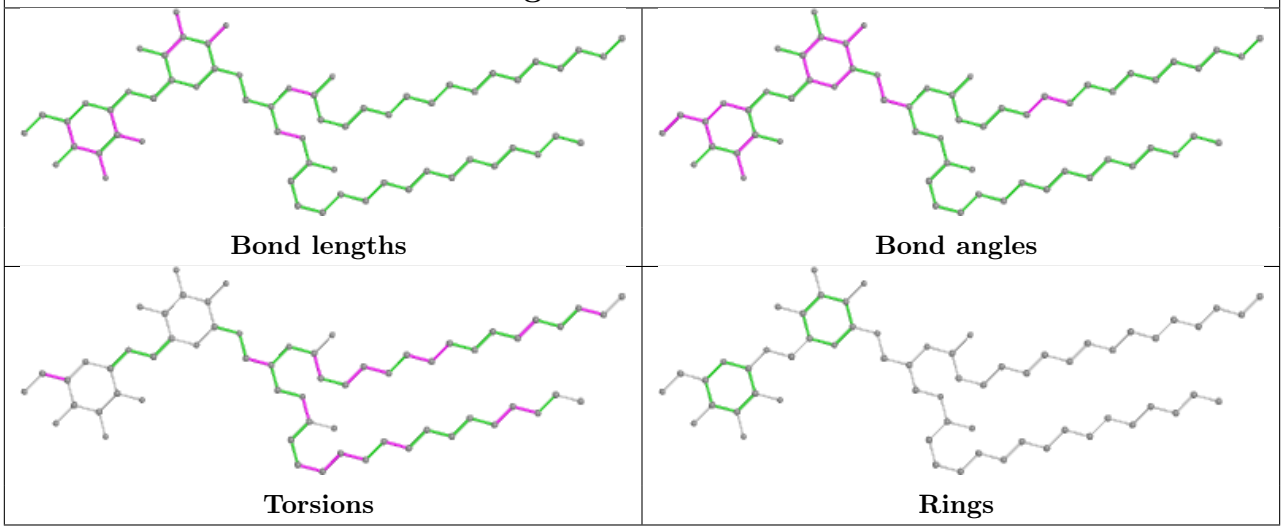


Torsions

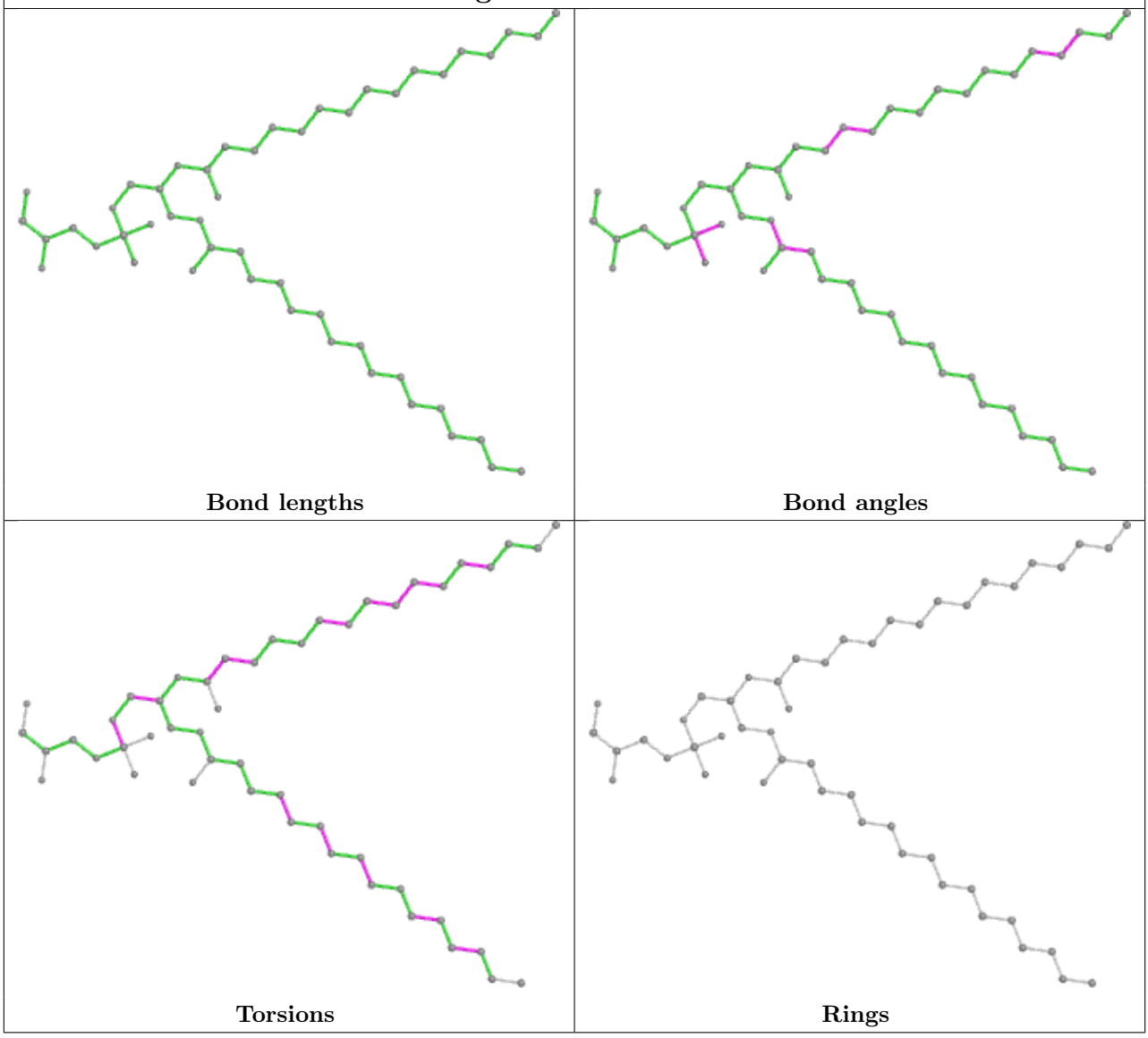


Rings

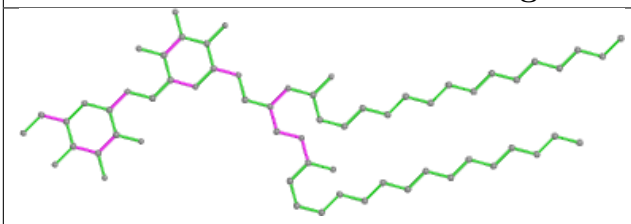
## Ligand DGD h 102



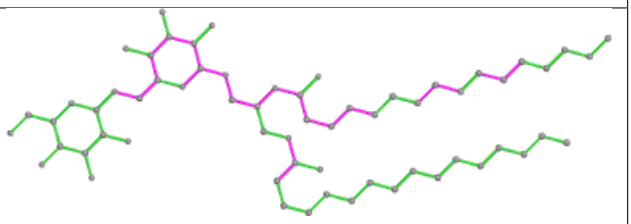

## Ligand LHG l 101



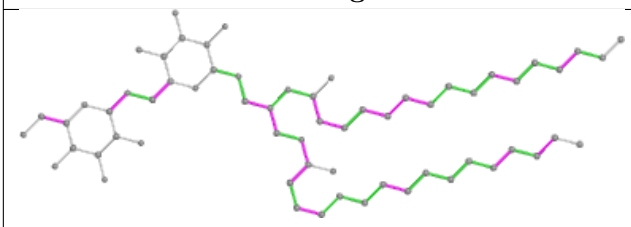
## Ligand DGD C 515



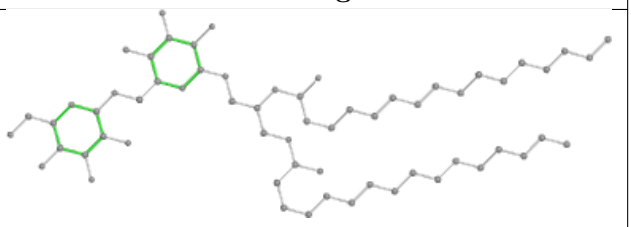
Bond lengths



Bond angles

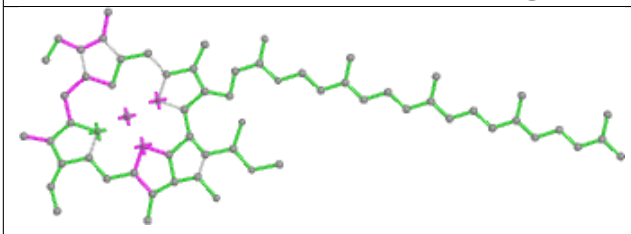


Torsions



Rings

## Ligand CLA H 101



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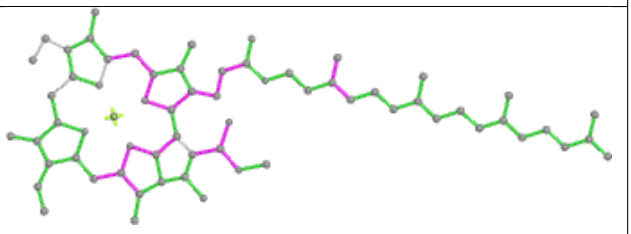
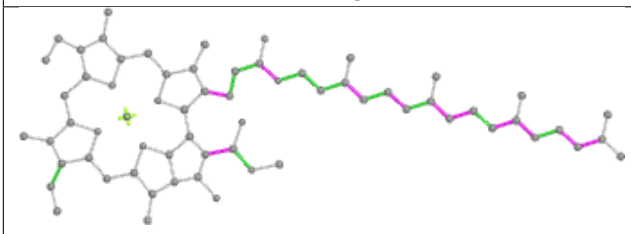
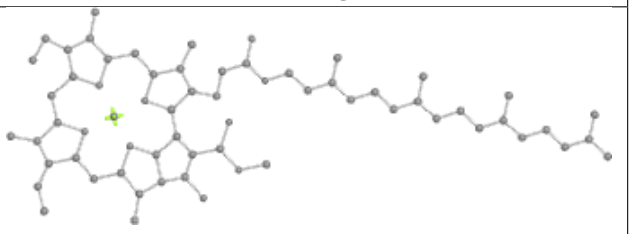


Bond angles

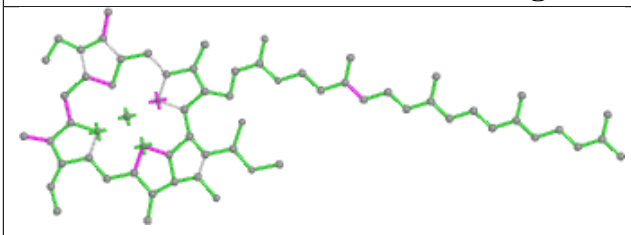


Torsions



Rings

## Ligand CLA c 511



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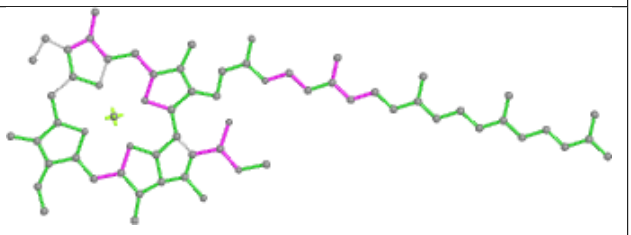
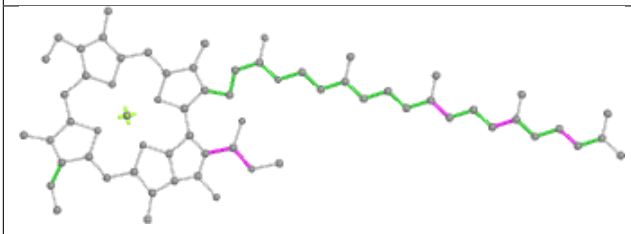
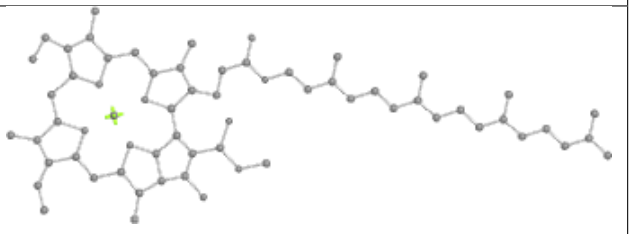


Bond angles

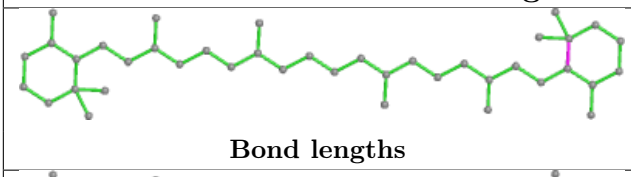


Torsions

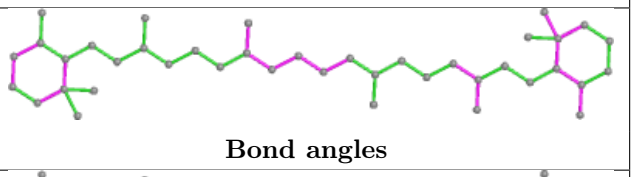


Rings

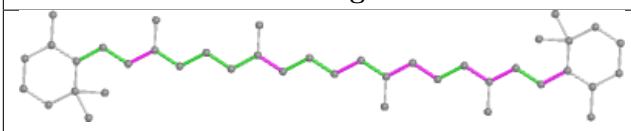
### Ligand BCR B 618



Bond lengths



Bond angles



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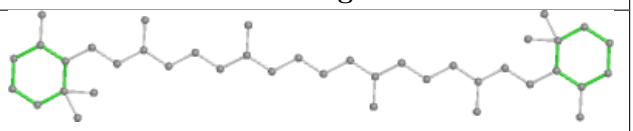
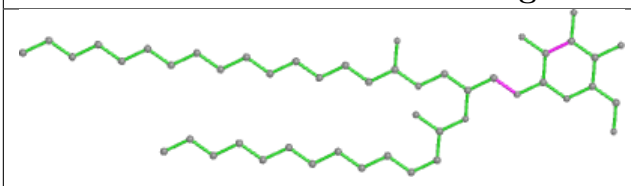
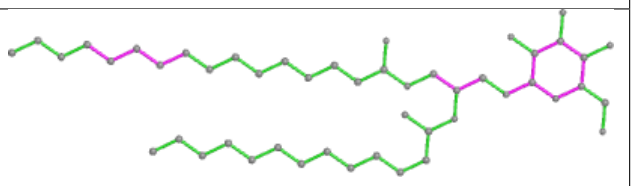


Rings

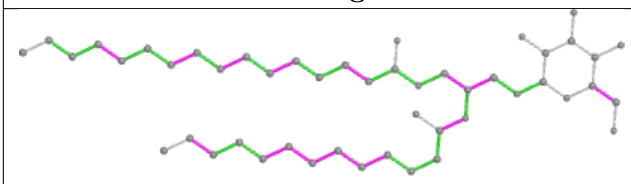
### Ligand LMG A 410



Bond lengths



Bond angles



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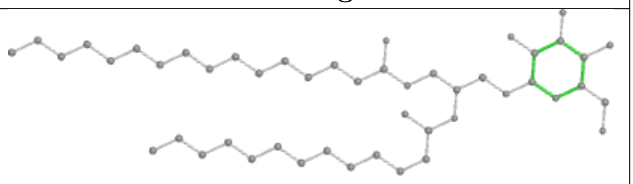
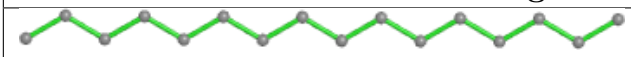


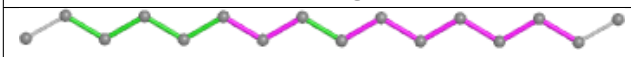
Rings

### Ligand STE B 626

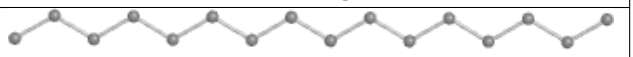


Bond lengths

Bond angles

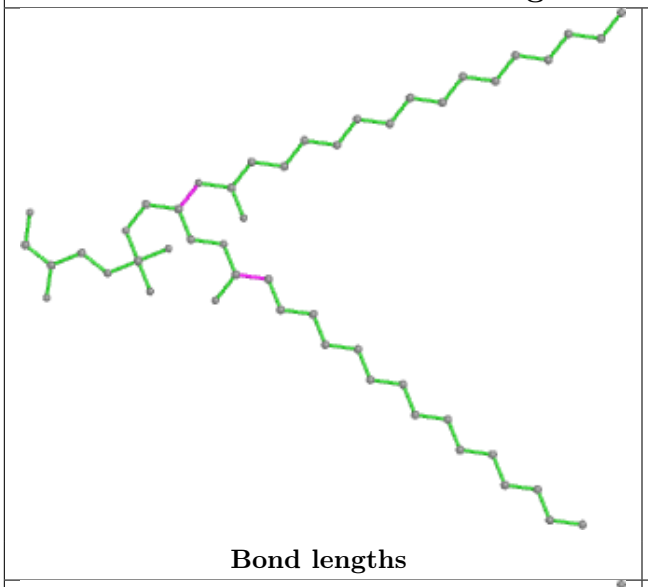


Torsions



Rings

### Ligand LHG d 407



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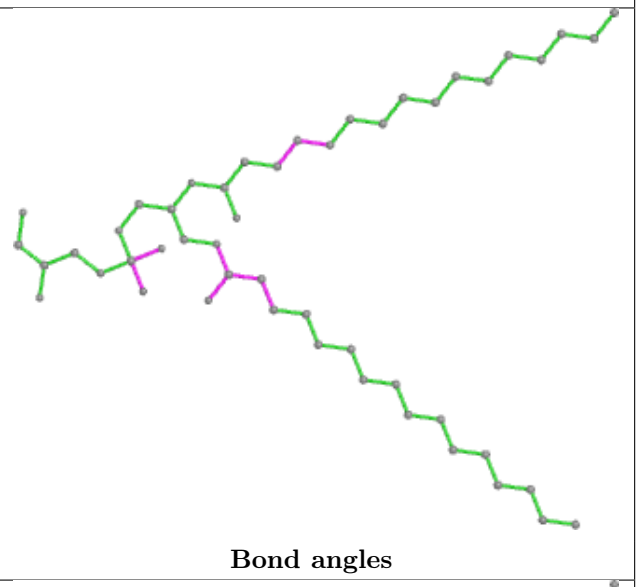
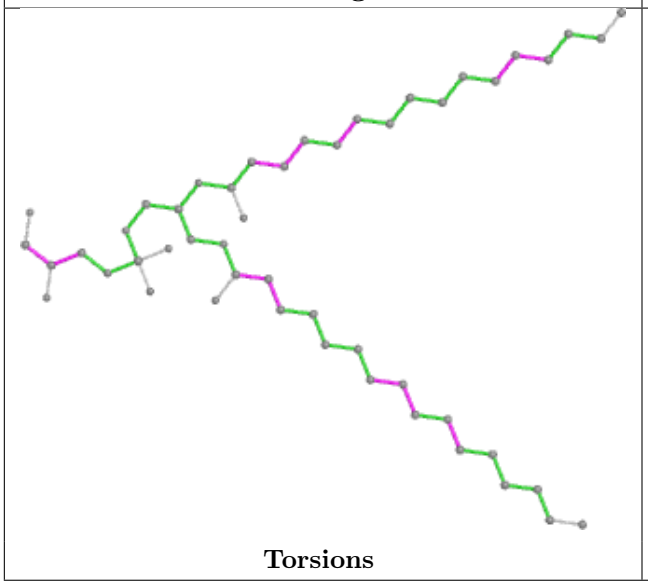
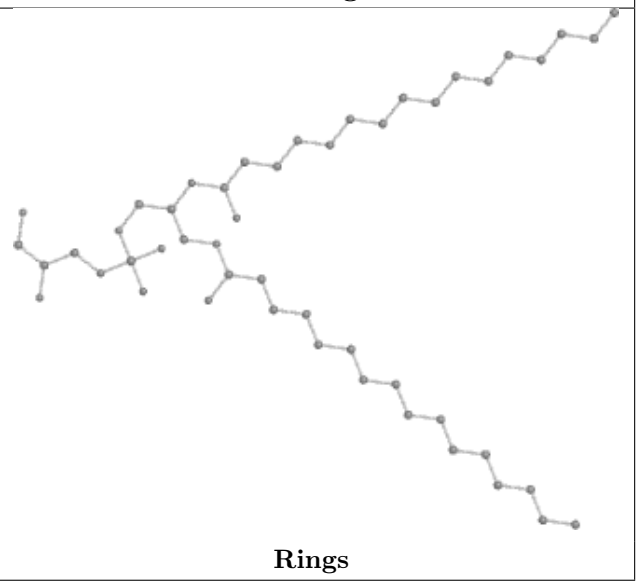


Bond angles

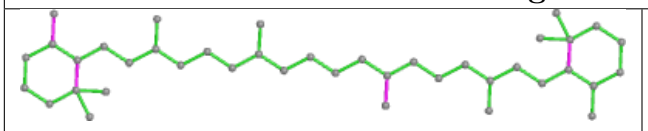


Torsions



Rings

### Ligand BCR c 516



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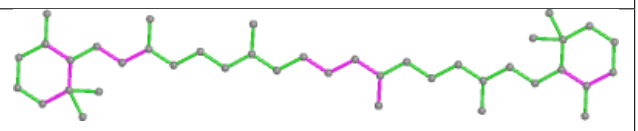
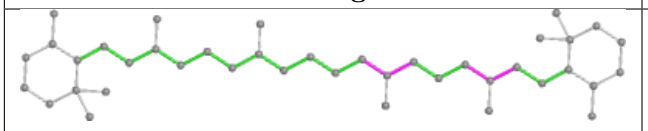
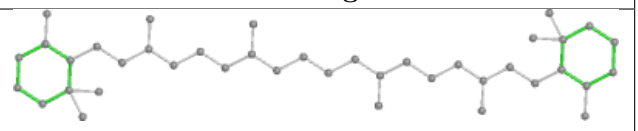


Bond angles

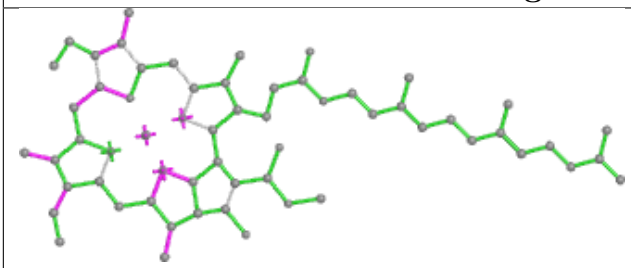


Torsions



Rings

### Ligand CLA B 616



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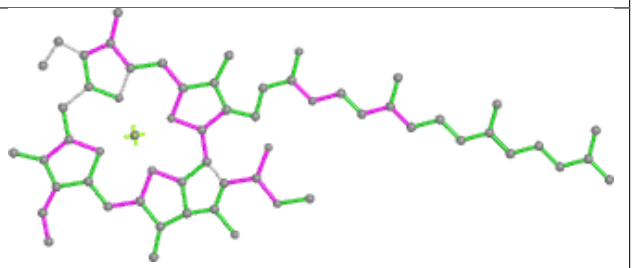
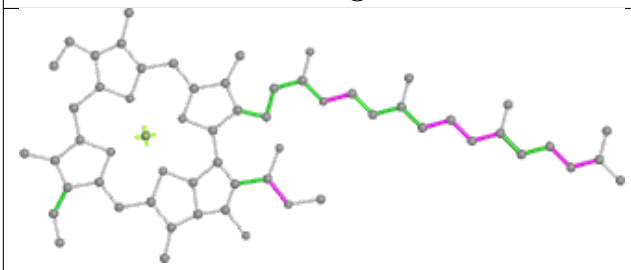


Bond angles



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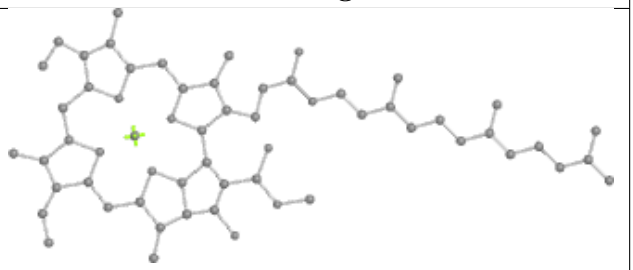
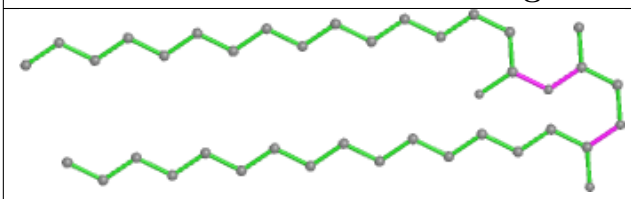


Rings

### Ligand SQD A 412



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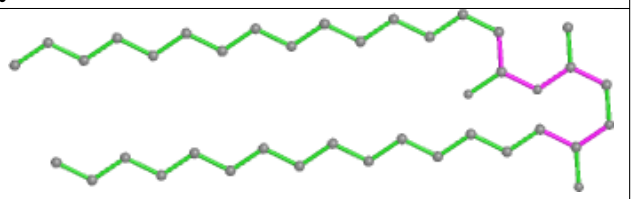
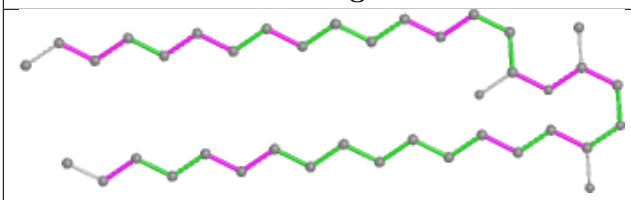
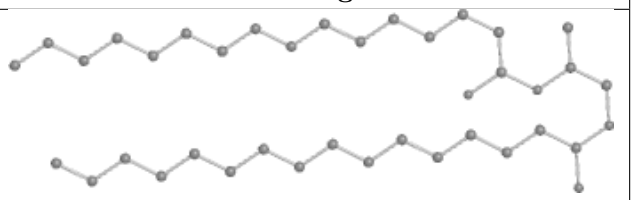


Bond angles

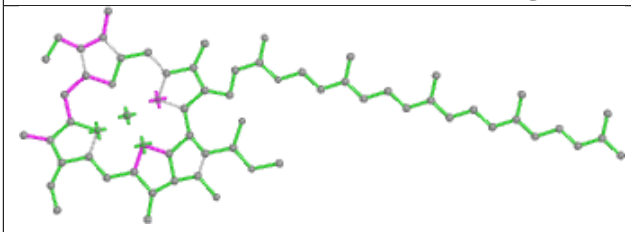


Torsions

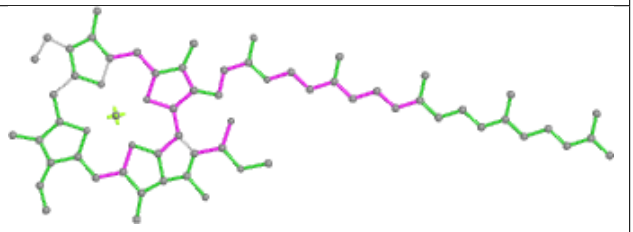


Rings

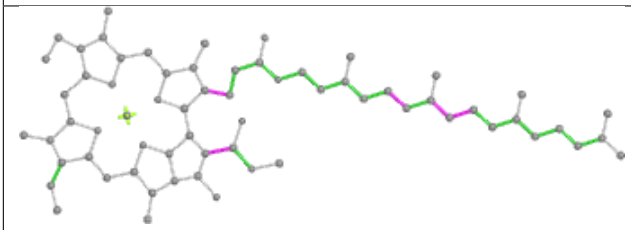
### Ligand CLA C 503



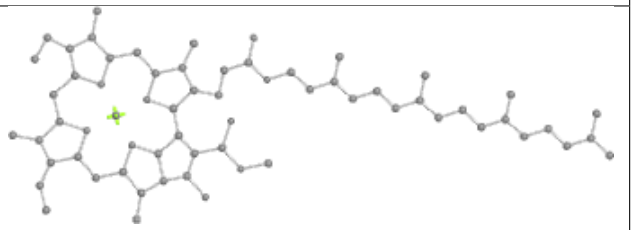
Bond lengths



Bond angles

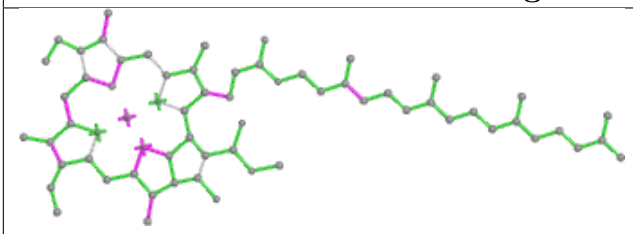


Torsions

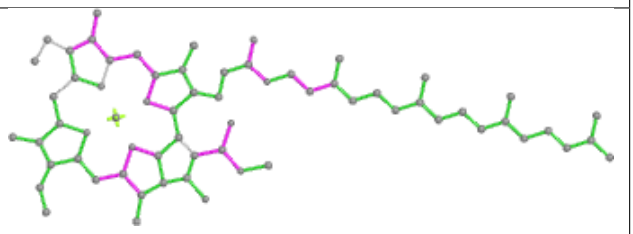


Rings

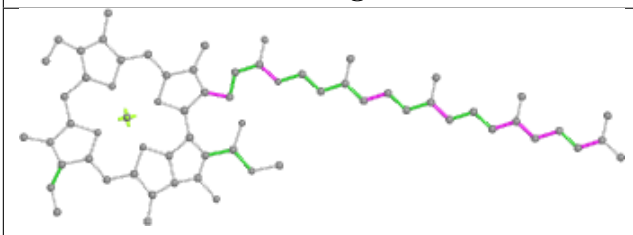
## Ligand CLA A 403



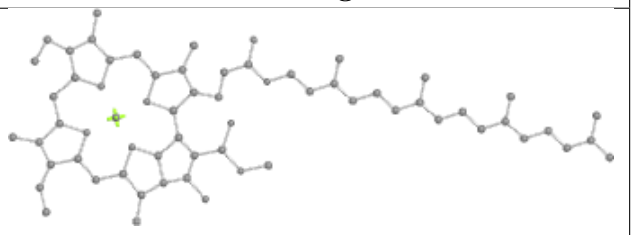
Bond lengths



Bond angles

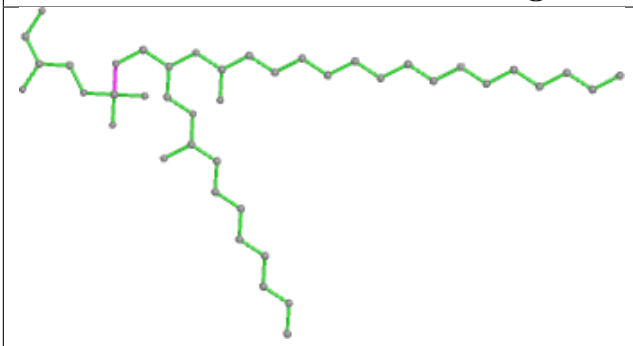


Torsions

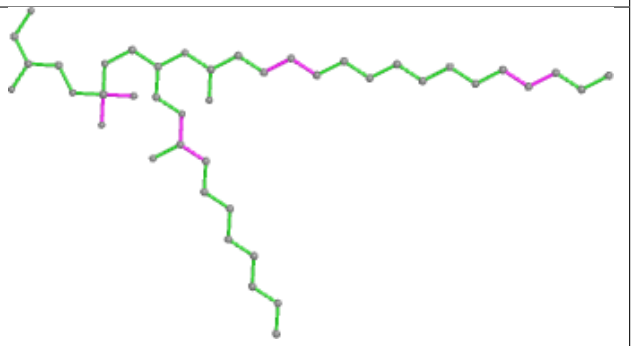


Rings

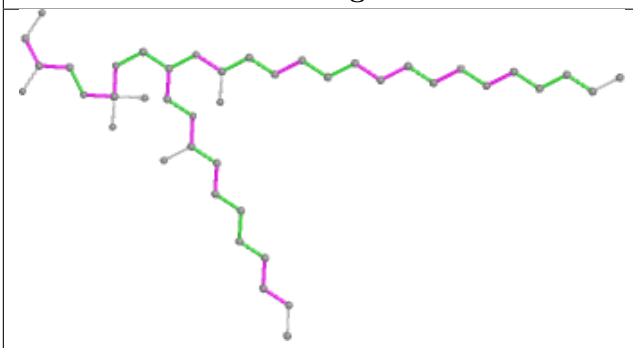
## Ligand LHG e 101



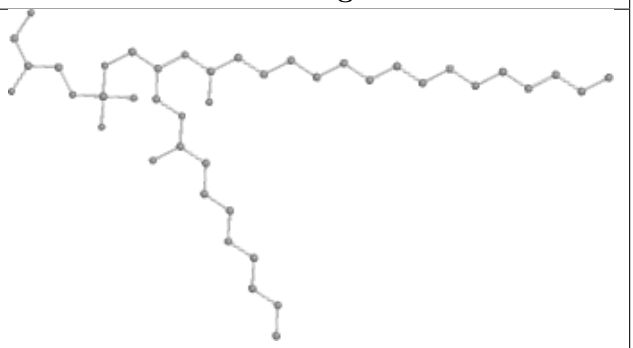
Bond lengths



Bond angles

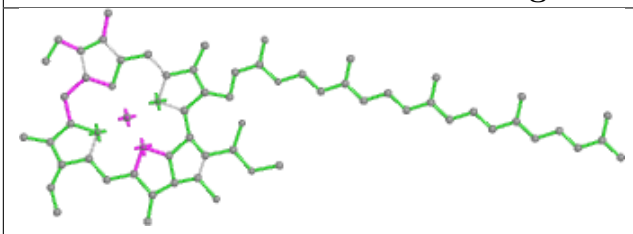


Torsions

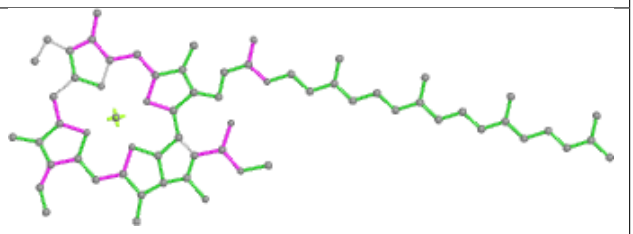


Rings

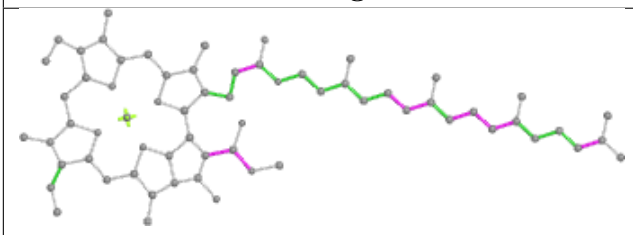
### Ligand CLA c 510



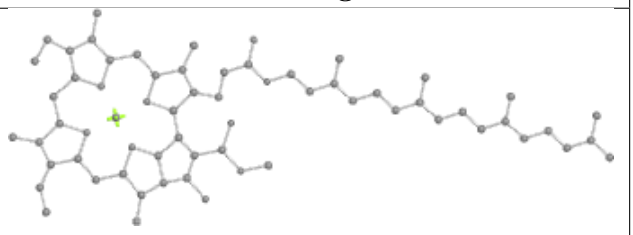
Bond lengths



Bond angles

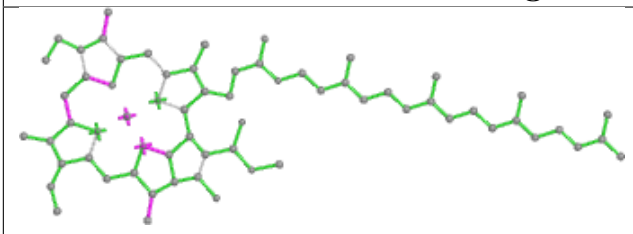


Torsions

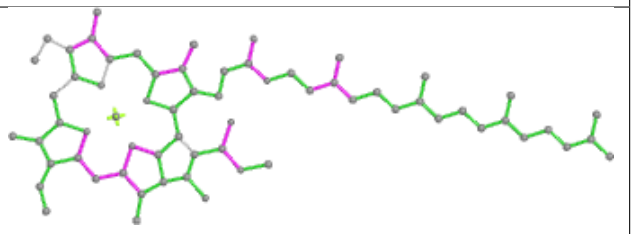


Rings

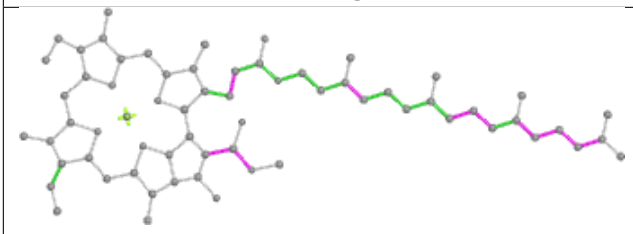
### Ligand CLA B 603



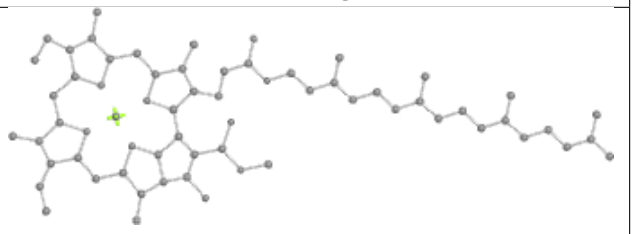
Bond lengths



Bond angles

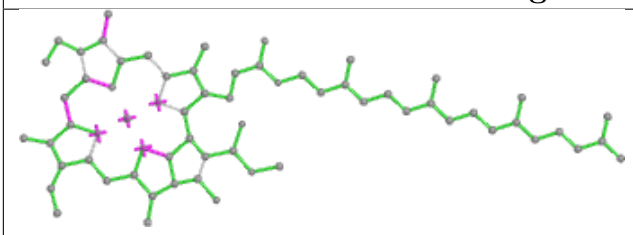


Torsions

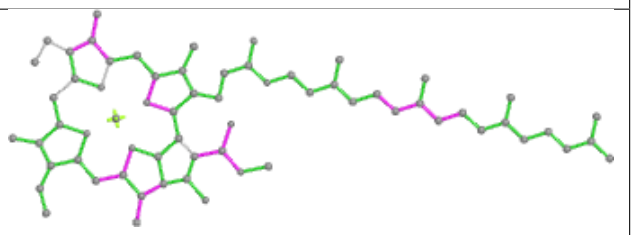


Rings

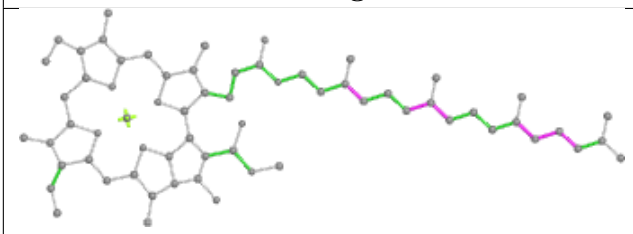
### Ligand CLA c 506



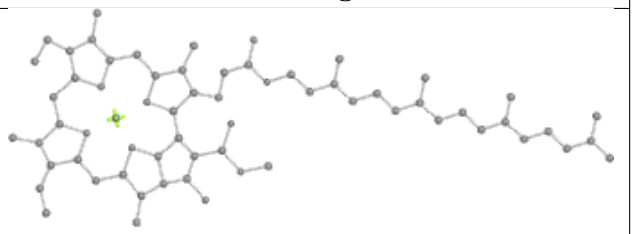
Bond lengths



Bond angles

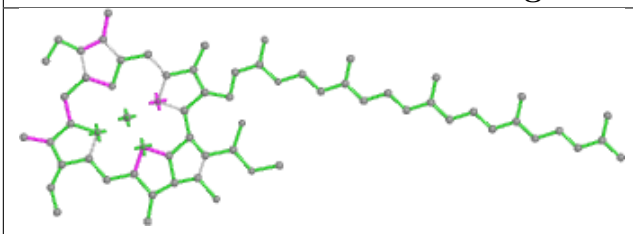


Torsions



Rings

### Ligand CLA C 511



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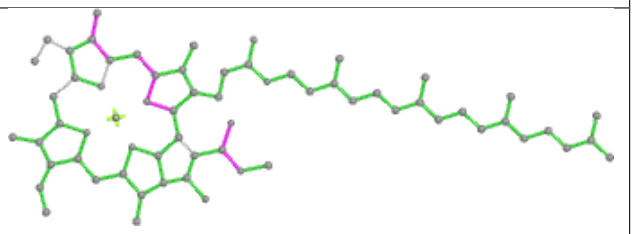
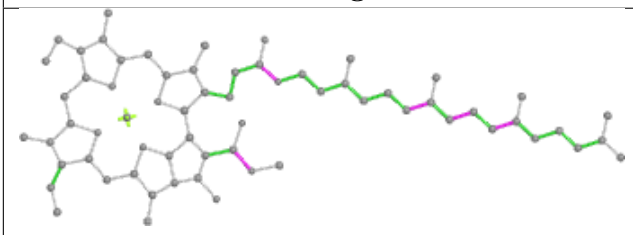
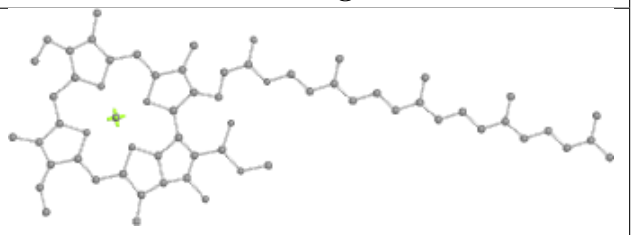


Bond angles

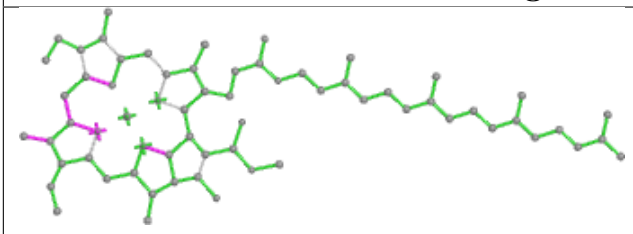


Torsions

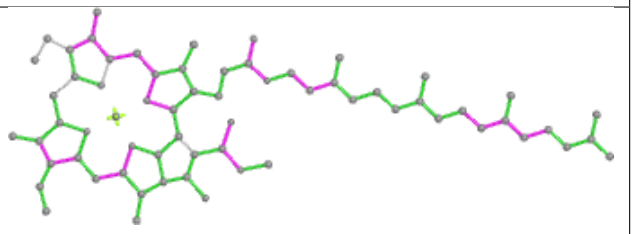


Rings

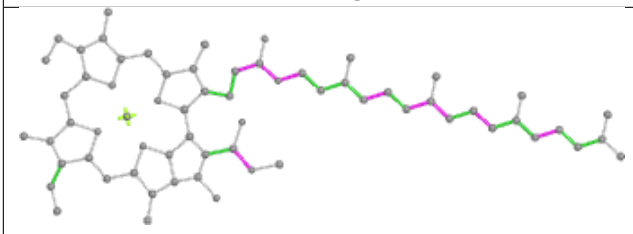
### Ligand CLA B 612



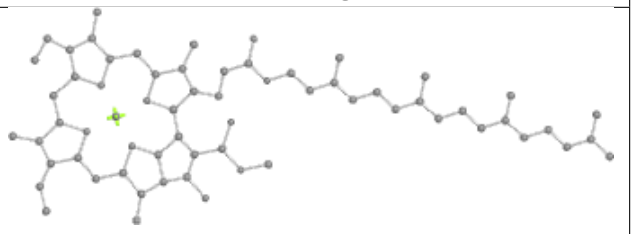
Bond lengths



Bond angles

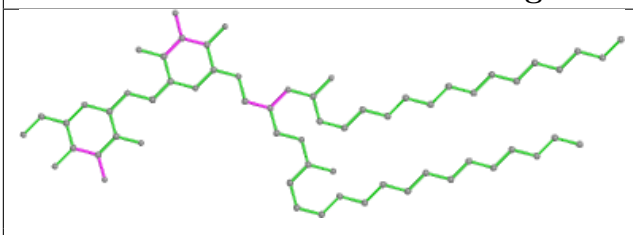


Torsions

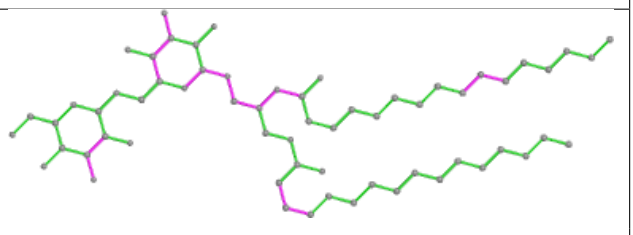


Rings

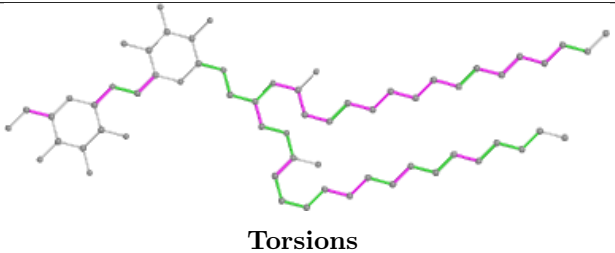
### Ligand DGD c 517



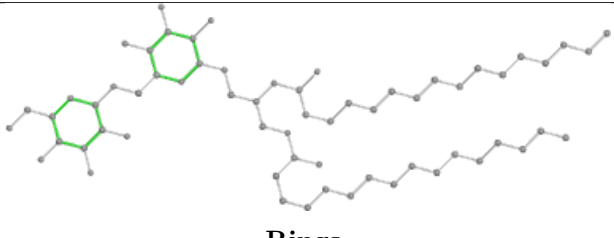
Bond lengths



Bond angles

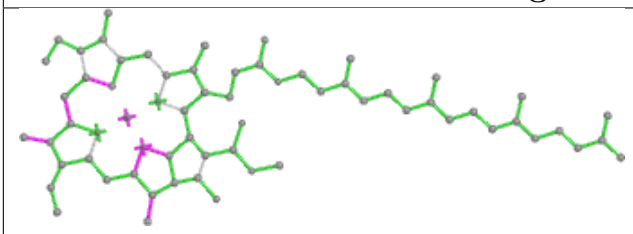


Torsions

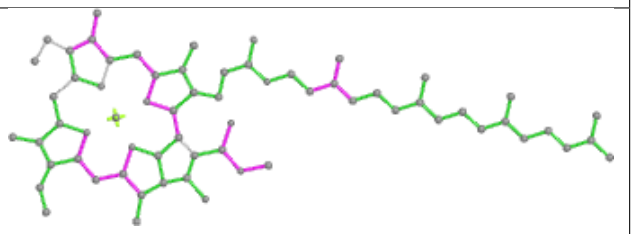


Rings

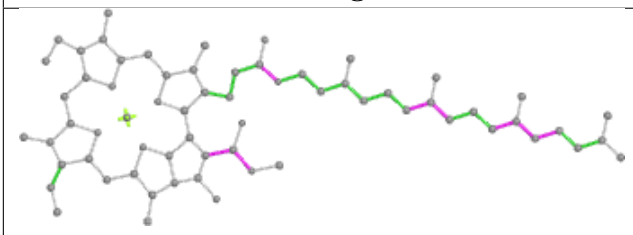
### Ligand CLA c 507



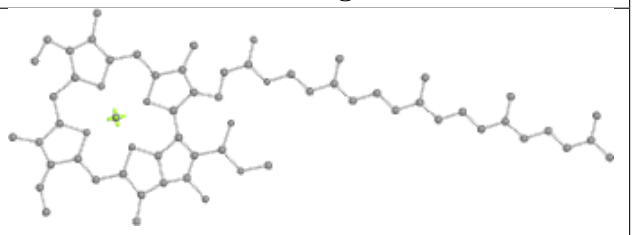
Bond lengths



Bond angles

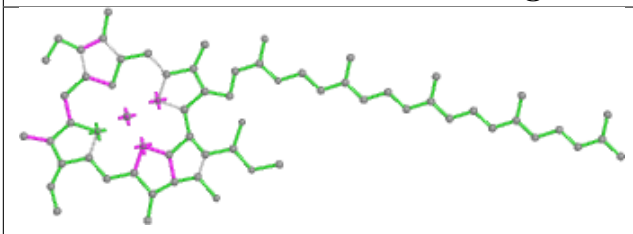


Torsions

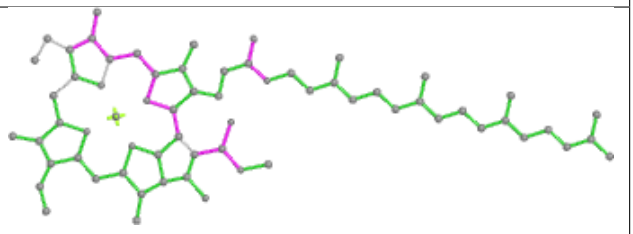


Rings

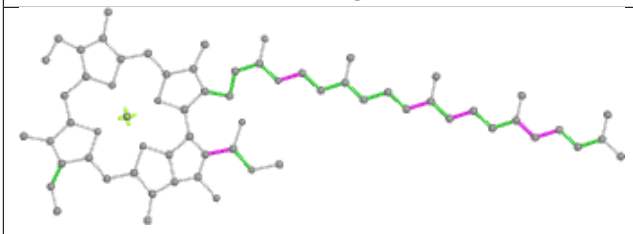
### Ligand CLA C 506



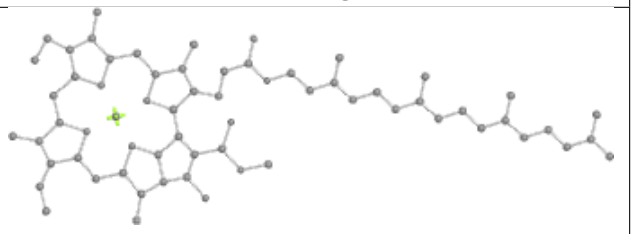
Bond lengths



Bond angles

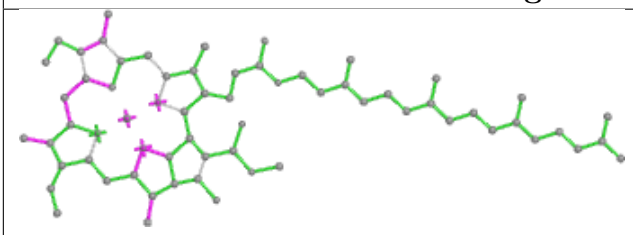


Torsions

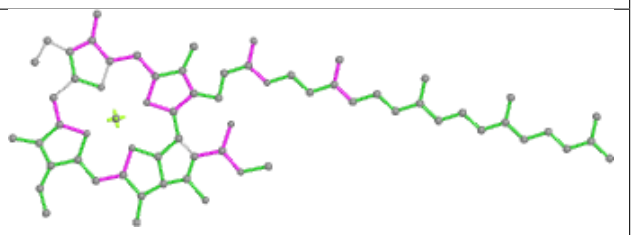


Rings

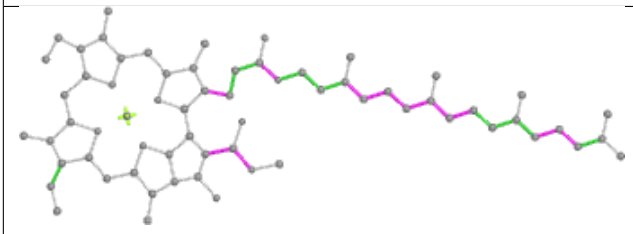
### Ligand CLA C 513



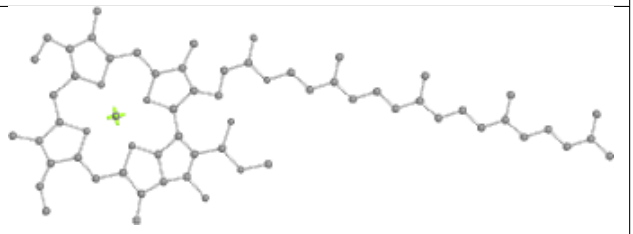
Bond lengths



Bond angles

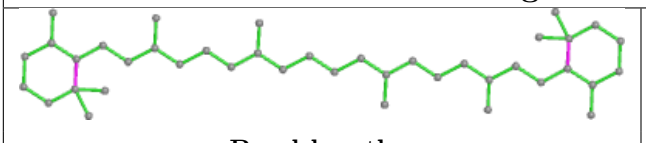


Torsions

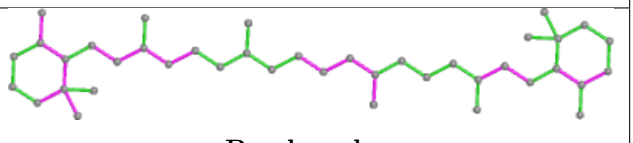


Rings

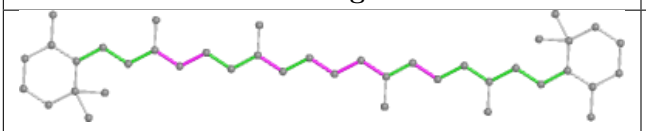
### Ligand BCR K 101



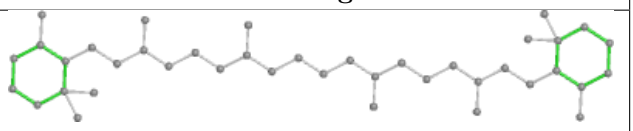
Bond lengths



Bond angles

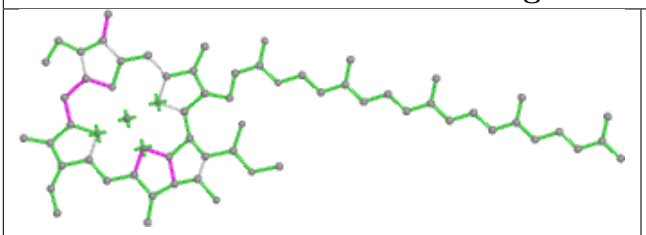


Torsions

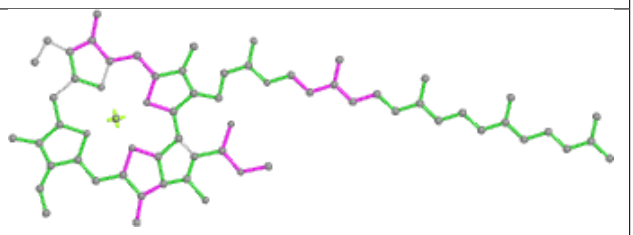


Rings

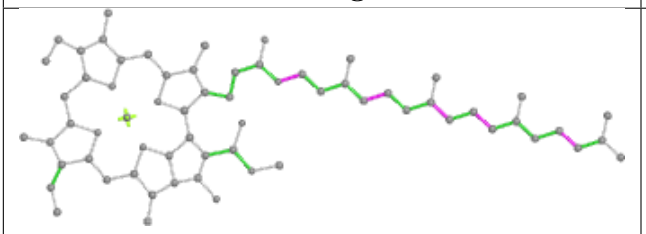
### Ligand CLA D 403



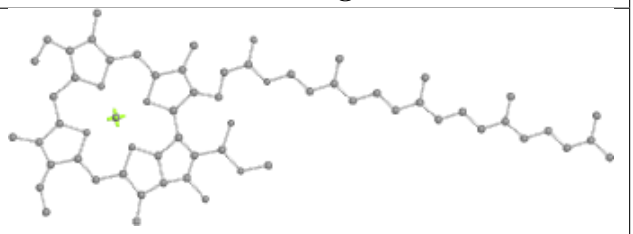
Bond lengths



Bond angles

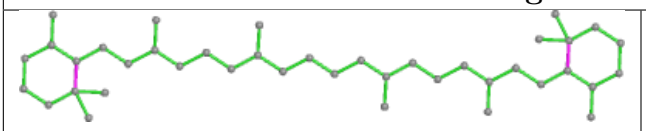


Torsions

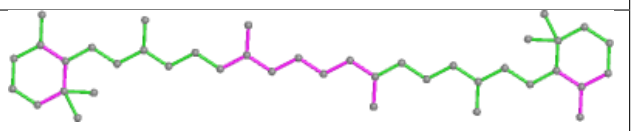


Rings

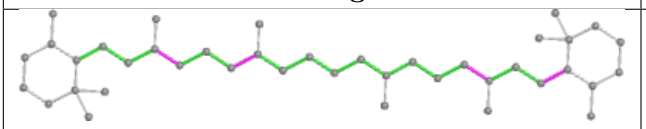
### Ligand BCR h 101



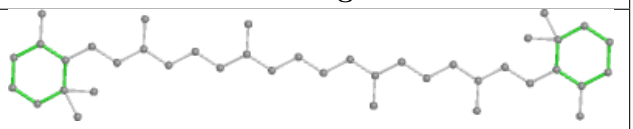
Bond lengths



Bond angles

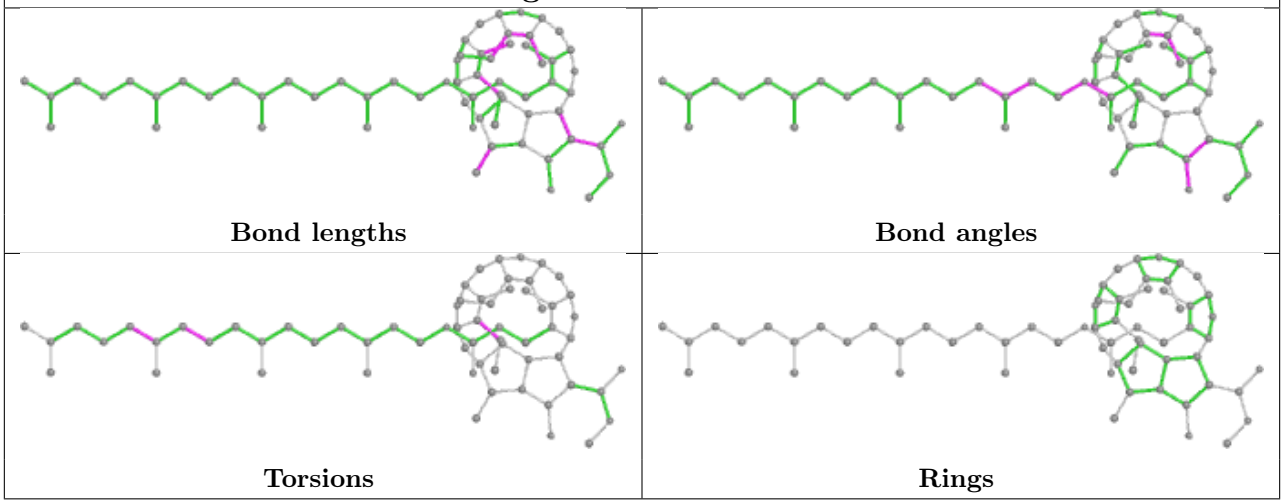


Torsions

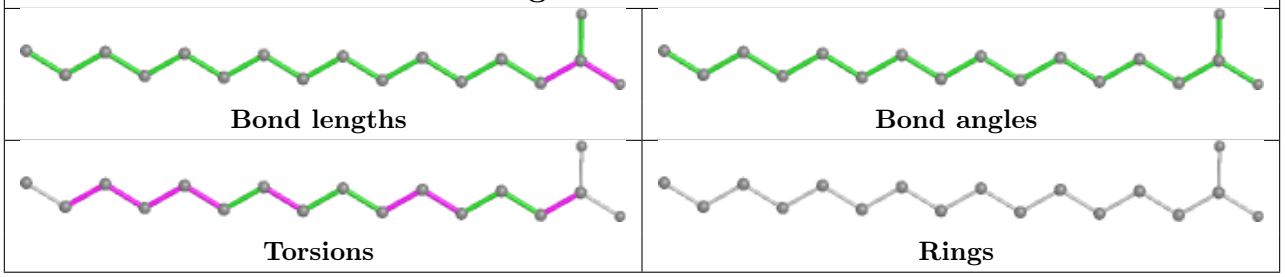


Rings

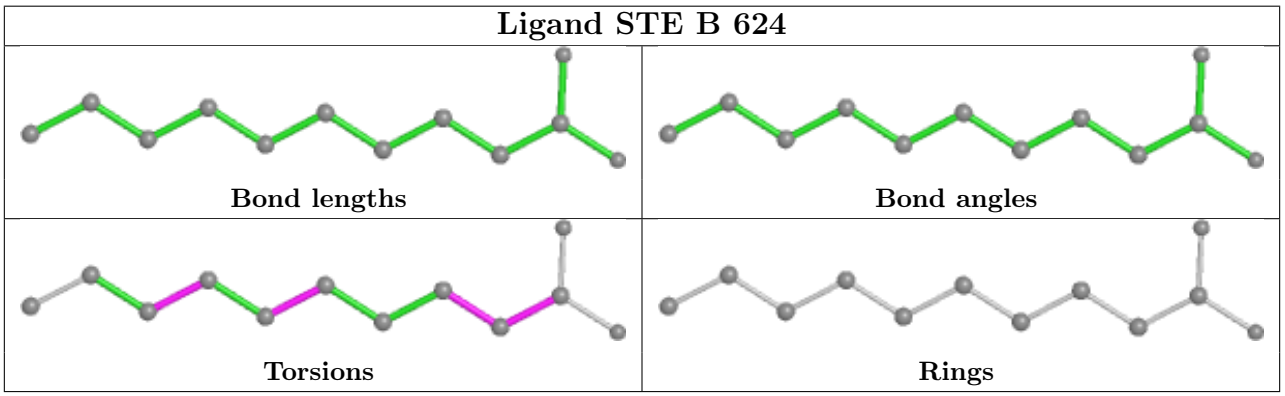
### Ligand PHO A 404



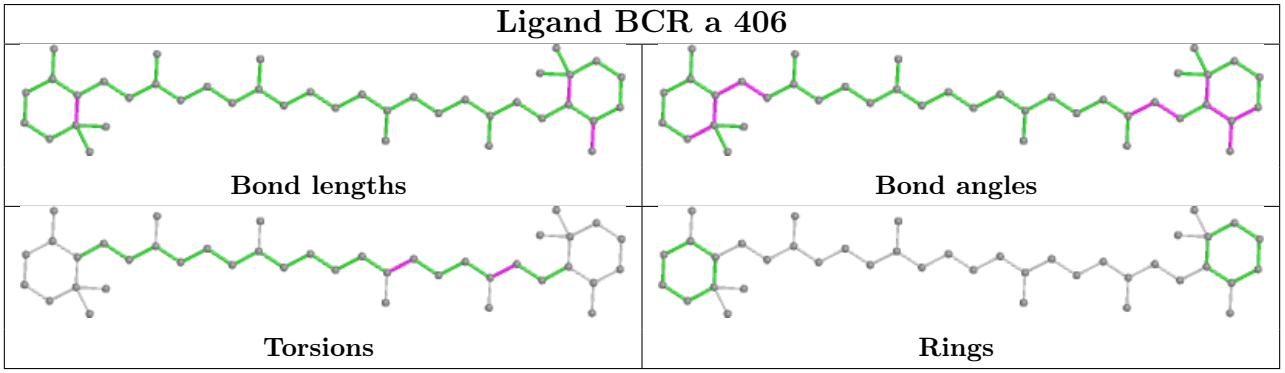

### Ligand STE B 620



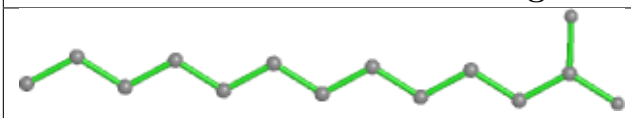

### Ligand STE B 624



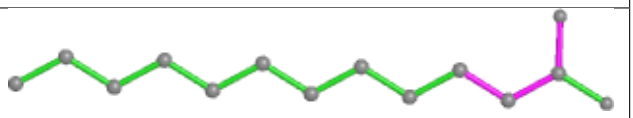

### Ligand BCR a 406



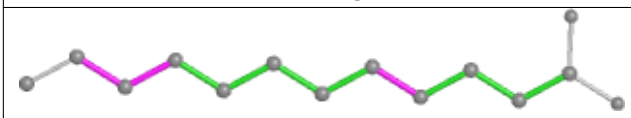
### Ligand STE B 623



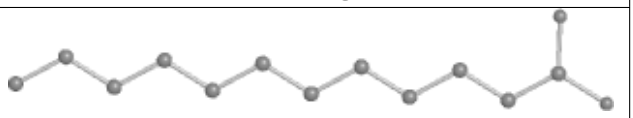
Bond lengths



Bond angles

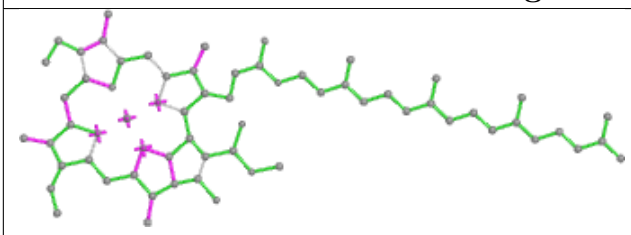


Torsions

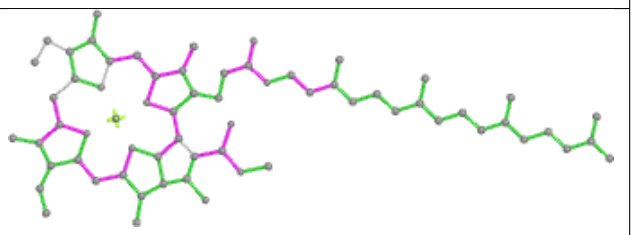


Rings

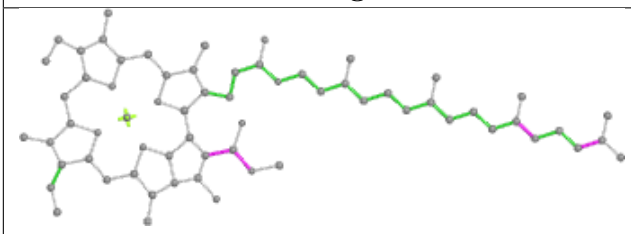
### Ligand CLA B 610



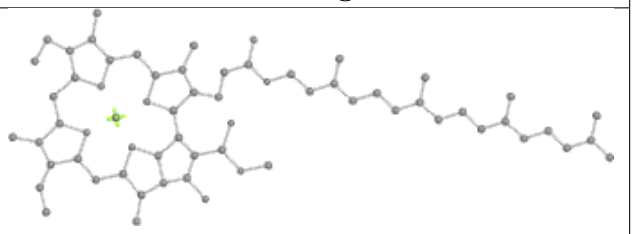
Bond lengths



Bond angles

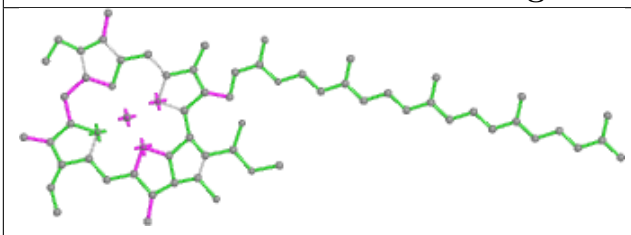


Torsions

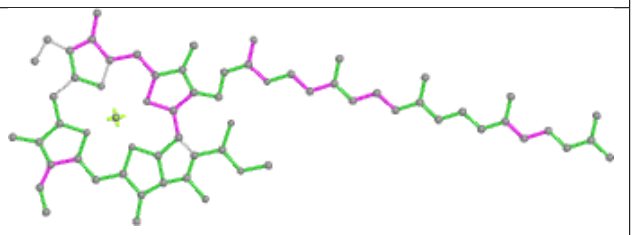


Rings

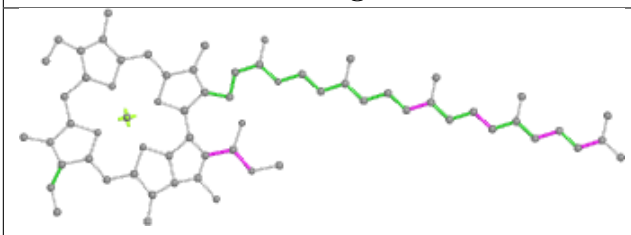
### Ligand CLA b 613



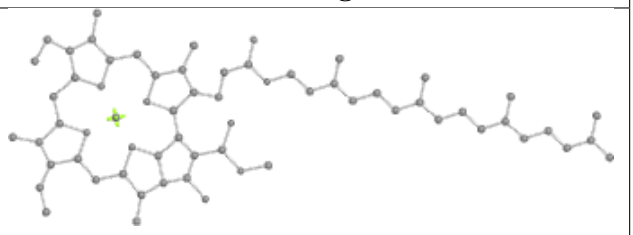
Bond lengths



Bond angles



Torsions



Rings

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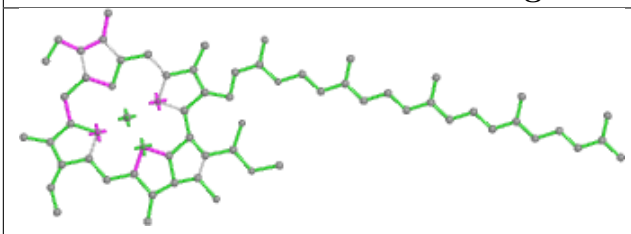

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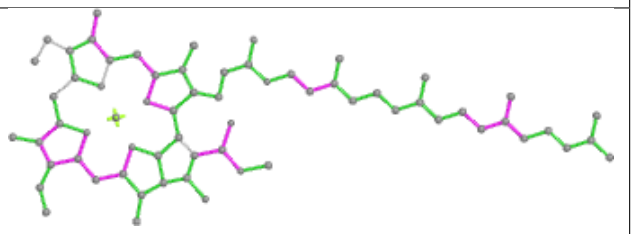
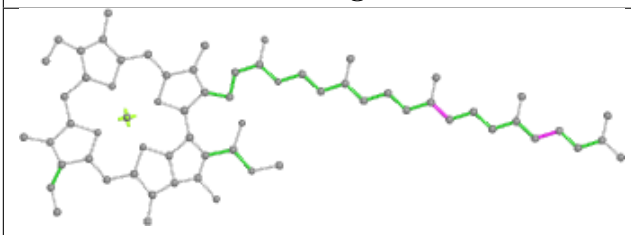
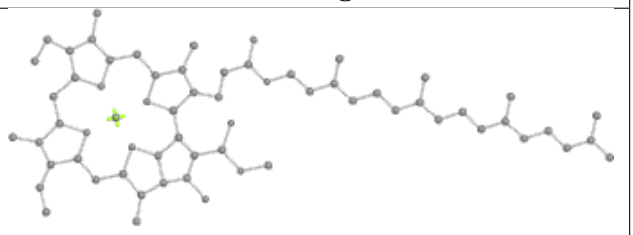


Bond angles

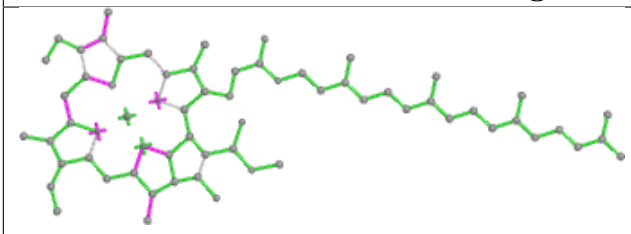


Torsions

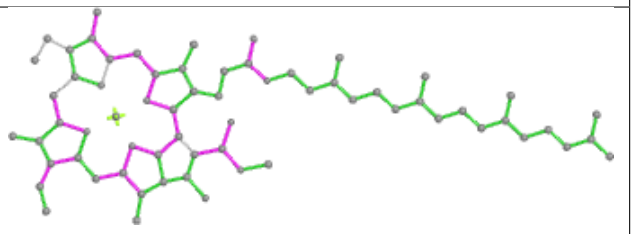


Rings

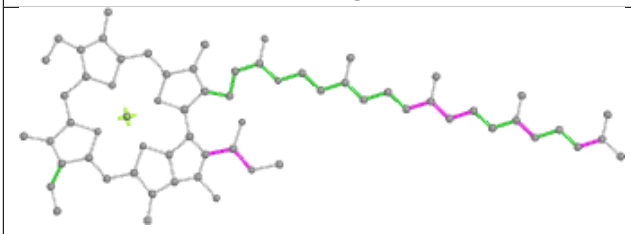
### Ligand CLA a 403



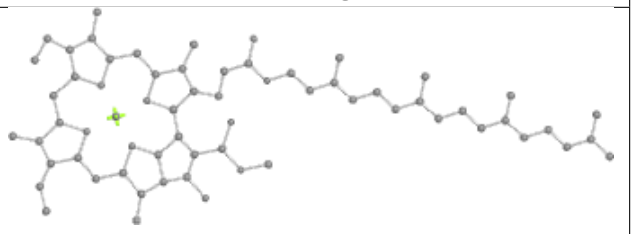
Bond lengths



Bond angles

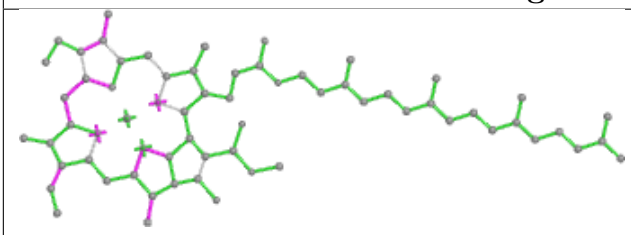


Torsions

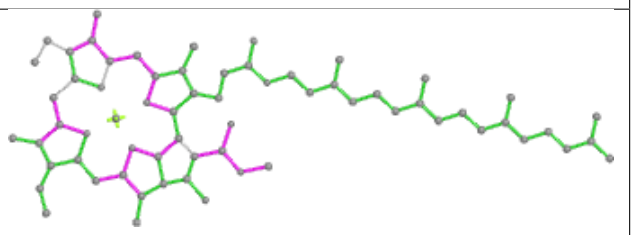


Rings

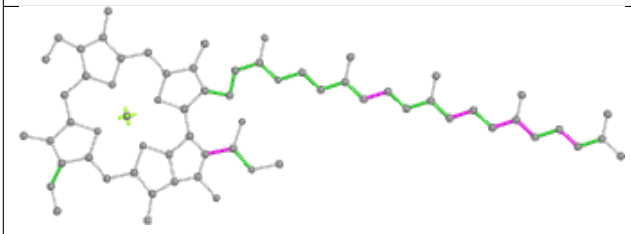
### Ligand CLA b 602



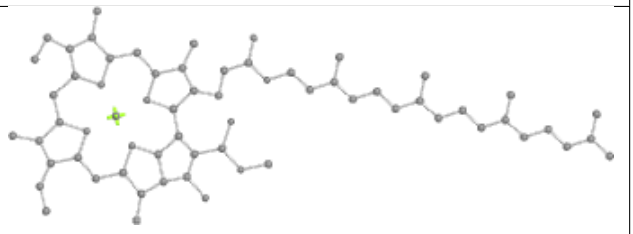
Bond lengths



Bond angles

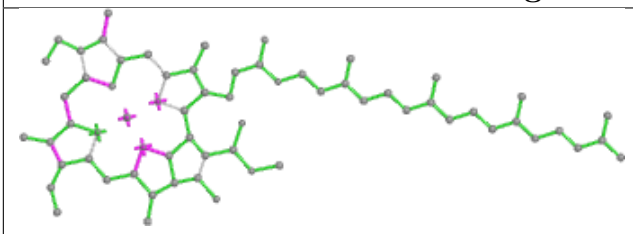


Torsions

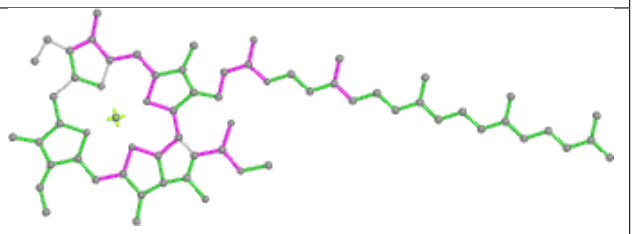


Rings

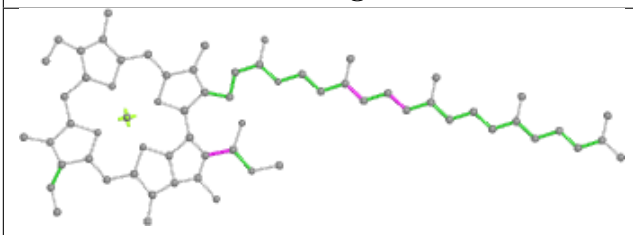
### Ligand CLA C 507



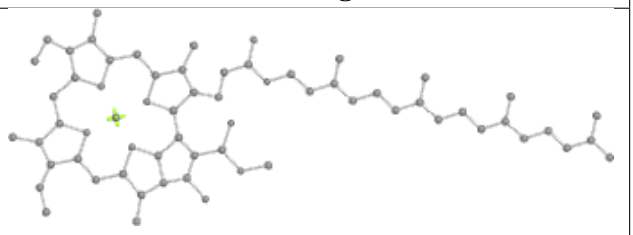
Bond lengths



Bond angles

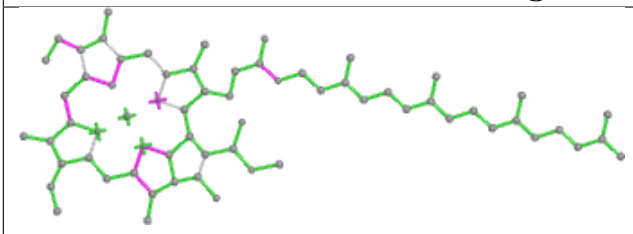


Torsions

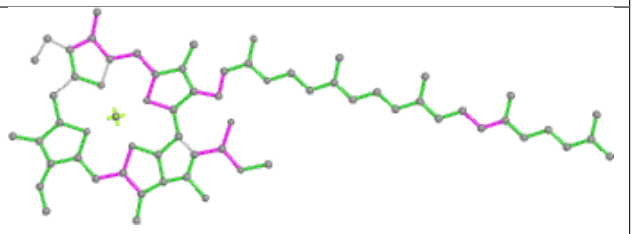


Rings

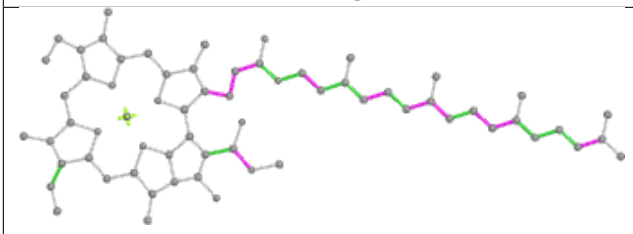
### Ligand CLA b 601



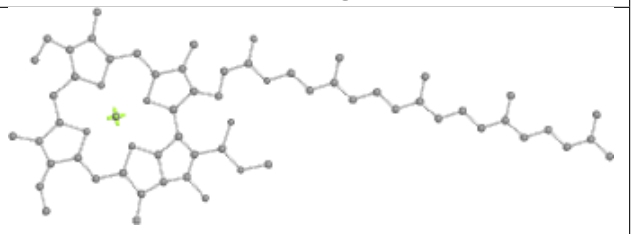
Bond lengths



Bond angles

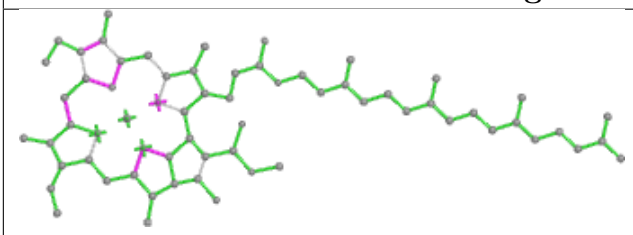


Torsions

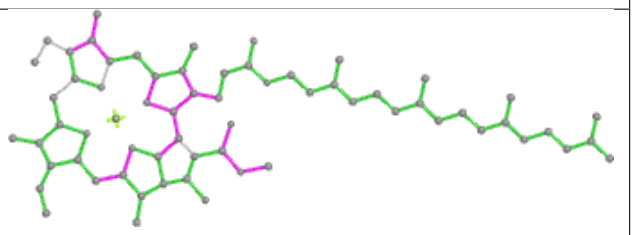


Rings

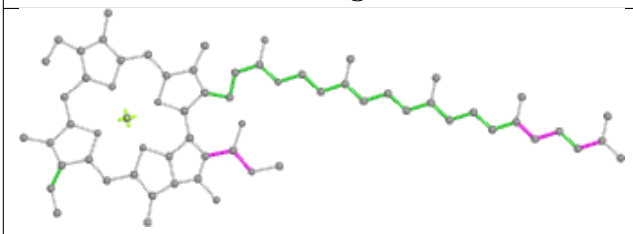
### Ligand CLA C 502



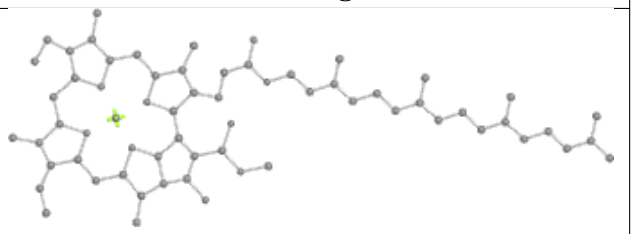
Bond lengths



Bond angles

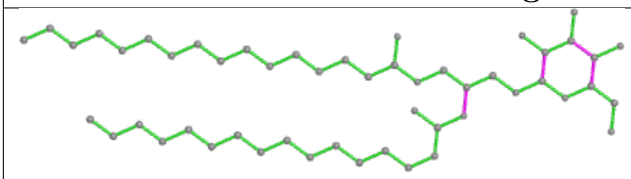


Torsions

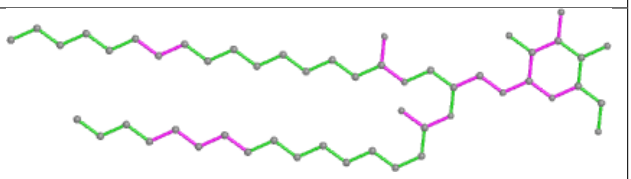


Rings

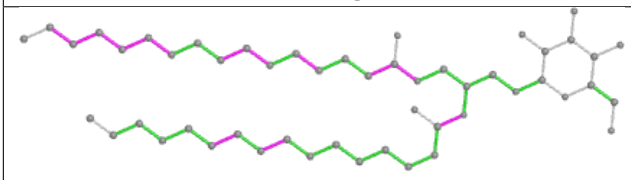
**Ligand LMG b 621**



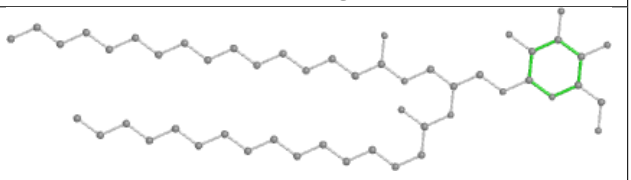
Bond lengths



Bond angles

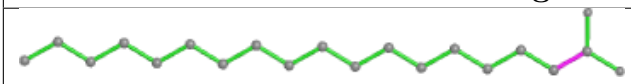


Torsions

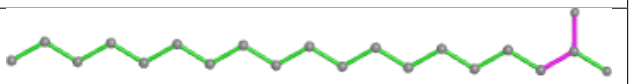


Rings

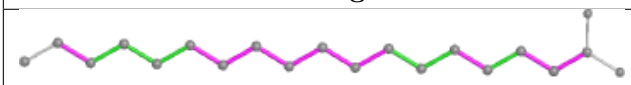
**Ligand STE c 521**



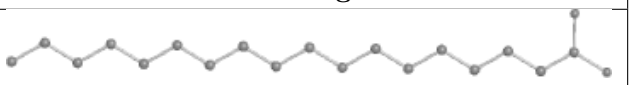
Bond lengths



Bond angles

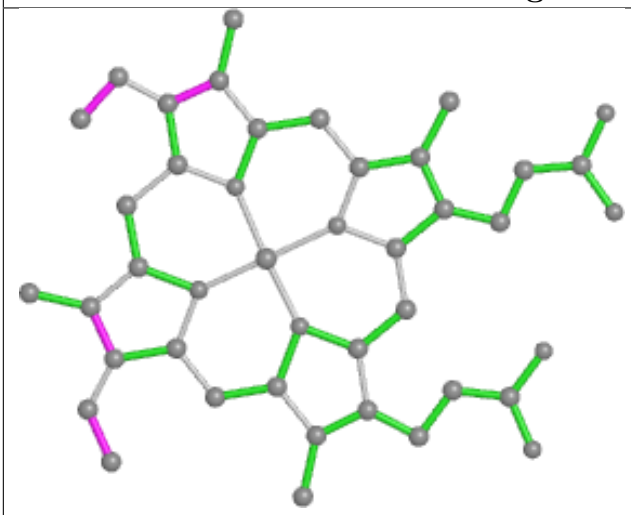


Torsions

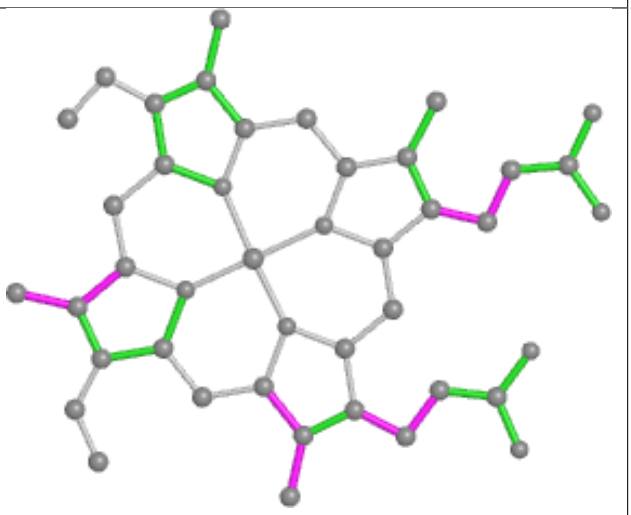


Rings

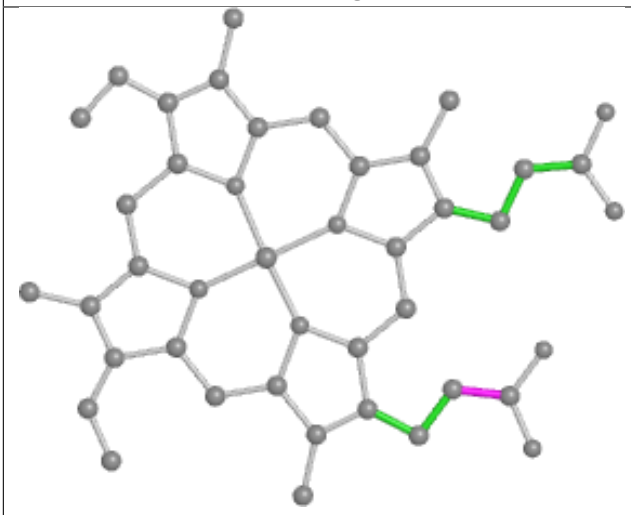
## Ligand HEC v 201



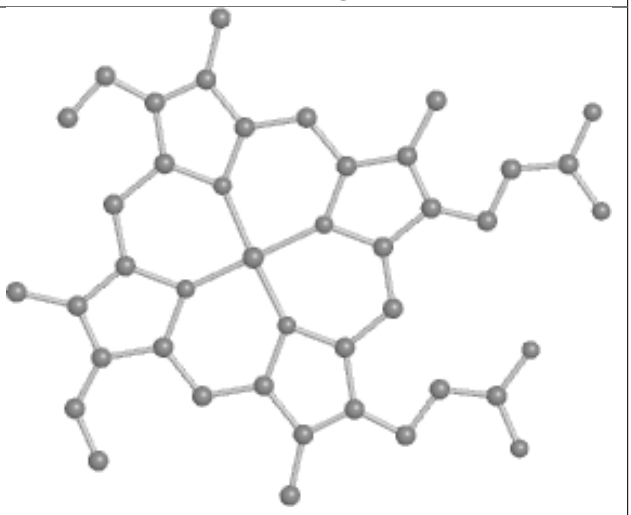
Bond lengths



Bond angles

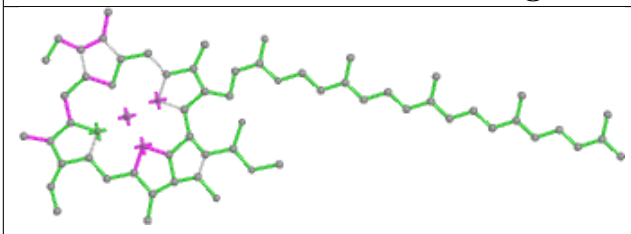


Torsions

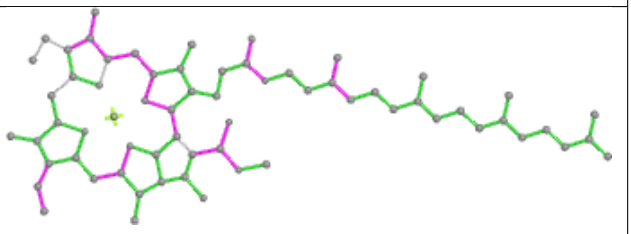


Rings

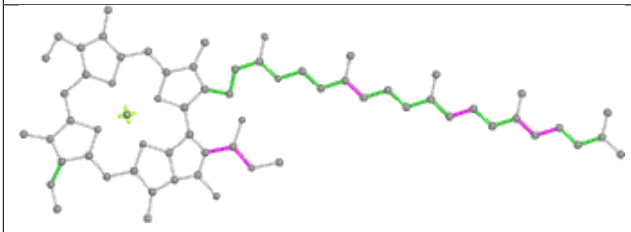
## Ligand CLA B 614



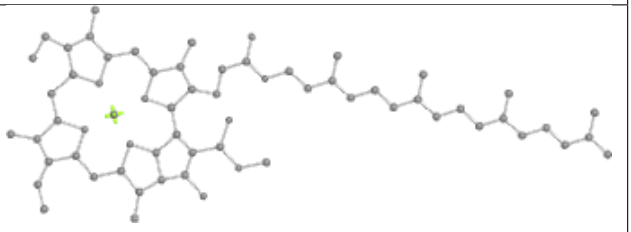
Bond lengths



Bond angles

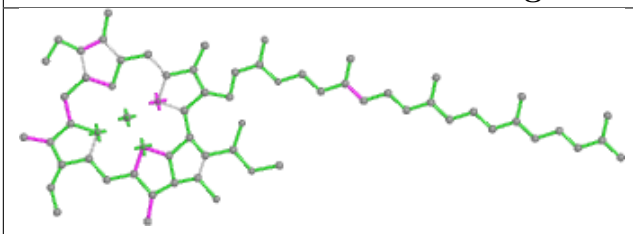


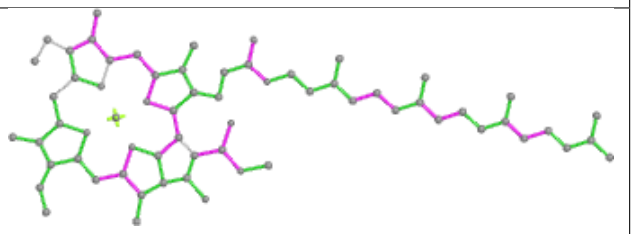
Torsions

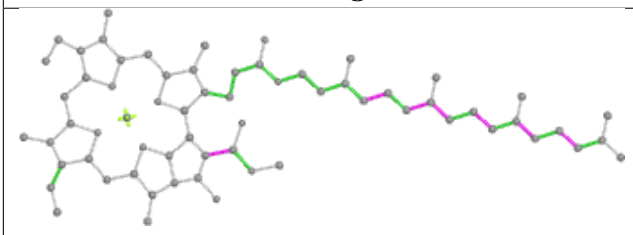


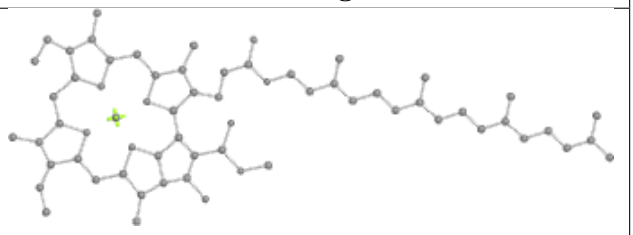
Rings

### Ligand CLA B 605

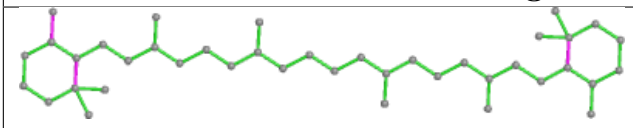

Bond lengths

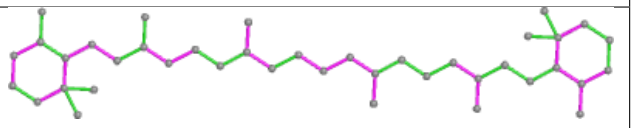

Bond angles

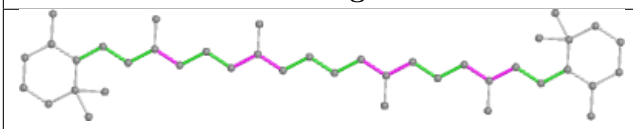

Torsions

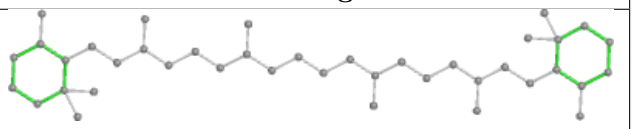

Rings

### Ligand BCR b 617

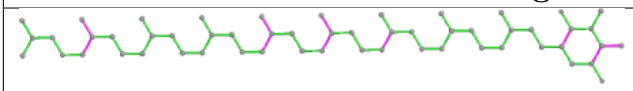

Bond lengths

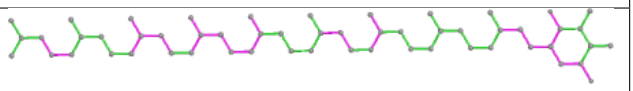

Bond angles

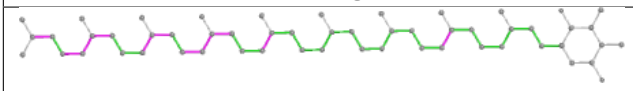

Torsions

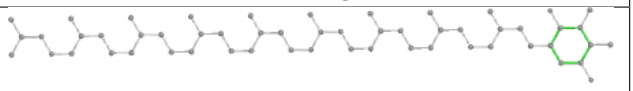

Rings

### Ligand PL9 d 406

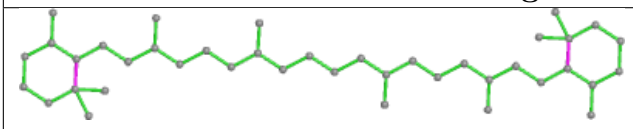

Bond lengths

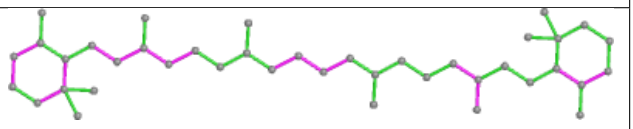

Bond angles

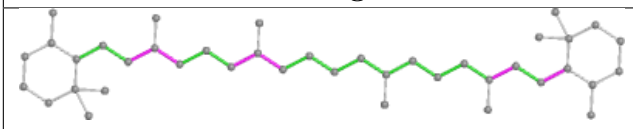

Torsions

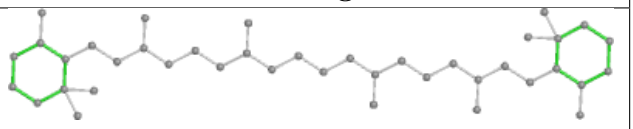

Rings

### Ligand BCR K 103

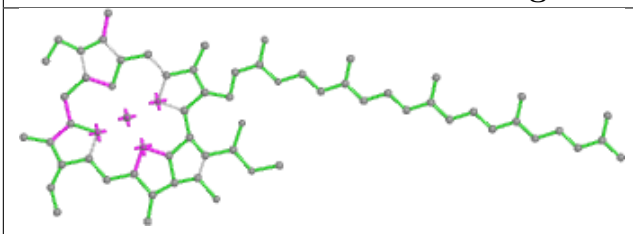

Bond lengths


Bond angles

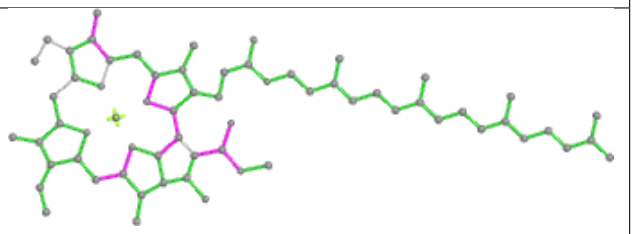

Torsions


Rings

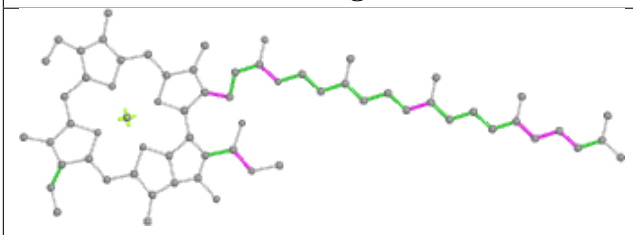
### Ligand CLA c 512



Bond lengths



Bond angles



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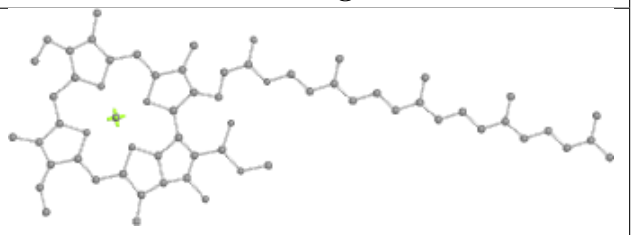
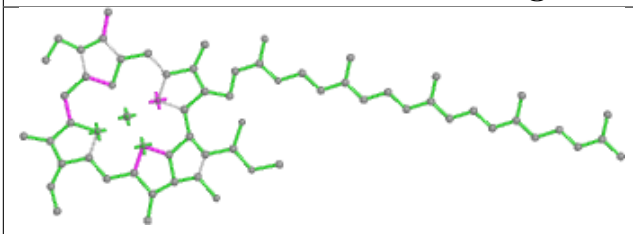


Rings

### Ligand CLA a 402



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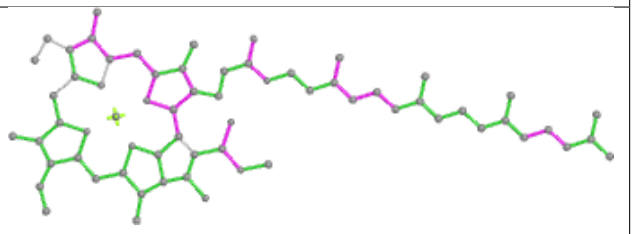
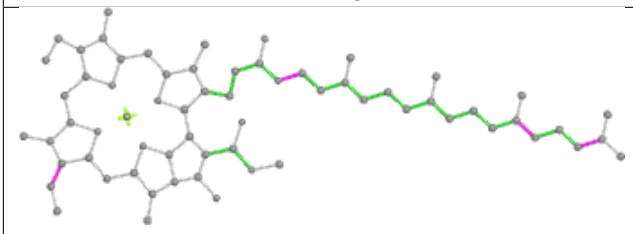
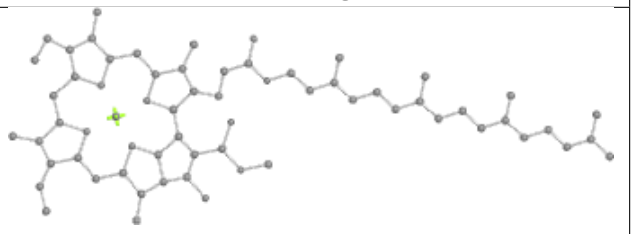


Bond angles

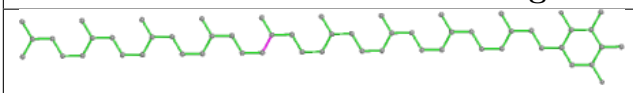


Torsions



Rings

### Ligand PL9 A 409



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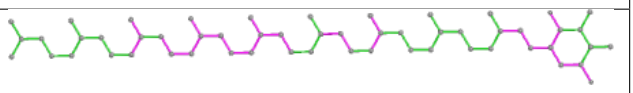
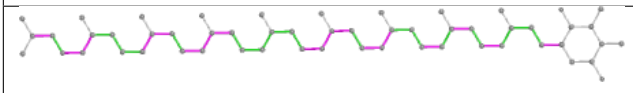
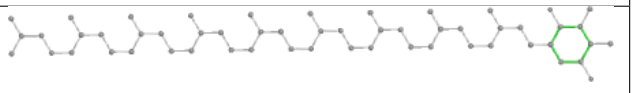


Bond angles

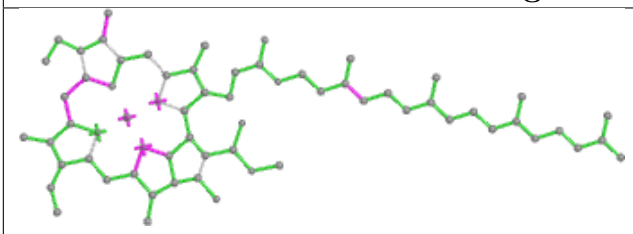


Torsions

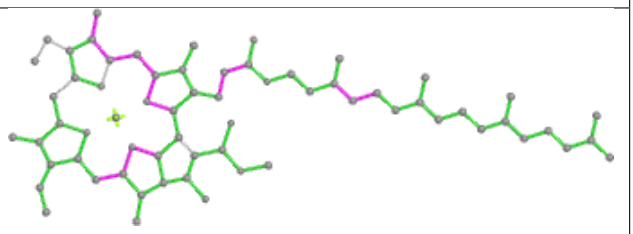


Rings

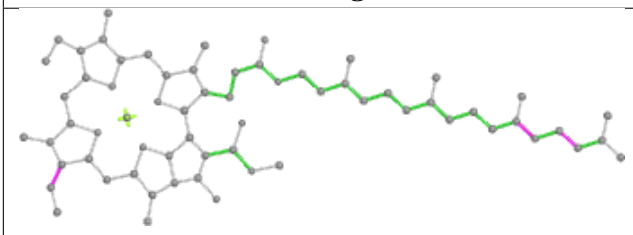
### Ligand CLA A 402



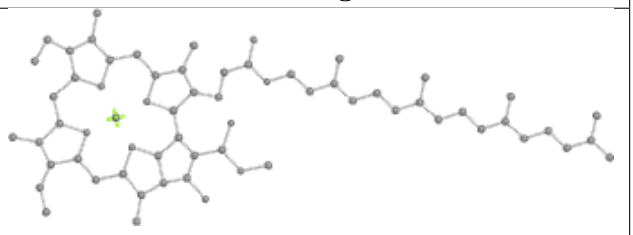
Bond lengths



Bond angles

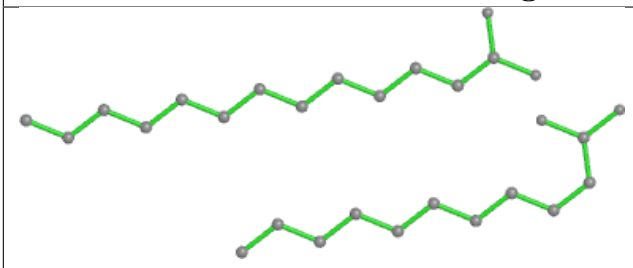


Torsions

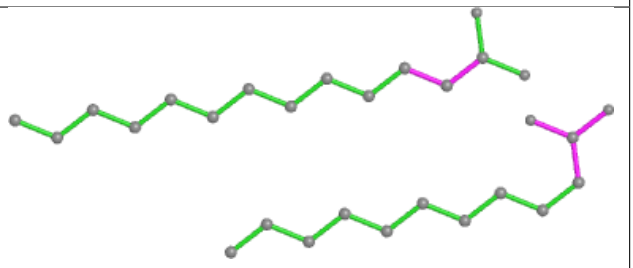


Rings

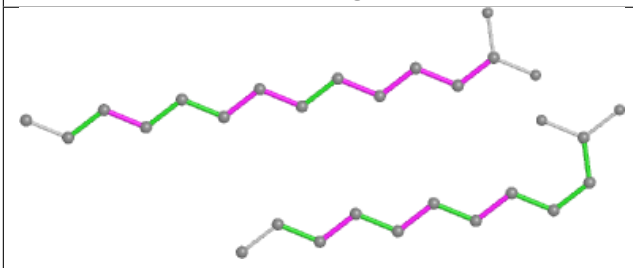
### Ligand LMG B 621



Bond lengths



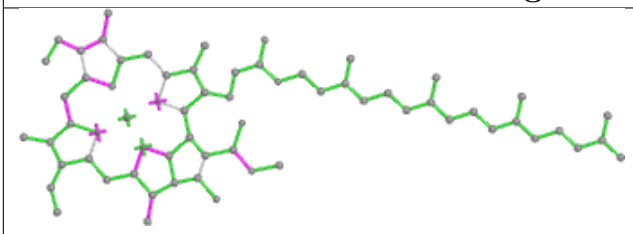
Bond angles



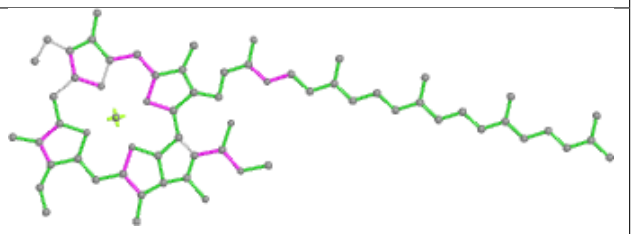
Torsions

Rings

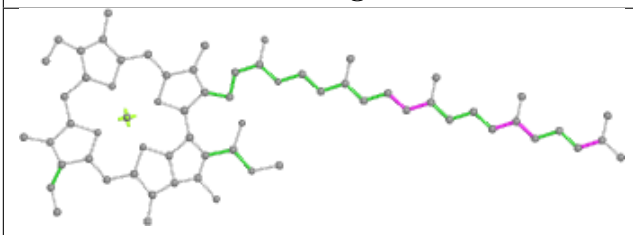
## Ligand CLA B 615



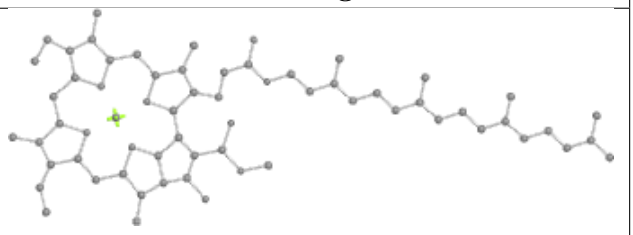
Bond lengths



Bond angles

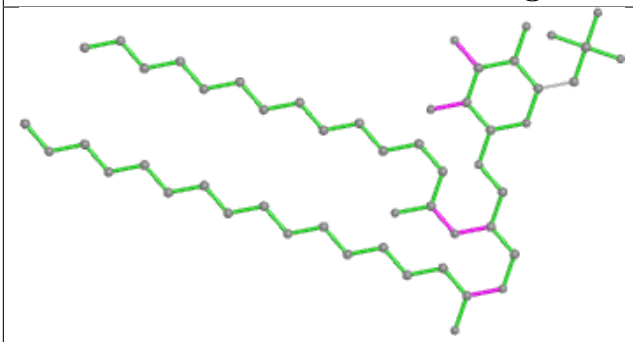


Torsions

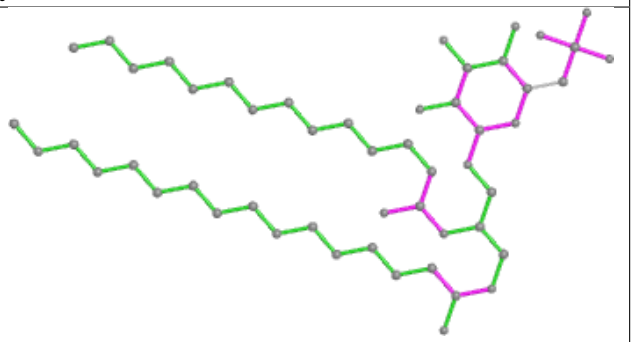


Rings

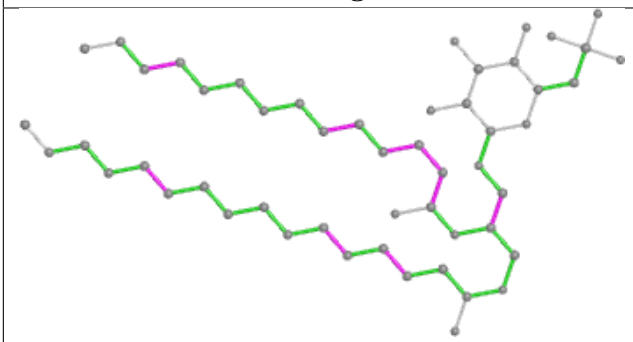
## Ligand SQD A 411



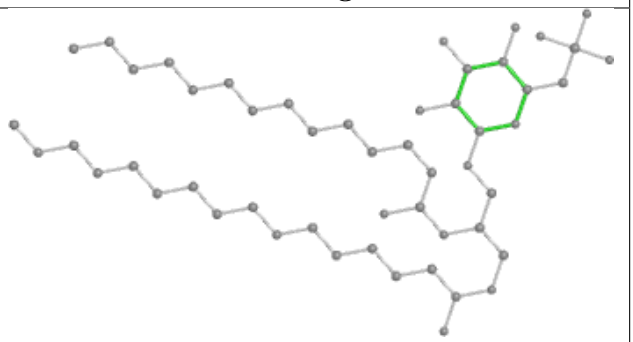
Bond lengths



Bond angles

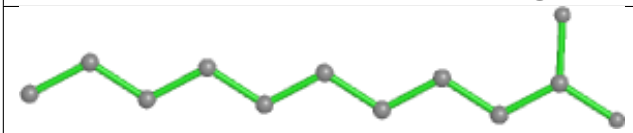


Torsions



Rings

## Ligand STE J 101



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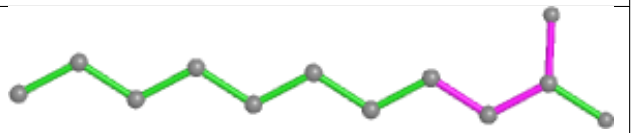
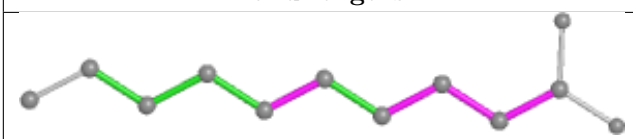
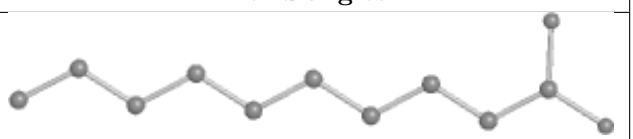


Bond angles

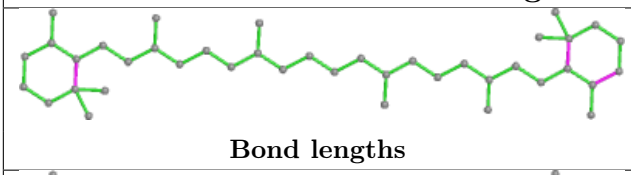


Torsions

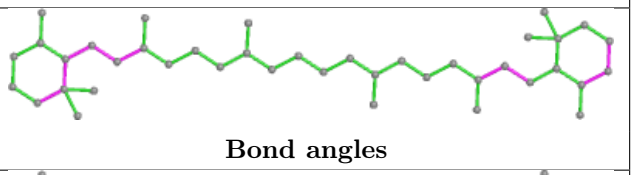


Rings

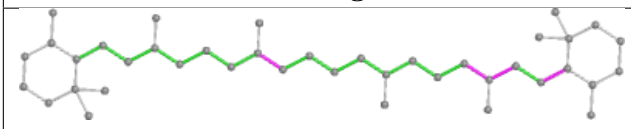
## Ligand BCR F 101



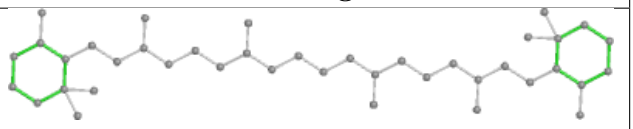
Bond lengths



Bond angles

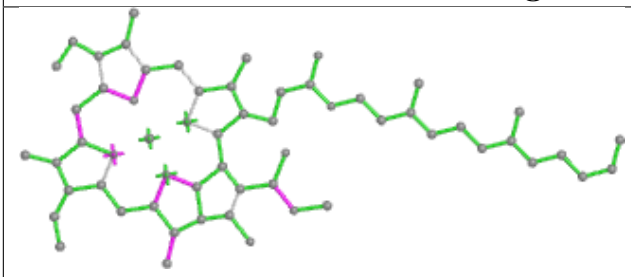


Torsions



Rings

## Ligand CLA C 504



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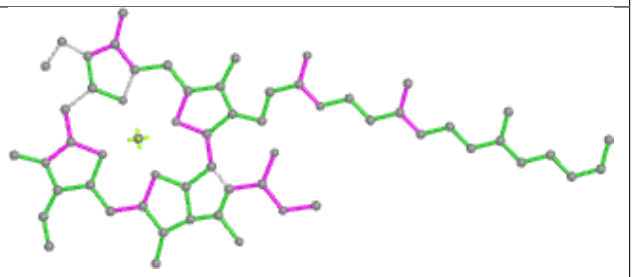
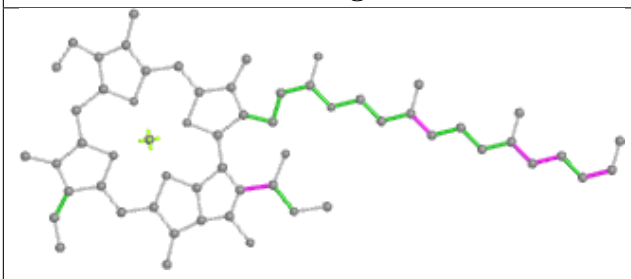
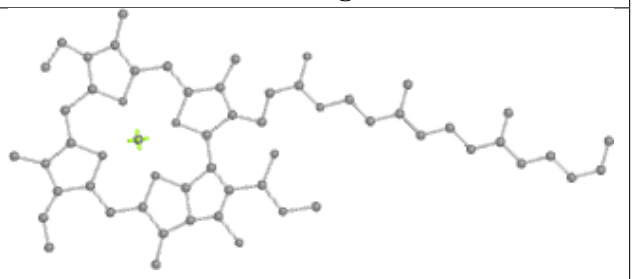


Bond angles

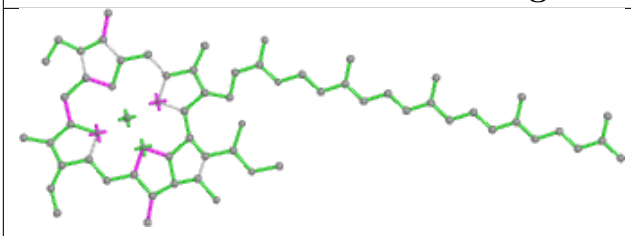


Torsions

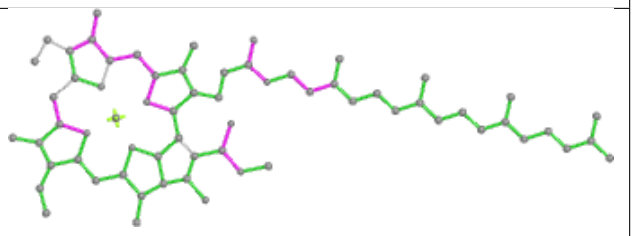


Rings

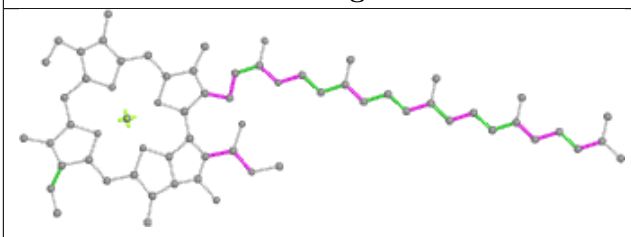
## Ligand CLA c 513



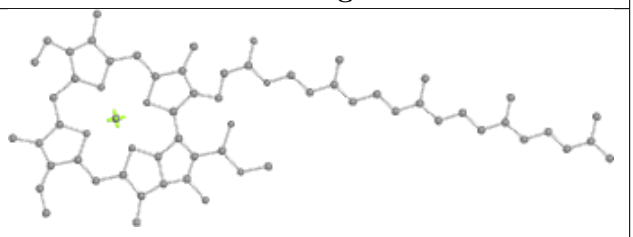
Bond lengths



Bond angles

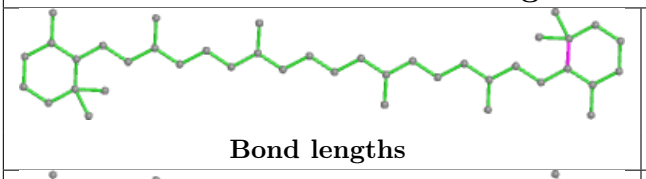


Torsions

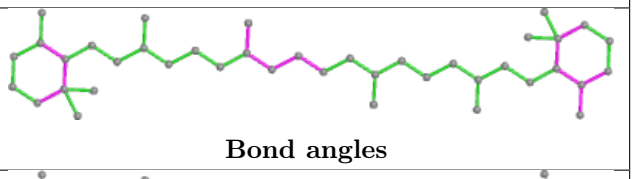


Rings

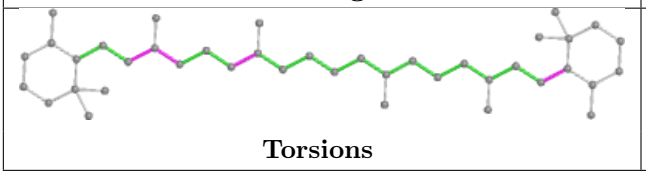
### Ligand BCR H 102



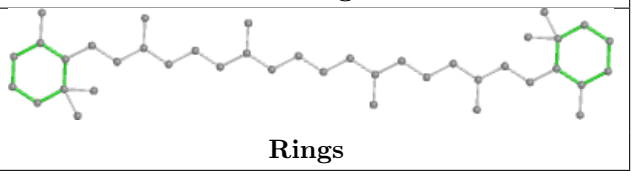
Bond lengths



Bond angles

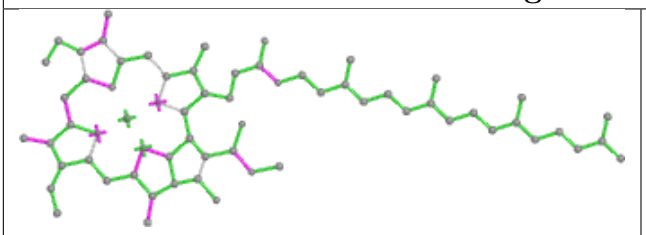


Torsions

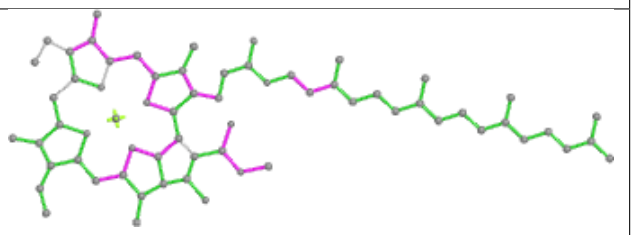


Rings

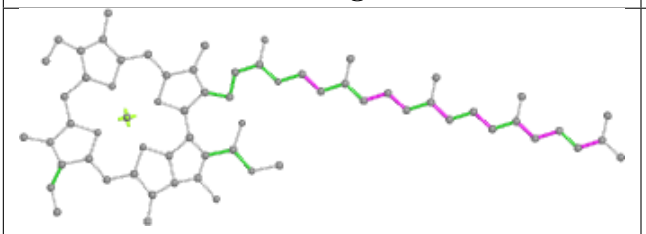
### Ligand CLA C 509



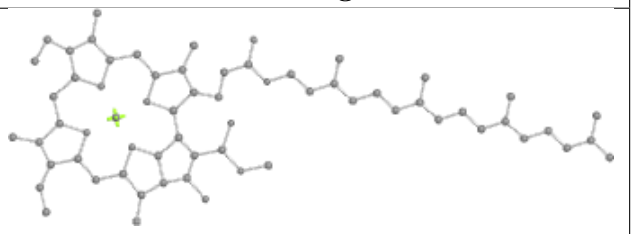
Bond lengths



Bond angles

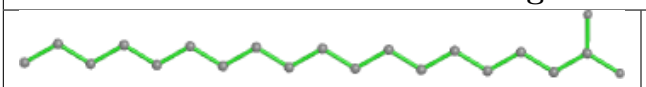


Torsions

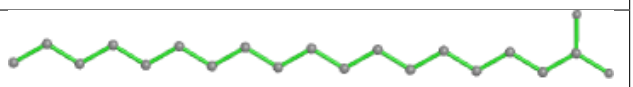


Rings

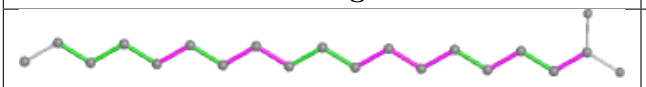
### Ligand STE D 413



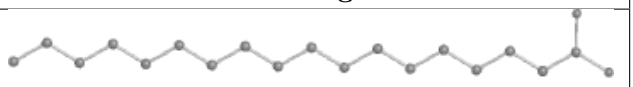
Bond lengths



Bond angles

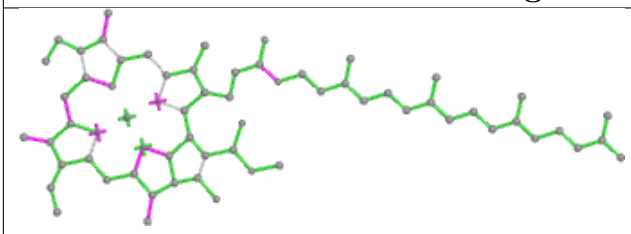


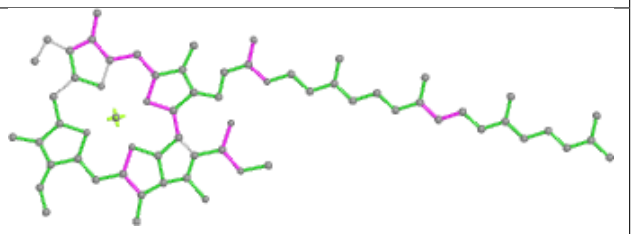
Torsions

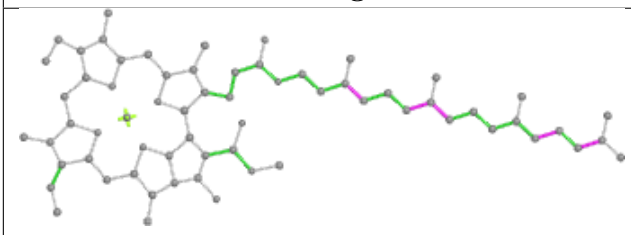


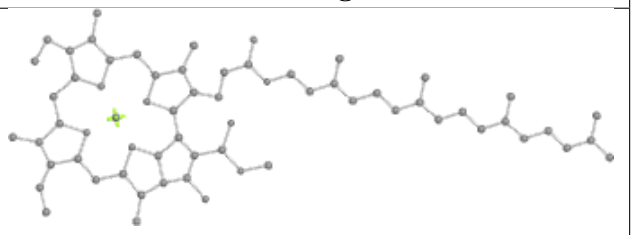
Rings

### Ligand CLA C 510


Bond lengths


Bond angles


Torsions

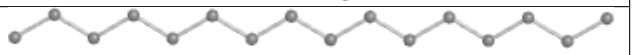

Rings

### Ligand STE b 620

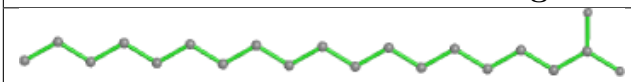
Bond lengths

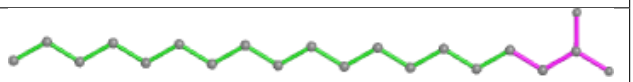
Bond angles

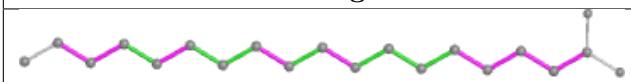
Torsions

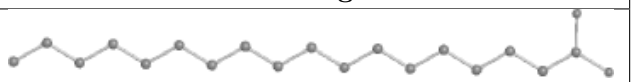

Rings

### Ligand STE b 624

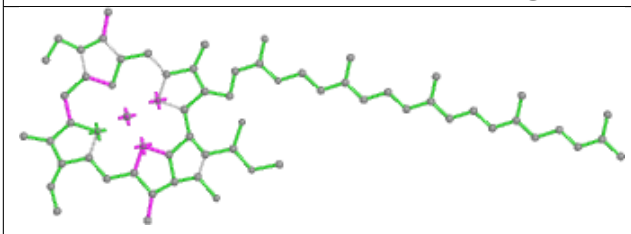

Bond lengths

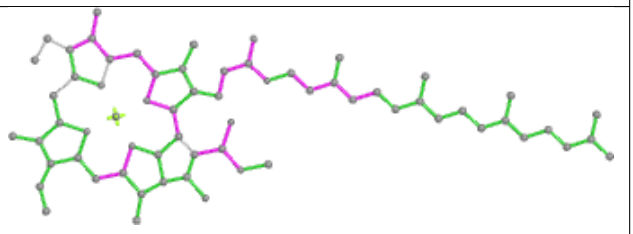

Bond angles

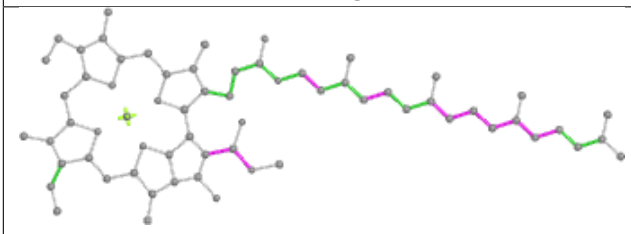

Torsions

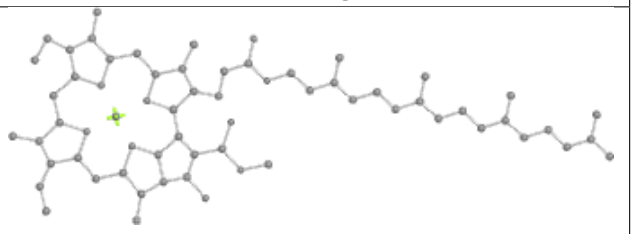

Rings

### Ligand CLA C 512

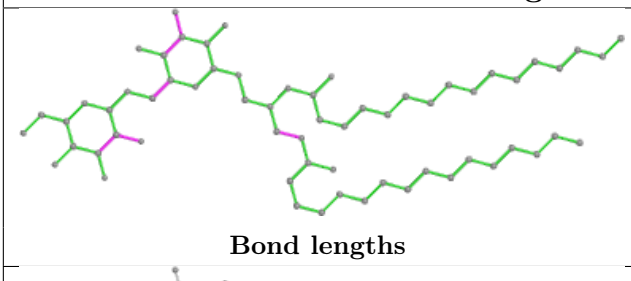

Bond lengths

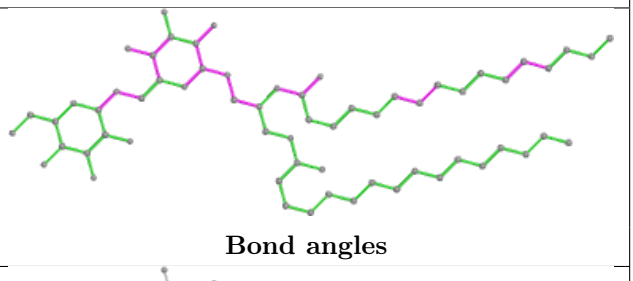

Bond angles

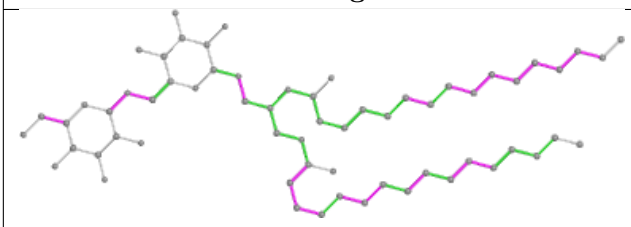

Torsions

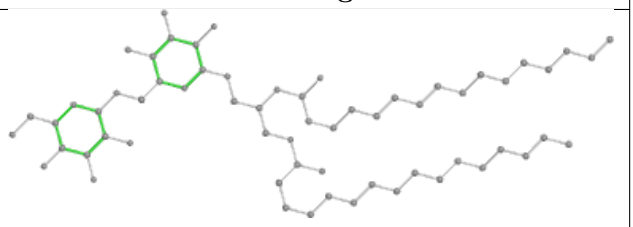

Rings

## Ligand DGD c 518

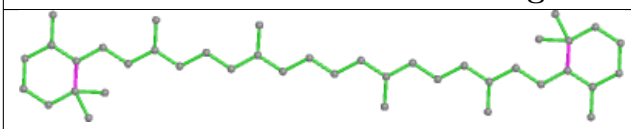

Bond lengths

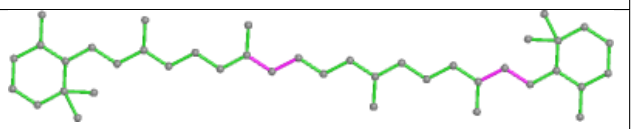

Bond angles

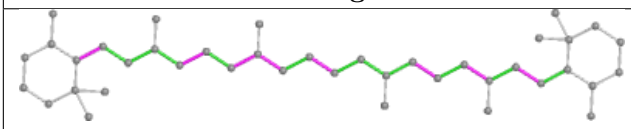

Torsions

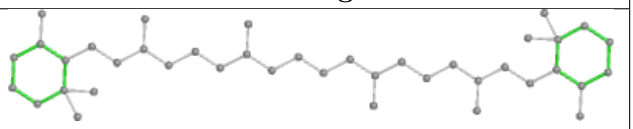

Rings

## Ligand BCR c 515

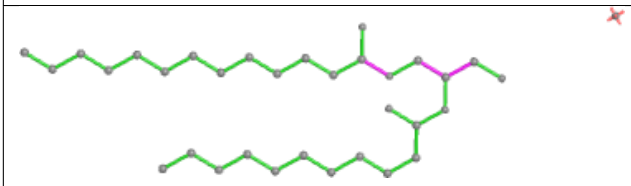

Bond lengths

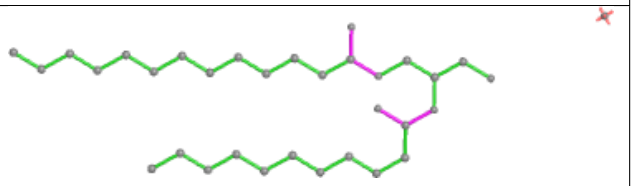

Bond angles

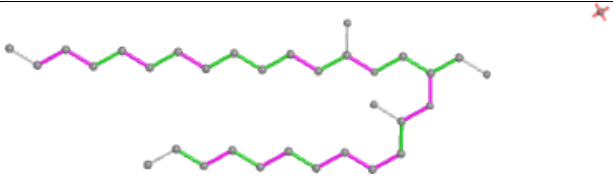

Torsions

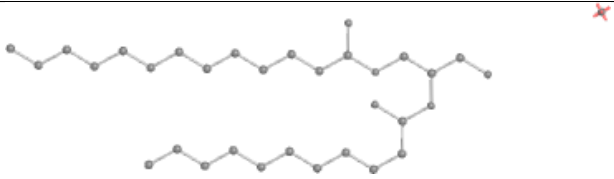

Rings

## Ligand LMG D 411


Bond lengths


Bond angles

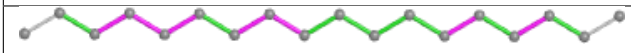

Torsions

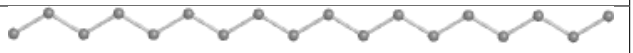

Rings

## Ligand STE m 101

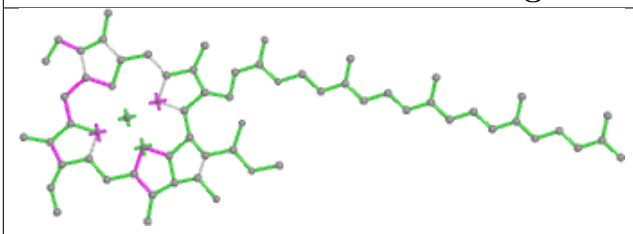
Bond lengths

Bond angles

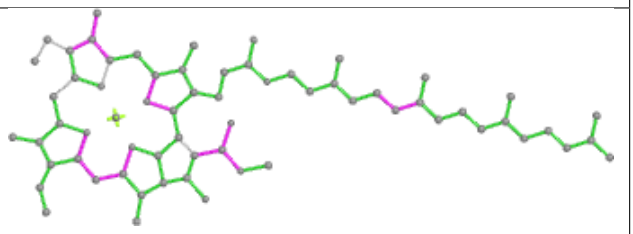

Torsions


Rings

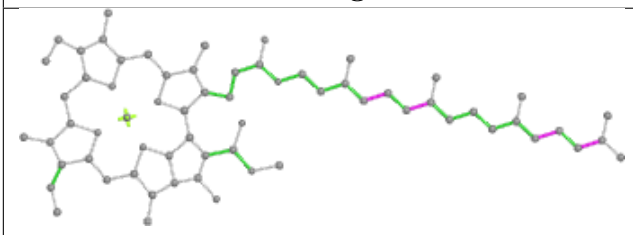
### Ligand CLA B 608



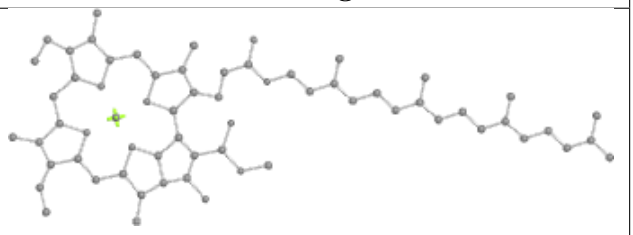
Bond lengths



Bond angles

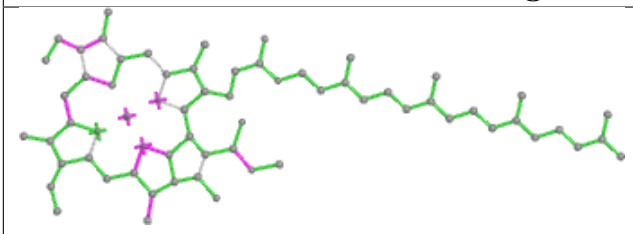


Torsions

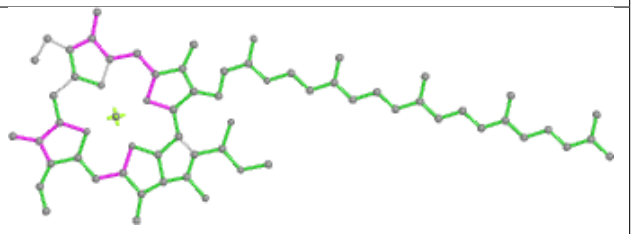


Rings

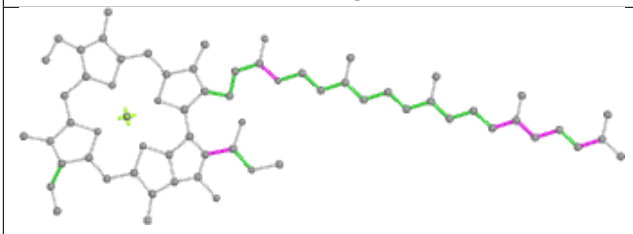
### Ligand CLA B 609



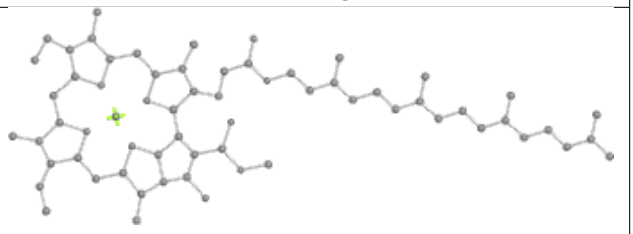
Bond lengths



Bond angles

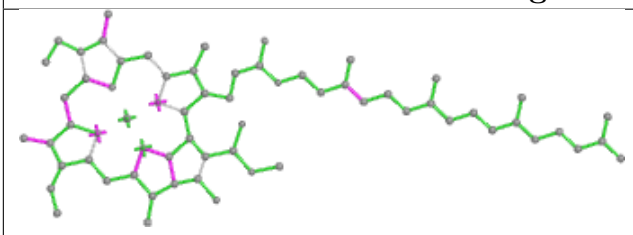


Torsions

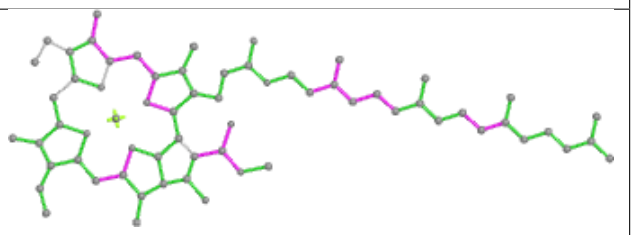


Rings

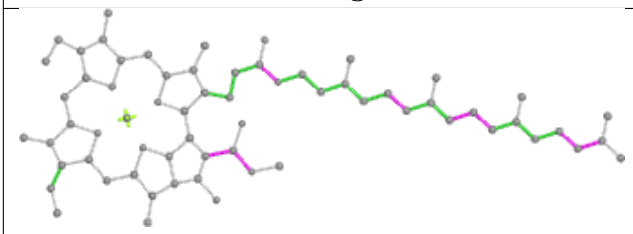
### Ligand CLA c 504



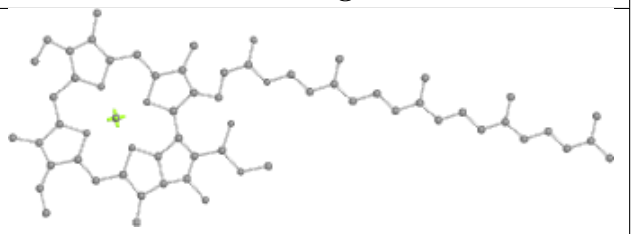
Bond lengths



Bond angles

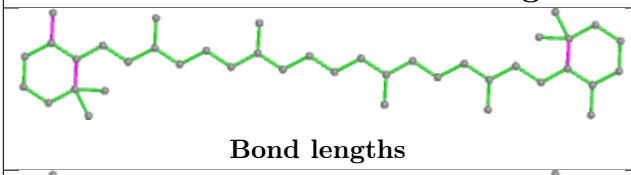


Torsions

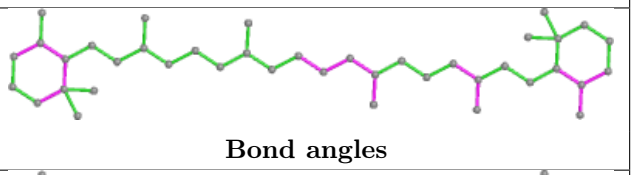


Rings

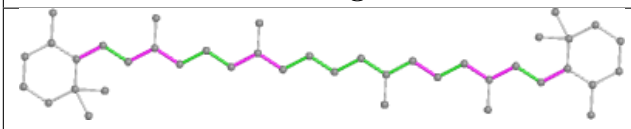
## Ligand BCR A 406



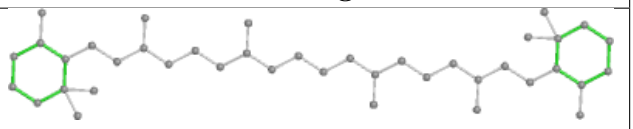
Bond lengths



Bond angles

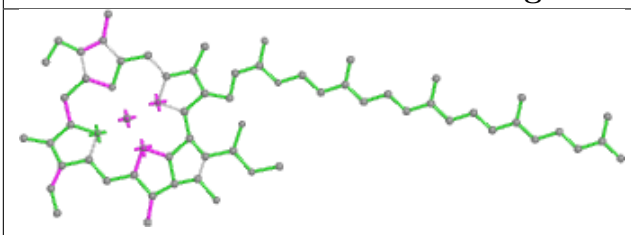


Torsions

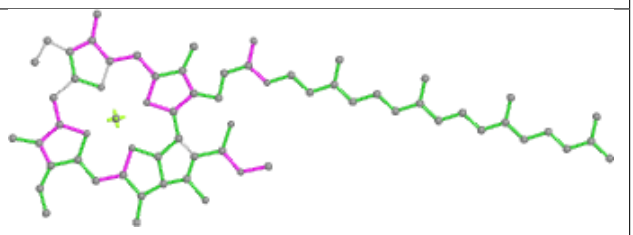


Rings

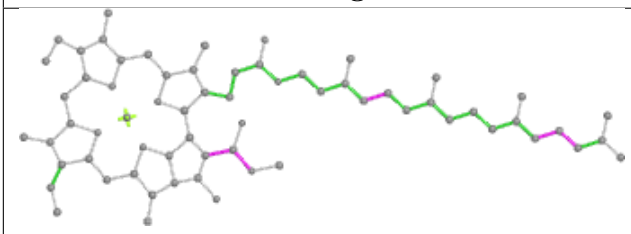
## Ligand CLA B 607



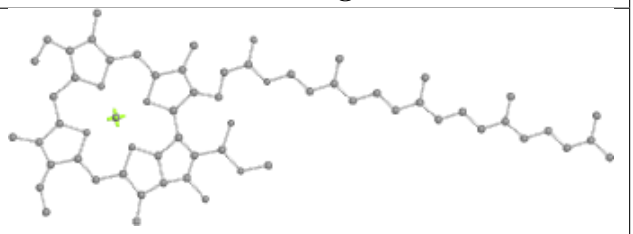
Bond lengths



Bond angles

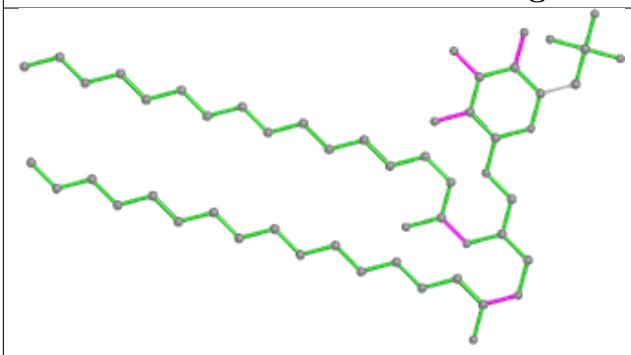


Torsions

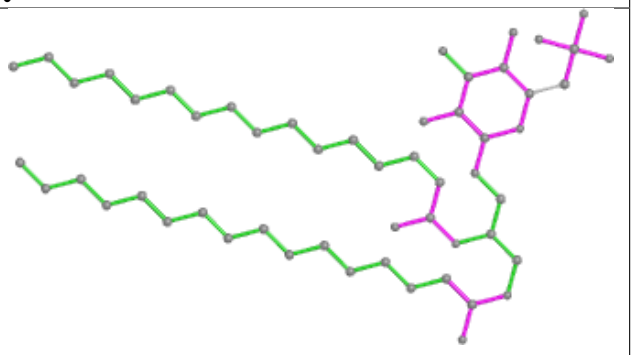


Rings

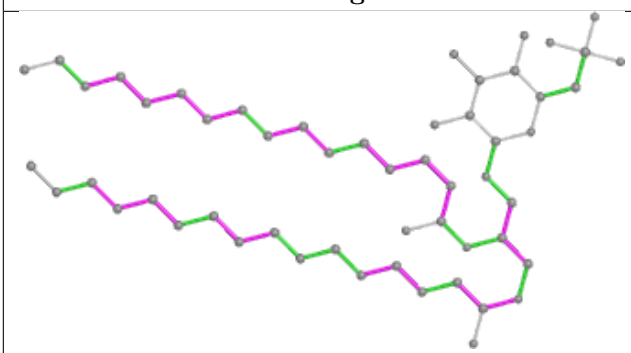
## Ligand SQD a 411



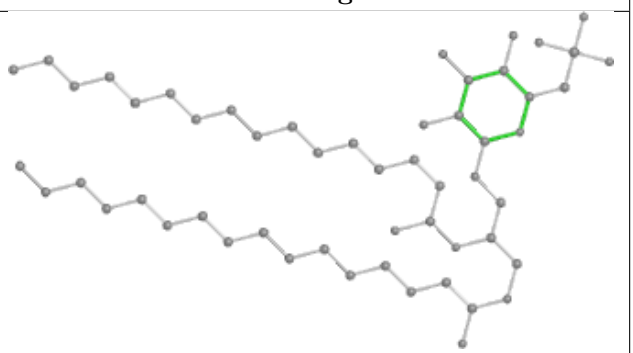
Bond lengths



Bond angles

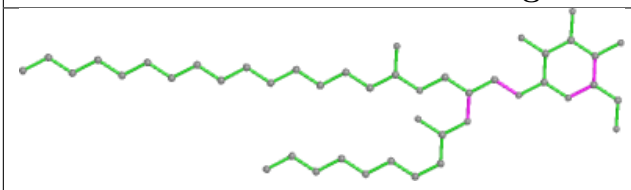


Torsions

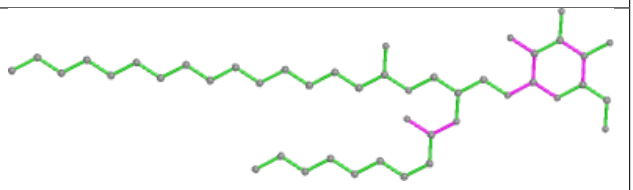


Rings

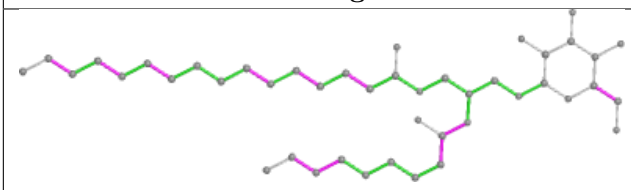
### Ligand LMG d 410



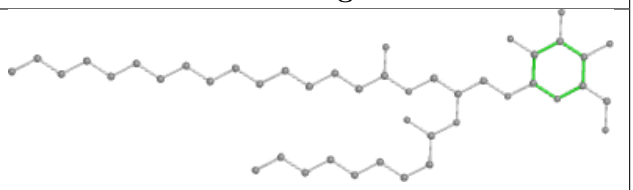
Bond lengths



Bond angles

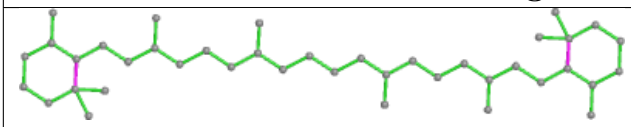


Torsions

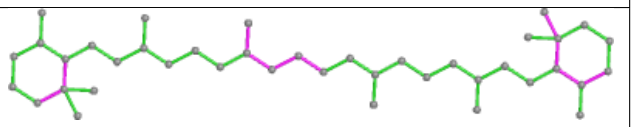


Rings

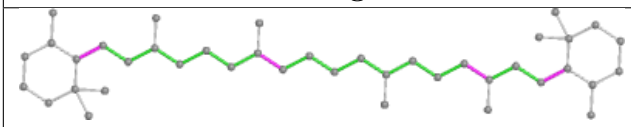
### Ligand BCR k 102



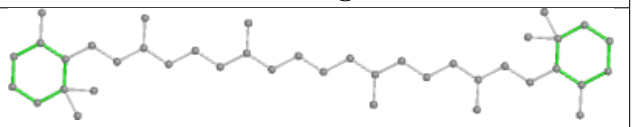
Bond lengths



Bond angles

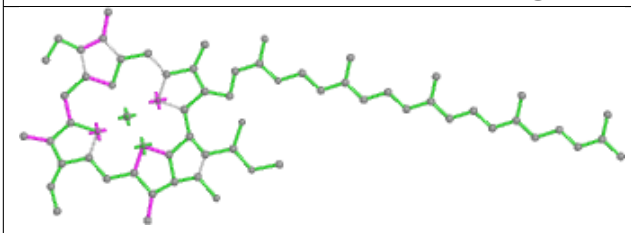


Torsions

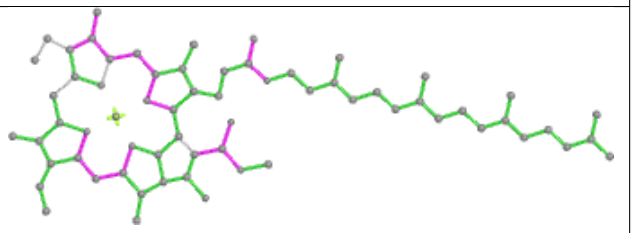


Rings

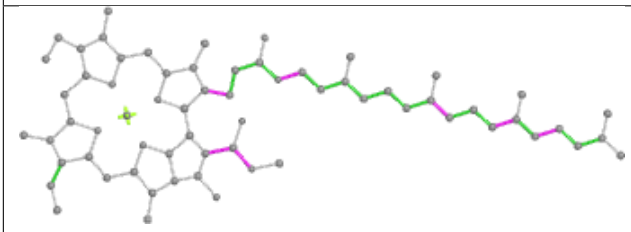
### Ligand CLA c 514



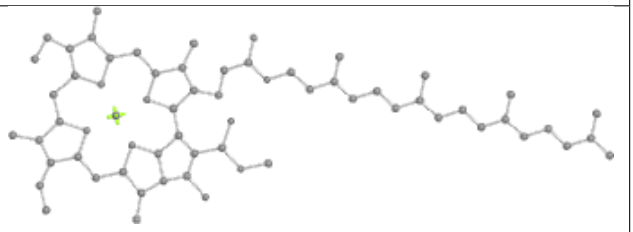
Bond lengths



Bond angles

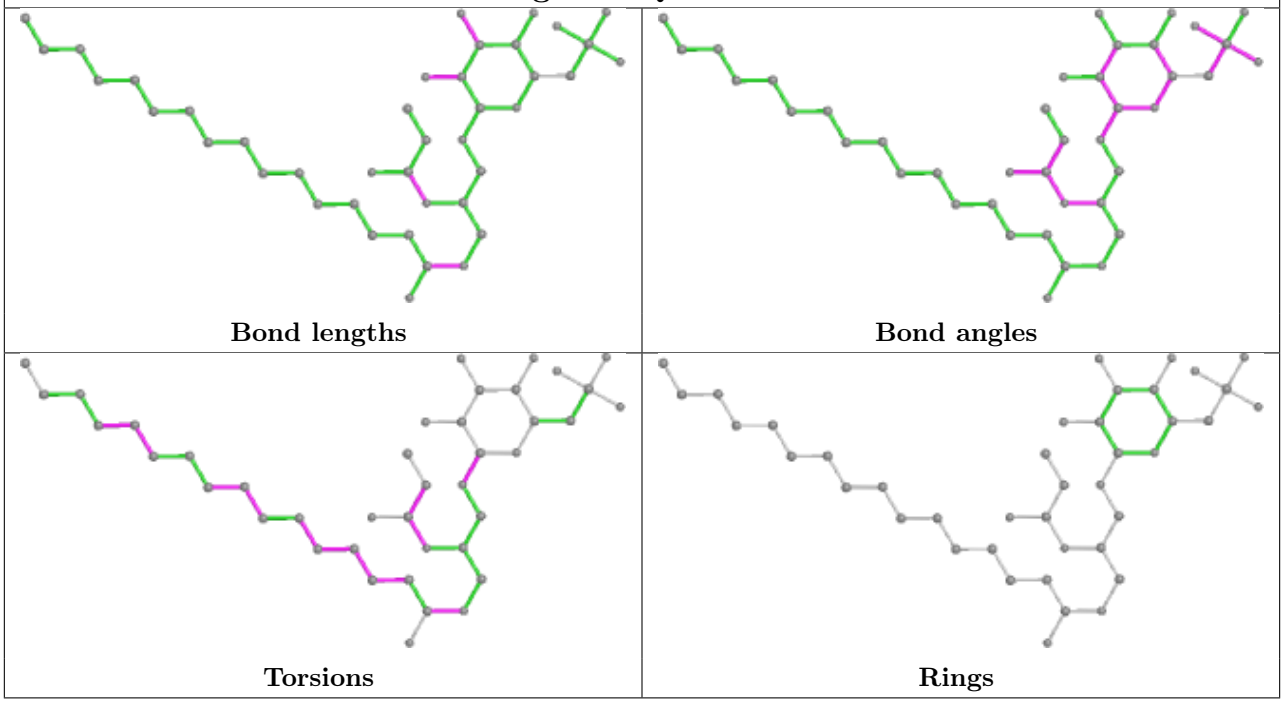


Torsions

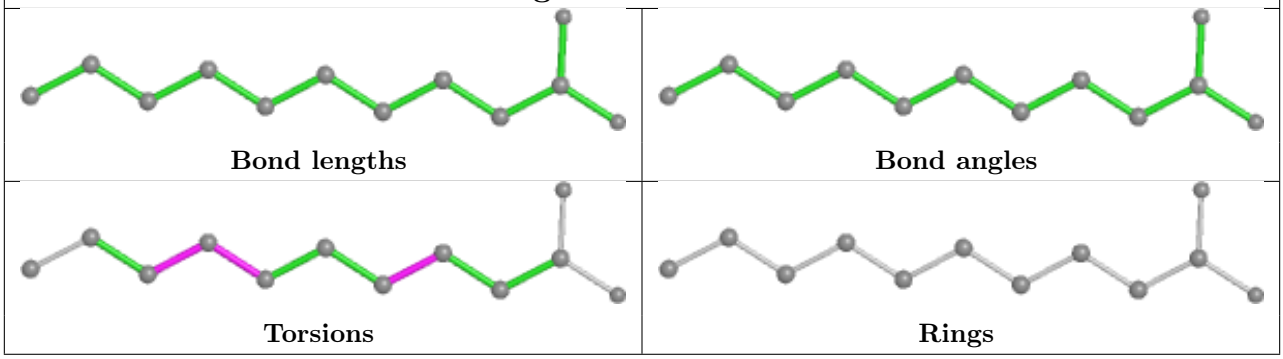


Rings

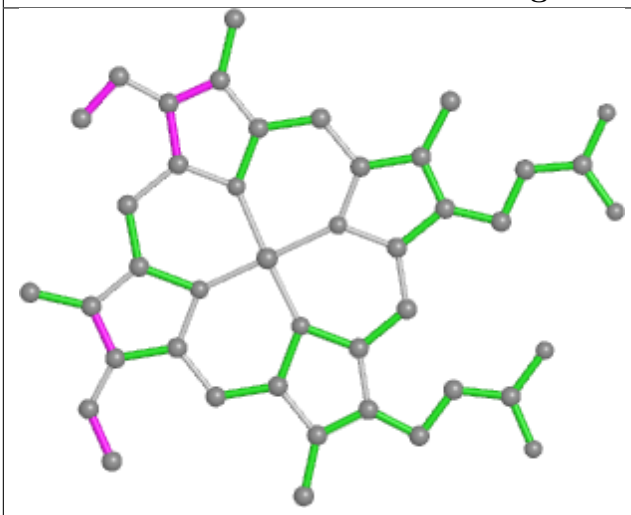
### Ligand SQD f 102



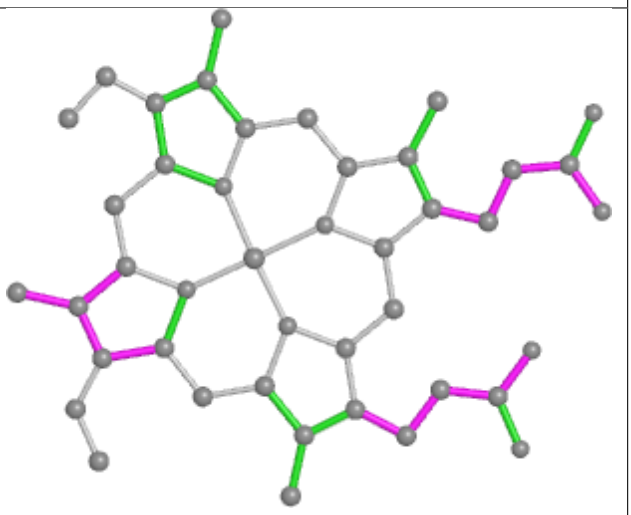

### Ligand STE c 501



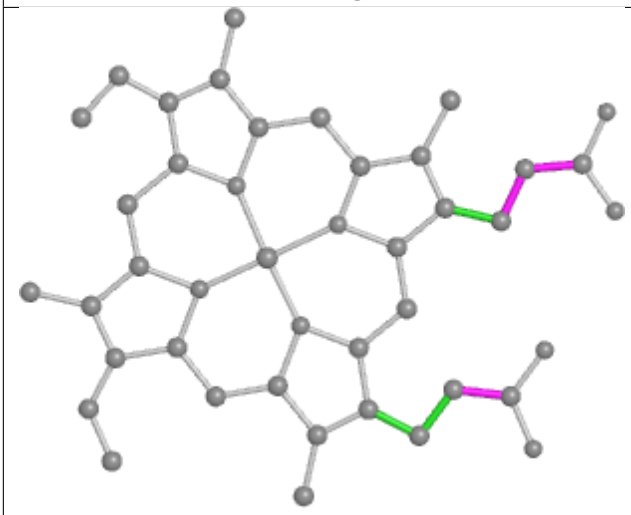
## Ligand HEC f 101



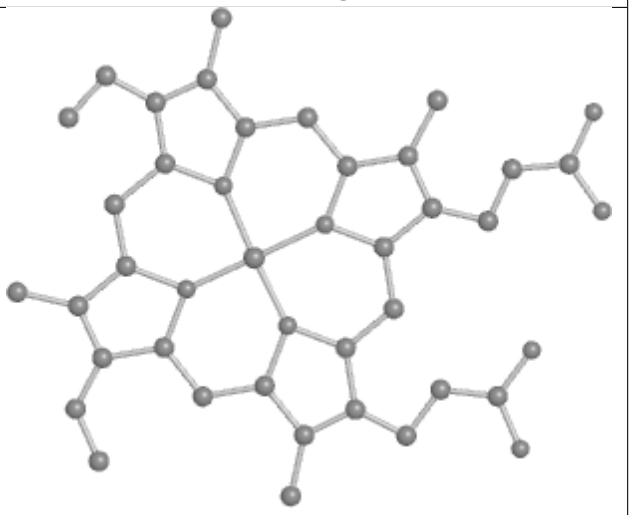
Bond lengths



Bond angles



Torsions

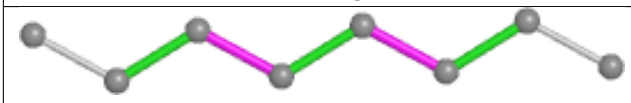


Rings

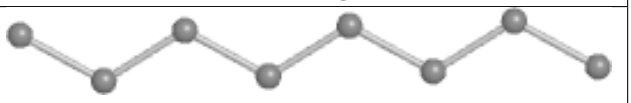
## Ligand STE Z 101

Bond lengths

Bond angles

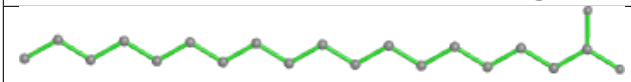


Torsions

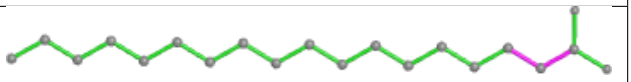


Rings

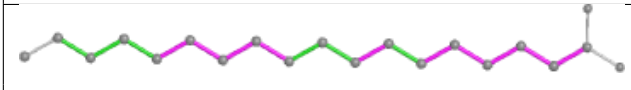
## Ligand STE d 413



Bond lengths



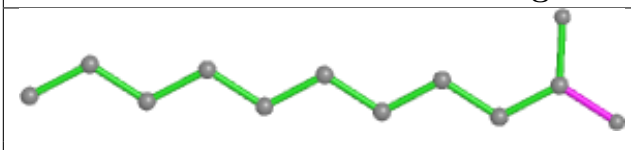
Bond angles

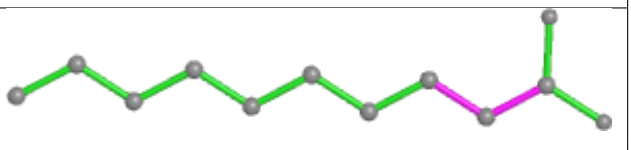


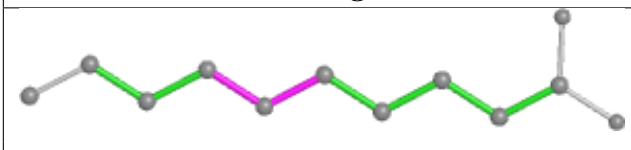
Torsions

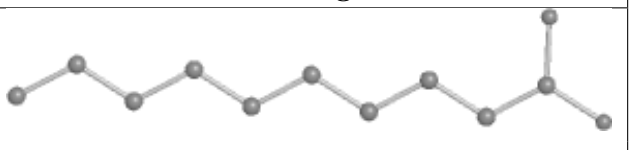
Rings

### Ligand STE a 414

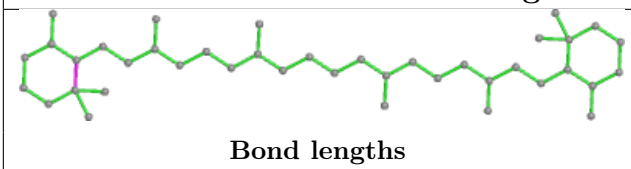

Bond lengths

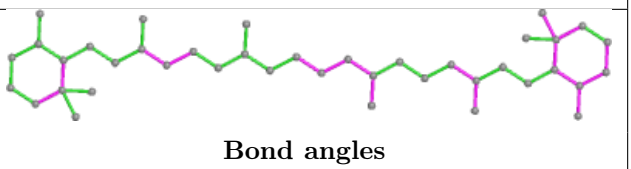

Bond angles

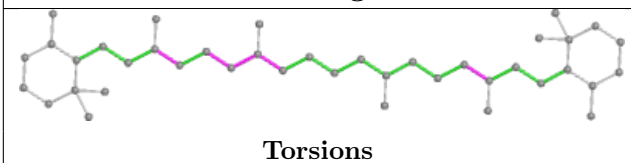

Torsions


Rings

### Ligand BCR B 619

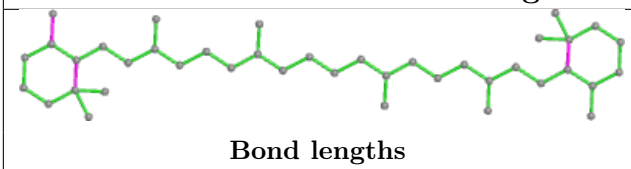

Bond lengths

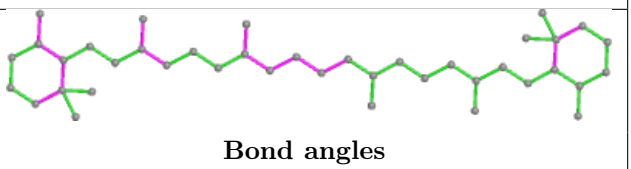

Bond angles

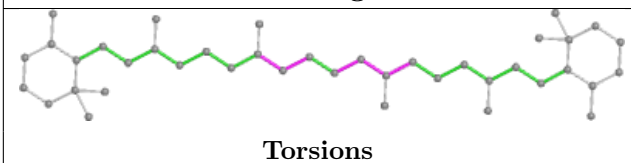

Torsions

Rings

### Ligand BCR C 514


Bond lengths

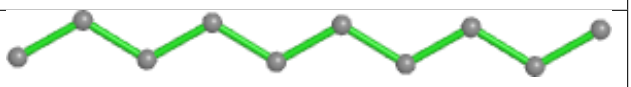

Bond angles


Torsions

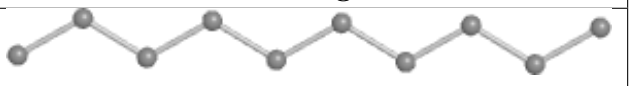
Rings

### Ligand STE M 103

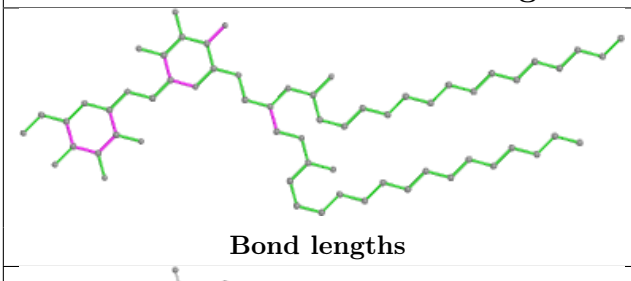
Bond lengths


Bond angles

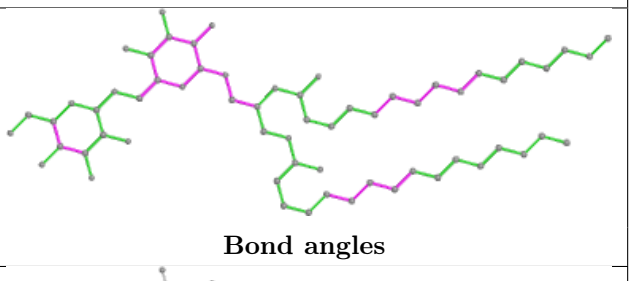
Torsions


Rings

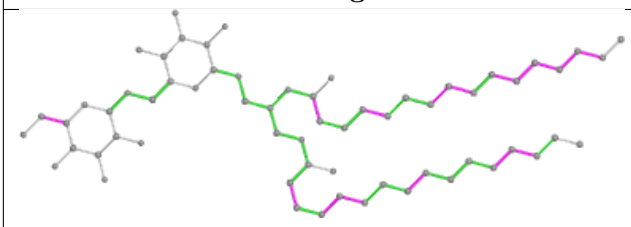
## Ligand DGD H 103



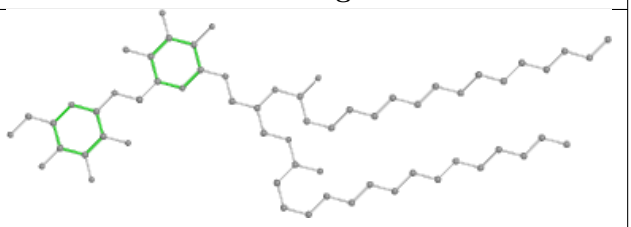
Bond lengths



Bond angles

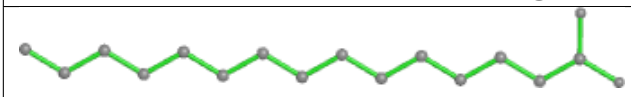


Torsions

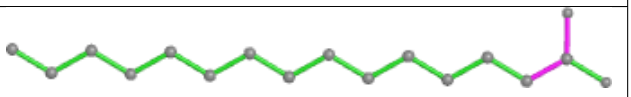


Rings

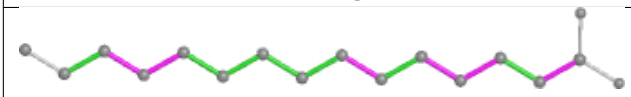
## Ligand STE d 412



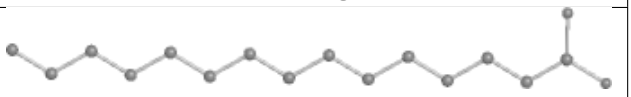
Bond lengths



Bond angles

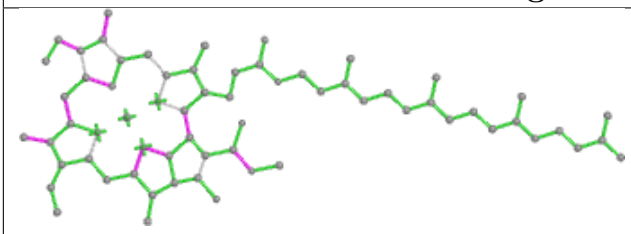


Torsions

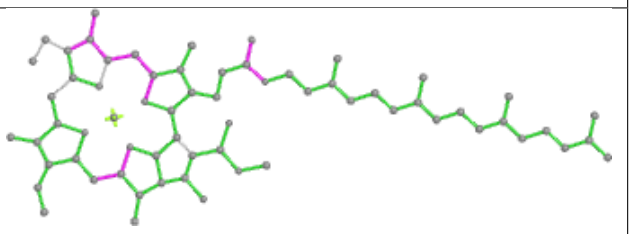


Rings

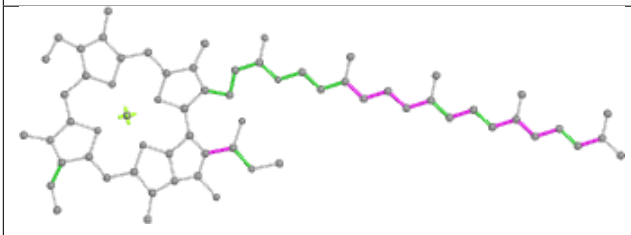
## Ligand CLA b 614



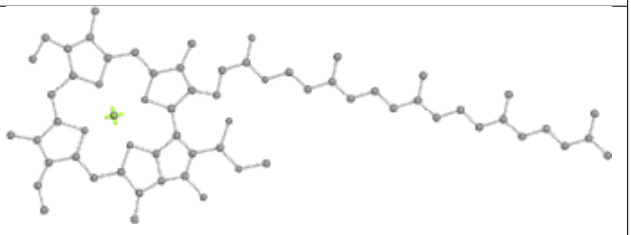
Bond lengths



Bond angles

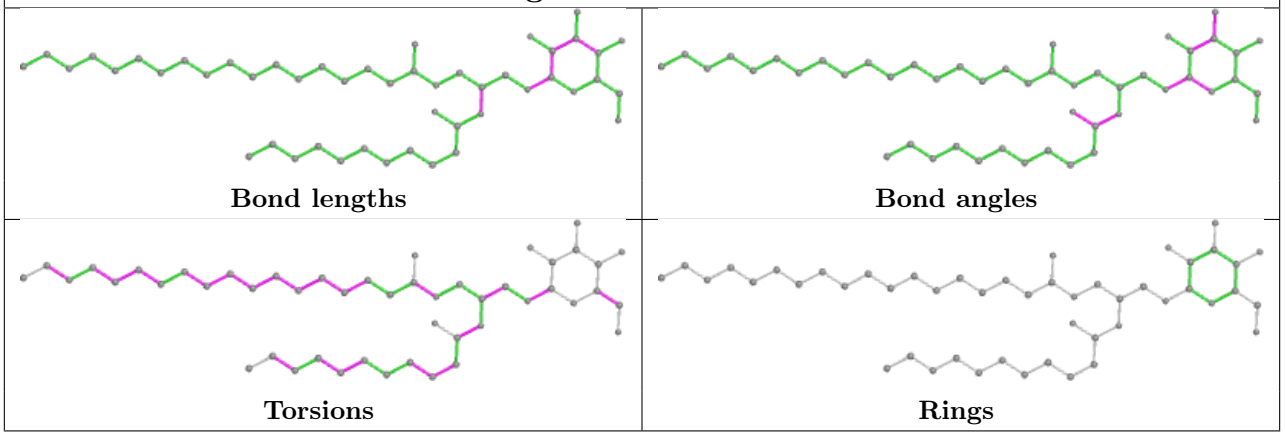


Torsions

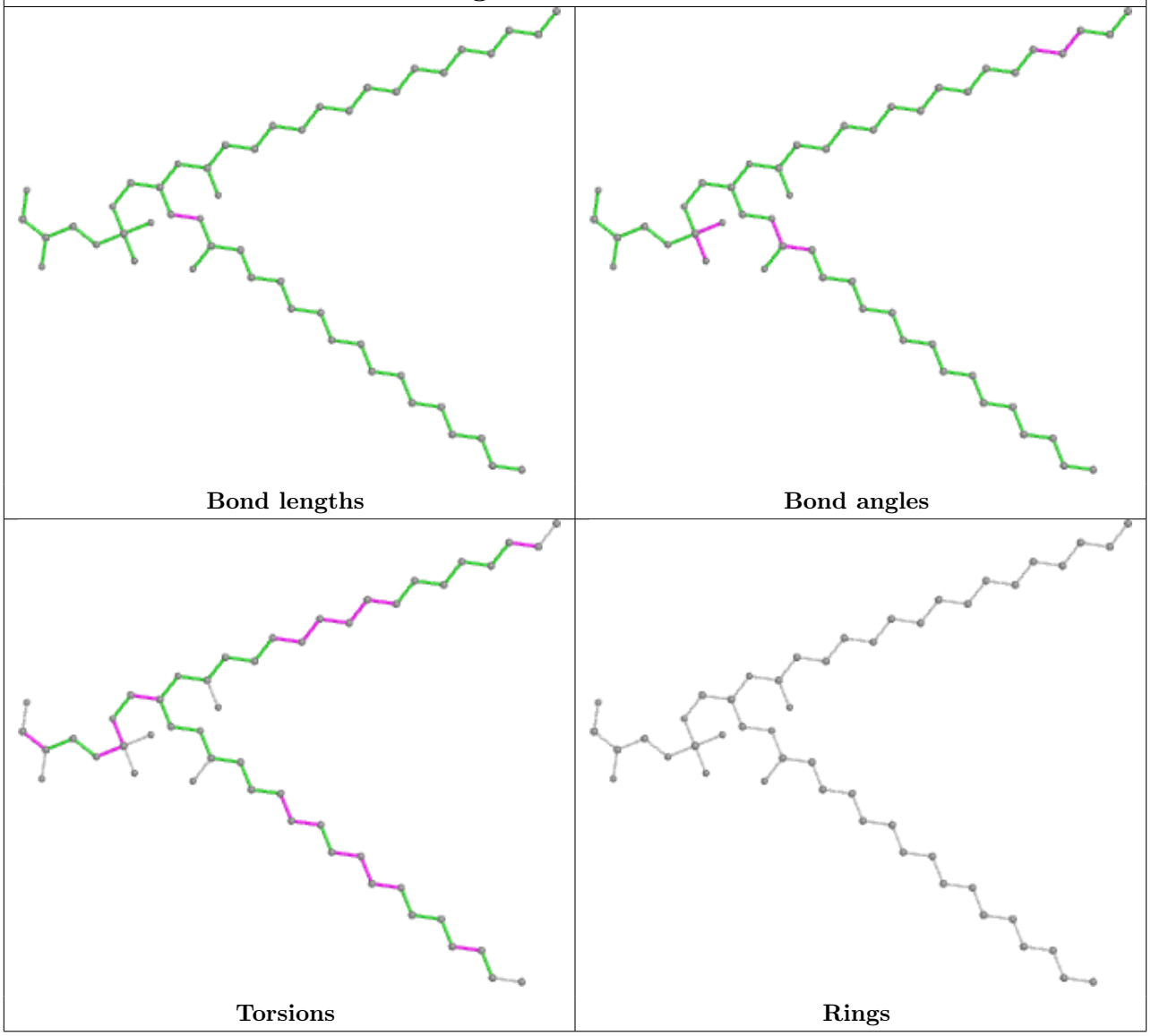


Rings

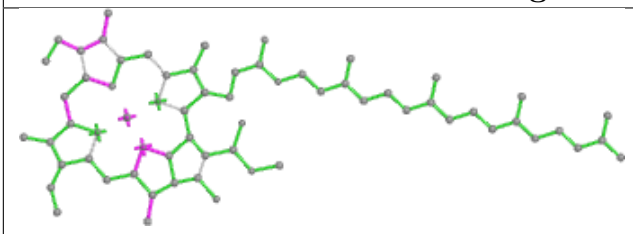
### Ligand LMG c 522



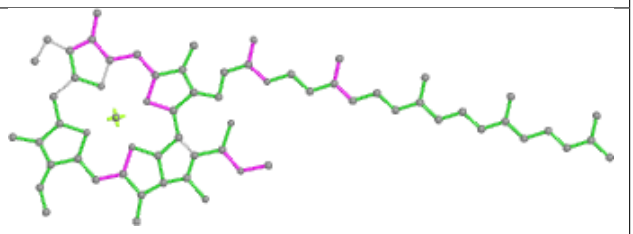

### Ligand LHG d 408



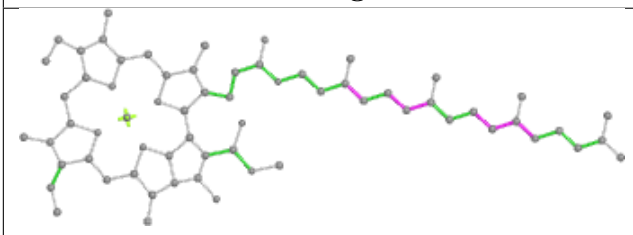
### Ligand CLA c 508



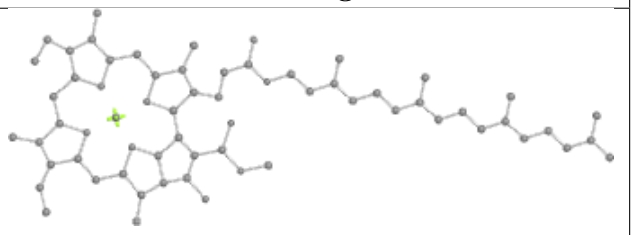
Bond lengths



Bond angles

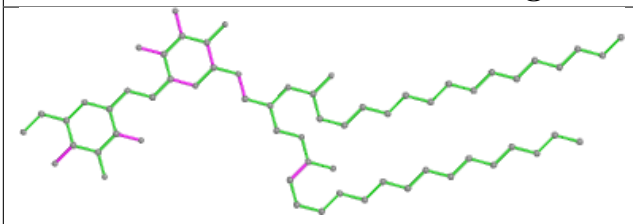


Torsions

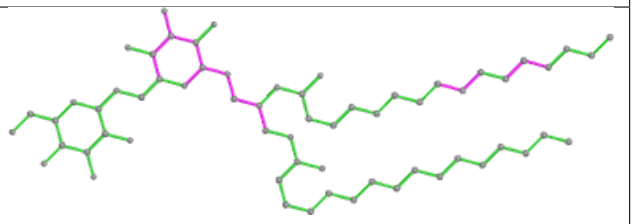


Rings

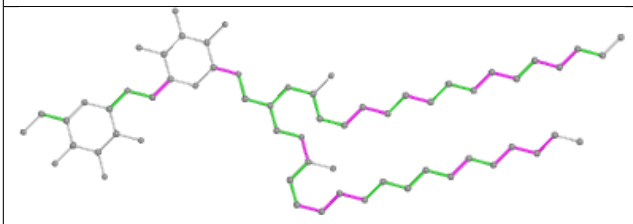
### Ligand DGD c 519



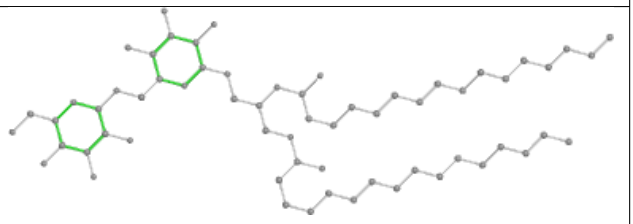
Bond lengths



Bond angles

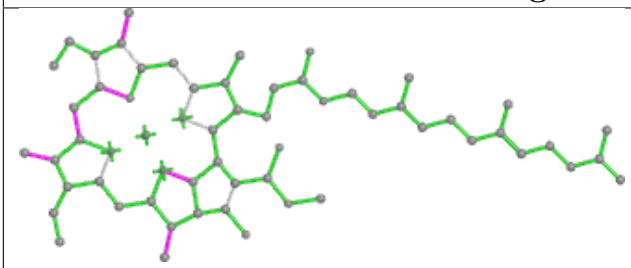


Torsions



Rings

### Ligand CLA c 505



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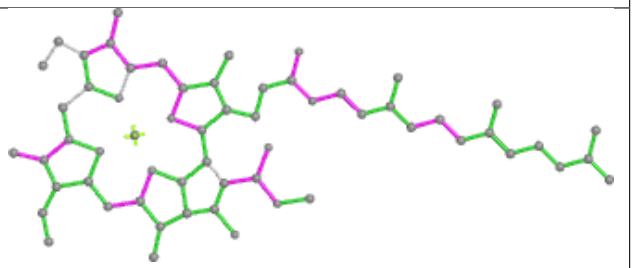
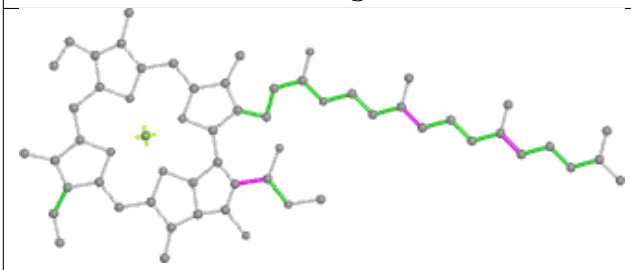
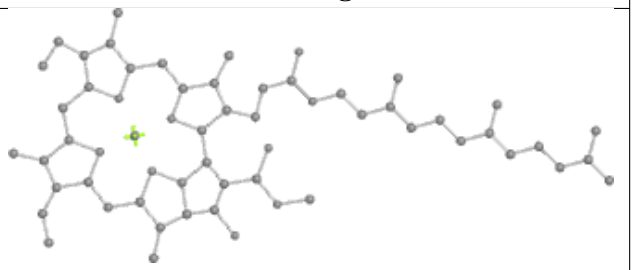


Bond angles

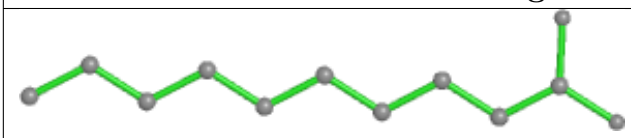


Torsions



Rings

### Ligand STE B 601



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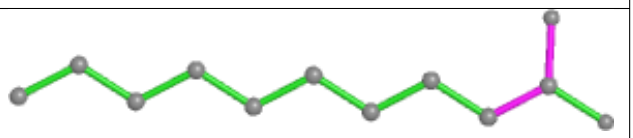
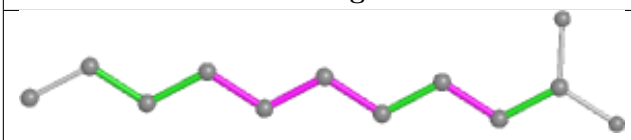
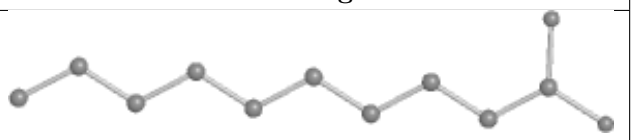


Bond angles

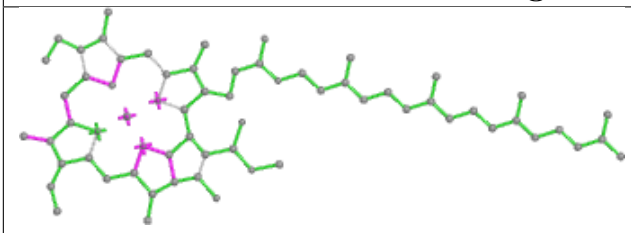


Torsions

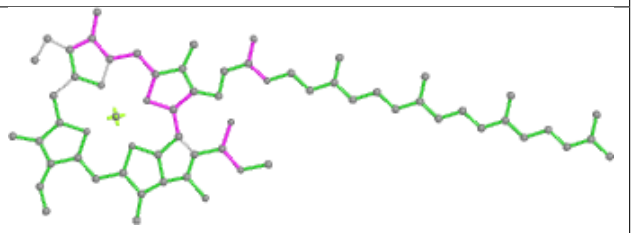


Rings

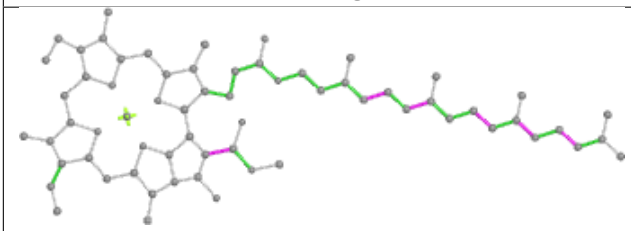
### Ligand CLA b 604



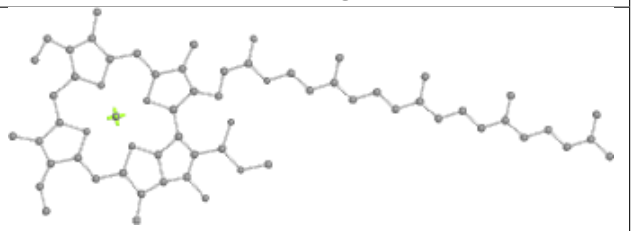
Bond lengths



Bond angles

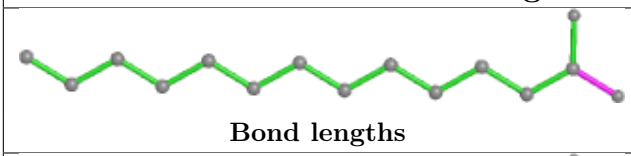


Torsions



Rings

### Ligand STE M 102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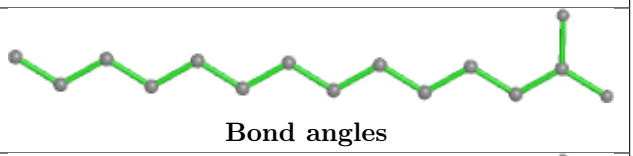
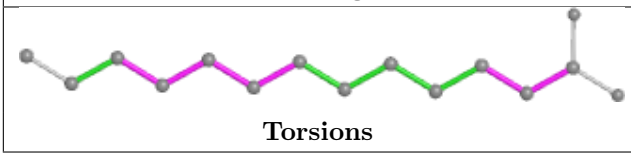
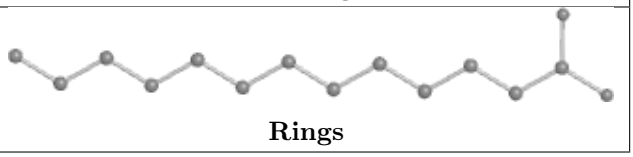
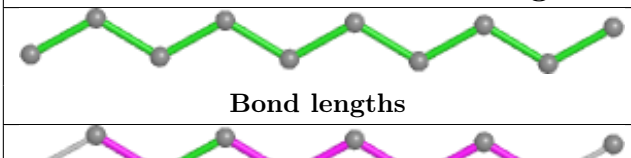
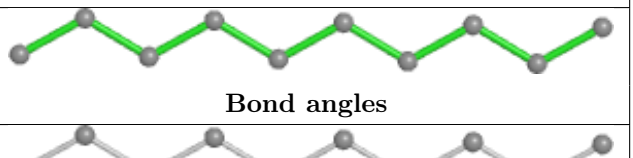

Bond angles

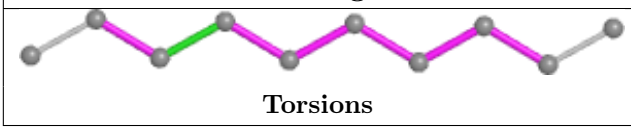

Torsions

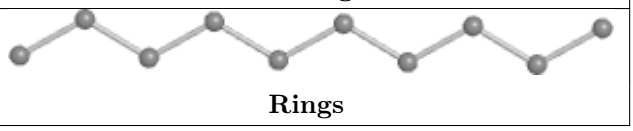

Rings

### Ligand STE b 625

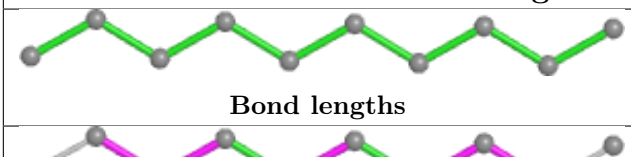

Bond lengths


Bond angles


Torsions


Rings

### Ligand STE a 413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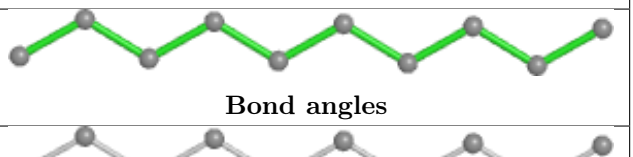
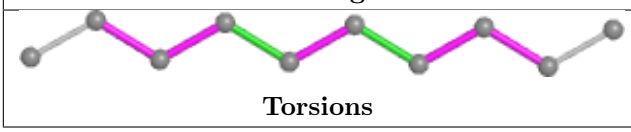
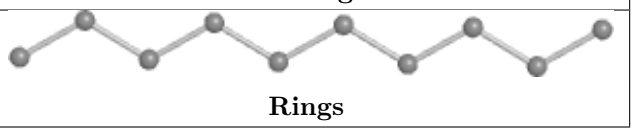
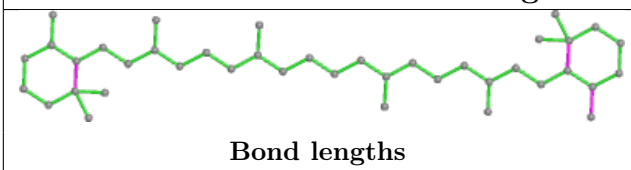

Bond angles


Torsions


Rings

### Ligand BCR K 102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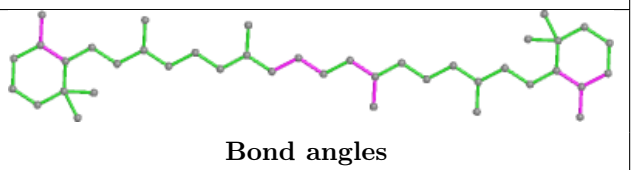
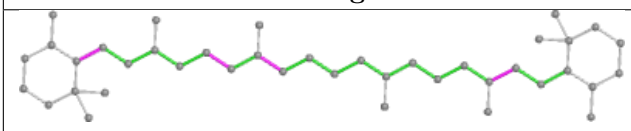
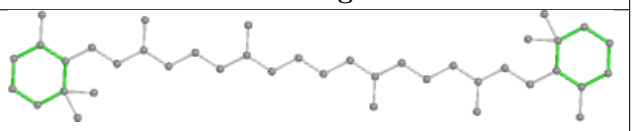
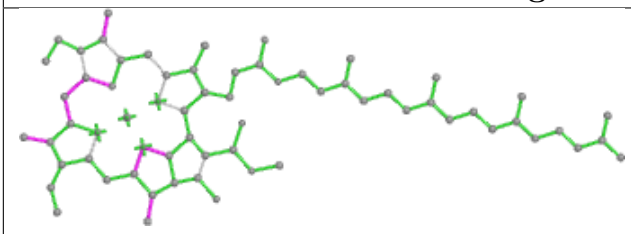

Bond angles

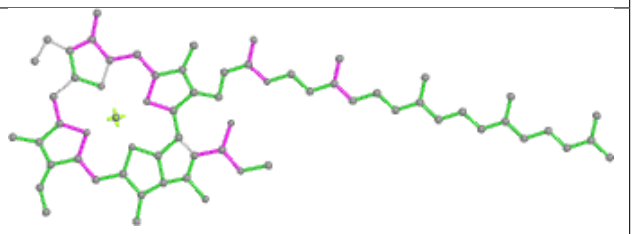

Torsions


Rings

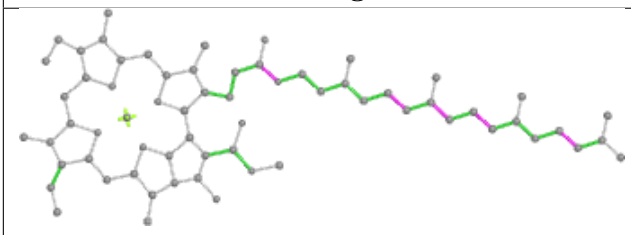
**Ligand CLA a 405**



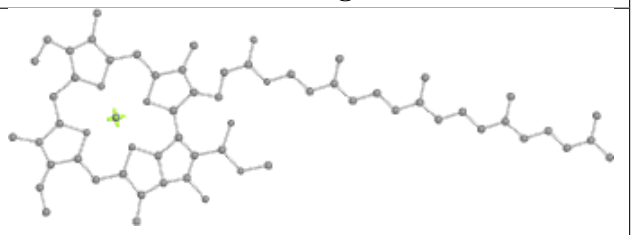
Bond lengths



Bond angles

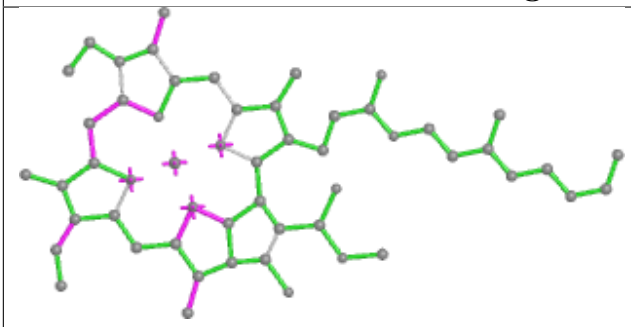


Torsions



Rings

**Ligand CLA A 405**



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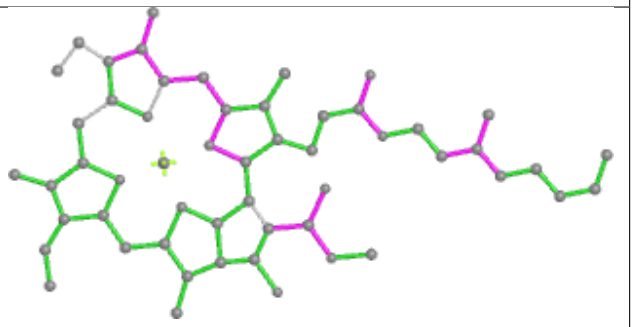
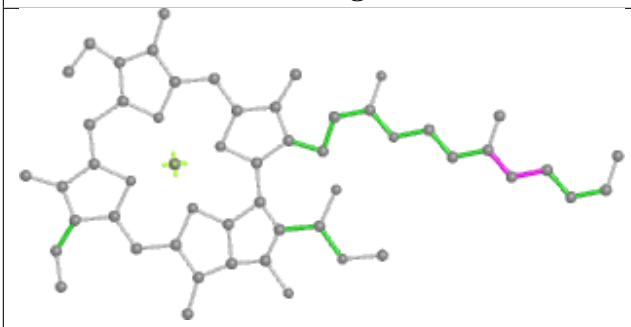
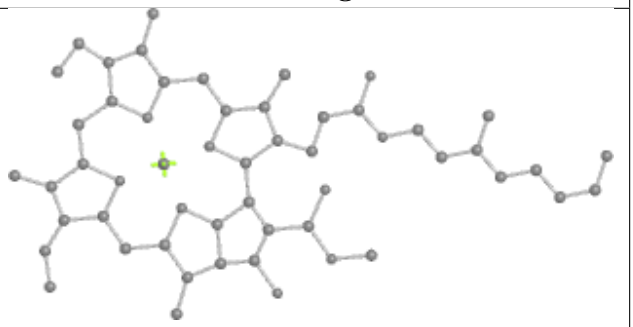


Bond angles

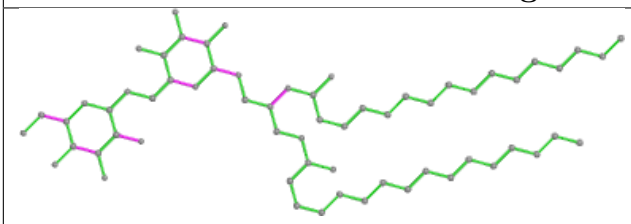


Torsions



Rings

## Ligand DGD C 517



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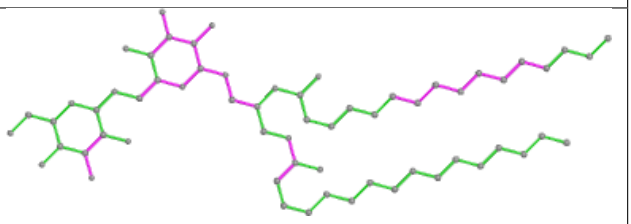
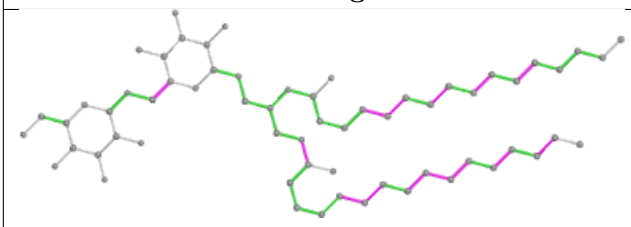
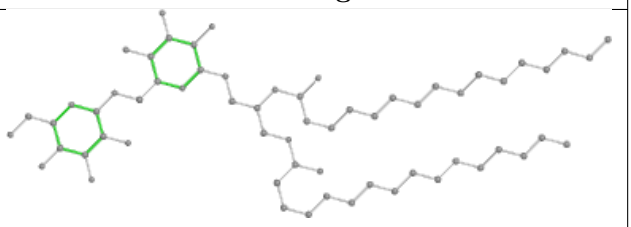


Bond angles

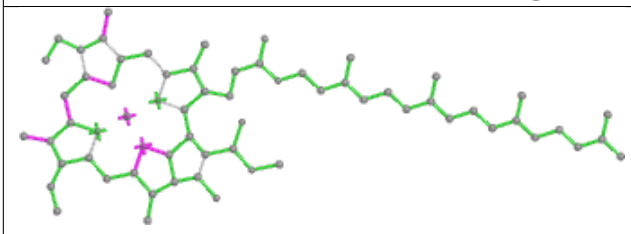


Torsions

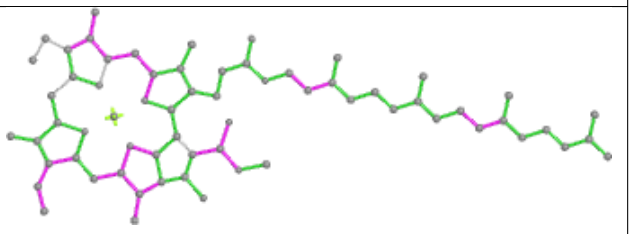


Rings

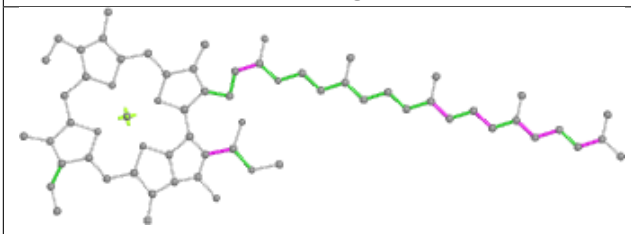
## Ligand CLA b 612



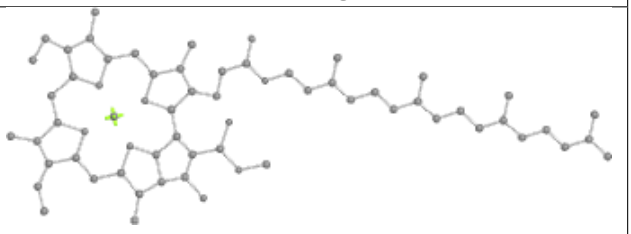
Bond lengths



Bond angles

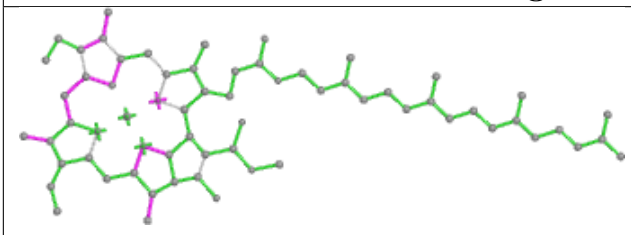


Torsions

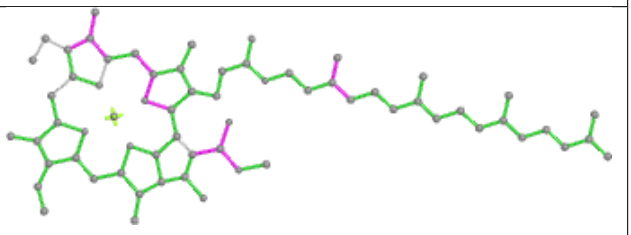


Rings

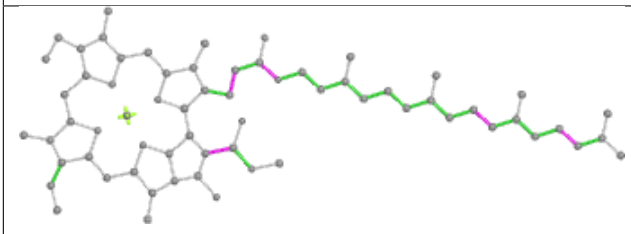
## Ligand CLA b 606



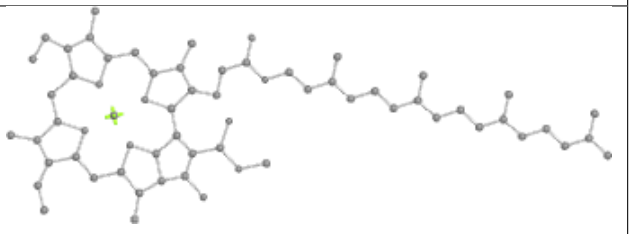
Bond lengths



Bond angles

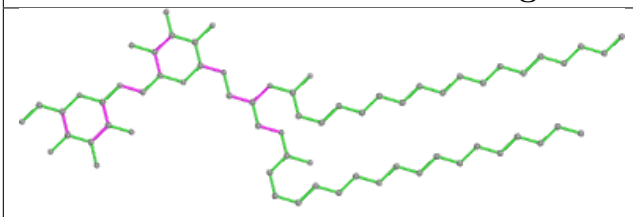


Torsions

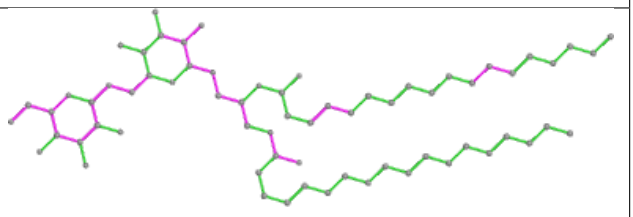


Rings

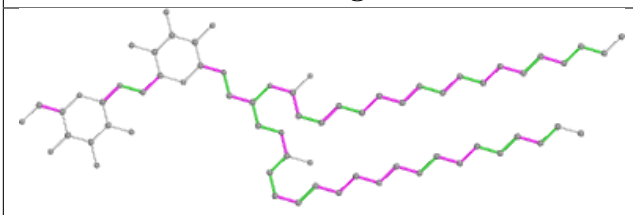
### Ligand DGD A 413



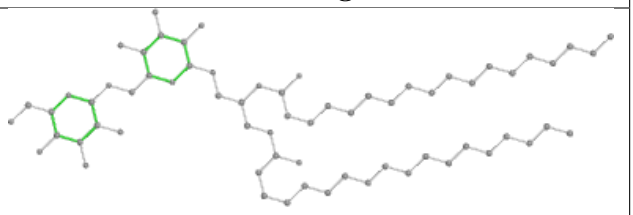
Bond lengths



Bond angles

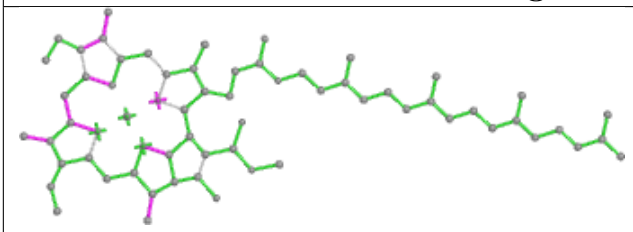


Torsions

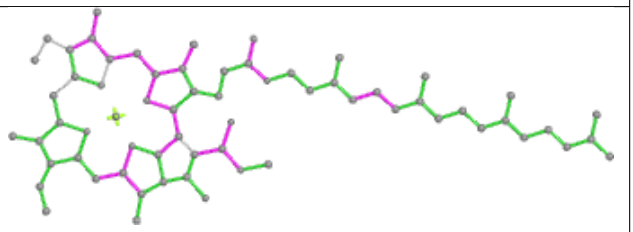


Rings

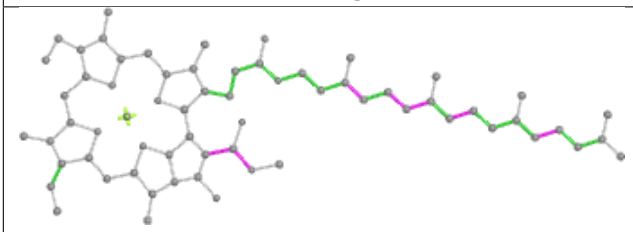
### Ligand CLA b 603



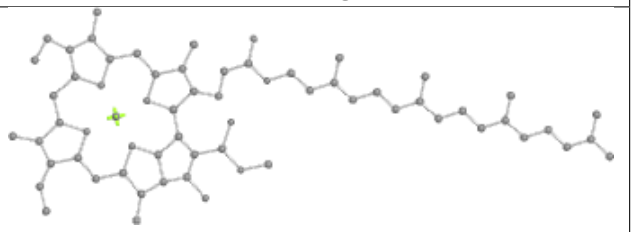
Bond lengths



Bond angles

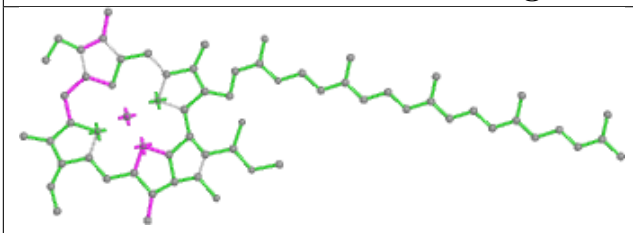


Torsions

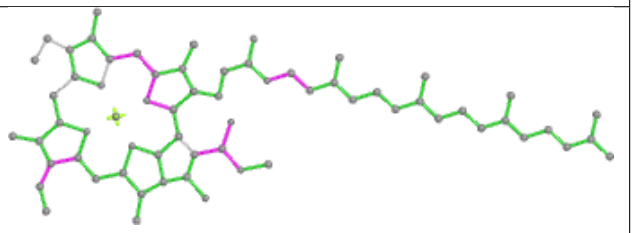


Rings

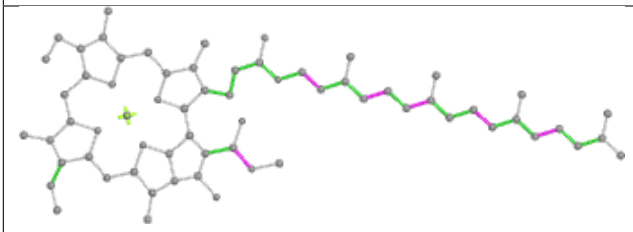
### Ligand CLA D 405



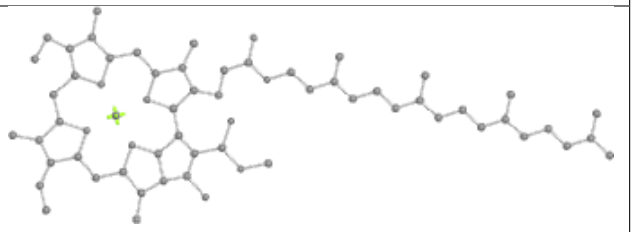
Bond lengths



Bond angles

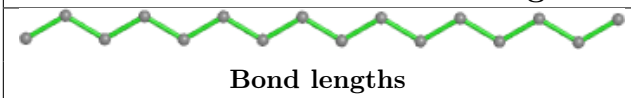


Torsions

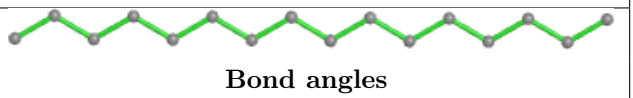


Rings

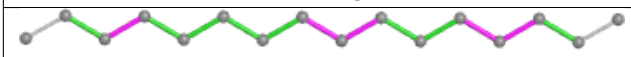
## Ligand STE C 519



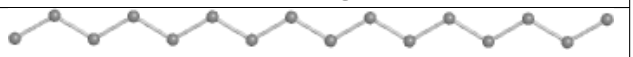
Bond lengths



Bond angles

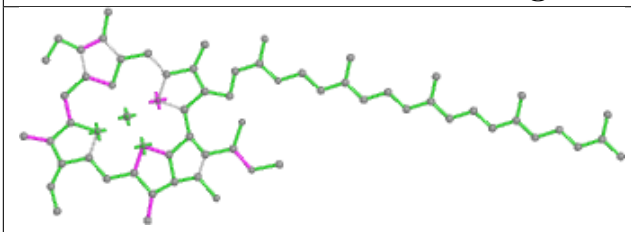


Torsions

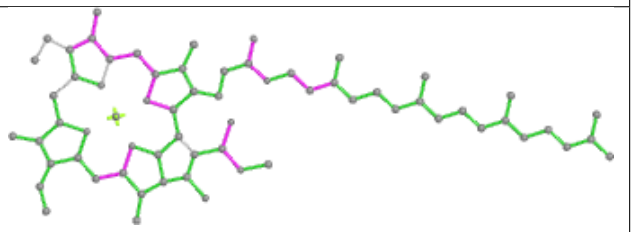


Rings

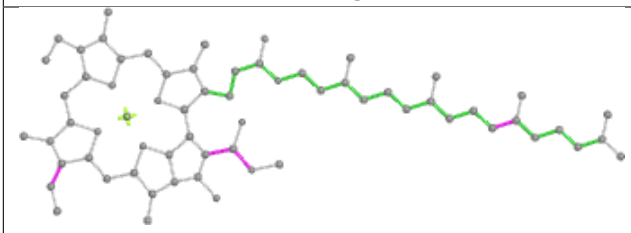
## Ligand CLA c 503



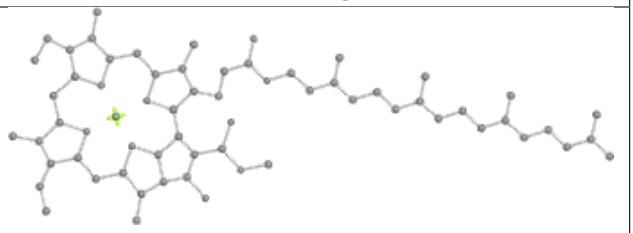
Bond lengths



Bond angles

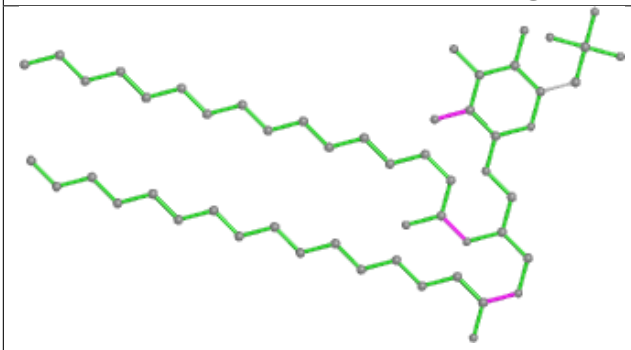


Torsions

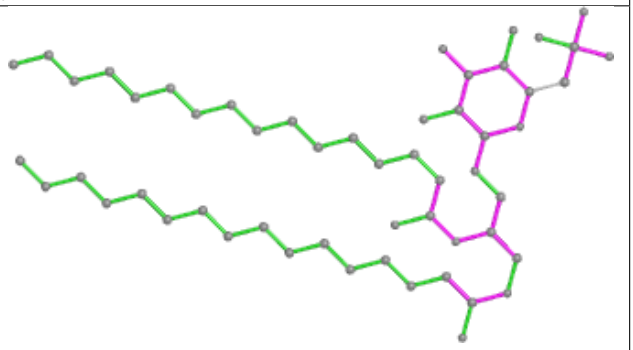


Rings

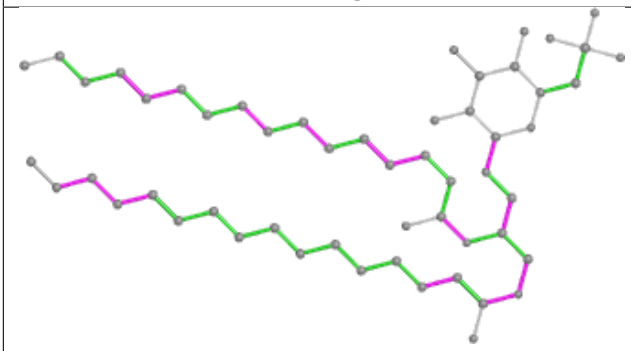
## Ligand SQD B 622



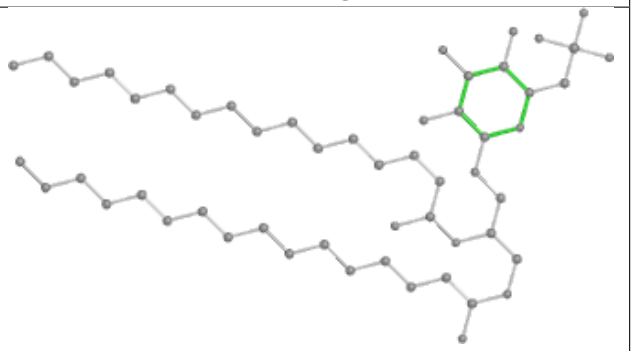
Bond lengths



Bond angles

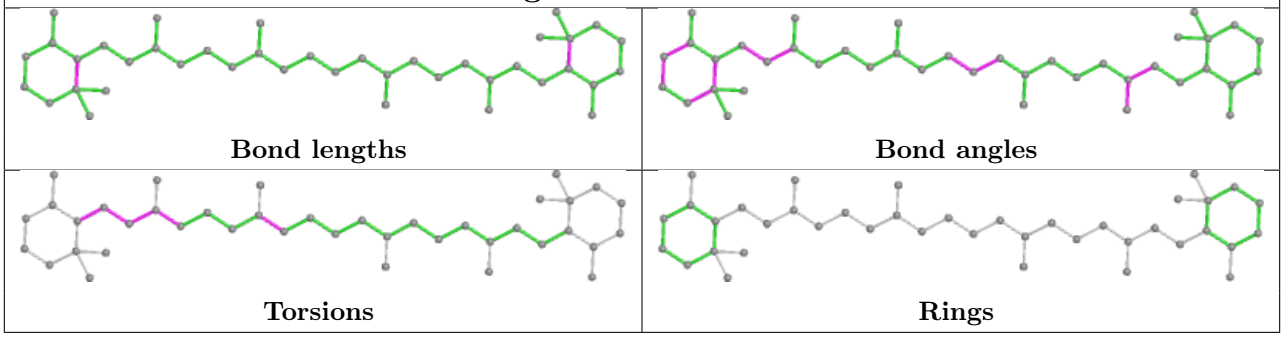


Torsions

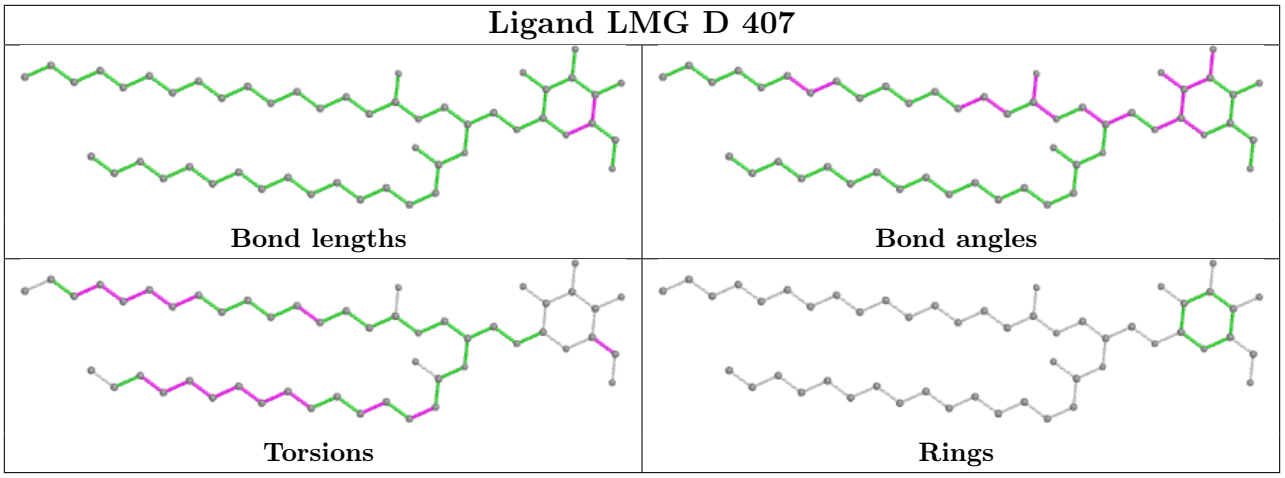


Rings

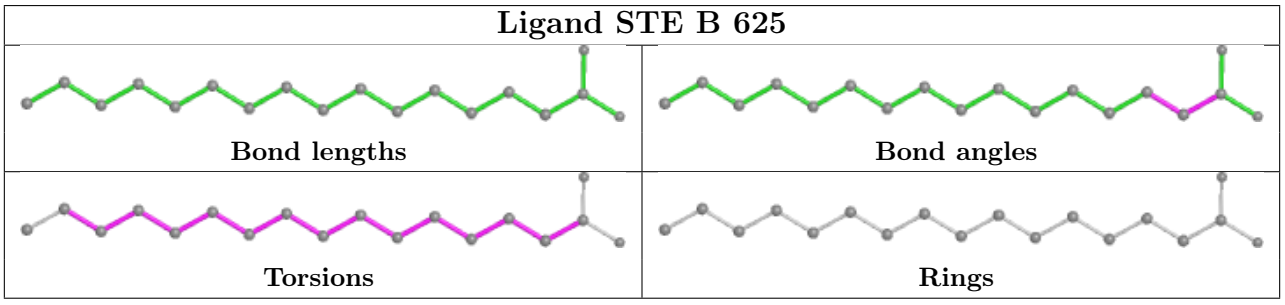
### Ligand BCR B 617



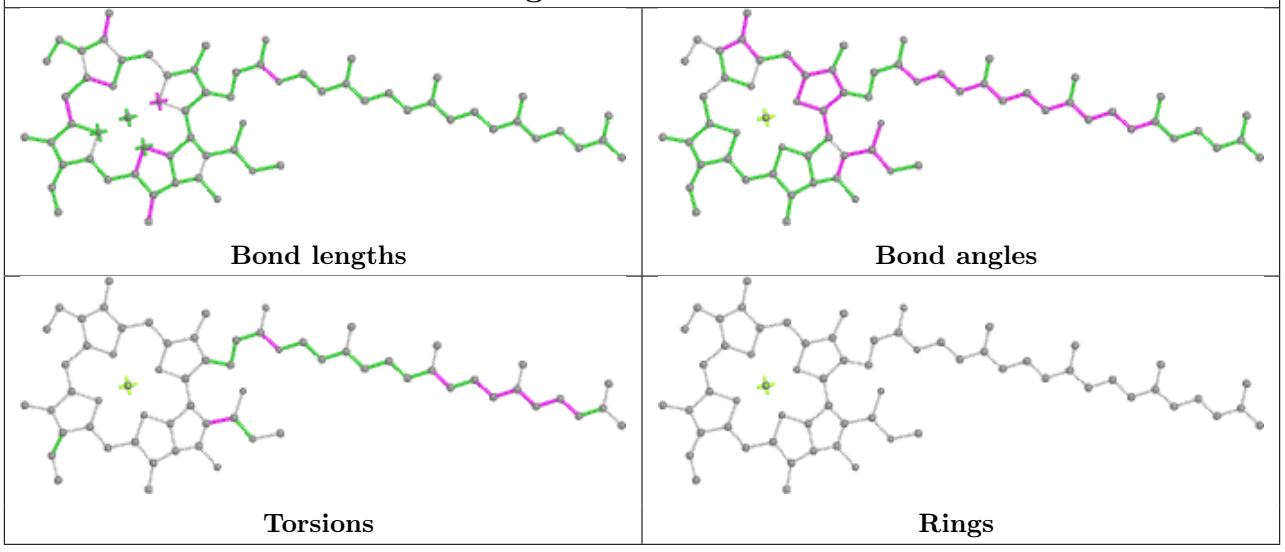

### Ligand LMG D 407



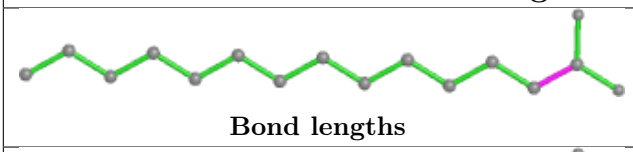

### Ligand STE B 625

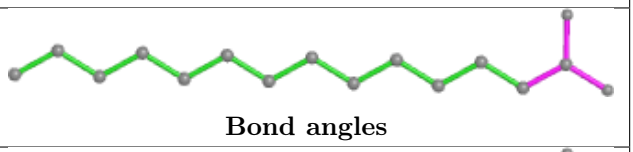


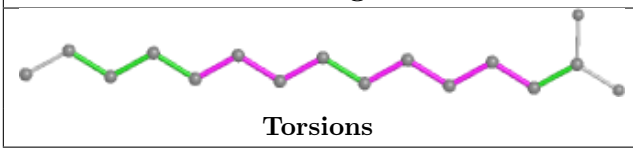

### Ligand CLA B 604

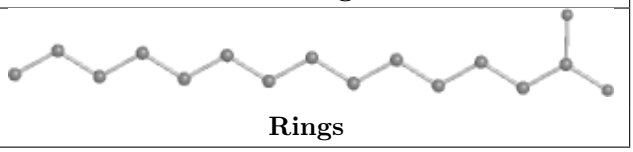


### Ligand STE d 411

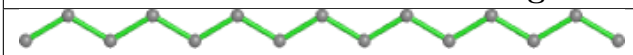

Bond lengths

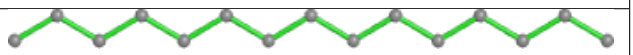

Bond angles

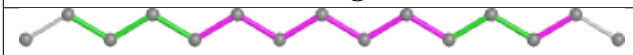

Torsions

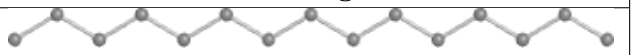

Rings

### Ligand STE T 102

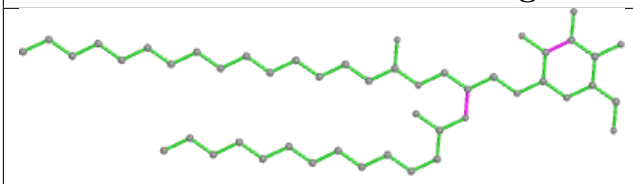

Bond lengths

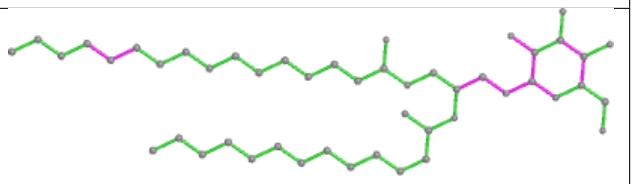

Bond angles

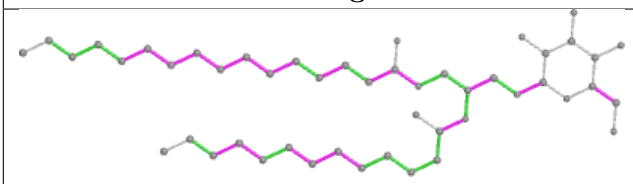

Torsions

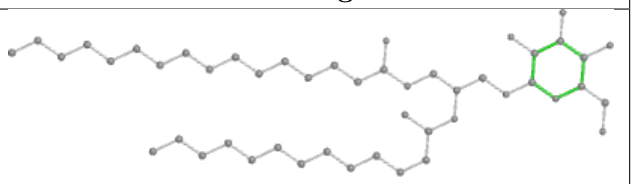

Rings

### Ligand LMG Y 101

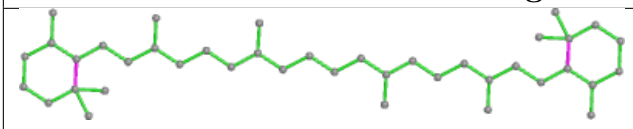

Bond lengths


Bond angles


Torsions


Rings

### Ligand BCR d 405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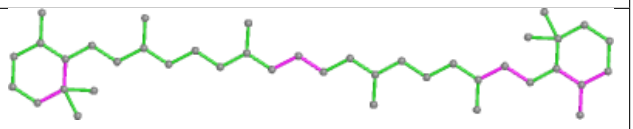
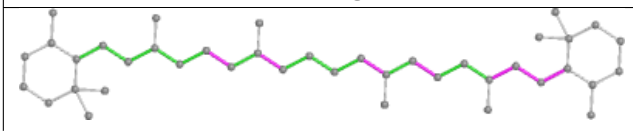
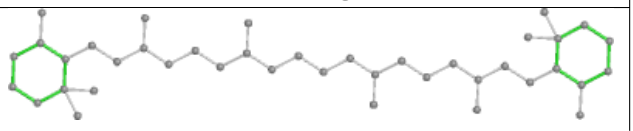
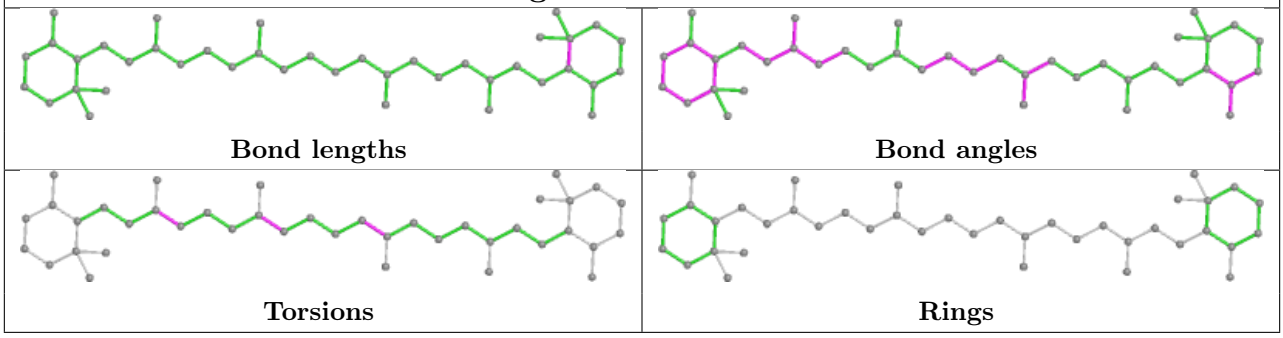

Bond angles

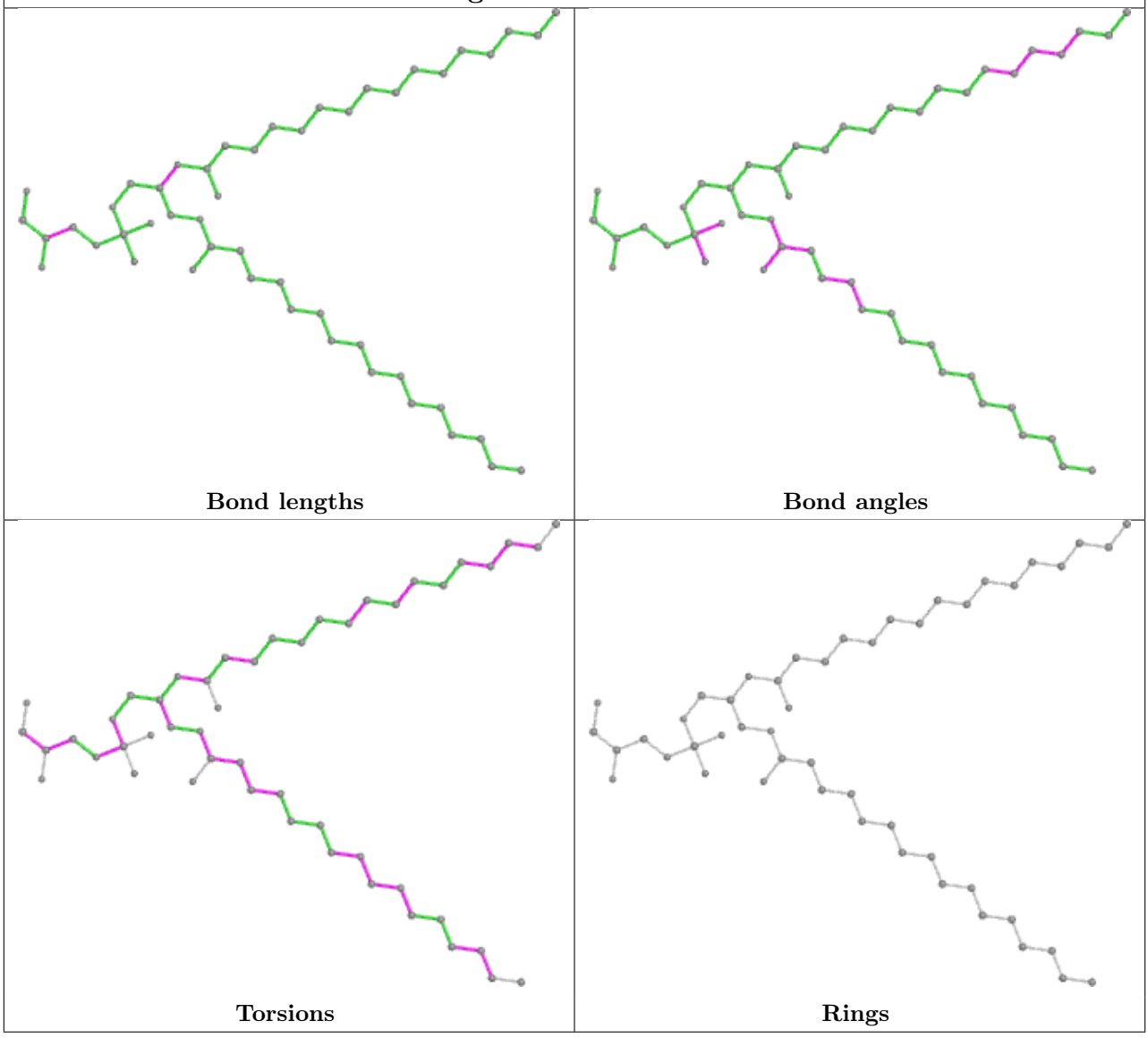

Torsions


Rings

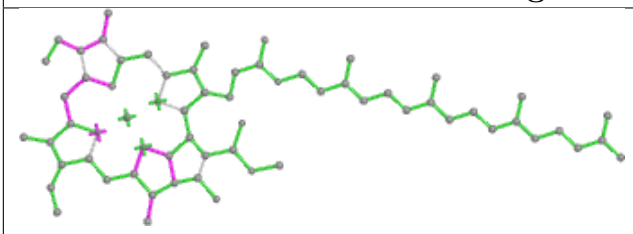
**Ligand BCR t 101**



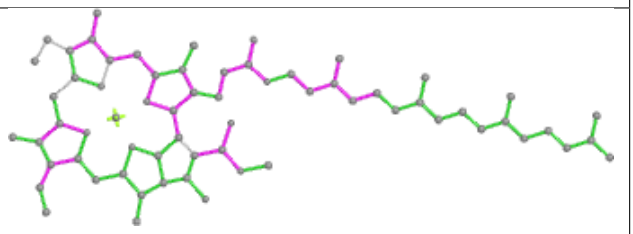

**Ligand LHG D 409**



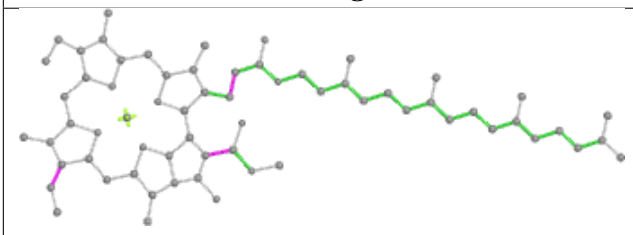
### Ligand CLA b 610



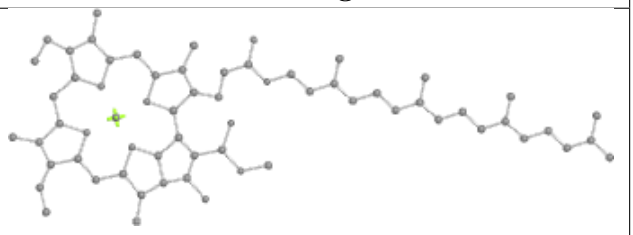
Bond lengths



Bond angles

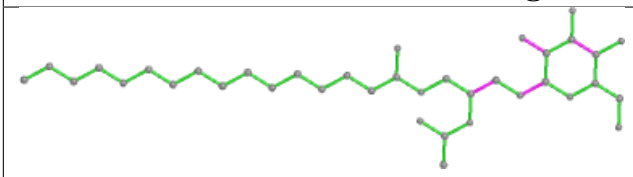


Torsions

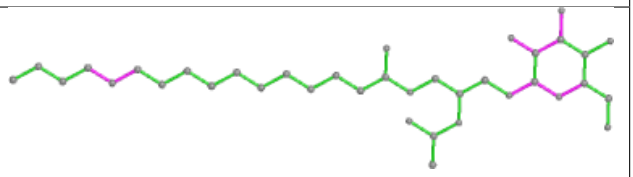


Rings

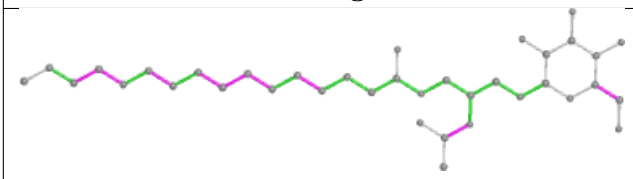
### Ligand LMG c 520



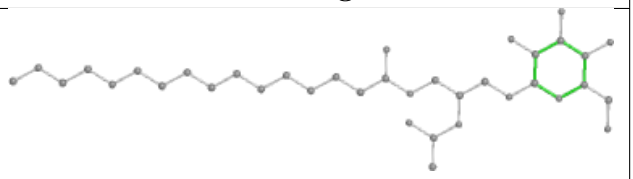
Bond lengths



Bond angles

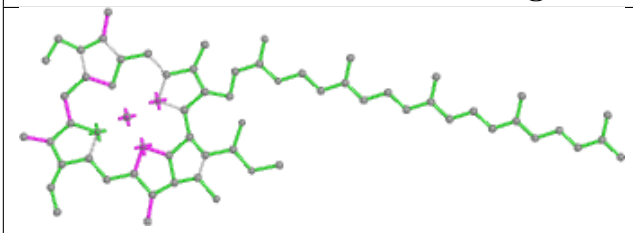


Torsions

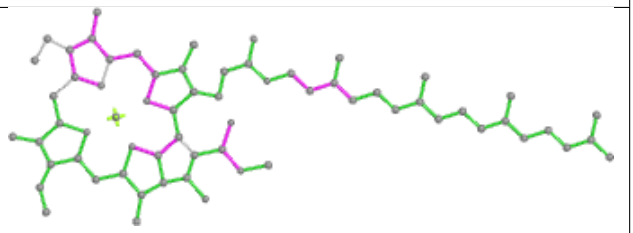


Rings

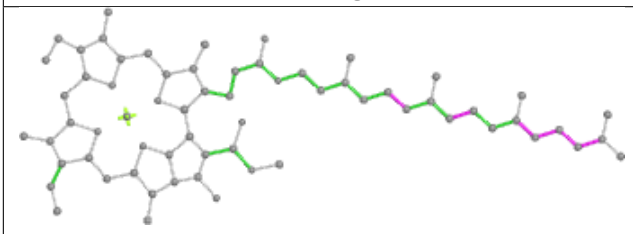
### Ligand CLA b 615



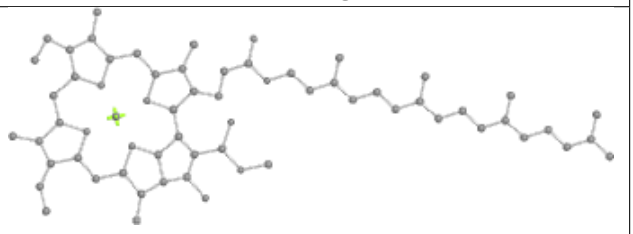
Bond lengths



Bond angles

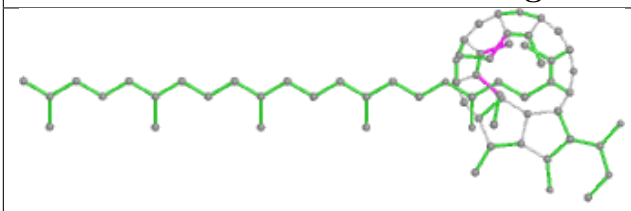


Torsions

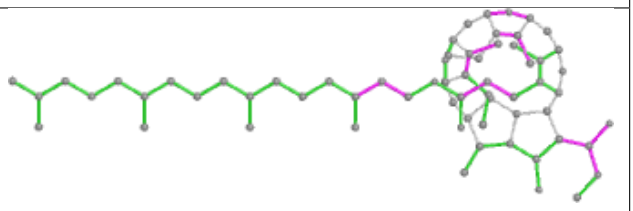


Rings

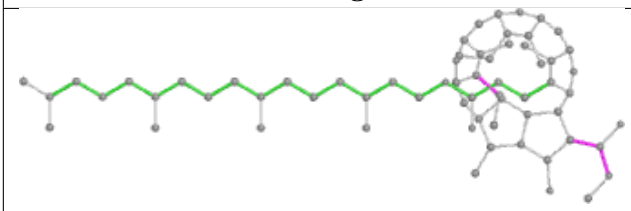
## Ligand PHO d 401



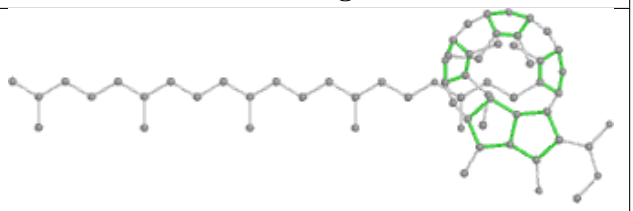
Bond lengths



Bond angles

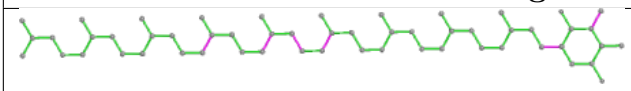


Torsions



Rings

## Ligand PL9 D 406



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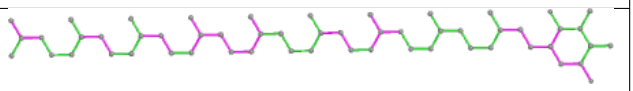
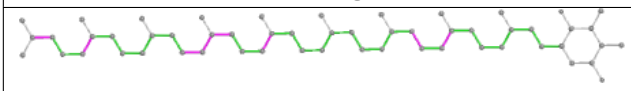
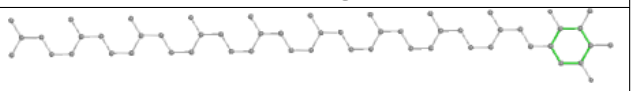


Bond angles

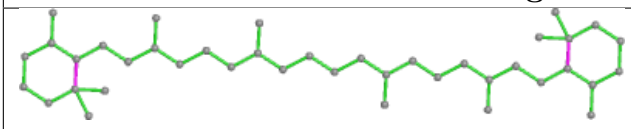


Torsions



Rings

## Ligand BCR k 101



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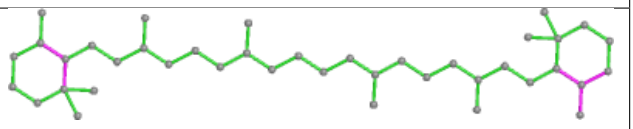
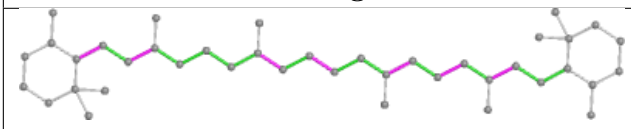


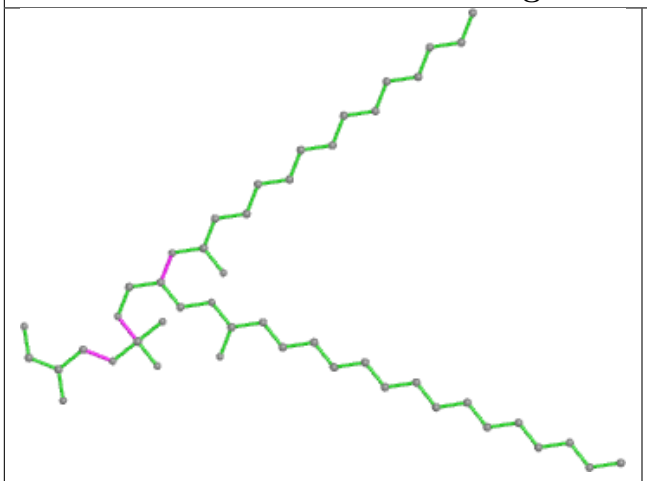
Bond angles



Torsions

Rings

## Ligand LHG D 410



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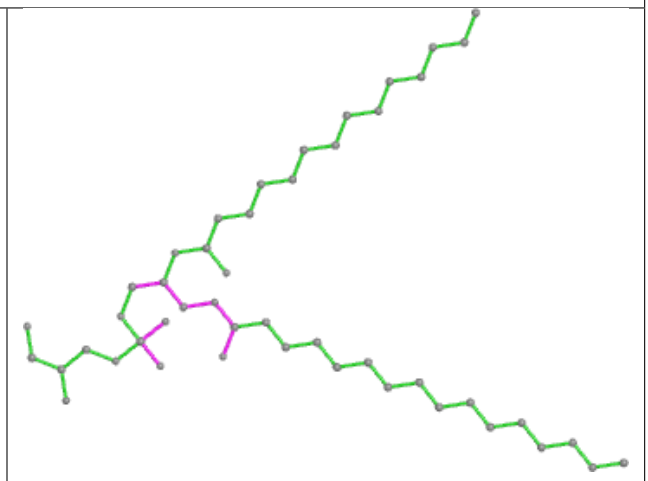
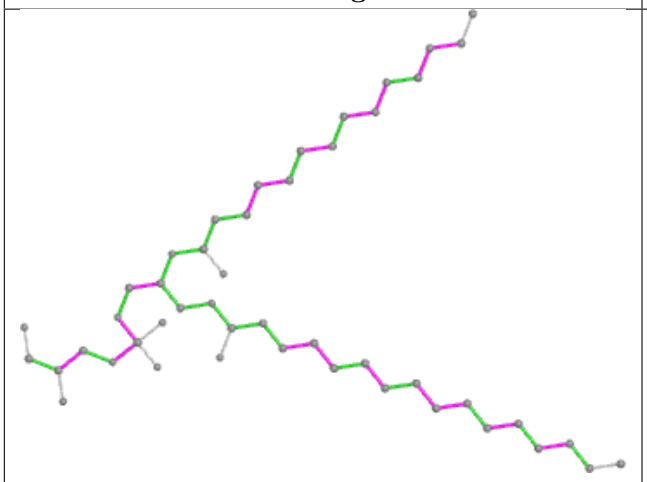
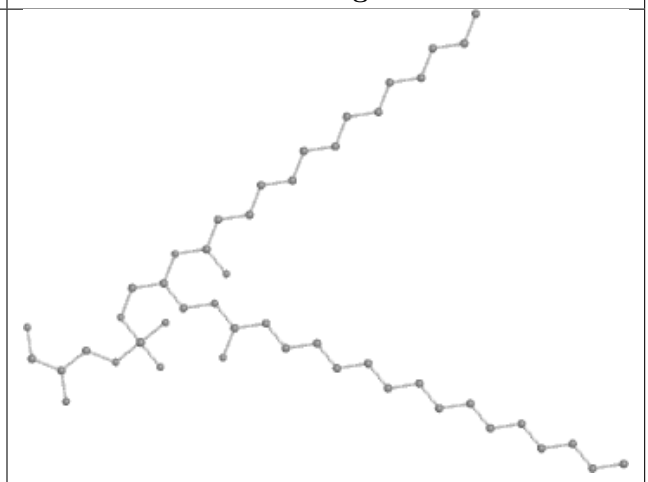


Bond angles

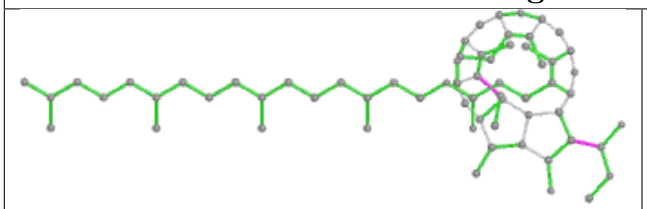


Torsions

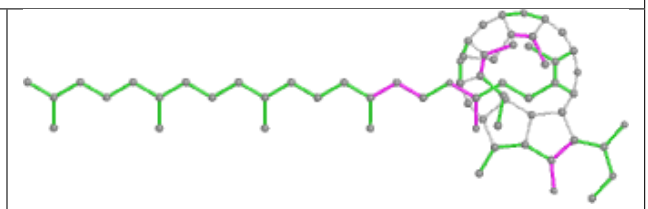


Rings

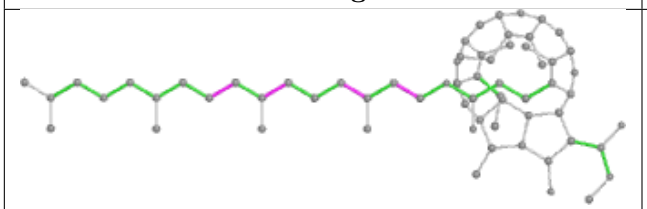
## Ligand PHO a 404



Bond lengths



Bond angles



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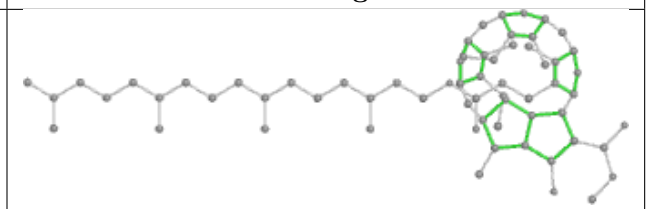
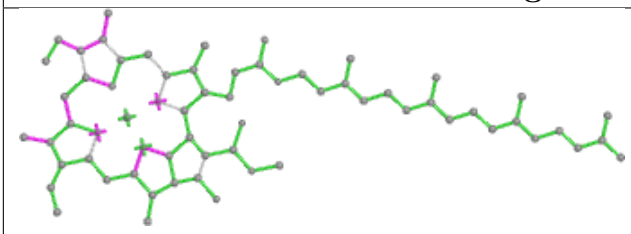


Rings

### Ligand CLA B 606



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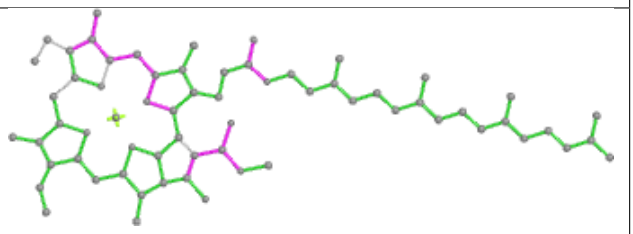
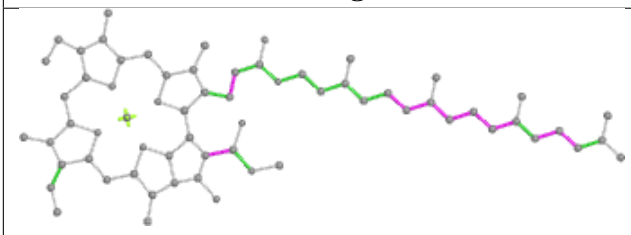
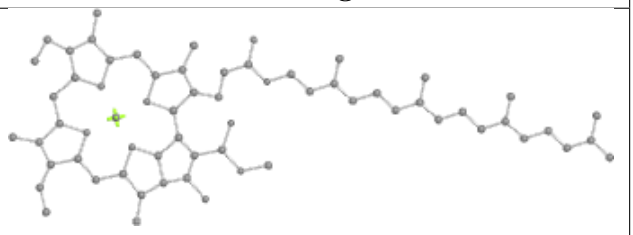


Bond angles

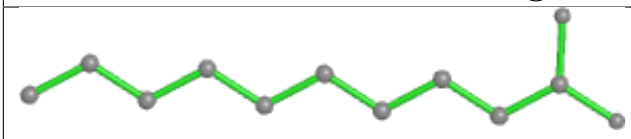


Torsions



Rings

### Ligand STE C 518



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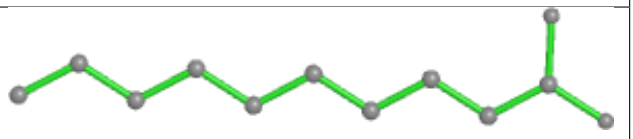
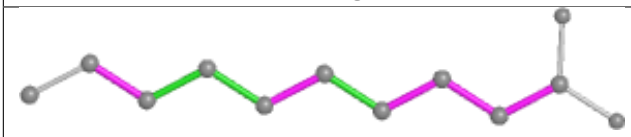
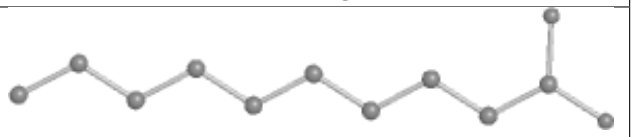


Bond angles

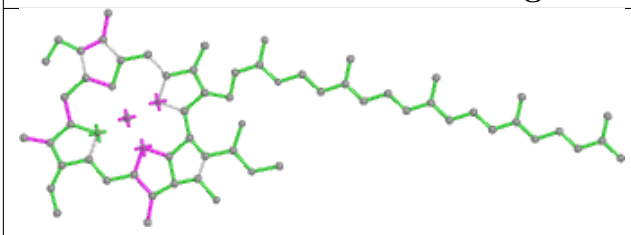


Torsions

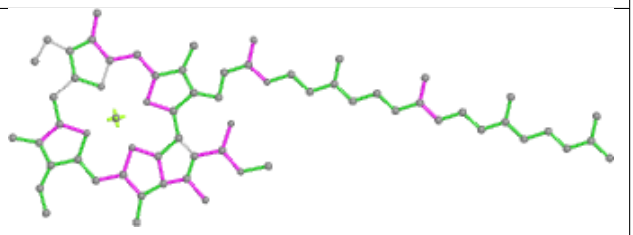


Rings

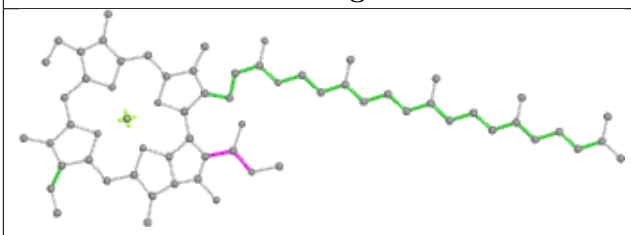
### Ligand CLA C 501



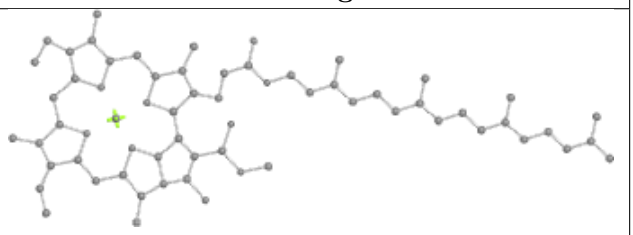
Bond lengths



Bond angles

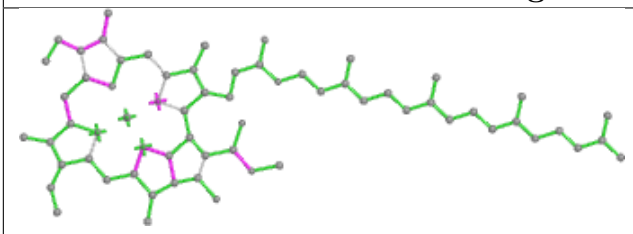


Torsions



Rings

## Ligand CLA b 609



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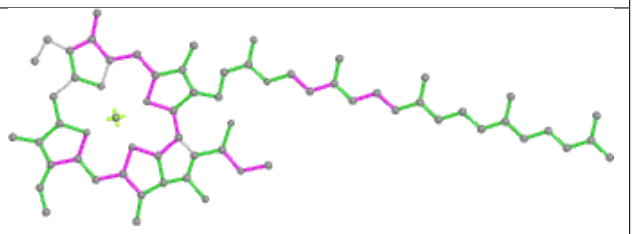
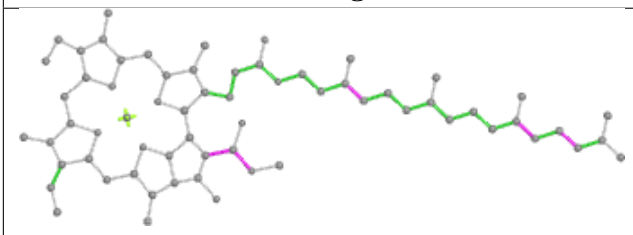
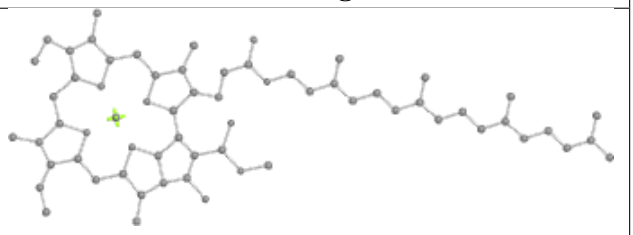


Bond angles

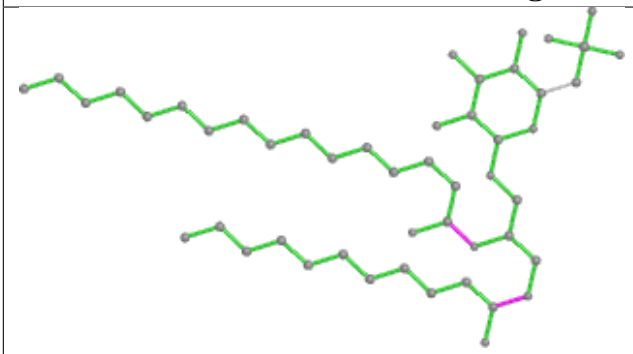


Torsions



Rings

## Ligand SQD L 101



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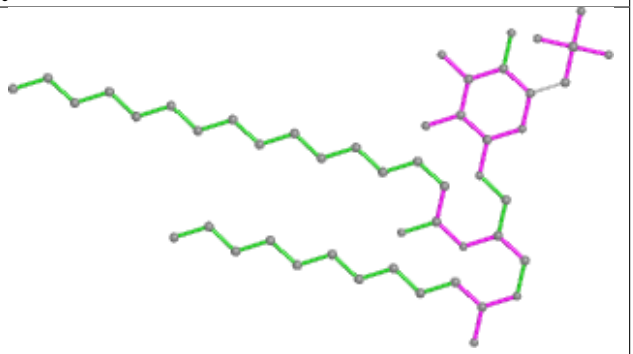
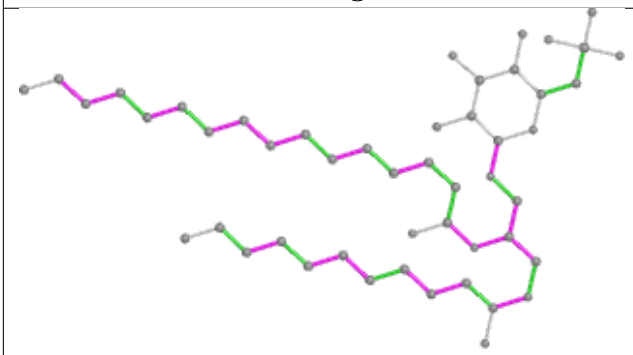
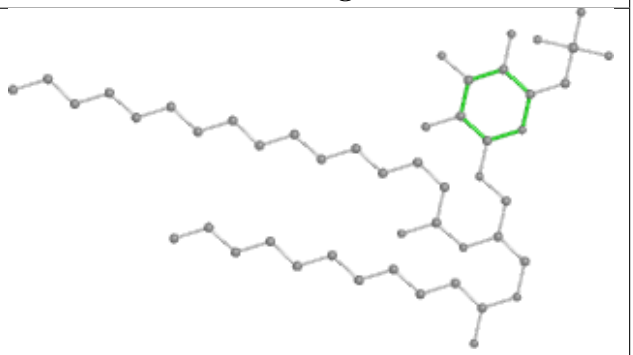


Bond angles

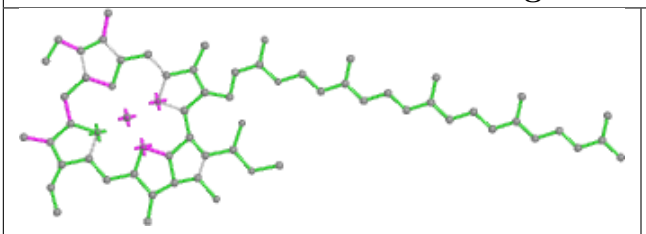


Torsions



Rings

## Ligand CLA C 505



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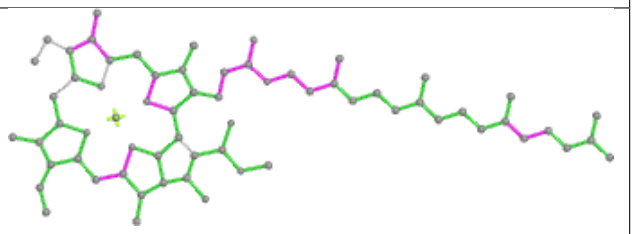
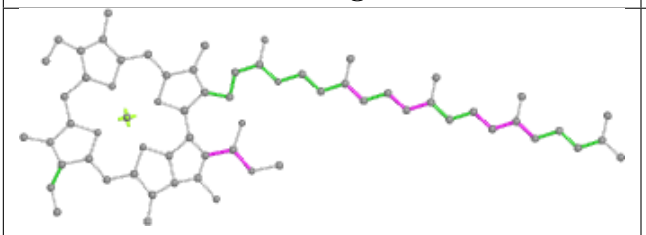
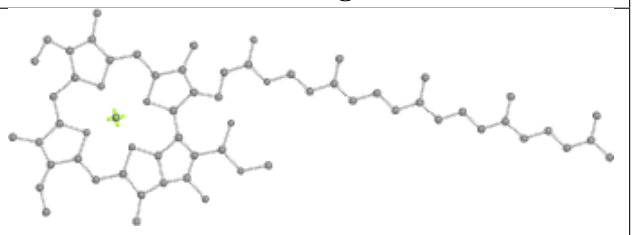


Bond angles

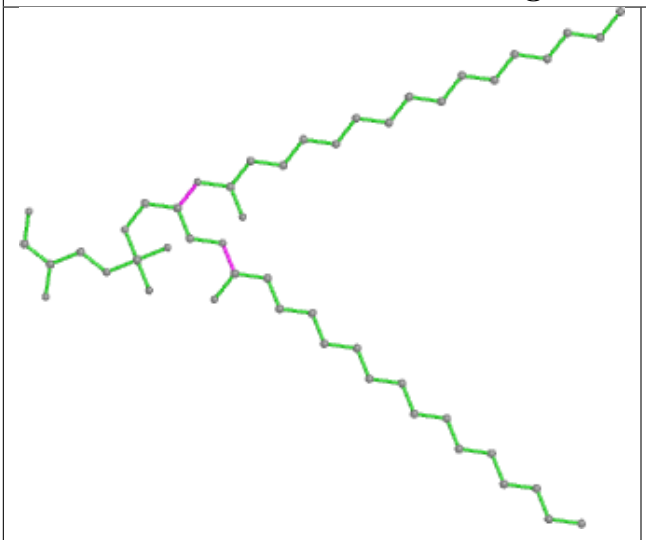


Torsions

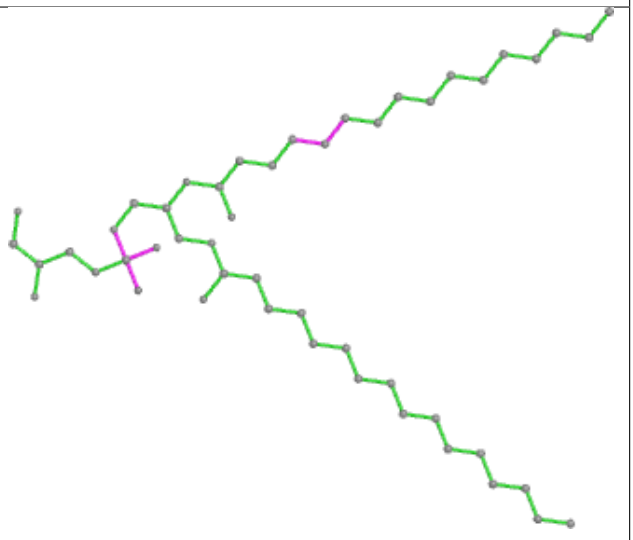


Rings

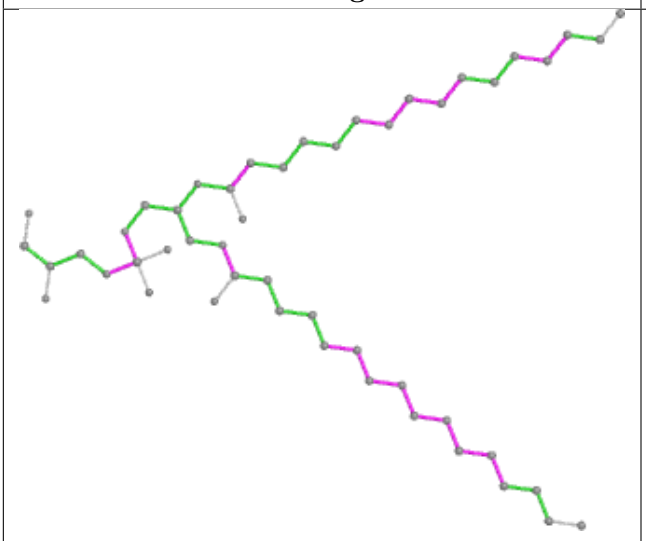
## Ligand LHG L 102



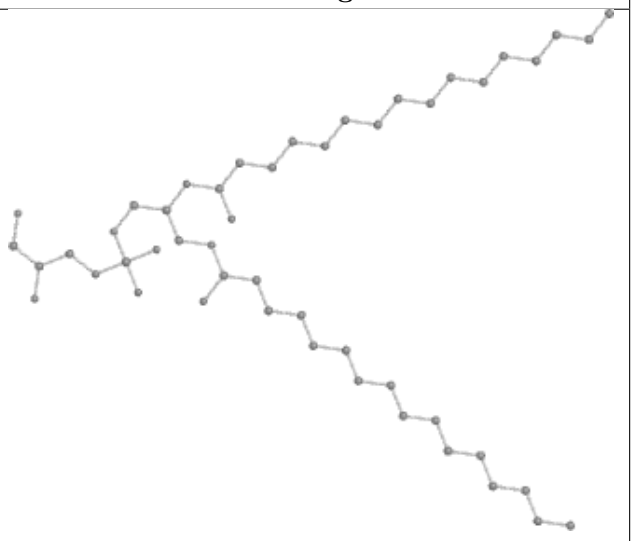
Bond lengths



Bond angles

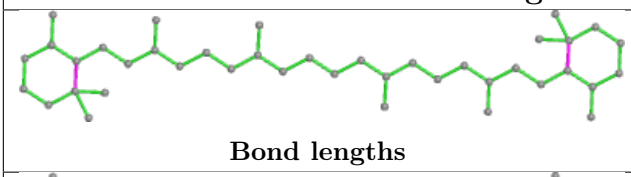


Torsions

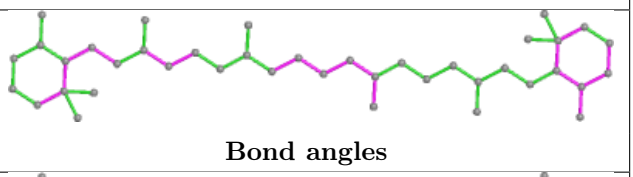


Rings

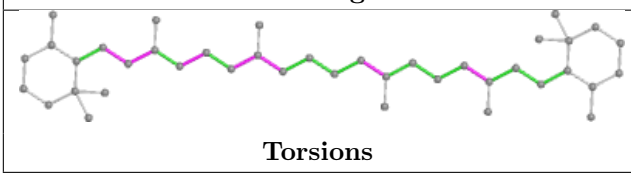
**Ligand BCR b 619**



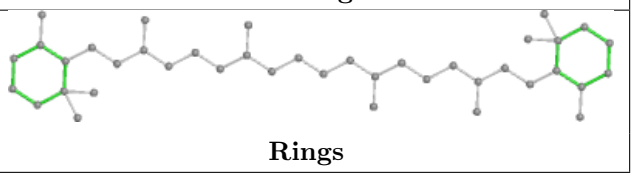
Bond lengths



Bond angles

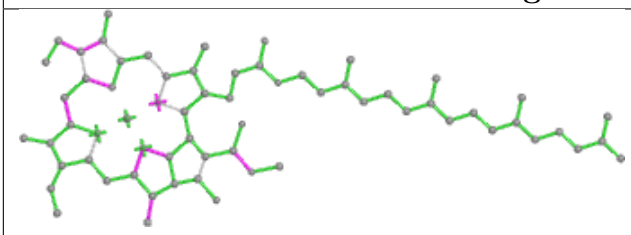


Torsions

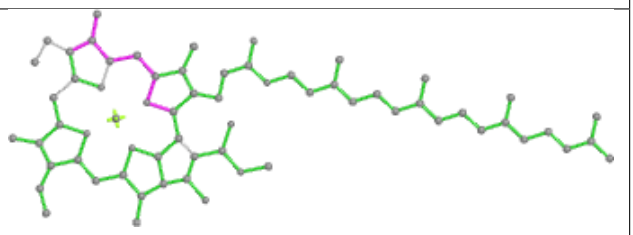


Rings

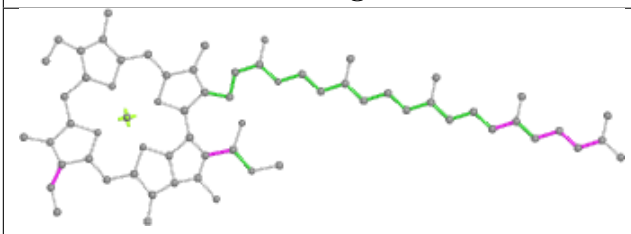
**Ligand CLA D 404**



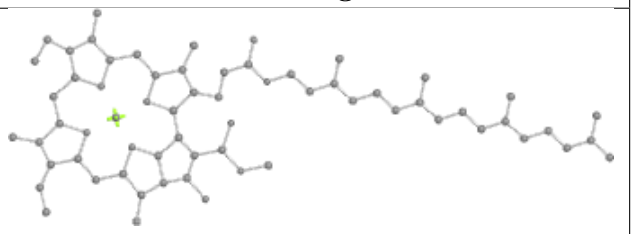
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 334/334 (100%) | -0.35 | 2 (0%) 89 91 | 21, 28, 49, 74 | 0 |
| 1 | a | 334/334 (100%) | -0.36 | 1 (0%) 94 94 | 22, 30, 56, 74 | 0 |
| 2 | B | 505/506 (99%) | -0.30 | 7 (1%) 75 78 | 22, 32, 61, 88 | 0 |
| 2 | b | 505/506 (99%) | -0.14 | 16 (3%) 47 53 | 20, 35, 69, 101 | 0 |
| 3 | C | 442/461 (95%) | -0.24 | 4 (0%) 84 86 | 23, 35, 51, 73 | 0 |
| 3 | c | 451/461 (97%) | -0.16 | 7 (1%) 72 75 | 25, 38, 59, 88 | 0 |
| 4 | D | 341/352 (96%) | -0.30 | 1 (0%) 94 94 | 20, 29, 48, 78 | 0 |
| 4 | d | 341/352 (96%) | -0.23 | 1 (0%) 94 94 | 22, 33, 55, 76 | 0 |
| 5 | E | 82/84 (97%) | 0.05 | 4 (4%) 29 34 | 32, 50, 69, 76 | 0 |
| 5 | e | 82/84 (97%) | 0.21 | 4 (4%) 29 34 | 38, 56, 76, 83 | 0 |
| 6 | F | 34/45 (75%) | -0.26 | 1 (2%) 51 56 | 34, 41, 62, 87 | 0 |
| 6 | f | 34/45 (75%) | -0.22 | 1 (2%) 51 56 | 41, 47, 74, 86 | 0 |
| 7 | H | 65/66 (98%) | -0.07 | 1 (1%) 73 76 | 30, 39, 57, 67 | 0 |
| 7 | h | 63/66 (95%) | 0.22 | 3 (4%) 30 35 | 40, 48, 59, 71 | 0 |
| 8 | I | 35/38 (92%) | -0.09 | 3 (8%) 10 12 | 29, 37, 68, 80 | 0 |
| 8 | i | 35/38 (92%) | -0.24 | 2 (5%) 23 28 | 30, 39, 73, 77 | 0 |
| 9 | J | 36/40 (90%) | 0.13 | 4 (11%) 5 6 | 33, 48, 73, 87 | 0 |
| 9 | j | 36/40 (90%) | 0.21 | 4 (11%) 5 6 | 38, 50, 79, 91 | 0 |
| 10 | K | 37/46 (80%) | 0.25 | 1 (2%) 54 59 | 42, 50, 66, 73 | 0 |
| 10 | k | 37/46 (80%) | 0.08 | 1 (2%) 54 59 | 48, 54, 65, 75 | 0 |
| 11 | L | 37/37 (100%) | -0.44 | 0 100 100 | 23, 29, 59, 67 | 0 |
| 11 | l | 36/37 (97%) | -0.23 | 2 (5%) 24 28 | 24, 29, 69, 80 | 0 |
| 12 | M | 32/36 (88%) | -0.09 | 1 (3%) 49 54 | 26, 31, 56, 65 | 0 |
| 12 | m | 31/36 (86%) | -0.15 | 0 100 100 | 25, 32, 50, 64 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | O | 244/272 (89%) | -0.03 | 14 (5%) 23 28 | 24, 39, 76, 124 | 0 |
| 13 | o | 244/272 (89%) | -0.12 | 12 (4%) 29 34 | 23, 38, 72, 104 | 0 |
| 14 | R | 34/40 (85%) | 2.46 | 19 (55%) 0 0 | 63, 73, 90, 102 | 0 |
| 14 | r | 31/40 (77%) | 4.42 | 28 (90%) 0 0 | 70, 93, 109, 116 | 0 |
| 15 | T | 29/30 (96%) | -0.47 | 2 (6%) 16 20 | 24, 29, 58, 75 | 0 |
| 15 | t | 29/30 (96%) | -0.21 | 2 (6%) 16 20 | 25, 31, 72, 88 | 0 |
| 16 | U | 97/134 (72%) | -0.26 | 1 (1%) 82 84 | 30, 42, 64, 84 | 0 |
| 16 | u | 97/134 (72%) | -0.42 | 0 100 100 | 29, 38, 56, 78 | 0 |
| 17 | V | 137/163 (84%) | -0.45 | 0 100 100 | 29, 39, 55, 76 | 0 |
| 17 | v | 137/163 (84%) | -0.14 | 3 (2%) 62 66 | 30, 45, 65, 85 | 0 |
| 18 | X | 38/41 (92%) | -0.03 | 2 (5%) 26 31 | 38, 49, 71, 78 | 0 |
| 18 | x | 39/41 (95%) | 0.54 | 5 (12%) 3 4 | 46, 57, 87, 100 | 0 |
| 19 | Y | 27/46 (58%) | 1.31 | 8 (29%) 0 0 | 50, 69, 85, 92 | 0 |
| 19 | y | 30/46 (65%) | 0.57 | 5 (16%) 1 1 | 58, 69, 81, 88 | 0 |
| 20 | Z | 62/62 (100%) | 1.06 | 18 (29%) 0 0 | 53, 66, 109, 121 | 0 |
| 20 | z | 62/62 (100%) | 0.95 | 12 (19%) 1 1 | 56, 67, 101, 116 | 0 |
| All | All | 5302/5666 (93%) | -0.11 | 202 (3%) 40 45 | 20, 36, 71, 124 | 0 |

All (202) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | r | 14 | LEU | 9.0 |
| 2 | b | 495 | PHE | 7.7 |
| 13 | o | 58 | ASN | 7.4 |
| 14 | r | 9 | LEU | 7.2 |
| 20 | z | 33 | TRP | 7.0 |
| 14 | r | 10 | LEU | 6.9 |
| 13 | O | 60 | ARG | 6.8 |
| 14 | r | 29 | LYS | 6.6 |
| 14 | r | 28 | VAL | 6.4 |
| 20 | Z | 33 | TRP | 5.9 |
| 14 | r | 6 | LEU | 5.9 |
| 15 | t | 30 | THR | 5.7 |
| 13 | O | 56 | PRO | 5.7 |
| 20 | z | 35 | ARG | 5.7 |
| 14 | r | 3 | TRP | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 13 | LEU | 5.6 |
| 13 | o | 4 | THR | 5.6 |
| 13 | O | 61 | GLN | 5.5 |
| 14 | r | 18 | TRP | 5.5 |
| 14 | r | 26 | TYR | 5.5 |
| 14 | R | 3 | TRP | 5.4 |
| 14 | r | 2 | ASP | 5.3 |
| 14 | R | 6 | LEU | 5.3 |
| 13 | O | 3 | GLN | 5.3 |
| 14 | r | 31 | VAL | 5.1 |
| 14 | r | 19 | ALA | 5.1 |
| 20 | Z | 7 | LEU | 5.1 |
| 14 | r | 13 | LEU | 5.1 |
| 20 | Z | 32 | ASP | 5.0 |
| 14 | R | 32 | GLN | 5.0 |
| 9 | J | 5 | GLY | 4.9 |
| 9 | j | 5 | GLY | 4.9 |
| 9 | j | 6 | GLY | 4.8 |
| 2 | b | 127 | ARG | 4.8 |
| 13 | O | 62 | GLU | 4.8 |
| 14 | r | 15 | ALA | 4.8 |
| 20 | Z | 62 | VAL | 4.7 |
| 14 | r | 25 | PRO | 4.6 |
| 20 | Z | 35 | ARG | 4.6 |
| 20 | Z | 34 | ASP | 4.6 |
| 13 | O | 59 | LYS | 4.5 |
| 13 | o | 3 | GLN | 4.5 |
| 14 | r | 7 | VAL | 4.4 |
| 14 | r | 11 | PRO | 4.4 |
| 13 | O | 4 | THR | 4.4 |
| 14 | r | 24 | LEU | 4.4 |
| 19 | Y | 41 | VAL | 4.4 |
| 3 | c | 147 | PHE | 4.3 |
| 2 | b | 487 | SER | 4.3 |
| 2 | B | 495 | PHE | 4.3 |
| 9 | j | 8 | ILE | 4.3 |
| 3 | c | 23 | ALA | 4.2 |
| 14 | r | 27 | ALA | 4.2 |
| 2 | b | 488 | PRO | 4.1 |
| 14 | R | 25 | PRO | 4.1 |
| 14 | R | 26 | TYR | 4.1 |
| 9 | j | 7 | ARG | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | r | 23 | ILE | 4.0 |
| 20 | Z | 42 | LEU | 3.9 |
| 14 | R | 21 | ARG | 3.9 |
| 19 | Y | 43 | ARG | 3.9 |
| 20 | Z | 61 | VAL | 3.9 |
| 7 | H | 66 | GLY | 3.9 |
| 3 | c | 146 | PHE | 3.9 |
| 5 | e | 79 | PHE | 3.9 |
| 13 | o | 61 | GLN | 3.8 |
| 18 | X | 2 | THR | 3.7 |
| 14 | r | 5 | VAL | 3.7 |
| 17 | v | 15 | GLU | 3.7 |
| 19 | Y | 42 | ARG | 3.6 |
| 20 | Z | 37 | LYS | 3.6 |
| 20 | Z | 3 | ILE | 3.5 |
| 14 | R | 2 | ASP | 3.5 |
| 5 | E | 79 | PHE | 3.5 |
| 2 | b | 505 | ARG | 3.5 |
| 8 | I | 36 | ASP | 3.5 |
| 19 | y | 37 | PHE | 3.5 |
| 13 | O | 63 | ALA | 3.5 |
| 13 | o | 59 | LYS | 3.5 |
| 10 | K | 17 | ILE | 3.5 |
| 20 | z | 1 | MET | 3.5 |
| 15 | T | 30 | THR | 3.4 |
| 9 | J | 7 | ARG | 3.4 |
| 14 | r | 16 | ALA | 3.4 |
| 19 | Y | 20 | ALA | 3.4 |
| 5 | E | 83 | LEU | 3.4 |
| 14 | R | 31 | VAL | 3.3 |
| 18 | x | 38 | GLN | 3.3 |
| 13 | o | 57 | LYS | 3.3 |
| 14 | r | 12 | VAL | 3.3 |
| 2 | b | 490 | GLN | 3.2 |
| 19 | Y | 37 | PHE | 3.2 |
| 7 | h | 6 | TRP | 3.2 |
| 14 | R | 24 | LEU | 3.1 |
| 9 | J | 8 | ILE | 3.1 |
| 6 | F | 12 | SER | 3.1 |
| 2 | B | 505 | ARG | 3.1 |
| 14 | r | 4 | ARG | 3.1 |
| 2 | B | 295 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 18 | x | 2 | THR | 3.1 |
| 13 | o | 5 | LEU | 3.1 |
| 20 | Z | 38 | GLN | 3.1 |
| 20 | z | 7 | LEU | 3.1 |
| 20 | Z | 59 | PHE | 3.1 |
| 14 | R | 10 | LEU | 3.0 |
| 14 | R | 18 | TRP | 3.0 |
| 14 | R | 13 | LEU | 3.0 |
| 14 | R | 29 | LYS | 3.0 |
| 2 | b | 502 | VAL | 3.0 |
| 8 | I | 34 | ARG | 3.0 |
| 2 | b | 85 | GLY | 3.0 |
| 19 | y | 19 | ILE | 3.0 |
| 16 | U | 8 | GLU | 3.0 |
| 2 | b | 491 | VAL | 2.9 |
| 20 | z | 3 | ILE | 2.9 |
| 2 | B | 293 | ALA | 2.9 |
| 18 | x | 40 | SER | 2.9 |
| 20 | z | 36 | SER | 2.9 |
| 20 | z | 37 | LYS | 2.9 |
| 20 | Z | 1 | MET | 2.9 |
| 19 | Y | 40 | ALA | 2.9 |
| 2 | b | 289 | GLN | 2.9 |
| 4 | D | 12 | ARG | 2.9 |
| 3 | C | 146 | PHE | 2.9 |
| 13 | o | 56 | PRO | 2.9 |
| 18 | x | 37 | VAL | 2.8 |
| 18 | x | 34 | ILE | 2.8 |
| 3 | c | 143 | TYR | 2.8 |
| 14 | R | 9 | LEU | 2.8 |
| 19 | y | 41 | VAL | 2.8 |
| 14 | R | 28 | VAL | 2.7 |
| 1 | A | 11 | ALA | 2.7 |
| 14 | R | 20 | VAL | 2.7 |
| 14 | r | 32 | GLN | 2.7 |
| 13 | o | 60 | ARG | 2.7 |
| 19 | Y | 25 | ILE | 2.7 |
| 13 | O | 57 | LYS | 2.7 |
| 2 | B | 127 | ARG | 2.7 |
| 18 | X | 3 | ILE | 2.7 |
| 19 | y | 18 | VAL | 2.6 |
| 2 | b | 295 | GLY | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 8 | i | 34 | ARG | 2.6 |
| 20 | Z | 60 | PHE | 2.6 |
| 2 | b | 161 | LEU | 2.6 |
| 5 | e | 61 | ARG | 2.6 |
| 13 | O | 35 | SER | 2.6 |
| 15 | t | 29 | ILE | 2.6 |
| 9 | J | 6 | GLY | 2.6 |
| 14 | r | 30 | GLN | 2.5 |
| 20 | z | 30 | PRO | 2.5 |
| 19 | y | 40 | ALA | 2.5 |
| 3 | c | 25 | ASN | 2.5 |
| 13 | O | 5 | LEU | 2.5 |
| 11 | l | 3 | PRO | 2.5 |
| 2 | b | 496 | TYR | 2.5 |
| 13 | o | 207 | ARG | 2.4 |
| 11 | l | 2 | GLU | 2.4 |
| 5 | E | 3 | GLY | 2.4 |
| 10 | k | 17 | ILE | 2.4 |
| 14 | r | 17 | GLY | 2.4 |
| 3 | C | 143 | TYR | 2.4 |
| 13 | o | 62 | GLU | 2.4 |
| 14 | R | 5 | VAL | 2.4 |
| 13 | O | 87 | VAL | 2.4 |
| 14 | R | 33 | LYS | 2.4 |
| 20 | Z | 4 | LEU | 2.3 |
| 20 | Z | 39 | LEU | 2.3 |
| 20 | z | 62 | VAL | 2.3 |
| 19 | Y | 21 | GLN | 2.3 |
| 17 | v | 17 | LYS | 2.3 |
| 20 | Z | 41 | PHE | 2.3 |
| 5 | E | 84 | LYS | 2.3 |
| 2 | b | 128 | THR | 2.3 |
| 2 | b | 486 | LEU | 2.2 |
| 3 | C | 61 | VAL | 2.2 |
| 3 | c | 262 | ARG | 2.2 |
| 20 | z | 32 | ASP | 2.2 |
| 8 | I | 35 | LYS | 2.2 |
| 17 | v | 22 | THR | 2.2 |
| 6 | f | 13 | TYR | 2.2 |
| 8 | i | 36 | ASP | 2.2 |
| 7 | h | 10 | ILE | 2.2 |
| 7 | h | 41 | PHE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | o | 63 | ALA | 2.2 |
| 20 | Z | 30 | PRO | 2.2 |
| 20 | z | 60 | PHE | 2.1 |
| 14 | r | 8 | VAL | 2.1 |
| 2 | b | 506 | ARG | 2.1 |
| 3 | C | 57 | ALA | 2.1 |
| 15 | T | 29 | ILE | 2.1 |
| 1 | a | 146 | ALA | 2.1 |
| 13 | O | 37 | THR | 2.1 |
| 14 | R | 34 | LEU | 2.0 |
| 20 | z | 34 | ASP | 2.0 |
| 13 | O | 246 | ALA | 2.0 |
| 4 | d | 239 | GLN | 2.0 |
| 12 | M | 33 | GLN | 2.0 |
| 2 | B | 486 | LEU | 2.0 |
| 3 | c | 261 | ARG | 2.0 |
| 2 | B | 487 | SER | 2.0 |
| 5 | e | 83 | LEU | 2.0 |
| 5 | e | 82 | GLN | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ 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 | 0.95 | 0.12 | 40,48,64,66 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.95 | 0.12 | 40,53,69,79 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.95 | 0.10 | 33,47,65,76 | 0 |
| 15 | FME | T | 1 | 10/11 | 0.95 | 0.09 | 29,44,67,67 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.96 | 0.18 | 40,50,65,66 | 0 |
| 15 | FME | t | 1 | 10/11 | 0.96 | 0.09 | 28,43,73,73 | 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, $95^{th}$ 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 |
|---|---|---|---|---|---|---|---|---|
| 31 | STE | E | 102 | 12/20 | 0.68 | 0.42 | 46,78,92,94 | 0 |
| 31 | STE | a | 414 | 12/20 | 0.71 | 0.26 | 40,65,71,75 | 0 |
| 31 | STE | b | 624 | 20/20 | 0.75 | 0.21 | 41,60,75,89 | 0 |
| 31 | STE | B | 627 | 15/20 | 0.76 | 0.16 | 36,61,74,77 | 0 |
| 31 | STE | B | 626 | 16/20 | 0.76 | 0.29 | 35,58,78,79 | 0 |
| 31 | STE | H | 104 | 18/20 | 0.77 | 0.27 | 44,73,89,94 | 0 |
| 26 | PL9 | A | 409 | 55/55 | 0.78 | 0.31 | 47,68,94,97 | 0 |
| 31 | STE | j | 101 | 12/20 | 0.78 | 0.17 | 42,56,74,75 | 0 |
| 31 | STE | c | 501 | 12/20 | 0.79 | 0.19 | 54,68,87,89 | 0 |
| 26 | PL9 | a | 409 | 55/55 | 0.79 | 0.25 | 47,74,93,96 | 0 |
| 24 | BCR | H | 102 | 40/40 | 0.80 | 0.16 | 30,50,66,75 | 0 |
| 27 | LMG | c | 522 | 48/55 | 0.80 | 0.23 | 46,80,104,108 | 0 |
| 31 | STE | C | 519 | 16/20 | 0.80 | 0.17 | 42,58,73,77 | 0 |
| 31 | STE | b | 625 | 10/20 | 0.81 | 0.22 | 44,53,61,73 | 0 |
| 28 | SQD | a | 412 | 36/54 | 0.81 | 0.19 | 29,63,90,97 | 0 |
| 27 | LMG | D | 411 | 33/55 | 0.81 | 0.19 | 34,56,84,89 | 0 |
| 33 | LHG | E | 101 | 49/49 | 0.81 | 0.25 | 50,83,110,126 | 0 |
| 33 | LHG | e | 101 | 42/49 | 0.81 | 0.27 | 65,87,116,127 | 0 |
| 31 | STE | B | 620 | 17/20 | 0.82 | 0.16 | 32,50,63,71 | 0 |
| 27 | LMG | a | 415 | 55/55 | 0.82 | 0.17 | 34,58,80,92 | 0 |
| 31 | STE | I | 101 | 15/20 | 0.82 | 0.17 | 37,55,73,76 | 0 |
| 24 | BCR | h | 101 | 40/40 | 0.82 | 0.15 | 35,54,73,79 | 0 |
| 22 | CLA | b | 601 | 65/65 | 0.82 | 0.17 | 43,68,89,92 | 0 |
| 31 | STE | a | 413 | 10/20 | 0.83 | 0.20 | 38,61,67,68 | 0 |
| 31 | STE | m | 101 | 18/20 | 0.83 | 0.13 | 34,51,78,79 | 0 |
| 31 | STE | d | 413 | 20/20 | 0.84 | 0.21 | 42,57,76,84 | 0 |
| 31 | STE | B | 624 | 12/20 | 0.84 | 0.11 | 32,48,63,76 | 0 |
| 27 | LMG | b | 623 | 55/55 | 0.84 | 0.27 | 42,70,95,101 | 0 |
| 29 | DGD | A | 413 | 66/66 | 0.84 | 0.18 | 44,62,78,99 | 0 |
| 22 | CLA | C | 512 | 65/65 | 0.84 | 0.17 | 35,55,82,95 | 0 |
| 31 | STE | T | 102 | 15/20 | 0.85 | 0.20 | 44,59,83,85 | 0 |
| 24 | BCR | K | 102 | 40/40 | 0.85 | 0.13 | 33,53,68,74 | 0 |
| 31 | STE | b | 626 | 14/20 | 0.85 | 0.22 | 51,65,84,88 | 0 |
| 31 | STE | m | 102 | 12/20 | 0.85 | 0.19 | 46,61,76,76 | 0 |
| 22 | CLA | c | 514 | 65/65 | 0.85 | 0.20 | 39,67,109,116 | 0 |
| 31 | STE | c | 521 | 20/20 | 0.85 | 0.20 | 37,55,93,103 | 0 |
| 22 | CLA | H | 101 | 65/65 | 0.86 | 0.16 | 33,63,91,110 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 31 | STE | b | 627 | 20/20 | 0.86 | 0.16 | 38,64,84,90 | 0 |
| 22 | CLA | c | 513 | 65/65 | 0.86 | 0.16 | 38,56,91,106 | 0 |
| 28 | SQD | A | 412 | 39/54 | 0.86 | 0.19 | 42,61,90,93 | 0 |
| 31 | STE | B | 623 | 14/20 | 0.86 | 0.13 | 36,47,56,62 | 0 |
| 28 | SQD | B | 622 | 54/54 | 0.87 | 0.14 | 37,61,91,101 | 0 |
| 31 | STE | d | 411 | 16/20 | 0.87 | 0.16 | 45,62,78,83 | 0 |
| 28 | SQD | L | 101 | 49/54 | 0.87 | 0.14 | 38,60,89,107 | 0 |
| 24 | BCR | K | 101 | 40/40 | 0.87 | 0.16 | 40,58,75,82 | 0 |
| 31 | STE | b | 622 | 20/20 | 0.88 | 0.24 | 36,54,79,85 | 0 |
| 31 | STE | B | 625 | 18/20 | 0.88 | 0.11 | 40,58,76,83 | 0 |
| 31 | STE | M | 102 | 15/20 | 0.88 | 0.17 | 32,48,69,74 | 0 |
| 31 | STE | D | 413 | 20/20 | 0.88 | 0.15 | 34,54,71,79 | 0 |
| 31 | STE | Z | 101 | 8/20 | 0.88 | 0.14 | 50,61,70,70 | 0 |
| 22 | CLA | C | 513 | 65/65 | 0.88 | 0.18 | 38,64,97,109 | 0 |
| 24 | BCR | k | 102 | 40/40 | 0.88 | 0.18 | 40,55,67,68 | 0 |
| 31 | STE | d | 412 | 17/20 | 0.89 | 0.14 | 41,56,67,74 | 0 |
| 28 | SQD | f | 102 | 41/54 | 0.89 | 0.20 | 55,91,113,119 | 0 |
| 24 | BCR | k | 101 | 40/40 | 0.89 | 0.13 | 42,60,81,85 | 0 |
| 31 | STE | B | 601 | 12/20 | 0.89 | 0.49 | 51,67,78,86 | 0 |
| 27 | LMG | c | 523 | 49/55 | 0.89 | 0.14 | 30,56,82,98 | 0 |
| 31 | STE | J | 101 | 12/20 | 0.89 | 0.11 | 45,59,69,77 | 0 |
| 27 | LMG | Y | 101 | 48/55 | 0.89 | 0.14 | 34,68,86,99 | 0 |
| 31 | STE | b | 620 | 16/20 | 0.90 | 0.14 | 35,46,64,71 | 0 |
| 22 | CLA | d | 404 | 65/65 | 0.90 | 0.17 | 32,49,89,106 | 0 |
| 31 | STE | C | 520 | 12/20 | 0.90 | 0.10 | 34,46,57,58 | 0 |
| 31 | STE | M | 103 | 10/20 | 0.90 | 0.13 | 34,47,64,70 | 0 |
| 22 | CLA | C | 502 | 65/65 | 0.90 | 0.14 | 26,42,52,53 | 0 |
| 22 | CLA | c | 503 | 65/65 | 0.90 | 0.16 | 29,41,62,66 | 0 |
| 27 | LMG | A | 410 | 48/55 | 0.90 | 0.14 | 38,57,72,87 | 0 |
| 27 | LMG | c | 520 | 37/55 | 0.90 | 0.16 | 40,67,80,83 | 0 |
| 24 | BCR | d | 405 | 40/40 | 0.91 | 0.12 | 28,54,85,95 | 0 |
| 29 | DGD | C | 516 | 62/66 | 0.91 | 0.13 | 34,51,97,119 | 0 |
| 27 | LMG | b | 621 | 51/55 | 0.91 | 0.12 | 32,53,76,97 | 0 |
| 22 | CLA | D | 405 | 65/65 | 0.91 | 0.13 | 22,42,107,119 | 0 |
| 22 | CLA | b | 616 | 60/65 | 0.91 | 0.12 | 24,42,86,88 | 0 |
| 24 | BCR | C | 514 | 40/40 | 0.91 | 0.11 | 23,38,55,63 | 0 |
| 24 | BCR | F | 101 | 40/40 | 0.91 | 0.12 | 21,44,82,90 | 0 |
| 22 | CLA | C | 507 | 65/65 | 0.91 | 0.14 | 20,40,56,66 | 0 |
| 22 | CLA | c | 509 | 64/65 | 0.91 | 0.14 | 27,46,86,103 | 0 |
| 31 | STE | C | 518 | 12/20 | 0.91 | 0.10 | 41,55,62,66 | 0 |
| 22 | CLA | a | 405 | 65/65 | 0.91 | 0.14 | 18,35,82,91 | 0 |
| 27 | LMG | M | 101 | 51/55 | 0.91 | 0.12 | 31,48,72,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 24 | BCR | c | 515 | 40/40 | 0.91 | 0.15 | 41,62,76,77 | 0 |
| 24 | BCR | B | 619 | 40/40 | 0.92 | 0.09 | 25,42,61,72 | 0 |
| 28 | SQD | D | 408 | 36/54 | 0.92 | 0.17 | 46,75,89,100 | 0 |
| 22 | CLA | b | 615 | 65/65 | 0.92 | 0.13 | 24,39,59,63 | 0 |
| 22 | CLA | c | 512 | 65/65 | 0.92 | 0.12 | 39,52,65,74 | 0 |
| 22 | CLA | B | 616 | 60/65 | 0.92 | 0.15 | 25,39,94,110 | 0 |
| 22 | CLA | b | 602 | 65/65 | 0.92 | 0.15 | 26,44,65,72 | 0 |
| 22 | CLA | c | 506 | 65/65 | 0.92 | 0.16 | 24,40,64,70 | 0 |
| 24 | BCR | K | 103 | 40/40 | 0.92 | 0.17 | 36,54,67,69 | 0 |
| 24 | BCR | b | 619 | 40/40 | 0.92 | 0.11 | 31,47,63,67 | 0 |
| 27 | LMG | B | 621 | 28/55 | 0.92 | 0.14 | 35,51,65,73 | 0 |
| 27 | LMG | D | 407 | 51/55 | 0.92 | 0.16 | 27,56,86,93 | 0 |
| 22 | CLA | C | 505 | 65/65 | 0.93 | 0.16 | 19,39,71,77 | 0 |
| 24 | BCR | T | 101 | 40/40 | 0.93 | 0.10 | 23,39,52,52 | 0 |
| 22 | CLA | C | 506 | 65/65 | 0.93 | 0.12 | 28,45,83,99 | 0 |
| 28 | SQD | a | 411 | 54/54 | 0.93 | 0.15 | 39,62,94,96 | 0 |
| 22 | CLA | c | 504 | 65/65 | 0.93 | 0.14 | 28,41,54,58 | 0 |
| 24 | BCR | c | 516 | 40/40 | 0.93 | 0.11 | 22,44,60,72 | 0 |
| 24 | BCR | B | 618 | 40/40 | 0.93 | 0.10 | 23,39,50,52 | 0 |
| 22 | CLA | B | 615 | 65/65 | 0.93 | 0.12 | 21,38,60,69 | 0 |
| 29 | DGD | H | 103 | 62/66 | 0.93 | 0.11 | 29,46,61,73 | 0 |
| 29 | DGD | c | 518 | 62/66 | 0.93 | 0.11 | 33,50,90,96 | 0 |
| 29 | DGD | h | 102 | 62/66 | 0.93 | 0.11 | 29,48,65,68 | 0 |
| 22 | CLA | c | 507 | 65/65 | 0.93 | 0.13 | 29,48,102,109 | 0 |
| 22 | CLA | c | 508 | 65/65 | 0.93 | 0.14 | 28,44,59,63 | 0 |
| 22 | CLA | b | 609 | 65/65 | 0.93 | 0.13 | 27,43,64,74 | 0 |
| 22 | CLA | c | 511 | 65/65 | 0.93 | 0.15 | 29,47,64,68 | 0 |
| 22 | CLA | C | 510 | 65/65 | 0.93 | 0.14 | 27,46,62,66 | 0 |
| 22 | CLA | c | 510 | 65/65 | 0.94 | 0.17 | 33,47,70,77 | 0 |
| 22 | CLA | B | 602 | 65/65 | 0.94 | 0.15 | 20,36,55,66 | 0 |
| 22 | CLA | a | 403 | 65/65 | 0.94 | 0.14 | 25,40,97,106 | 0 |
| 22 | CLA | C | 503 | 65/65 | 0.94 | 0.13 | 32,42,51,61 | 0 |
| 22 | CLA | a | 410 | 65/65 | 0.94 | 0.12 | 17,29,48,54 | 0 |
| 22 | CLA | C | 504 | 59/65 | 0.94 | 0.12 | 27,41,81,83 | 0 |
| 24 | BCR | A | 406 | 40/40 | 0.94 | 0.09 | 23,35,43,47 | 0 |
| 22 | CLA | B | 604 | 65/65 | 0.94 | 0.12 | 19,32,79,84 | 0 |
| 22 | CLA | b | 606 | 65/65 | 0.94 | 0.11 | 22,37,73,77 | 0 |
| 22 | CLA | b | 608 | 65/65 | 0.94 | 0.15 | 25,42,60,69 | 0 |
| 22 | CLA | B | 606 | 65/65 | 0.94 | 0.10 | 23,36,69,86 | 0 |
| 22 | CLA | b | 610 | 65/65 | 0.94 | 0.18 | 23,36,50,56 | 0 |
| 22 | CLA | b | 612 | 65/65 | 0.94 | 0.17 | 15,33,48,57 | 0 |
| 27 | LMG | d | 410 | 44/55 | 0.94 | 0.13 | 31,51,89,104 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 22 | CLA | b | 613 | 65/65 | 0.94 | 0.14 | 17,34,73,87 | 0 |
| 22 | CLA | b | 614 | 65/65 | 0.94 | 0.12 | 21,38,78,86 | 0 |
| 22 | CLA | B | 609 | 65/65 | 0.94 | 0.13 | 24,39,57,69 | 0 |
| 24 | BCR | a | 406 | 40/40 | 0.94 | 0.09 | 19,32,50,55 | 0 |
| 24 | BCR | b | 617 | 40/40 | 0.94 | 0.11 | 25,41,54,59 | 0 |
| 24 | BCR | b | 618 | 40/40 | 0.94 | 0.10 | 22,38,51,52 | 0 |
| 22 | CLA | C | 508 | 65/65 | 0.94 | 0.11 | 25,42,97,107 | 0 |
| 22 | CLA | C | 509 | 65/65 | 0.94 | 0.17 | 25,46,62,69 | 0 |
| 29 | DGD | C | 515 | 62/66 | 0.94 | 0.12 | 21,40,73,87 | 0 |
| 22 | CLA | B | 613 | 65/65 | 0.94 | 0.14 | 17,31,71,73 | 0 |
| 29 | DGD | C | 517 | 62/66 | 0.94 | 0.11 | 26,46,77,87 | 0 |
| 22 | CLA | c | 505 | 60/65 | 0.94 | 0.11 | 32,45,76,89 | 0 |
| 22 | CLA | C | 511 | 65/65 | 0.94 | 0.11 | 27,49,66,77 | 0 |
| 29 | DGD | c | 519 | 62/66 | 0.94 | 0.13 | 28,54,83,91 | 0 |
| 22 | CLA | B | 614 | 65/65 | 0.94 | 0.15 | 20,36,75,87 | 0 |
| 22 | CLA | A | 403 | 65/65 | 0.94 | 0.14 | 21,34,97,110 | 0 |
| 24 | BCR | t | 101 | 40/40 | 0.94 | 0.09 | 23,38,51,52 | 0 |
| 22 | CLA | A | 405 | 54/65 | 0.94 | 0.11 | 18,31,66,72 | 0 |
| 26 | PL9 | D | 406 | 55/55 | 0.94 | 0.10 | 21,34,49,54 | 0 |
| 23 | PHO | A | 404 | 64/64 | 0.95 | 0.10 | 18,28,40,48 | 0 |
| 23 | PHO | a | 404 | 64/64 | 0.95 | 0.13 | 19,29,40,44 | 0 |
| 22 | CLA | b | 604 | 65/65 | 0.95 | 0.12 | 20,33,81,91 | 0 |
| 24 | BCR | B | 617 | 40/40 | 0.95 | 0.11 | 24,38,59,60 | 0 |
| 22 | CLA | b | 605 | 65/65 | 0.95 | 0.11 | 21,34,49,53 | 0 |
| 22 | CLA | D | 403 | 65/65 | 0.95 | 0.12 | 15,29,52,61 | 0 |
| 28 | SQD | A | 411 | 52/54 | 0.95 | 0.14 | 34,59,84,88 | 0 |
| 22 | CLA | D | 404 | 65/65 | 0.95 | 0.10 | 19,28,52,62 | 0 |
| 22 | CLA | B | 610 | 65/65 | 0.95 | 0.15 | 18,33,46,50 | 0 |
| 22 | CLA | C | 501 | 65/65 | 0.95 | 0.12 | 19,36,51,56 | 0 |
| 22 | CLA | b | 611 | 65/65 | 0.95 | 0.13 | 19,34,53,61 | 0 |
| 26 | PL9 | d | 406 | 55/55 | 0.95 | 0.10 | 22,33,42,53 | 0 |
| 22 | CLA | B | 611 | 65/65 | 0.95 | 0.13 | 19,30,46,50 | 0 |
| 22 | CLA | B | 612 | 65/65 | 0.95 | 0.14 | 19,31,47,56 | 0 |
| 22 | CLA | B | 603 | 65/65 | 0.95 | 0.14 | 15,32,63,67 | 0 |
| 22 | CLA | B | 608 | 65/65 | 0.95 | 0.12 | 20,34,56,61 | 0 |
| 22 | CLA | B | 605 | 65/65 | 0.95 | 0.14 | 19,31,47,52 | 0 |
| 22 | CLA | d | 403 | 65/65 | 0.95 | 0.11 | 19,34,54,65 | 0 |
| 33 | LHG | D | 410 | 47/49 | 0.95 | 0.12 | 24,46,82,99 | 0 |
| 22 | CLA | c | 502 | 65/65 | 0.95 | 0.13 | 26,41,53,57 | 0 |
| 33 | LHG | d | 407 | 49/49 | 0.95 | 0.12 | 33,49,76,80 | 0 |
| 33 | LHG | d | 409 | 39/49 | 0.95 | 0.10 | 29,45,72,80 | 0 |
| 29 | DGD | c | 517 | 62/66 | 0.95 | 0.11 | 24,42,84,94 | 0 |

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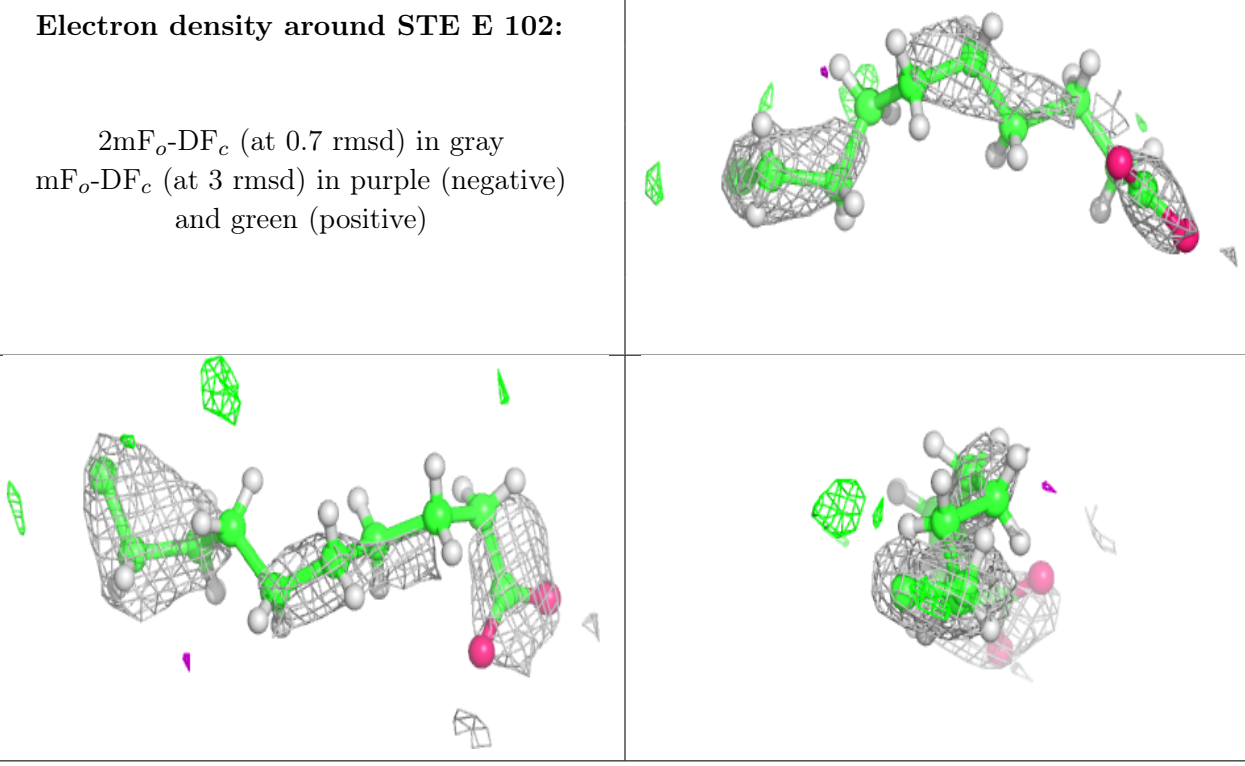
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 34 | HEC | F | 102 | 43/43 | 0.95 | 0.12 | 37,48,64,66 | 0 |
| 23 | PHO | d | 401 | 64/64 | 0.96 | 0.11 | 20,37,47,61 | 0 |
| 22 | CLA | a | 402 | 65/65 | 0.96 | 0.10 | 19,29,46,56 | 0 |
| 33 | LHG | D | 412 | 49/49 | 0.96 | 0.11 | 30,44,65,76 | 0 |
| 22 | CLA | A | 402 | 65/65 | 0.96 | 0.10 | 16,26,46,49 | 0 |
| 33 | LHG | L | 102 | 49/49 | 0.96 | 0.10 | 26,41,53,60 | 0 |
| 22 | CLA | B | 607 | 65/65 | 0.96 | 0.10 | 14,34,62,66 | 0 |
| 22 | CLA | b | 607 | 65/65 | 0.96 | 0.12 | 18,35,69,78 | 0 |
| 23 | PHO | D | 401 | 64/64 | 0.96 | 0.13 | 21,32,44,48 | 0 |
| 33 | LHG | l | 101 | 49/49 | 0.96 | 0.10 | 26,45,55,64 | 0 |
| 22 | CLA | b | 603 | 65/65 | 0.96 | 0.12 | 18,36,65,76 | 0 |
| 34 | HEC | f | 101 | 43/43 | 0.96 | 0.12 | 42,58,81,84 | 0 |
| 33 | LHG | d | 408 | 49/49 | 0.97 | 0.09 | 23,42,57,68 | 0 |
| 34 | HEC | V | 201 | 43/43 | 0.97 | 0.13 | 19,35,43,44 | 0 |
| 33 | LHG | D | 409 | 49/49 | 0.97 | 0.09 | 26,41,53,56 | 0 |
| 34 | HEC | v | 201 | 43/43 | 0.97 | 0.12 | 27,37,50,51 | 0 |
| 32 | BCT | d | 402 | 4/4 | 0.98 | 0.17 | 31,35,44,53 | 0 |
| 25 | CL | A | 407 | 1/1 | 0.98 | 0.06 | 29,29,29,29 | 0 |
| 32 | BCT | D | 402 | 4/4 | 0.98 | 0.17 | 22,26,32,36 | 0 |
| 21 | FE2 | A | 401 | 1/1 | 0.99 | 0.10 | 26,26,26,26 | 0 |
| 25 | CL | A | 408 | 1/1 | 0.99 | 0.03 | 30,30,30,30 | 0 |
| 25 | CL | a | 407 | 1/1 | 0.99 | 0.02 | 28,28,28,28 | 0 |
| 30 | OEX | A | 414 | 10/10 | 0.99 | 0.11 | 22,26,28,29 | 0 |
| 30 | OEX | a | 416 | 10/10 | 0.99 | 0.12 | 23,26,30,31 | 0 |
| 25 | CL | a | 408 | 1/1 | 0.99 | 0.05 | 28,28,28,28 | 0 |
| 21 | FE2 | a | 401 | 1/1 | 0.99 | 0.08 | 34,34,34,34 | 0 |

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

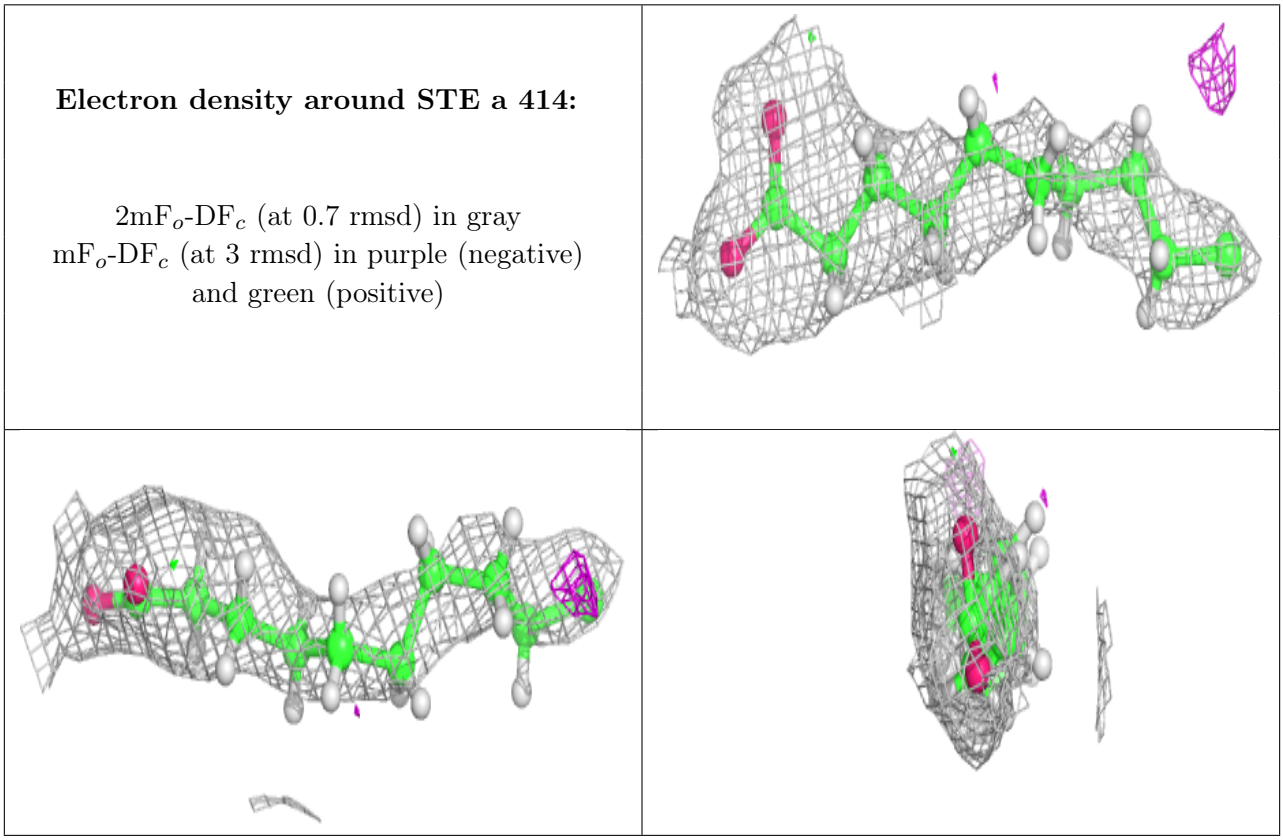
**Electron density around STE E 102:**

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



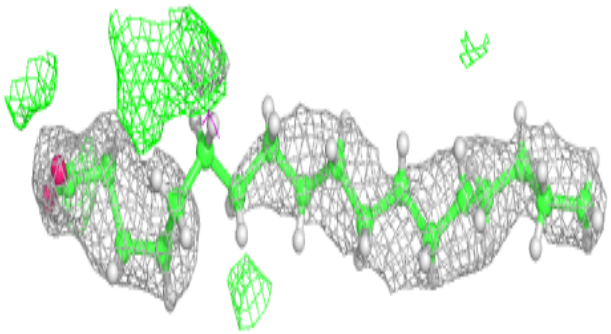
**Electron density around STE a 414:**

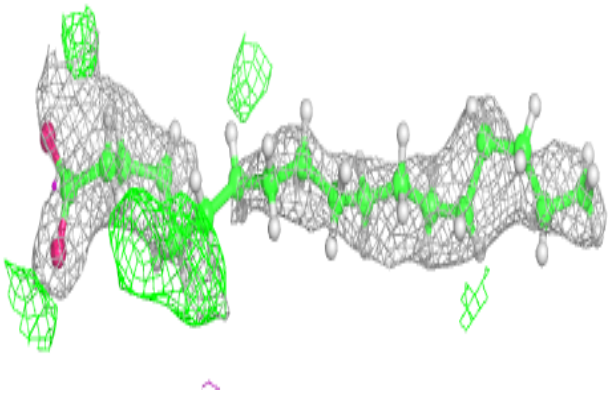
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

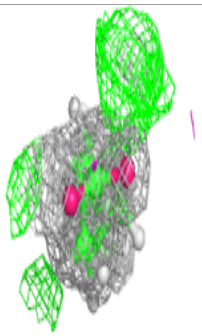


**Electron density around STE b 624:**

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

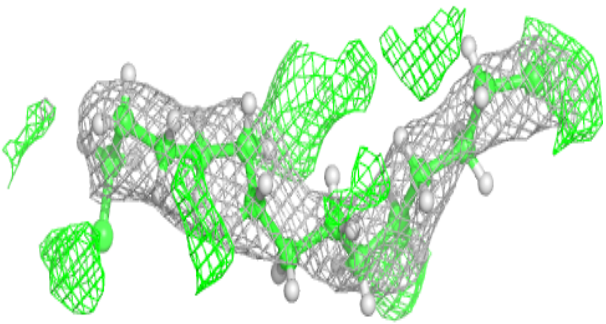


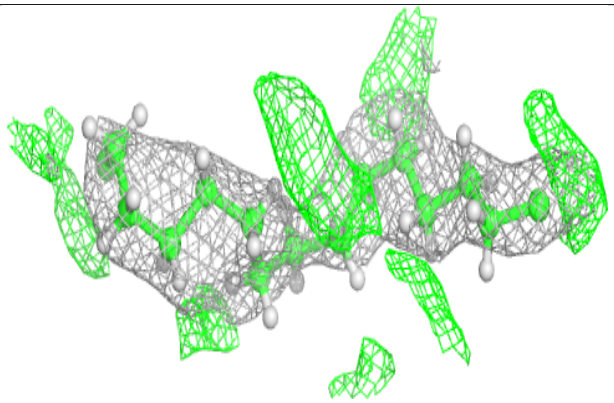


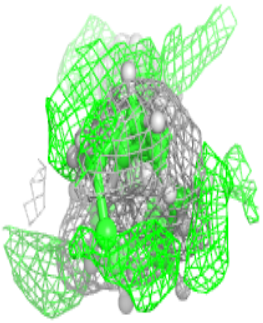


**Electron density around STE B 627:**

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

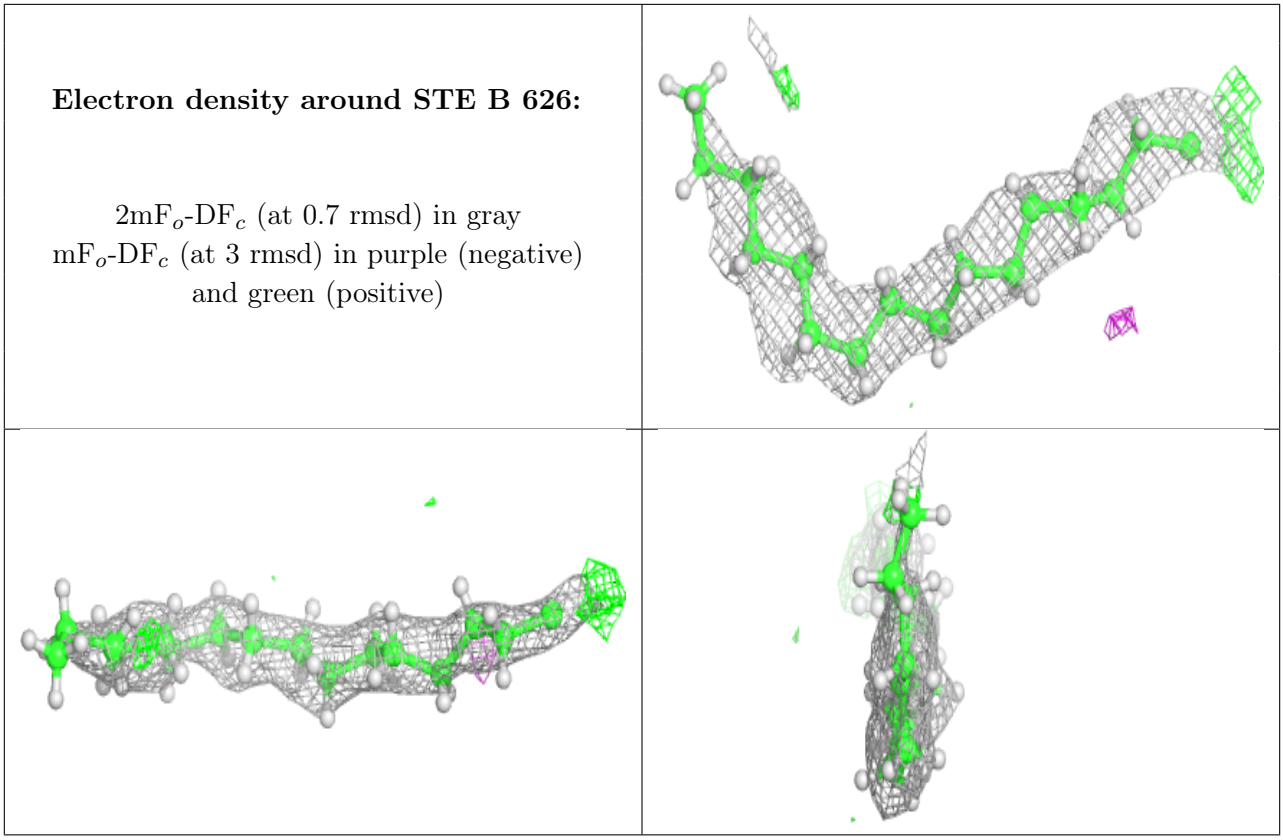






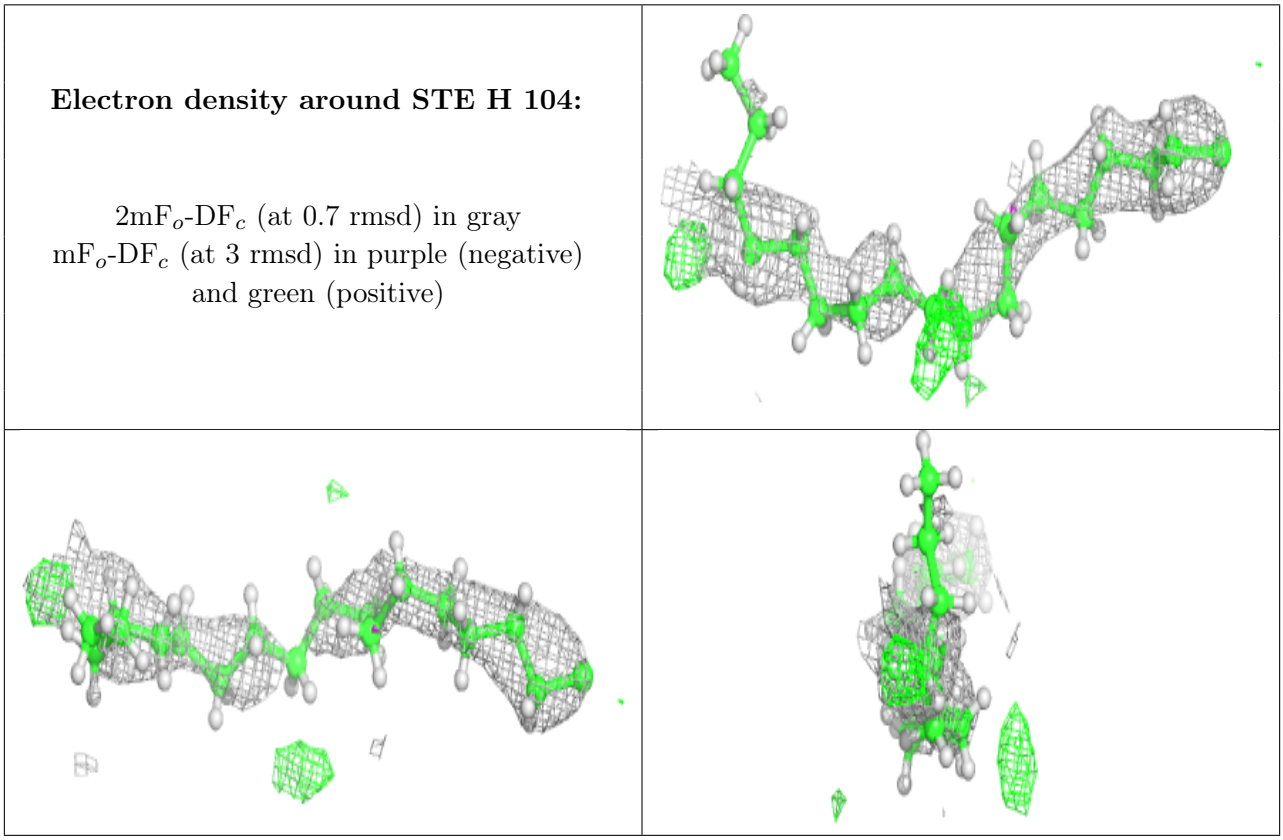
**Electron density around STE B 626:**

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



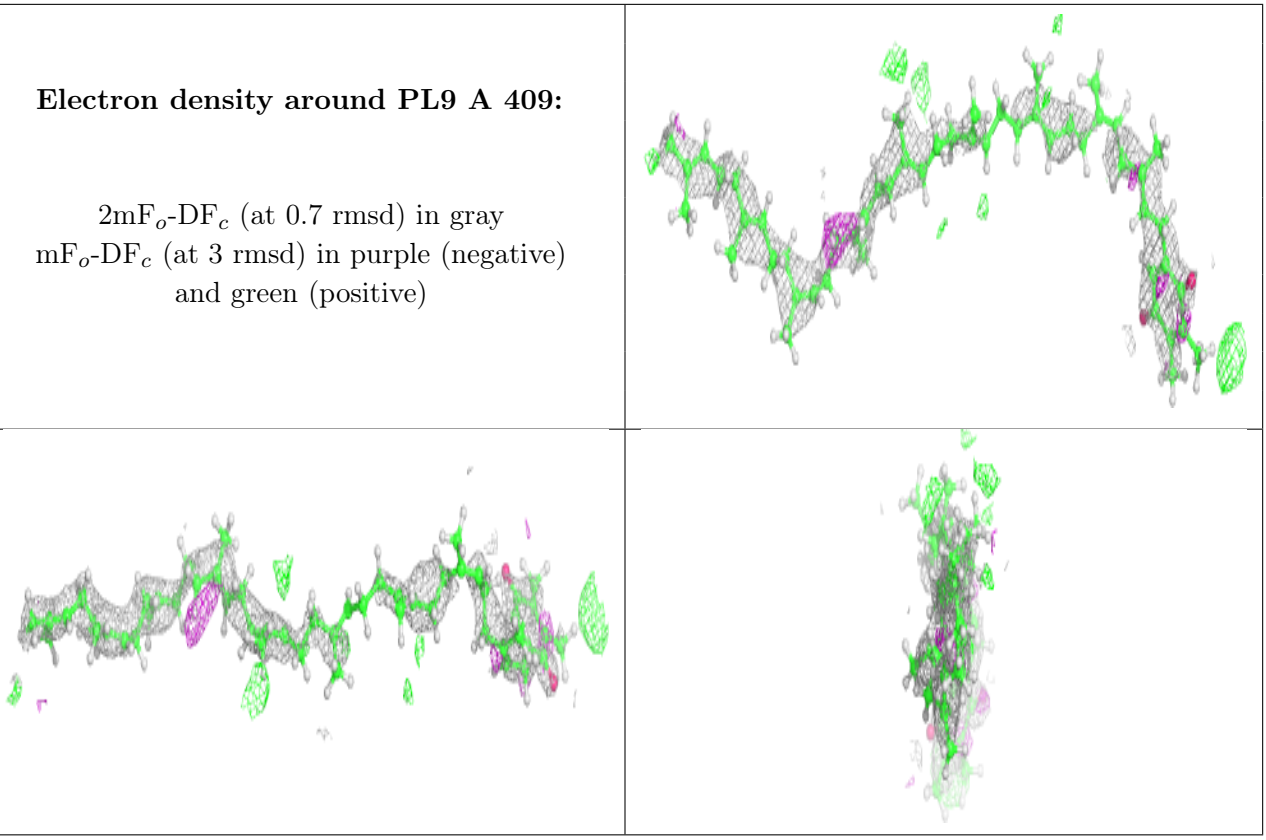
**Electron density around STE H 104:**

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



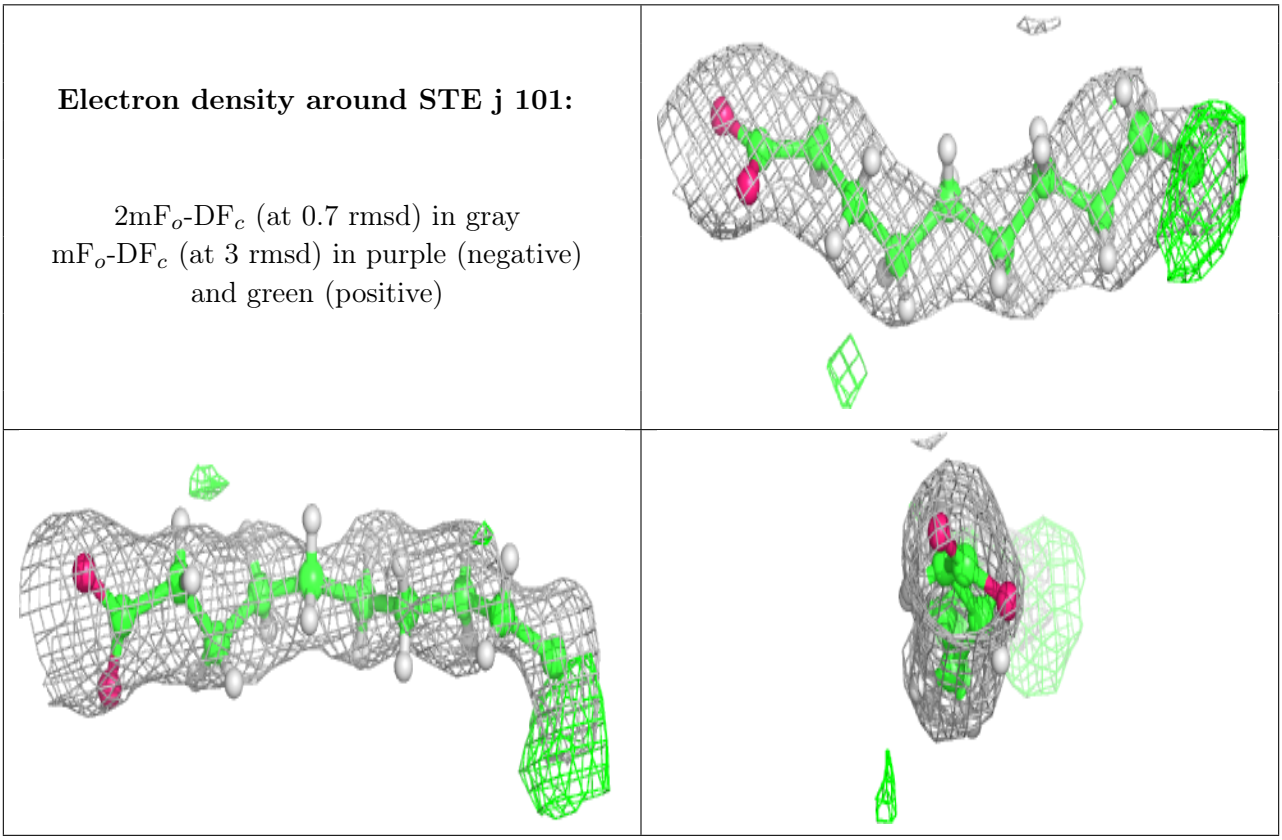
**Electron density around PL9 A 409:**

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



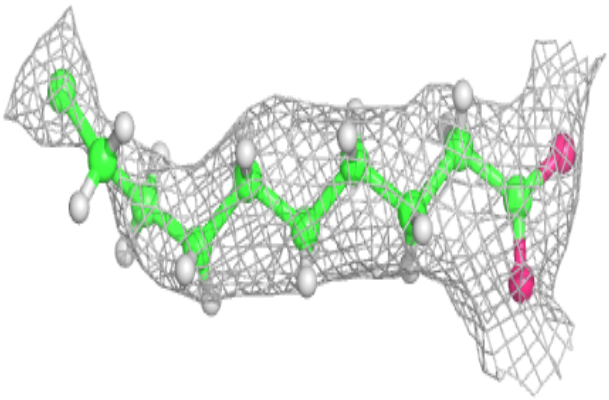
**Electron density around STE j 101:**

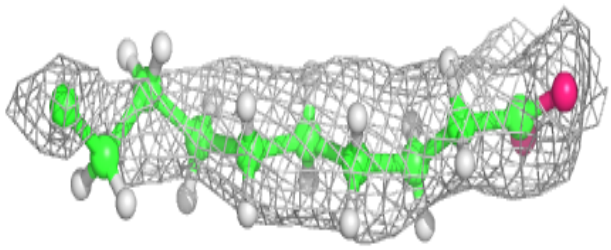
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

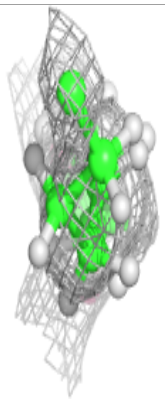


**Electron density around STE c 501:**

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

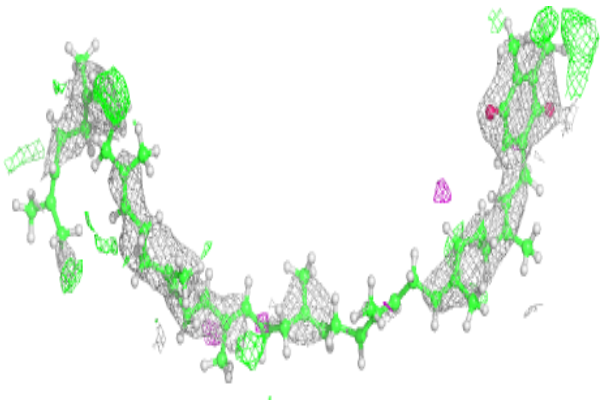


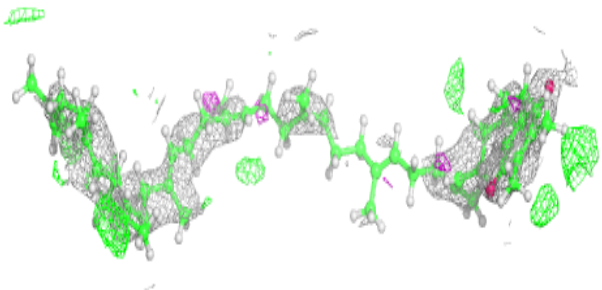


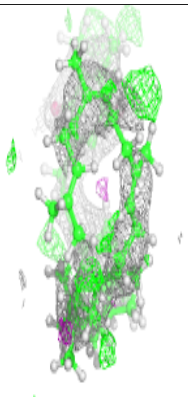


**Electron density around PL9 a 409:**

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

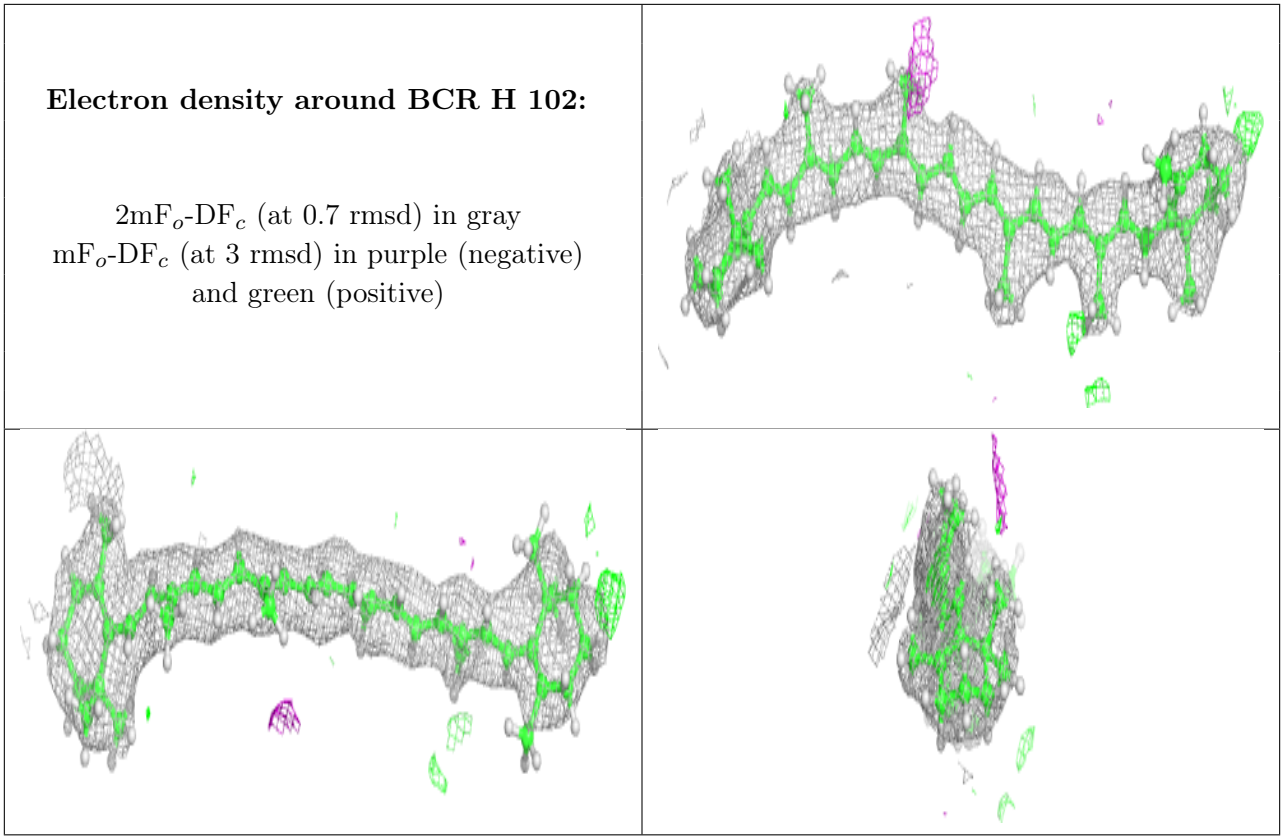






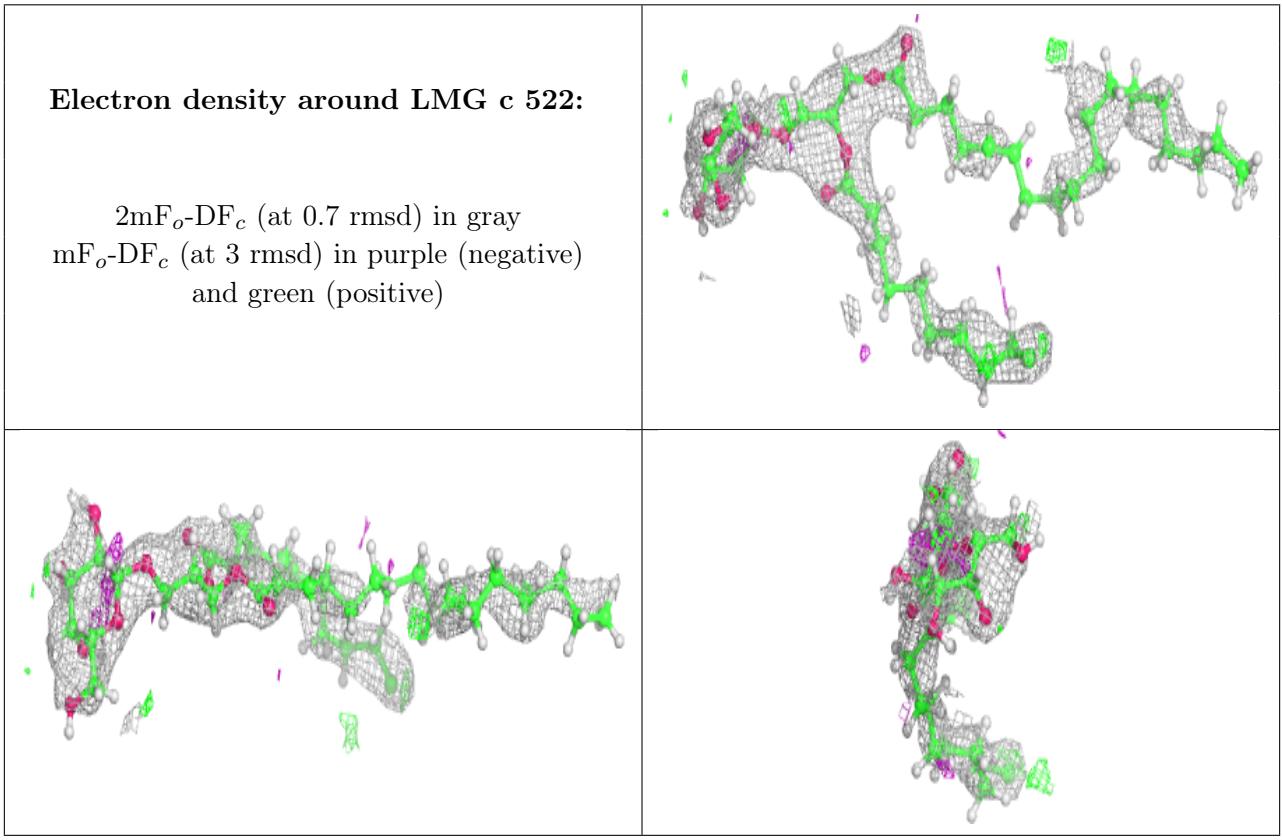
**Electron density around BCR H 102:**

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



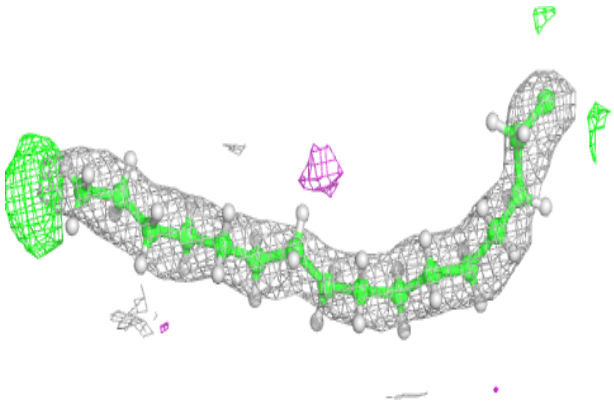
**Electron density around LMG c 522:**

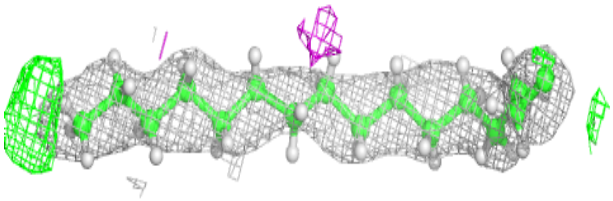
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

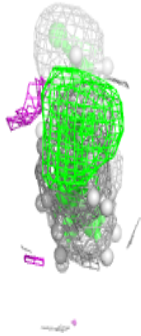


**Electron density around STE C 519:**

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

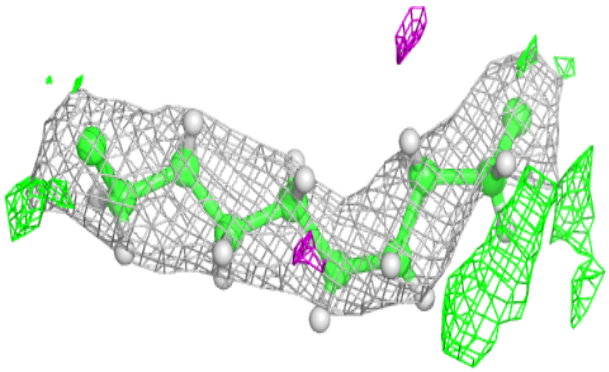


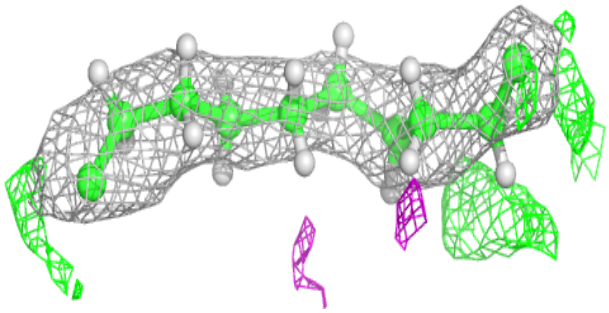


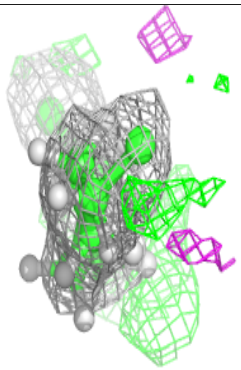


**Electron density around STE b 625:**

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

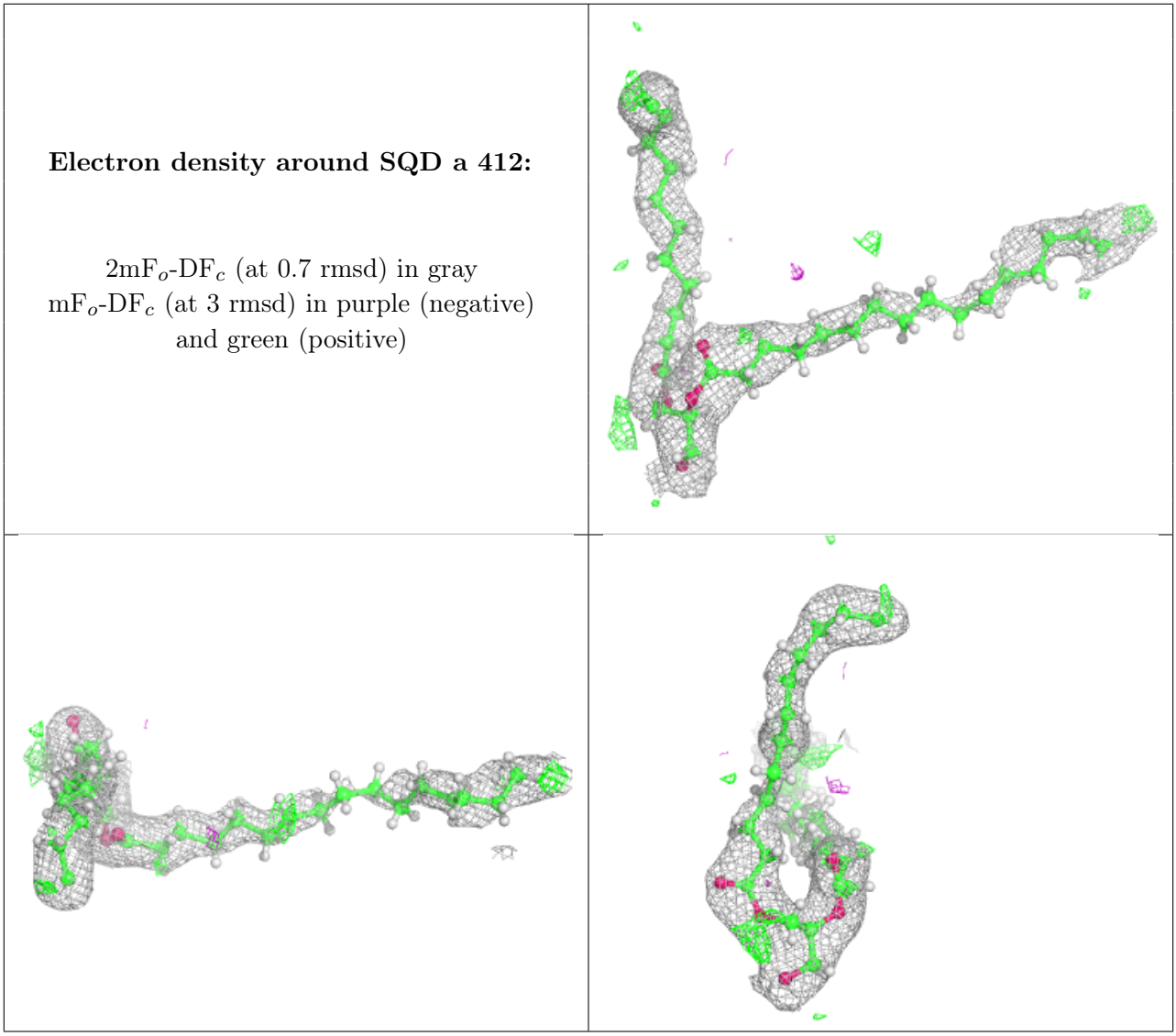






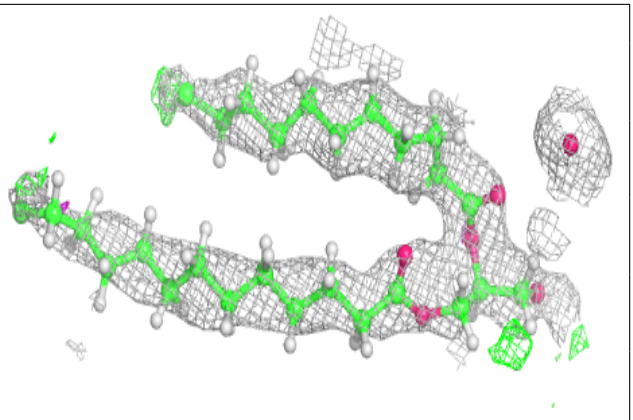
**Electron density around SQD a 412:**

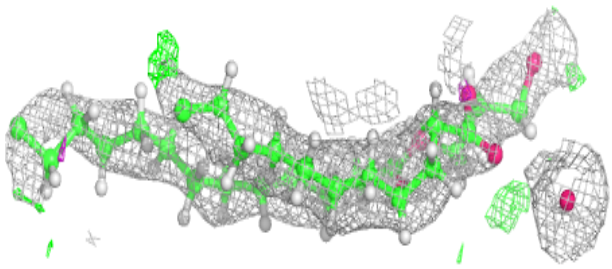
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

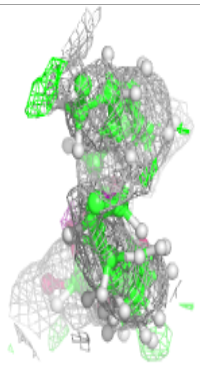


**Electron density around LMG D 411:**

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

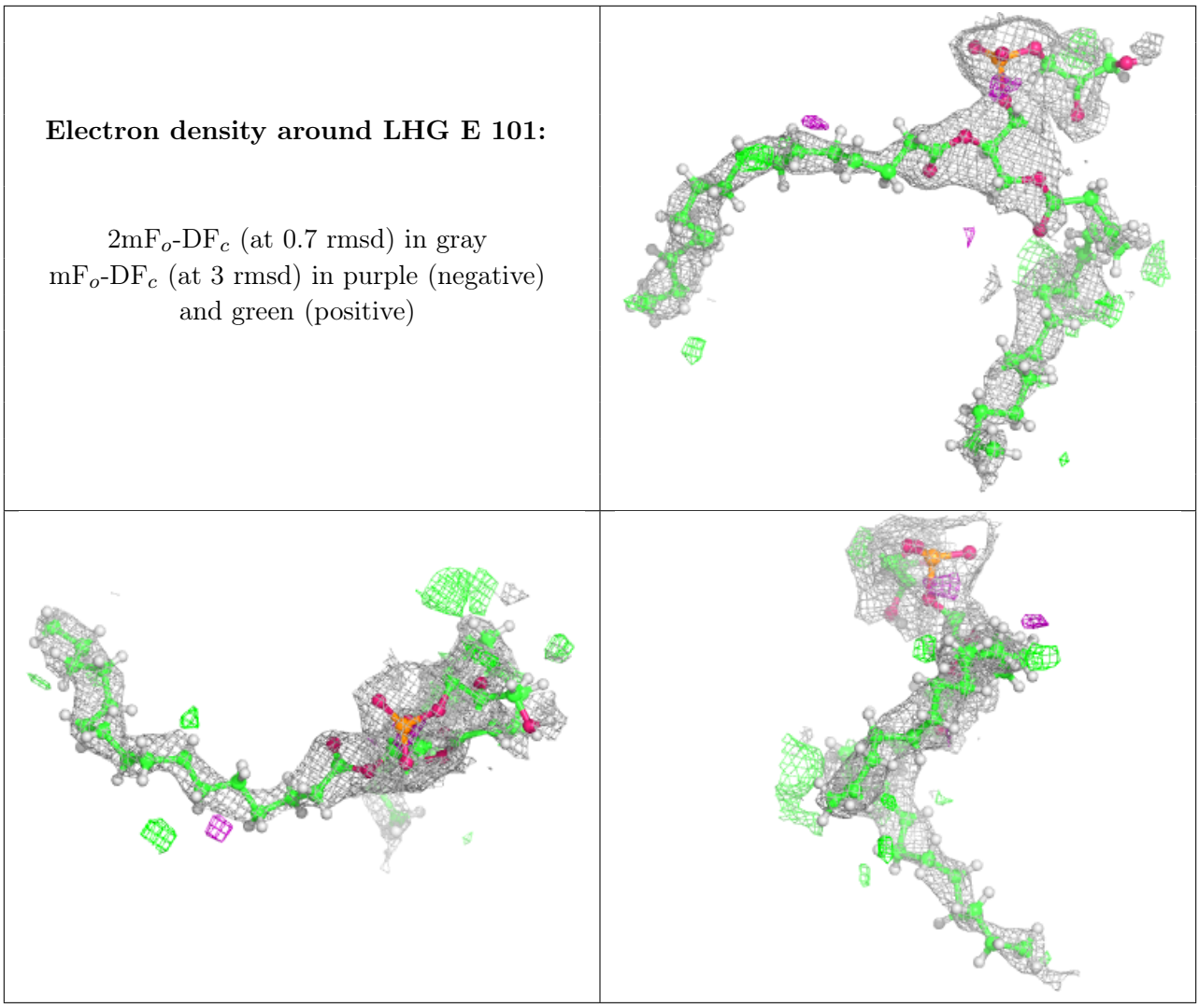






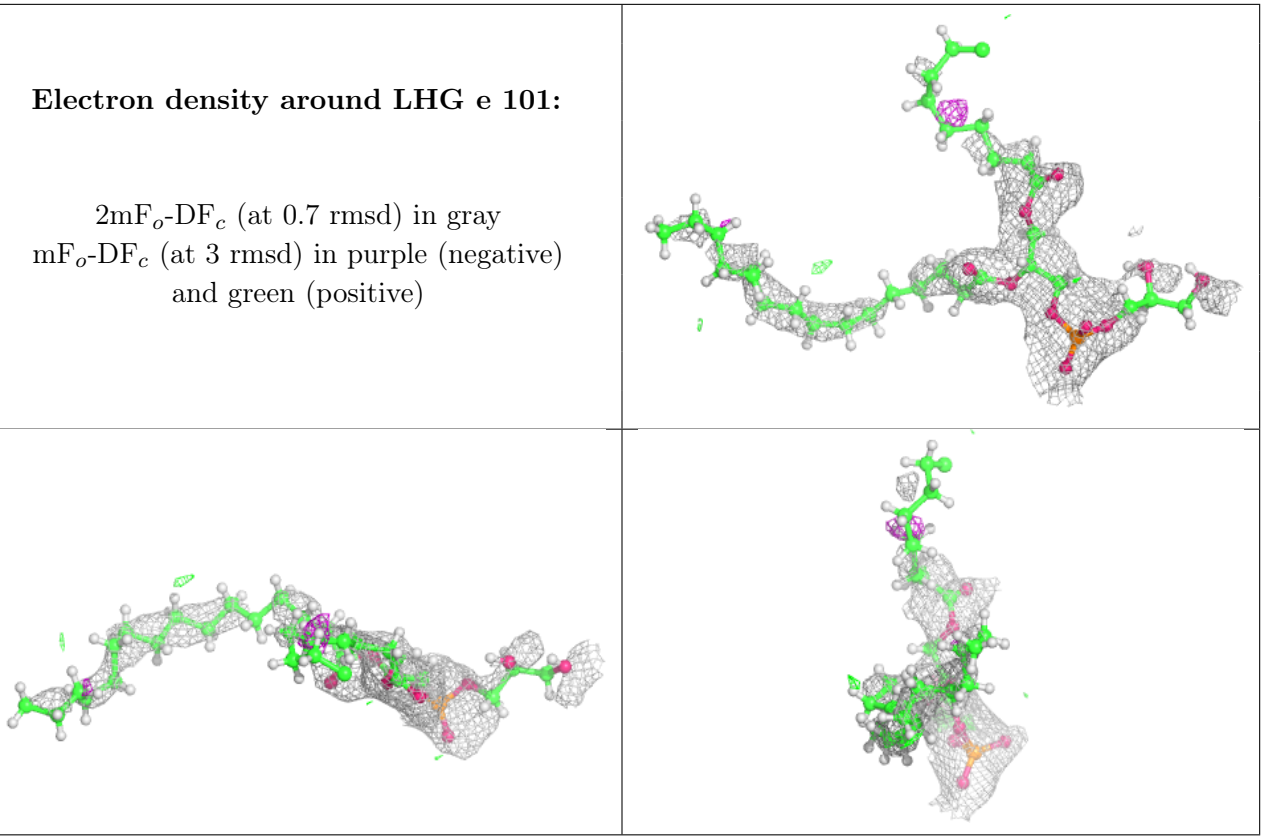
**Electron density around LHG E 101:**

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



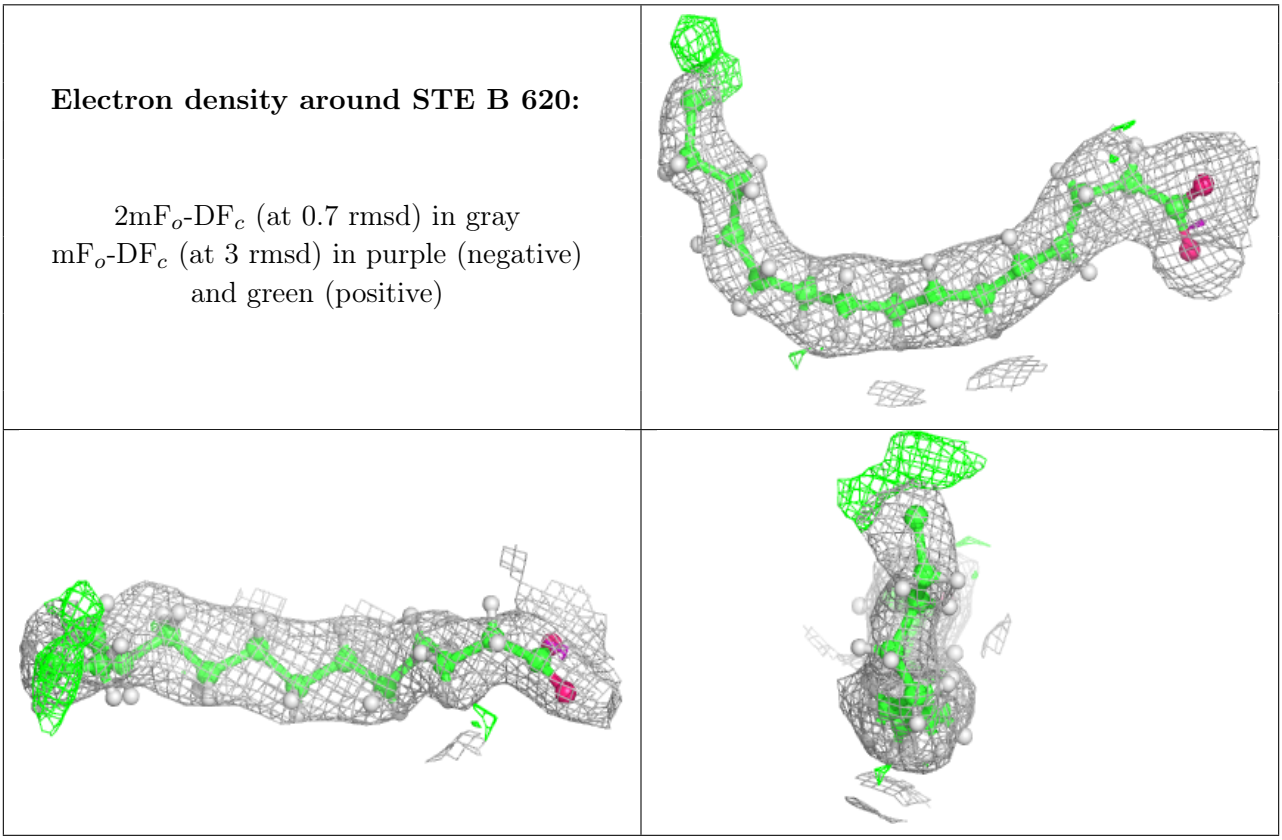
**Electron density around LHG e 101:**

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



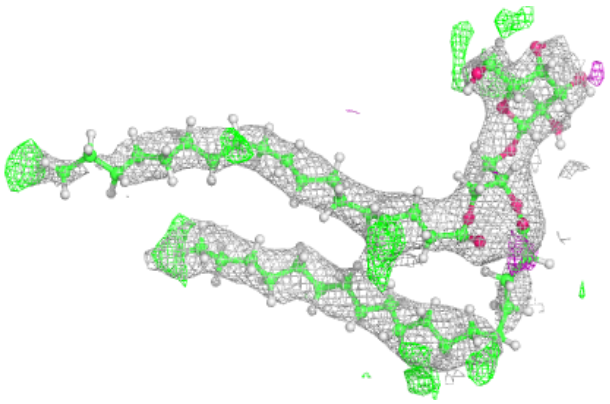
**Electron density around STE B 620:**

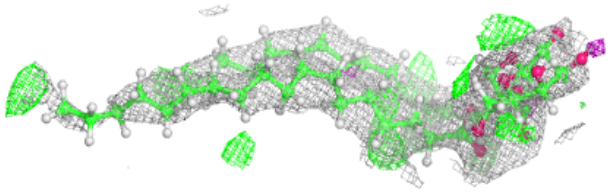
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

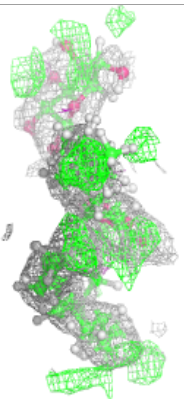


**Electron density around LMG a 415:**

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

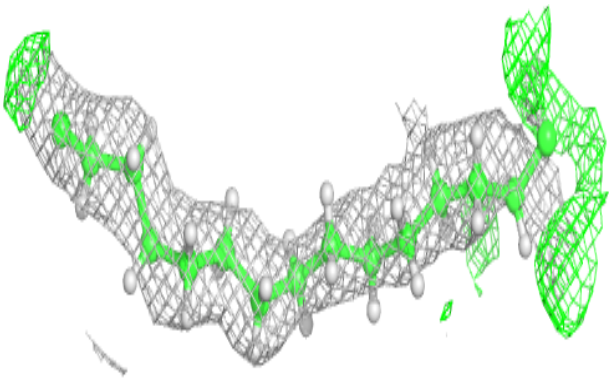


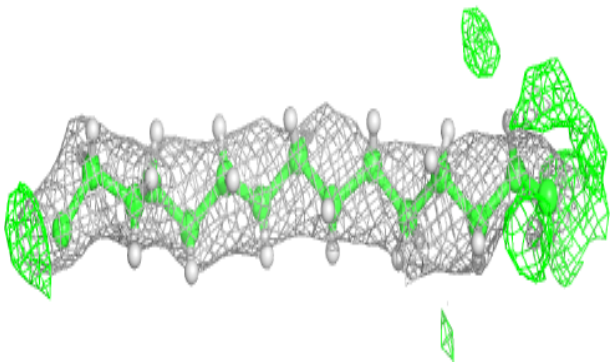


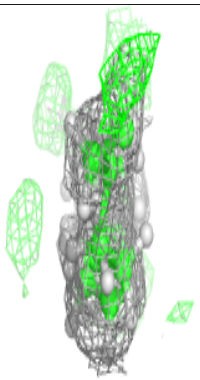


**Electron density around STE I 101:**

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

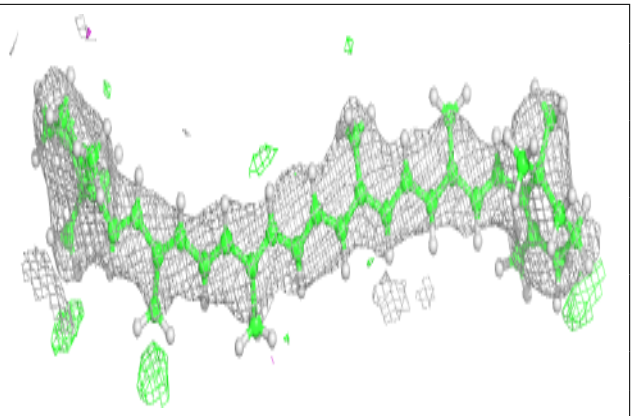


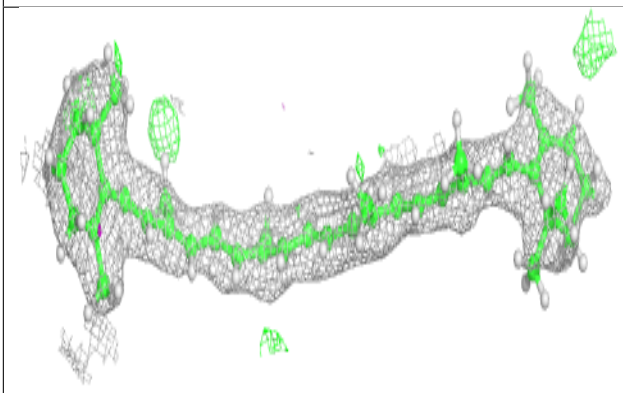


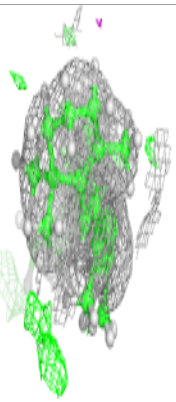


**Electron density around BCR h 101:**

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

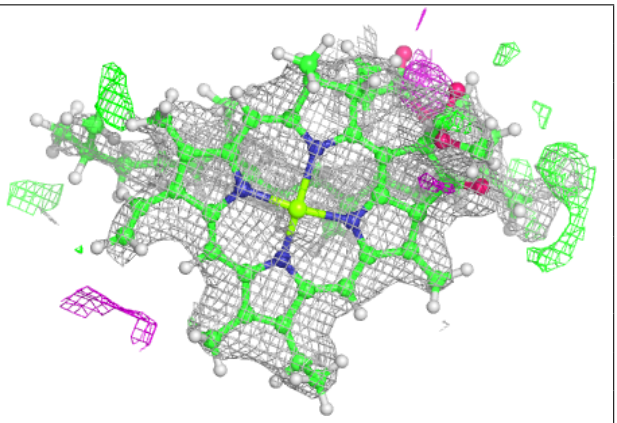


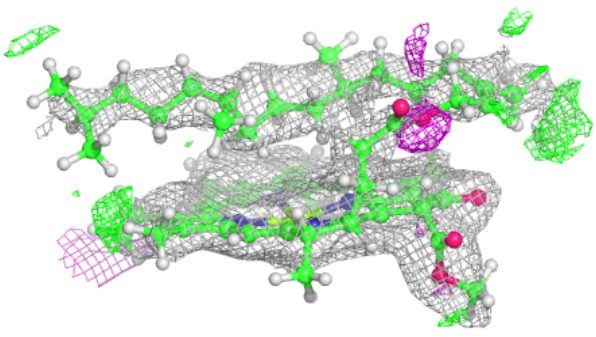




**Electron density around CLA b 601:**

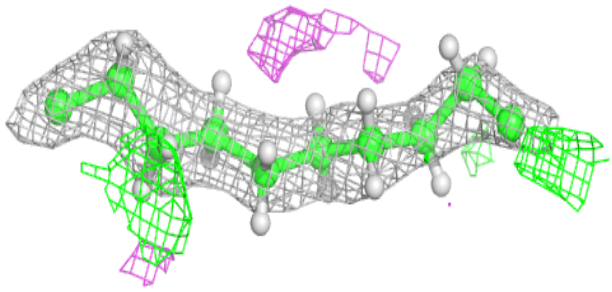
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

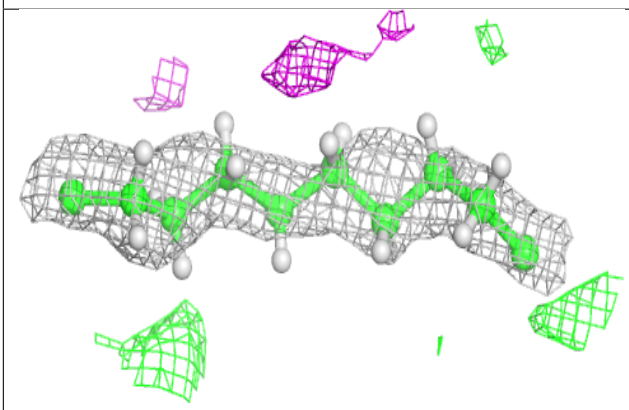


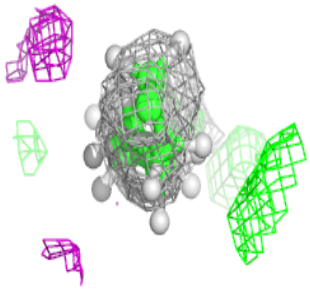


**Electron density around STE a 413:**

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

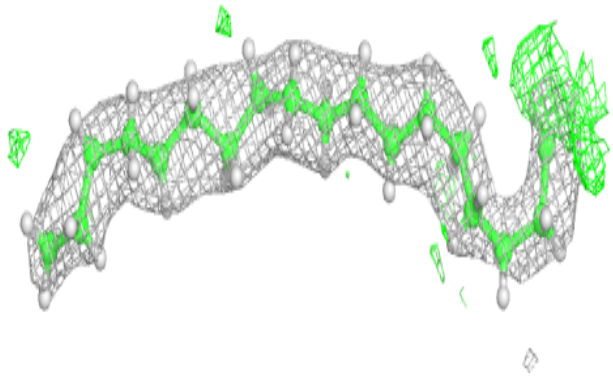


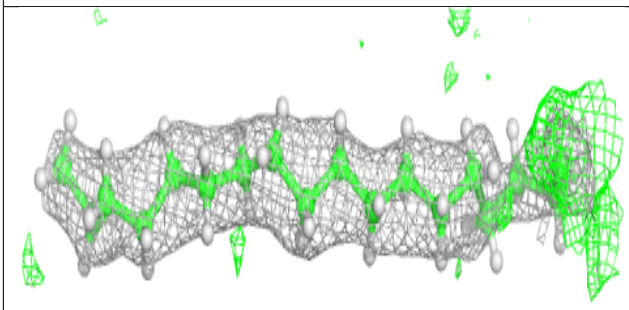


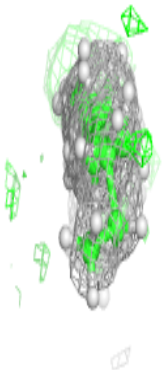


**Electron density around STE m 101:**

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

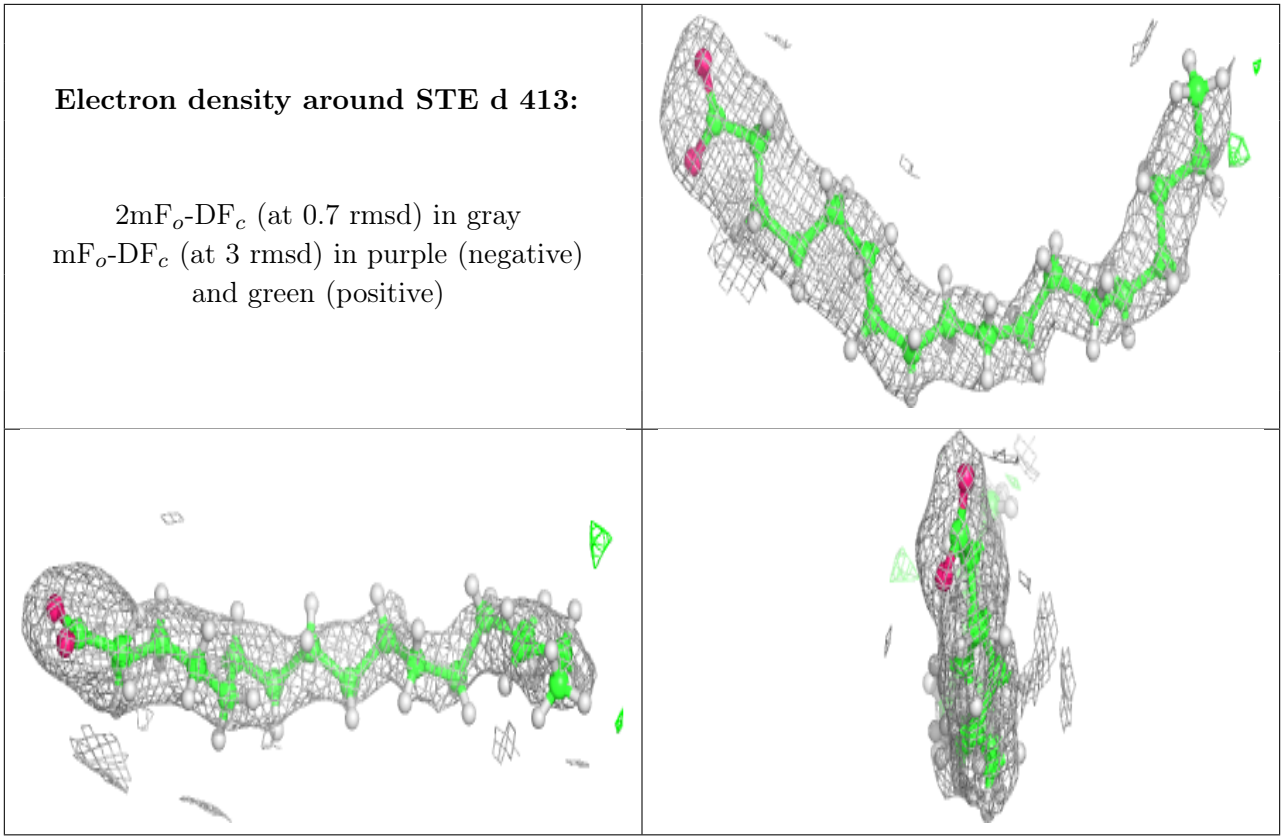






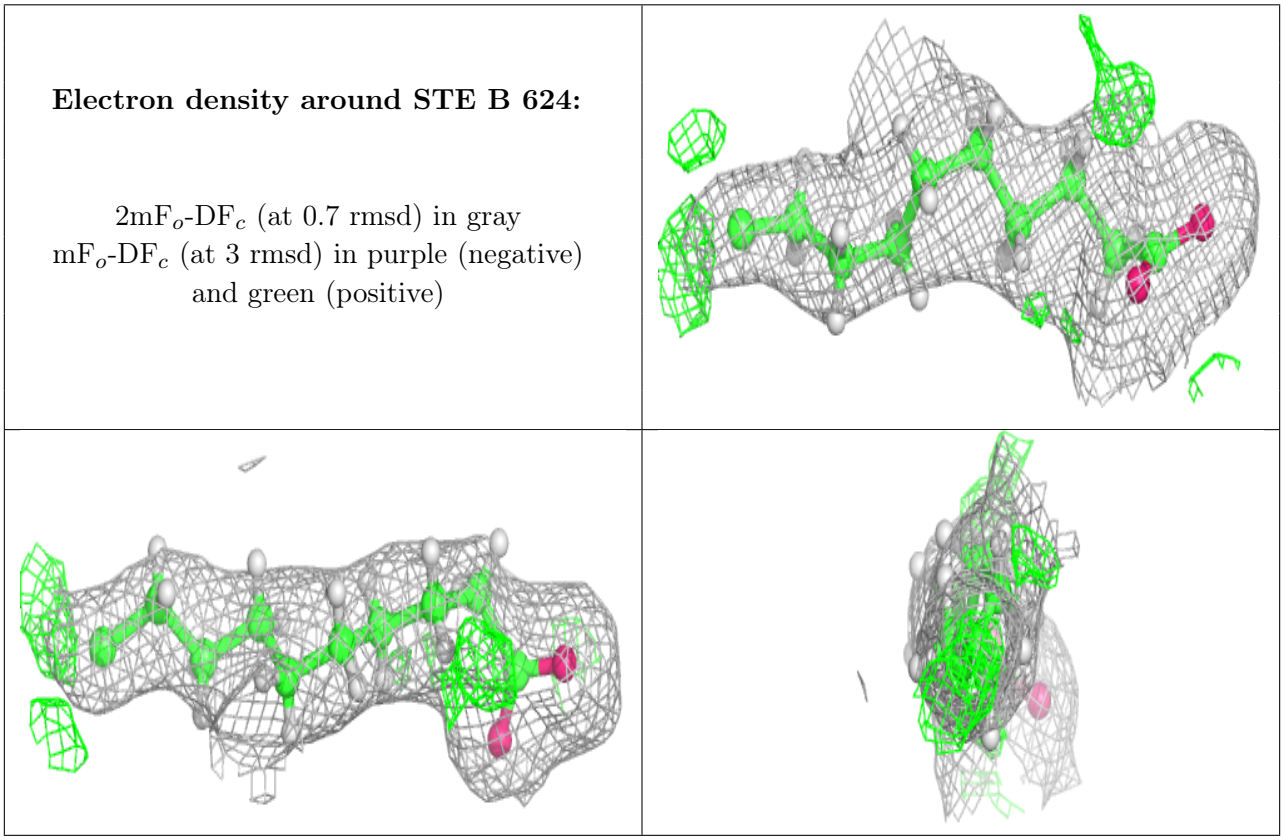
**Electron density around STE d 413:**

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



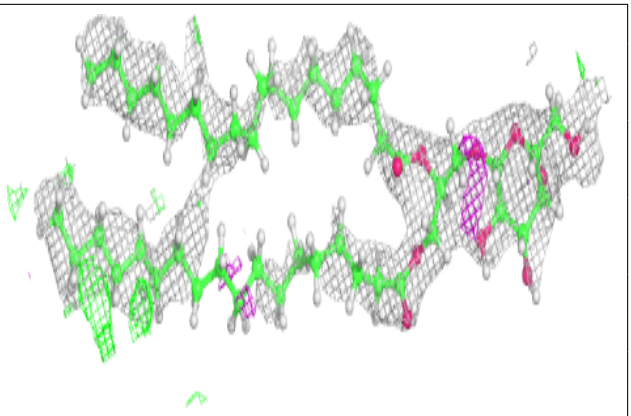
**Electron density around STE B 624:**

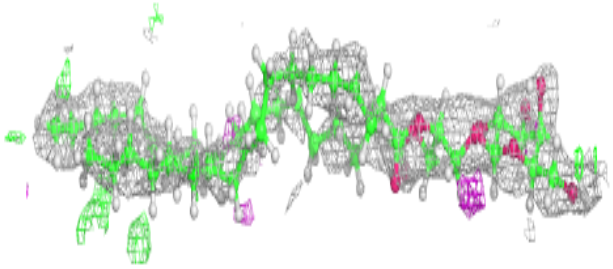
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

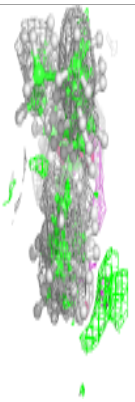


**Electron density around LMG b 623:**

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

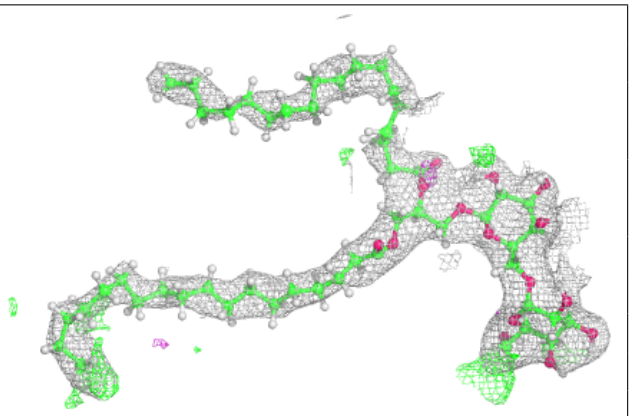


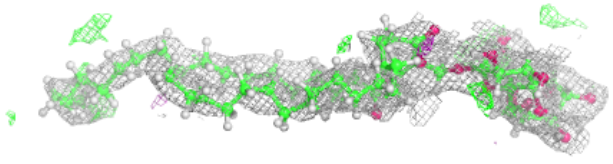


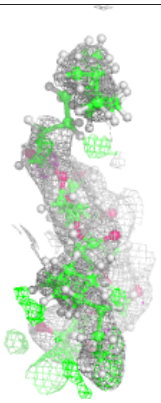


**Electron density around DGD A 413:**

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

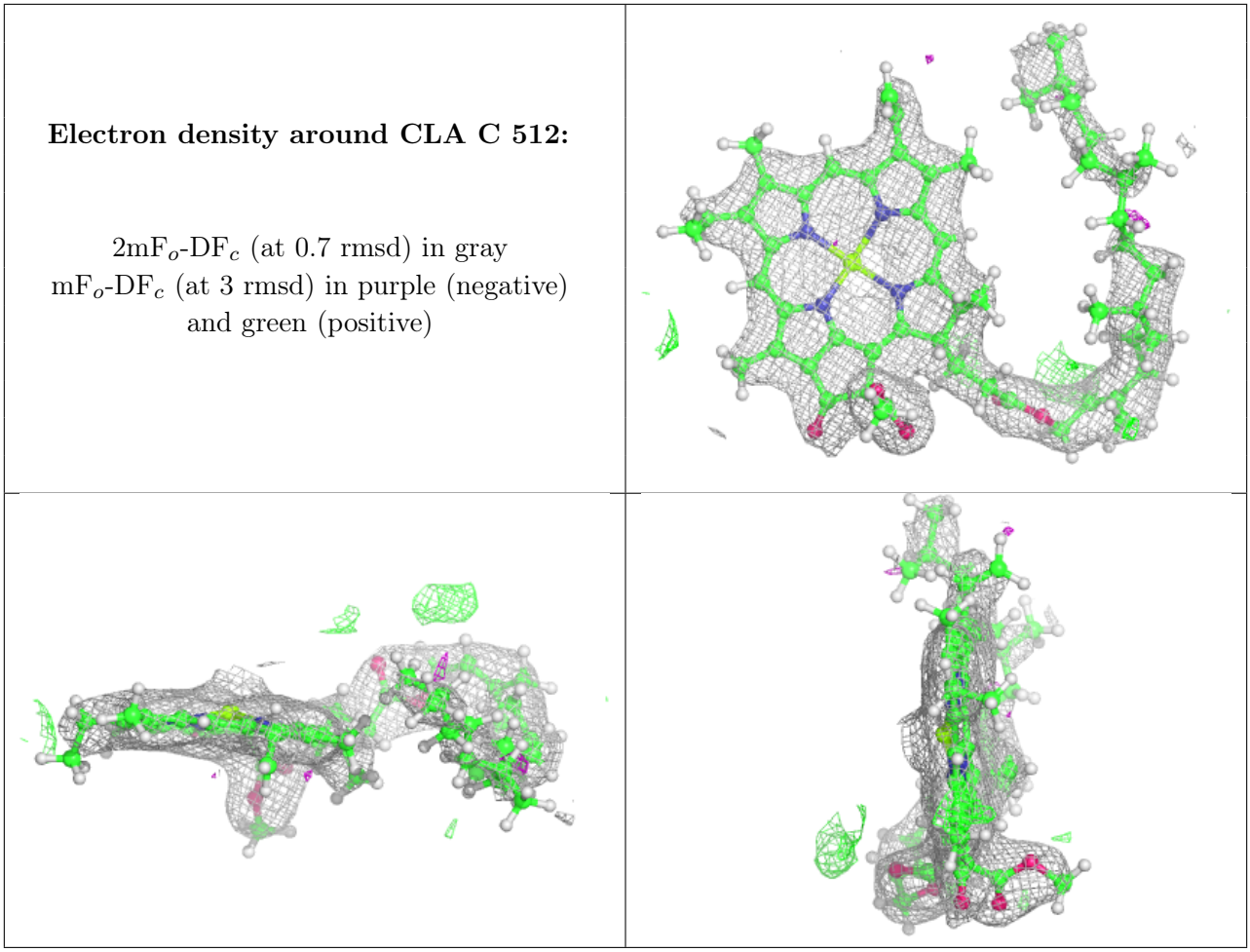






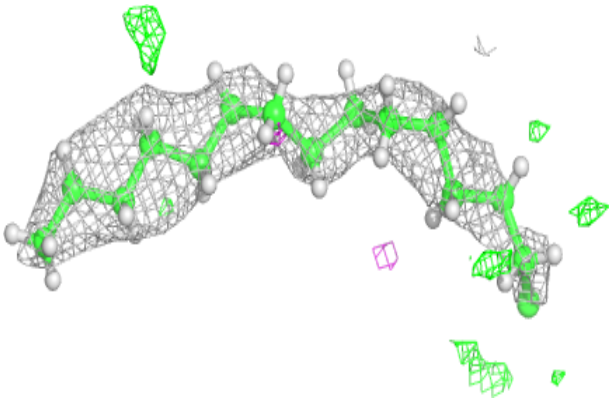
**Electron density around CLA C 512:**

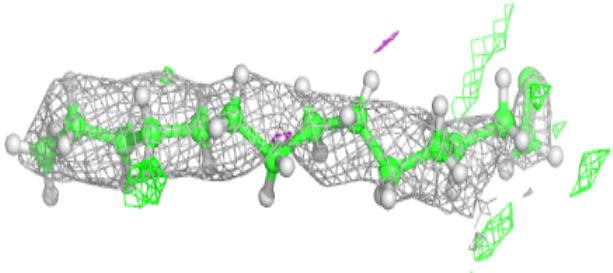
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

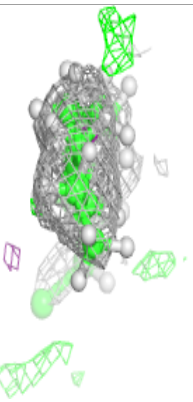


**Electron density around STE T 102:**

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

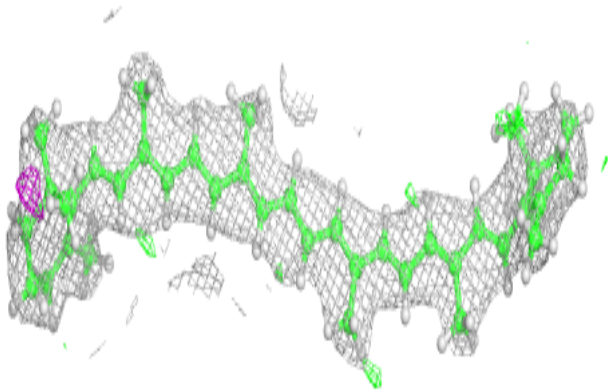


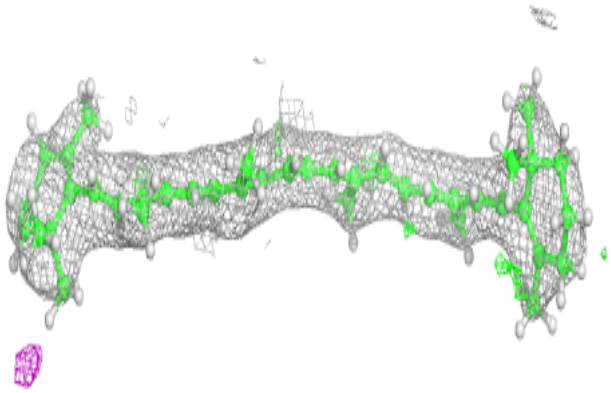


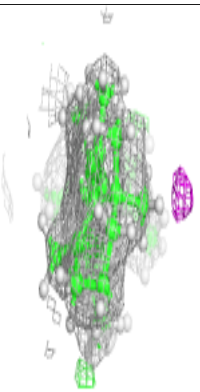


**Electron density around BCR K 102:**

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

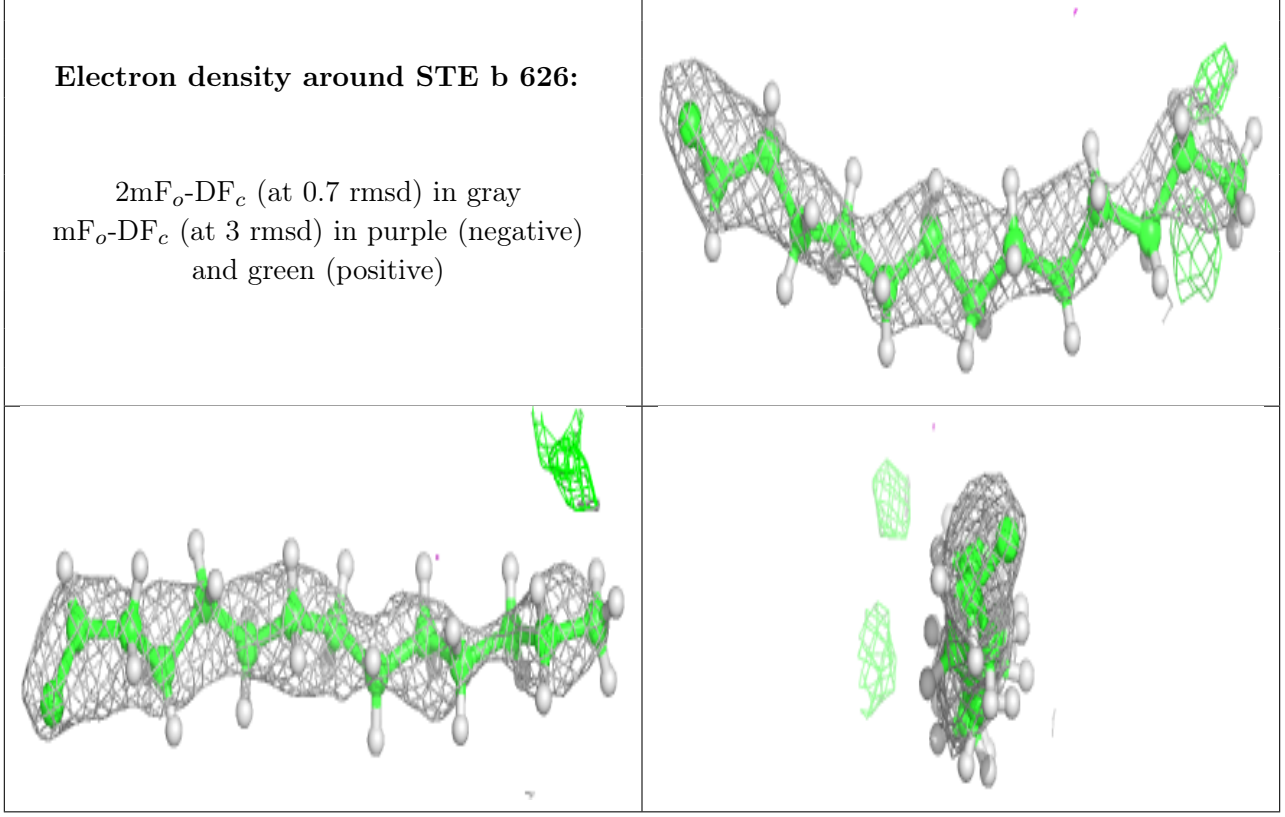






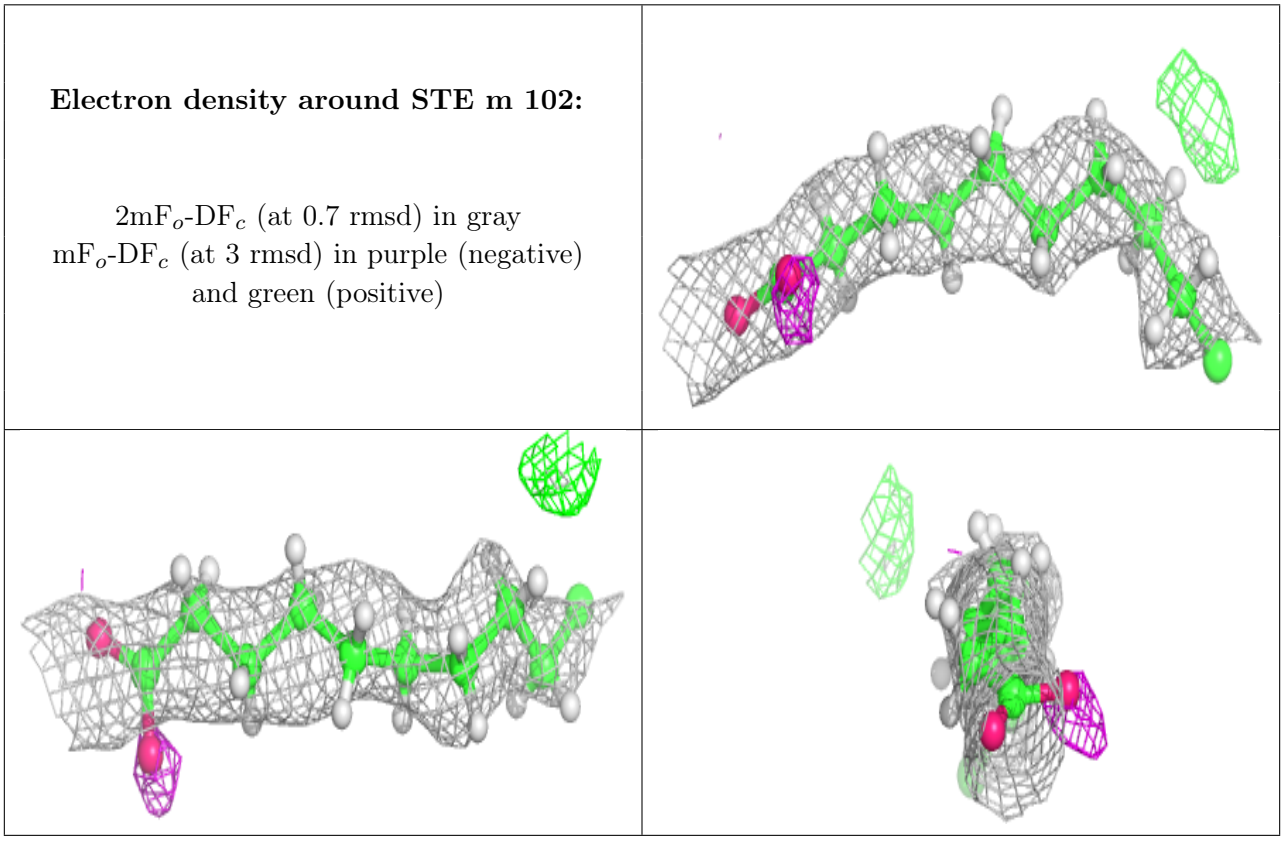
**Electron density around STE b 626:**

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



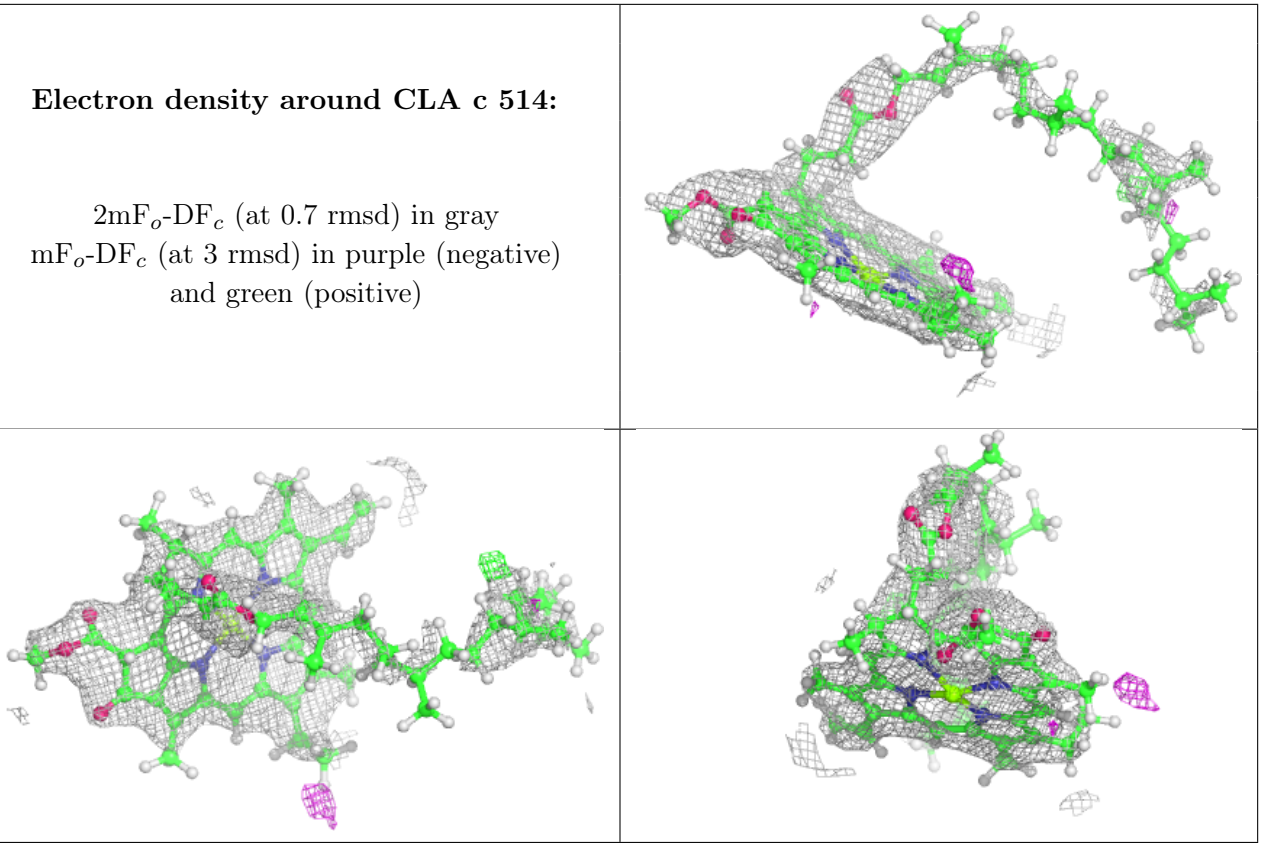
**Electron density around STE m 102:**

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



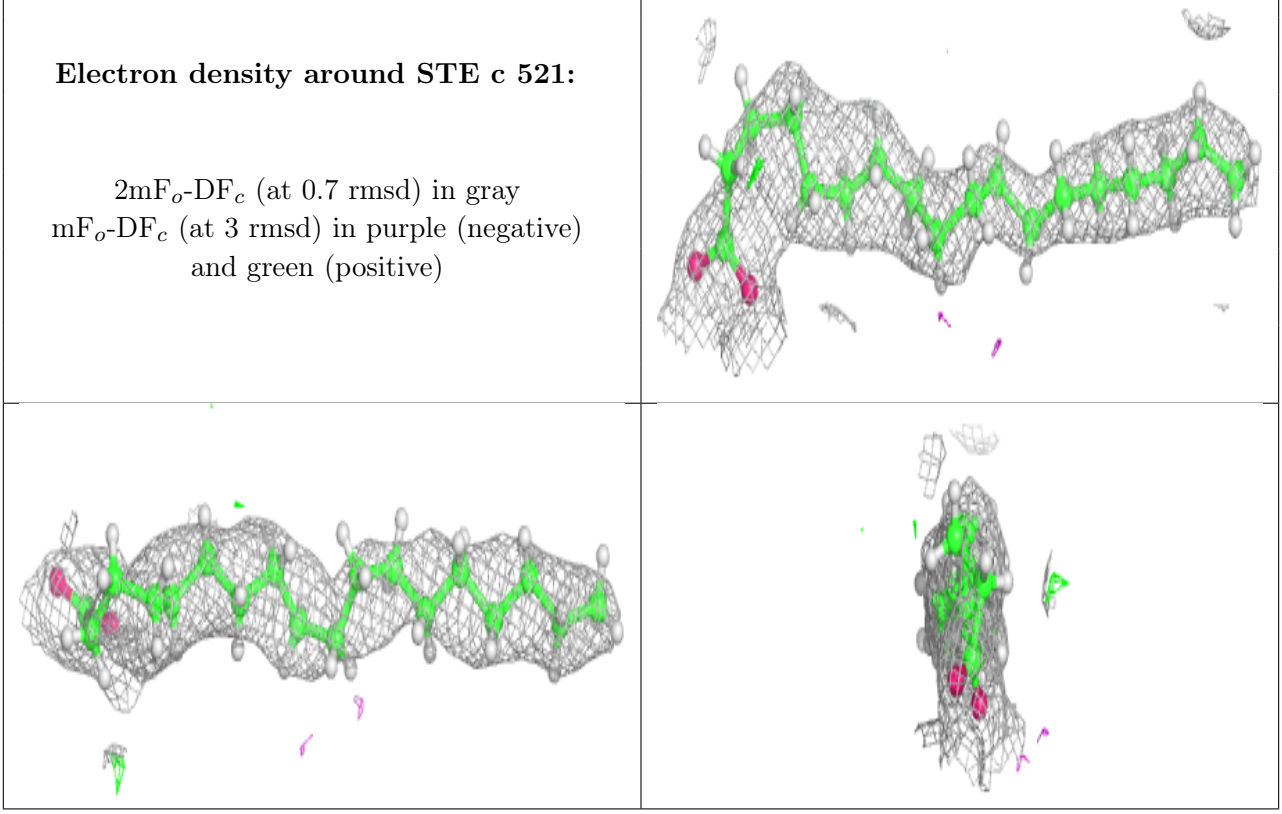
**Electron density around CLA c 514:**

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



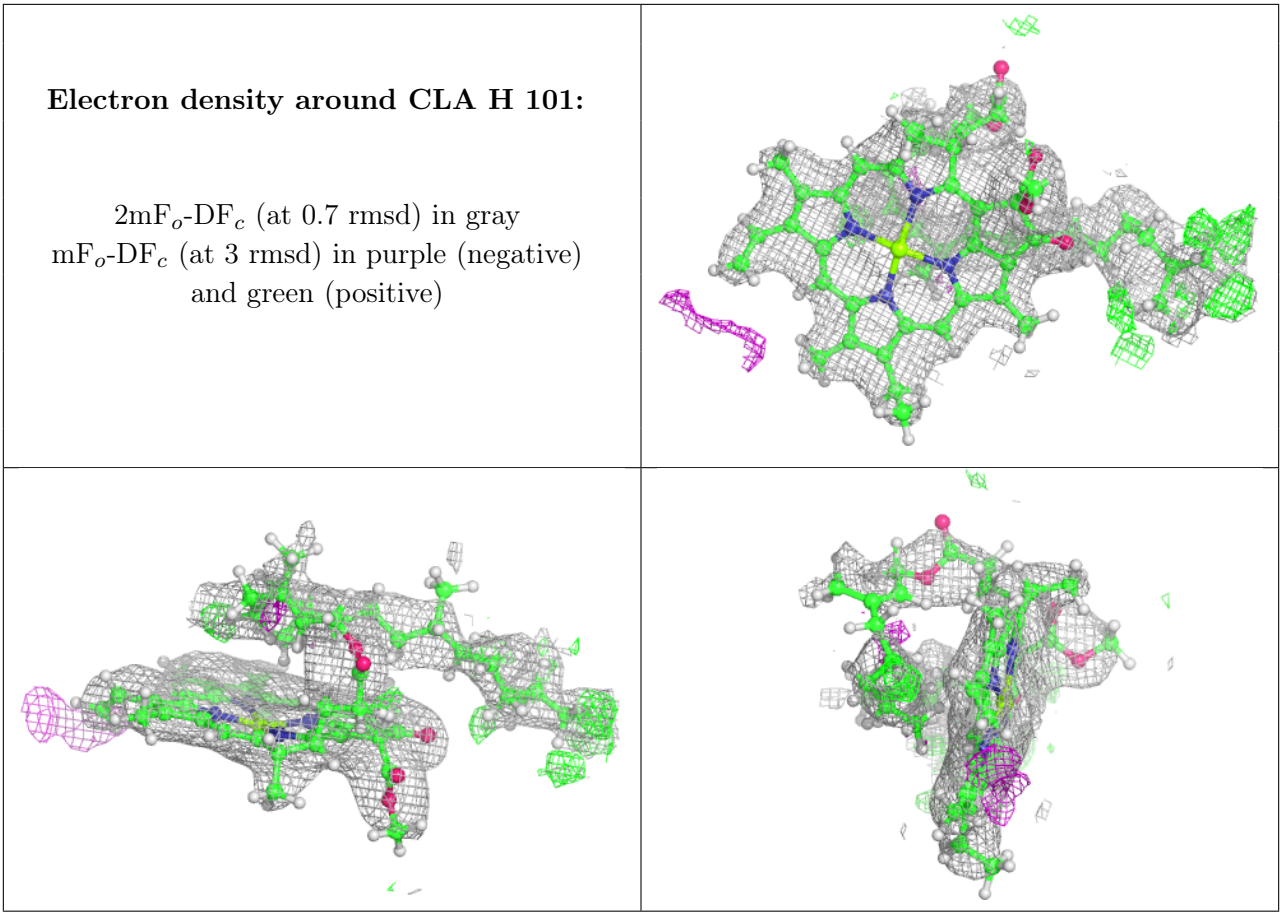
**Electron density around STE c 521:**

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



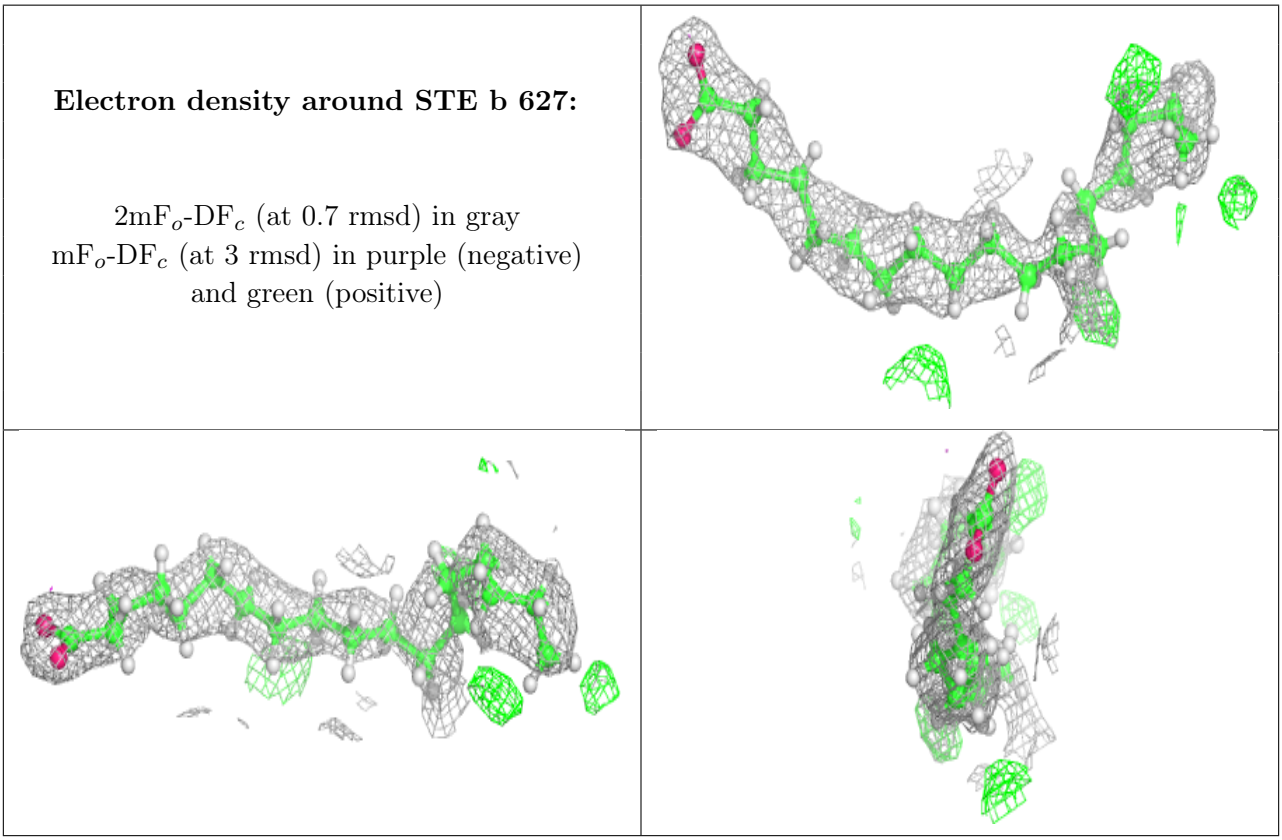
**Electron density around CLA H 101:**

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



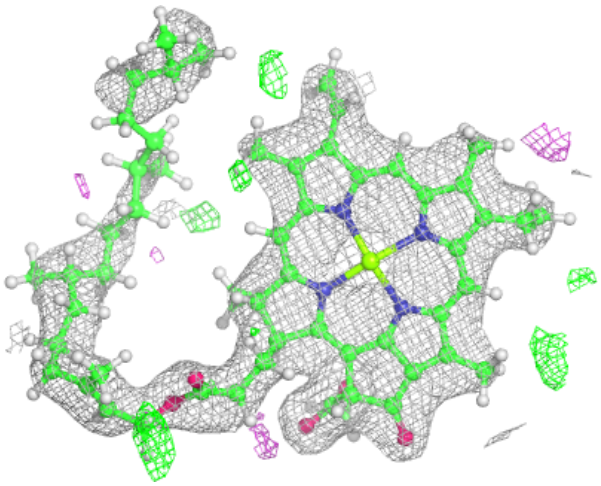
**Electron density around STE b 627:**

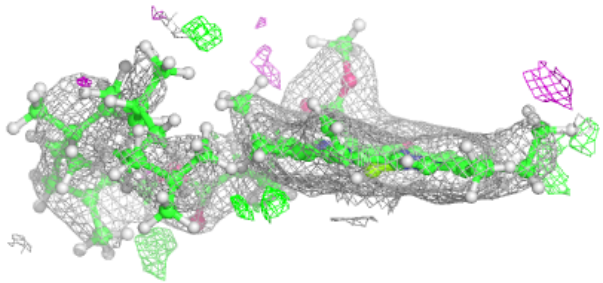
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

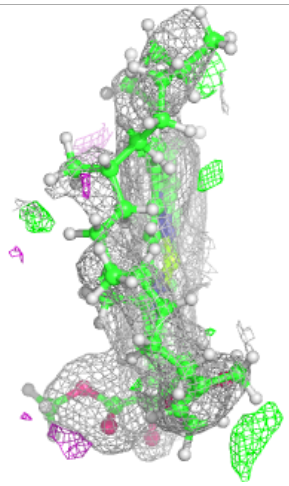


**Electron density around CLA c 513:**

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

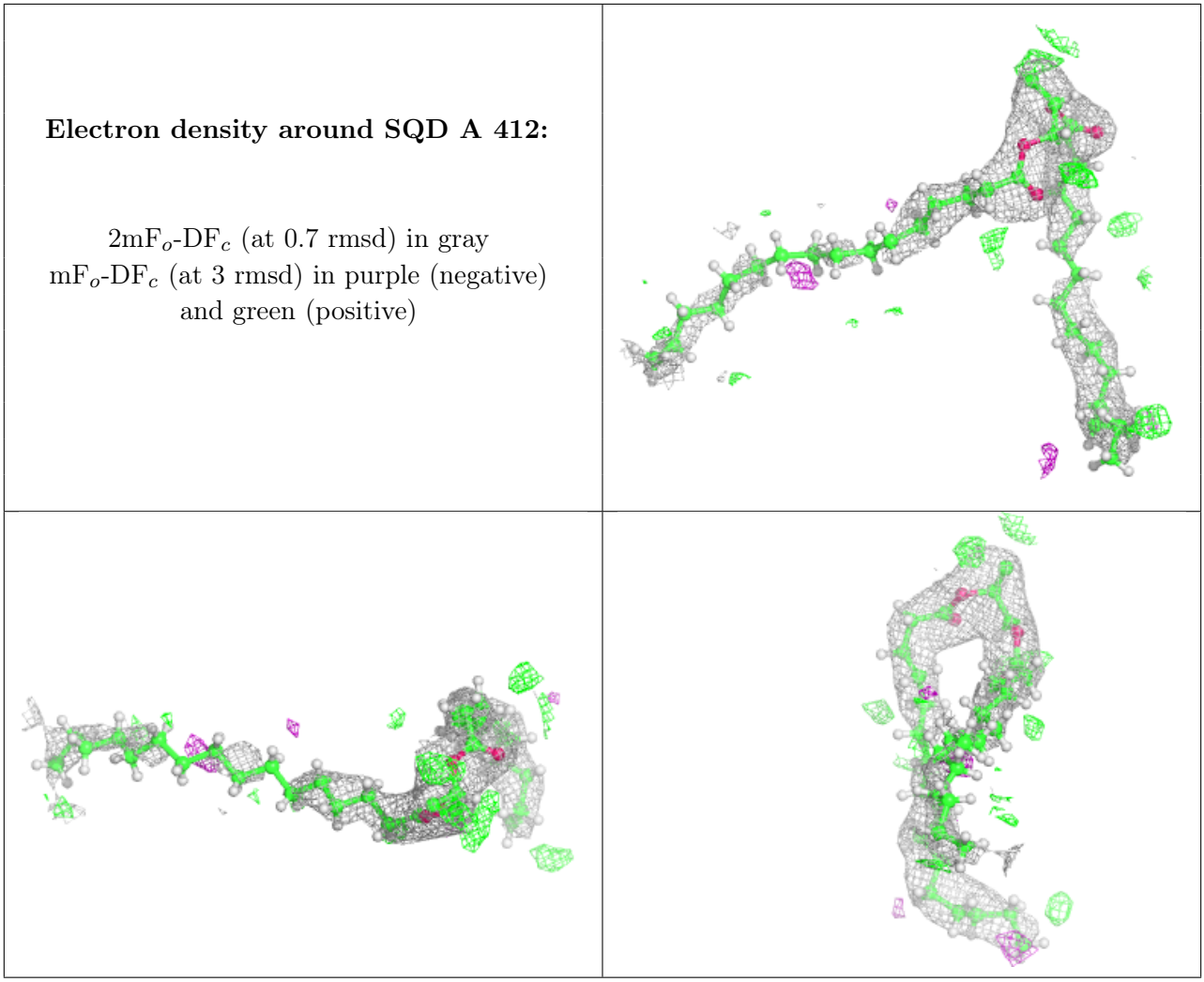






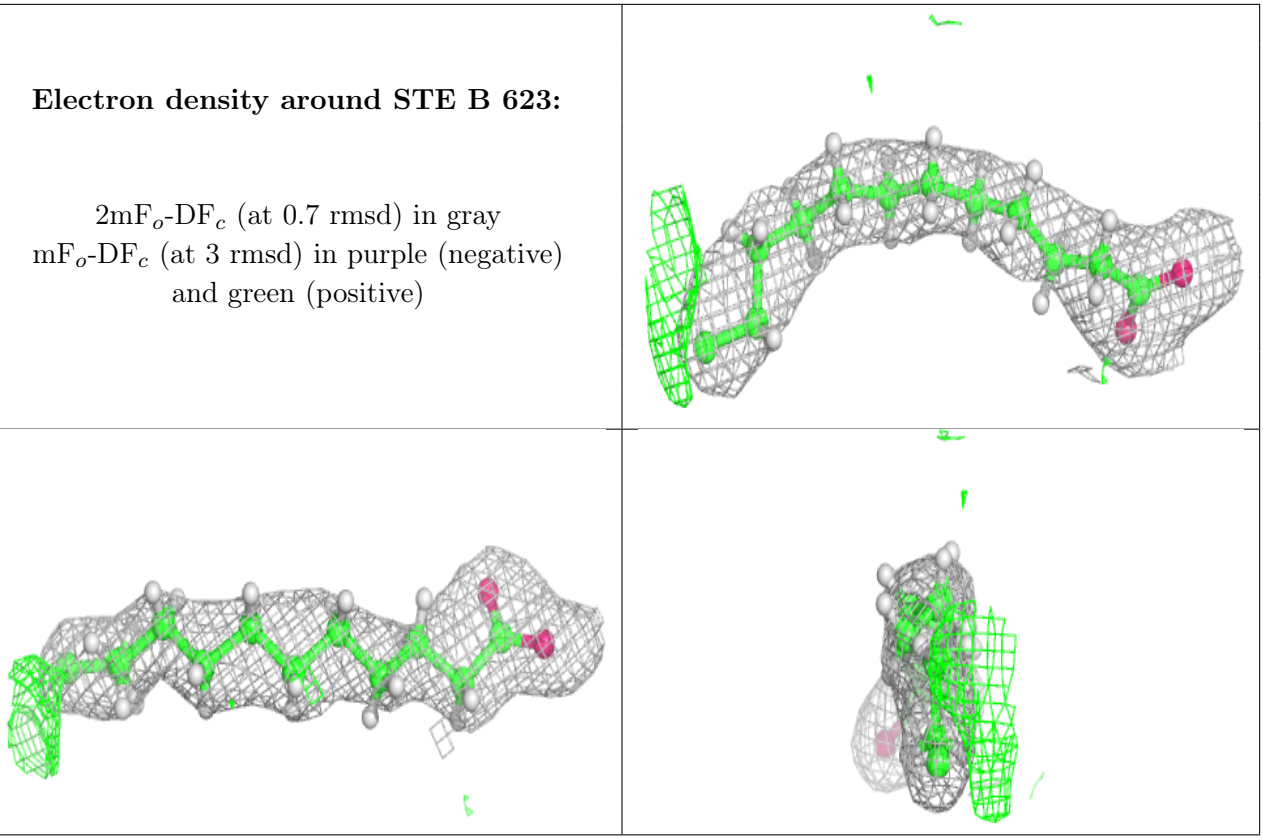
**Electron density around SQD A 412:**

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



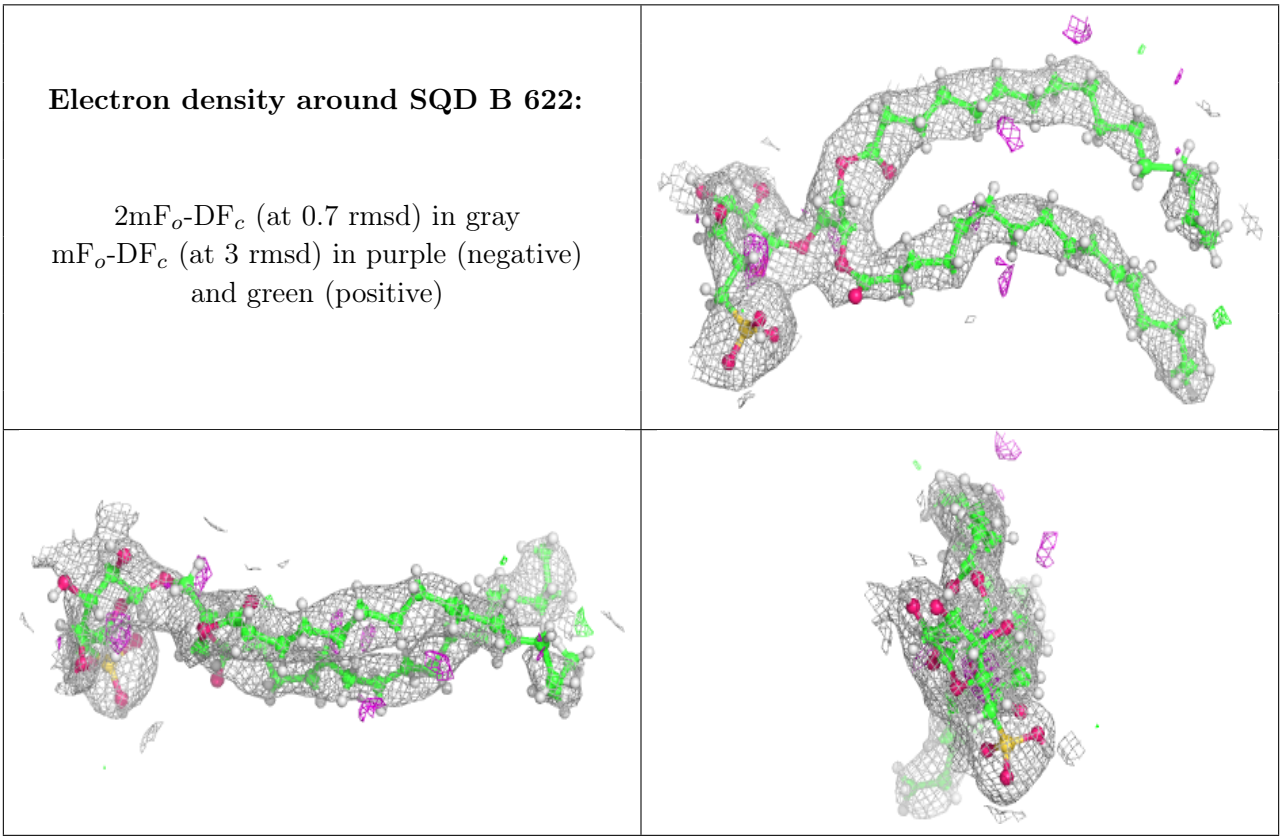
**Electron density around STE B 623:**

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



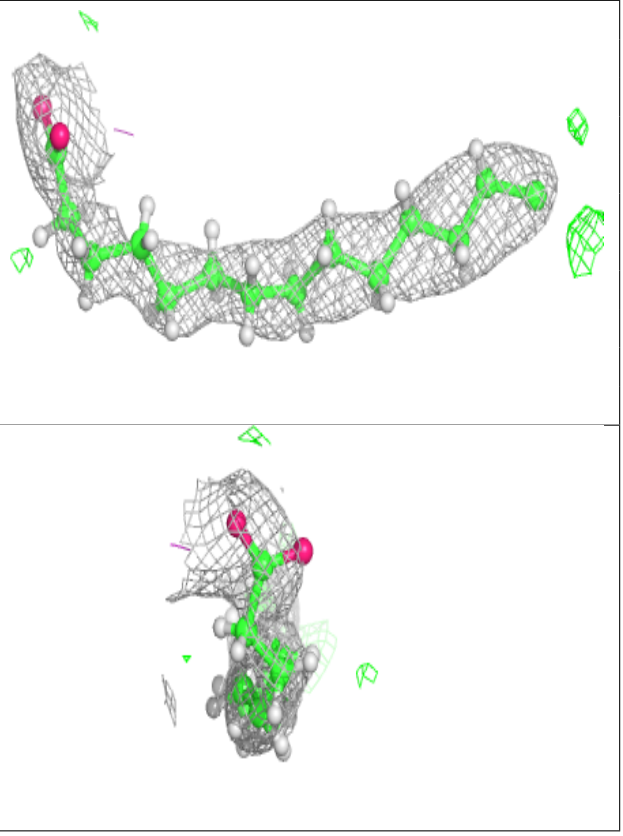
**Electron density around SQD B 622:**

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



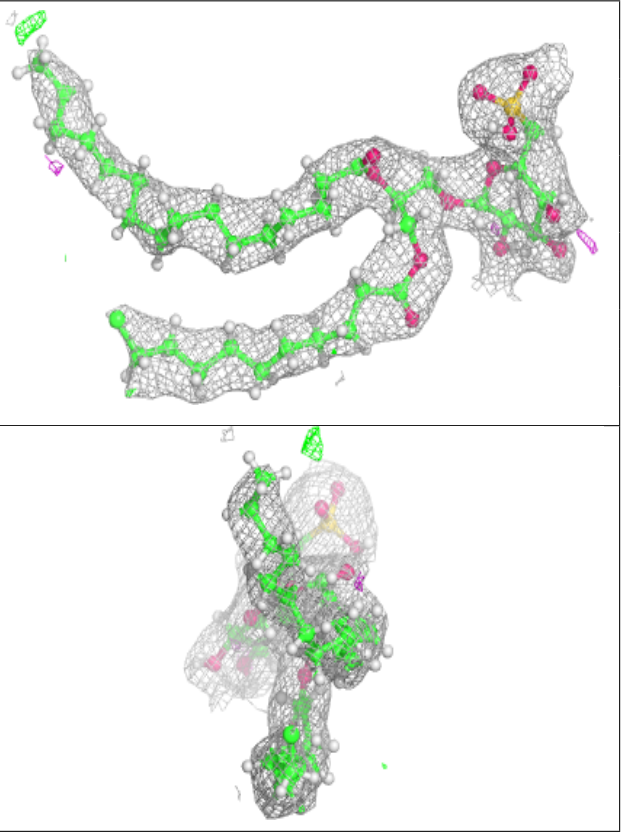
**Electron density around STE d 411:**

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



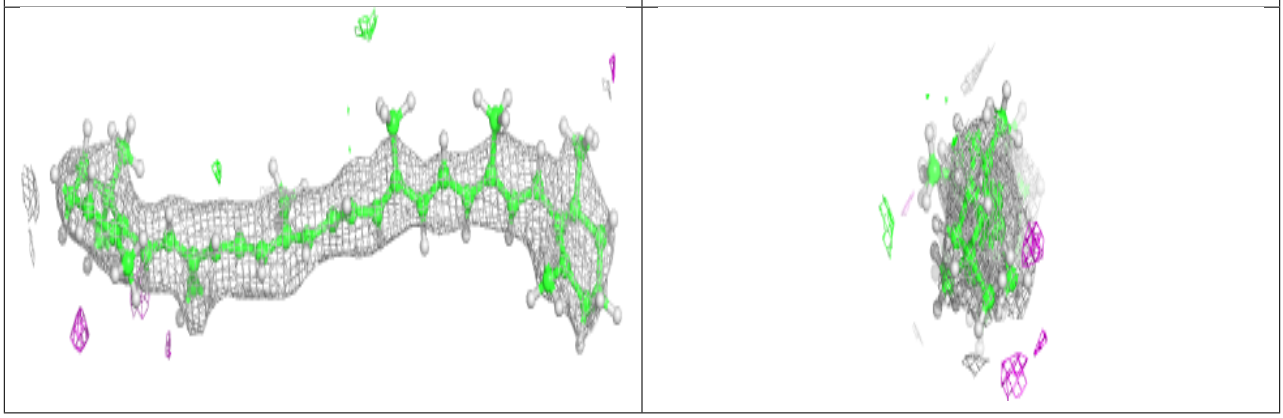
**Electron density around SQD L 101:**

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



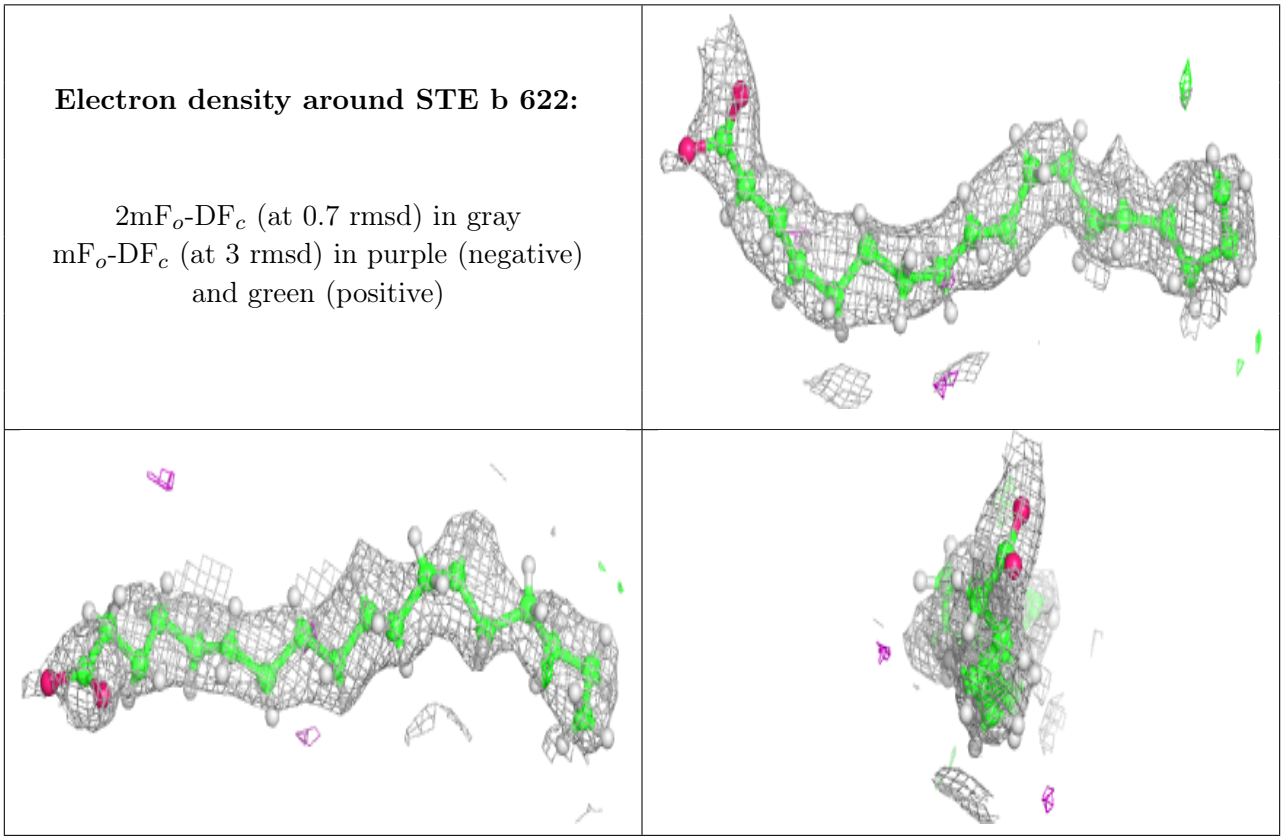
**Electron density around BCR K 101:**

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



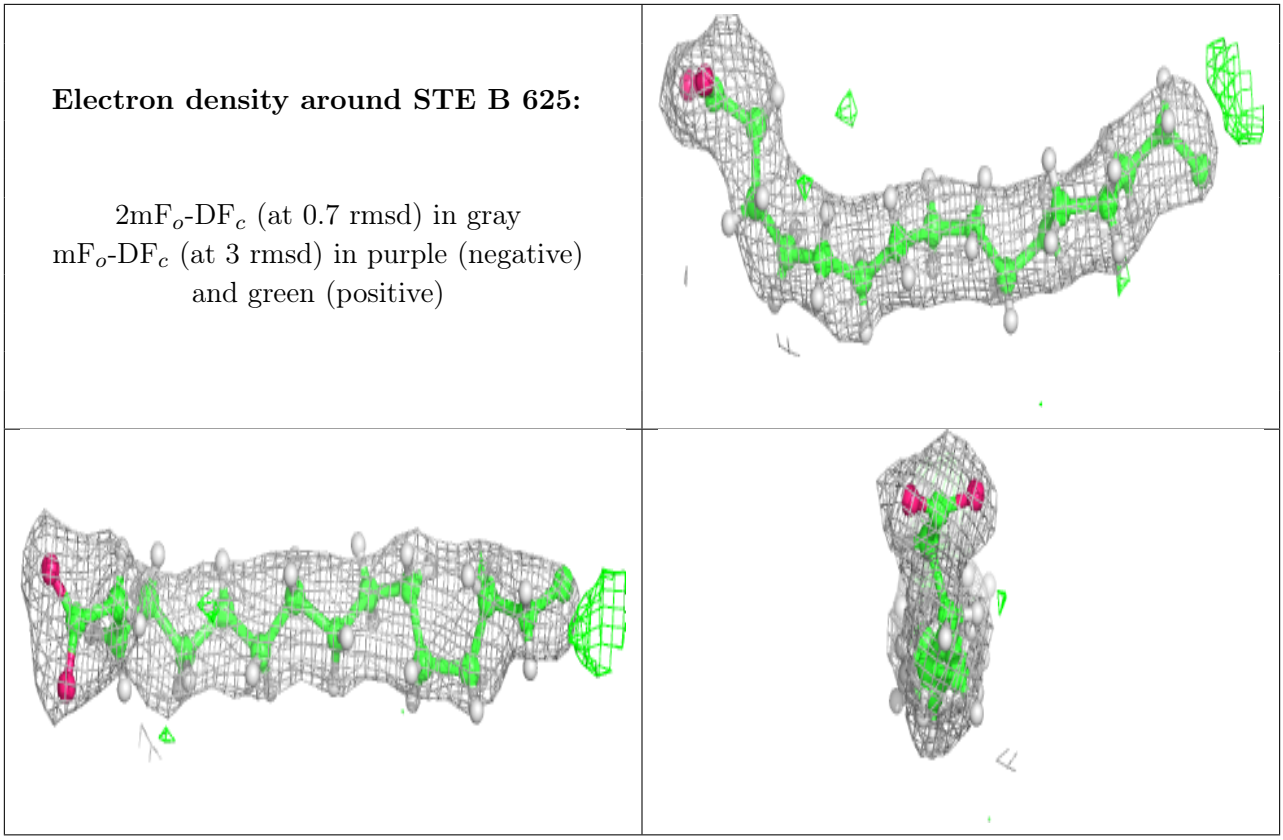
**Electron density around STE b 622:**

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



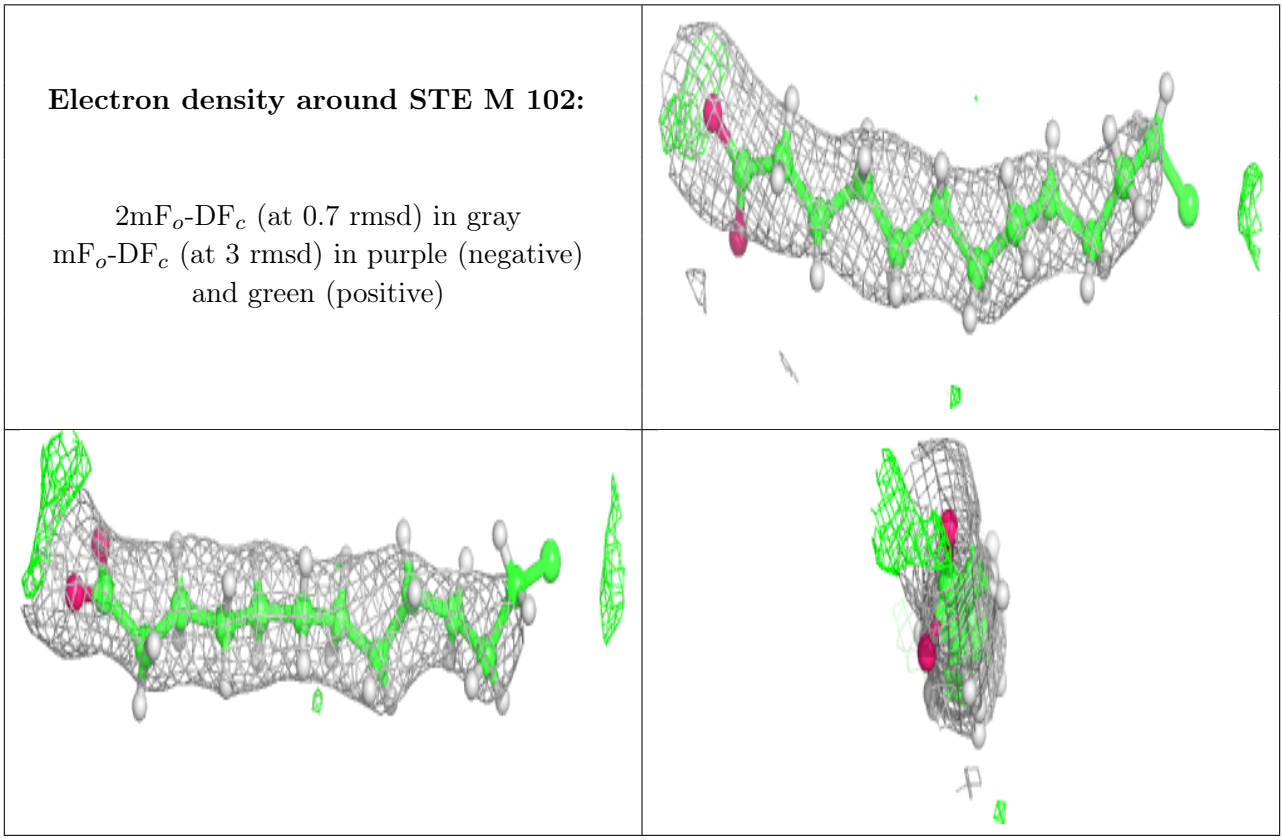
**Electron density around STE B 625:**

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



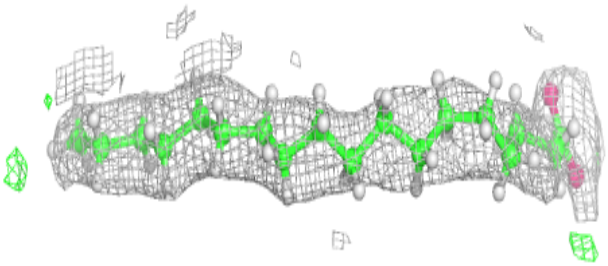
**Electron density around STE M 102:**

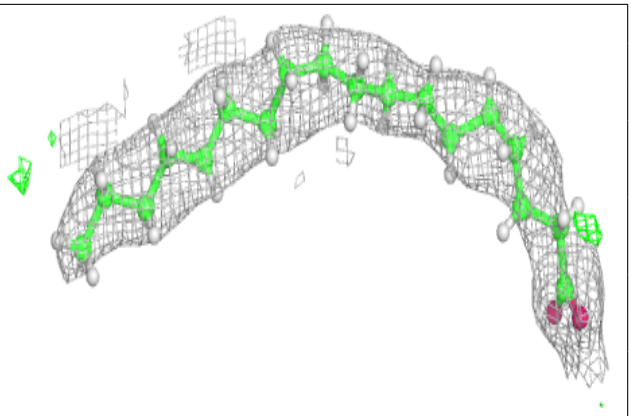
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

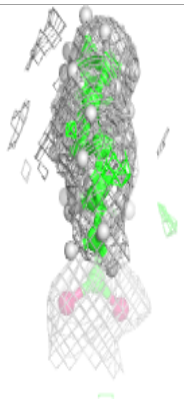


**Electron density around STE D 413:**

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

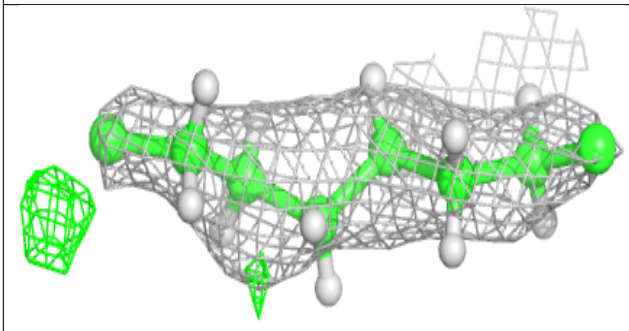


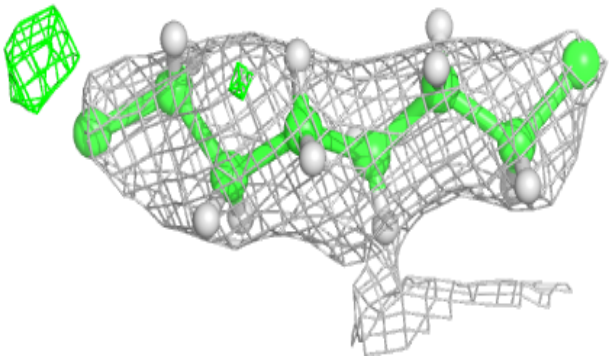


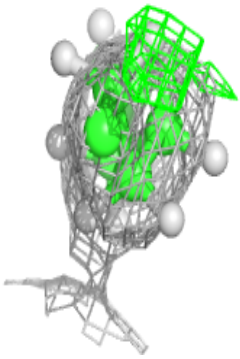


**Electron density around STE Z 101:**

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

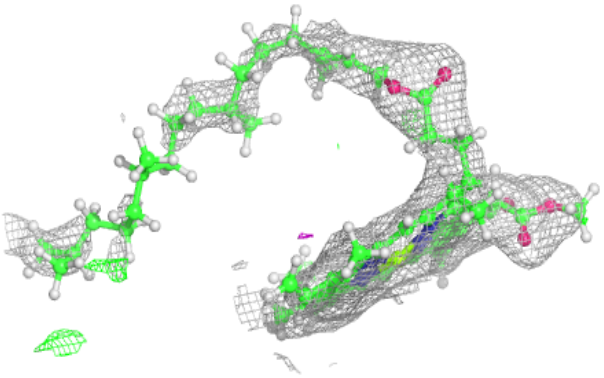


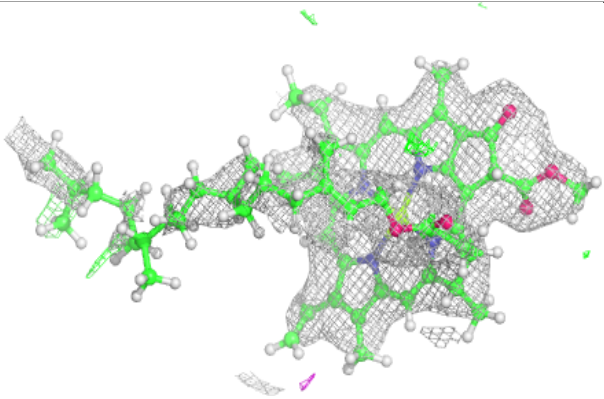


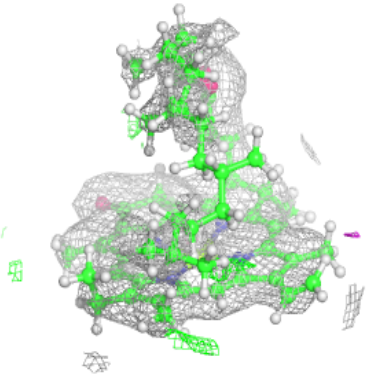


**Electron density around CLA C 513:**

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

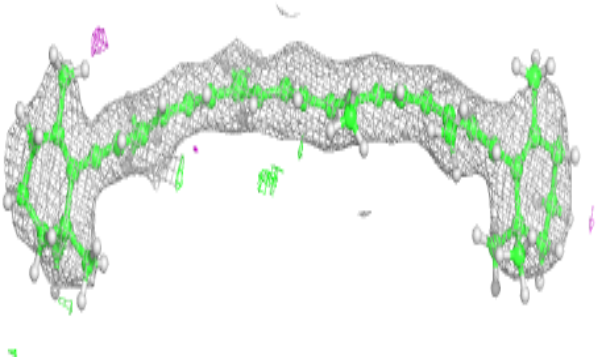


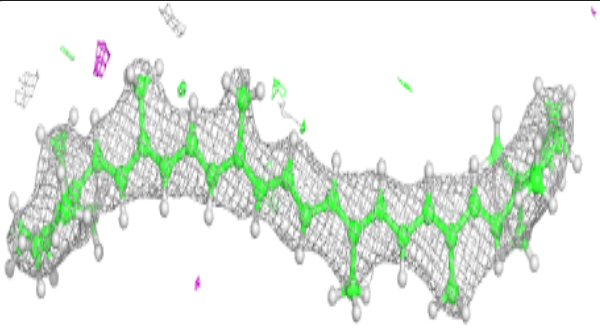


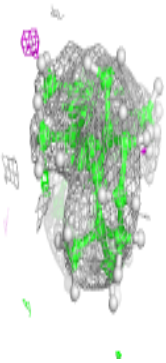


**Electron density around BCR k 102:**

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

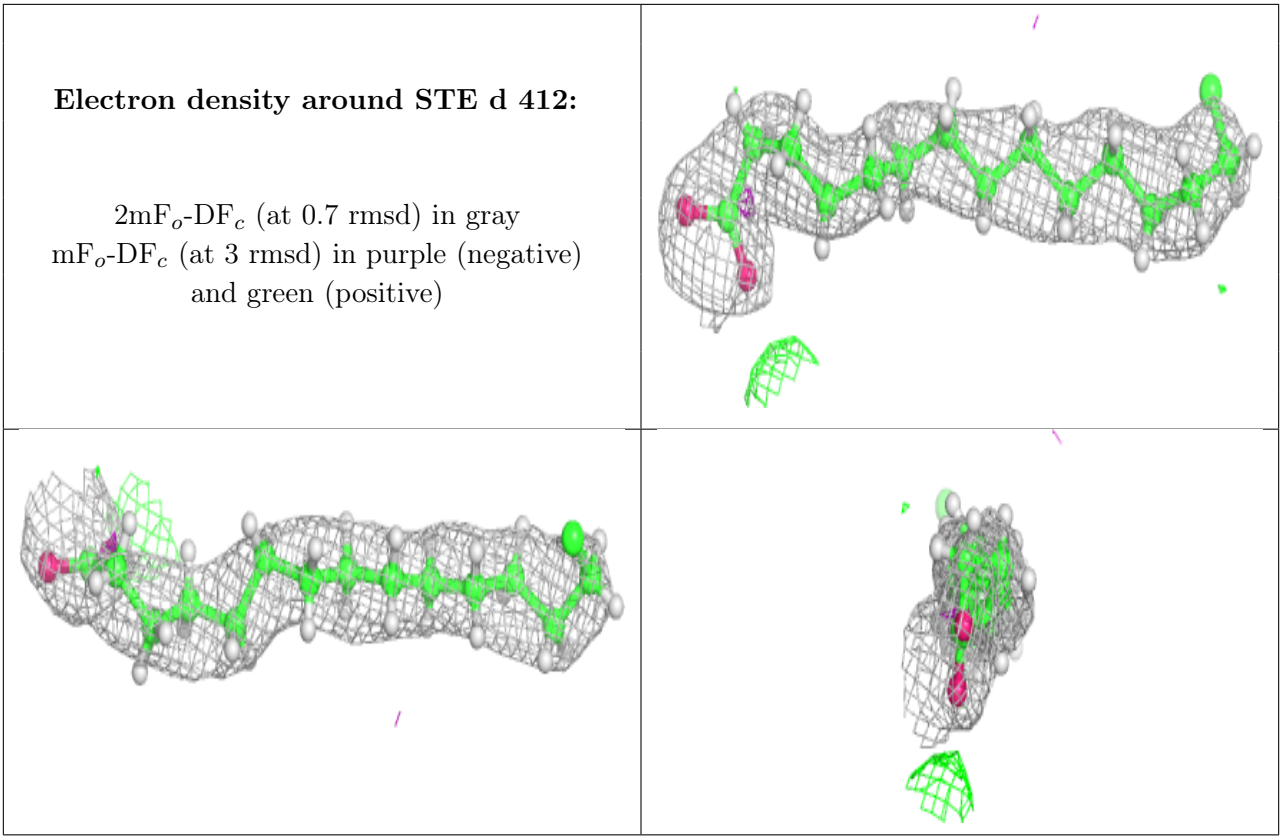






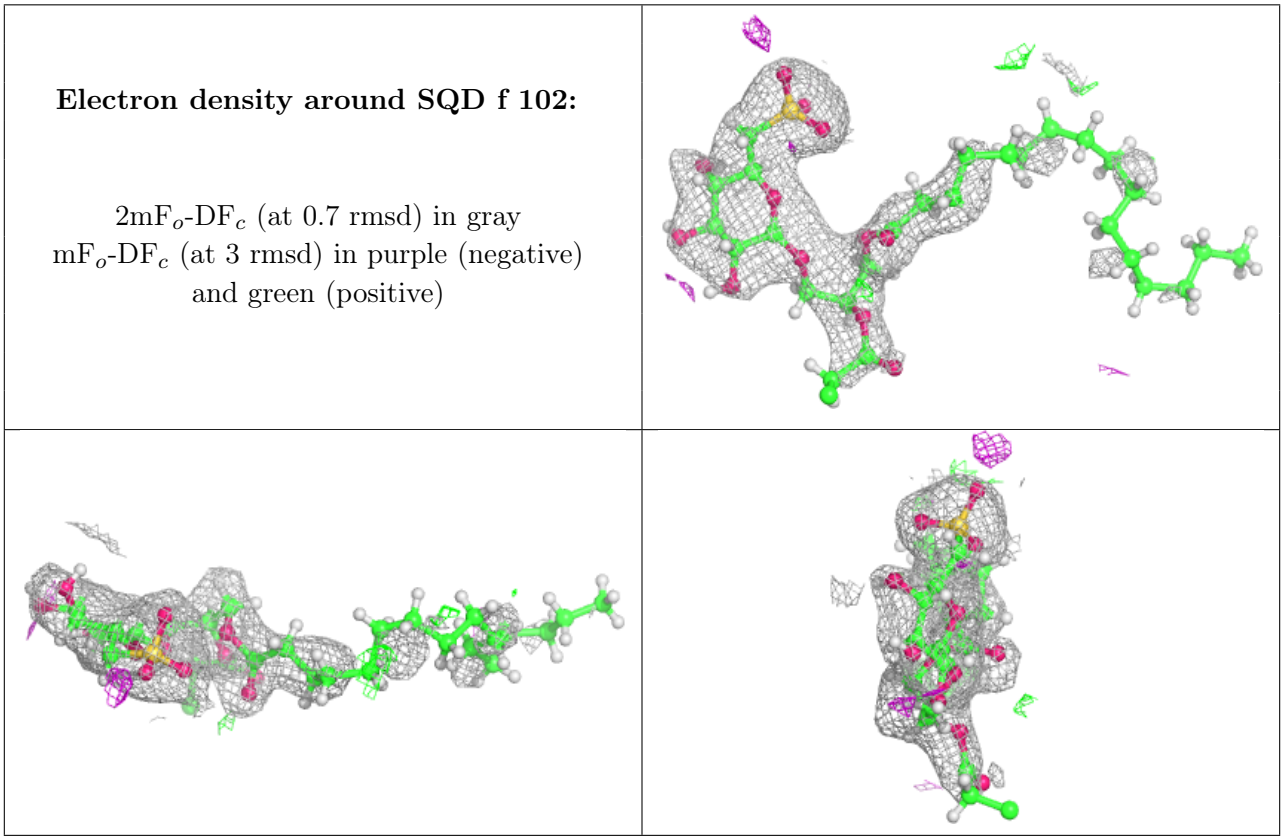
**Electron density around STE d 412:**

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



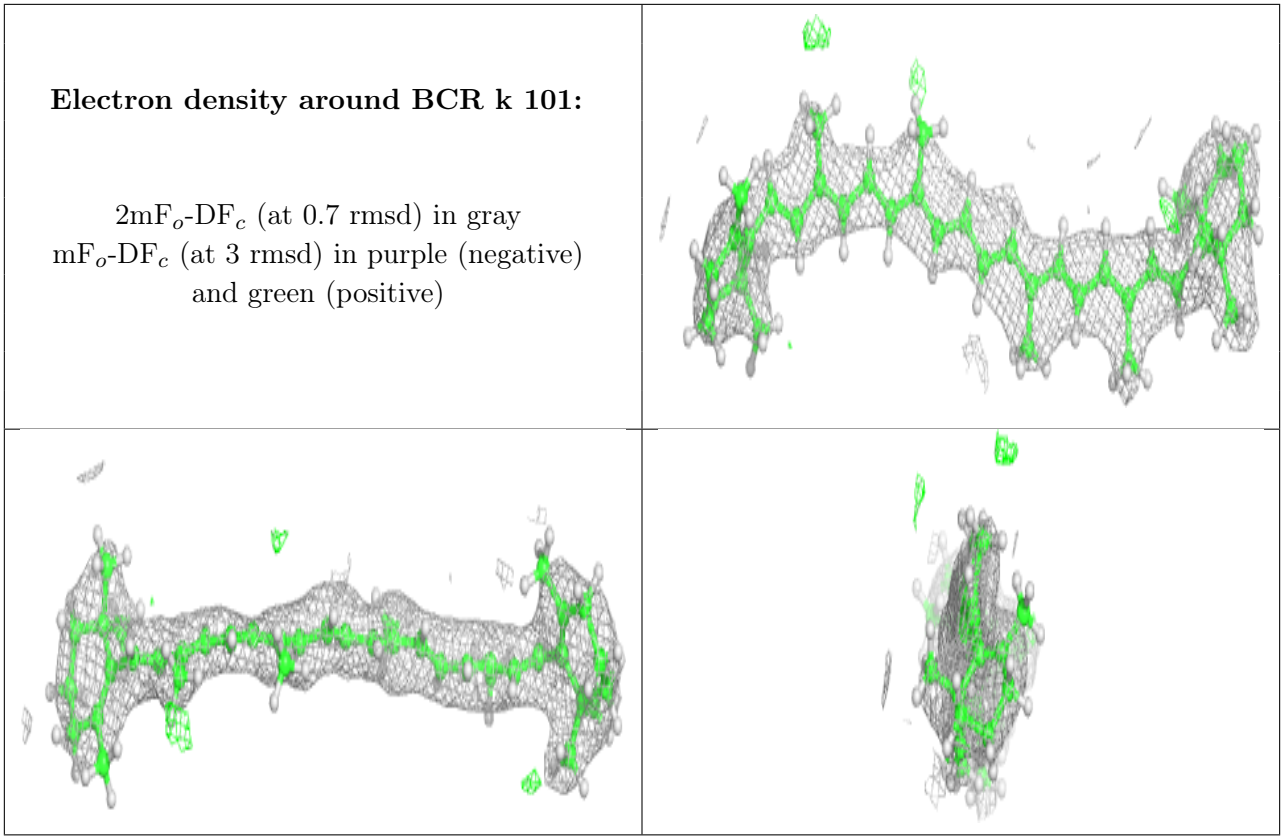
**Electron density around SQD f 102:**

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



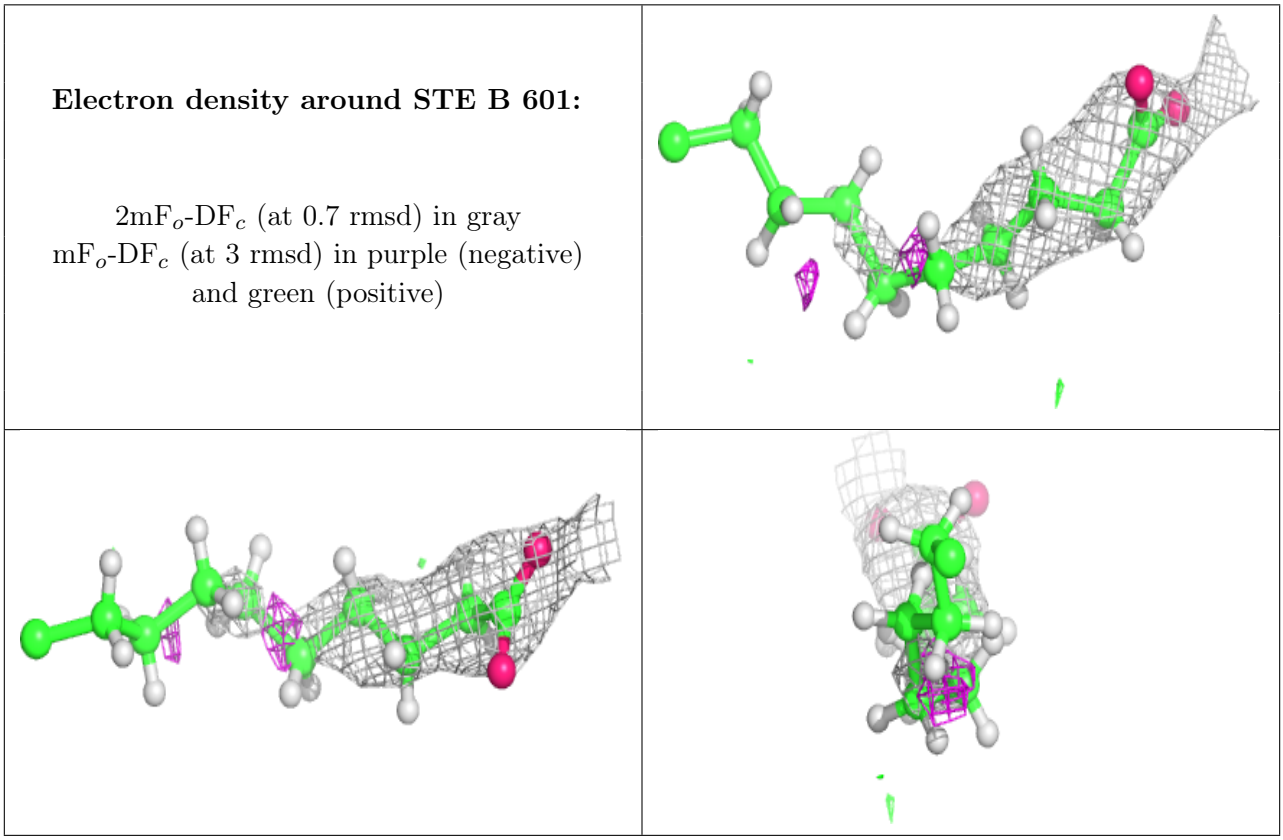
**Electron density around BCR k 101:**

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



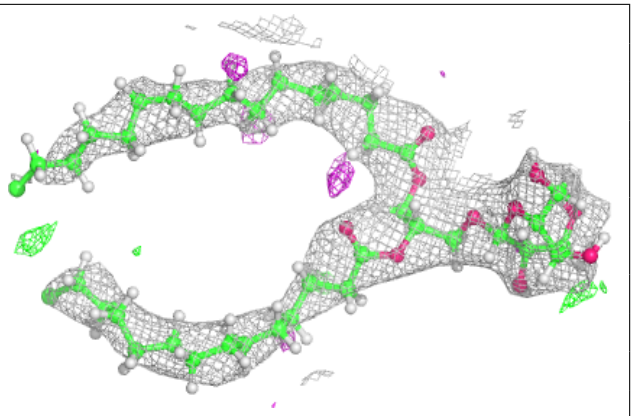
**Electron density around STE B 601:**

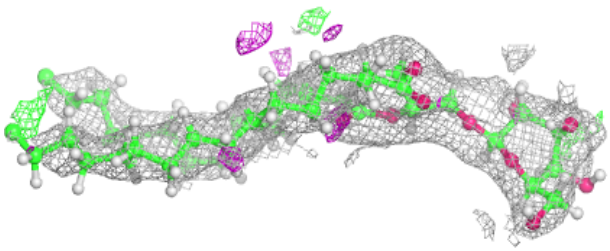
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

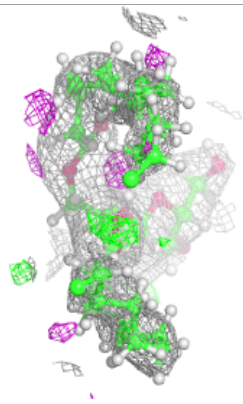


**Electron density around LMG c 523:**

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

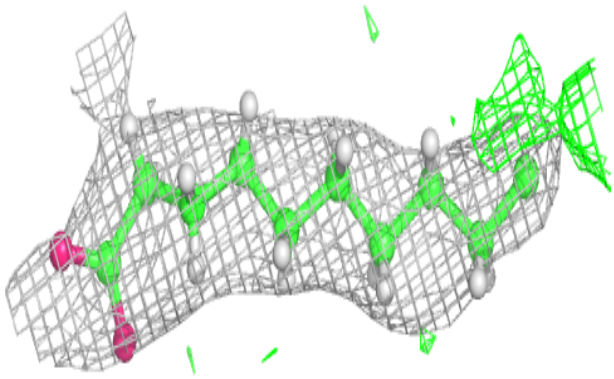


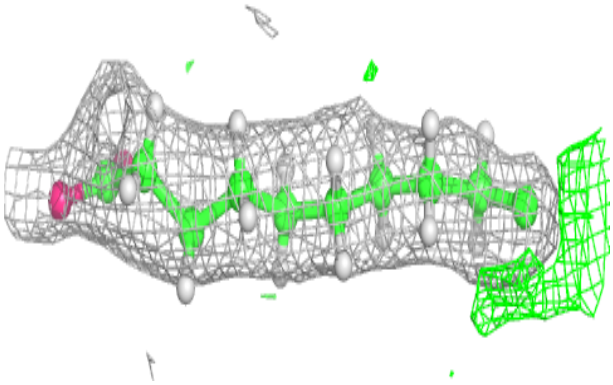


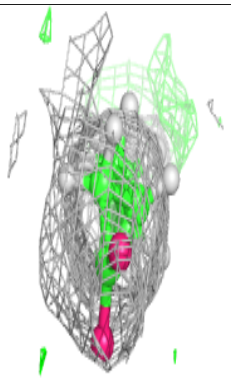


**Electron density around STE J 101:**

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

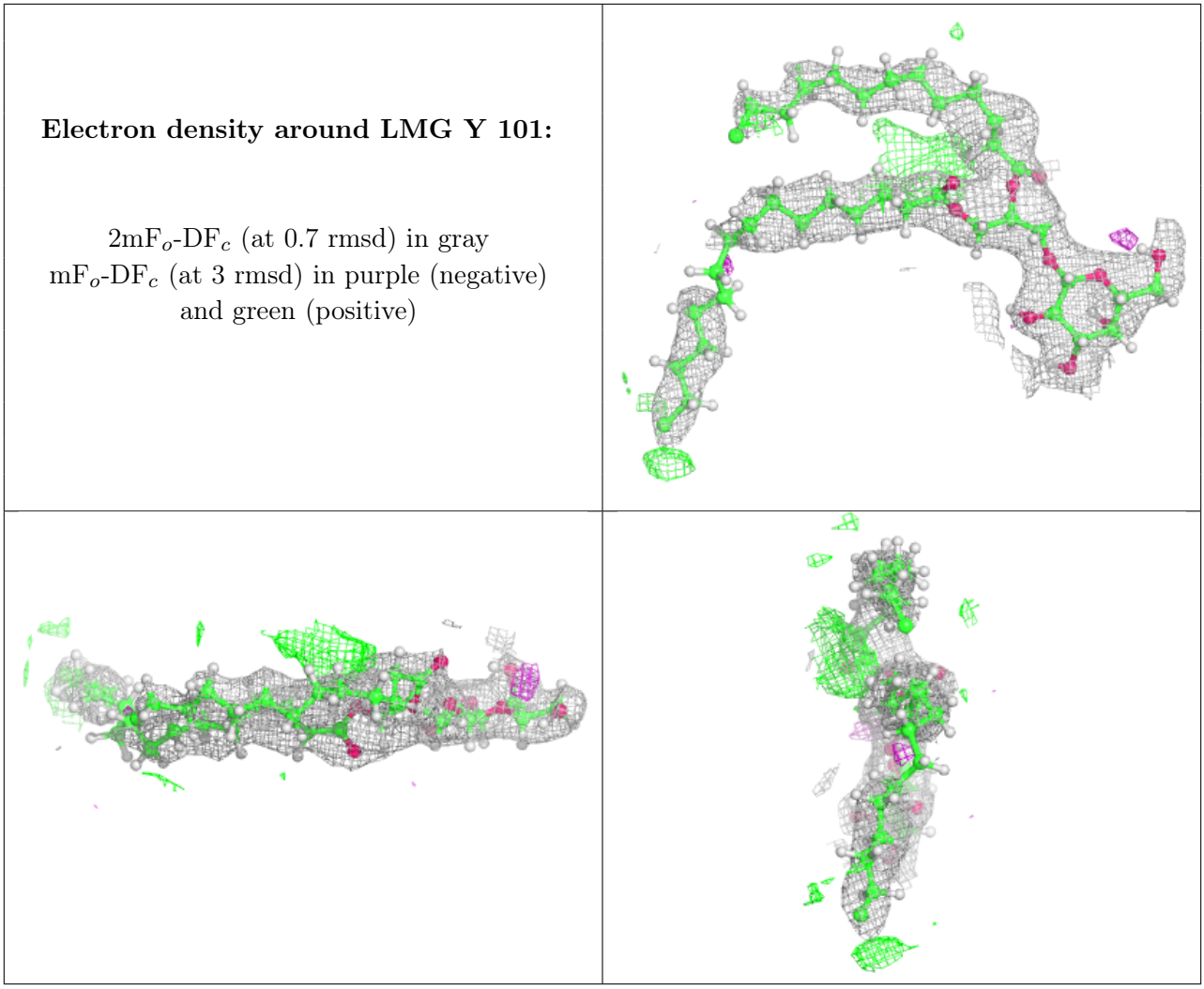






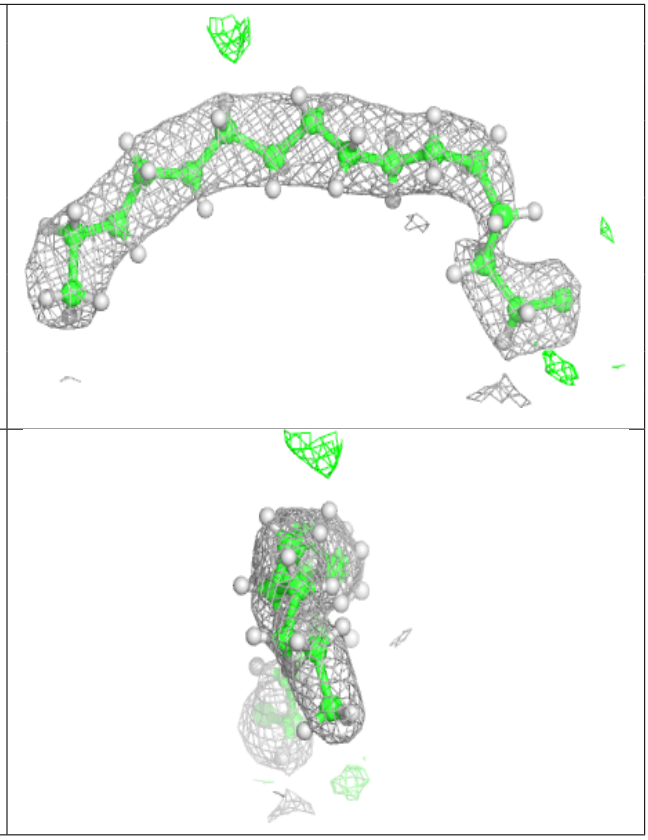
**Electron density around LMG Y 101:**

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



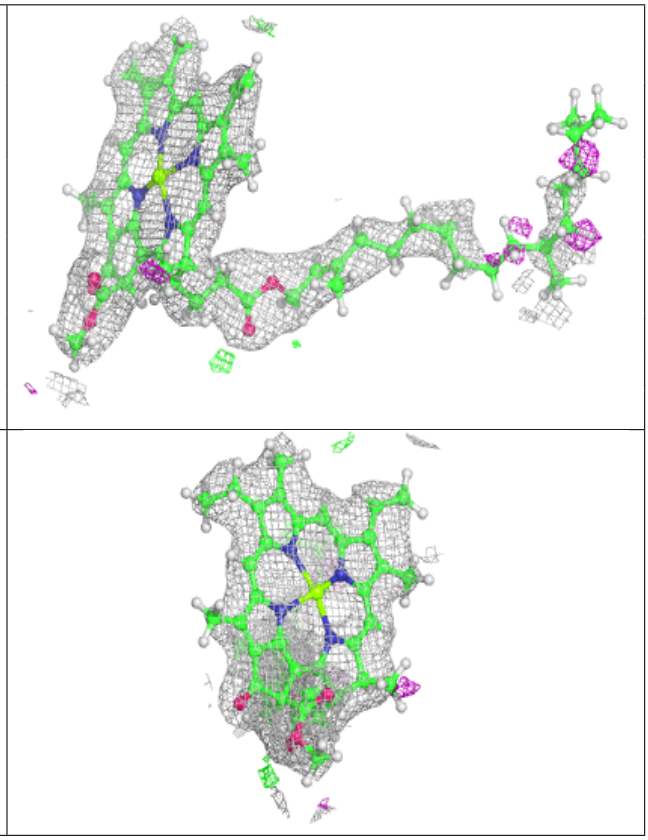
**Electron density around STE b 620:**

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



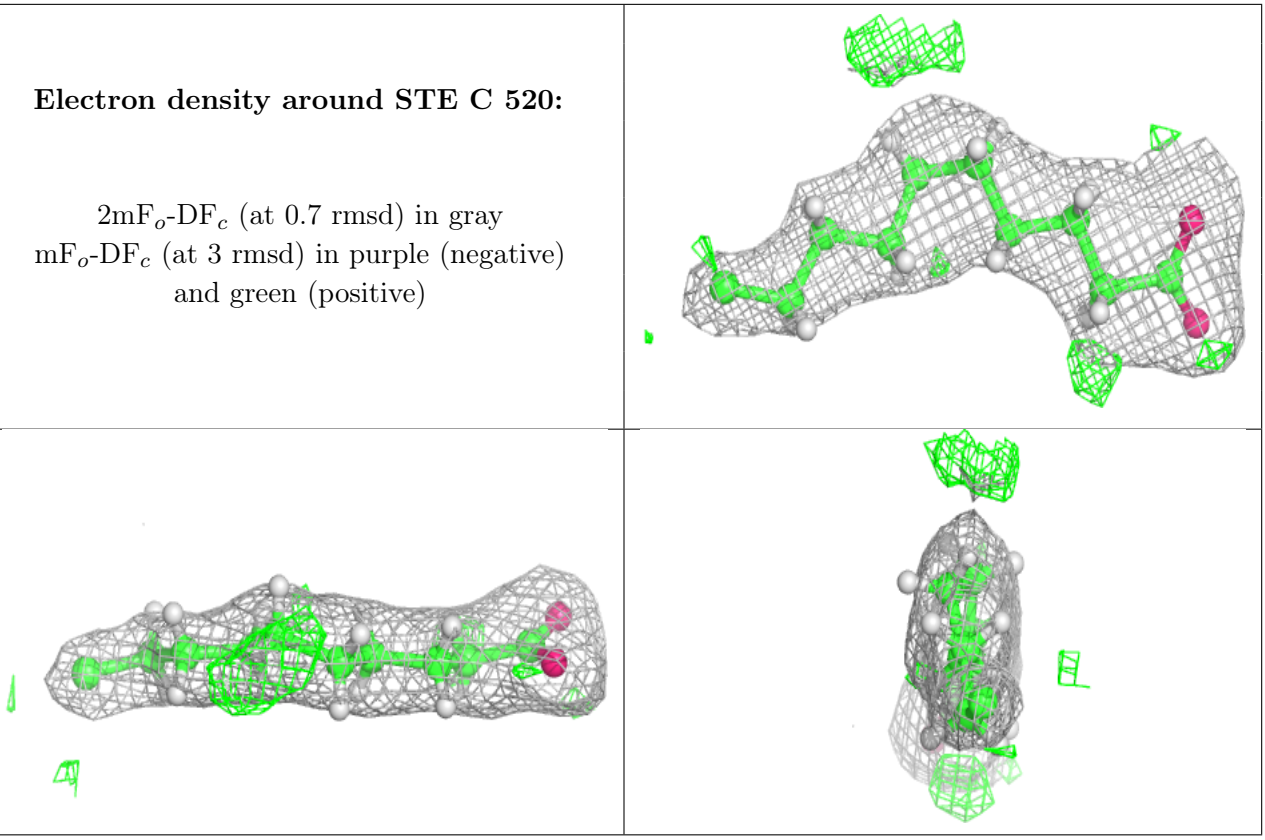
**Electron density around CLA d 404:**

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



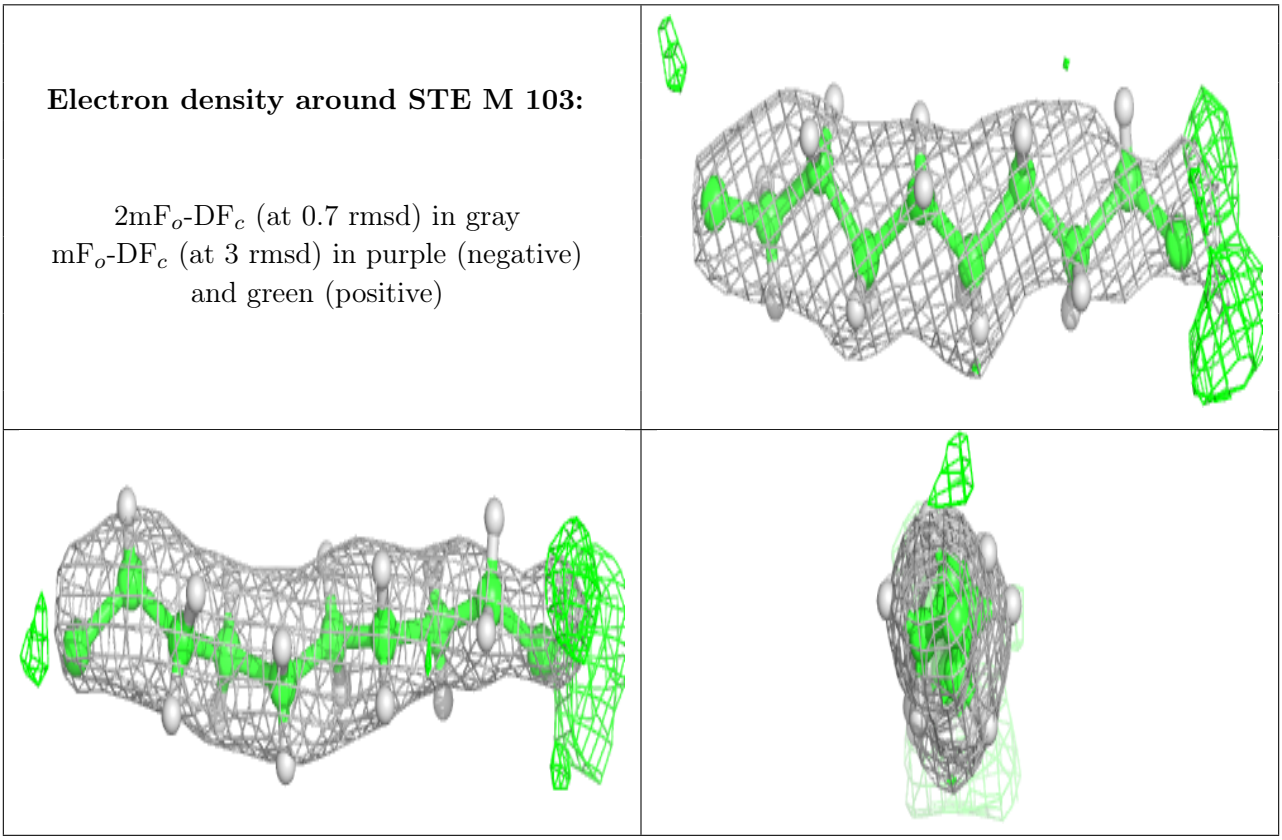
**Electron density around STE C 520:**

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



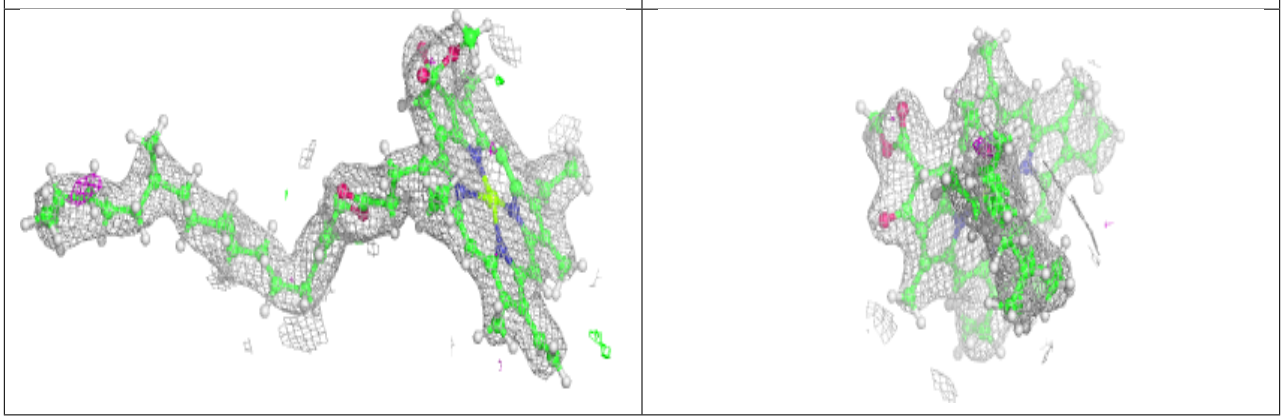
**Electron density around STE M 103:**

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



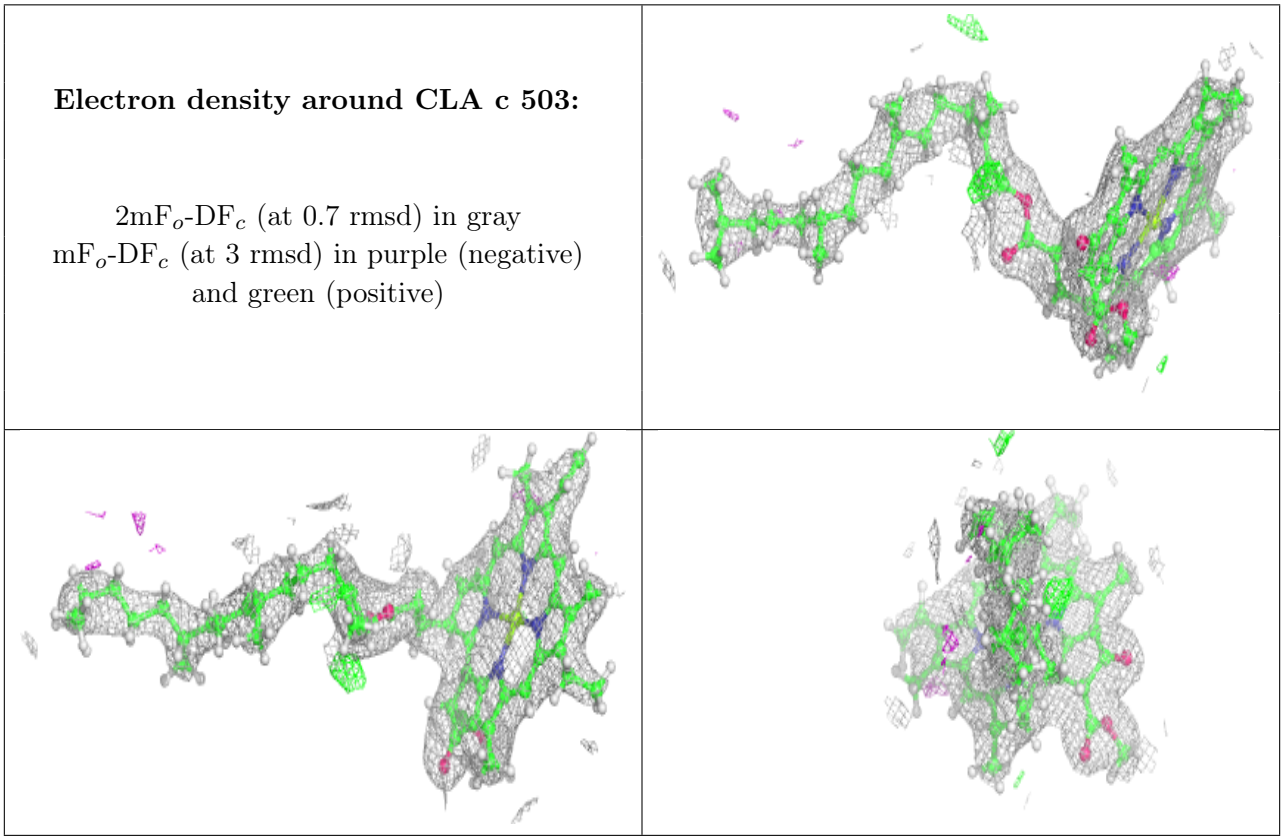
**Electron density around CLA C 502:**

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



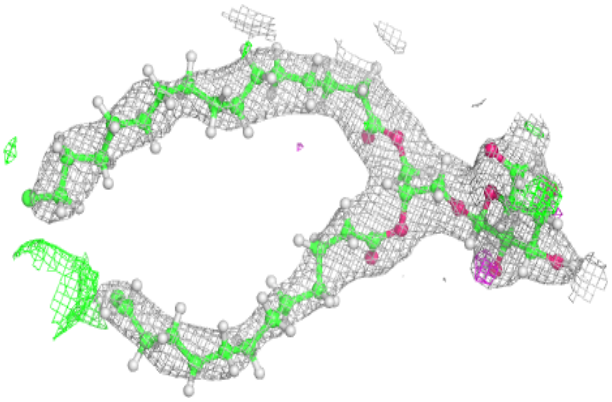
**Electron density around CLA c 503:**

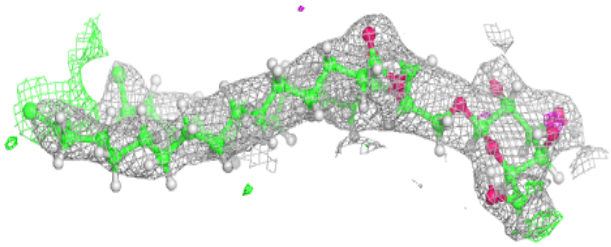
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

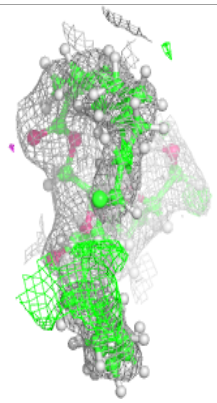


**Electron density around LMG A 410:**

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

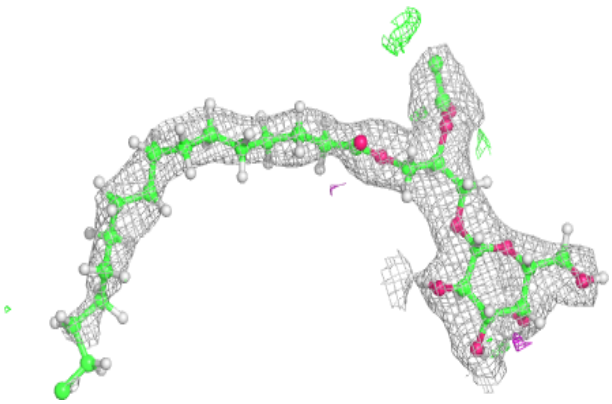


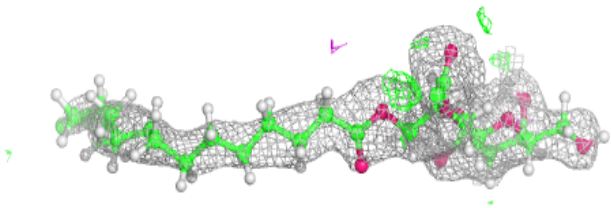


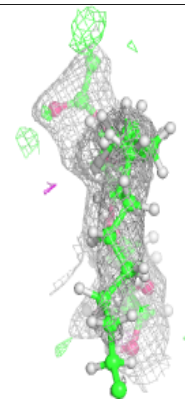


**Electron density around LMG c 520:**

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

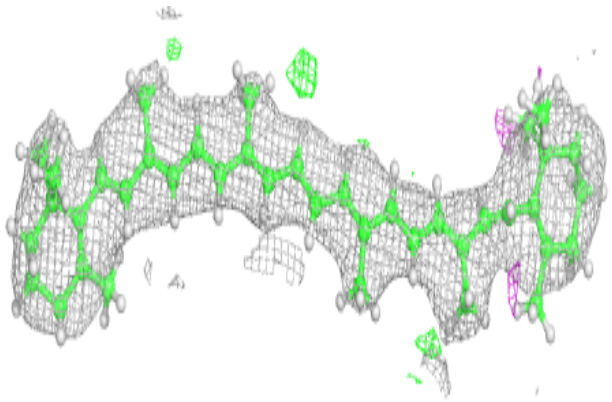


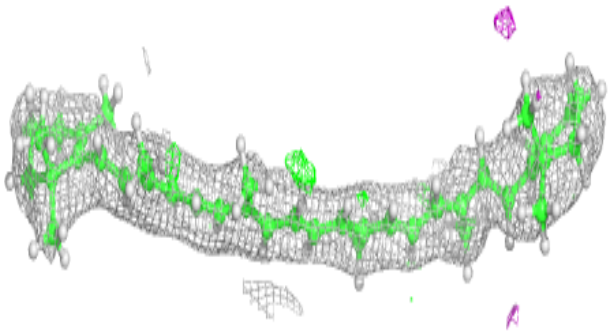


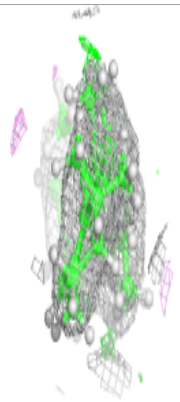


**Electron density around BCR d 405:**

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

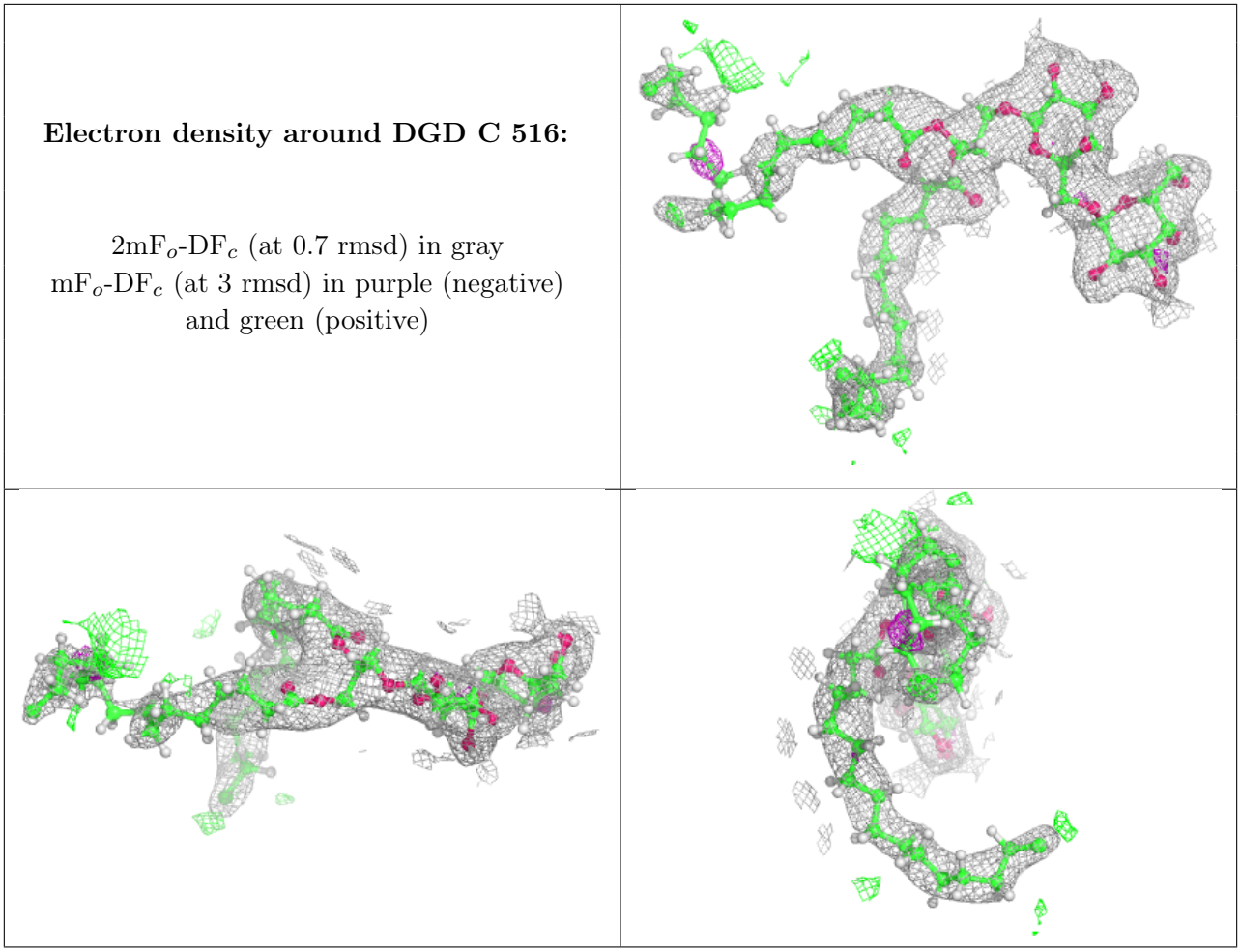






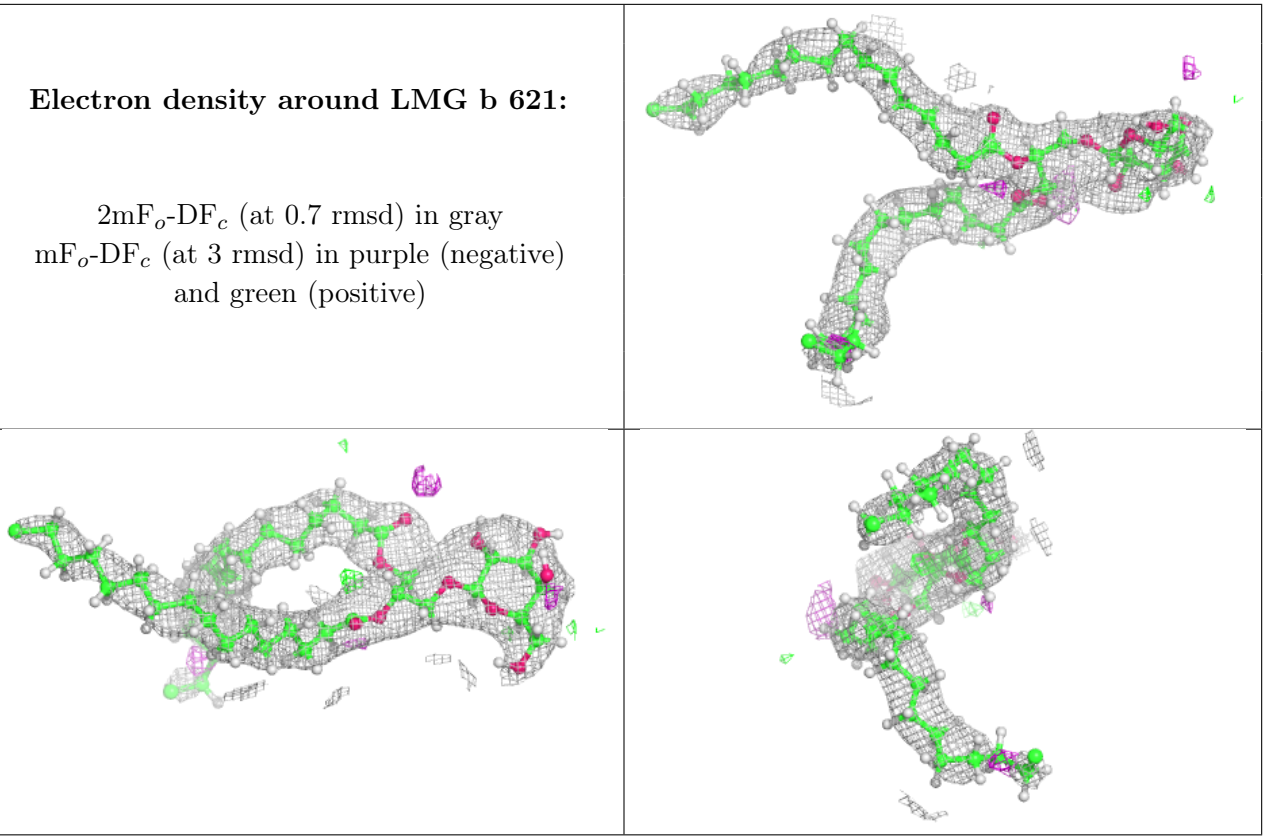
**Electron density around DGD C 516:**

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



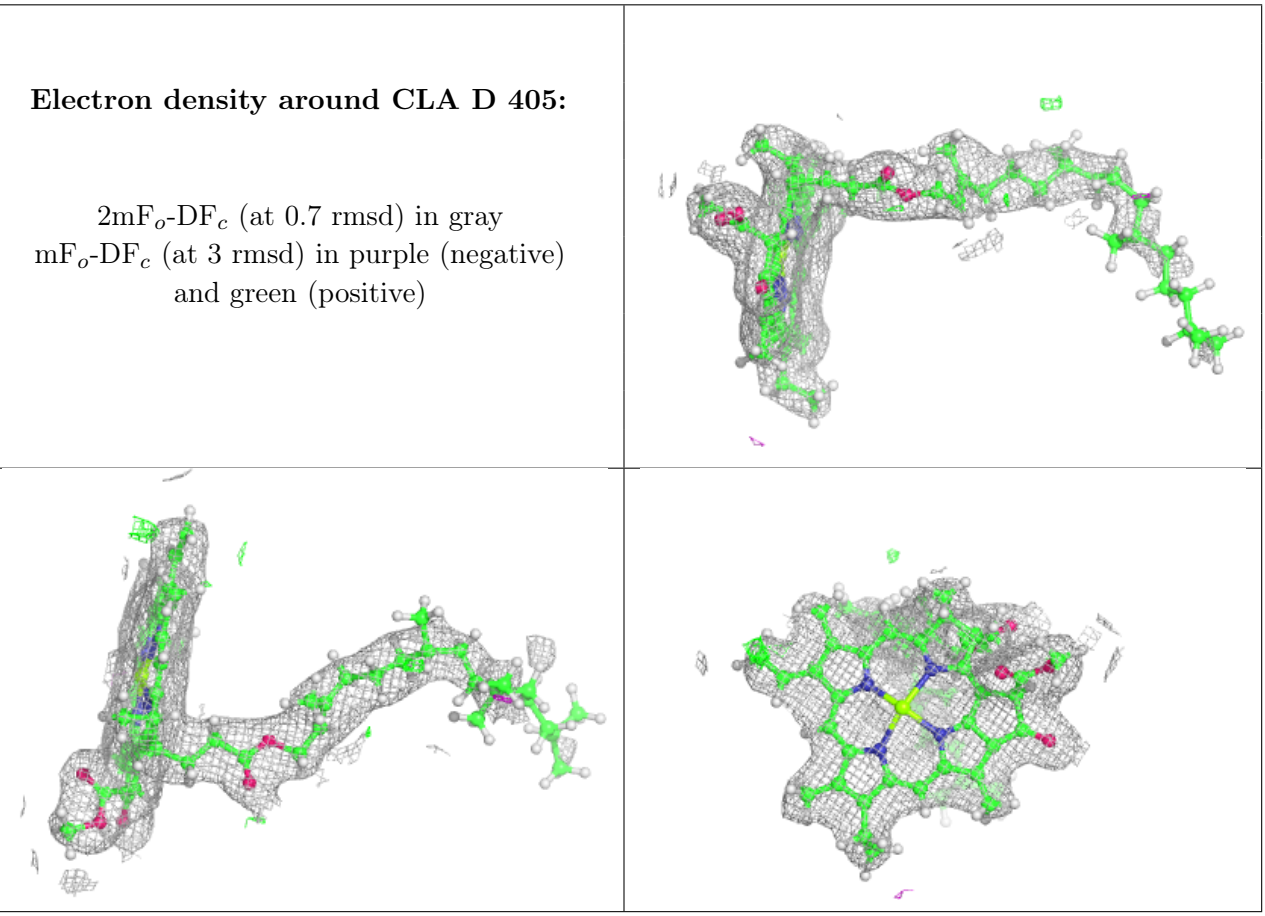
**Electron density around LMG b 621:**

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



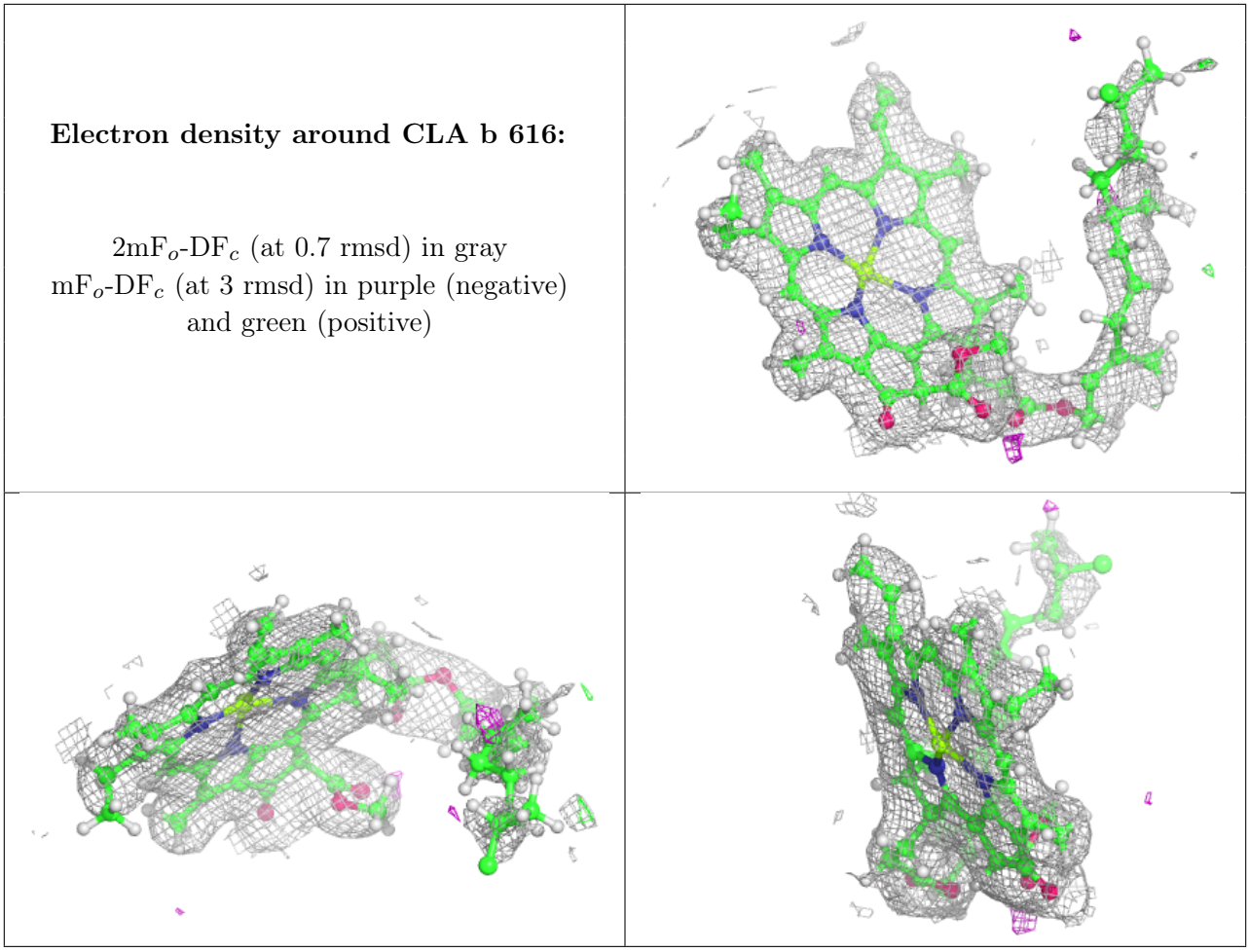
**Electron density around CLA D 405:**

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



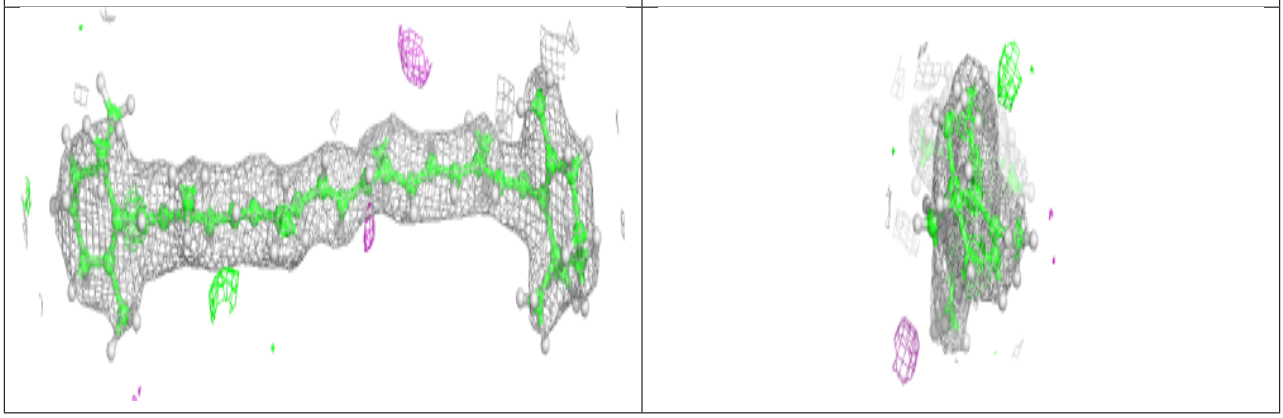
**Electron density around CLA b 616:**

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



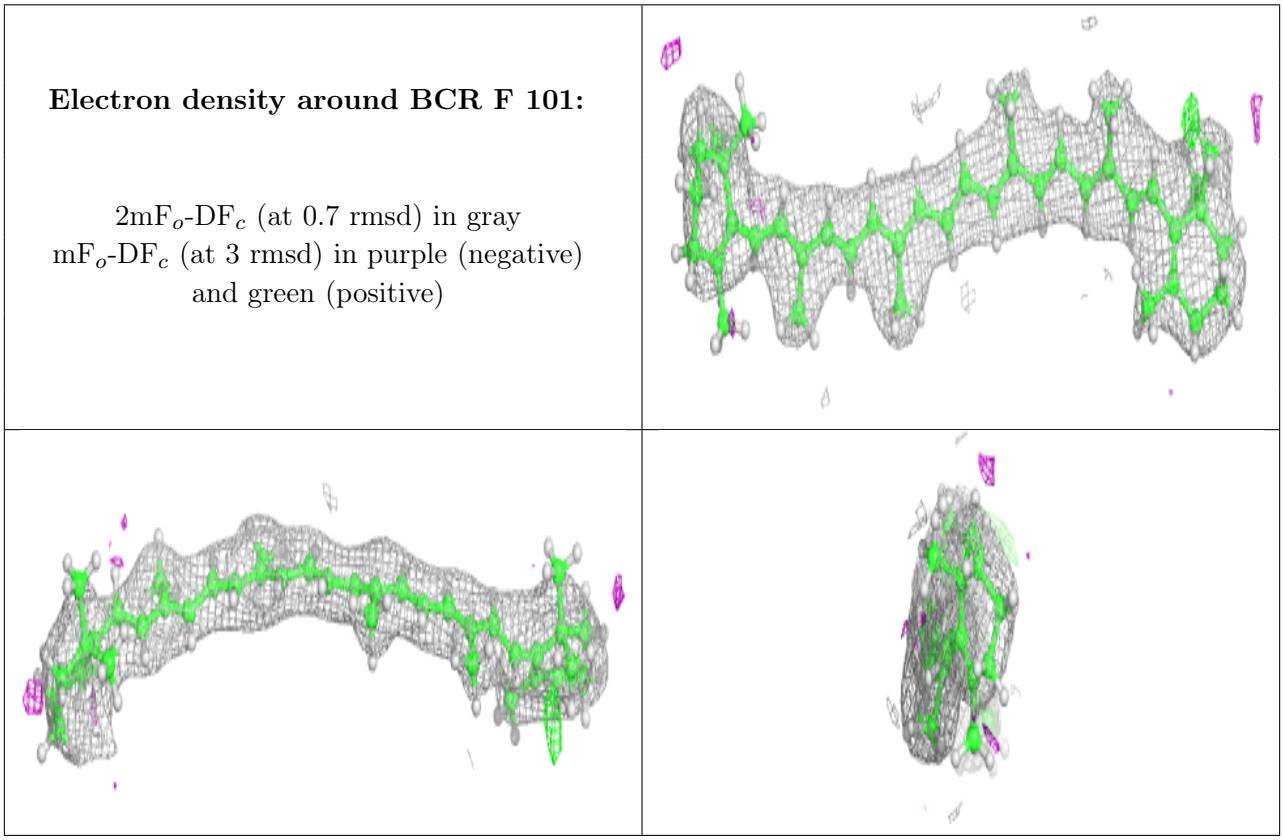
**Electron density around BCR C 514:**

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



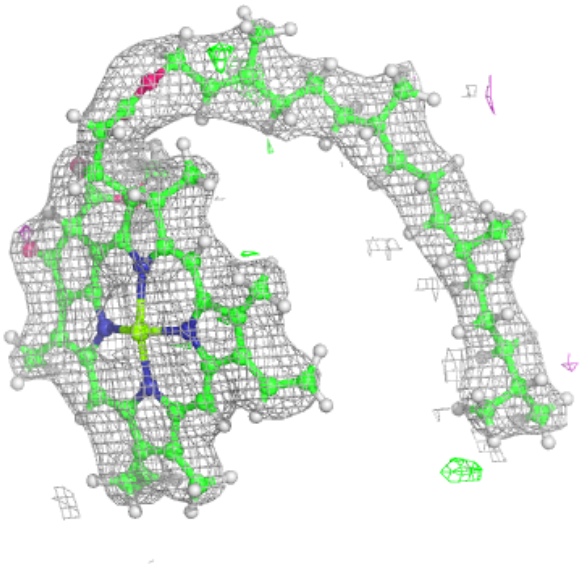
**Electron density around BCR F 101:**

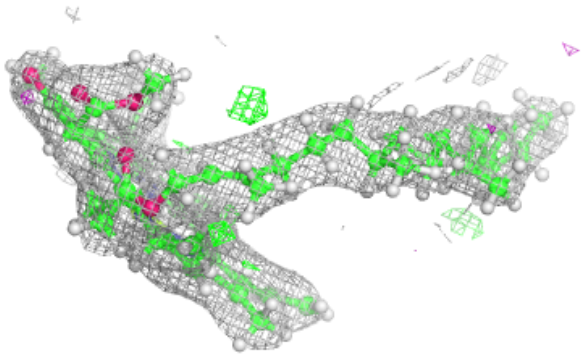
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

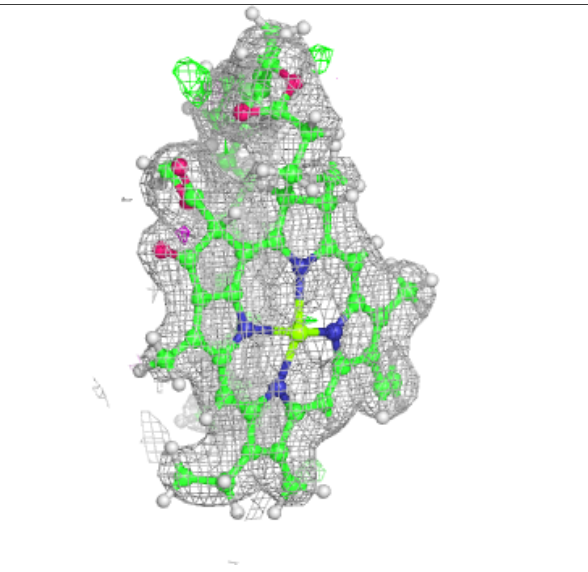


**Electron density around CLA C 507:**

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

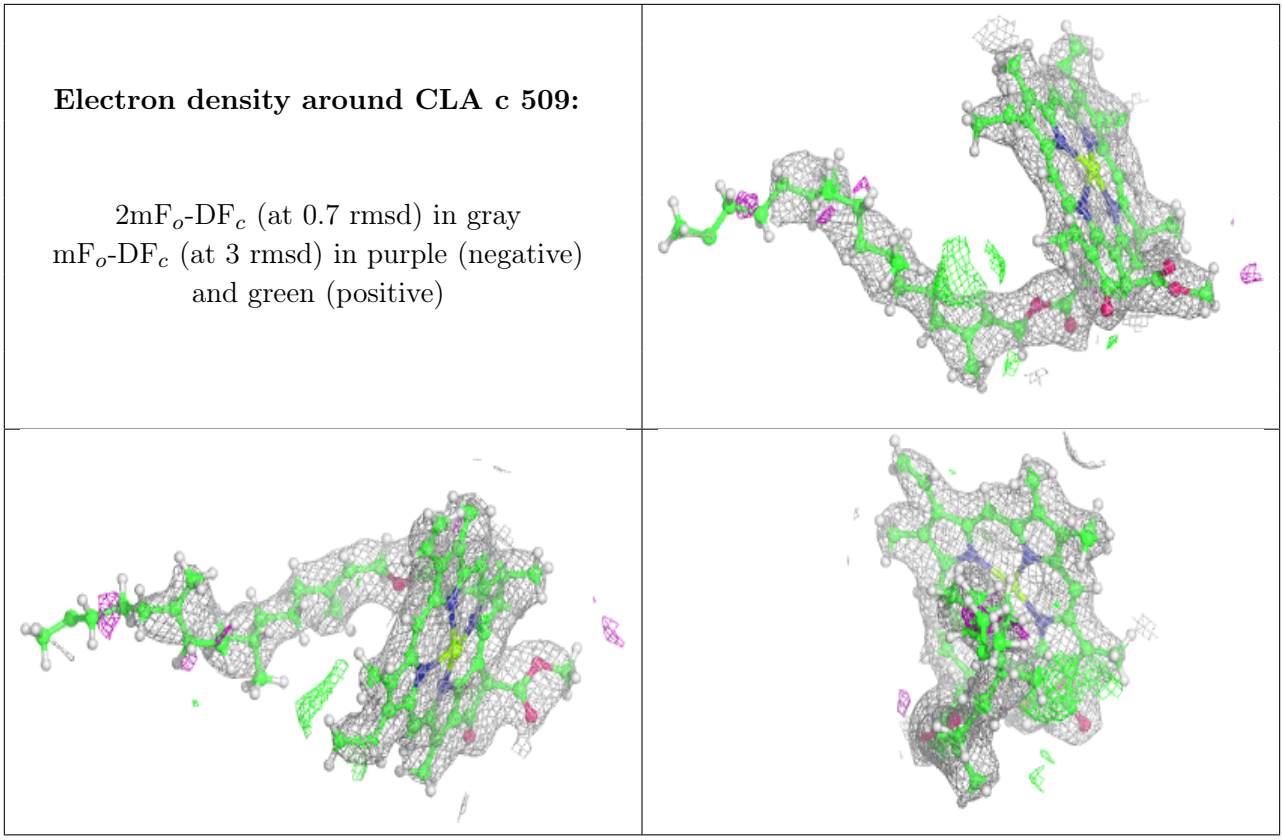






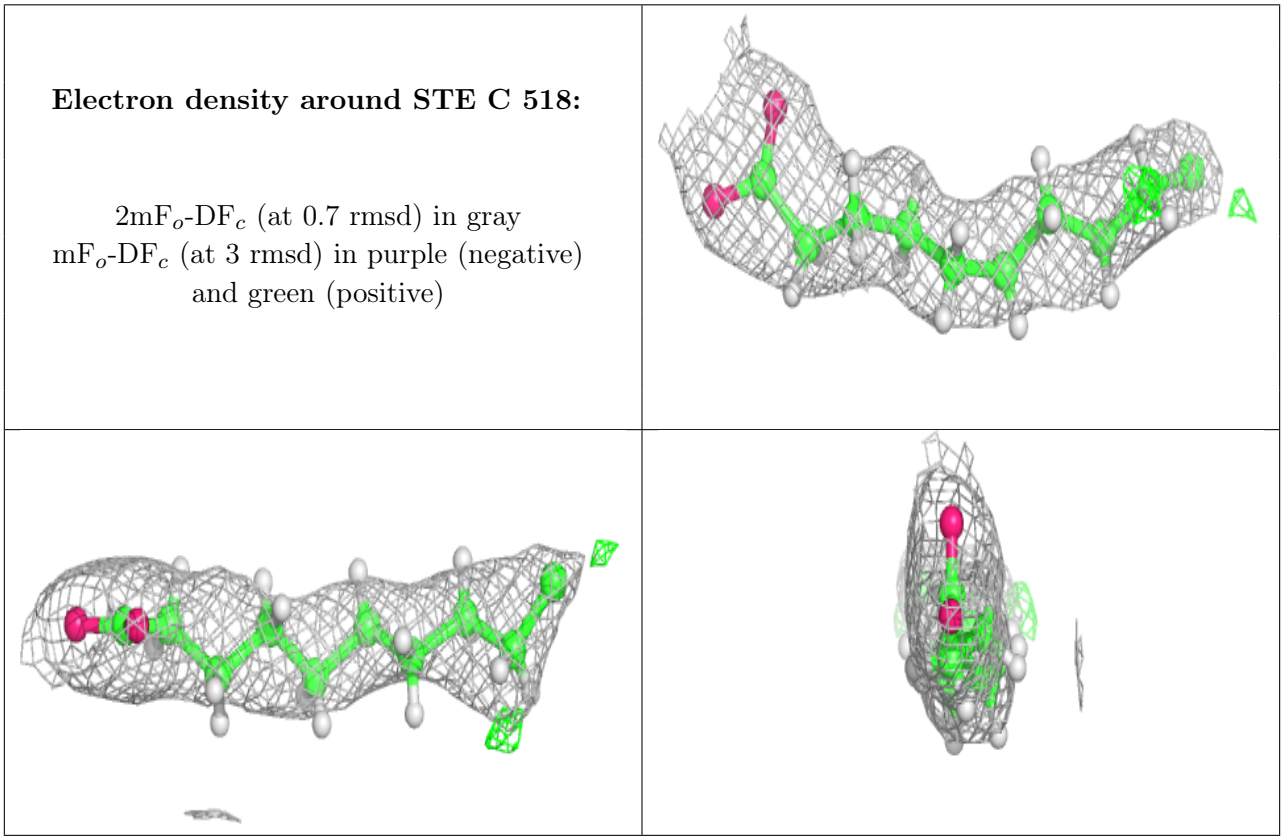
**Electron density around CLA c 509:**

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



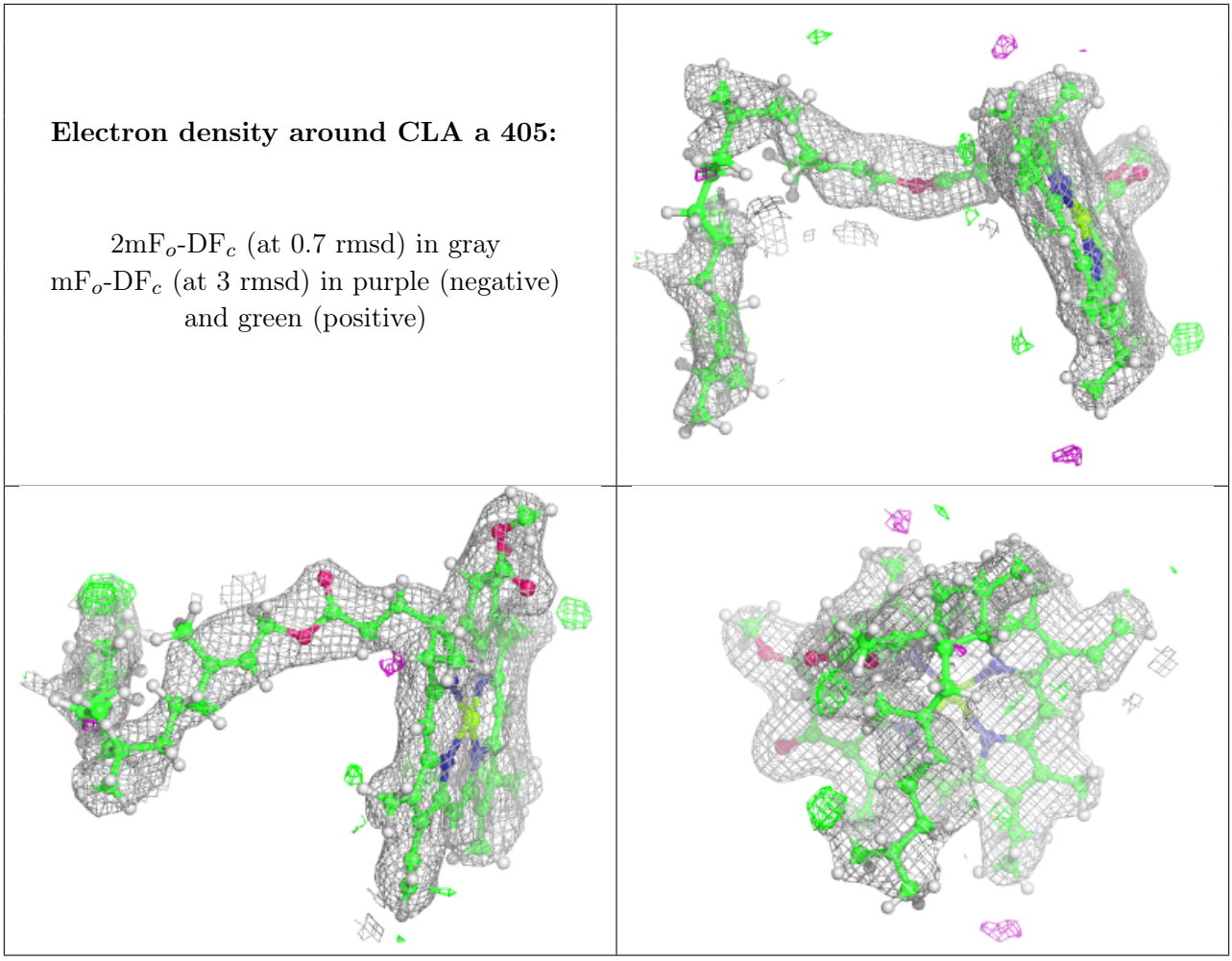
**Electron density around STE C 518:**

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



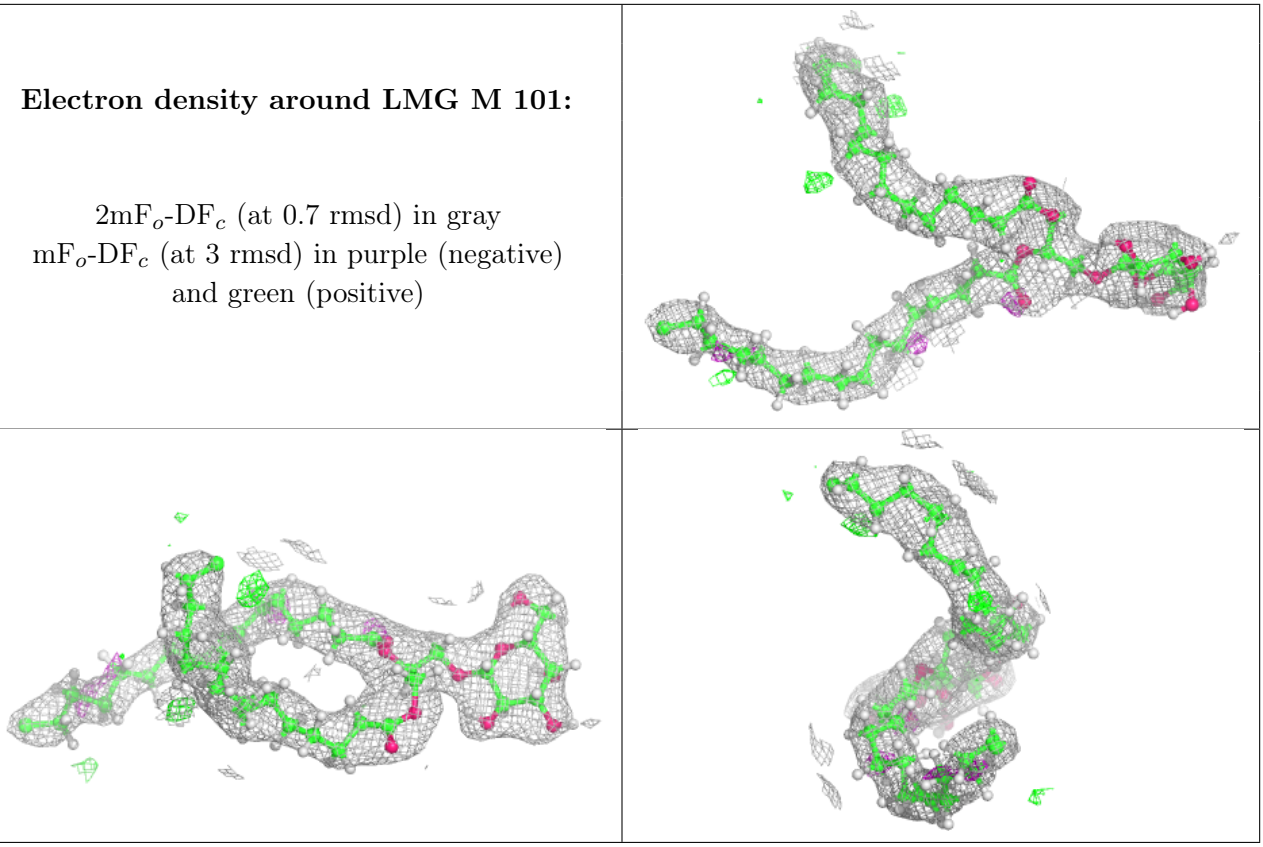
**Electron density around CLA a 405:**

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



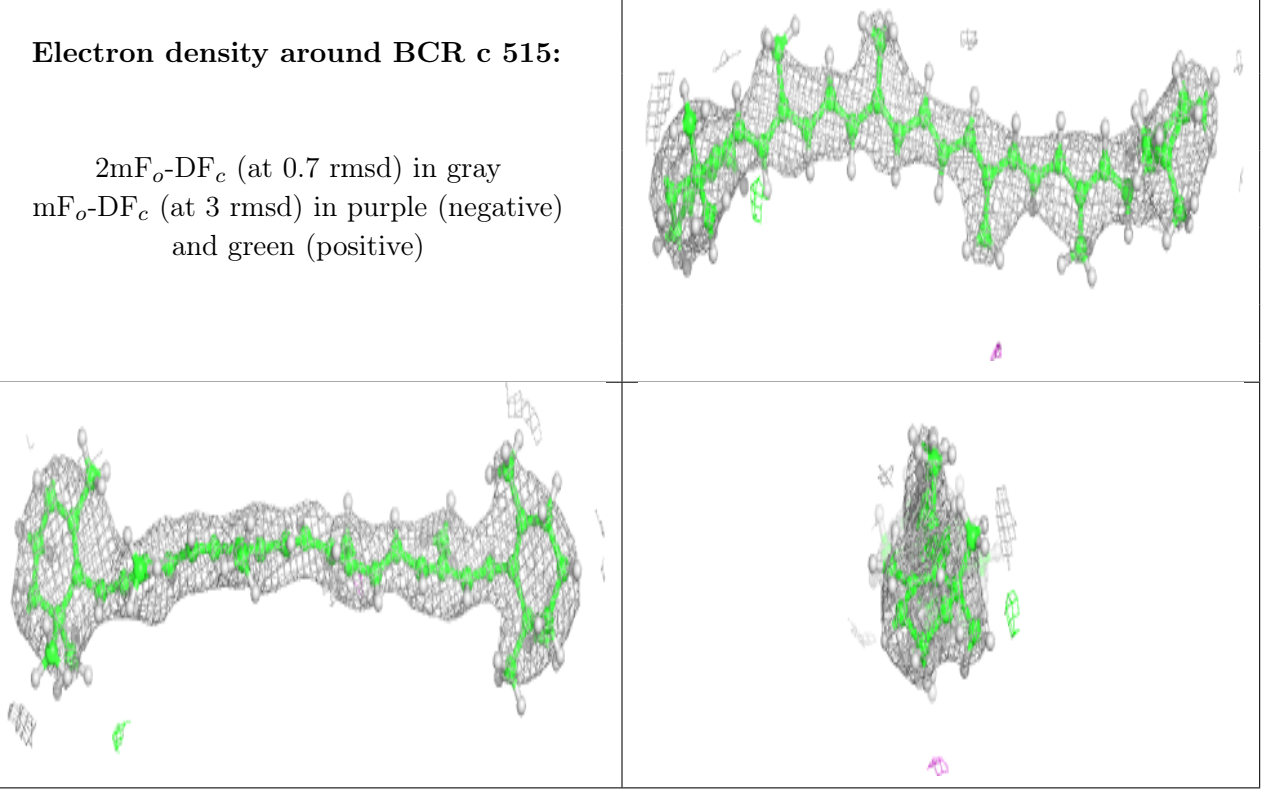
**Electron density around LMG M 101:**

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



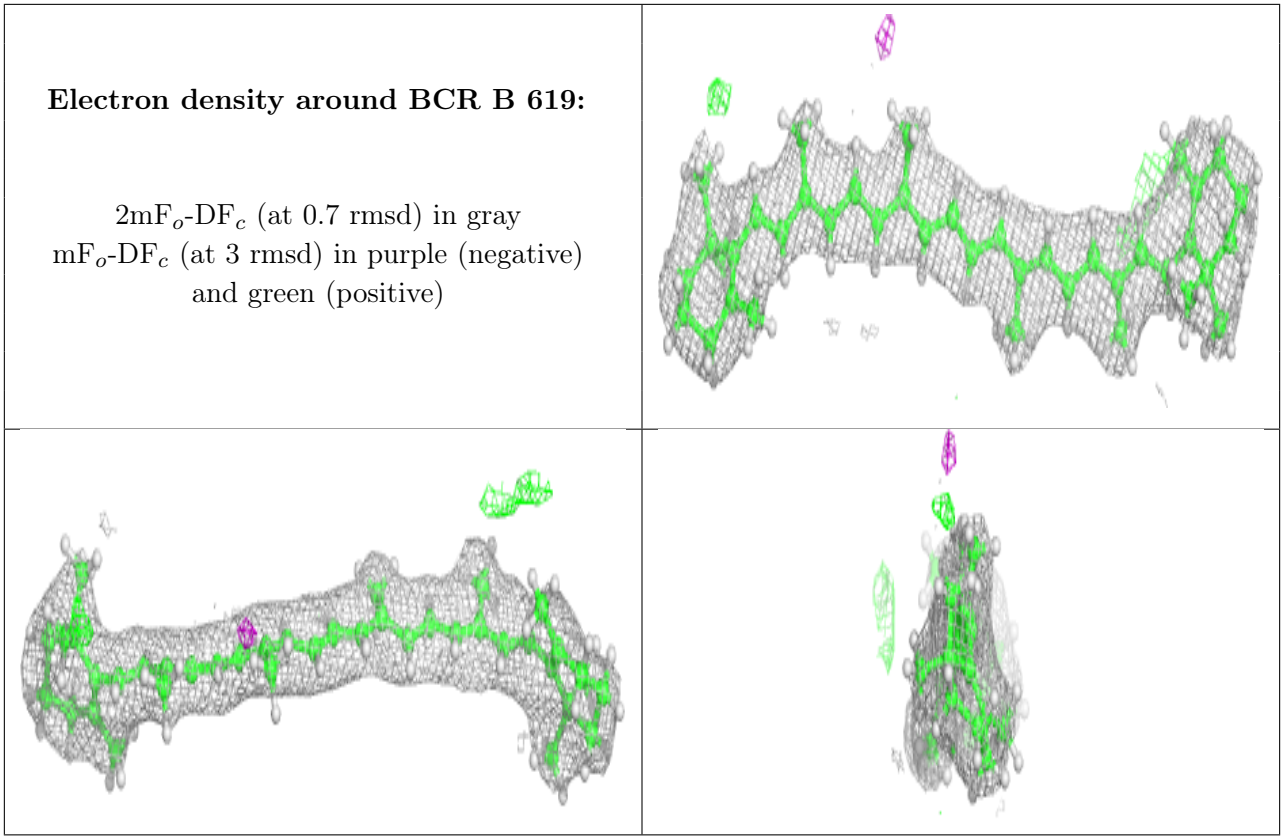
**Electron density around BCR c 515:**

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



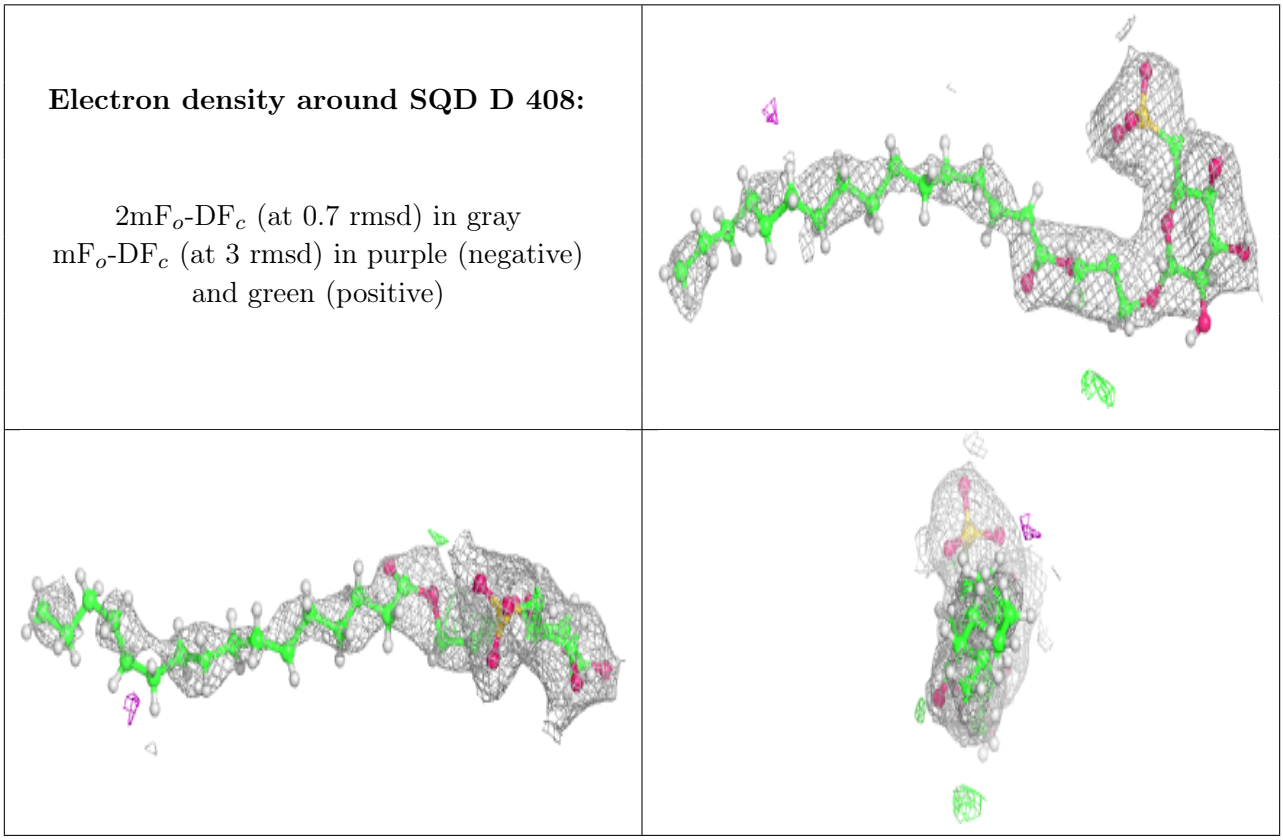
**Electron density around BCR B 619:**

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



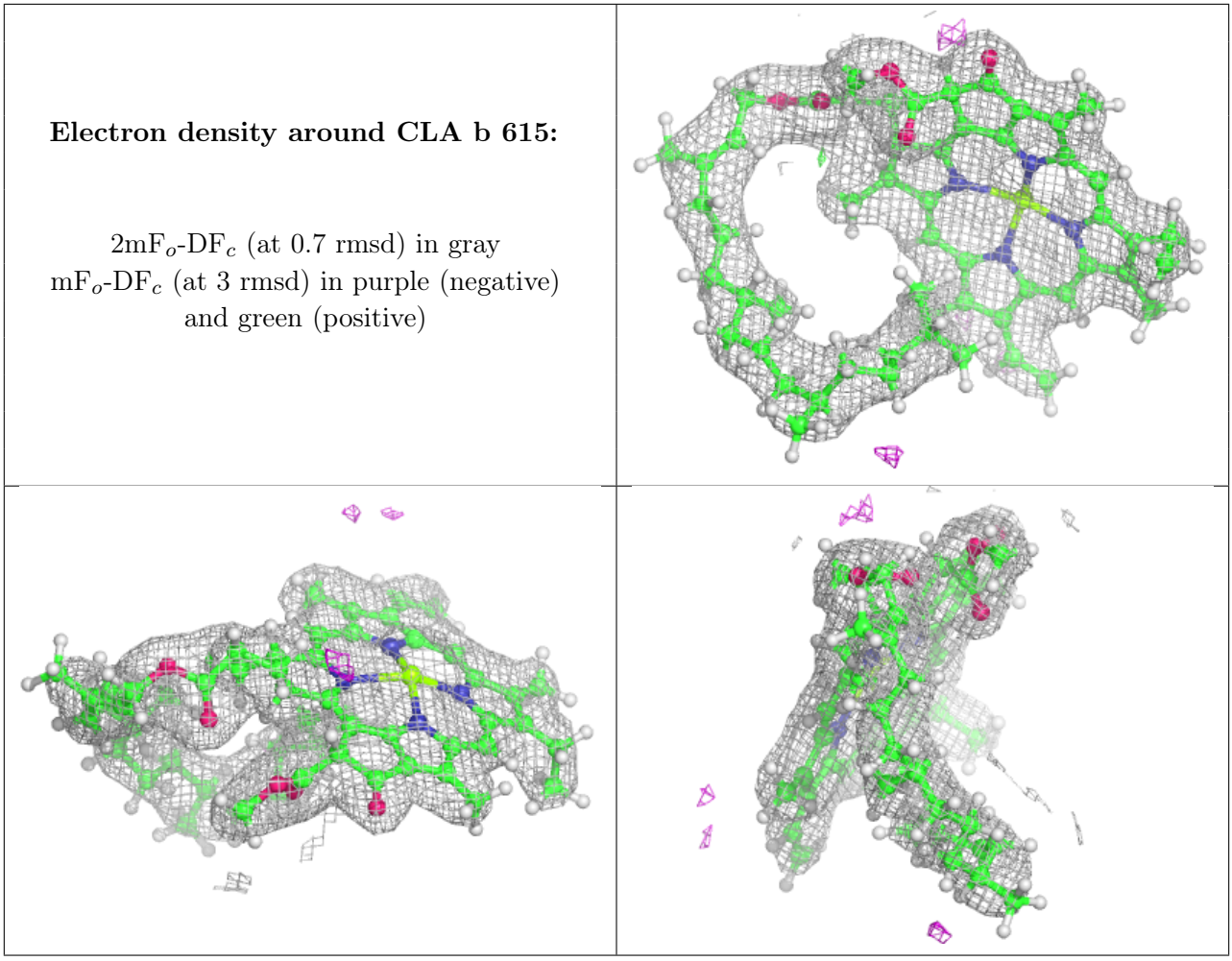
**Electron density around SQD D 408:**

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



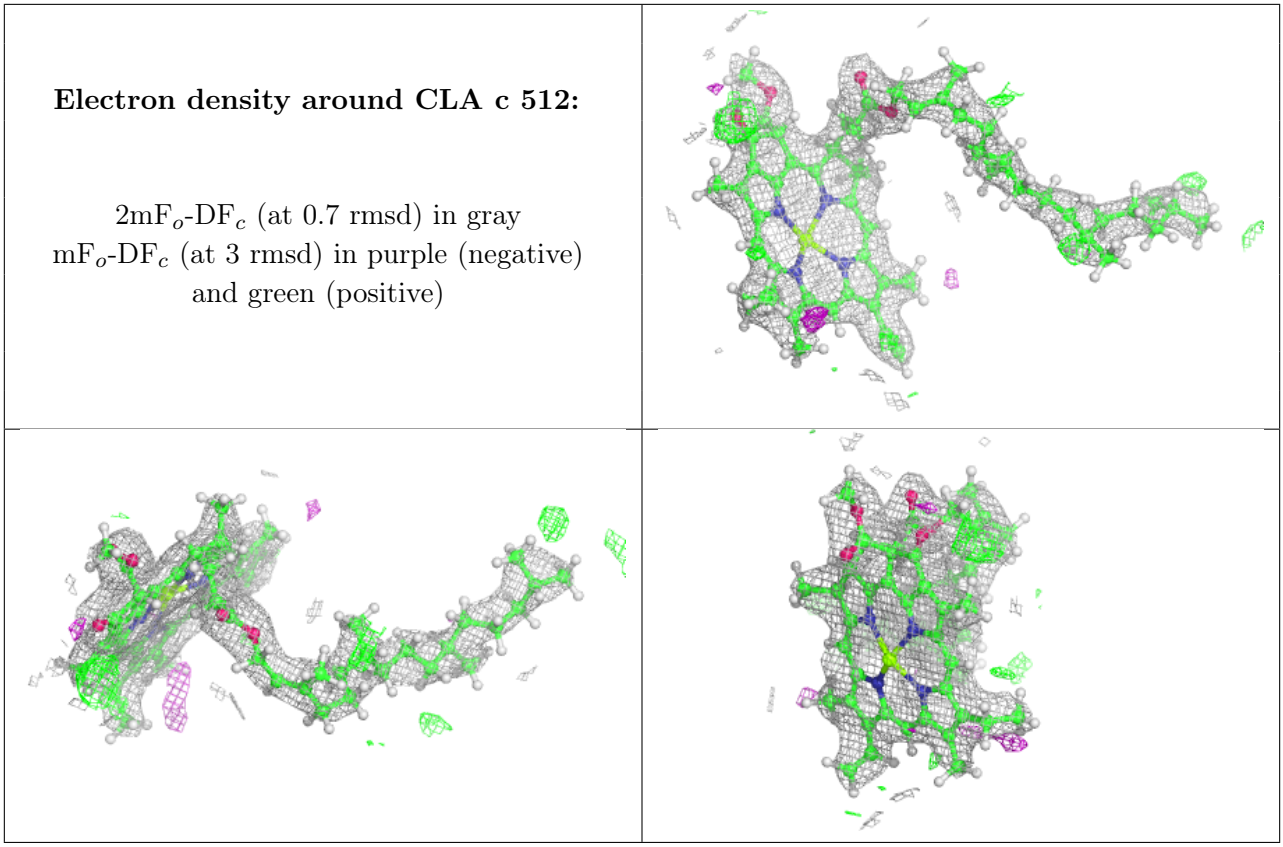
**Electron density around CLA b 615:**

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



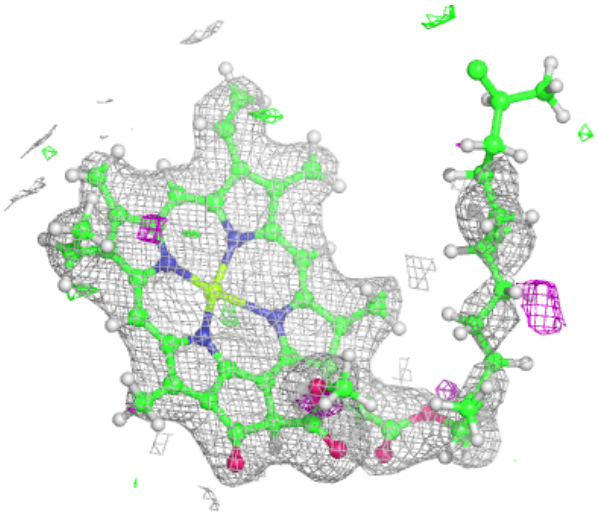
**Electron density around CLA c 512:**

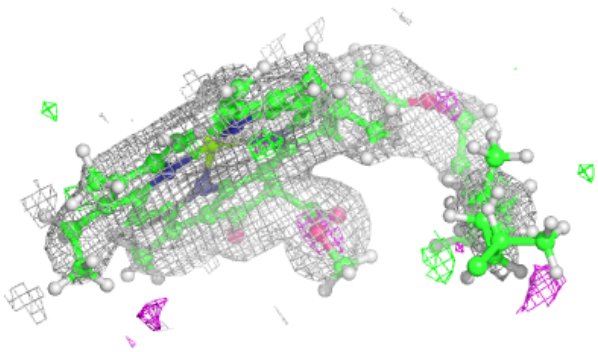
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

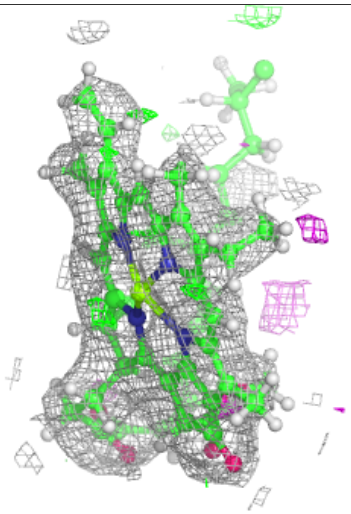


**Electron density around CLA B 616:**

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

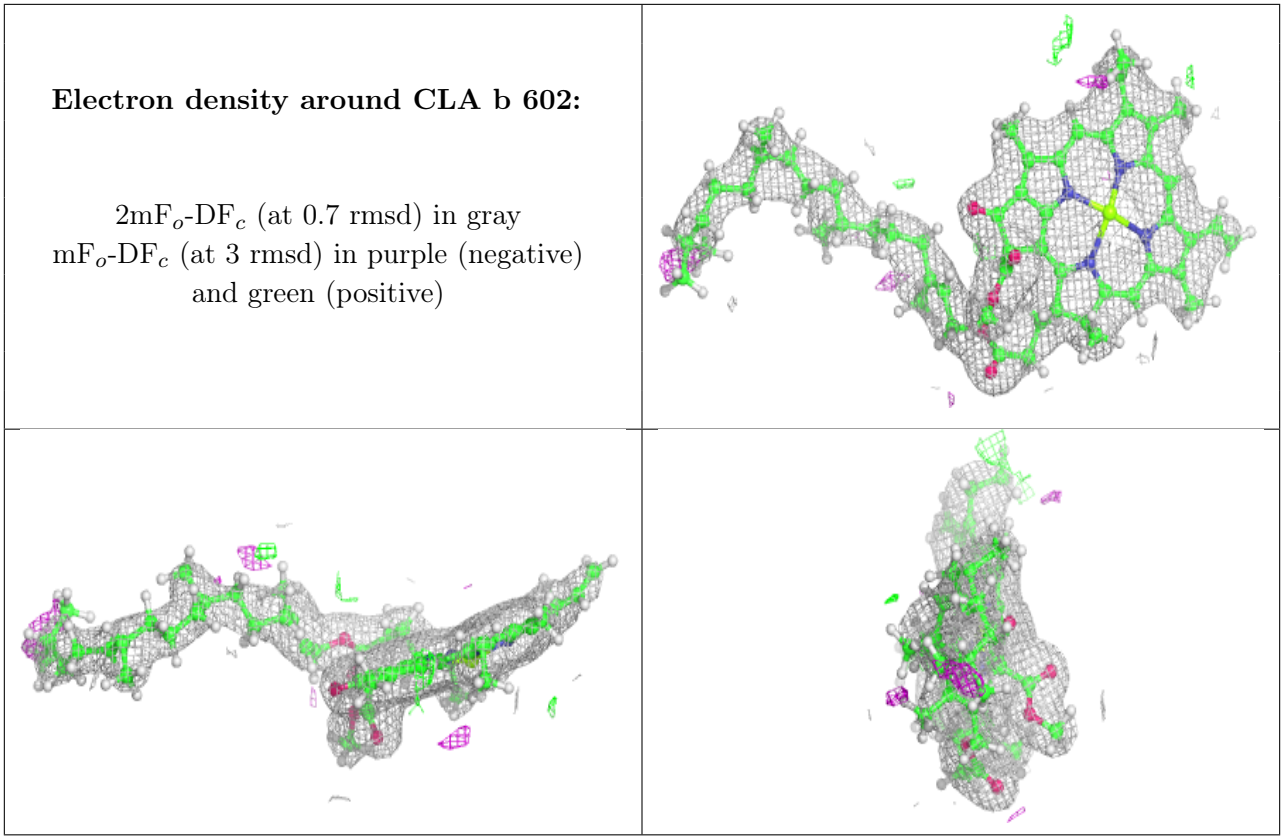






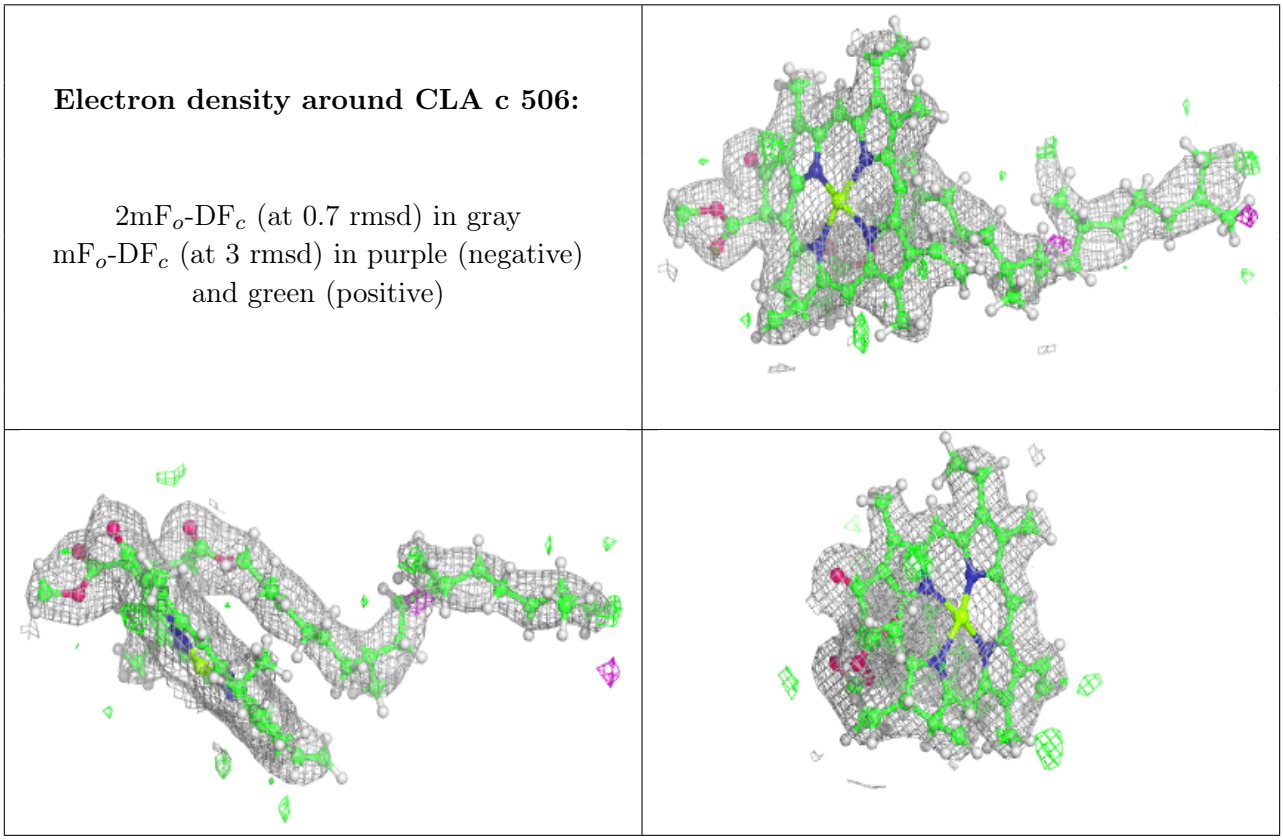
**Electron density around CLA b 602:**

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



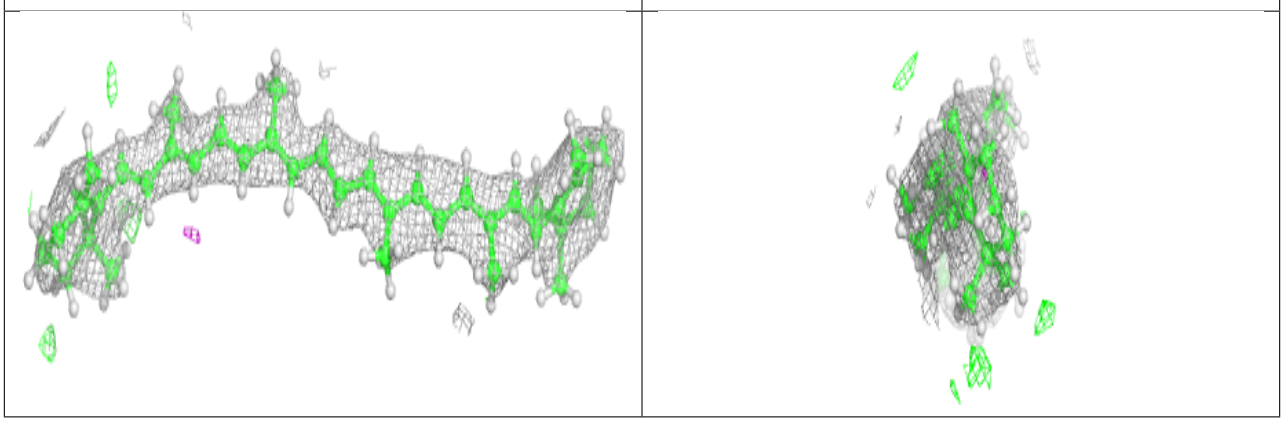
**Electron density around CLA c 506:**

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



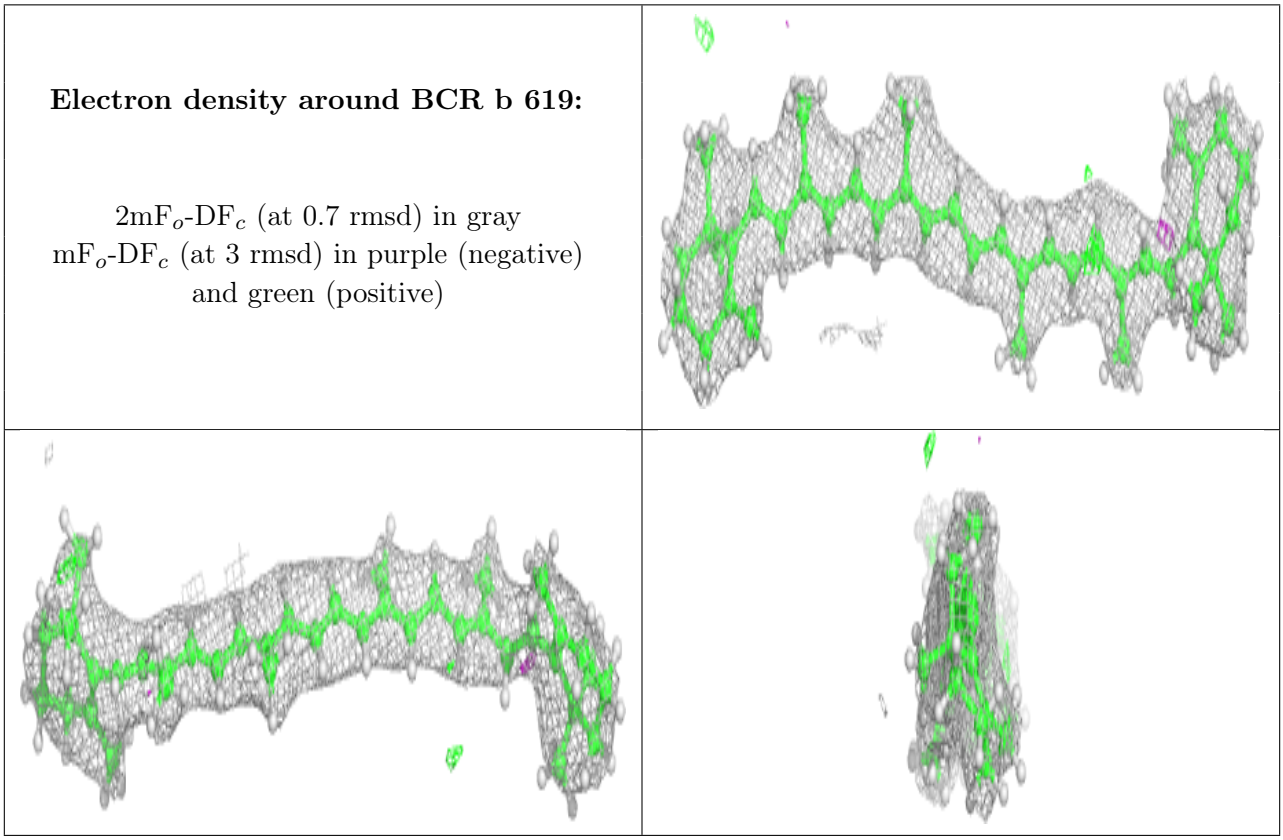
**Electron density around BCR K 103:**

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



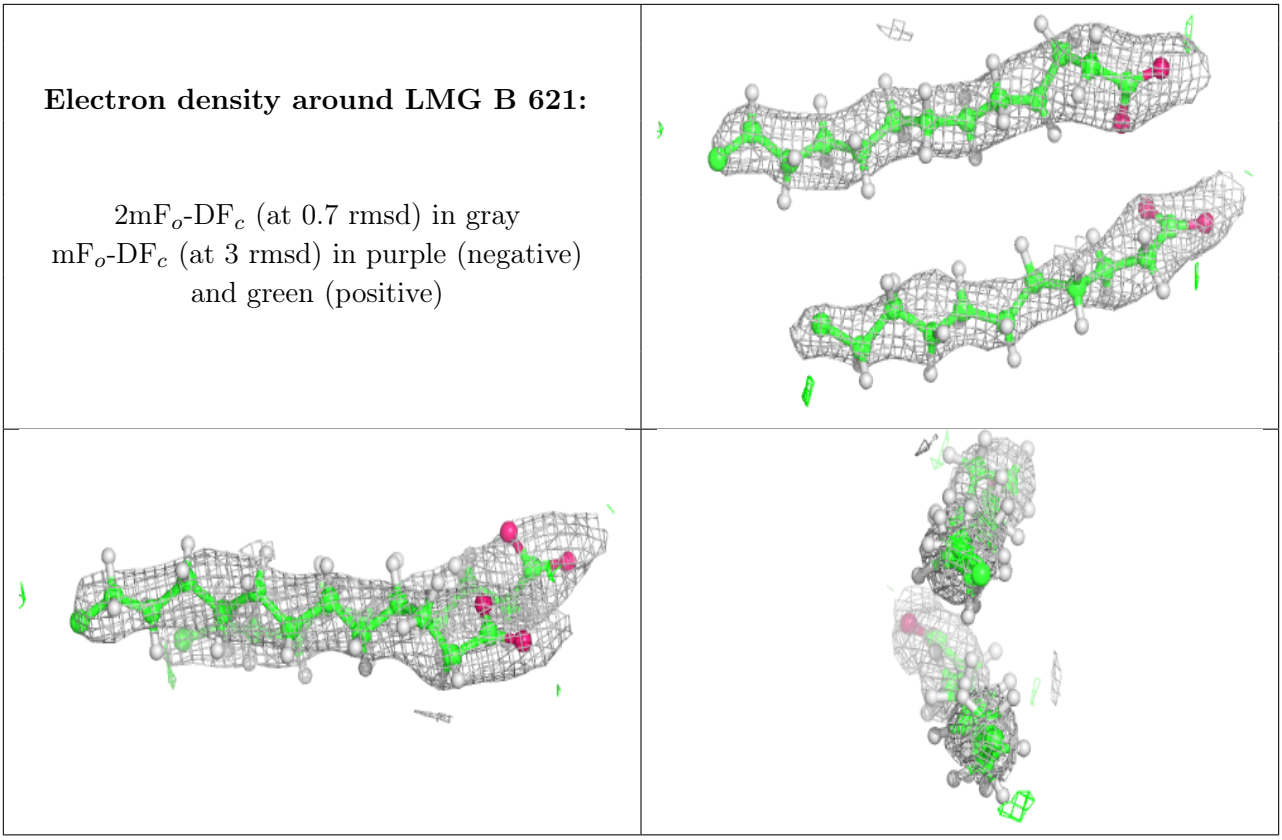
**Electron density around BCR b 619:**

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



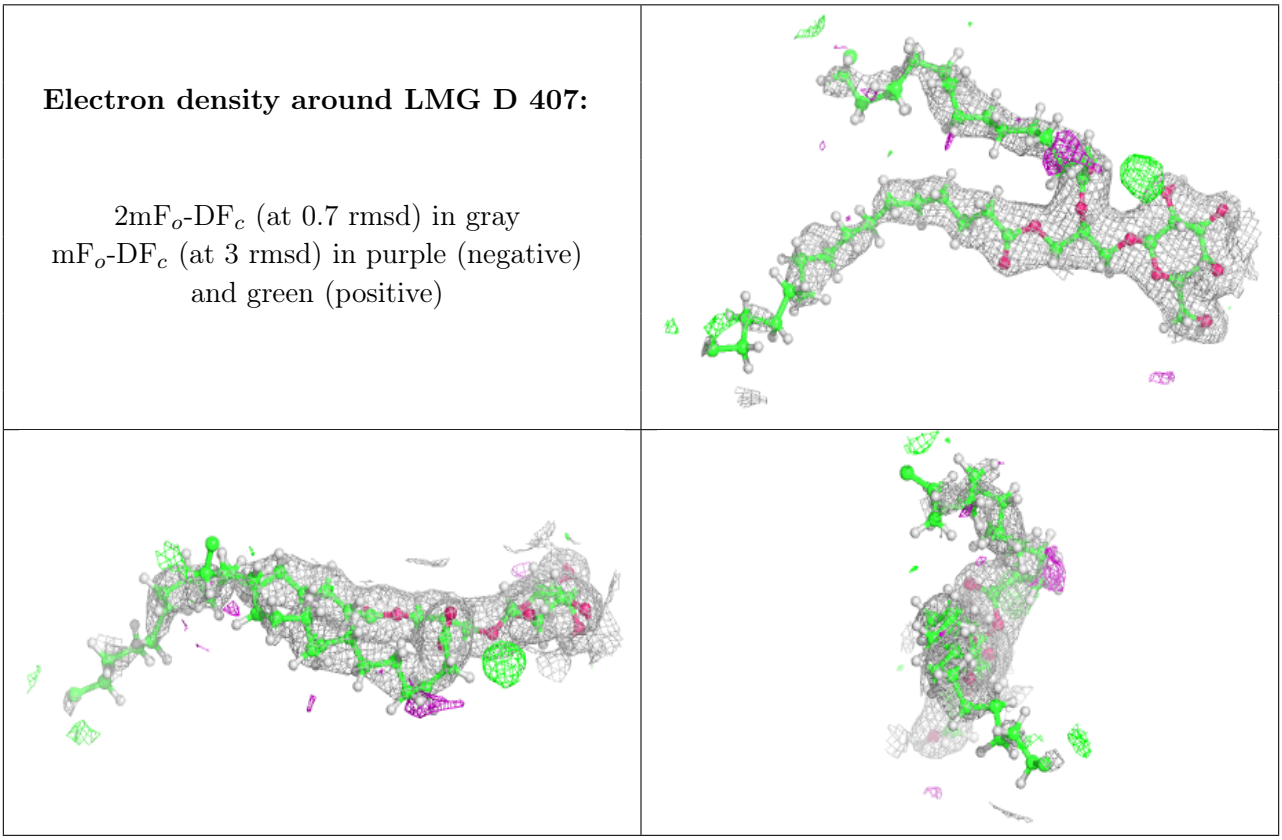
**Electron density around LMG B 621:**

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



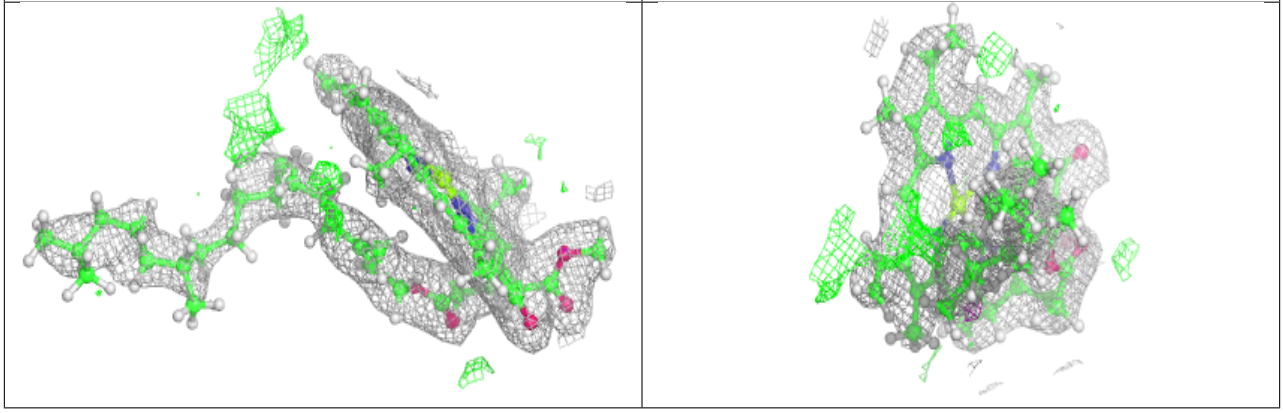
**Electron density around LMG D 407:**

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



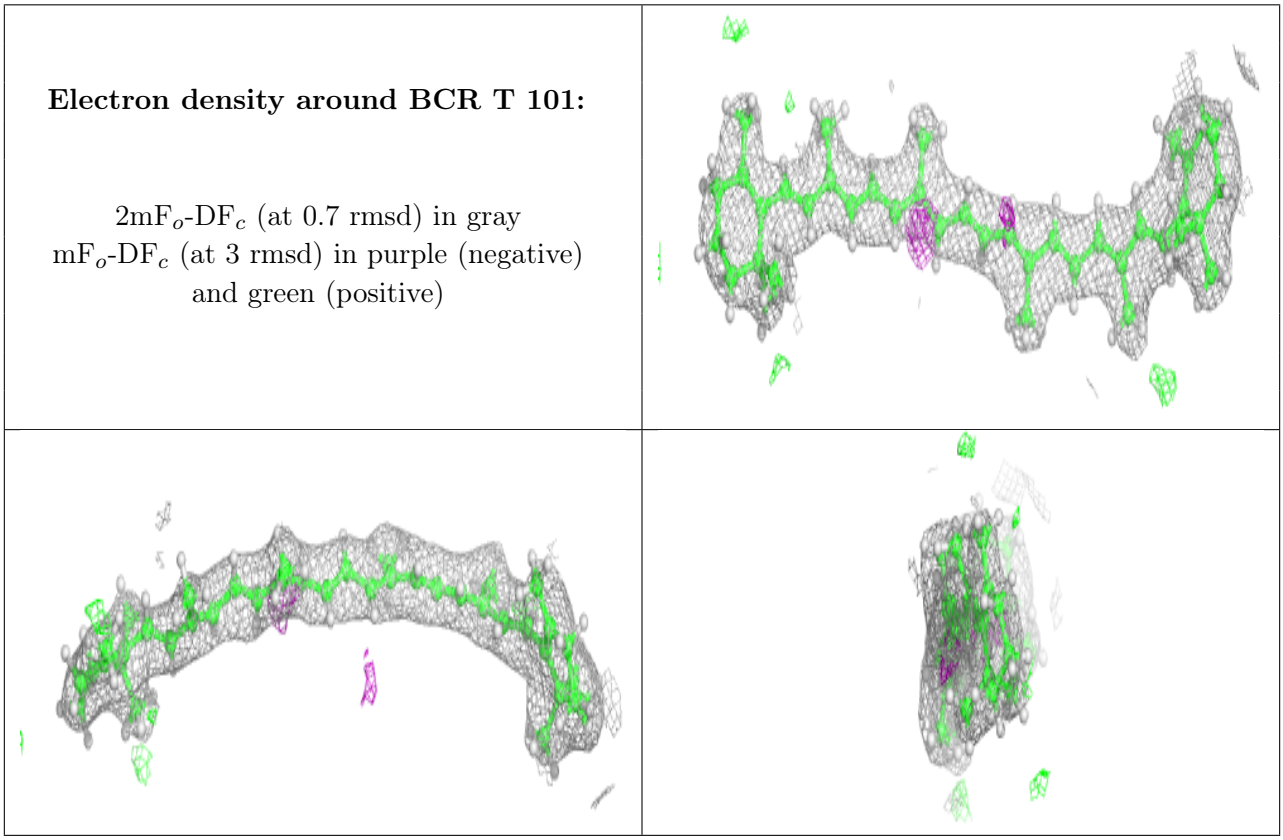
**Electron density around CLA C 505:**

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



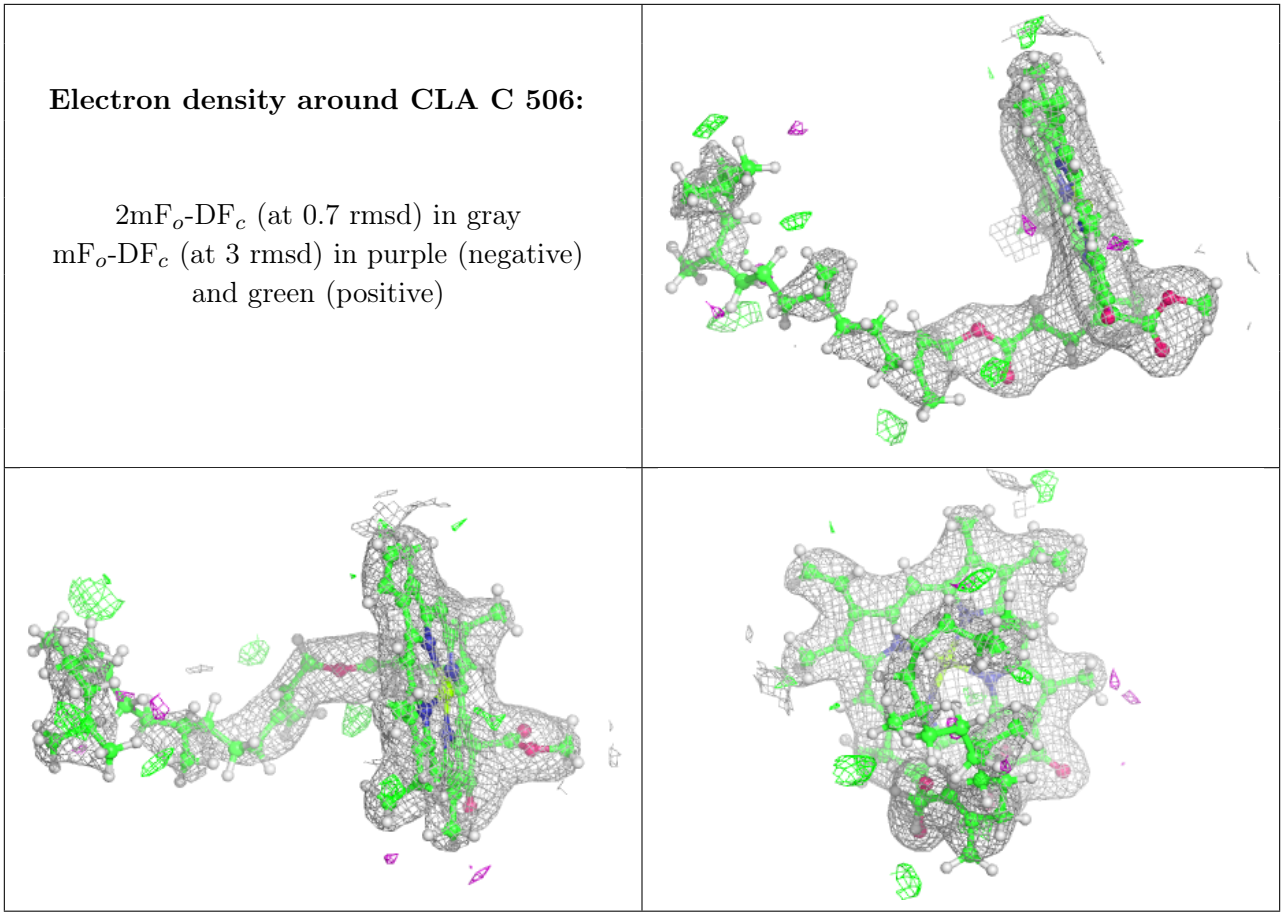
**Electron density around BCR T 101:**

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



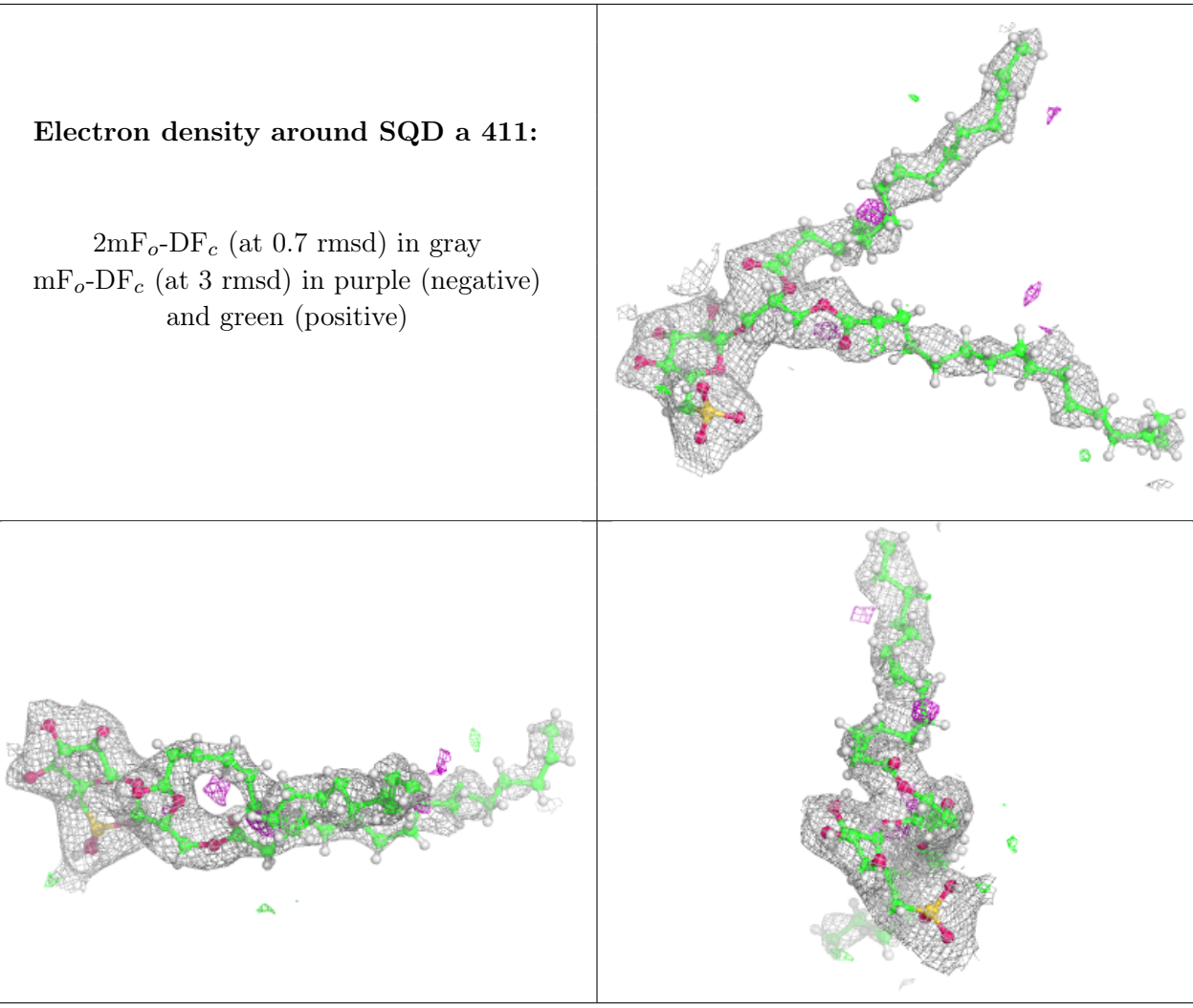
**Electron density around CLA C 506:**

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



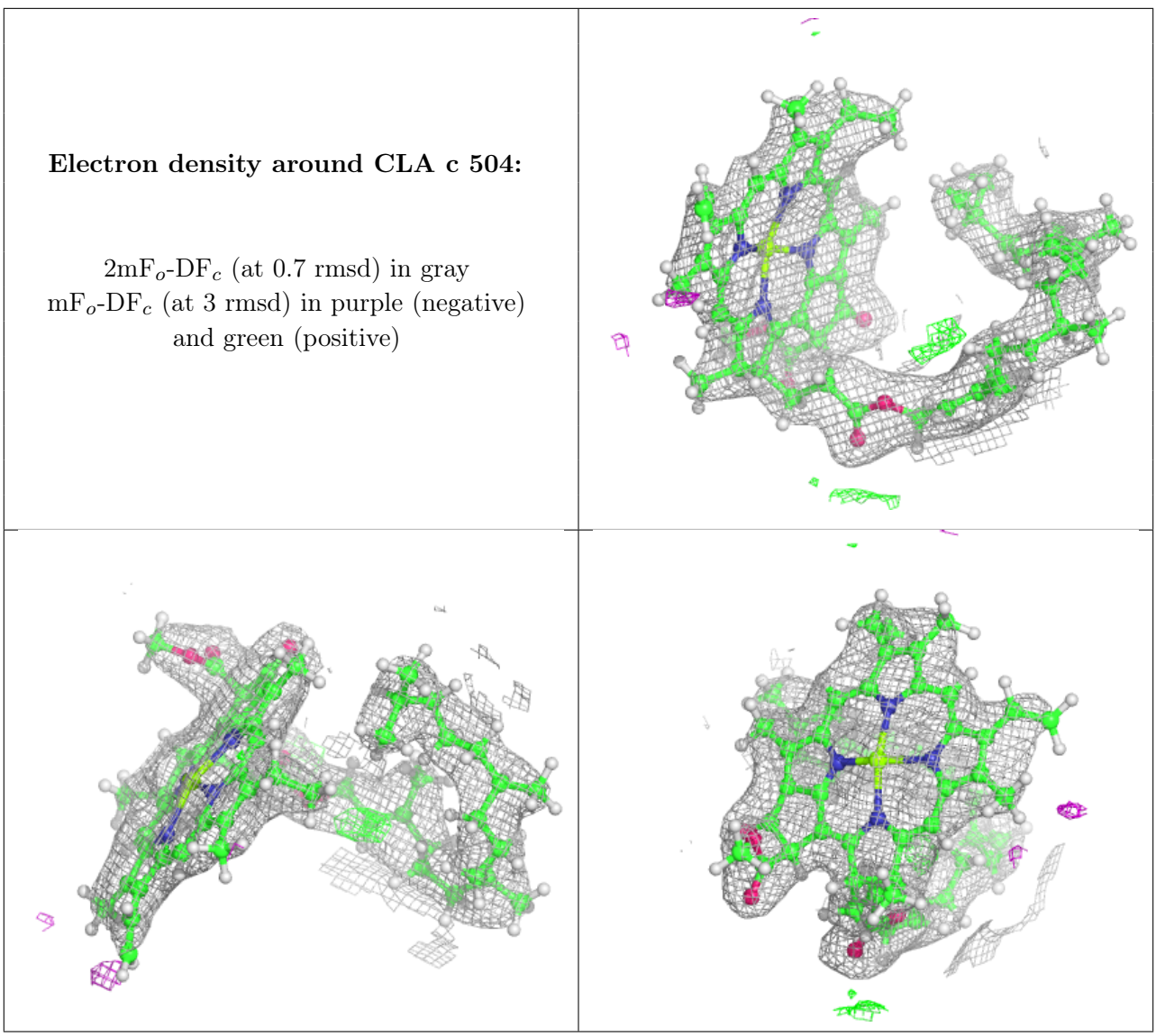
**Electron density around SQD a 411:**

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



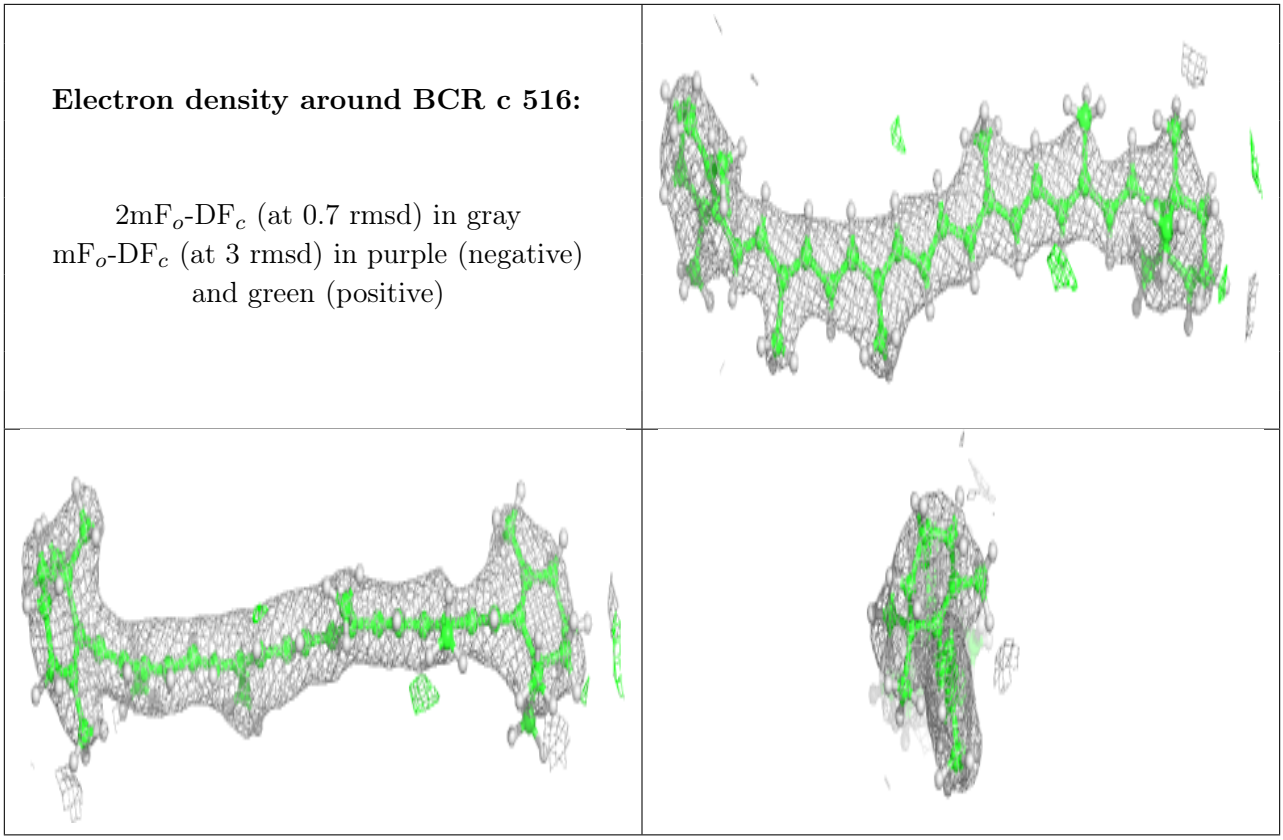
**Electron density around CLA c 504:**

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



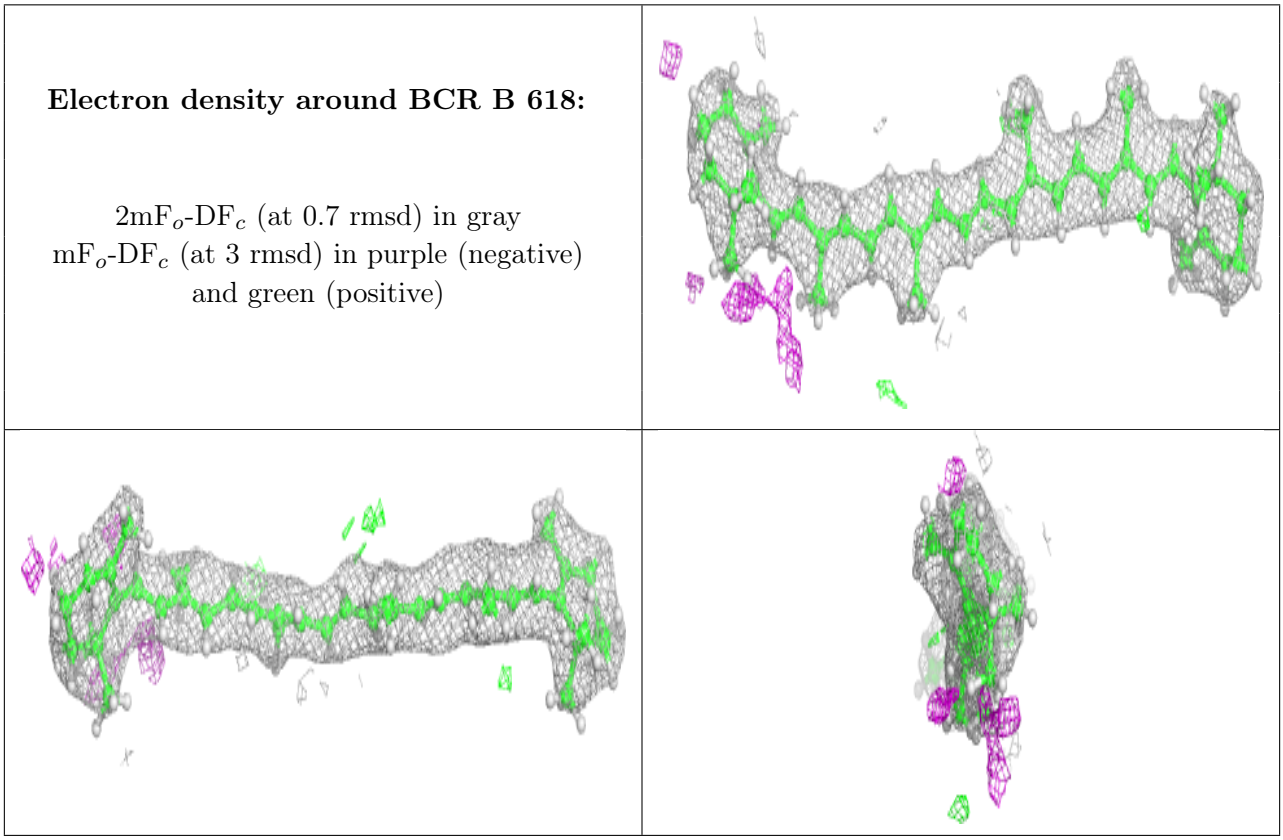
**Electron density around BCR c 516:**

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



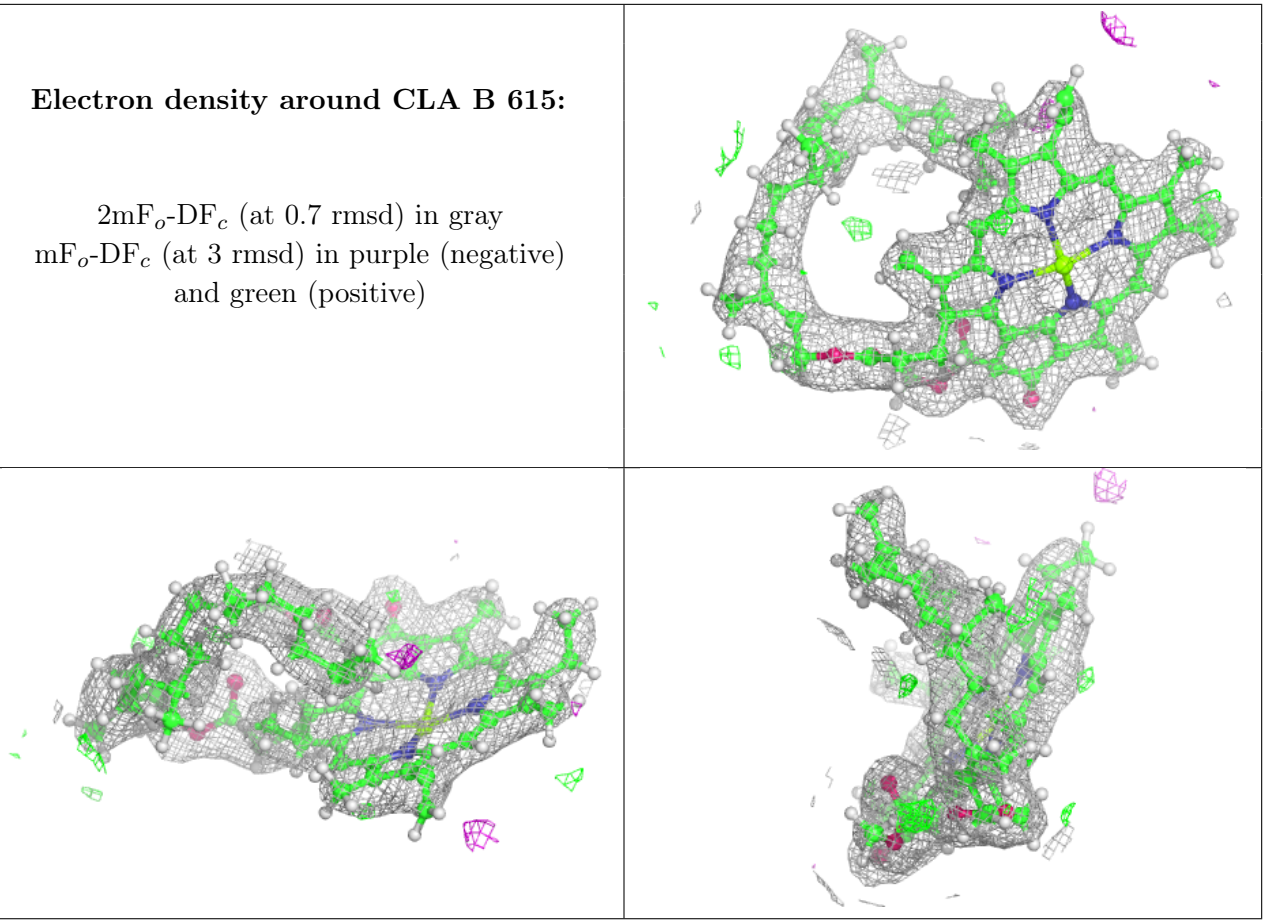
**Electron density around BCR B 618:**

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



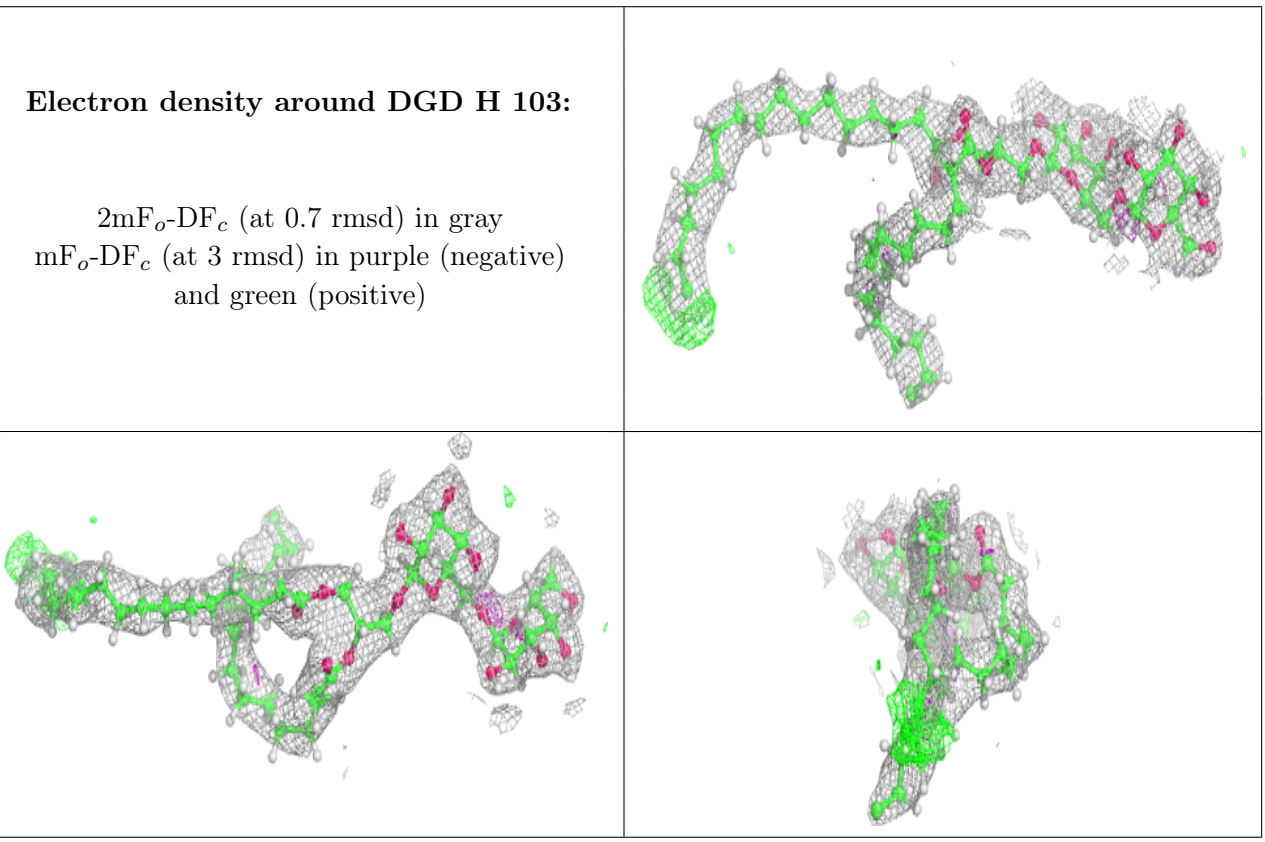
**Electron density around CLA B 615:**

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



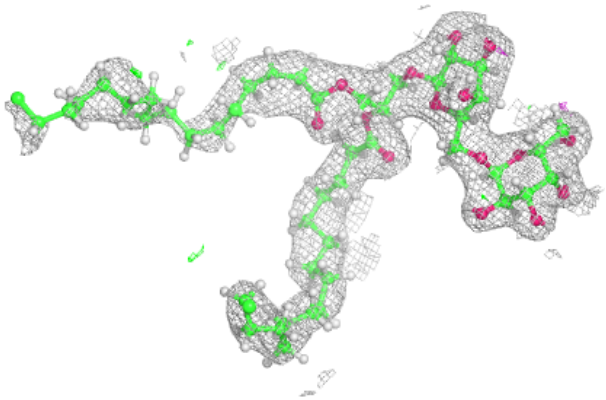
**Electron density around DGD H 103:**

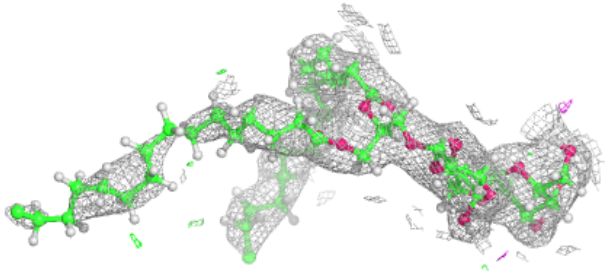
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

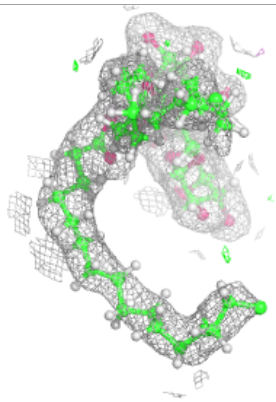


**Electron density around DGD c 518:**

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

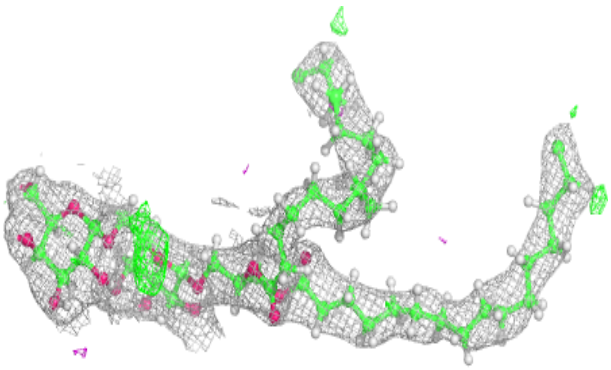


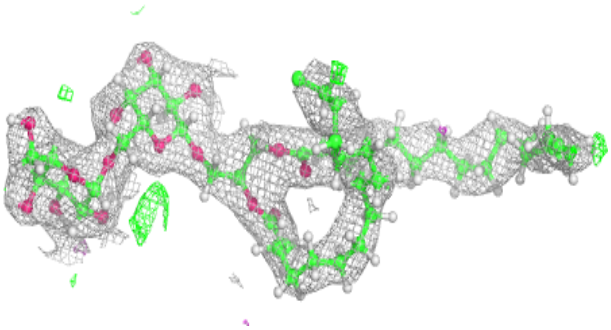


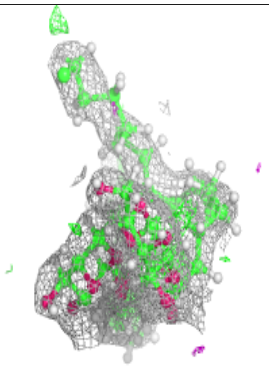


**Electron density around DGD h 102:**

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

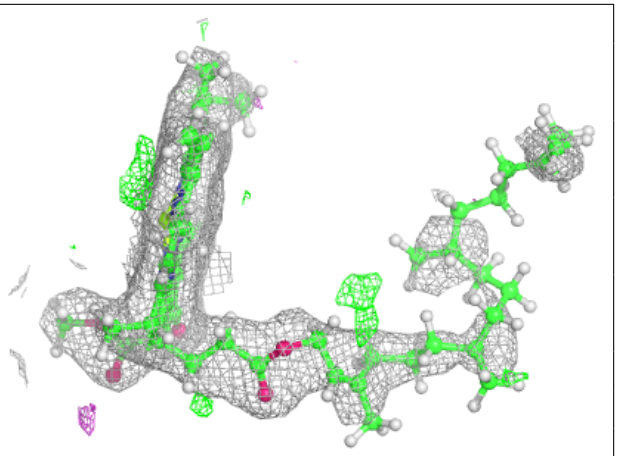


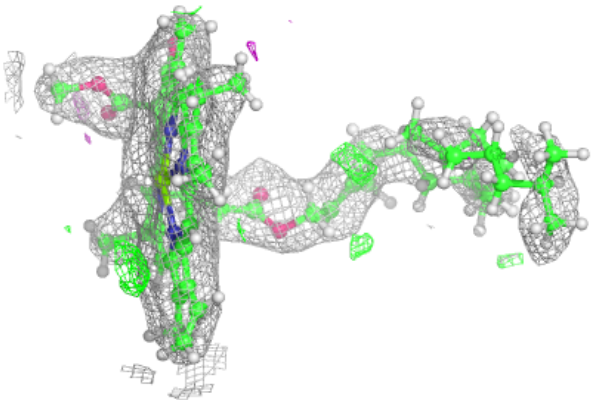


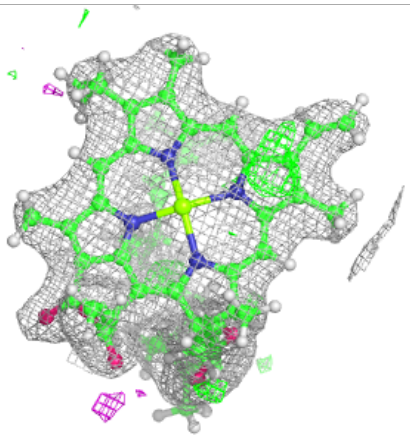


**Electron density around CLA c 507:**

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

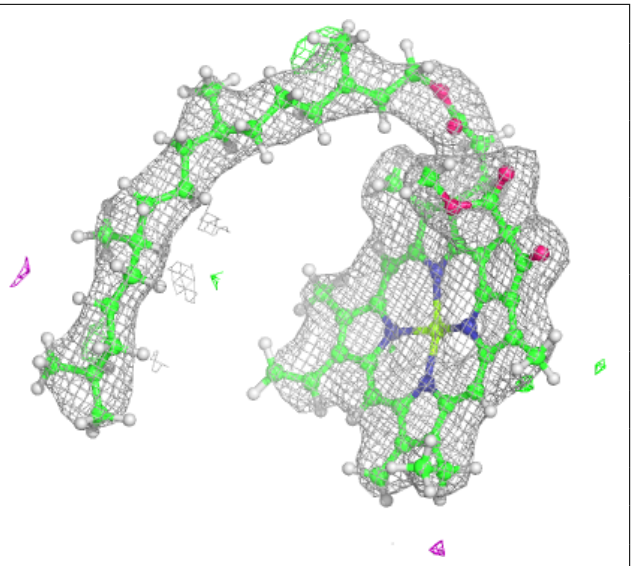


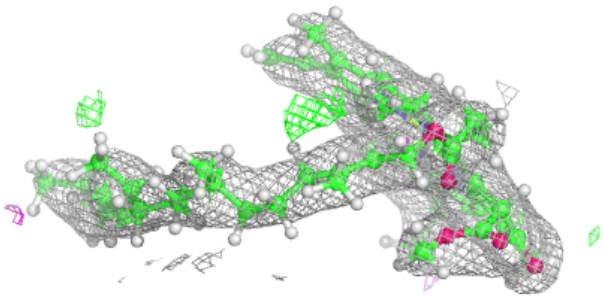


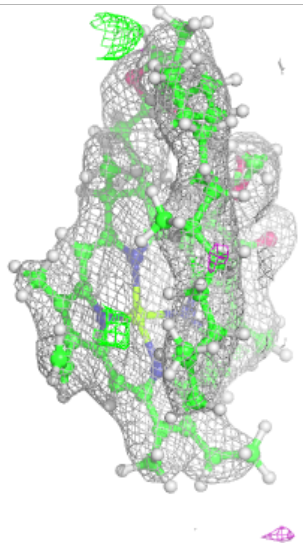


**Electron density around CLA c 508:**

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

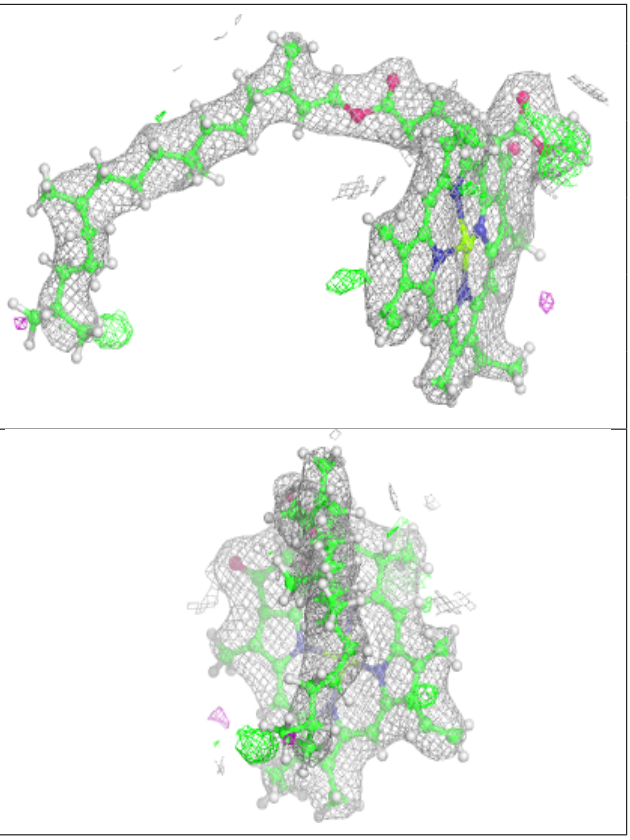






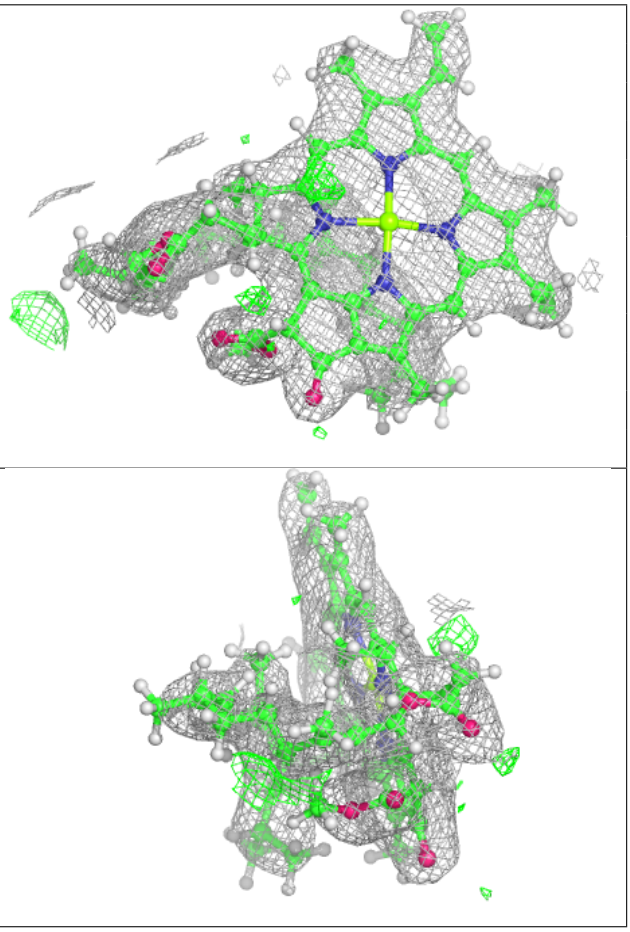
**Electron density around CLA b 609:**

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



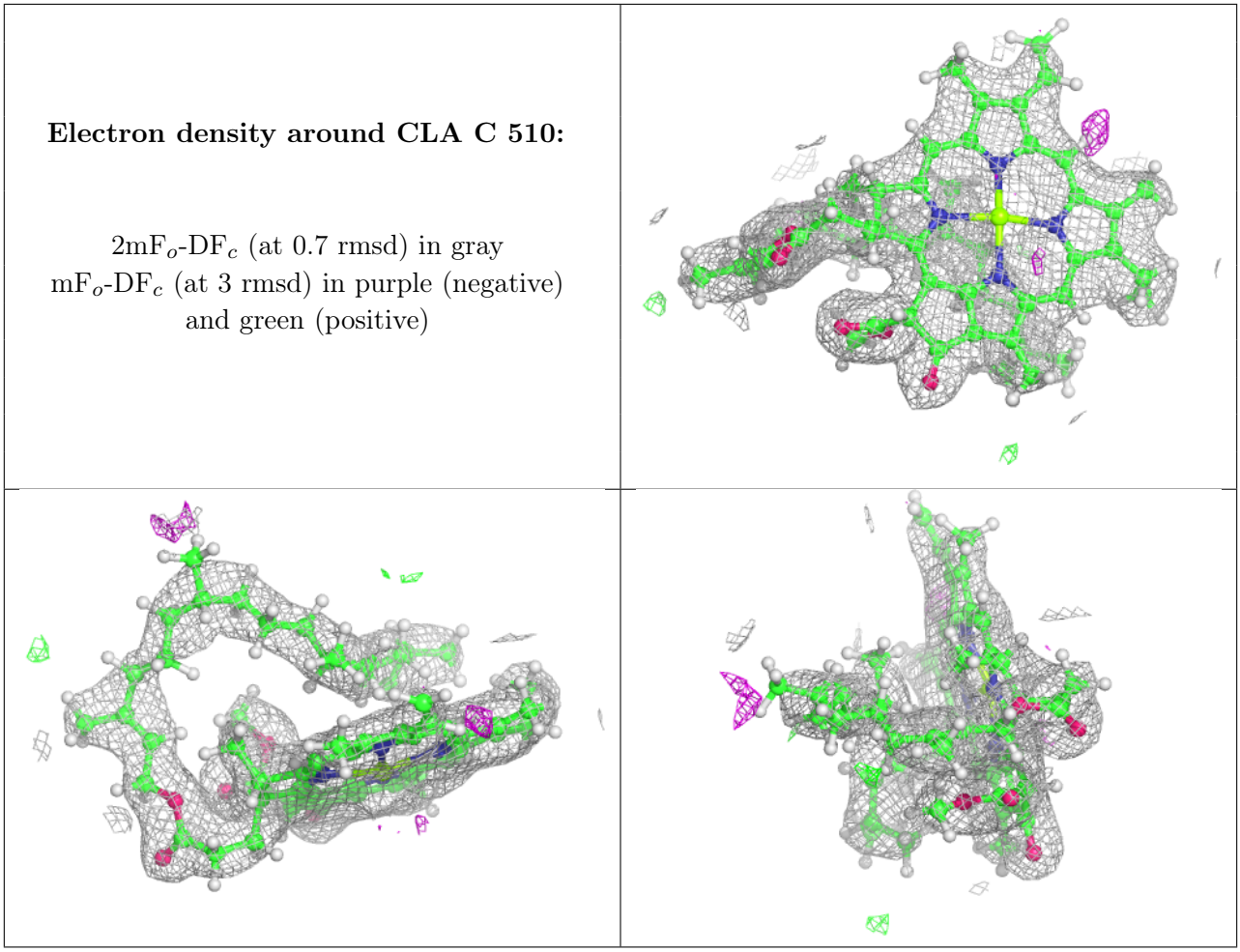
**Electron density around CLA c 511:**

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



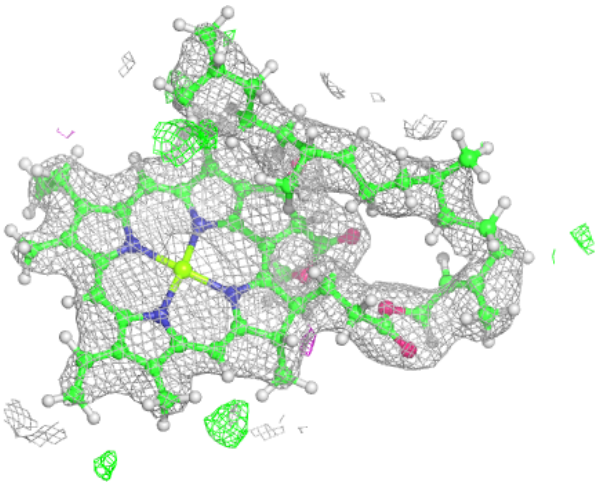
**Electron density around CLA C 510:**

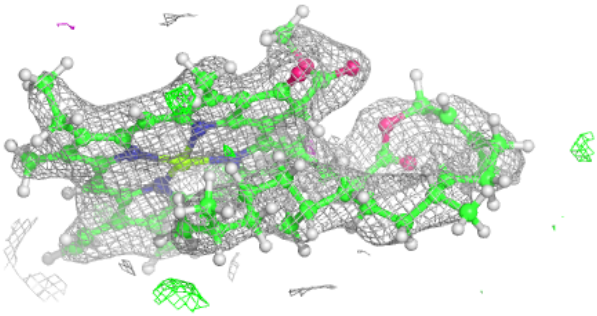
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

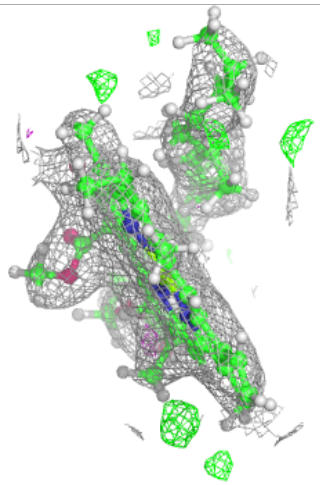


**Electron density around CLA c 510:**

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

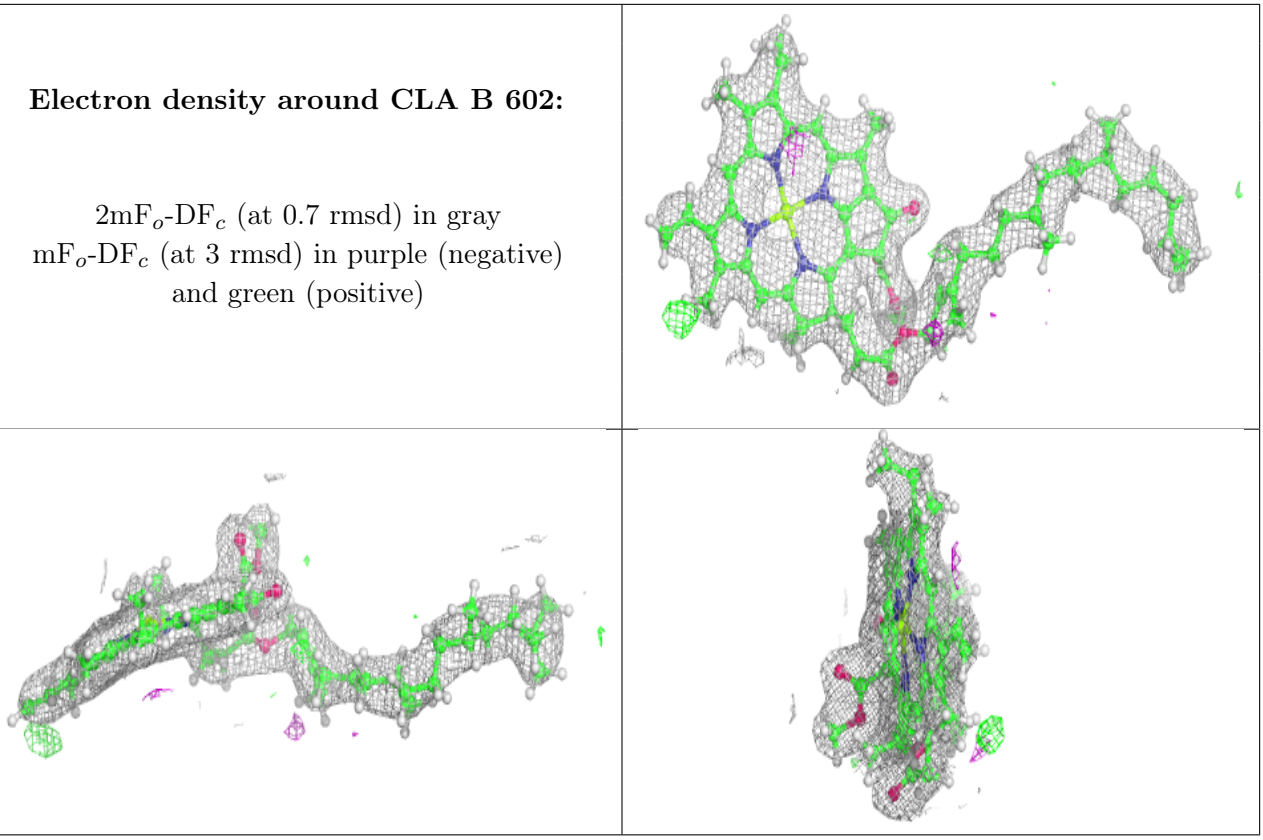






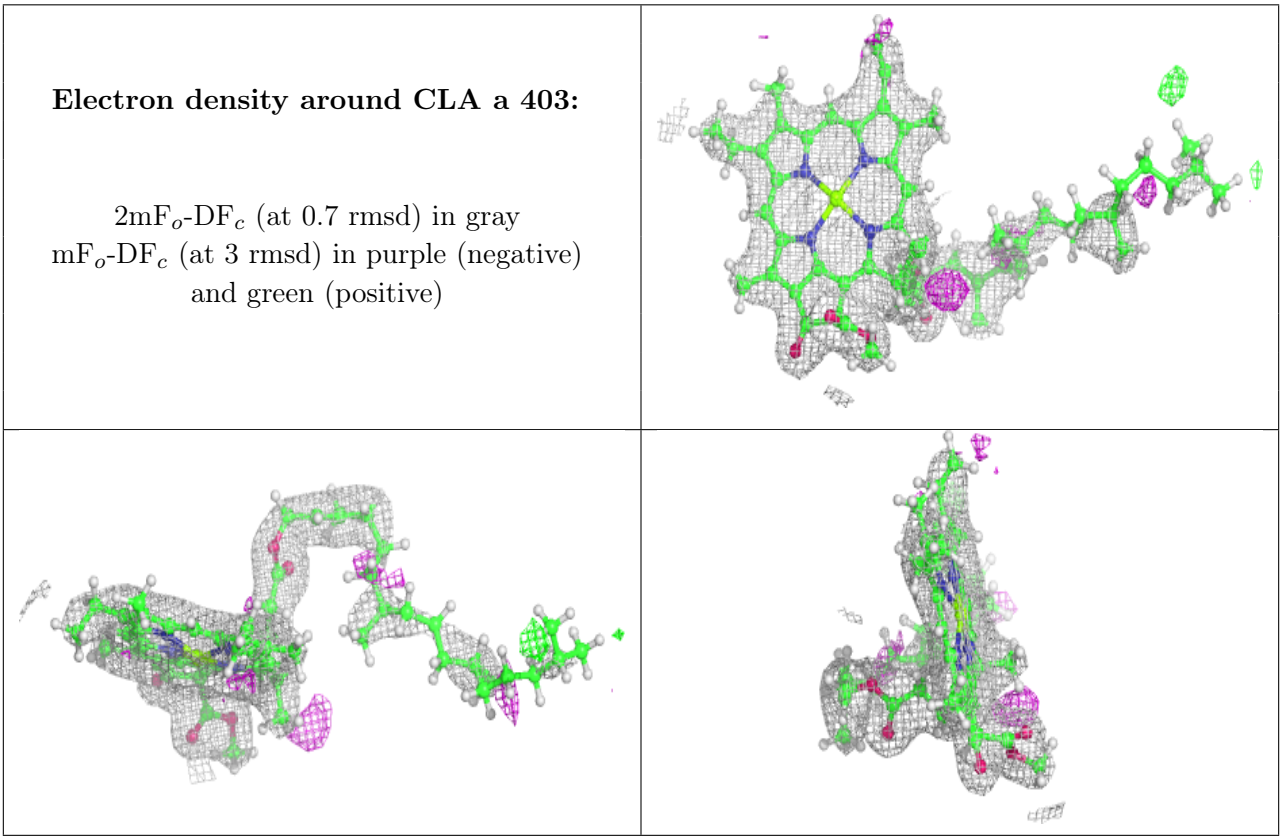
**Electron density around CLA B 602:**

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



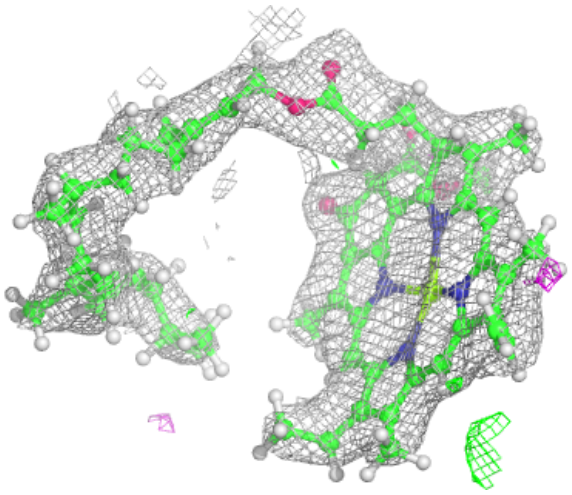
**Electron density around CLA a 403:**

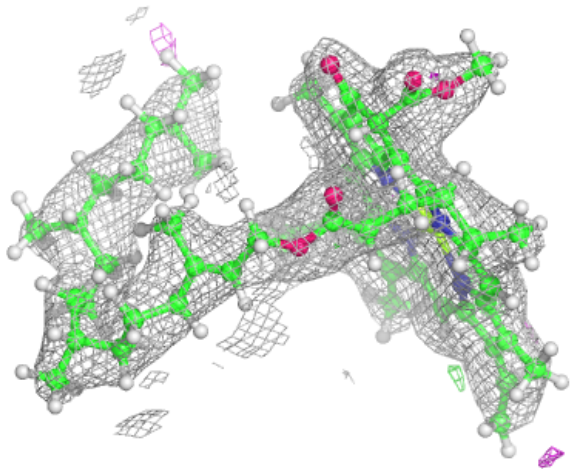
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

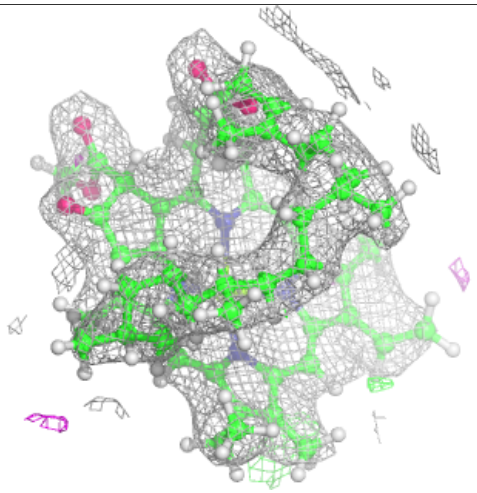


**Electron density around CLA C 503:**

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

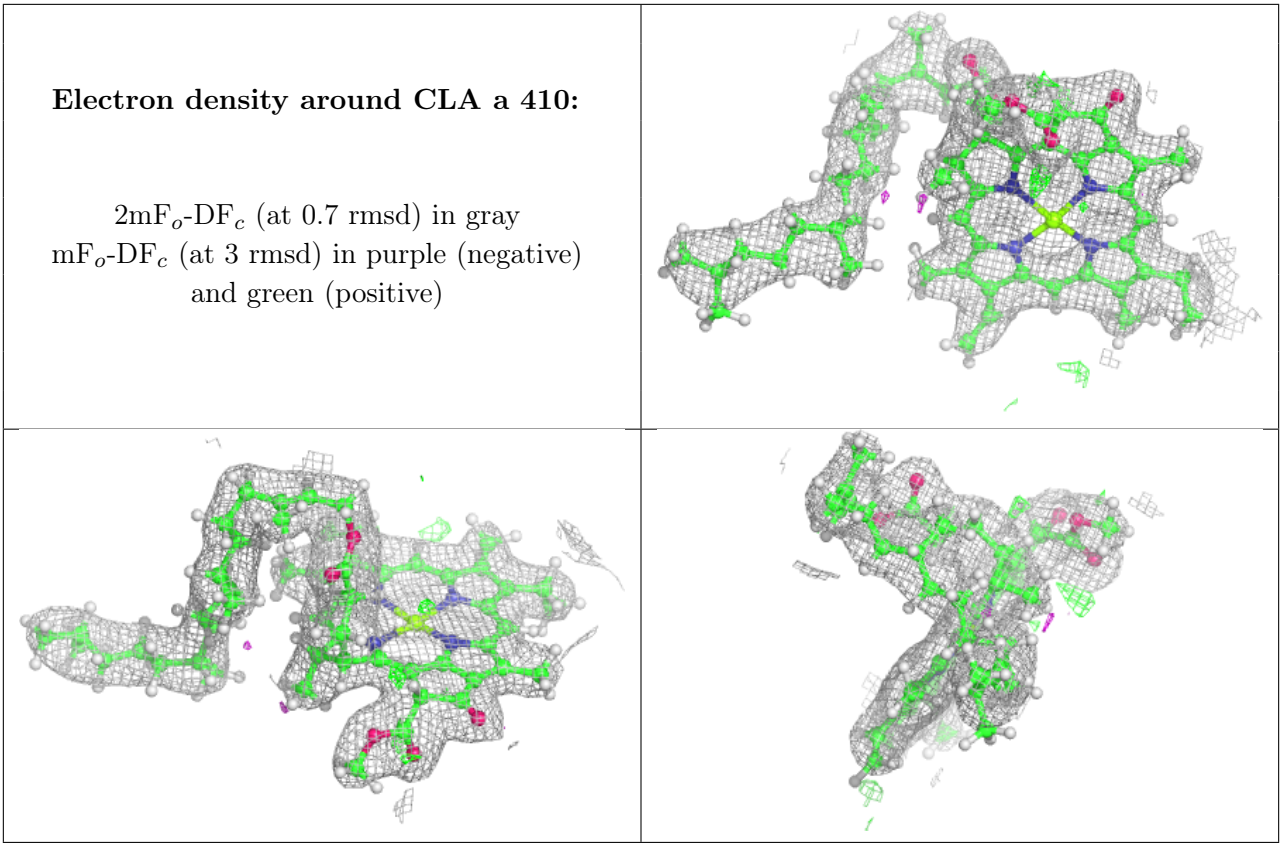






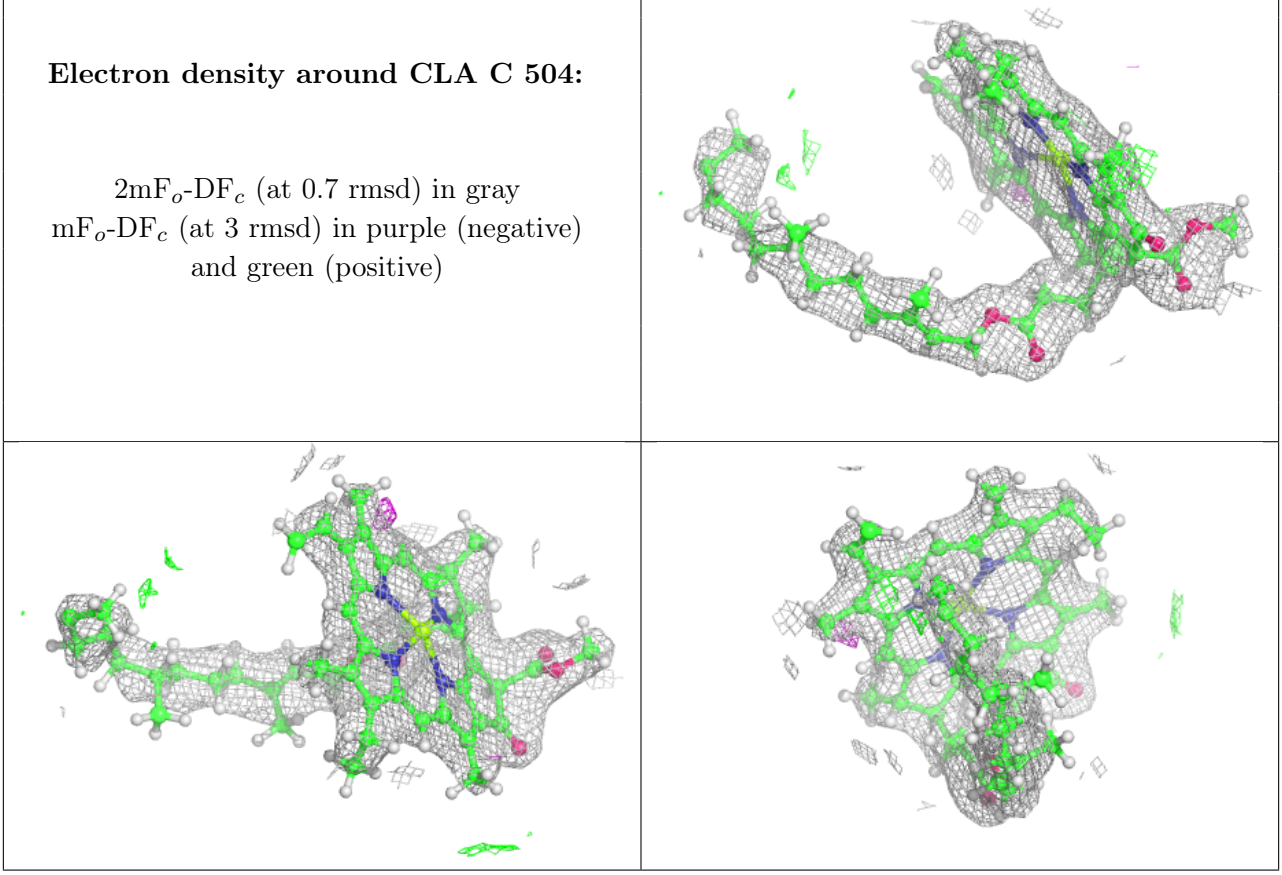
**Electron density around CLA a 410:**

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



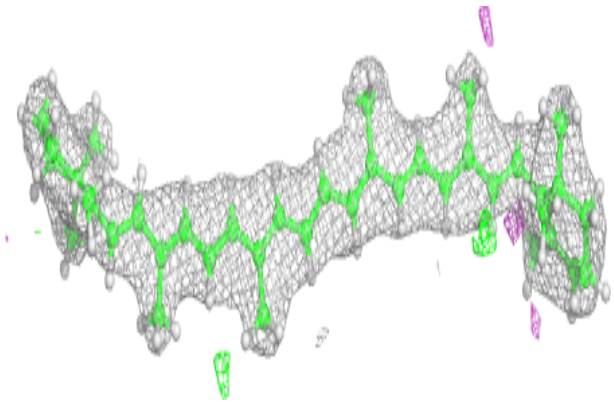
**Electron density around CLA C 504:**

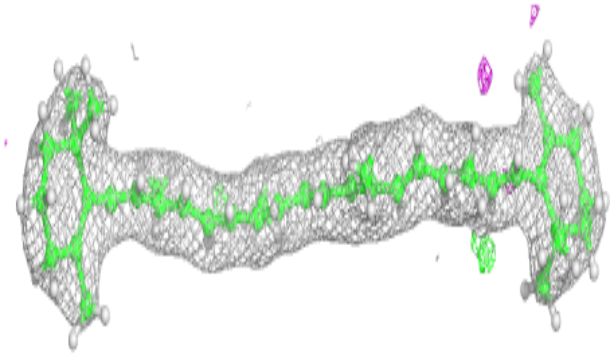
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

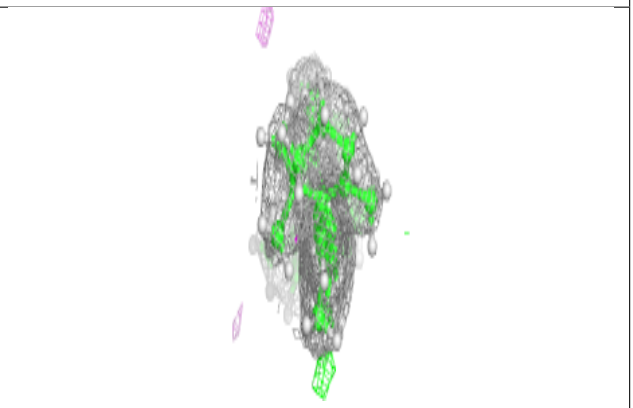


**Electron density around BCR A 406:**

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

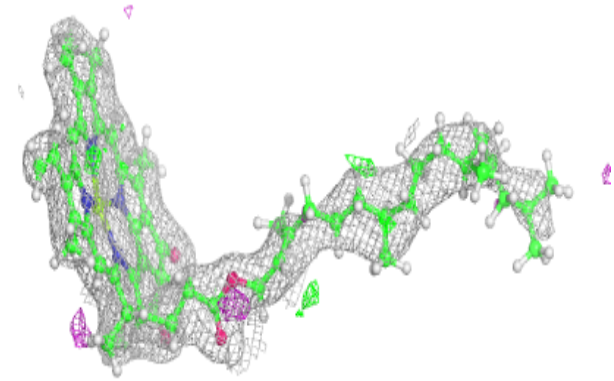


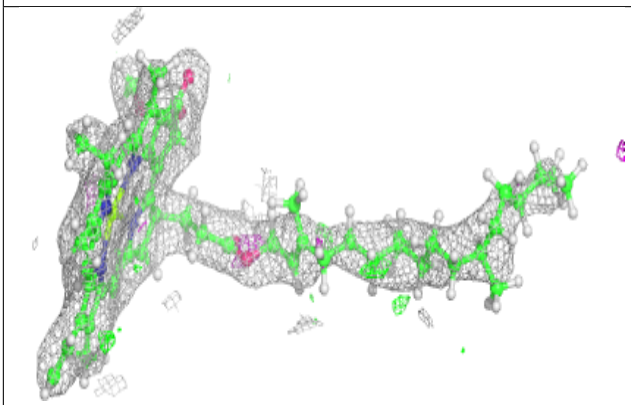


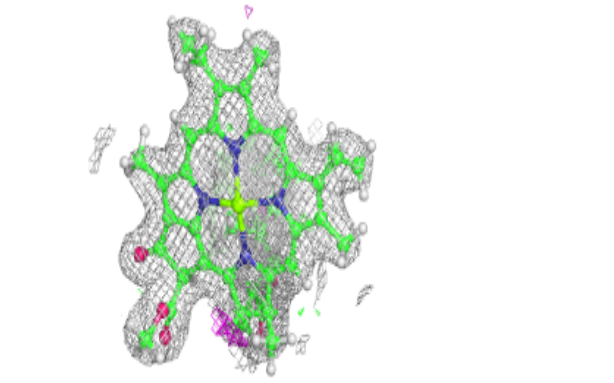


**Electron density around CLA B 604:**

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

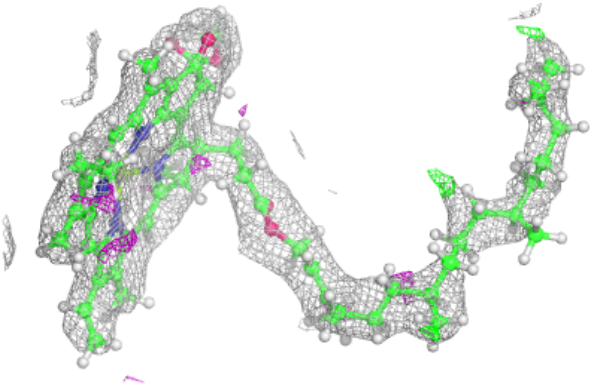


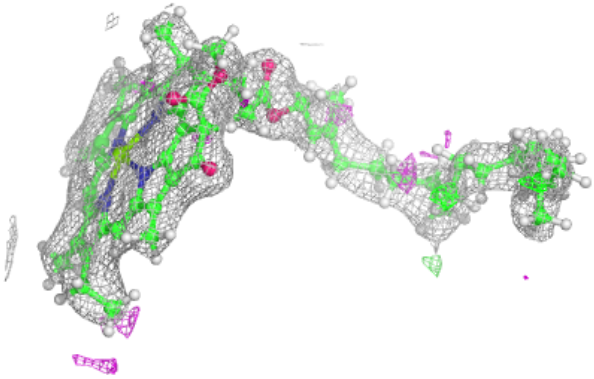


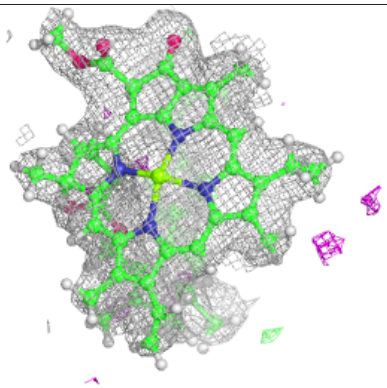


**Electron density around CLA b 606:**

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

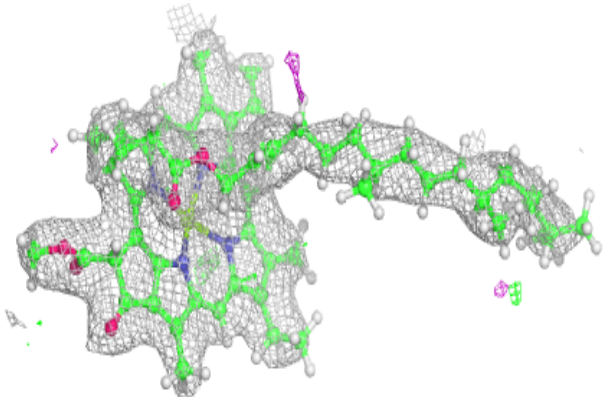


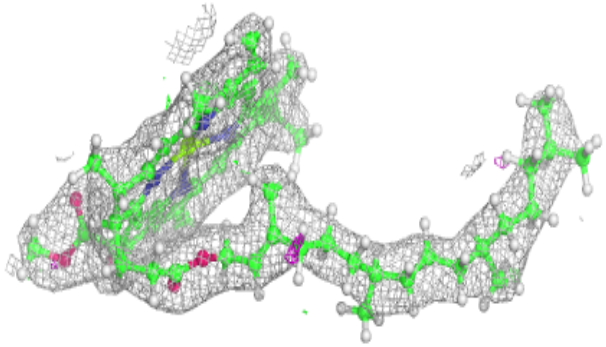


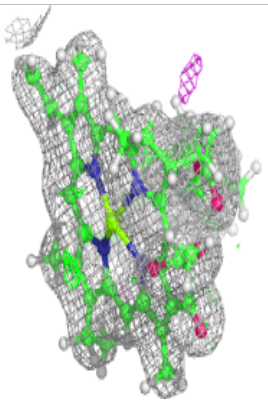


**Electron density around CLA b 608:**

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

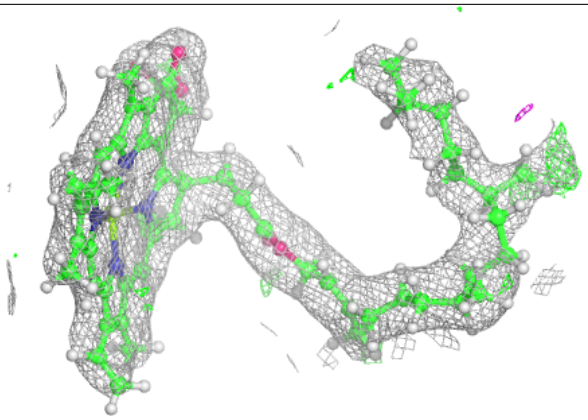


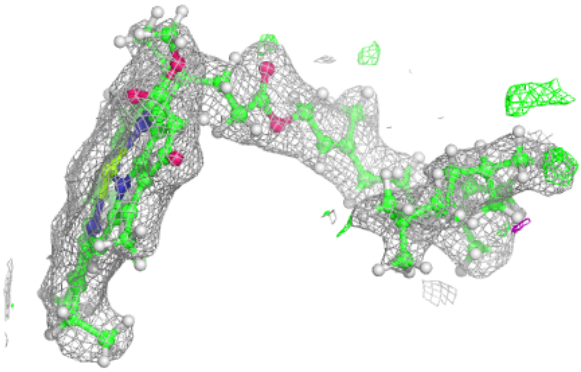


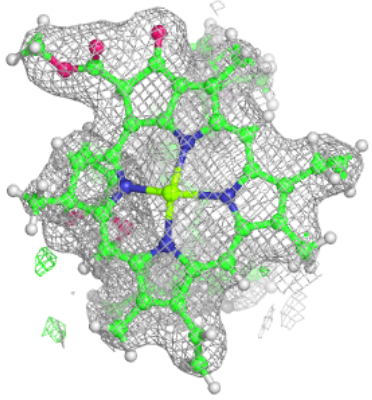


**Electron density around CLA B 606:**

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

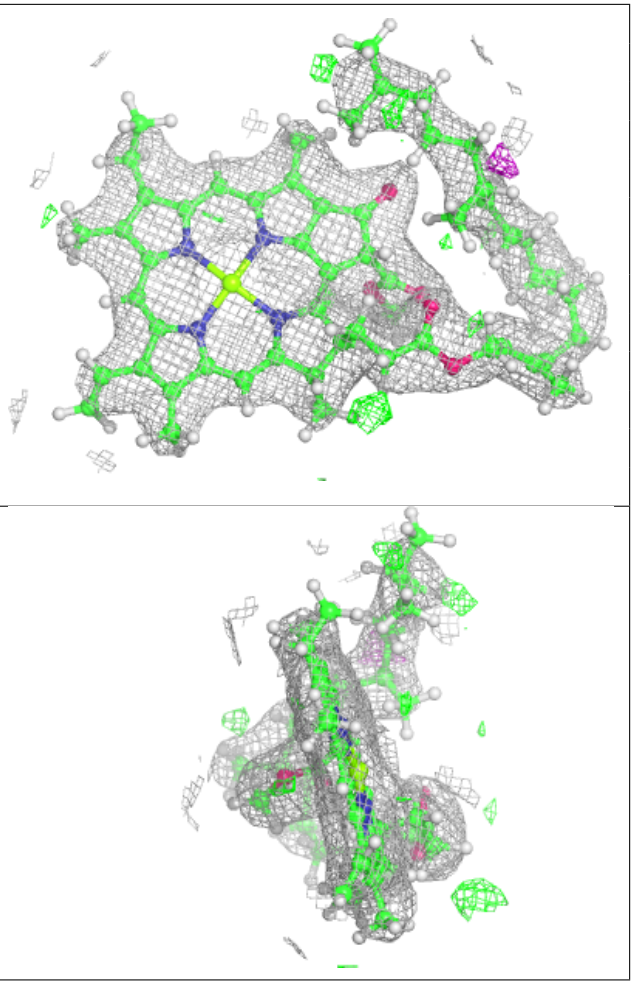






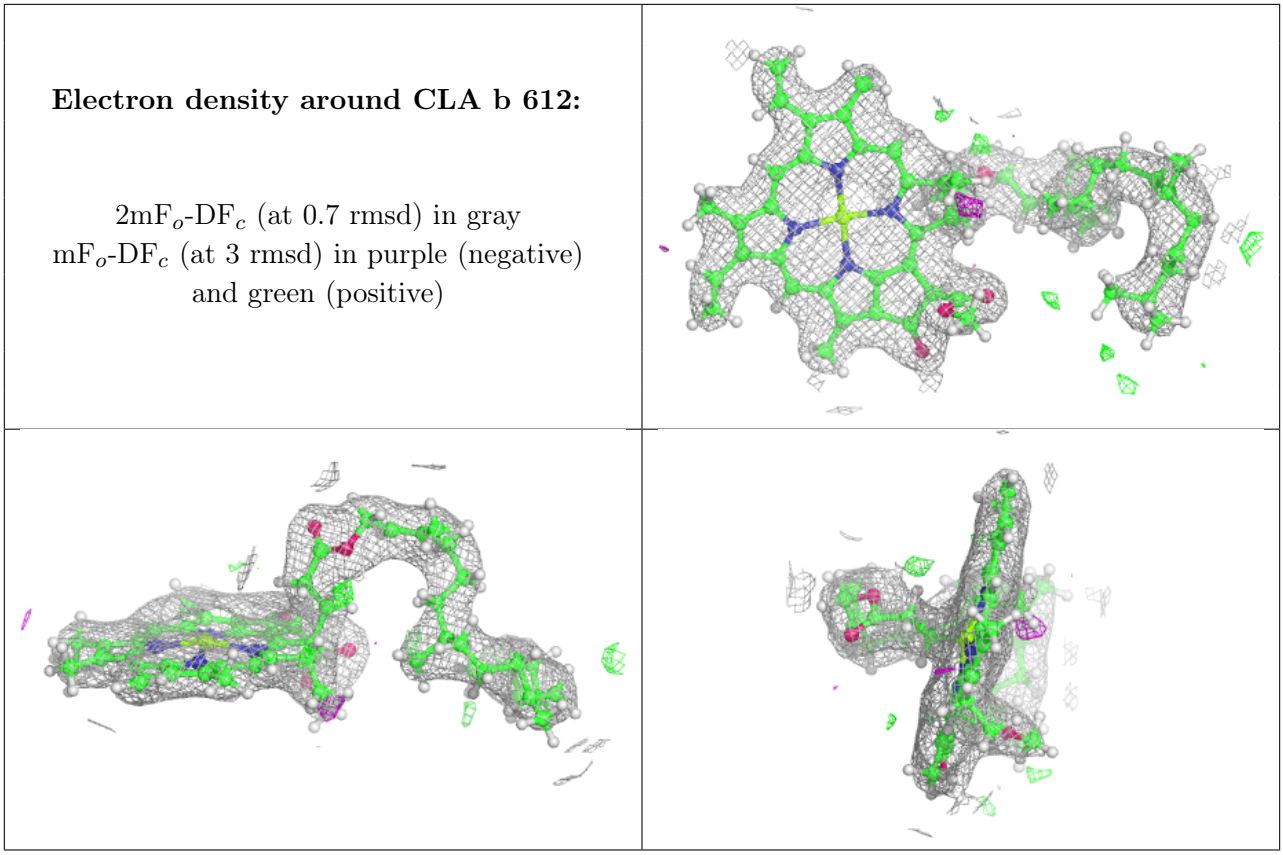
**Electron density around CLA b 610:**

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



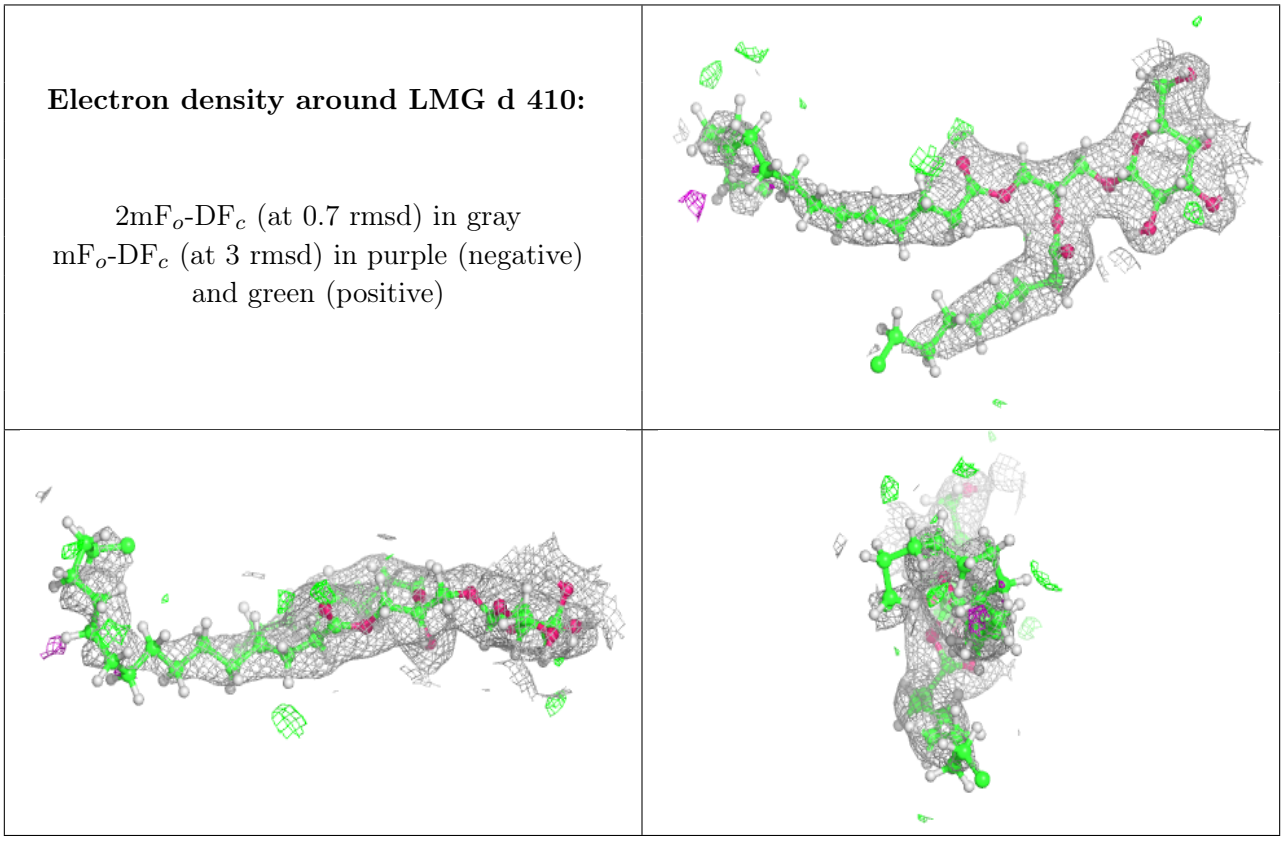
**Electron density around CLA b 612:**

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



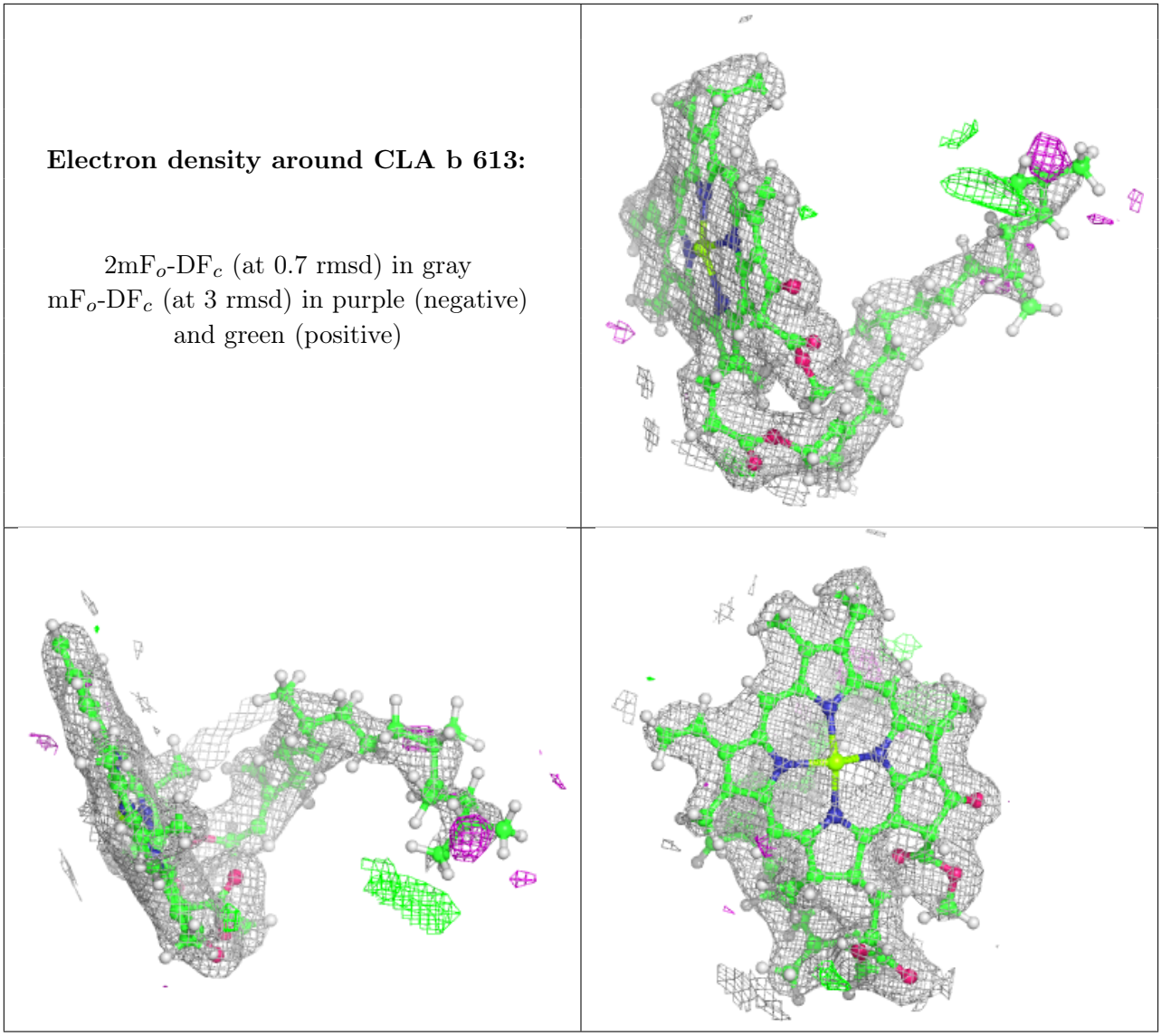
**Electron density around LMG d 410:**

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



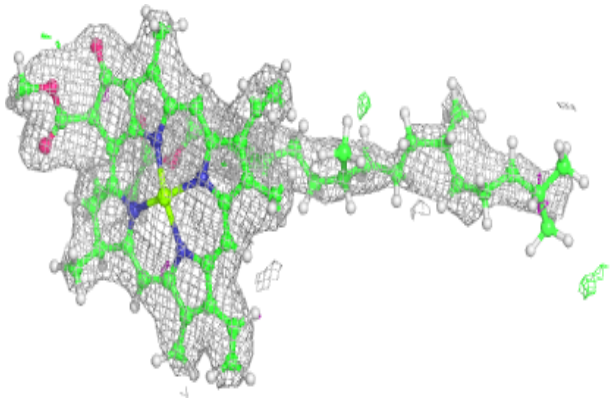
**Electron density around CLA b 613:**

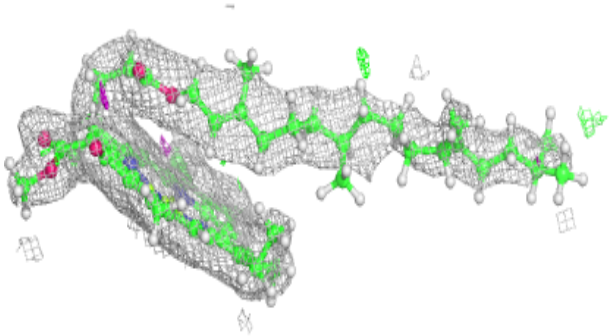
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

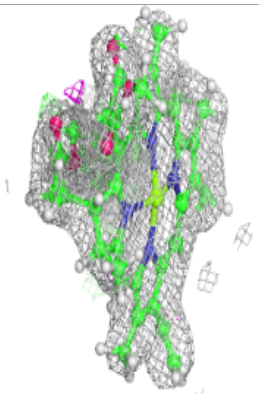


**Electron density around CLA b 614:**

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

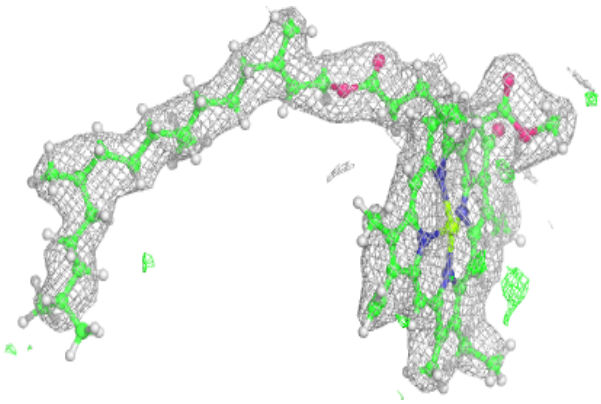


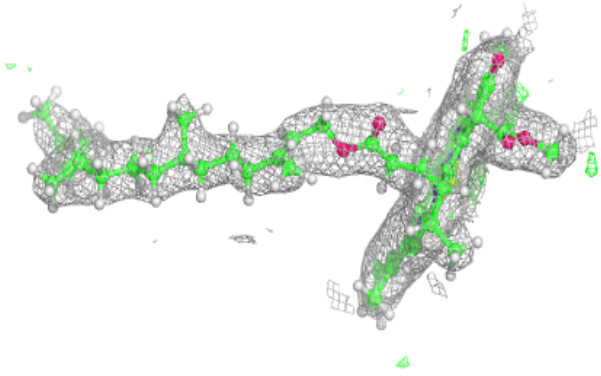


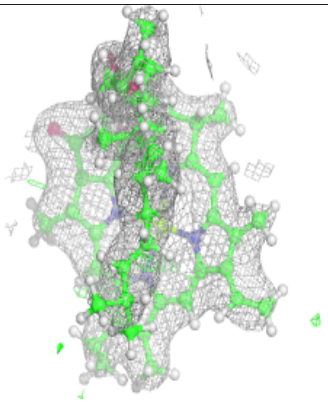


**Electron density around CLA B 609:**

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

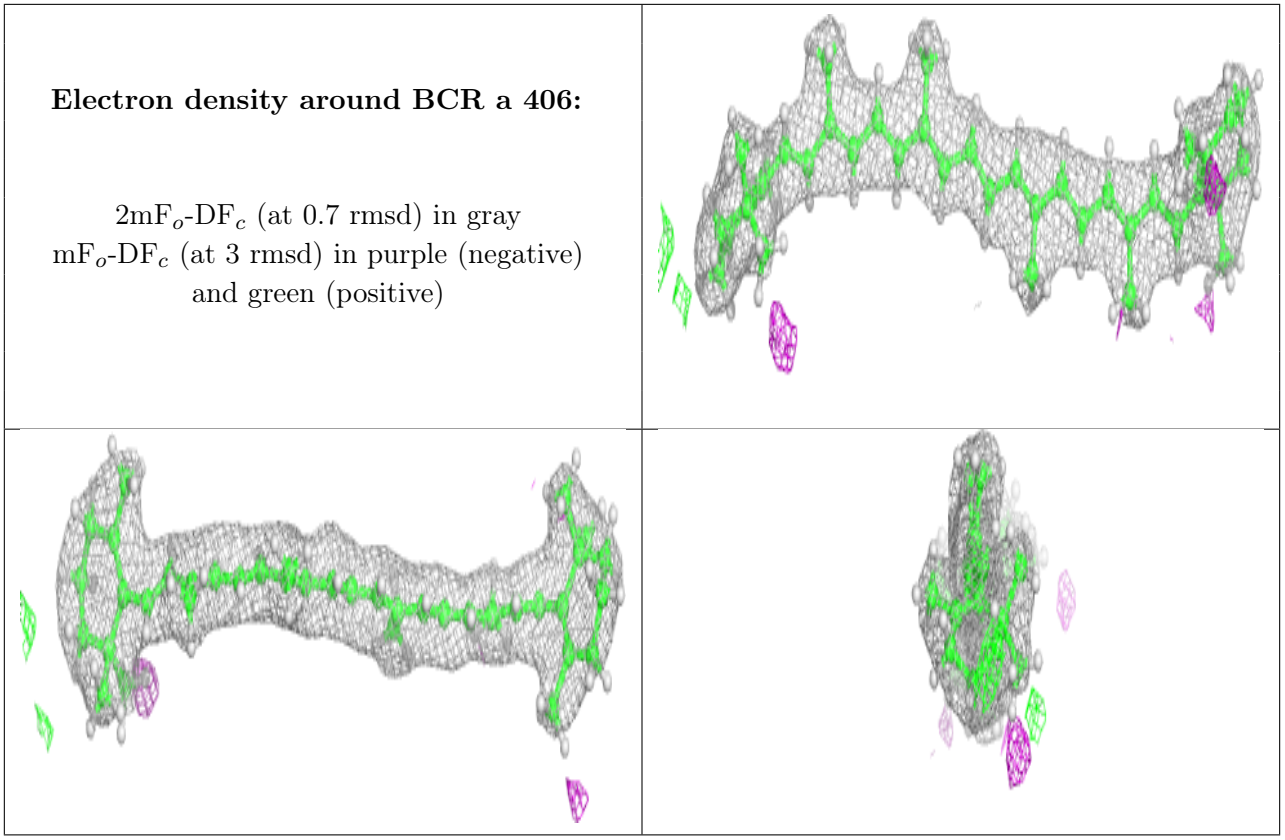






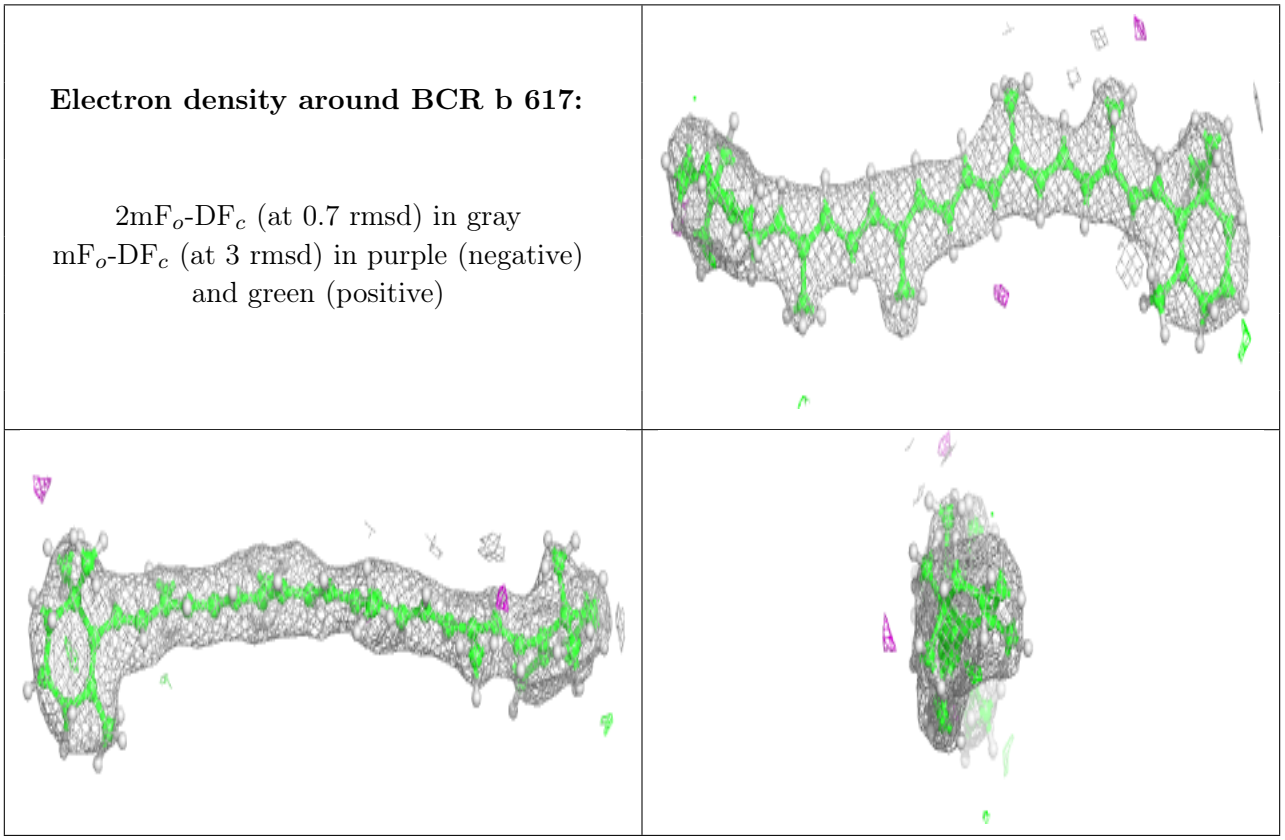
**Electron density around BCR a 406:**

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



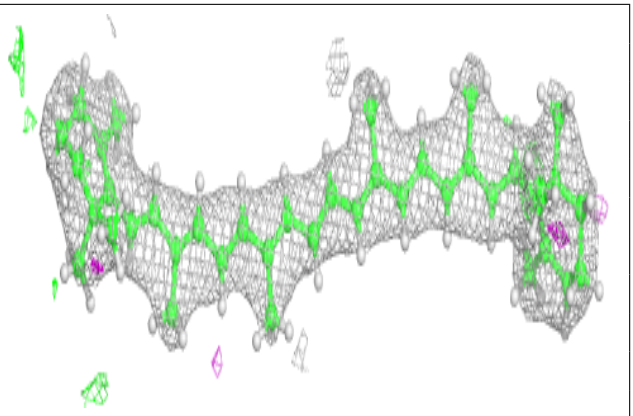
**Electron density around BCR b 617:**

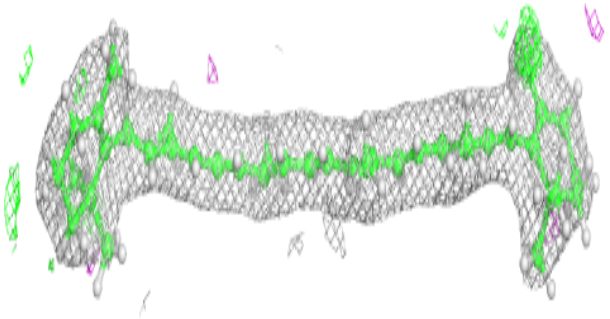
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

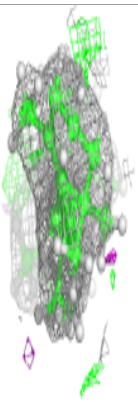


**Electron density around BCR b 618:**

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

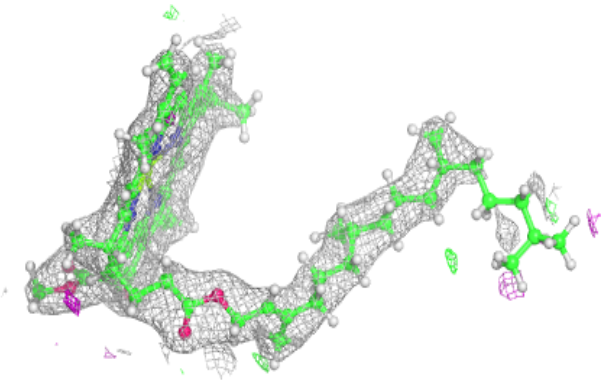


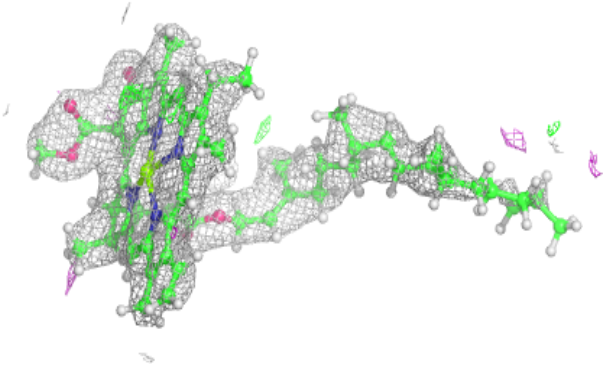


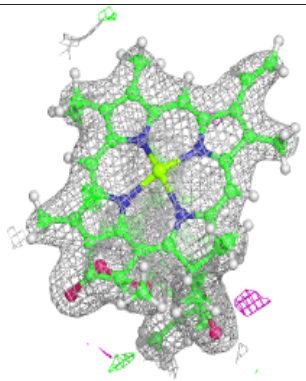


**Electron density around CLA C 508:**

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

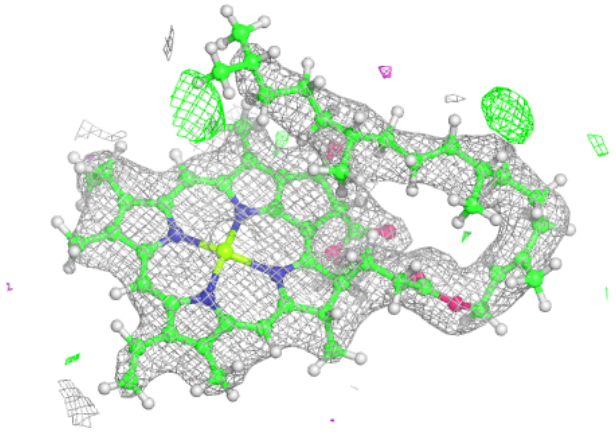


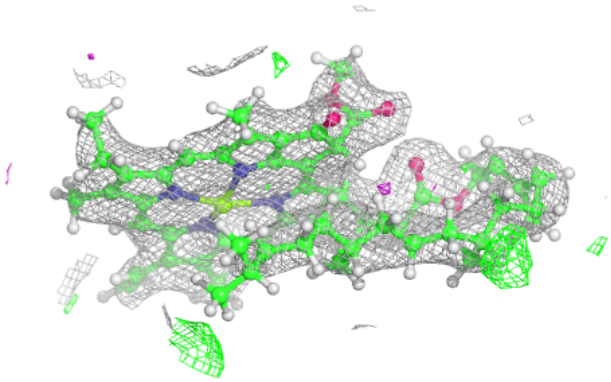


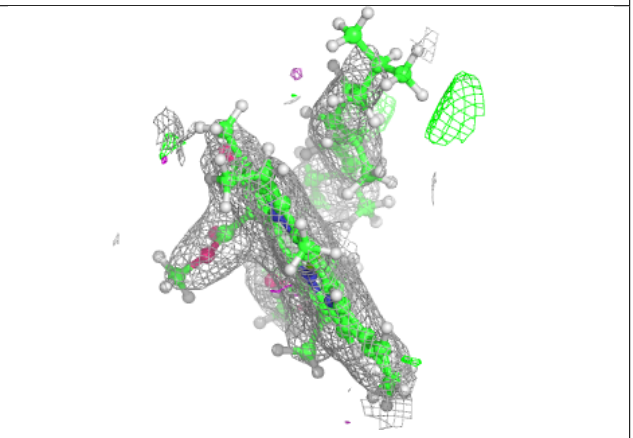


**Electron density around CLA C 509:**

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

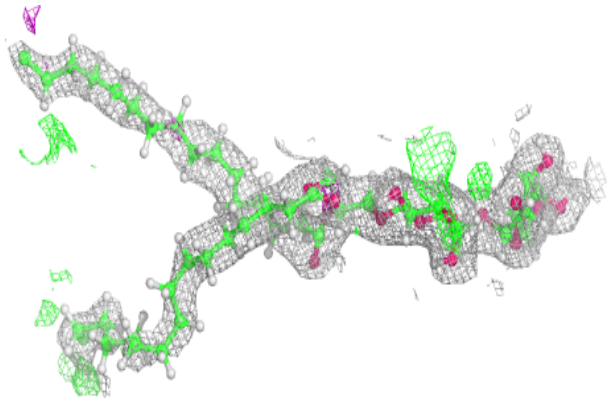


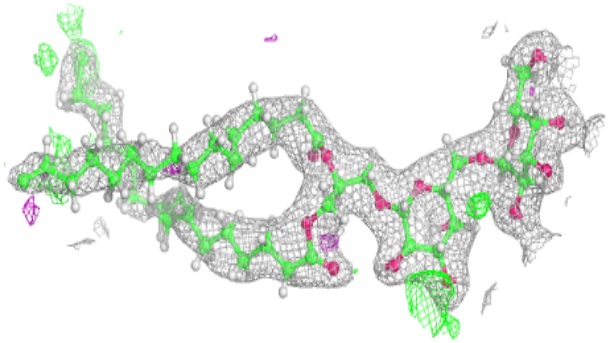


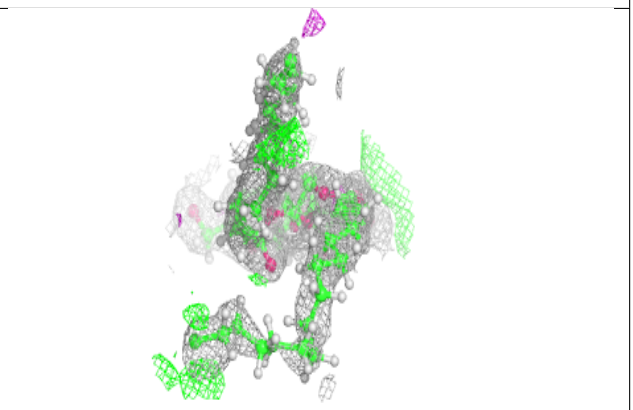


**Electron density around DGD C 515:**

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

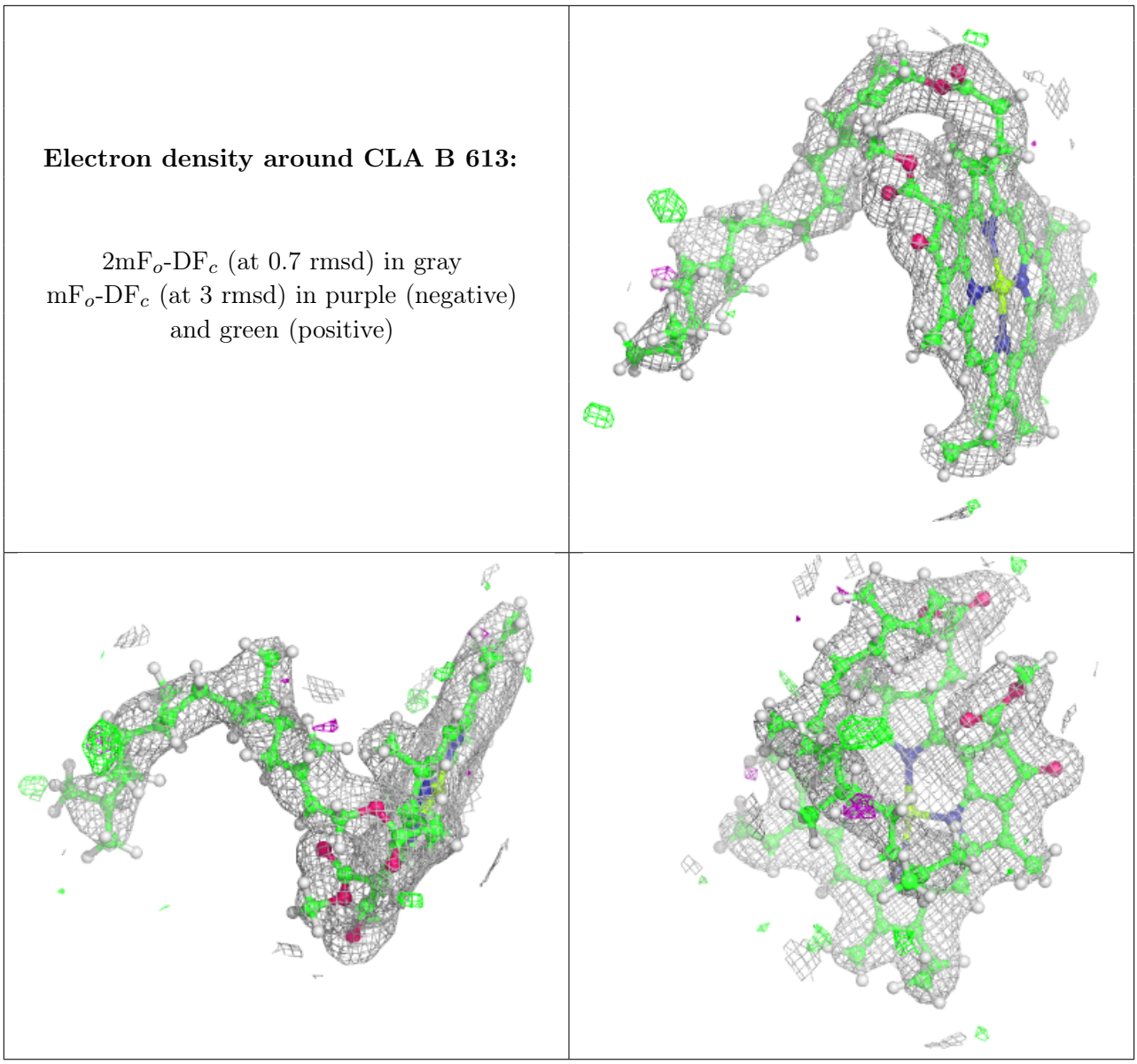






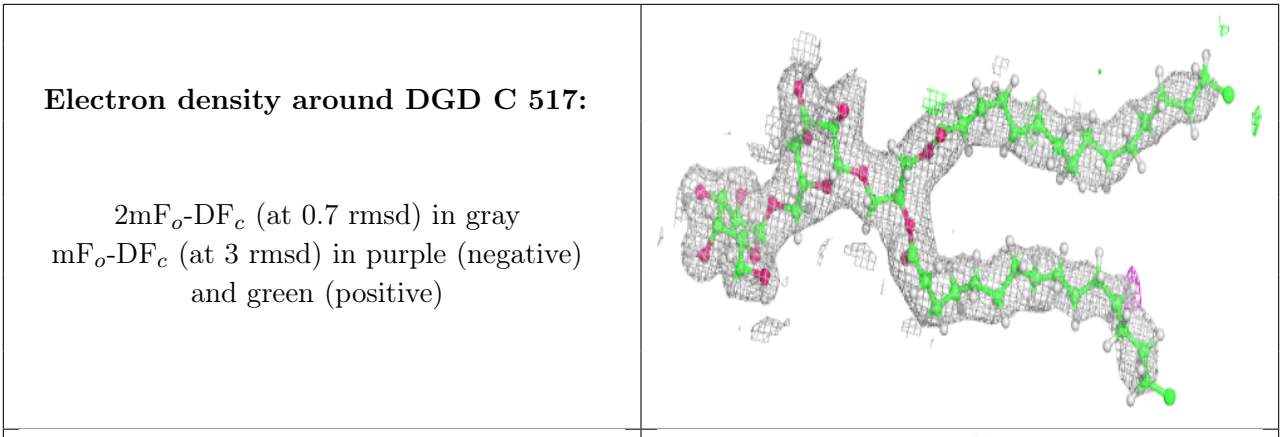
**Electron density around CLA B 613:**

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



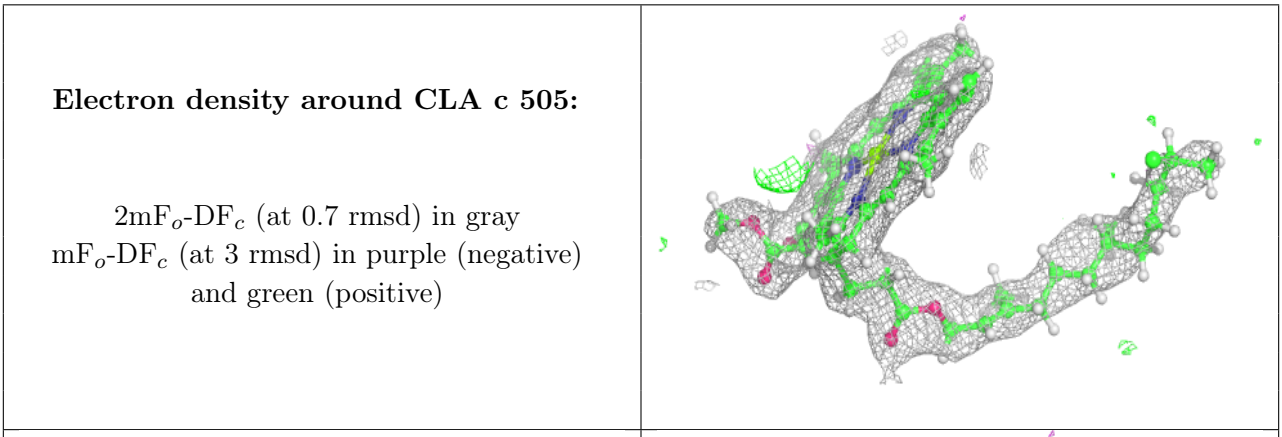
**Electron density around DGD C 517:**

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



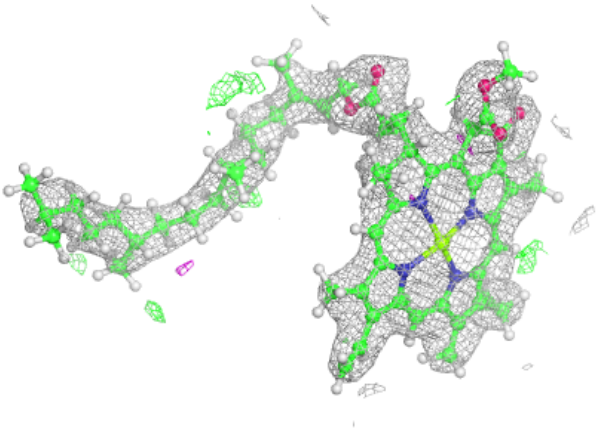
**Electron density around CLA c 505:**

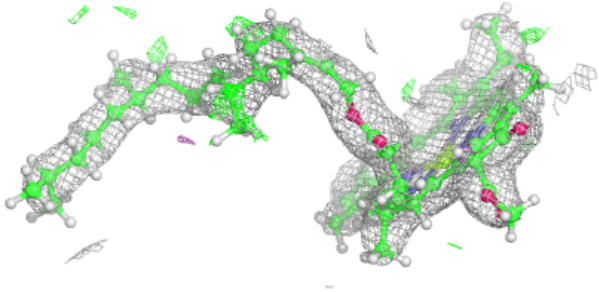
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

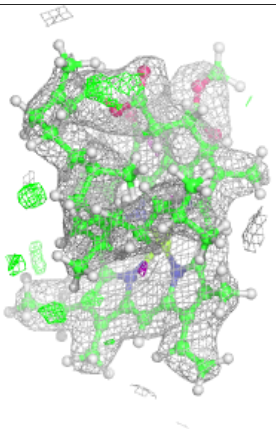


**Electron density around CLA C 511:**

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

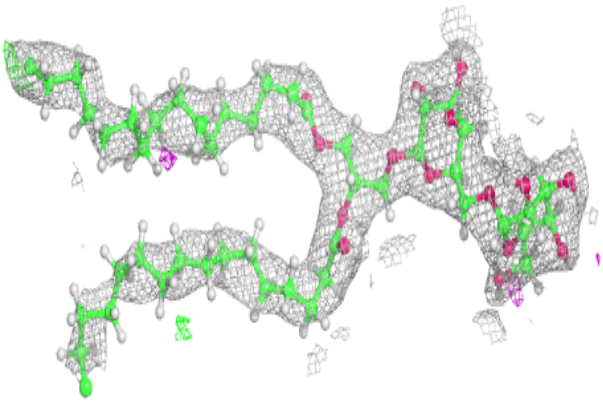


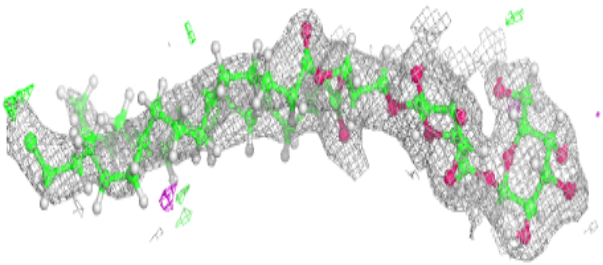


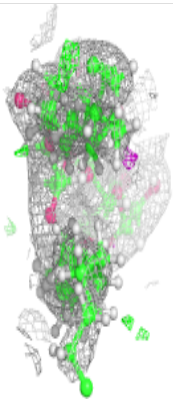


**Electron density around DGD c 519:**

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

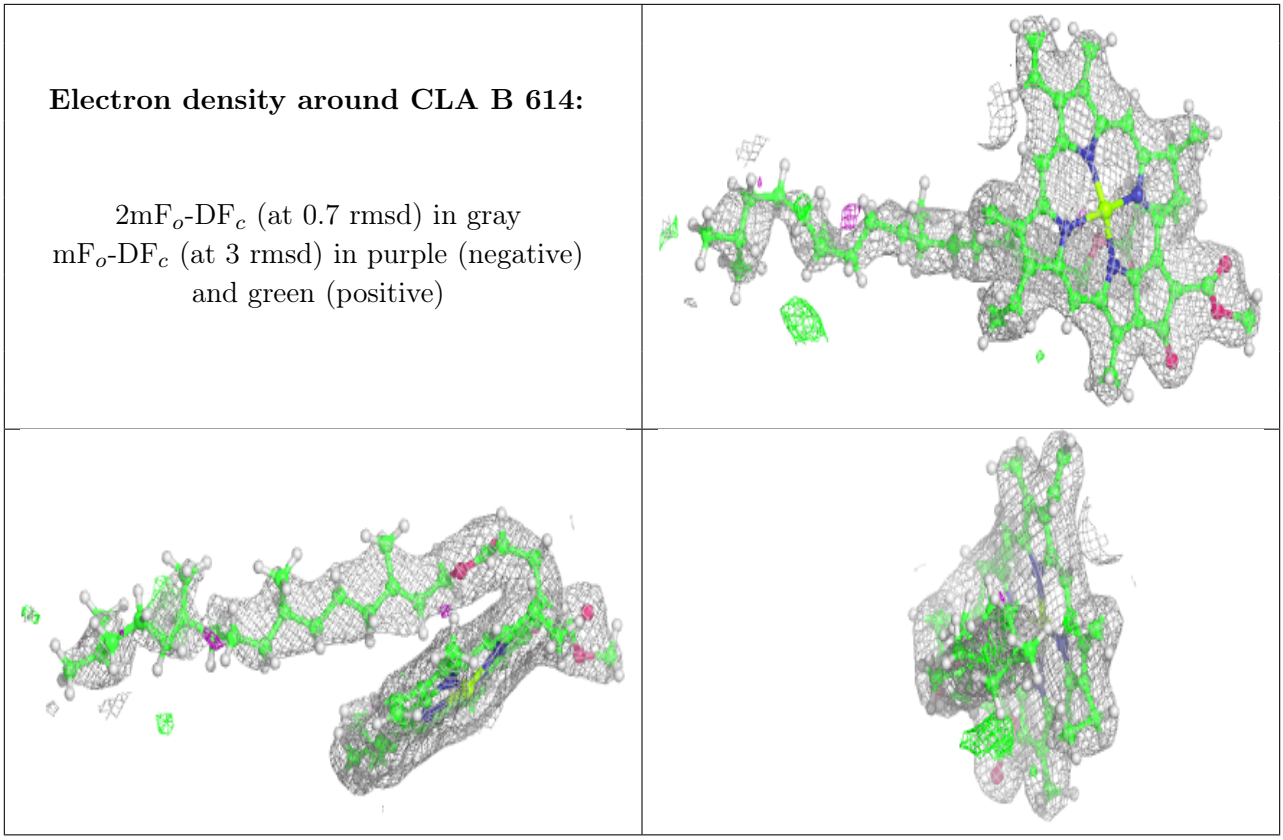






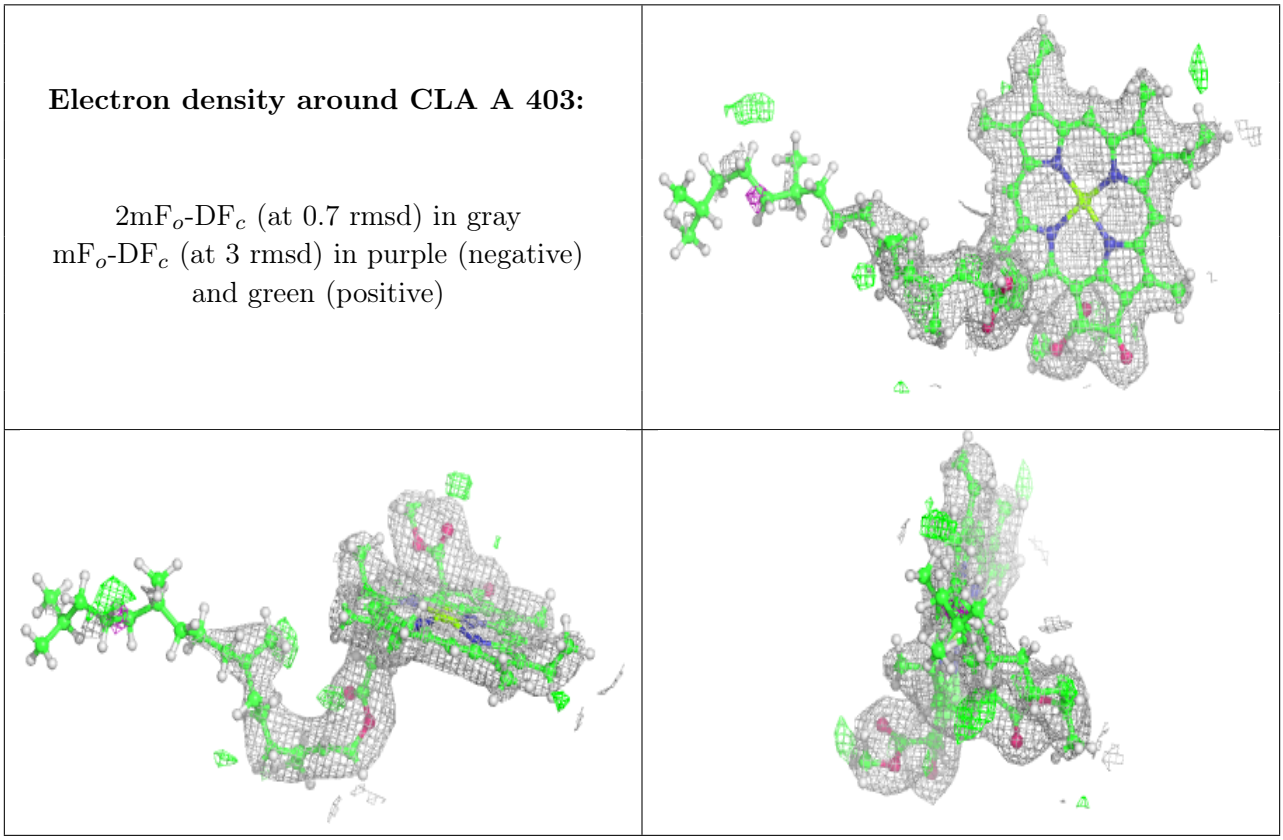
**Electron density around CLA B 614:**

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



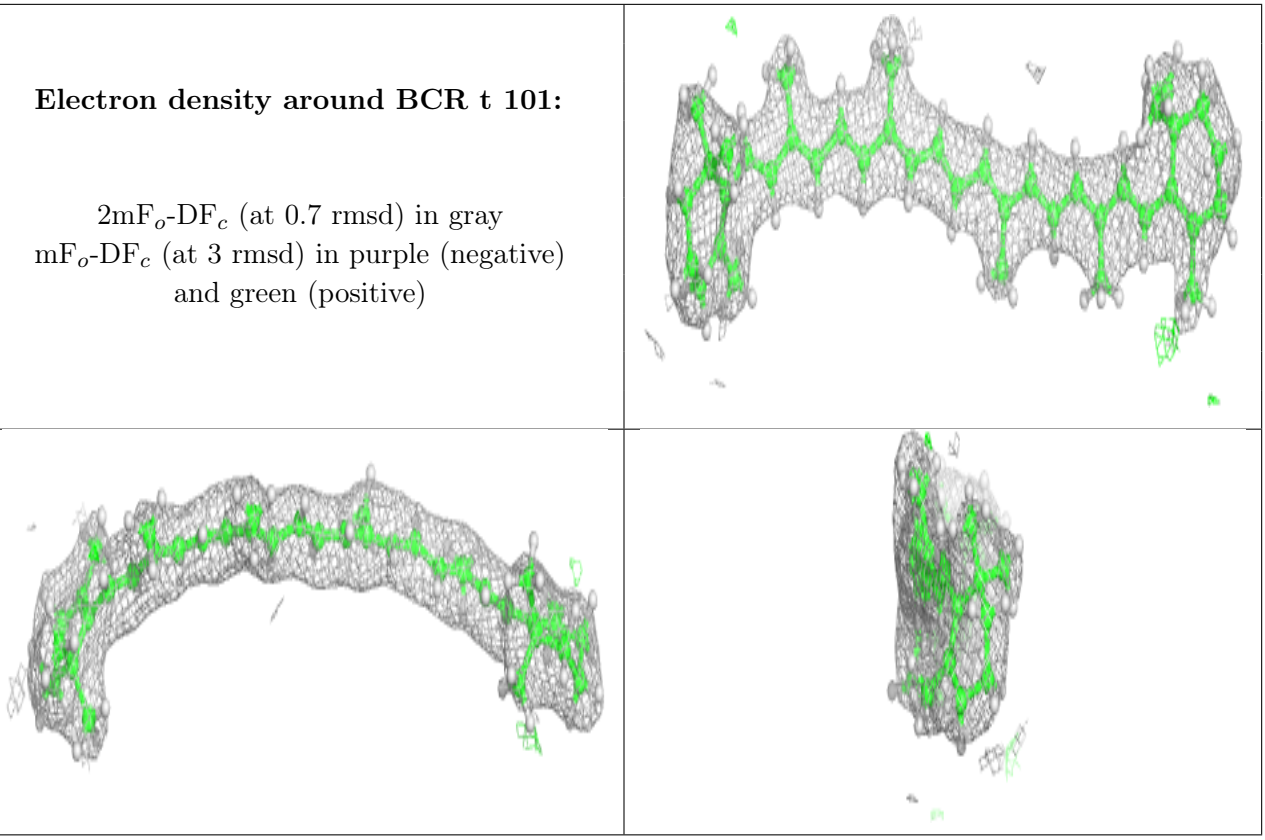
**Electron density around CLA A 403:**

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



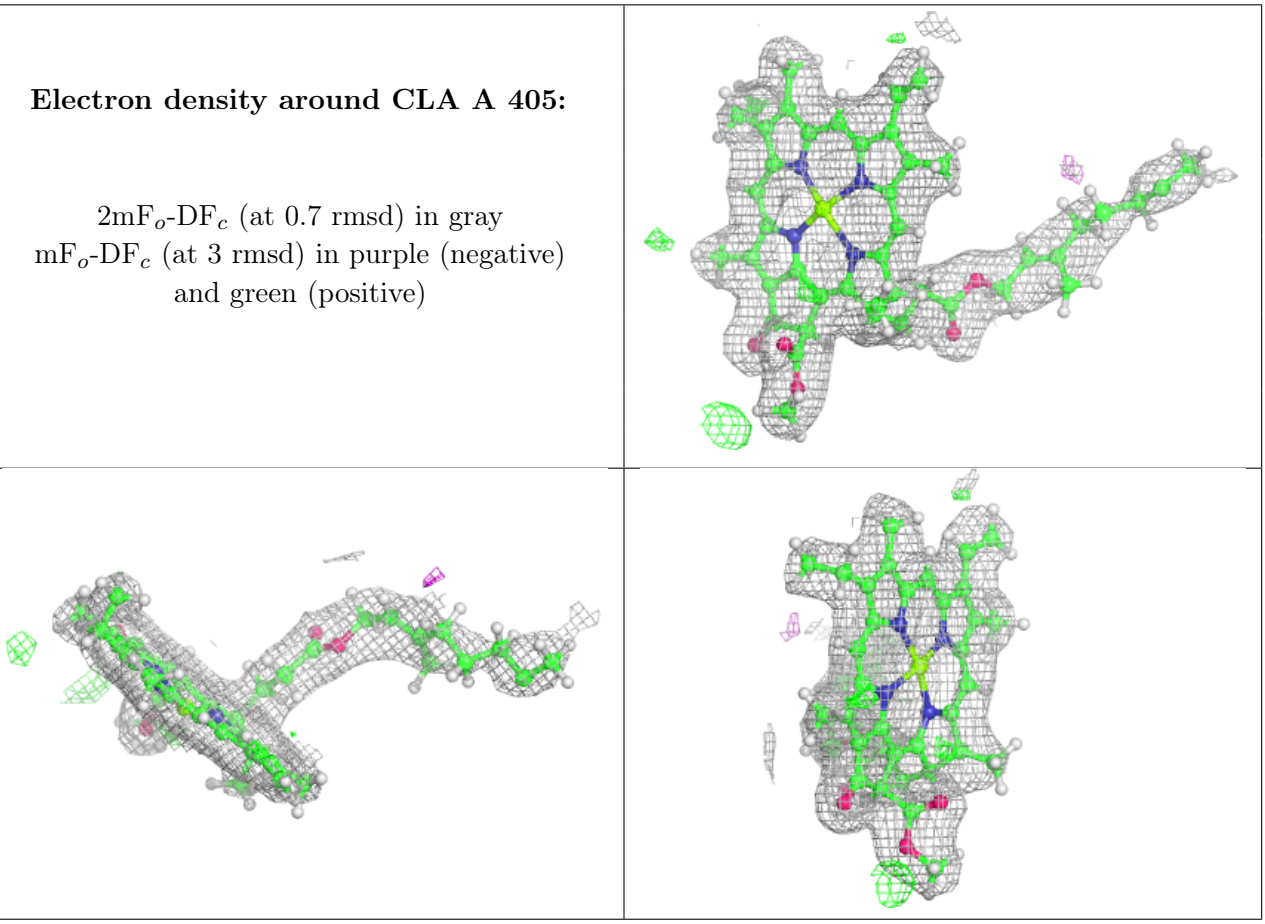
**Electron density around BCR t 101:**

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



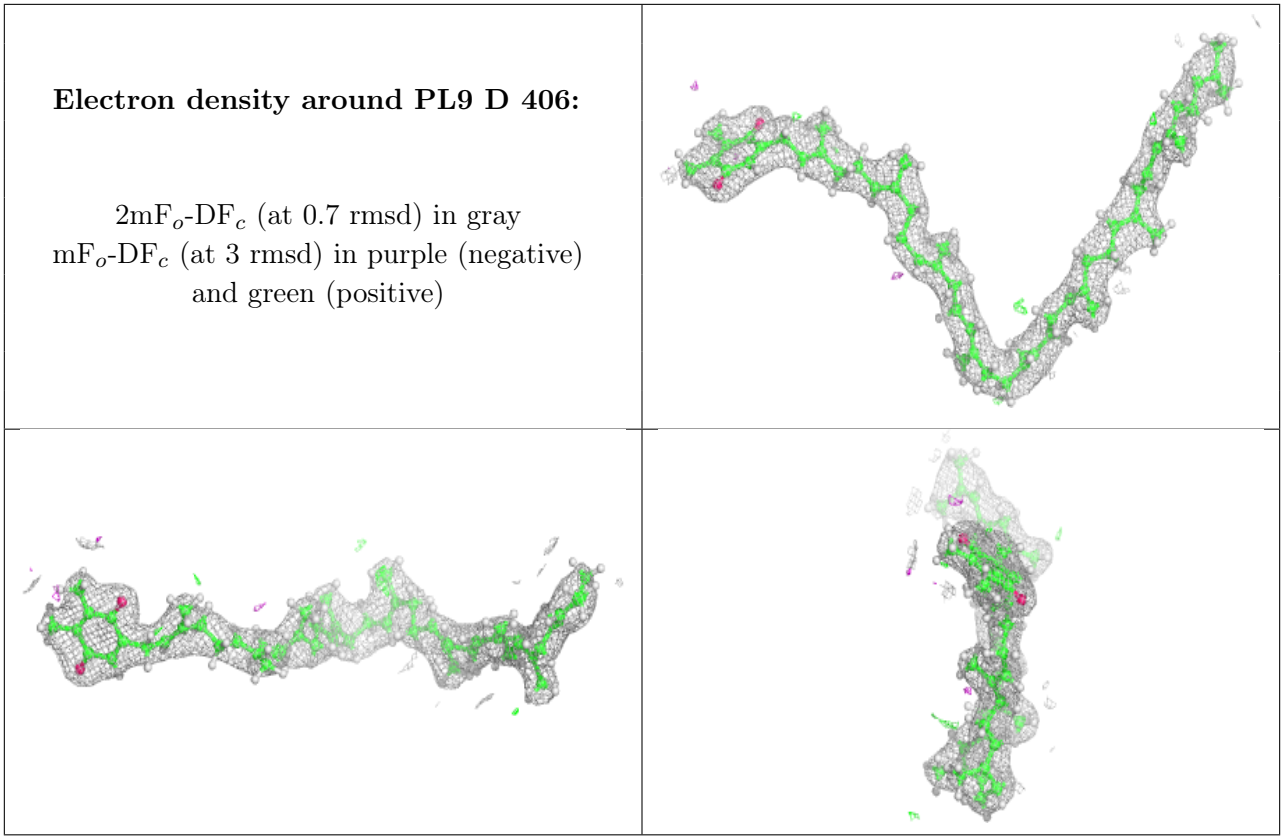
**Electron density around CLA A 405:**

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



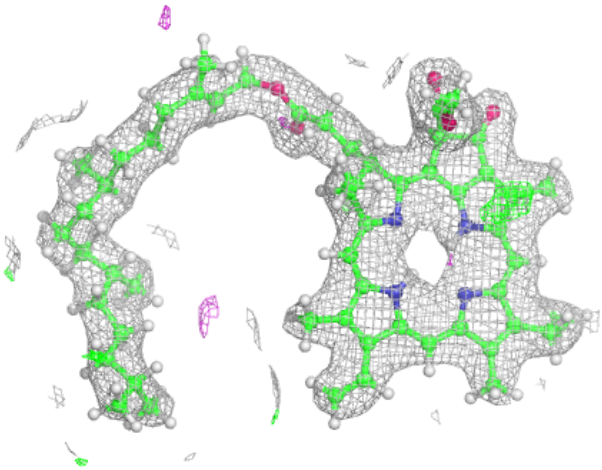
**Electron density around PL9 D 406:**

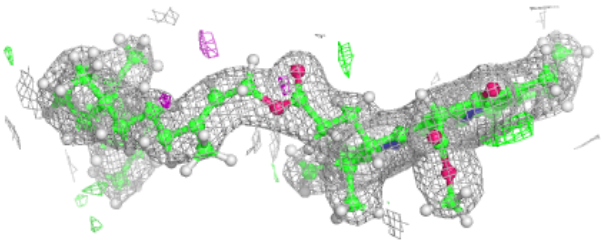
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

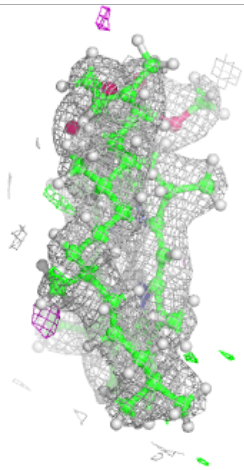


**Electron density around PHO A 404:**

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

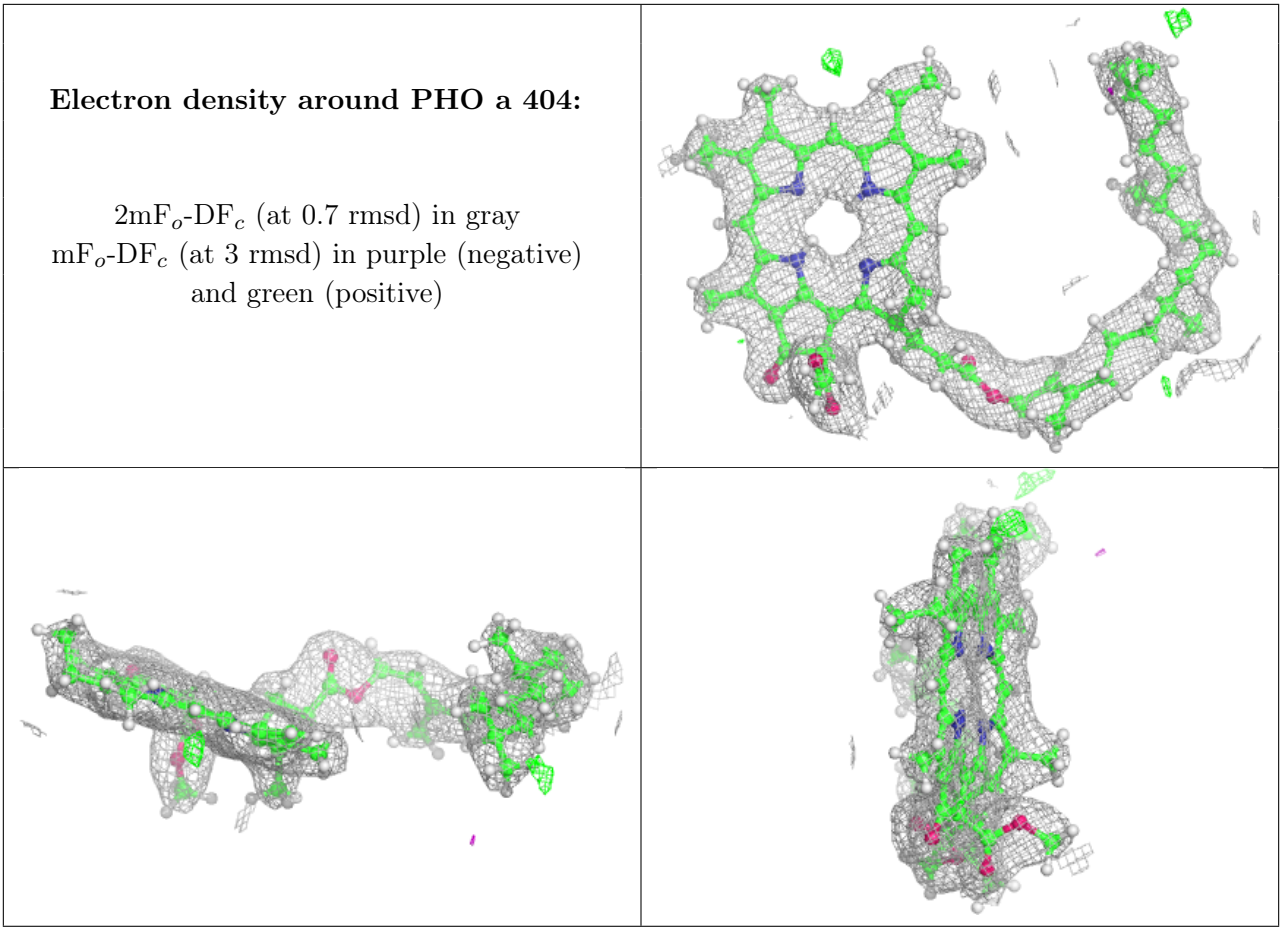






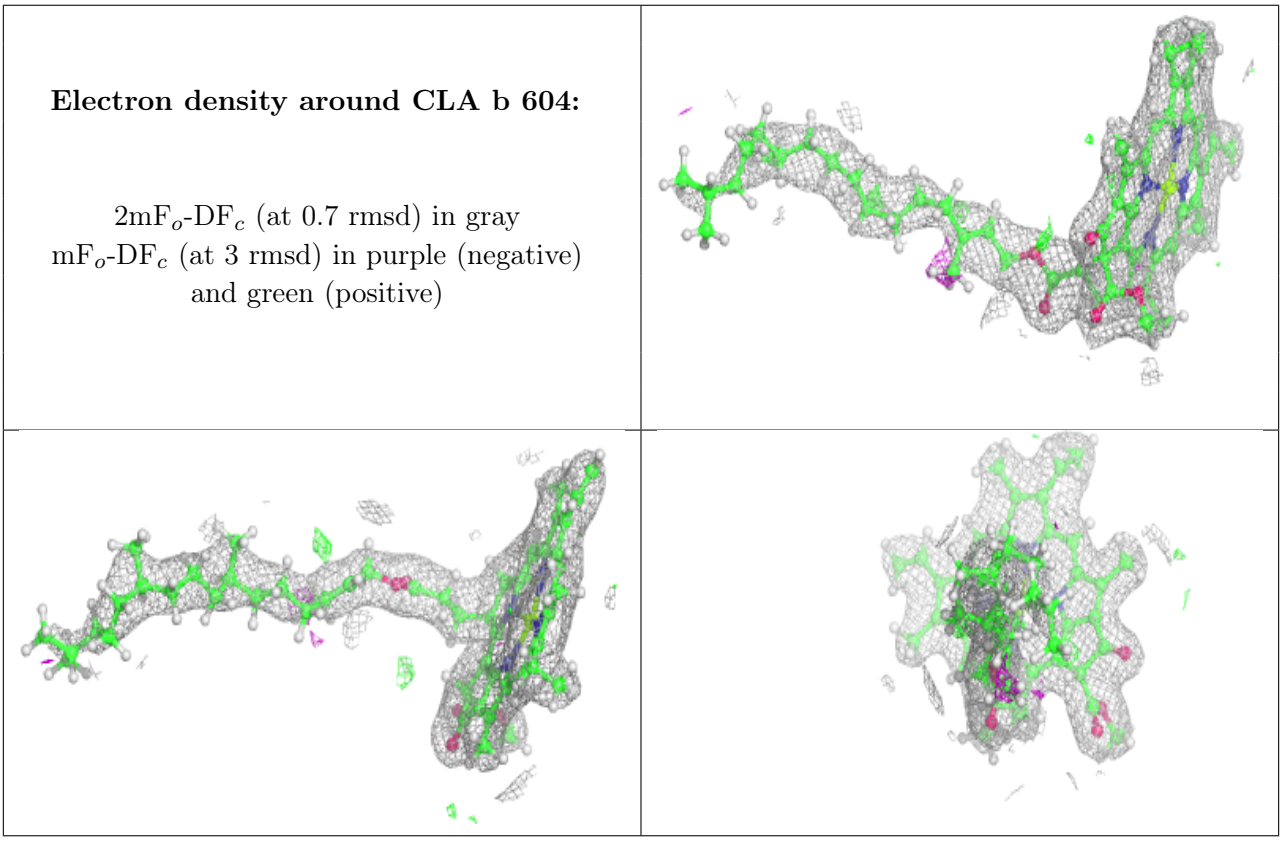
**Electron density around PHO a 404:**

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



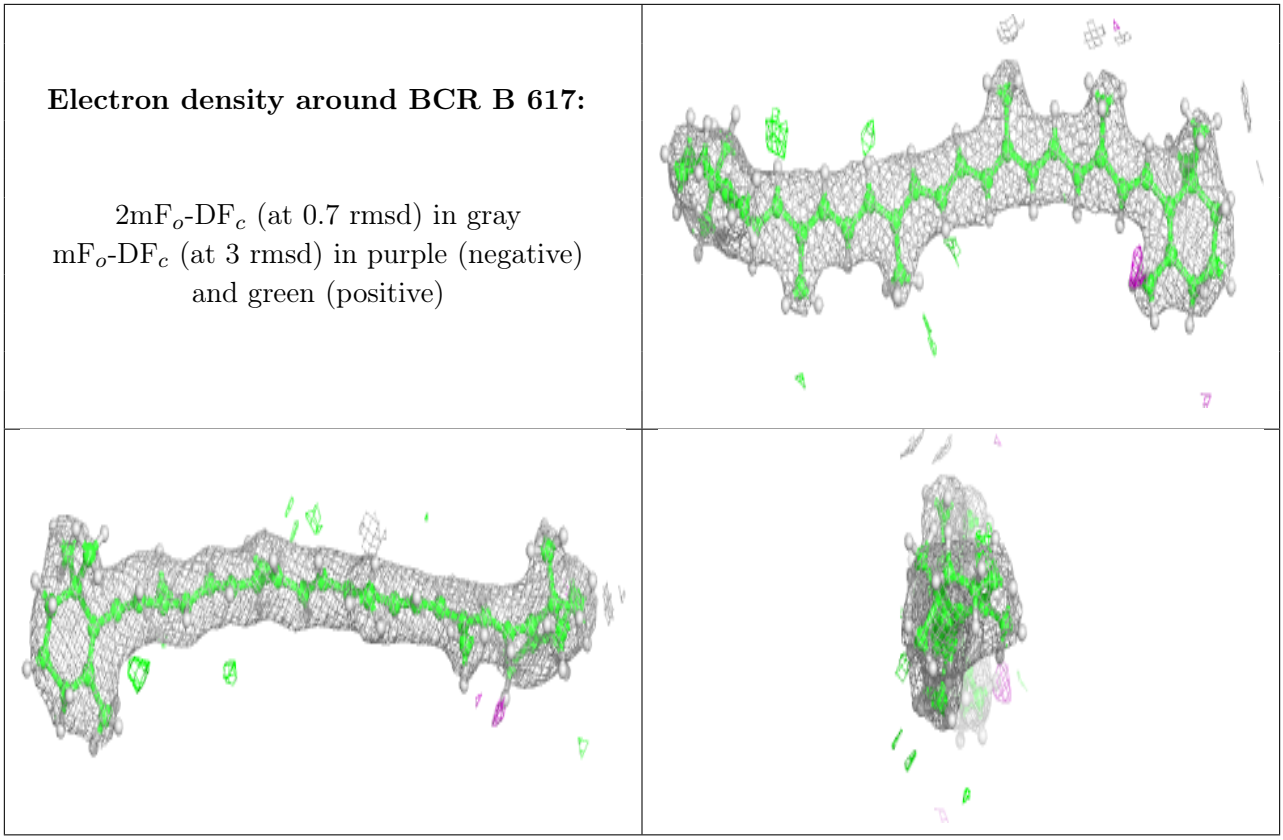
**Electron density around CLA b 604:**

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



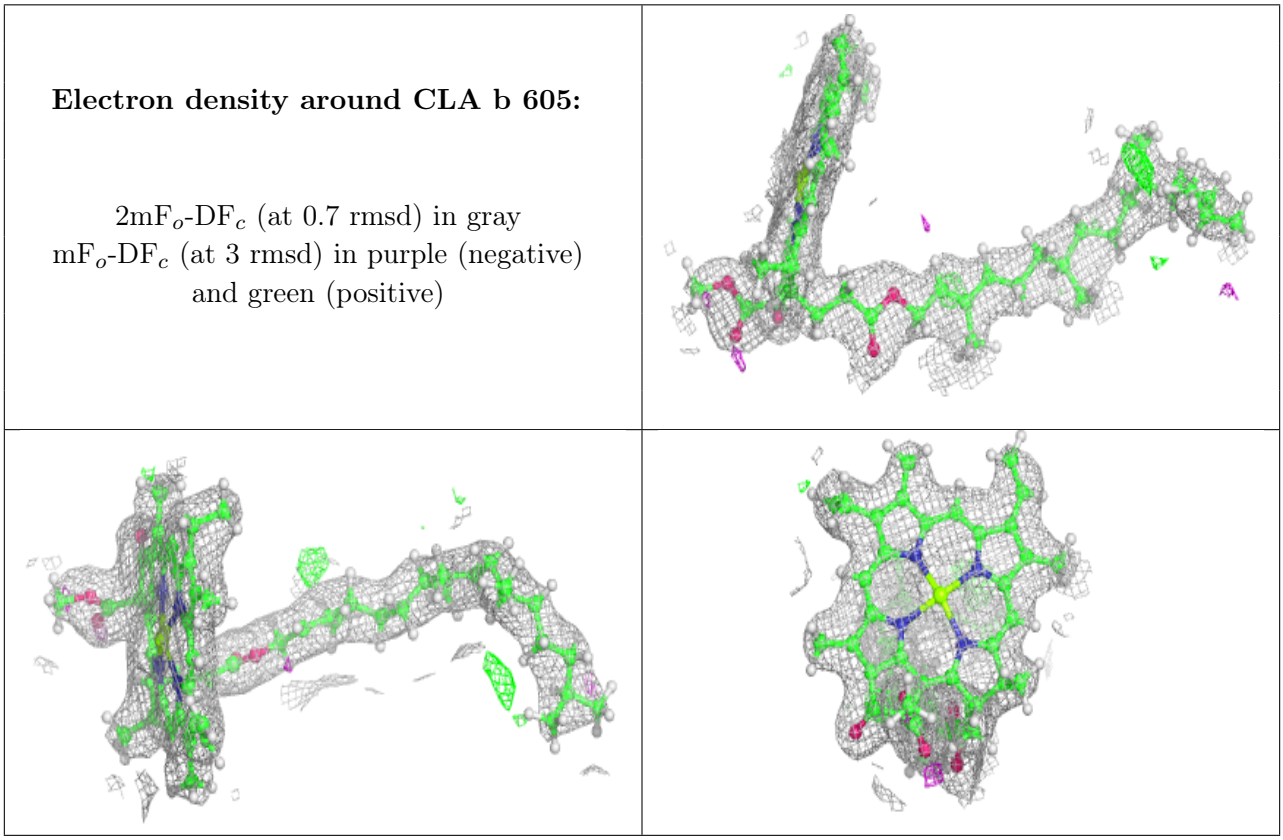
**Electron density around BCR B 617:**

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



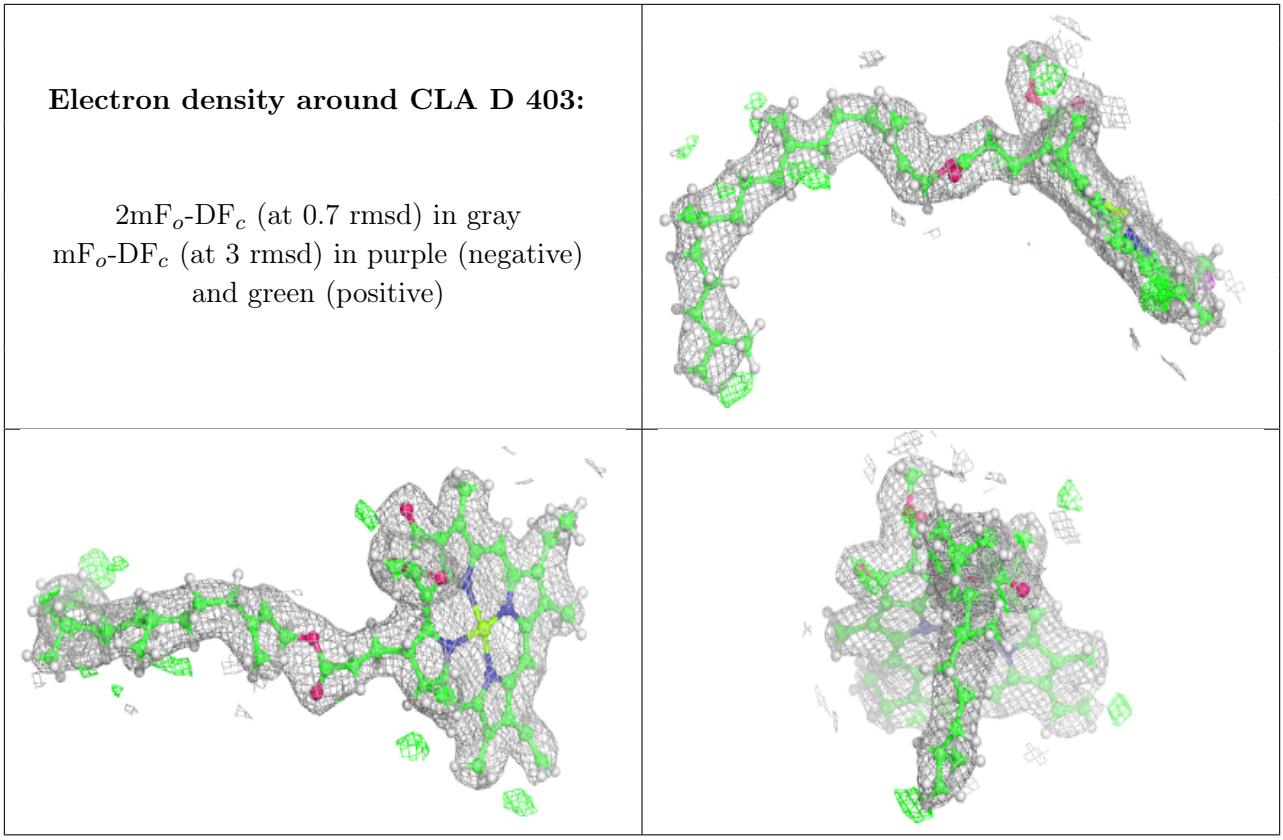
**Electron density around CLA b 605:**

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



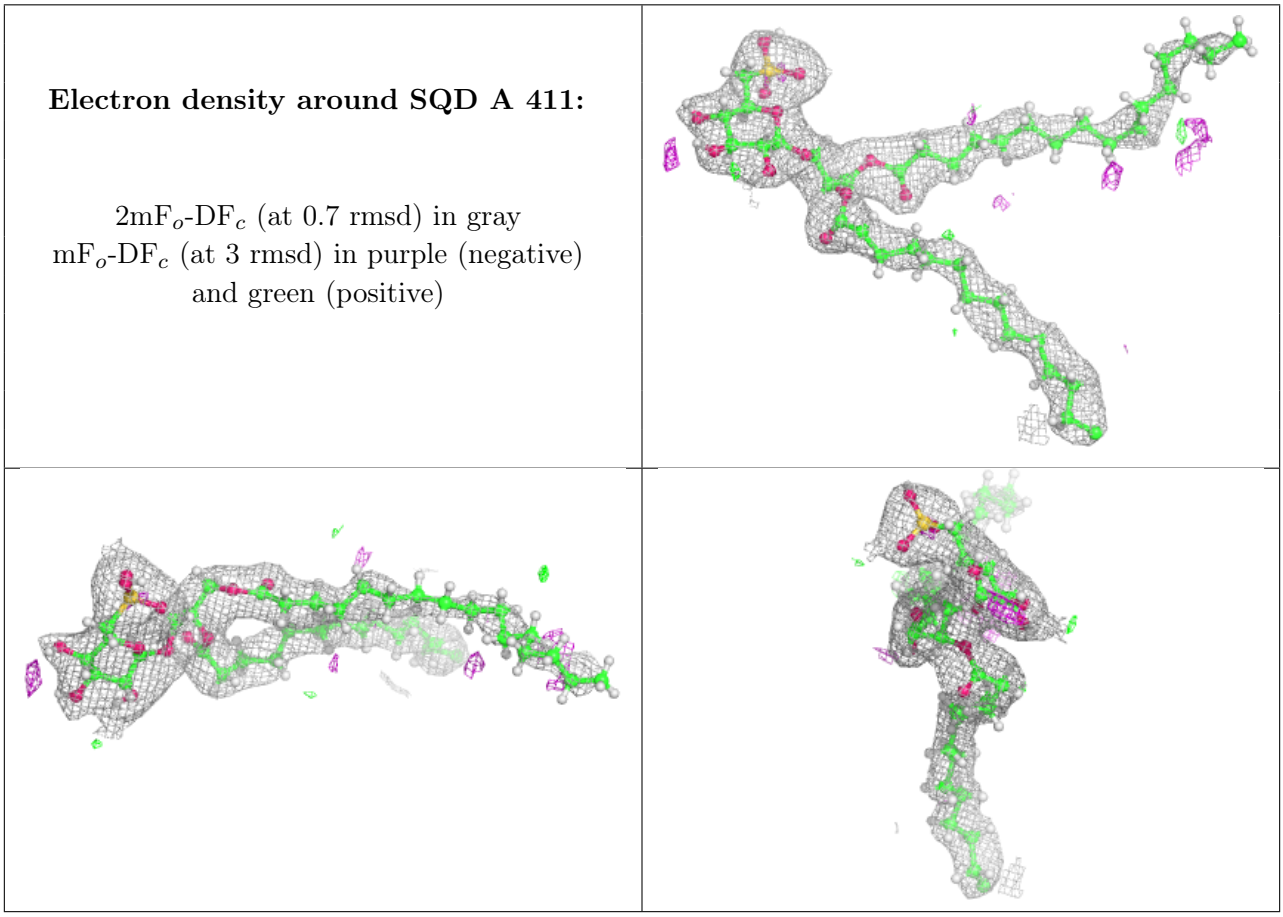
**Electron density around CLA D 403:**

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



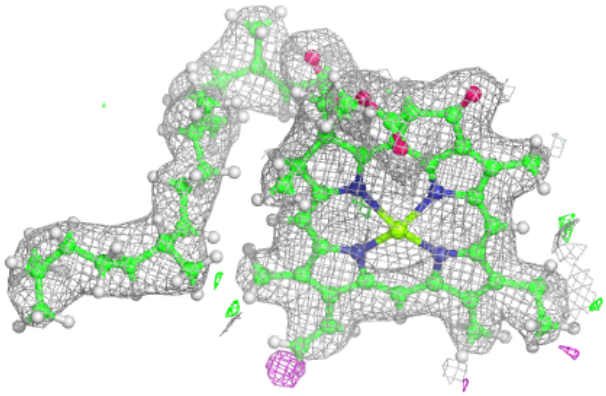
**Electron density around SQD A 411:**

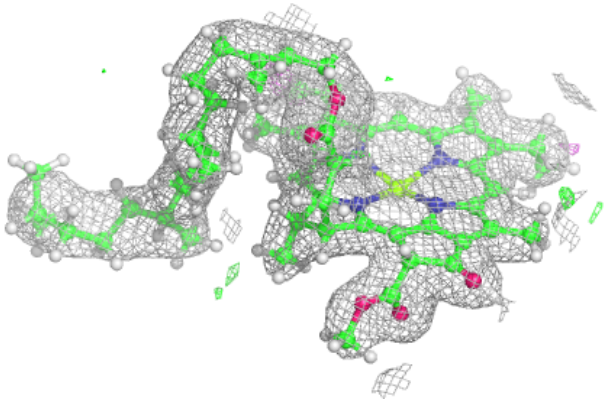
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

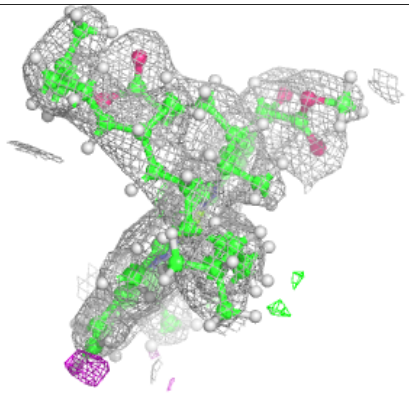


**Electron density around CLA D 404:**

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

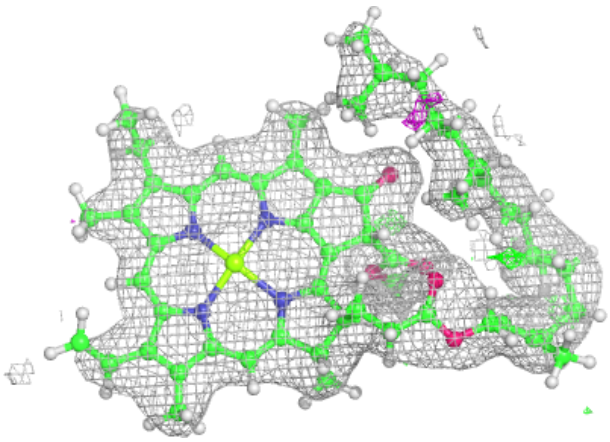


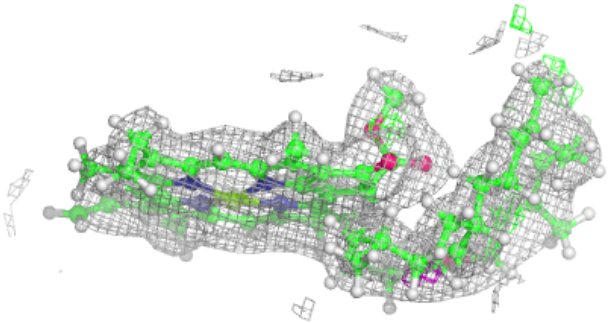


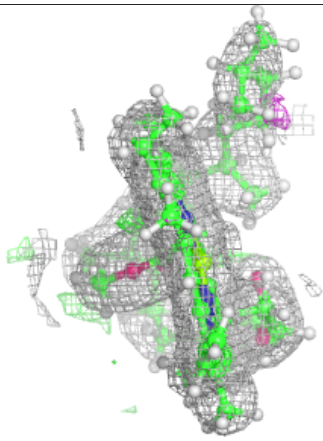


**Electron density around CLA B 610:**

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

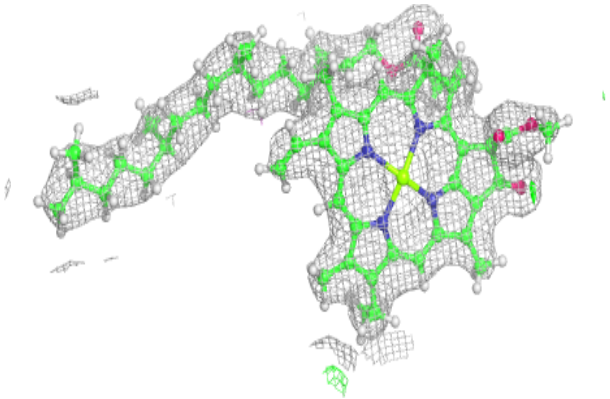


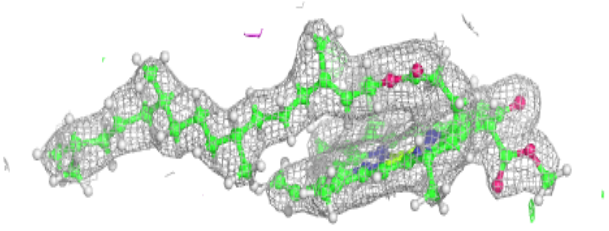


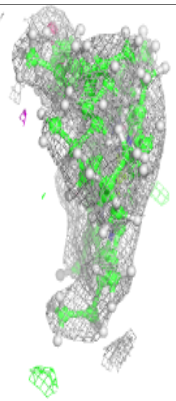


**Electron density around CLA C 501:**

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

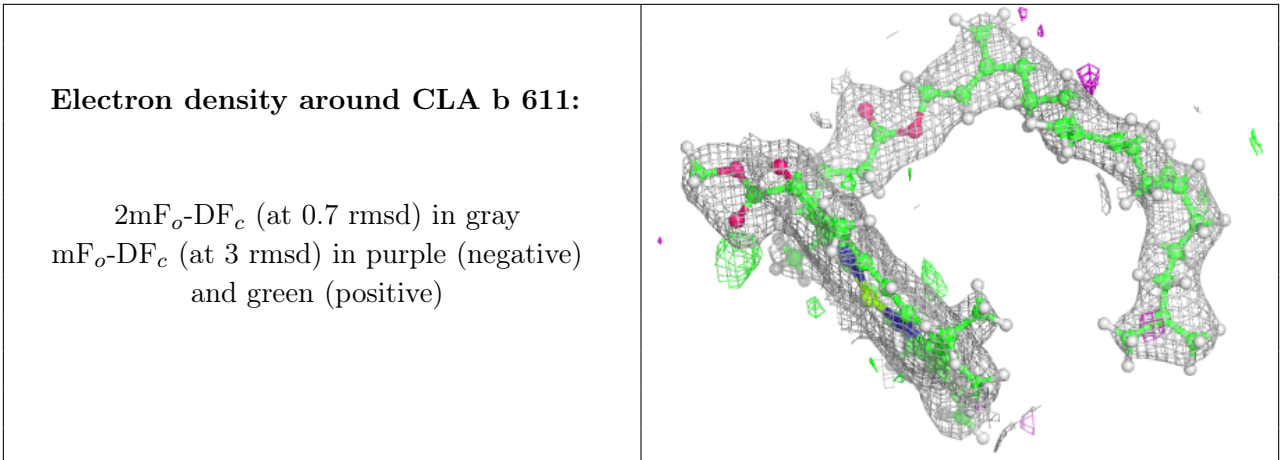


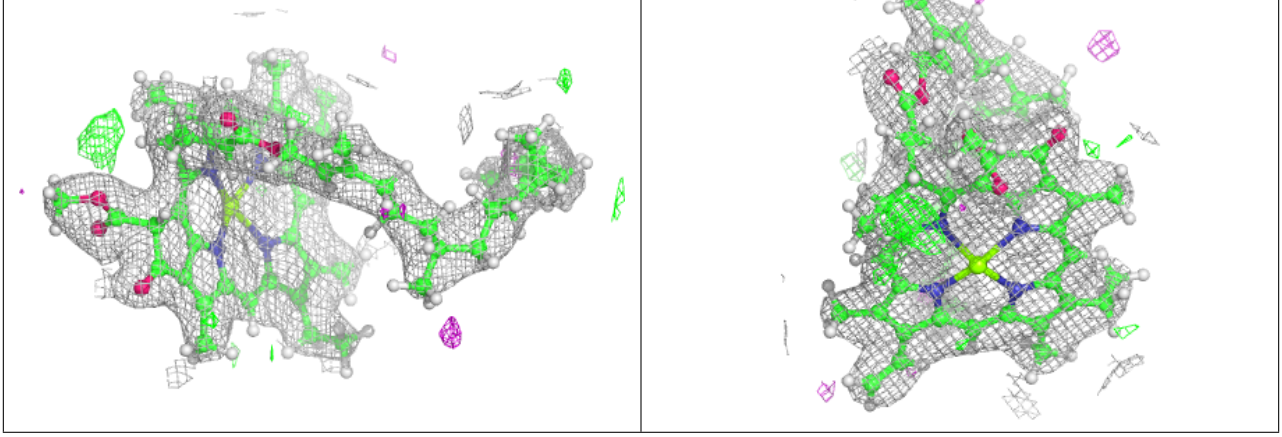




**Electron density around CLA b 611:**

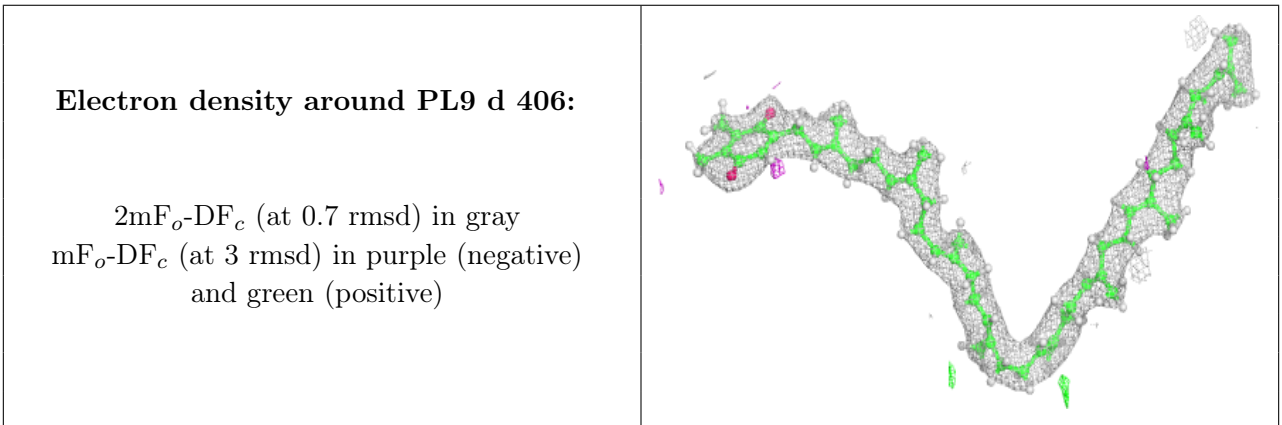
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

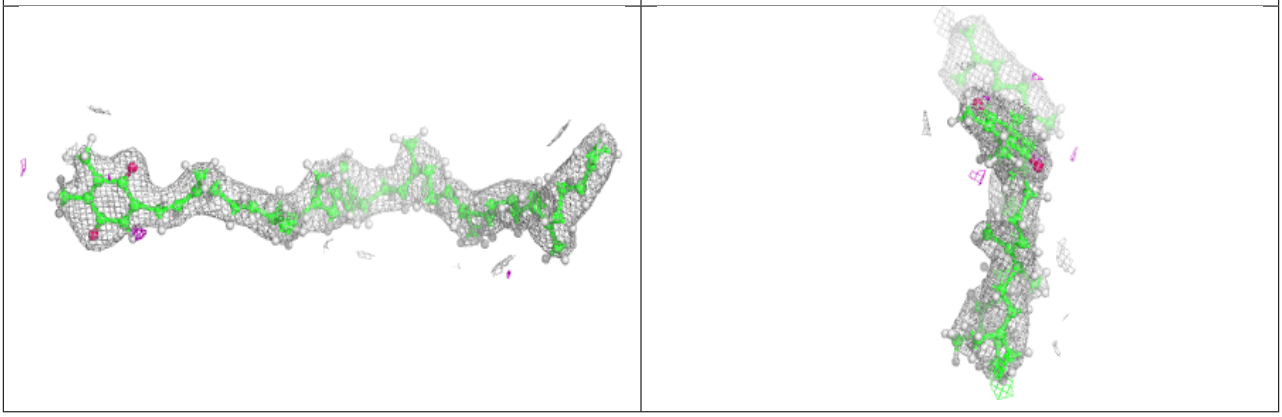




**Electron density around PL9 d 406:**

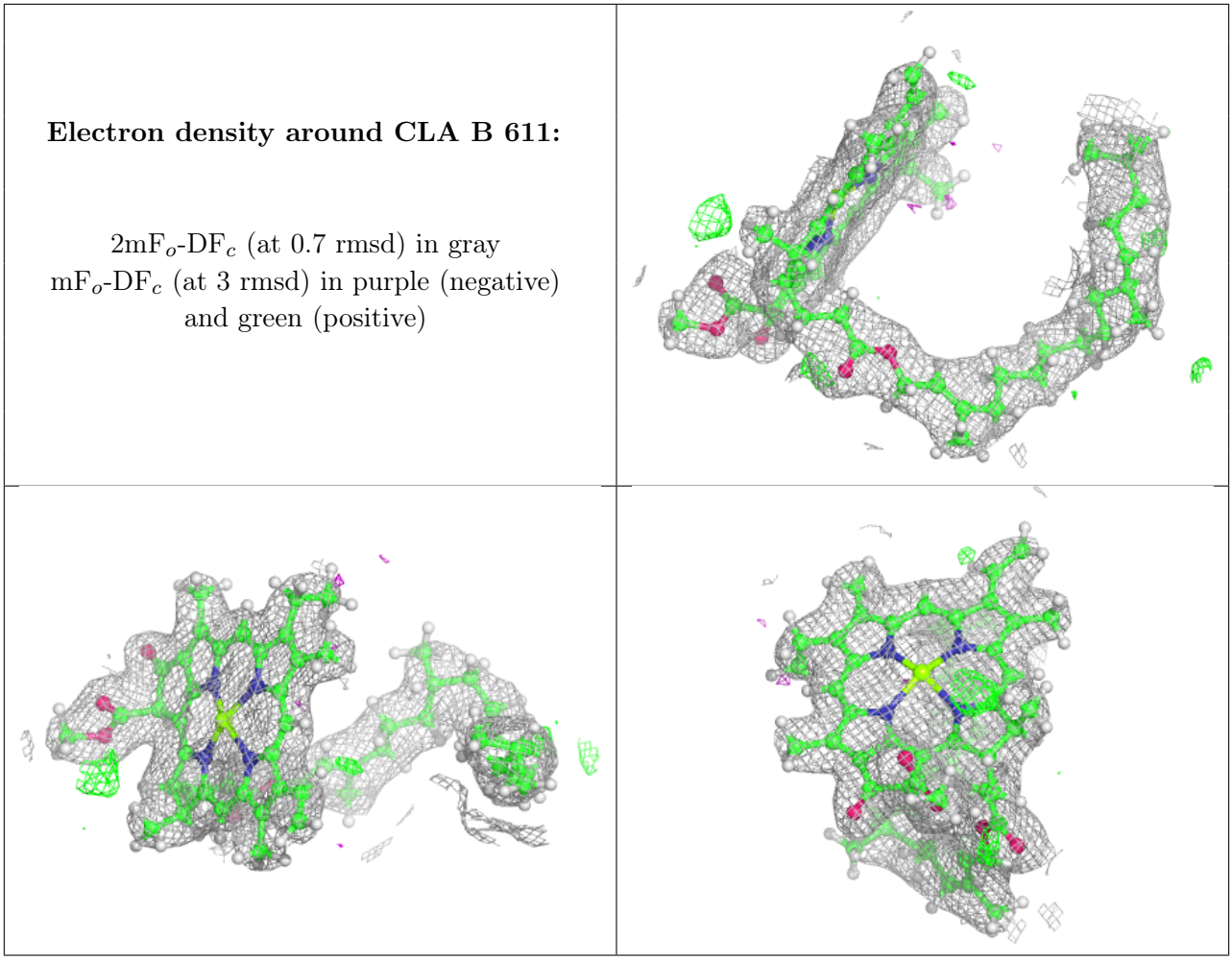
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)





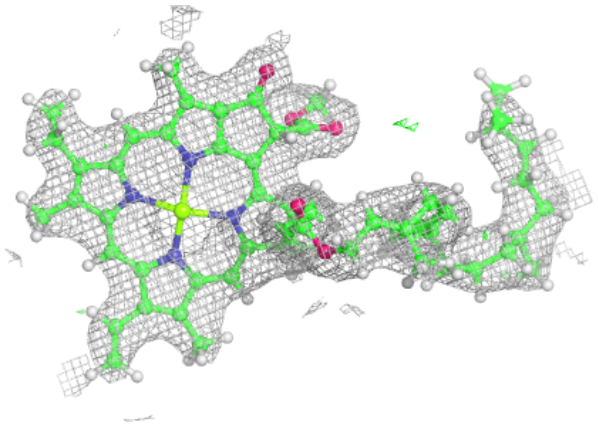
**Electron density around CLA B 611:**

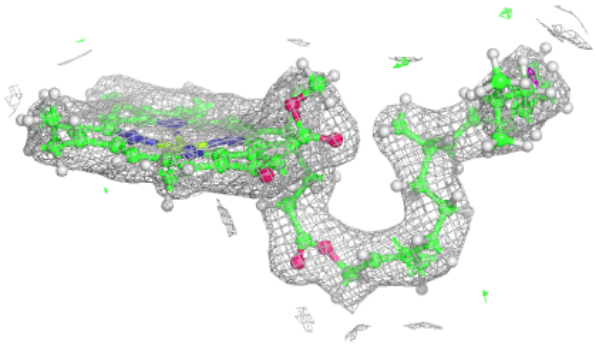
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

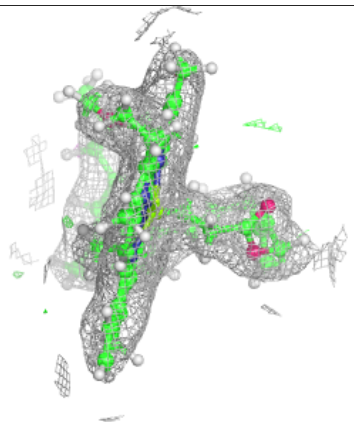


**Electron density around CLA B 612:**

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

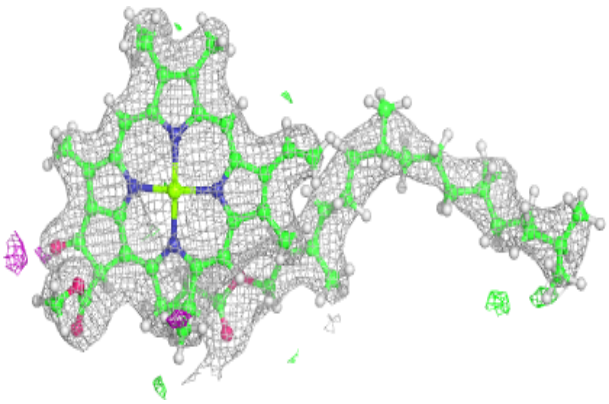


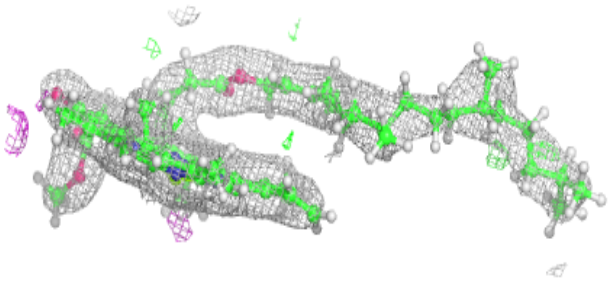


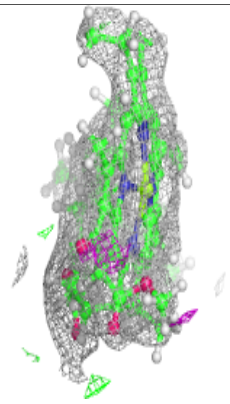


**Electron density around CLA B 603:**

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

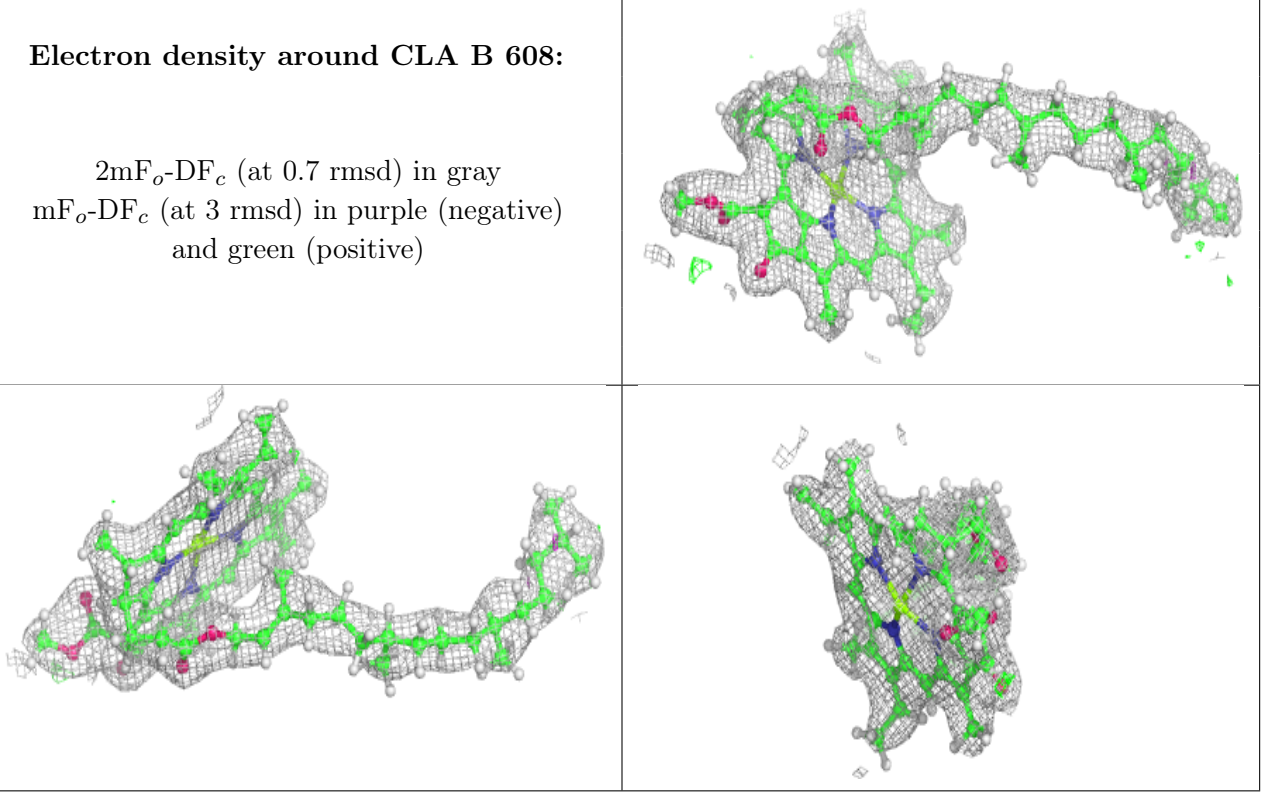






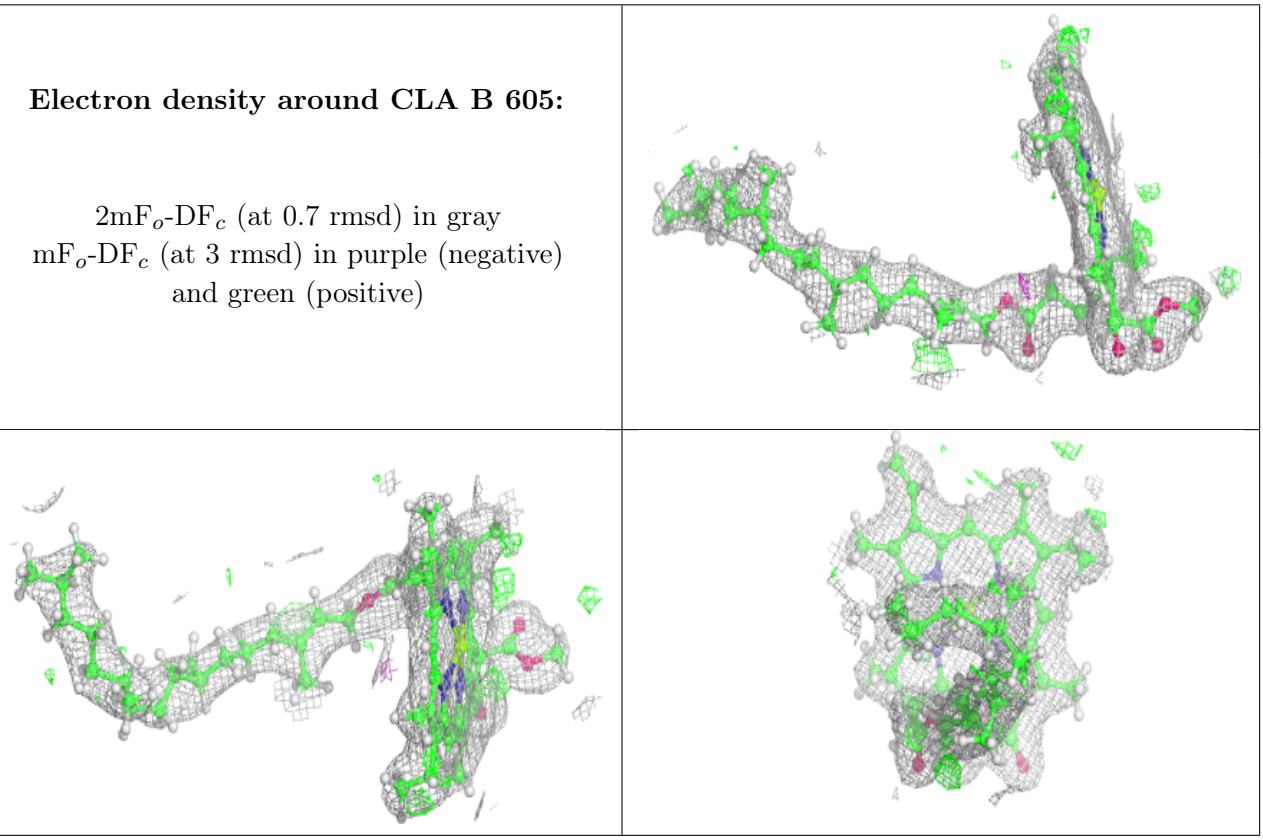
**Electron density around CLA B 608:**

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



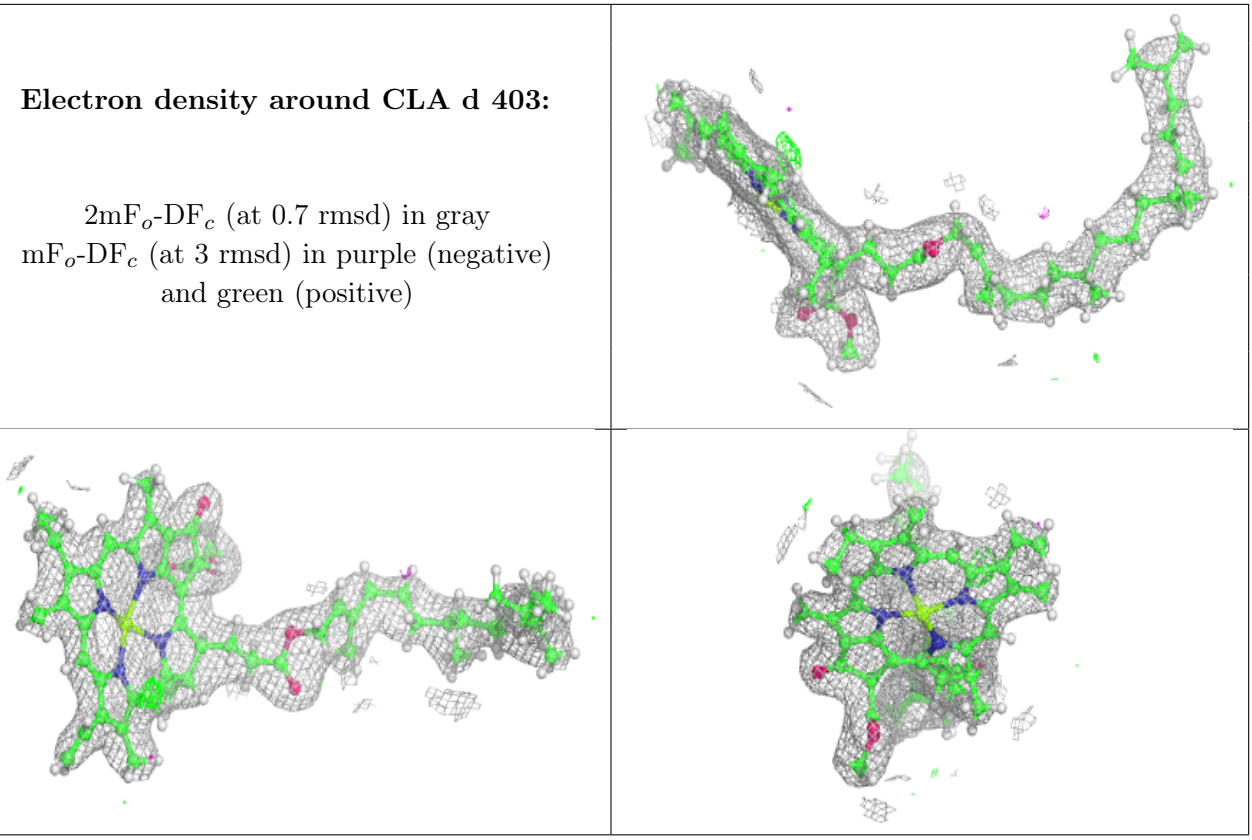
**Electron density around CLA B 605:**

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



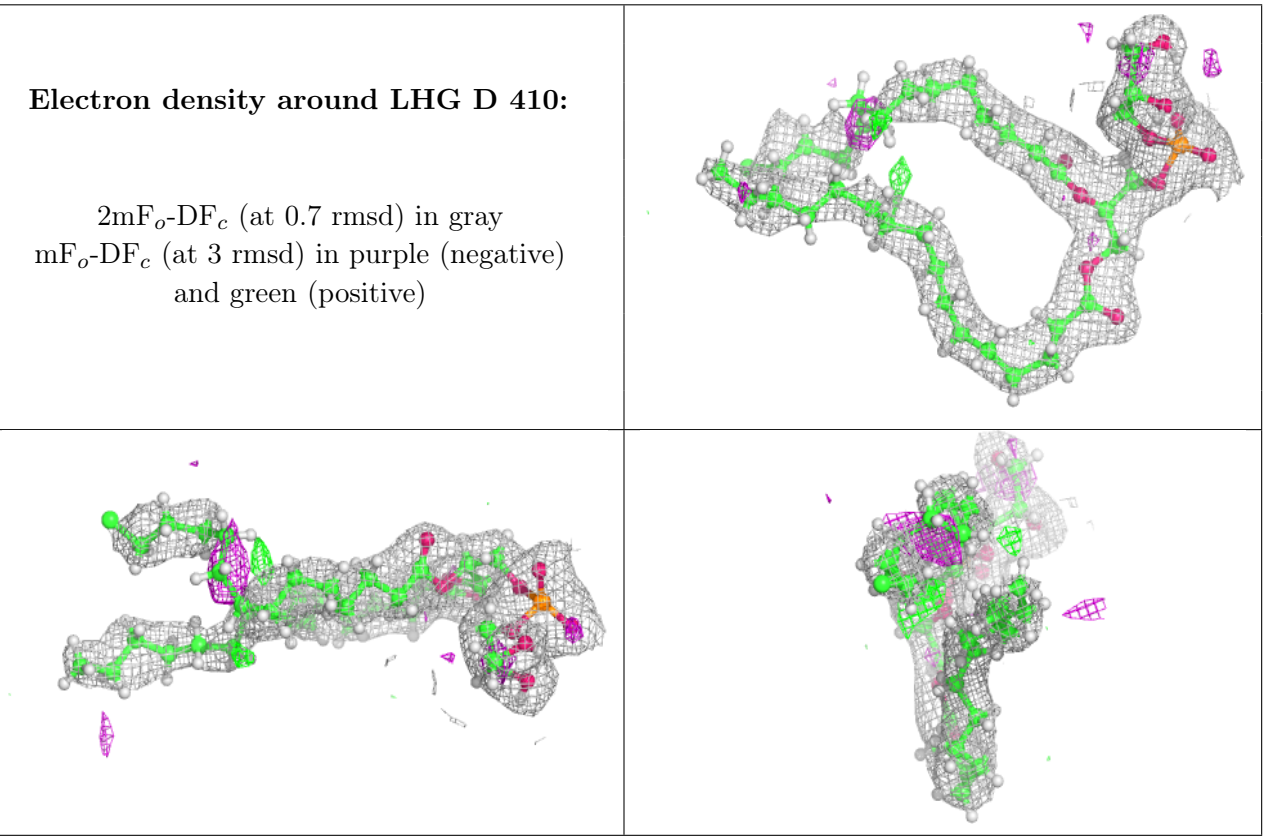
**Electron density around CLA d 403:**

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



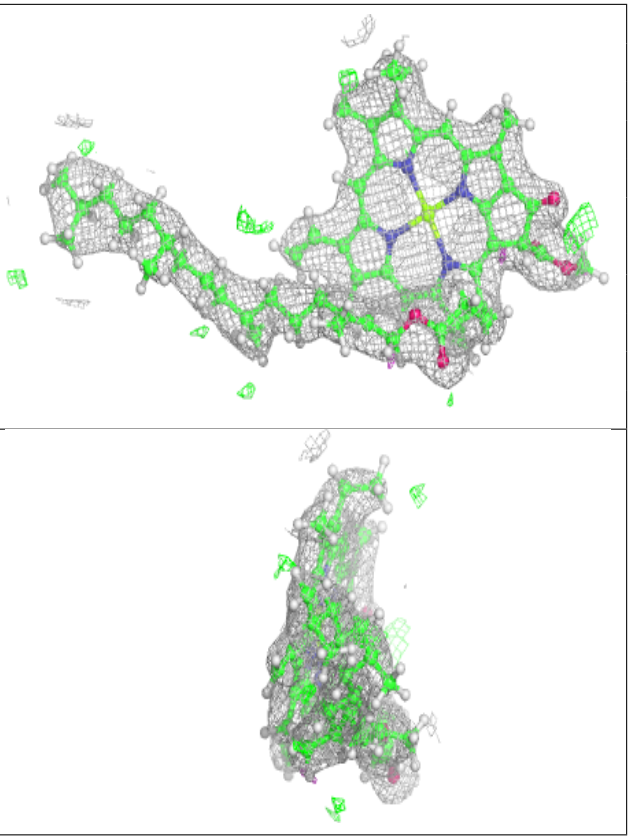
**Electron density around LHG D 410:**

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



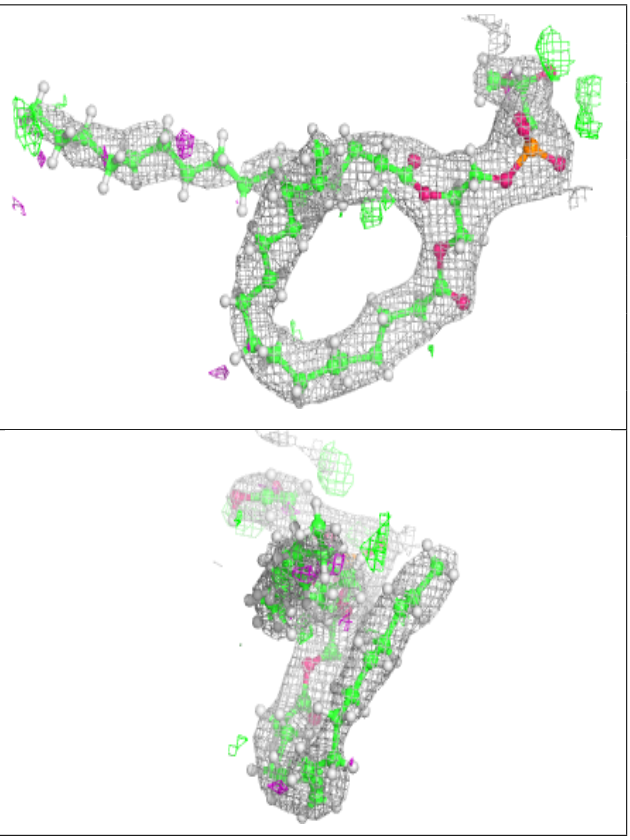
**Electron density around CLA c 502:**

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



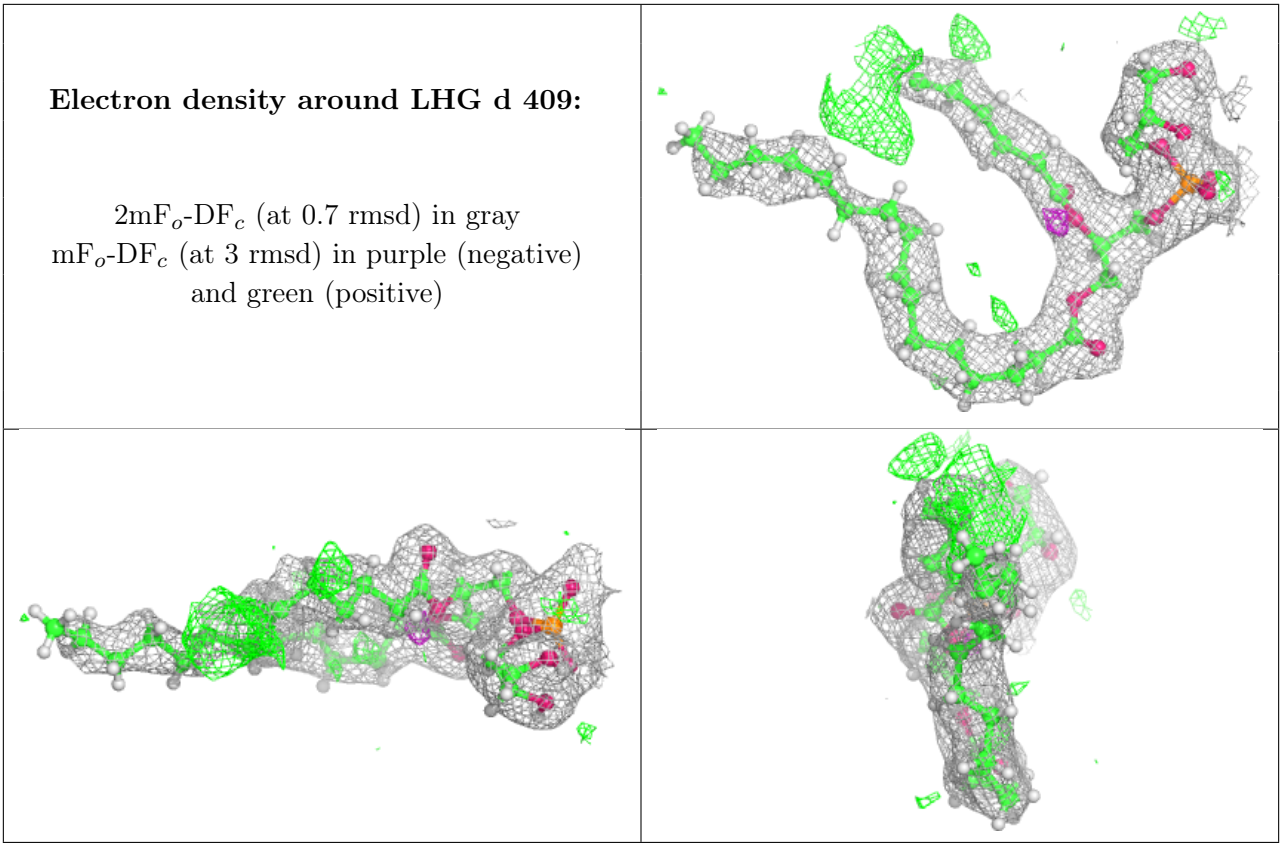
**Electron density around LHG d 407:**

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



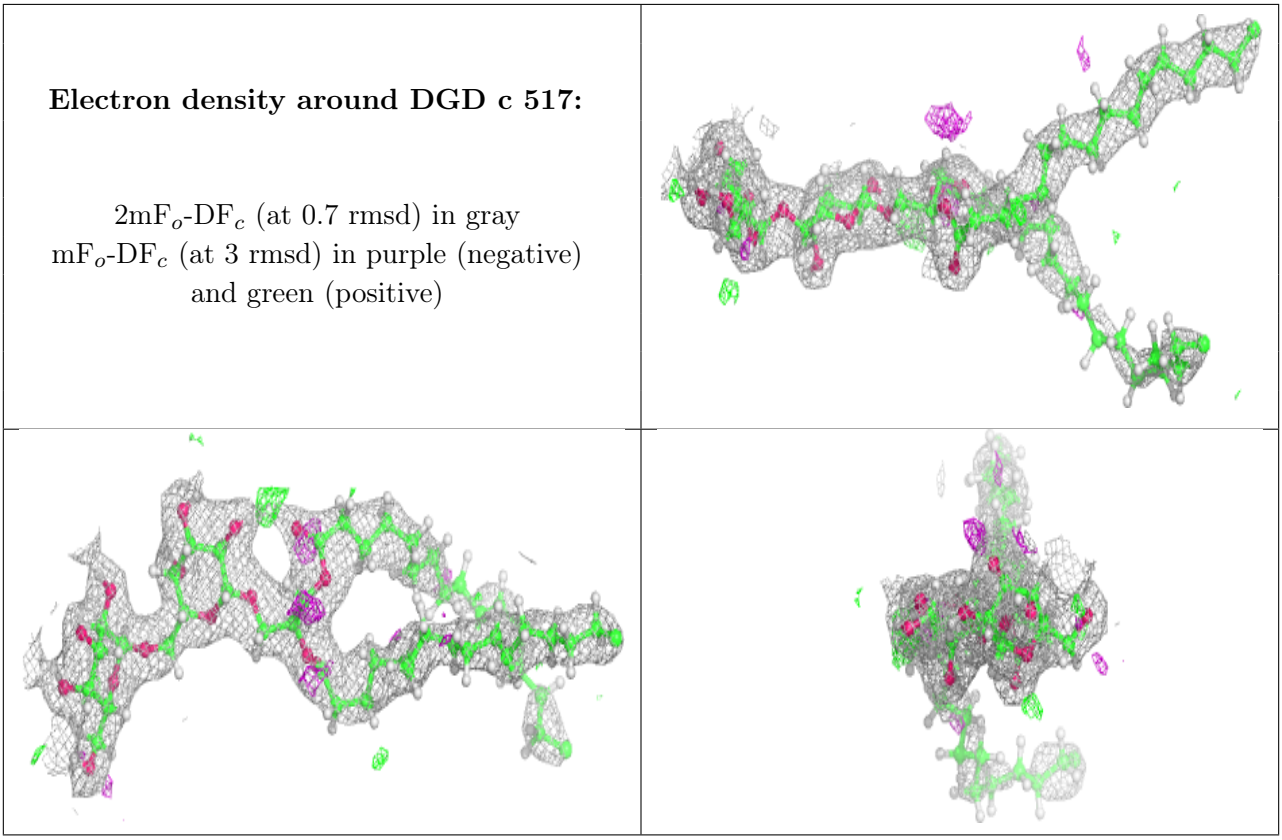
**Electron density around LHG d 409:**

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



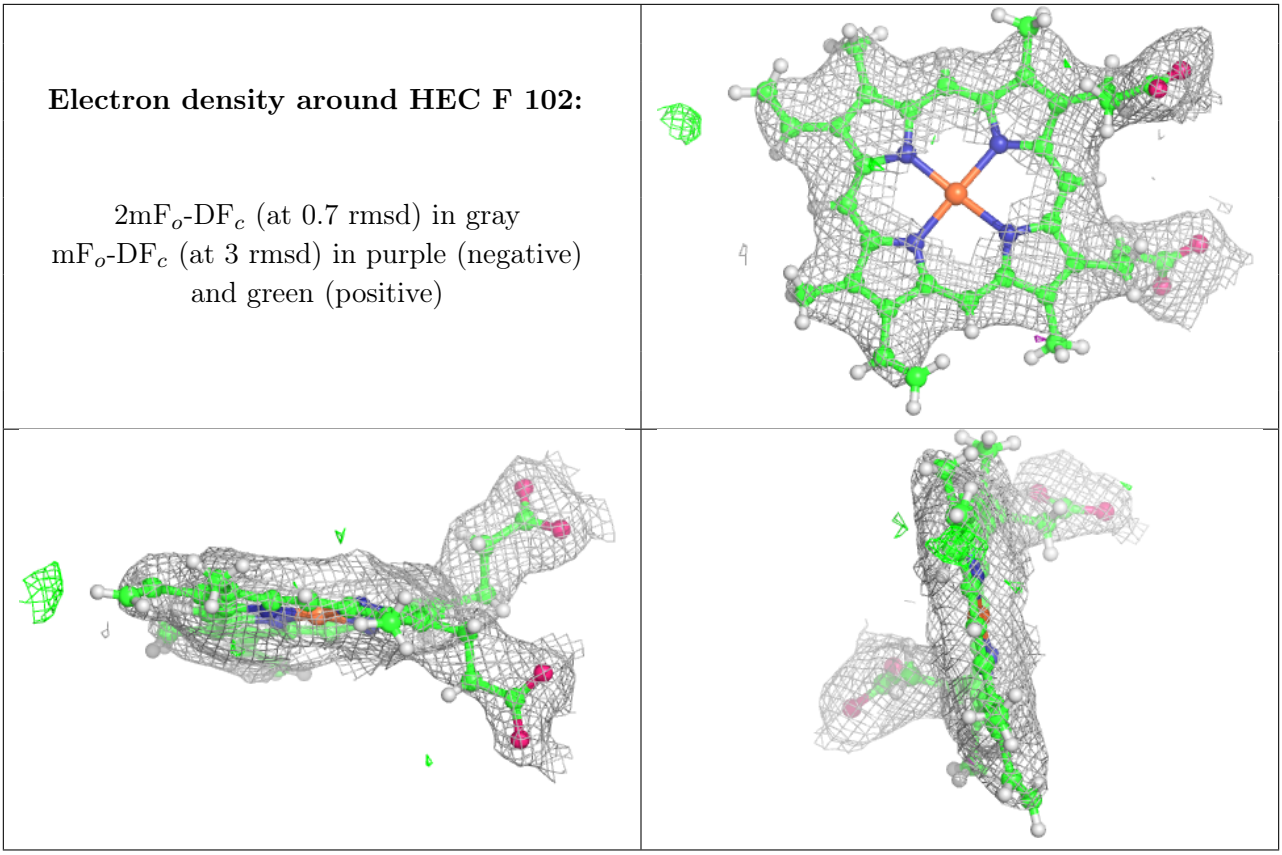
**Electron density around DGD c 517:**

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



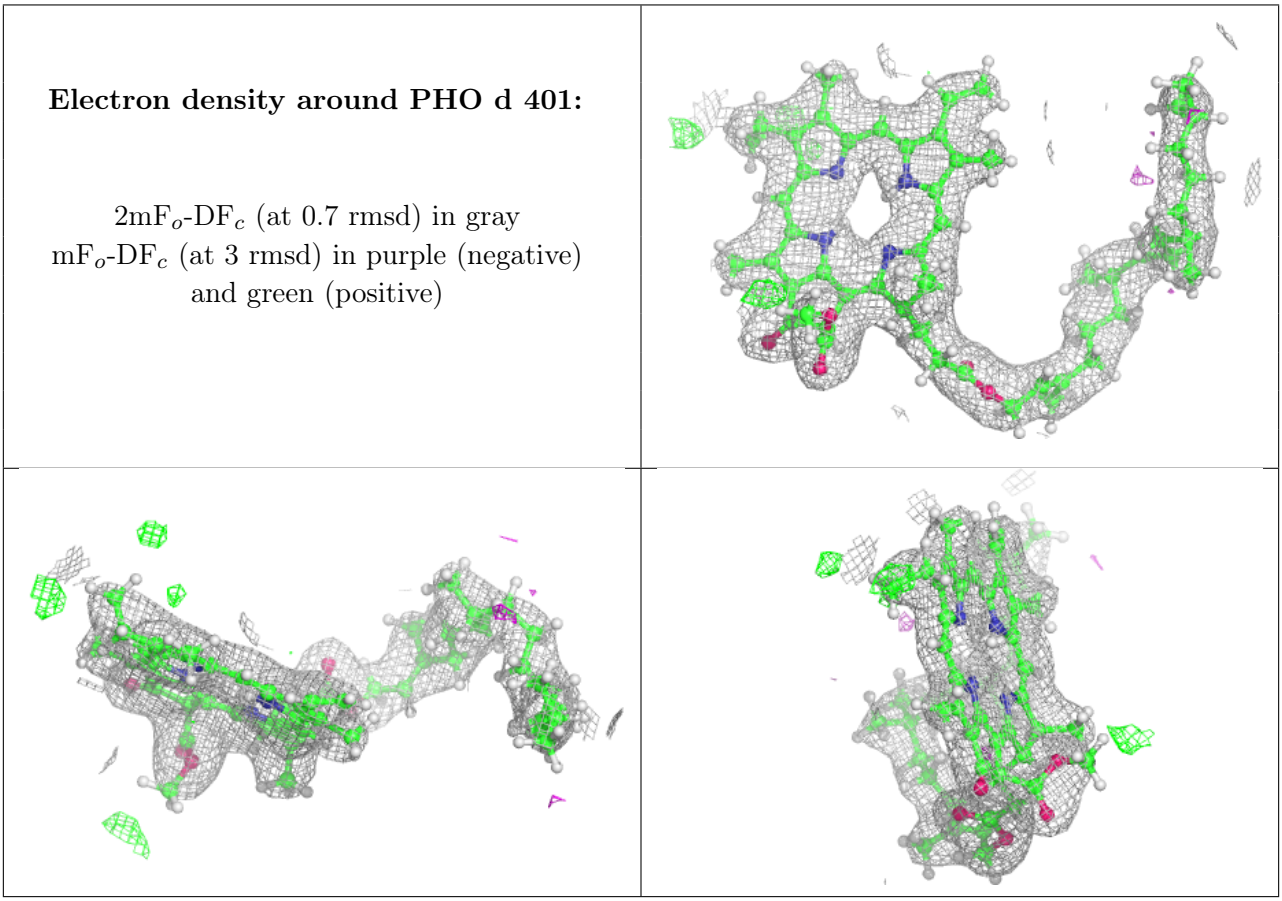
**Electron density around HEC F 102:**

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



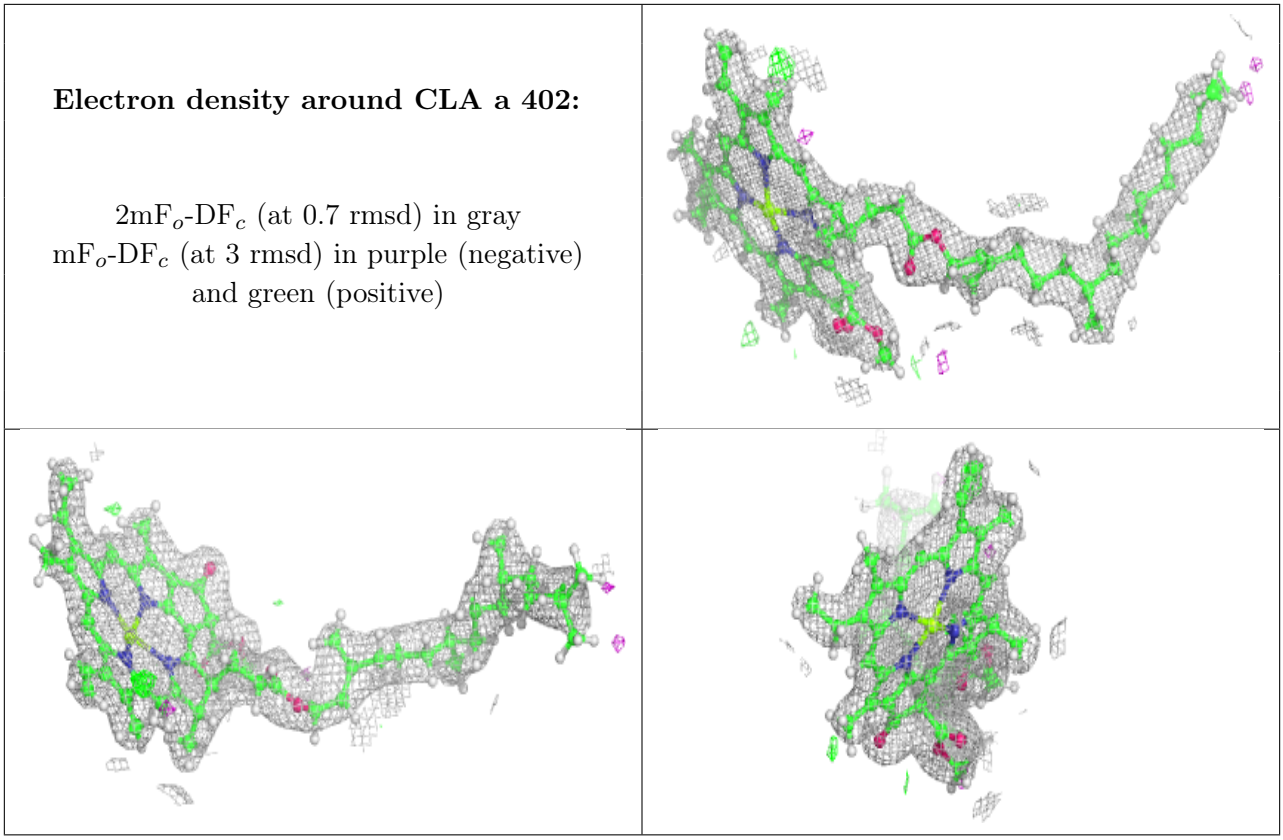
**Electron density around PHO d 401:**

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



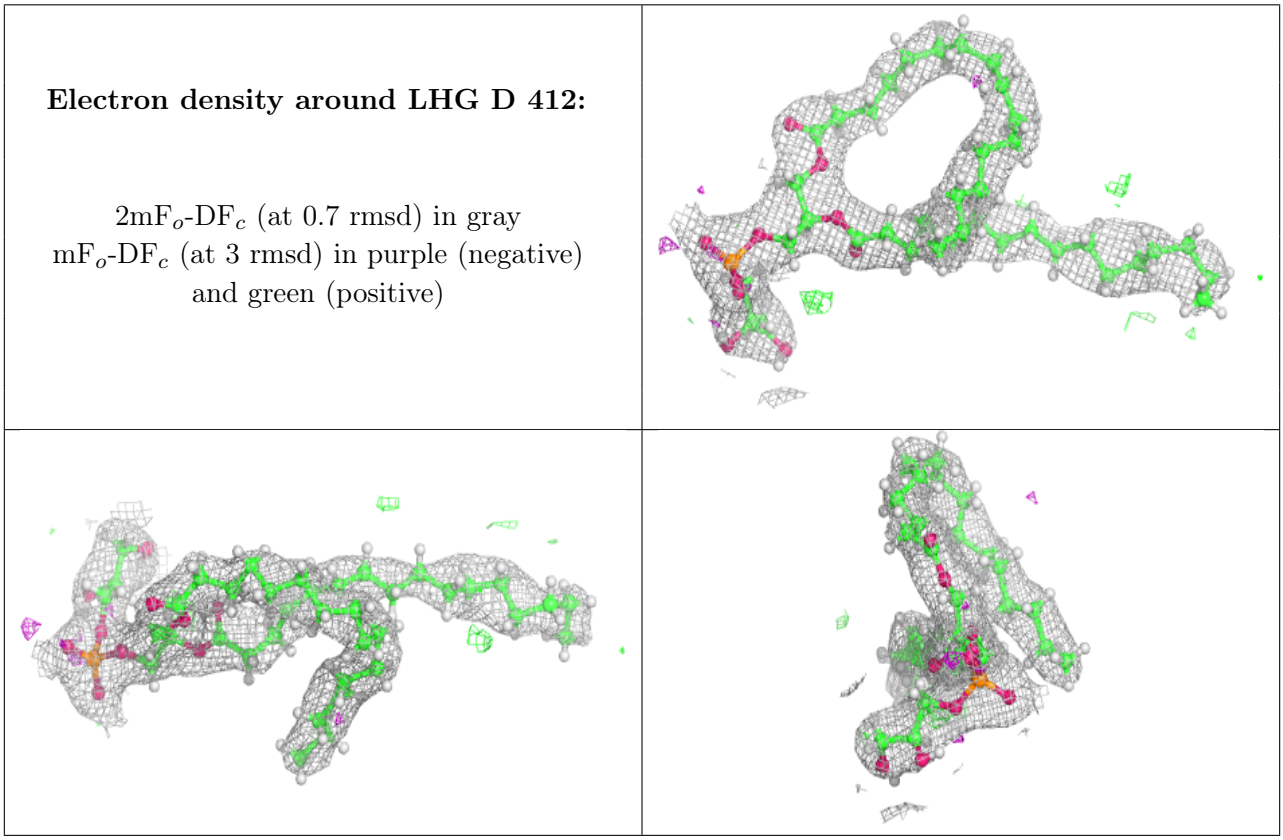
**Electron density around CLA a 402:**

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



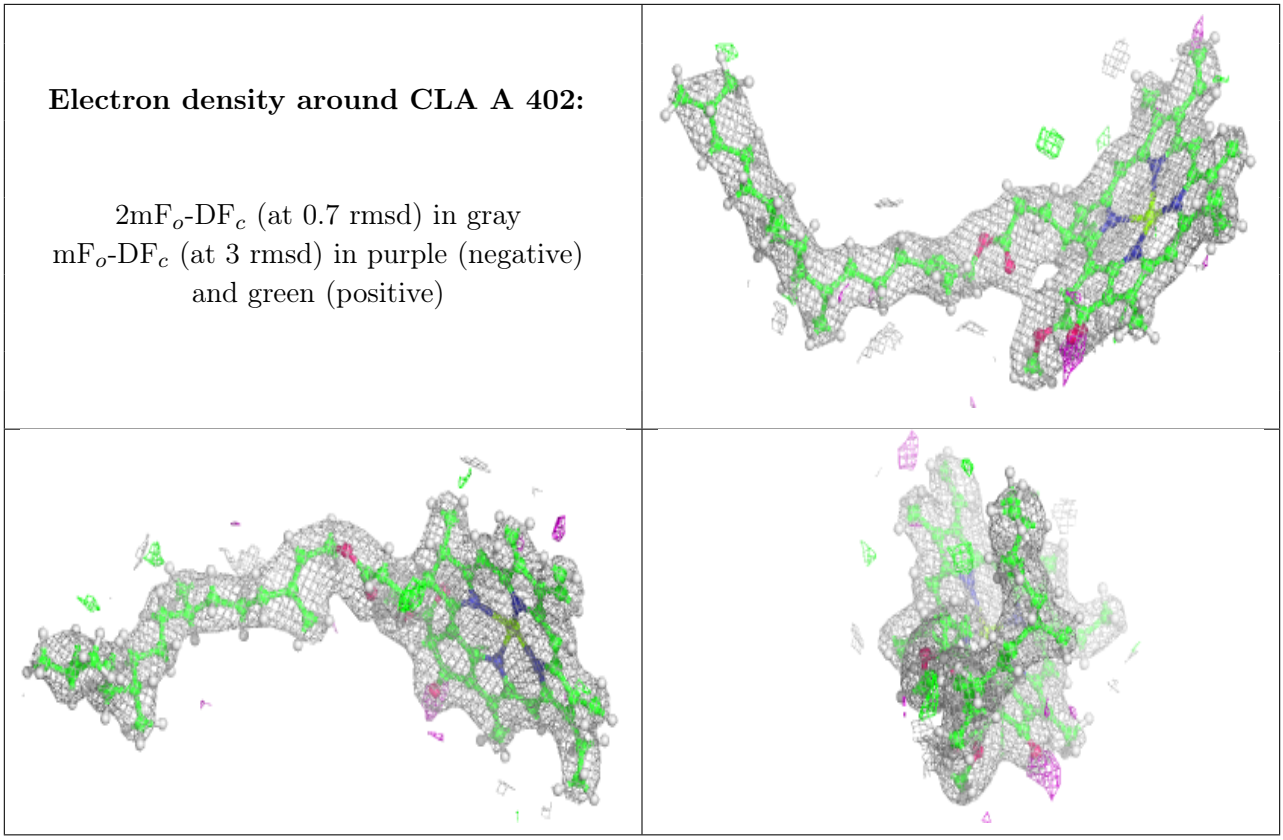
**Electron density around LHG D 412:**

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



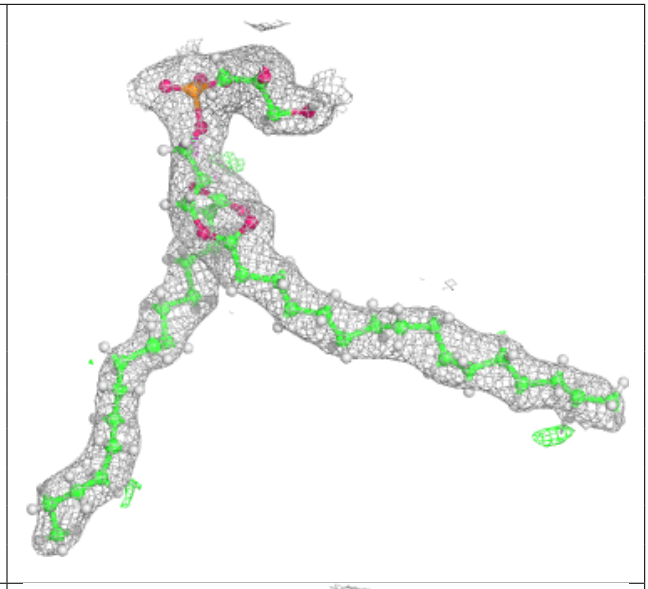
**Electron density around CLA A 402:**

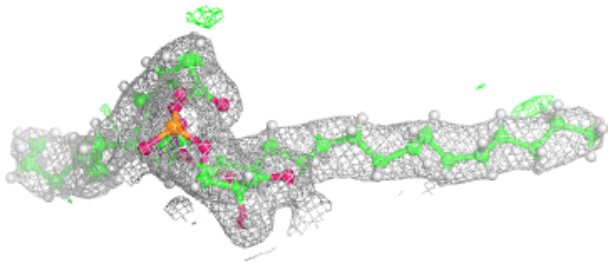
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

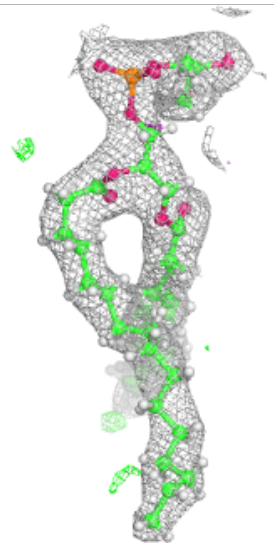


**Electron density around LHG L 102:**

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

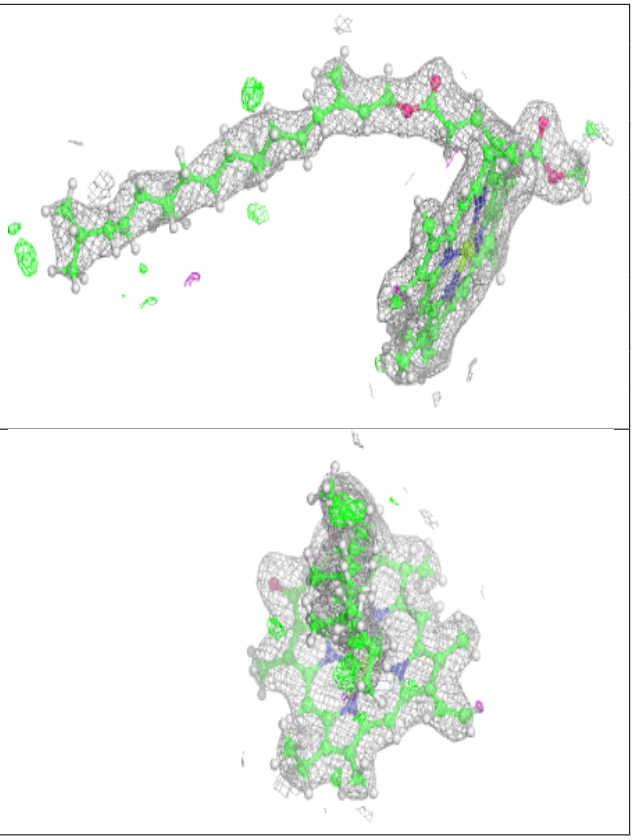






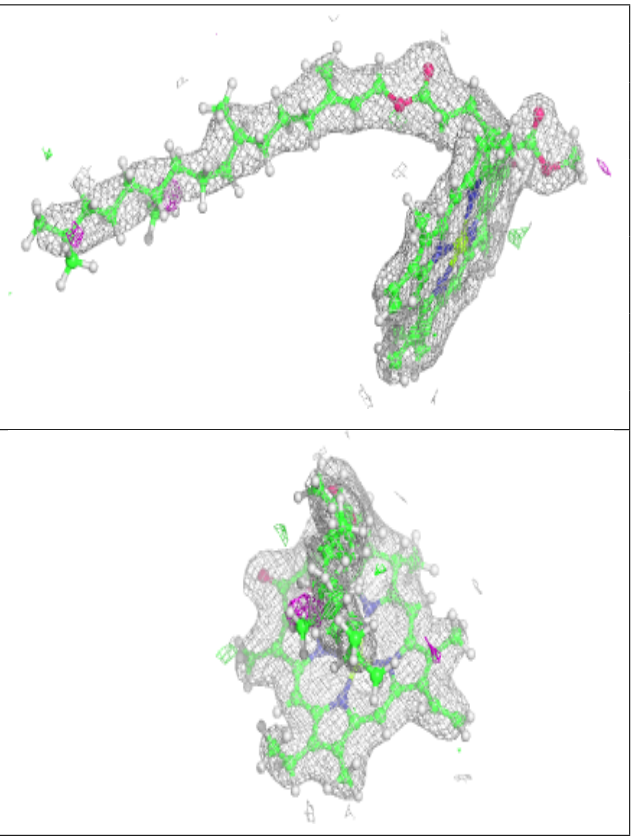
**Electron density around CLA B 607:**

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



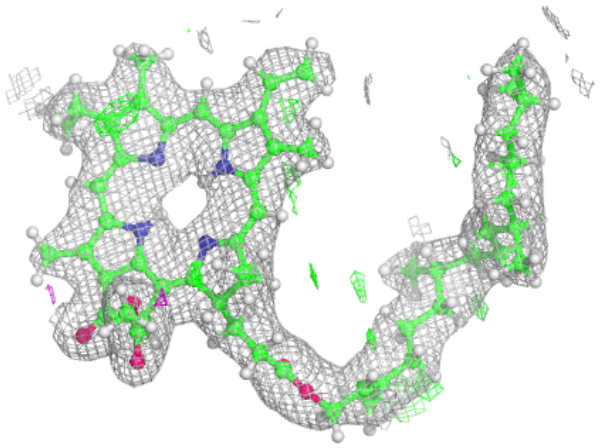
**Electron density around CLA b 607:**

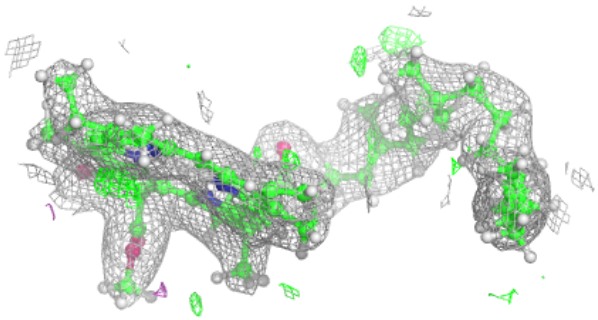
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

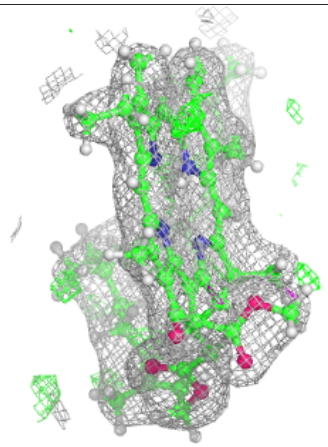


**Electron density around PHO D 401:**

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

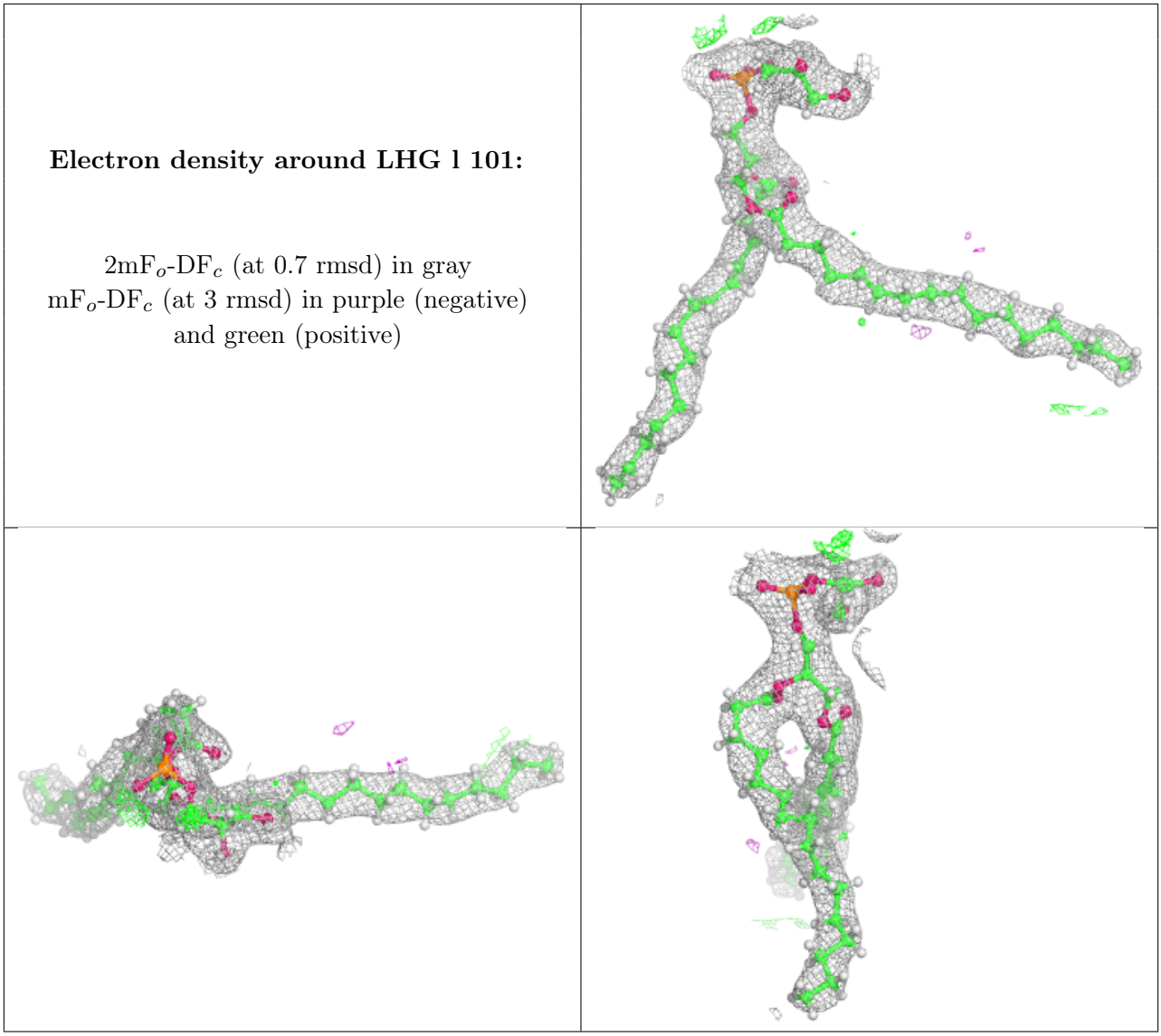






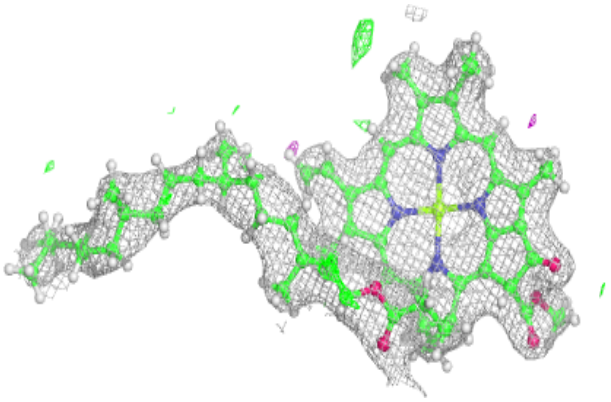
**Electron density around LHG l 101:**

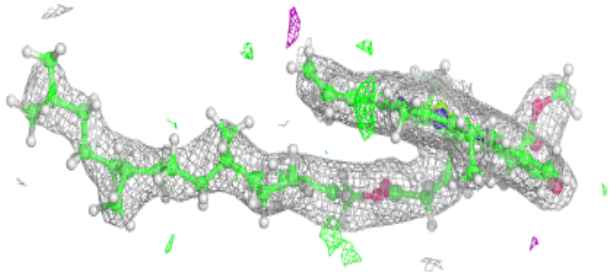
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

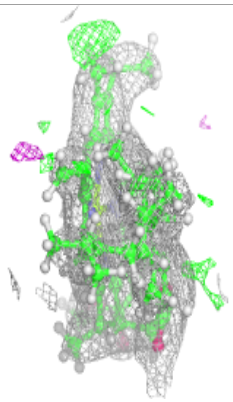


**Electron density around CLA b 603:**

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

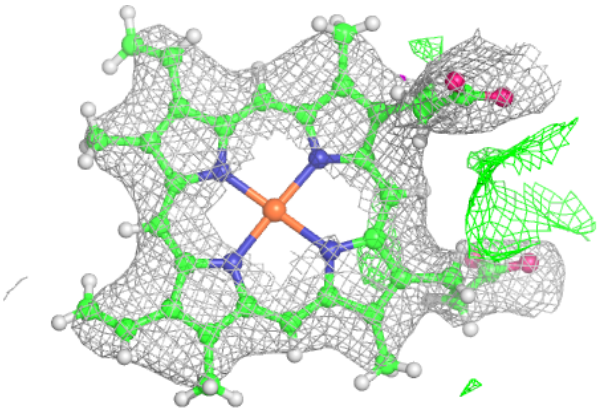


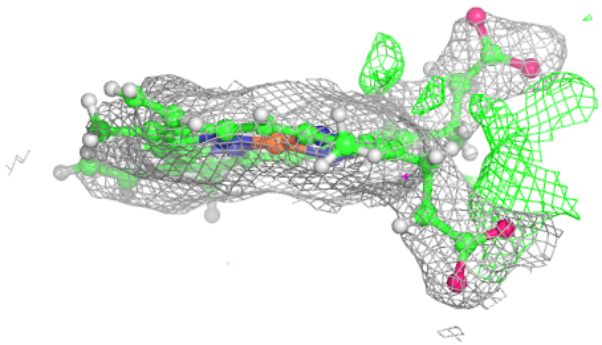


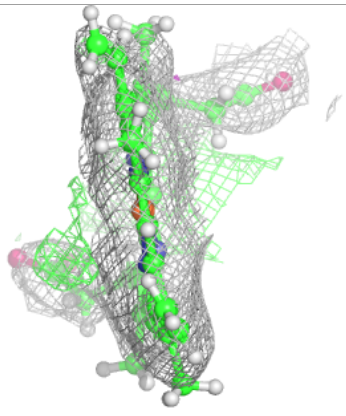


**Electron density around HEC f 101:**

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

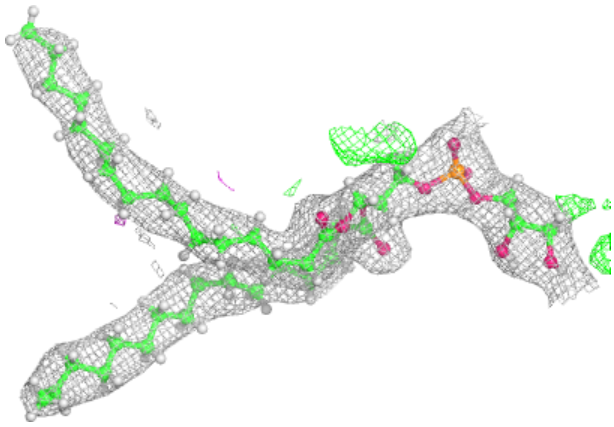


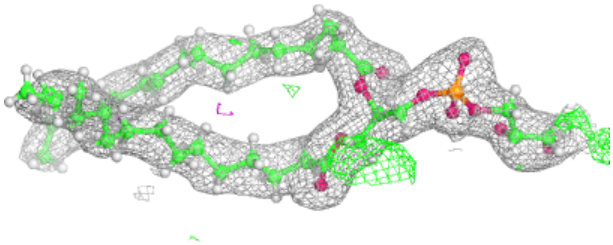


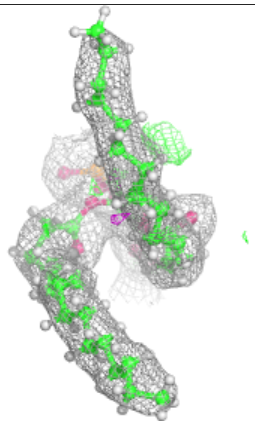


**Electron density around LHG d 408:**

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

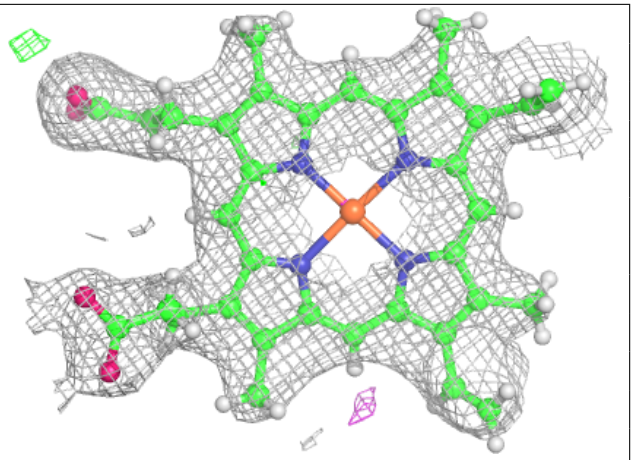


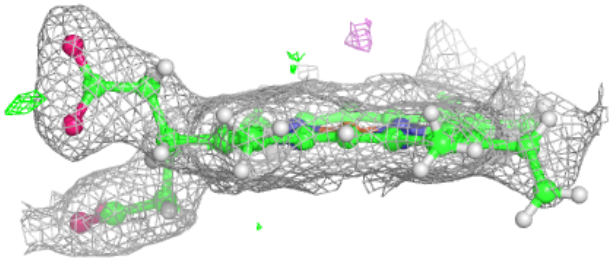


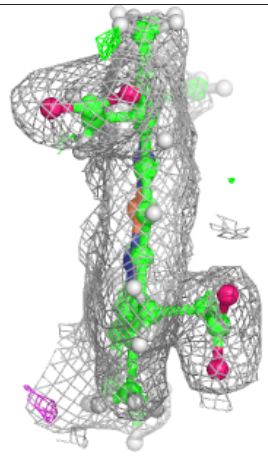


**Electron density around HEC V 201:**

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

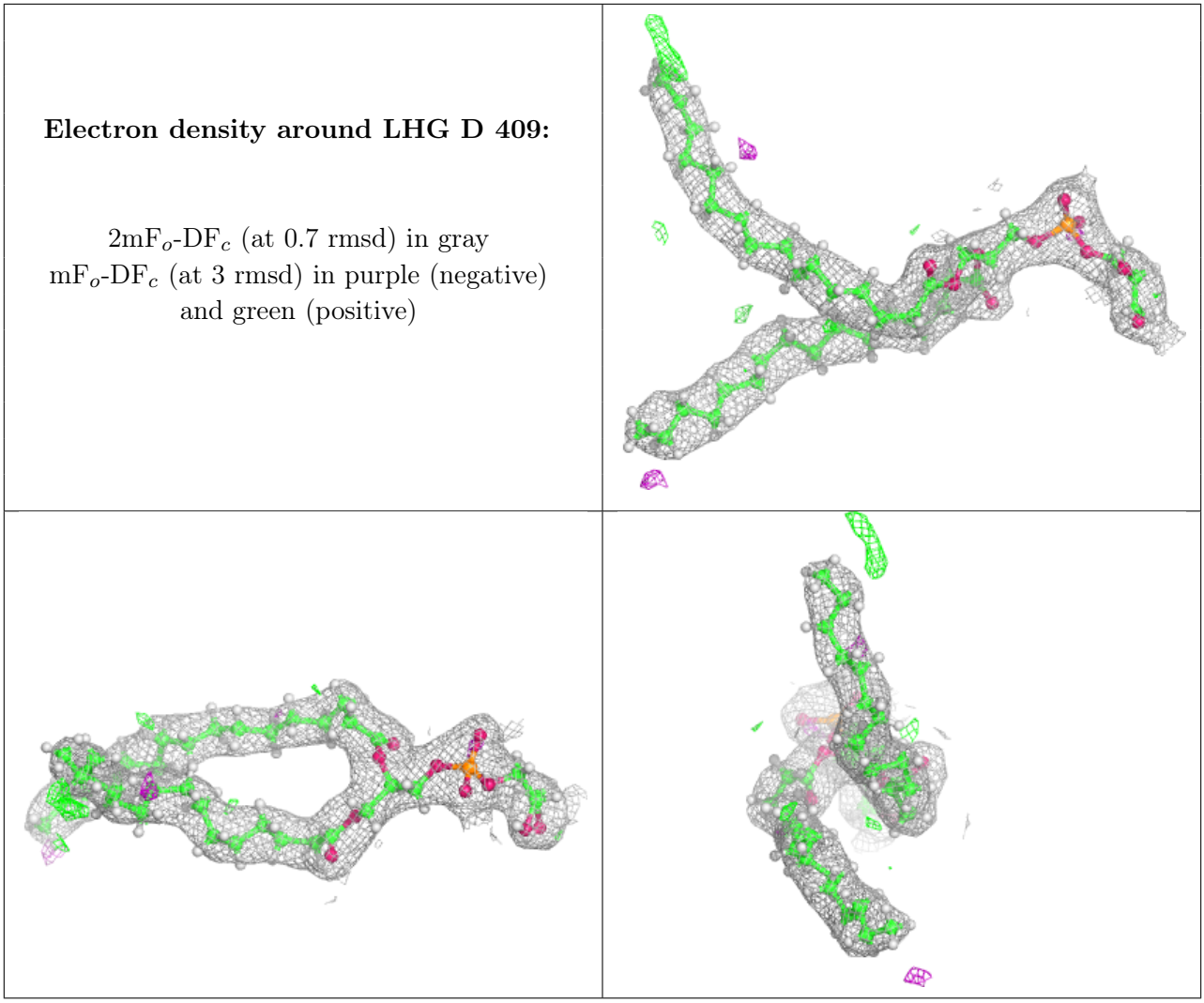






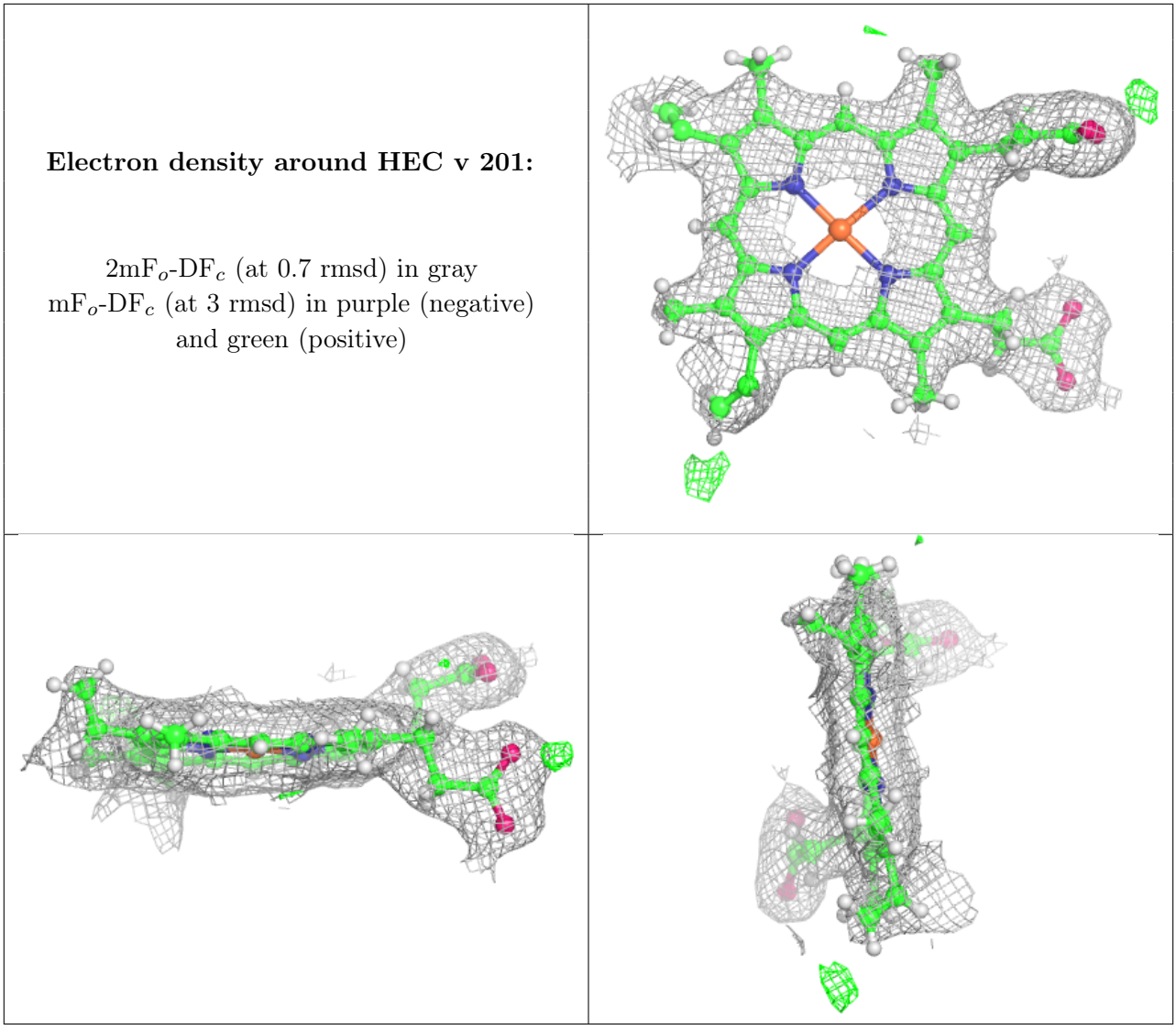
**Electron density around LHG D 409:**

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



**Electron density around HEC v 201:**

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



## 6.5 Other polymers

There are no such residues in this entry.